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(73) Titular/es:

NOVOZYMES A/S (100.0%)
Krogshøjvej 36
2880 Bagsvaerd, DK

(72) Inventor/es:

DE MARIA, LEONARDO;
SVENDSEN, ALLAN;
BORCHERT, TORBEN VEDEL;
CHRISTENSEN, LARS LEHMANN HYLLING;
LARSEN, SINE y
RYTTERSGAARD, CARSTEN

(74) Agente/Representante:

TOMAS GIL, Tesifonte Enrique

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DESCRIPCIÓN

Variantes de galactanasas

Campo de la invención

[0001] La presente invención se refiere a variantes de galactanasas de la familia glicósido hidrolasa 53, su producción y su uso en la industria láctea. Antecedentes de la invención

Estado de la técnica

[0002] La cristalización y estudios de rayos X preliminares de la galactanasa de Aspergillus aculeatus son descritos por Ryttersgaard et al en Acta.Cryst. (1999), 055, 929930.

[0003] La WO 97/32014 A divulga una galactanasa de M. thermophila y una galactanasa de H. insoles.

[0004] La WO 00/47711 A divulga una galactanasa de B. licheniformis.

Resumen de la invención

[0005] La invención proporciona una variante de una galactanasa de la familia glicósido hidrolasa 53 original que tiene un cambio en el perfil de la actividad del pH en comparación con la original; dicha variante comprende al menos una de las siguientes sustituciones: H91 N,L;D; A9OS+H91 D; DI8IN;
donde la variante tiene actividad de galactanasa;
donde la galactanasa original tiene cualquiera de las SEC ID nº: 1-4;
donde la variante tiene al menos 80% de identidad con la galactanasa original; y
donde la numeración se define por alineamiento con SEC ID nº: 1 utilizando el programa Clus-talw con la opción alineamiento de perfil con el alineamiento múltiple de la figura 5 como perfil 1, y cualquier secuencia no presente en la fig. 5 como perfil 2 para ser alineado con el primer perfil," usando los parámetros: Parámetros de alineamiento múltiple = Lento/Exacto; Penalización por apertura de espacio = 10,00; Penalización por extensión de espacio = 0,20; Secuencias divergentes de retraso = 30%; Peso de transiciones de ADN: 0,50; Matriz de peso de proteína = series Gonnet; Matriz de peso de ADN = IUB; Uso matriz negativa = OFF; Parámetros de espacio de proteína: Alternar sanciones específicas de residuos = ON; Alternar sanciones hidrofílicas = ON; Residuos hidrofílicos = GPSNDQEKR; Distancia de separación de espacio = 4; Alternar separación de espacio final = OFF.

Breve descripción de dibujos

[0006]

La fig. 1 muestra las coordenadas para la estructura 3D de una galactanasa de familia GH 53 de Myceliophthora thermophila con SEC ID nº: 1;
La fig. 2 muestra las coordenadas para la estructura 3D de una galactanasa de la familia GH 53 de Humicola insolens con SEC ID nº: 2;
La fig. 3 muestra las coordenadas para la estructura 3D de una galactanasa de la familia GH 53 de Aspergillus aculeatus con SEC ID nº: 3;
La fig. 4 muestra las coordenadas para la estructura 3D de una galactanasa de la familia GH 53 de Bacillus licheniformis con SEC ID nº: 4;
La fig. 5 muestra un alineamiento múltiple de SEC ID nº: 1-4; y
La fig. 6 muestra el alineamiento de la figura 5 con tres secuencias de galactanasa adicionales añadidas.

Descripción detallada de la invención

Determinación de la estructura 3D

[0007] La cristalización y los estudios de rayos X preliminares de la galactanasa de Aspergillus aculeatus (AAGAL) son descritos por Ryttersgaard et al. en Acta. Cryst. (1999), 055, 929930. Las galactanasas de Myceliophthora thermophila (MTGAL) y Humicola insolens (HIGAL) (WO 97/32014), y la galactanasa de Bacillus licheniformis (BLGAL) (WO 00/47711) fueron cristalizadas utilizando principios similares.

[0008] Las estructuras 3D se resolvieron conforme a los principios para métodos cristalográficos de rayos X como se dan, por ejemplo, en XRay Structure Determination, Stout, G.K. y Jensen, L.H., John Wiley & Sons, Inc. NY, 1989. Las coordenadas estructurales para la estructura cristalina de la galactanasa de Aspergillus aculeatus (AAGAL), como se determina por sustitución isomorfa múltiple a 1,8 A resolución en 100 K se dan en la fig. 1 en formato de PDB estándar (Protein Data Bank, Brookhaven National Laboratory, Brookhaven, CT).

[0009] Las estructuras de las otras tres galactanasas se resolvieron por sustitución molecular, usando la estructura AAGAL293 (a 2,3 A resolución en 293K) como modelo de búsqueda. Datos de 20-2,55 A, 18-2,14 A y 19,67-2,60 A se usaron para HIGAL, MTGAL y BLGAL, respectivamente, dentro de AMoRe (J. Navaza: AMoRe: an Automated package for Molecular Replacement. Acta Crystallogr., A50:157163, 1994). Las coordenadas respectivas se dan en las figuras 2-4 en formato de PDB estándar.

Variante

[0010] El término "variante de galactanasa" o simplemente "variante" se refiere a galactanasa que comprende una o más alteración(es), tal como sustitución(es), inserción(es), deleción(es) y/o truncamiento(s) de uno o varios residuos de aminoácidos específicos de una o más posiciones específicas en una galactanasa original.

[0011] El número total de tales alteraciones es típicamente no mayor de treinta, por ejemplo uno, dos, tres, cuatro, cinco, seis, siete, ocho, nueve, diez, once, doce, trece, catorce, quince, dieciséis, diez, dieciocho, diecinueve, veinte, veintiuno, veintidós, veintitrés, veinticuatro, veinticinco, veintiséis, veintisiete, veintiocho, veintinueve, o treinta de dichas alteraciones. Además, la variante de la invención puede incluir otras modificaciones de la enzima original, típicamente no mayor de 10, por ejemplo no mayor de 5 de tales modificaciones.

Nomenclatura y convenios para la designación de variantes

[0012] Una sustitución en una variante se indica como "aminoácido original – posición – aminoácido sustituido". Se usa preferiblemente el código de una letra, pero por supuesto se puede traducir en el código de tres letras como se desee. Los códigos X (o Xaa) se pueden utilizar para indicar cualquier residuo de aminoácido. Por consiguiente, la notación "D182N" o significa que la variante comprende una sustitución de ácido aspártico con ácido de asparagina en la posición de aminoácido variante que corresponde al aminoácido de la posición 182 en MTGAL, cuando los dos se alinean como se indica en la fig. 5.

[0013] Donde el residuo de aminoácido original puede ser cualquier residuo de aminoácido, una notación a mano corta se puede usar a veces indicando sólo la posición, y el aminoácido sustituido, por ejemplo: "Posición - aminoácido sustituido" o "182N". Esta notación es particularmente importante en relación con la modificación(es) de una serie de polipéptidos homólogos, tales como las galactanasas de la familia GH 53. De forma similar, cuando la identidad de los residuos de aminoácidos de substitución es irrelevante: "aminoácido original - posición" o "D182".

[0014] Cuando tanto los aminoácidos originales como los aminoácidos sustituidos pueden ser cualquier aminoácido, entonces sólo se indica la posición, por ejemplo "182".

[0015] Cuando los aminoácidos originales y/o aminoácidos sustituidos pueden comprender más de uno, pero no todos los aminoácidos, entonces los aminoácidos se catalogan, separados por comas: "aminoácido original - número de posición - aminoácido sustituido"; por ejemplo "H9ID,L,N".

[0016] Varios ejemplos de esta nomenclatura se enumeran a continuación:

La sustitución de ácido aspártico por asparagina en la posición 182 se designa como D182N.

[0017] La sustitución de cualquier residuo de aminoácido por serina en la posición 131 se designa como S131X o S131.

[0018] La sustitución de prolina por cualquier residuo de aminoácido en la posición 29 se denominaría así X29P o 29P.

[0019] Para una modificación donde el o los aminoácidos originales y/o aminoácidos sustituidos pueden comprender más de uno, pero no todos los aminoácidos, la sustitución de ácido aspártico, leucina o asparagina por histidina en la posición 91 se indicaría por H91 D,L,N lo que indica las variantes específicas H91 D, H91 L o H91 N.

[0020] Una eliminación de ácido glutámico en la posición 288a se indicará por E288a*. Correspondientemente, la eliminación de más de un residuo de aminoácido, tal como la eliminación de ácido glutámico y ácido aspártico en las posiciones 252a y 252b será designará “E252a*+D252b*”.

[0021] Un truncamiento se refiere a un encogimiento N o C-terminal de la secuencia de aminoácidos completa, es decir una eliminación de uno, o normalmente más, aminoácidos y el extremo N o C-terminal del péptido. En cuanto a la designación de variantes truncadas, se puede utilizar la regla general para deleciones.

[0022] La inserción de un residuo de aminoácido adicional tal como por ejemplo una valina después de F216 se indica por "F216FV"; o, cuando más de un residuo de aminoácido se inserta, tal como por ejemplo una valina, alanina, serina, treonina y una glicina después de F216 se indicará como: "F216FVASTG".

[0023] En tales casos el o los residuos de aminoácido insertados se numeran por la adición de letras minúsculas al número de posición del residuo de aminoácido precedente al residuo o residuos de aminoácido insertados.

En el ejemplo anterior las secuencias serían entonces:

Original:	Variante:						
216	216	216a	216b	216c	216d	216e	217
F	F	V	A	S	T	G	Y

[0024] Una vez que se han utilizado todas las letras minúsculas de la a a la z (a, b, c, d, e, f, g, h, i, j, k, l, m, n, o, p, q, r, s, t, u, v, x, y, z) para este propósito, se utilizan letras dobles aa, bb, cc, etc. hasta zz, véase por ejemplo el alineamiento de la figura 5, entre las posiciones 302 y 303.

[0025] En los casos donde se inserta un residuo de aminoácido idéntico al residuo de aminoácido existente, está claro que se produce degeneración en la nomenclatura. Si por ejemplo una fenilalanina se insertara después de la fenilalanina en el ejemplo anterior esto se indicaría por "F216FF'.

[0026] Suponiendo que una prolina esté presente en la posición 215, el mismo cambio actual podría también indicarse como "P215PF":

	Original:		Variante:		
Numeración I:	215	216	215	216	216a
Secuencia:	P	F	P	F	F
Numeración II:			215	215a	216

[0027] Tales casos serán aparentes para el experto en la materia, y la indicación "F216FF" y las correspondientes indicaciones para este tipo de inserciones se entiende de este modo que comprenden tales equivalentes indicaciones degeneradas.

[0028] Por analogía, si segmentos de secuencia de aminoácidos se repiten en la galactanasa original y/o en la variante, será aparente para el experto en la materia que las indicaciones degeneradas equivalente están comprendidas, también cuando otras alteraciones diferentes de las inserciones se enumeran tal como deleciones y/o sustituciones. Por ejemplo, la eliminación de dos aminoácidos consecutivos "DG" en la secuencia “DGDG” de la posición 252b-252e, se puede escribir como “D252b*+G252c*” o “D252d*+G252e*” o “G252c*+D252d*”:

	Original:				Variante:	
Numeración I:	252b	252c	252d	252e	252b	252c
Secuencia:	D	G	D	G	D	G
Numeración II:					252d	252e
Numeración III:					252b	252e

[0029] Variantes que comprenden modificaciones múltiples se separan con el signo más, por ejemplo "A9OS+H91 D" representa modificaciones en las posiciones 90 y 91 sustituyendo tirosina y ácido glutámico por arginina y glicina, respectivamente. Así, "A9OS+H91 D,N,L" designa las siguientes variantes: A90S+H91D, A90S+H91 N y A90S+H91 L. Asimismo, N303D,H+N305D,H,P designa las siguientes variantes: N303D+N305D; N303D+N305H; N303D+N305P; N303H+N305D; N303H+N305H y N303H+N305P.

[0030] Esta nomenclatura es especialmente pertinente en relación con las modificaciones dirigidas a substituir, insertar o borrar residuos de aminoácidos que tienen propiedades comunes específicas, tales modificaciones se denominan modificación(es) de aminoácidos conservadoras. Ejemplos de modificaciones conservadoras están en el grupo de los aminoácidos básicos (arginina, lisina e histidina), aminoácidos ácidos (ácido glutámico y ácido aspártico), aminoácidos polares (glutamina y asparagina), aminoácidos hidrofóbicos (leucina, isoleucina y valina), aminoácidos aromáticos (fenilalanina, triptófano y tirosina) y aminoácidos pequeños (glicina, alanina, serina, treonina y metionina). Modificaciones de aminoácidos que generalmente no alterar la actividad específica se conocen en la técnica y son descritas, por ejemplo, por H. Neurath y R.L. Hill, 1979, en, The Proteins, Academic Press, New York. Los intercambios que se producen más frecuentemente son Ala/Ser, Val/Ile, Asp/Glu, Thr/Ser, Ala/Gly, Ala/Thr, Ser/Asn, Ala/Val, Ser/Gly, Tyr/Phe, Ala/Pro, Lys/Arg, Asp/Asn, Leu/Ile, Leu/Val, Ala/Glu y Asp/Gly al igual que a la inversa.

[0031] Para los fines presentes, la secuencia de MTGAL (SEC ID nº: 1) se ha seleccionado como marco de referencia, lo que significa que todas las variantes serán definidas basándose en la secuencia de aminoácidos de MTGAL. En particular, a cada residuo de aminoácido en una secuencia de galactanasa se le asigna un número, una posición o un número de posición, por referencia a la fig. 5 presente, es decir, el número del residuo de aminoácido correspondiente en la estructura de galactanasa de Myceliophthora thermophila (MT; la línea superior del alineamiento de la figura 5). En

este contexto, el término "correspondiente" se refiere al aminoácido que, según el alineamiento, está en la misma columna que el residuo de aminoácido en cuestión, pero en la primera fila designada "MT".

[0032] Por ejemplo, la variante de la galactanasa de Bacillus licheniformis (BL) que por referencia a SEC ID nº: 4 quizá se puede designar S39C se designará, para los fines presentes, SI8C, porque S39 de BL corresponde a A18 de MT. Como otro ejemplo, la variante de la galactanasa de Aspergillus aculeatus que por referencia a SEC ID nº: 3 se puede designar D1 82N se designará, para los fines presentes, 0181 N, porque D182 de AA corresponde a N181 de MT. Como otro ejemplo más, la variante K16P de BL se puede designar *-6p porque K16P de BL corresponde a un aminoácido que falta o eliminado en la posición -6 de MT, todavía por referencia formal estricta a la fig. 5.

[0033] No obstante, si se desea, las variantes de la invención también se pueden definir por referencia a sus respectivas estructuras "propias", por ejemplo con referencia a SEC ID nº: 1, SEC ID nº: 2, SEC ID nº: 3 o SEC ID nº: 4. Los números de la posición correspondiente se deducen fácilmente, de la misma manera que se ha descrito anteriormente, de las figuras 5-6 o, para secuencias de galactanasa adicionales, de una figura que se puede preparar según los principios aquí descritos.

Dinámica Molecular (MD)

[0034] Las simulaciones de Dinámica Molecular (MD) son indicativas de la movilidad de los aminoácidos en una estructura de proteína (véase McCammon, JA y Harvey, SC., (1987), "Dynamics of proteins and nucleic acids", Cambridge University Press). Tales dinámicas de proteína se comparan frecuentemente con los B-factores cristalográficos (véase Stout, GH y Jensen, LH, (1989), "Xray structure determination", Wiley). Al llevar a cabo la de MD en, por ejemplo, temperaturas diferentes, la movilidad relacionada con la temperatura de los residuos se simula. Regiones que tienen la máxima movilidad o flexibilidad (aquí fluctuaciones isotrópicas) se pueden sugerir para mutagénesis aleatoria. Se entiende aquí que la alta movilidad encontrada en áreas determinadas de la proteína puede ser térmicamente mejorada por substitución de estos residuos.

Variantes de propiedades enmendadas

[0035] Basadas en la estructura 3D de la galactanasa de Myceliophthora thermophila de SEC ID nº: 1, las siguientes variantes se contemplan, donde al menos uno de los residuos abajo mencionados se ha enmendados y/o al menos una de las alteraciones abajo mencionadas se han introducido:

i) variantes de una actividad específica enmendada, dentro de 10A del sitio activo: Y4, G6, V7, D8, W9, SI 0, R45, 046, R47, W49, Y77, 079, F80, H81, Y82, W86, A87, D88, P89, A90, H91, 092, T93, S131,1132, G133, N134, E135,1136, R137,A138, G139, L140, L141, W142, G145, R146, T147, I153, L157, M176,1177, H178, L179, D180, N181, G182, W183, T187, Q188, W191, Y192, M209, G210, V211, S212, F213, Y214, P215, F216, Y217, A221, L226, 1241, A242, V243, V244, E245, T246, N247, W248, F276, I277, V280, V284, G292, L293, F294, Y295, W296, E297, P298, W300, L306, G307, F329;

ii) variantes de una actividad enmendada en la lactosa, dentro de 10A del sitio activo: Y214S,N+N247Y+L306Q; Y214A; F216FVASTGY217; P89W+W86N;

iii) variantes de un perfil de actividad de pH enmendado: H91 N,L,D; N313D; N303D,H; N305D,H; A9OS+H91 D;

iv) variantes de una termoestabilidad enmendada, por inserción de prolinas: Y22P, N24P, T25P, A29P, A53P, N56P, T93P, DIOIP, W142P, T147P, Q1 98P, L203P, S204P, S219P; S258P, S288P, A304P, A3I1P, Q318P, A322P, S324P, S325P, S327P;

v) variantes de una termoestabilidad enmendada, mediante el aumento de la hidrofobicidad de superficie: W1O7S,H;

vi) variantes de una termoestabilidad enmendada, por enmendado del potencial electroestático de superficie: Q126E;

vii) variantes de una termoestabilidad enmendada, por puentes disulfuro (mutaciones dobles a cisteínas): V2OC+G320C, N39C+L326C, Yl I OC+G I 63C, WI 50C+N1 94C, T274C+V328C, 1301 C+F31 6C

viii) variantes de termoestabilidad enmendada, por empaquetado de cadena lateral mejorado: 9F,Y,W; 12V, 80F, 82Y, 191Y,W; 213F; 9W+12V; 80F+82Y.

[0036] Basadas en la estructura 3D de la galactanasa de Humicola insolens, las siguientes variantes se contemplan, donde al menos uno de los residuos abajo mencionados se han enmendado y/o al menos una de las alteraciones abajo mencionadas se han introducido:

i) variantes de una termoestabilidad enmendada, por inserción de prolinas: V20P, V25P, E29P, V41P, V50P, W53P, N56P, T94P, A96P, W142P, L169P, W185P, Q198P, M203P, A219P, A221P, T222P, Q258P, A261P, D262P, S288P, N305P, A311P, A322P, S324P, S325P.

ii) variantes de una termoestabilidad enmendada, por puentes disulfuro (mutaciones dobles a cisteínas): T113C+G163C, W185C+S229C, S218C+A221C, R227C+V283C.

[0037] Basadas en la estructura 3D de la galactanasa de Aspergillus aculeatus, las siguientes variantes son contempladas, donde al menos uno de los residuos abajo mencionados se ha enmendado y/o al menos una de las alteraciones abajo mencionadas se ha introducido:

i) variantes de un perfil de actividad de pH enmendado: D18IN;

ii) variantes de una termoestabilidad enmendada, por inserción de prolinas: T3P, Y20P, N24P, L25P, T29P, A31 P, V50P, S53P, S56P, T93P, T94P, S96P, W142P, L144P, E146P, T147P, T172 P, E200P, S203P, A219P, A256P, A258P, S261 P, S264P, I266P, T288P, 1301P, A304P, Y318P, E324P;

iii) variantes de una termoestabilidad enmendada, por puentes disulfuro (mutaciones dobles a cisteínas): L13C+L65C, N24C+Q300, S218C+A221C, A304C+Y318C.

[0038] Basadas en la estructura 3D de la galactanasa de Bacillus licheniformis, las siguientes variantes son contempladas, donde al menos uno de los residuos abajo mencionados ha sido enmendado y/o al menos una de las alteraciones abajo mencionadas ha sido introducida:

i) variantes de una termoestabilidad enmendada, por inserción de prolinas: K6P, S4P, L2P, K1P, V20P, S26P, K29P, D31P, A54aP, G54eP, N57P, K93P, A97P, N101P, S171P, S185P, T256P, N260P, N266P, D286P, E288aP, A289P, A302dP, S302yP, Y302zP, A302bbP, E302ccP, E302ggP, F305P, 0311 F, F318P;

ii) variantes de una termoestabilidad enmendada, por puentes disulfuro (mutaciones dobles a cisteínas): S18C+Y302qC, G40C+Q330C, V44C+A69C, 148C+A62C, N5OC+D84C, G54gC+T302xC, N56C+G302rC, A62C+G146C, K106C+A159C, K114C+A163C, E183C+G221C, T227C+A283C, A234C+V241C, Y250C+Q273C, A302aaC+A302iiC.

[0039] Variantes adicionales descritas aquí que pueden mostrar propiedades enmendadas con respecto a la unión de sustrato y/o la especificidad de sustrato se enumeran por debajo.

[0040] Según "Nomenclature for sugarbinding subsites in glycosyl hydrolases", G.J. Davis, KS. Wilson and B. Henrissart, Biochemical Journal, Volume 321, páginas 557 a 559 (1997), los llamados subsitios se pueden determinar. Tales subsitios se pueden marcar desde -N a +N (donde N es un número entero). -N representa el extremo de no reducción y +N el extremo de reducción del polisacárido. La escisión tiene lugar entre los subsitios -1 y +1. El constituyente principal de un subsitio de unión de azúcar también se denomina una plataforma aromática. Esto es un residuo aromático, es decir, uno de los siguientes: W, H, Y o F.

[0041] Basado en las figuras 1-4 los inventores identificaron subsitios de la siguiente manera:

Para MTGAL, HIGAl y AAGAL los siguientes subsitios fueron identificados, haciendo referencia aquí a la numeración de posición de SEC ID nº: 1, 2 y 3, respectivamente (no al residuo correspondiente en SEC ID nº: 1):

Subsitio -4: MTGAL ninguno; HIGAL W53; AAGAL ninguno.
Subsitio -2: MTGAL W86; W300; HIGAL W86; W300; AAGAL W86; W301.
Subsitio -1: MTGAL W296; HIGAL W296; AAGAL W297.
Subsitio +1: MTGALY2I7,Y214; HIGALY2I7,Y214;AAGALY2I8,Y215.
Subsitio +2: MT WI83; HIGAL W183; AAGALWI84.

Para BLGAL los siguientes subsitios fueron identificados, haciendo referencia aquí a la numeración de posición de SEC ID nº: 4 (no al residuo correspondiente en SEC ID nº: 1):

Subsitio -4: W363.
Subsitio -3: W347.
Subsitio -2: W115.
Subsitio -1: W320.
Subsitio +1: W237; Y234.

[0042] También los residuos en la proximidad (5 A) de los residuos anteriores se pueden alterar y pueden proporcionar una especificidad de sustrato enmendado y/o unión de sustrato. Estos residuos son los siguiente, haciendo referencia aquí a la numeración de posición de SEC ID nº: 1, 2, 3 y 4, respectivamente (no al residuo correspondiente en SEC ID nº: 1):

MTGAL (SEC ID nº: 1): G6, V7, D8, W9, SlO, S1 1, V12, V13, V14, E15, E16, A18, V20, Y22, L32, L36, T43, V44, R45, Q46, R47, V48, W49, V50, N51, P52, D54, N56, Y57, Y61, Y77, D79, F80, H81, Y82, S83, D84, T85, W86, A87, D88,

P89, A90, H91, 092, T93, M94, P95, G133, N134, E135,1136, R137, G139, L140, L141, W142, H178, L179, D180, N181, 0182, W183, D184, W185, G186, T187, 0188, Nl89, 0210, V211, S212, F213, Y214, P215, F216, Y217, S218, S219, S220, A221, T222, L223, S224, A225, L226, K227, S228, S229, L230, D231, N232, M233, 1241, A242, V243, V244, E245, T246, N247, W248, P249,1250, C252, P255, R256, Y257, S258, F259, P260, 0262, V263, Q273, F276,1277, V280,1283, L293, F294, Y295, W296, E297, P298, A299, W300,1301, H302, N303, A304, N305, L306, G307, S308, S309, C310, A311, D312, N313, T314, M315, F316, S317, Q318, S319, G320, 0321, L326, F329.

HIGAL (SEC ID nº: 2): G6, V7, D8, W9, S10, S11, V12, M13, V14, E15, E16, Ai8, V20, Y22, L32, L36, M43, V44, R45, 046, R47, V48, W49, V50, N51, P52, W53, D54, G55, N56, Y57, N58, Y61, Y77, N79, F80, H81, Y82, S83, D84, T85, W86, A87, D88, P89, A90, H91, Q92, T93, T94, A96, G133, N134, El 35, 1136, T137, Gi39, L141, W142, H178, L179, 0180, N181, G182, W183, N184, W185, D186, T187, Q188, N189, G210, V211, S212, F213, Y214,P215,F216,Y217,5218,A219,S220,A221,T222,L223, D224,S225,L226, R227,R228,S229,L230, N231, N232, M233, V241, A242, V243, V244, E245, T246, N247, W248, P249, C252, P255, R256, Y257, 0258, F259, P260, 0262, V263, 0273, Y276, 1277, V280, V283, L293, F294, Y295, W296, E297, P298, A299, W300, I301, H302, N303, A304, N305, L306, G307, S308, S309, C310, A311, D312, N313, T314, M315, F316, T317, P318, S319, G320, Q321, L326, F329.

AAGAL (SEC ID nº: 3): R5, G6, A7, D8, 19, S10, S11, L12, L13, L14, L15, E16, E18, Y20, Y22, L32, L36, S43, 144, R45, 046, R47, V48, W49, V50, N51, P52, 054, S56, Y57, Y61, Y77, 079, L80, H81, L82, S83, 084, T85, W86, A87, 088, P89, S90, D91, 092, T93, T94, P95, G134, N135, E136,1137, R138, G140, L142, W143, H179, L180, D181, D182, G183, W184, S185, W186, D187, 0188, 0189, N190, G211, V212, S213, Y214, Y215, P216, F217, Y218, S219, A220, S221, A222, T223, L224, A225, S226, L227, K228, T229, S230, L231, A232, N233, L234, V243, V244, V245, E246, 1247, N248, W249, P250, C253, P256, A257, Y258, A259, F260, P261, 0263, L264, 0274, F277, L278, L281, V284, V294, Y295, Y296, W297, E298, P299, A300, W301, 302, G303, N304, A305, G306, L307, G308, S309, S310, C311, A312, D313, N314, L315, M316, V317, D318, Y319, T320, D322, V324, Y325, 1328, L331.

BLGAL (SEC ID nº: 4): K26, G27, V28, 029, V30, S31, S32, A35, L36, Y64, V65, R66, V67, R68,169, W70, N71, D72, P73, Y74, G80, Y81, G82, G83, G84, N85, N86, L106, 0108, F109, H110, Y111, S112, 0113, F114, W115, A116, Q117, P118, A119, k120, 0121, k122, A123, P124, 0161, G163, N164, E165, T166, G169, A171, 0172, H202, F203, T204, N205, P206, E207, T208, R211, Y212, S231, S232, Y233, Y234, P235, F236, W237, H238, G239, T240, L241, N243, L244, V261, A262, E263, T264, S265, Y266, T267, 0274, G275, H276, G277, N278, T279, A280, P281, K282, N283, G284, 0285, T286, L287, N288, 0296, A299, V300, V303, V317, F318, Y319, W320, E321, P322, A323, W324,1325, V327, N336, K337, L339, W340, E341, Y343, G344, S345, G346, W347, A348, T349, S350, Y351, A352, A353, Y355, 0356, P357, E358, 0359, A360, G361, K362, W363, F364, G365, G366, S367, A368, V369, D370, N371, Q372, A373, L374, F375, F388.

[0043] Los aminoácidos anteriores se pueden sustituir con cualquier otro aminoácido, por ejemplo cualquiera de los 19 aminoácidos naturales restantes. En las variantes descritas aquí, al menos uno de los residuos anteriormente mencionados se han enmendado para introducir cualquiera de los otros diecinueves residuos de aminoácidos.

Alineamientos

[0044] El programa ClustalW (CLUSTALW: improving the sensitivity of progressive multiple sequence alignment through sequence weighting, position specific gap penalties and weight matrix choice." Julie D. Thompson, Desmond G. Higgins, and Toby J. Gibson, Nucleic Acids Research, 22(22):46734680 (1994)) se usa para los fines de la presente invención para alineaciones de secuencia de proteína de pares, alineaciones de secuencia de proteína múltiple y alineaciones de perfil de proteína (versión 1.82, parámetros predeterminados).

[0045] Para comparación de secuencia de pares y cálculo de identidad de porcentaje, los parámetros de alineamiento de pares fueron: Lento/Preciso; Penalización por apertura de espacio = 10,00; Penalización por extensión de espacio = 0,10; Matriz de peso de proteína = Gonnet serie; Matriz de peso de ADN = IUB.

[0046] La longitud de consenso es calculada automáticamente por el programa. El número de residuos idénticos (identificados con un asterisco) se cuenta. El porcentaje de identidad de secuencia se calcula de la siguiente manera: el número de residuos idénticos se divide por la longitud de consenso y se multiplica por 100.

[0047] El alineamiento múltiple de la figura 5 se basa en un alineamiento múltiple de las cuatro secuencias usando ClustalW, pero, de manera importante, se combina con información derivada de las estructuras 3D, cada posición de cada estructura se evalúa cuidadosamente, y el alineamiento es modificado por los presentes inventores. En otras palabras, el alineamiento múltiple de la figura 5 no es un simple alineamiento múltiple de ClustalW que refleja sólo las homologías de secuencia, también refleja las similitudes estructurales.

[0048] El alineamiento de la figura 5 se puede usar por lo tanto para deducir las variantes correspondientes en otras estructuras, y estas variantes es posible que también muestren la propiedad enmendada en cuestión. Por ejemplo, la variante anteriormente mencionada A90S+H91 D de MT es transferible a las otras galactanasas originales o estructuras mostradas en la fig. 5 de la siguiente manera: según el alineamiento de la fig. 5, esta variante correspondería a: A90S+H91 D de HI; y A90S+K91 D de BL. Debido a que AA ya tiene la secuencia de S90D91, esta variante no es

pertinente para AA. Otro ejemplo es la variante T288P de AA, que, usando el alineamiento de la figura 5, traduce en S288P en MT y HI, y G288P en BL.

[0049] Otras estructuras de galactanasa de la familia de glicósido 53 se conocen (véase más abajo en originales), y se pueden añadir al alineamiento de la figura 5 como se describe abajo, y así variantes correspondientes se pueden deducir también para estas estructuras, como se acaba de describir anteriormente.

[0050] Para alinear una nueva secuencia al alineamiento múltiple de la figura 5, la opción de ClustalW denominada alineamiento de perfil se usa de la siguiente manera: el alineamiento múltiple de la fig. 5 se usa como perfil 1, y luego la nueva secuencia como perfil 2. Luego el programa pide "alinear secuencia a primer perfil" usando los siguientes parámetros:

Parámetros de alineamiento múltiple = Lento/Preciso; Penalización por apertura de espacio = 10,00; Penalización por extensión de espacio = 0,20; Secuencias divergentes de retraso = 30%; Peso de transiciones de ADN: 0,50; Matriz de peso de proteína = Gonnet series; Matriz de peso de ADN = IUB; Usar matriz negativa = OFF;
Parámetros de espacio de proteína: Alternar penalizaciones específicas de residuo = ON; Alternar penalizaciones hidrofílicas = ON; Residuos hidrofílicos = GPSNDQEKR; Distancia de separación de espacio = 4; Alternar separación de espacio final = OFF.

[0051] En la fig. 6, como un ejemplo, tres secuencias de galactanasa nuevas se han añadido al alineamiento de la fig. 5. Las muevas galactanasas se añaden a la parte inferior del alineamiento, como las filas número 5, 6 y 7. Las galactanasas son: AT (la galactanasa de Aspergillus tubigensis, (SEC ID nº: 7)); BS (la galactanasa de Bacillus subtilis (SEC ID nº: 8)); y PF (la galactanasa de Pseudomonas fluorescens (SEC ID nº: 9)). Así, usando la fig. 6, la variante anteriormente mencionada A90S+H91 D de MT traduce en A9OS+K91 D de BS y E9OS+K91 D de PR. Debido a que AT ya tiene la secuencia de S90D91, esta variante no es importante para AT. Otro ejemplo es la variante T288P de AA, que, usando el alineamiento de la figura 6, traduce en las variantes T288P de AT, G288P de BS y G288P de PF.

[0052] Alternativamente, los alineamientos de secuencias y el cálculo de grado de % de identidad se pueden realizar usando un alineamiento de Smith-Waterman completo, útil tanto para alineamientos de proteína como de ADN. Las matrices de puntuación por defecto BLOSUM5O y la matriz de identidad se usan para alineamientos de proteína y ADN respectivamente. La penalización para el primer residuo en un espacio es 12 para proteínas y 16 para ADN, mientras que la penalización para residuos adicionales en un espacio es 2 para proteínas y 4 para ADN. El alineamiento se puede hacer con el paquete FASTA versión v20u6 (W. R. Pearson and D. J. Lipman (1988), "Improved Tools for Biological Sequence Analysis", PNAS 85:24442448, and W. R. Pearson (1990) "Rapid and Sensitive Sequence Comparison with FASTP and FASTA", Methods in Enzymology, 183:6398).

Original

[0053] El término "galactanasa original" o simplemente "original" se refiere a la galactanasa en la que la variante estaba basada, y también a la galactanasa con la que la variante es comparada y alineada.

[0054] La original puede ser una galactanasa de origen natural (tipo salvaje) o puede sucesivamente incluso ser una variante de la misma preparada por cualquiera de los medios adecuados. Por ejemplo, la galactanasa original puede ser una variante de una galactanasa de origen natural que haya sido modificada o alterada en la secuencia de aminoácidos. Una original también puede ser una variante alélica que es cualquiera de dos o más formas alternativas de un gen que ocupa el mismo locus cromosómico. La variación alélica surge naturalmente a través de la mutación, y puede resultar en polimorfismo dentro de poblaciones como bien se describa en la técnica. Una variante alélica de un polipéptido es un polipéptido codificado por la variante alélica correspondiente de un gen.

Galactanasa

[0055] Esta sección es aplicable a las galactanasas originales, al igual que las galactanasas variantes de la invención.

[0056] Las galactanasas catalizan la endohidrólisis de los enlaces 1,4-beta-D-galactosídicos en arabinogalactanos de tipo I y/o galactanos (véase la estructura de ramnogalacturonano I como se describe en Carpita et al. in Plant J:, 3:130, 1993).

[0057] En el presente contexto, una galactanasa es un polipéptido que tiene actividad de galactanasa. La actividad de galactanasa se puede medir utilizando un sustrato que incluye enlaces 1,4-beta-D-galactosídicos. Ejemplos de sustratos de galactanasa son los arabinogalactanos de tipo I y galactanos. Sustratos especialmente adecuados son i) galactano de altramuz y galactano de patata (disponible comercialmente de, por ejemplo, MegaZyme, Australia); al igual que ii) sustratos de galactano AWL tal como galactano de patata AZCL y galactano de altramuz AWL (también disponible comercialmente de, MegaZyme Australia). Para los sustratos abajo mencionados i) por encima, la actividad de galactanasa se puede medir como liberación de azúcares reductores, mientras que para los sustratos AWL, la actividad de galactanasa se mide espectrofotométricamente (formación de un color azul). En una forma de realización particular, el ensayo de galactanasa se basa en el galactano AWL de altramuces de sustrato.

[0058] El experto en la técnica sabrá adaptar el pH de ensayo y la temperatura de ensayo a la galactanasa en cuestión. Ejemplos de valores de pH de ensayo son pH 2, 3, 4, 5, 6, 7, 8, 9, 10 o 11. Ejemplos de temperaturas de ensayo son 20, 25, 30, 35, 37, 40, 45, 50, 55, 60, 65, 70, 75, 80 o 90°C.

[0059] Un ensayo de galactanasa preferido se describe en el ejemplo 2 aquí.

[0060] En una forma de realización particular, la galactanasa es una enzima clasificada como EC 3.2.1.89, cuyo nombre oficial es arabinogalactano-endo-1,4-beta-galactosidasa. Nombres alternativos son endo-1,4-betagalactanasa, galactanasa o arabinogalactanasa. EC se refiere para Clase de Enzima como se describe en a) http:Ilwww.chem.amul.ac.uk/iubmblenzvmel y/o en b) Enzyme Nomenclature 1992 from NCIUBMB, Academic Press, San Diego, California, publicado por Academic Press para IUBMB en 1992 (ISBN 0122271645), según se ha suplementado y actualizado regularmente. Para suplementos y actualizaciones, por favor consulte http:l/www.chem.cimul.ac.uk/iubmb/enzyme/supplements/ que da detalles con respecto a los suplementos siguientes: Supplement 1(1993) (Eur. J. Biochem., 1994 223,115); Supplement 2 (1994) (Eur. J. Biochem., 1995 232, 16); Supplement 3 (1995) (Eur. J. Biochem., 1996 237, 15); Supplement 4 (1997) (Eur. J. Biochem., 1997, 250, 16); Supplement 5 (1999). (Eur. J. Biochem., 1999, 264, 610650): Supplement 6 (2000); Supplement 7 (2001) y Supplement 8 (2002).

Familia glicósido hidrolasa (GH) 53

[0061] El clasificación EC clasificación anteriormente mencionada se basa principalmente en la especificidad de sustrato de las enzimas, y por lo tanto no refleja las características estructurales de estas enzimas. Una clasificación de glicósido hidrolasas en familias basada en similitudes de secuencia de aminoácidos se propuso hace años; véase el sitio CAZy(ModO) en Internet:

Coutinho, P.M. & Henrissat, B. (1999) Carbohydrate Active Enzymes server at URL: hfto://afmb.cnrs-mrs.fr/-cazy/CAZY/index.htmL and/or Coutinho, P.M. & Henrissat, B. (1999) Carbohydrateactive enzymes: an integrated database approach. In "Recent Advances in Carbohydrate Bioengineering", H.J. Gilbert, G. Davies, B. Henrissat and B. Svensson eds., The Royal Society of Chemistry, Cambridge, pp. 312; Coutinho, P.M. & Henrissat, B. (1999) The modular structure of cellulases and other carbohydrateactive enzymes: an integrated database approach. In "Genetics, Biochemistry and Ecology of Cellulose Degradation"., K. Ohmiya, K. Hayashi, K. Sakka, Y. Kobayashi, S. Karita and T. Kimura eds., Uni Publishers Co., Tokyo, pp. 1523; Henrissat B., A classification of glycosyl hydrolases based on aminoacid sequence similarities. Biochem. J. 280:309316(1991); Henrissat B., Bairoch A. New families in the classification of glycosyl hydrolases based on amino acid sequence similarities. Biochem. J. 293:781788(1993); Henrissat B., Bairoch A. Updating the sequence based classification of glycosyl hydrolases. Biochem. J. 316:695696(1996); and/or Davies G., Henrissat B. Structures and mechanisms of glycosyl hydrolases. Structure 3:853859(1995).

[0062] La familia glicósido hidrolasa 53 se encuentra bajo la entrada acerca de las glicosidasas y las transglicosidasas (o glicósido hidrolasas).

[0063] Estas son formas de realización particulares de la galactanasa de la familia GH 53,

i) es una endo-1,4-beta-galactanasa (EC 3.2.1.89);
ii) tiene un mecanismo catalítico de retención;
iii) tiene Glu como un nucleófilo catalítico o base;
iv) tiene Glu como un donante de protón catalítico;
v) su estructura 3D tiene un pliegue (beta/alfa)8; y/o
vi) pertenece a GHA del clan GH.

[0064] Para los fines de la presente divulgación, las glicósido hidrolasas más abajo de la familia 53 son ejemplos no limitativos de una galactanasa original:

Proteína	Organismo	GenBank	GenPept	SwissProt	Publicación
galactanasa I	Aspergillus aculeatus	L34599	AAA32692.1	P48842	Christgau et al, Curr. Genet. 27:135-141(1995)
endo-1,4-beta-galactanasa (GalA)	Aspergillus niger	AJ305303	CAC83735.1	Q8X168	-
galactanasa GalA	Aspergillus tubingensis	AJ01231 6	CAB40555. 1	Q9Y7F8	Van der Vlugt-Bergmans et al, Biotechnol. Tech. 13:87-92(1999)
ORF 1	Bacillus circulans	L03425	AAA22259.1	P48843	SEC ID nº:10 de WO 00/47711
ORF BH2023	Bacillus halodurans	AP001514 NC_002570	8AB05742.1 NP_242889.1	Q9KBA5	Takami et al, Extremophiles 3(1), 21-28 (1999)
ORF yvfO	Bacillus subtilis	Z94043 Z99121	CABO8009.1 CAB15417.1	007013 007013 032260	SEQ ID NO: 14 of WO 00/47711
YvfO	Bifidobacterium longum	AE014643 NC_004307	AAN24099.1 NP_695463.1		Schell et al, Proc. Natl. Acad. Sci. U.S.A. 99 (22), 14422-14427 (2002)
galactanasa	Cellvibrio japonicus (Pseudomonas cellulosa)	X91885	CAA62990.1	P48841	Braithwaite et al, Biochemistry 36:15489-15500(1997)
ORF CAC2570	Clostridium acetobutylicum	AE007755	AAK80519.1	Q97G04	Nolling et al, J. Bacterial. 183 (16), 4823-4838(2001)
ORF TM1201	Thermotoga maritima	AE001777 NC_000853	AAD36276.1 NP_229006.1	Q9XOS8	Nelson et al, Nature 399:323-329(1999)
Secuencia 2 de la patente US 6242237	Myceliophthora thermophila	AAE73520	AAE73520.1		US 6242237
Secuencia 4 de la patente US6242237	Humicola insolens	AAE73521	AAE73521.1		US 6242237
ORF GalA	Xanthomonas axonopodis pv. citri	AE011762 NC_003919	AAM36180.1 NP_641644.1		da Silva et al, Nature 417 (6887), 459-463 (2002)
ORF XAC0575	Xanthomonas axonopodis pv. citri	AEO11684 NC_003919	AAM35464.1 NP_640928.1		da Silva et al, Nature 417 (6887), 459-463 (2002)
ORF GalA	Xanthomonas campestris pv. campestris	AEO12224 NC_003902	AAM40555.1 NP_636631.1		da Silva et al, Nature 417 (6887), 459-463 (2002)
ORF GalA	Xanthomonas campestris pv. campestris	AE012483 NC_003902	AAM42894.1 NP_638970.1		da Silva et al, Nature 417 (6887), 459-463 (2002)
ORF YP00853	Yersinia pestis	AJ414145 NC_003143	CAC89700.1 NP_404474. 1	Q8ZHN7	Parkhill et al, Nature 413:523-527(2001)
ORF Y3238	Yersinia pestis	AEO13925 NC_004088	AAM86788.1 NP_670537.1		Deng et al J. Bacteriol. 184 (16), 4601-4611 (2002)

[0065] Ejemplos adicionales de una galactanasa original de la invención son las galactanasas derivadas de Meripilus giganteus (SEC ID nº: 2 de WO 97/32013), Pseudomonas fluorescens, Bacillus agaradhaerens (SEC ID nº: 12 de WO 00/47711) y Bacillus licheniformis (SEC ID nº: 8 de WO 00/47711).

[0066] La presente divulgación específicamente incluye variantes de cada una de las galactanasas originales específicas anteriores de la familia GH 53 que corresponden a las variantes reivindicadas de MTGAL, HIGAL, AAGAL y BLGAL, tales variantes son derivables por adición de la secuencia de galactanasa original en cuestión al alineamiento de la fig. 5 como se ha descrito anteriormente para la construcción de la figura 6, y traducción de cada variante MTGAL, HIGAL, AAGAL o BLGAL en la galactanasa original en cuestión, usando el concepto del residuo de aminoácido correspondiente tal como se ha definido anteriormente.

[0067] En una primera divulgación, la galactanasa de la familia GH original 53 es una galactanasa fúngica. La galactanasa fúngica se puede derivar a partir de una levadura o de un hongo filamentoso. La galactanasa de levadura se puede derivar de Yersinia, por ejemplo de Yersinia pestis. La galactanasa fúngica filamentosa se puede derivar a partir de una cepa de Aspergillus, Humicola, Meripilus, Myceliophthora o Thermomyces. Ejemplos de estas cepas son Aspergillus aculeatus, Aspergillus niger, Aspergillus tubingensis, Humicola insolens, Meripilus giganteus y Myceliophthora thermophila.

[0068] En una segunda divulgación, la galactanasa de la familia GH 53 original es una galactanasa bacteriana. La galactanasa bacteriana se puede derivar a partir de una cepa de Bifidobacterium, Cellvibrio, Clostridium, Pseudomonas, Thermotoga o Xanthomonas. Ejemplos de tales cepas son Bacillus agaradhaerens, Bacillus circulans, Bacillus halodurans, Bacillus licheniformis, Bacillus subtilis, Bifidobacterium longum, Cellvibrio japonicus, Clostridium acetobutylicum, Pseudomonas fluorescens, Pseudomonas cellulosa, Thermotoga maritime, Xanthomonas axonopodis pv. citri y Xanthomonas campestris pv. campestris.

[0069] Galactanasas originales particularmente preferidas son aquellas con los números de registro del GenBank, GenPept o SwissProt anteriormente mencionados y aquellas con los números de SEC ID anteriormente mencionados.

[0070] Además, galactanasas originales de familia GH 53 particularmente preferidas son las siguientes:

Cepa de origen	Número de secuencia (aquí)	Abreviaturas usadas aquí
Myceliophthora thermophila	SEC ID nº: 1	MTGAL o MT
Humicola insolens	SEC ID nº: 2	HIGAL o HI
Aspergillus aculeatus	SEC ID nº: 3	AAGAL o AA
Bacillus licheniformis	SEC ID nº: 4	BLGAL o BL

[0071] Subgrupos preferidos de lo anterior son a) MTGAL, HIGAL, AAGAL; b) MTGAL, HIGAL, BLGAL; y c) MTGAL, HIGAL.

[0072] En una tercera divulgación, la galactanasa original tiene un porcentaje de identidad con SEC ID nº: 1 de al menos 25%, utilizando el programa ClustalW y los ajustes mencionados anteriormente. En otras descripciones particulares, el porcentaje de identidad es al menos 30, 35, 40, 45, 50, 55, 60, 65, 70, 75, 80, 85, 90, o al menos 95%.

[0073] En una cuarta divulgación, la variante de galactanasa tiene un porcentaje de identidad con SEC ID nº: 1 de al menos 50%, usando el programa ClustalW y los ajustes mencionados anteriormente. En otras descripciones particulares, el porcentaje de identidad es al menos 55, 60, 65, 70, 75, 80, 85, 90, 95, 97 o al menos 99%.

[0074] En una quinta divulgación, la galactanasa original tiene un porcentaje de identidad con SEC ID nº: 2 de al menos 25%, usando el programa ClustalW y los ajustes mencionados anteriormente. En otras descripciones particulares, el porcentaje de identidad es al menos 30, 35, 40, 45, 50, 55, 60, 65, 70, 75, 80, 85, 90 o al menos 95%.

[0075] En una sexta divulgación, la variante de galactanasa tiene un porcentaje de identidad con SEC ID nº: 2 de al menos 50%, usando el programa ClustalW y los ajustes mencionados anteriormente. En otras descripciones particulares, el porcentaje de identidad es al menos 55, 60, 65, 70, 75, 80, 85, 90, 95, 97 o al menos 99%.

[0076] En una séptima divulgación, la galactanasa original tiene un porcentaje de identidad con SEC ID nº: 3 de al menos 25%, usando el programa ClustalW y los ajustes mencionados anteriormente. En otras descripciones particulares, el porcentaje de identidad es al menos 30, 35, 40, 45, 50, 55, 60, 65, 70, 75, 80, 85, 90 o al menos 95%.

[0077] En una octava divulgación, la variante de galactanasa tiene un porcentaje de identidad con SEC ID nº: 3 de al menos 50%, usando el programa ClustalW y los ajustes mencionados anteriormente. En otras descripciones particulares, el porcentaje de identidad es al menos 55, 60, 65, 70, 75, 80, 85, 90, 95, 97 o al menos 99%.

[0078] En una novena divulgación, la galactanasa original tiene un porcentaje de identidad con SEC ID nº: 4 de al menos 25%, usando el programa ClustalW y los ajustes mencionados anteriormente. En otras descripciones particulares, el porcentaje de identidad es al menos 30, 35, 40, 45, 50, 55, 60, 65, 70, 75, 80, 85, 90 o al menos 95%.

[0079] En una décima divulgación, la variante de galactanasa tiene un porcentaje de identidad con SEC ID nº: 4 de al menos 50%, usando el programa ClustalW y los ajustes mencionados anteriormente. En otras descripciones particulares, el porcentaje de identidad es al menos 55, 60, 65, 70, 75, 80, 85, 90, 95, 97 o al menos 99%.

[0080] En otras descripciones particulares, de cada una de las anteriores primera a décima descripciones, el alineamiento es un alineamiento de Smith-Waterman completo con los ajustes mencionados anteriormente, preferiblemente hecho con el paquete FASTA también mencionado anteriormente.

[0081] Debe entenderse que también las variantes de galactanasas se contemplan como la enzima original.

Preparación de variantes de galactanasa

[0082] Las variantes de galactanasa se pueden preparar por cualquier método conocido en la técnica, véase por ejemplo el ejemplo 1 de la presente. Típicamente, se prepara una biblioteca de variantes de galactanasa. El término "biblioteca aleatorizada", "biblioteca de variantes" o simplemente "biblioteca" se refiere a tal biblioteca de variantes de galactanasa. La diversidad en la biblioteca de variantes se puede generar a través de mutagénesis de los genes que codifican las variantes en el nivel de triplete de ADN, de manera que los codones individuales se diversifiquen, por ejemplo, usando cebadores de secuencia parcialmente aleatorizada en una reacción por PCR. Diferentes técnicas se han descrito, por las que uno puede crear una biblioteca combinatoria diversa diversificando diferentes posiciones de nucleótidos en un gen y recombinando éstos, por ejemplo donde estas posiciones están demasiado separadas para ser cubiertas por un único cebador oligonucleótido (enriquecido o dopado). Estas técnicas incluyen el uso de recombinación in vivo de los segmentos génicos individualmente diversificados tal y como se describe en la WO 97/07205 en la página 3, líneas 8 a 29 (Novozymes A/S). También incluyen el uso de técnicas de redistribución de ADN para crear una biblioteca de genes de longitud total, donde diferentes segmentos génicos son combinados, y donde cada segmento se puede diversificar por ejemplo por mutagénesis enriquecida (Stemmer, Nature 370, pp. 389391, 1994 y US 5.811.238; US 5.605.793; y US 5.830.721). Uno puede usar un gen que codifica una "estructura" de galactanasa (galactanasa original de tipo salvaje) como un polinucleótido modelo, y combinar éste con uno o varios oligonucleótidos mono o bicatenarios tal y como se describe en la WO 98/41623 y en la WO 98/41622 (Novozymes A/S). Los oligonucleótidos monocatenarios se podrían aleatorizar parcialmente durante la síntesis. Los oligonucleótidos bicatenarios podrían ser productos de PCR que incorporan diversidad en una zona específica. En ambos casos, uno puede diluir la diversidad con los segmentos correspondientes que codifican la secuencia de la galactanasa de estructura para limitar el número medio de cambios que son introducidos.

[0083] También se han establecido métodos para el diseño de las proporciones de mezclas de nucleótidos (A; C; T; G) que se van a insertar en las posiciones de codón específicas durante la síntesis de oligo o polinucleótidos, para introducir un margen de error para aproximar una distribución de frecuencia deseada hacia un conjunto de uno o varios aminoácidos deseados que serán codificados por los codones particulares. Puede ser de interés producir una biblioteca de variantes que comprenda permutaciones de un número de modificaciones de aminoácidos conocidas en diferentes ubicaciones de la secuencia primaria del polipéptido. Estos podrían ser introducidos de forma post traduccional o por sitios de modificación química, o podrían ser introducidos a través de mutaciones en los genes de codificación. Las modificaciones en sí mismas pueden haberse probado previamente como beneficiosas para una razón u otra (por ejemplo, disminución de antigenicidad o mejora de actividad específica, rendimiento, estabilidad u otras características). En tales casos, puede ser deseable primero crear una biblioteca de combinaciones diversas de secuencias conocidas. Por ejemplo, si doce mutaciones individuales se conocen, se podría combinar (al menos) doce segmentos del gen de codificación de la proteína original, donde cada segmento está presente en dos formas: una con y una sin la mutación deseada. Mediante la variación de las cantidades relativas de esos segmentos, se podría diseñar una biblioteca (de tamaño 212) para que el número medio de mutaciones por gen se pueda predecir. Esta puede ser una forma útil de combinar mutaciones, que por ellas mismas den algo, pero no suficiente efecto, sin recurrir a mu bibliotecas y grandes, como suele ser el caso cuando se usa "mutagénesis enriquecida". Otra forma de combinar estas "mutaciones conocidas" podría ser el uso de la redistribución de familia de ADN oligomérico que codifica las mutaciones conocidas con fragmentos de la secuencia de tipo salvaje de longitud total.

[0084] El ADN mutado se puede expresar por cualquier método conocido en la técnica, véase, por ejemplo, el ejemplo 1. Generalmente, la célula huésped puede ser un microorganismo unicelular, por ejemplo, un procariota, o un microorganismo no unicelular, por ejemplo, un eucariota.

[0085] Células unicelulares útiles son bacterias tales como Bacillus, Streptomyces, E. coli, Pseudomonas sp., Lactococcus, Lactobacillus, Leuconostoc, Streptococcus, Pediococcus y Enterococcus.

[0086] Ejemplos de células eucariotas son células animales no humanas, células de insecto, células vegetales o células fúngicas. Ejemplos de células fúngicas son Candida, Hansenula, Kluyveromyces, Pichia, Saccharomyces, Schizosaccharomyces, Yarrowia, Acremonium, Aspergillus, Fusariurn, Humicola, Mucor, Myceliophthora, Neurospora, Penicillium, Thielavia, Tolypocladium y Trichoderma.

Aplicaciones

[0087] Las variantes de galactanasa de la invención son útiles en piensos para animales, véase, por ejemplo, la WO 97116982. Ejemplos no limitativos de características deseables de variantes de galactanasa para aplicaciones de alimentación son: estabilidad a altas temperaturas, estabilidad ácida y alta actividad específica.

[0088] Las variantes de galactanasa de la invención también se puede usar para preparar galactooligosacáridos y para la hidrólisis de lactosa, ambos pertinentes para, por ejemplo, la industria láctea. Por ejemplo, el método del ejemplo 5 se puede usar para selección de variantes de galactanasa para actividad mejorada en la lactosa, en particular para transglicosilación mejorada y/o actividad hidrolítica en la lactosa.

[0089] Las reacciones de transglicosilación observadas con ONPG (ejemplo 4) se pueden usar para selección de variantes de galactanasa para afinidades de aceptor adecuadas. La selección puede ser una selección de alto rendimiento. Esto proporciona conocimiento valioso de las afinidades de los subsitios individuales (tales como los subsitios +1, +2, +3, +4) para varios aceptores, por ejemplo galactosa (Gal), β-1,4-galactobiosa (Gal2) (Megazyme), β-1,4-galactotriosa (Gal3), β-1,4-galactotetraosa (Gal4), glucosa (Glu), arabinosa (Ara), ácido galacturónico (GalA), maltosa (Mal) o maltotriosa (Mal3).

[0090] Los resultados de ejemplo 3 proporcionan conocimiento de subsitios individuales para galactosa (-3 a +3), al igual que conocimiento de las tendencias para transglicosilato en vez de hidrolizar sustratos. Este conocimiento es útil para el diseño de variantes de galactanasa de propiedades deseadas.

Ejemplos

Ejemplo 1: Preparación de variantes de galactanasa

[0091] La mutación D181N se introdujo en el gen de codificación AAGAL por el uso del oligonucleótido mutagénico 5'-CAT TTG GAC AAC GGC TGG AGC -3' (SEC ID nº: 5) y el método de megacebado descrito por Sarkar, G. y Sommer, S.S., 1990. The "Megaprimer" Method of Site Directed Mutagenesis. BioTechniques, 8: 404407. Las mutaciones D181N+S9OA+D91H fueron introducidas de manera similar.

[0092] Los genes de variantes resultantes fueron clonados en el plásmido pHD464 como se describe en Dalbøge H., Heldt-Hansen H. 1994. A novel method for efficient expression cloning of fungal enzyme genes. Mol. Gen. Genet. 243: 253260, y la introducción correcta de las mutaciones se verificó por secuenciación del ADN.

[0093] La doble mutación A90S+H91 D fue introducida en el gen de codificación MTGAL esencialmente como se ha descrito anteriormente por el uso del oligonucleótido mutagénico 5'- GCC GAT CCT TCT GAT CAG ACC ATG CC -3' (SEC ID nº: 6).

[0094] Las proteínas fueron expresadas en, y segregadas a partir de Aspergillus oryzae esencialmente como se describe en Christensen, T., Wöldike, H., Boel, E., Mortensen, SR, Hjortshøj, K., Thim, L., Hansen, MT., 1988. High level expression of recombinant genes in Aspergillus oryzae. Bio/Technology 6, 14191422_.

Ejemplo 2: Purificación y caracterización de variantes de galactanasa

Purificación de variantes de galactanasa de Aspergillus aculeatus

[0095] El sobrenadante del cultivo de una fermentación de la cepa de Aspergillus oryzae que expresa la variante de galactanasa de Aspergillus aculeatus recombinante dirigida al sitio D181N (descrita en el ejemplo 1) fue filtrado a través de un filtro de 0,22 m para eliminar los micelios. Al filtrado de 1200 ml se añadió sulfato de amonio a una concentración de 1,6 M, cargado sobre una columna de 50 ml de butilo equilibrada con 25 mM de acetato sódico, 1,6 M de sulfato de amonio pH 5,0 y eluido utilizando un sulfato de amonio lineal decreciente de 1,6 M a 0 M sobre 10 volúmenes de columna. La actividad de galactanasa se midió mediante la mezcla de 40 µl de fracciones con 200 µl 10 mg/ml de AWL-galactano de altramuces (Megazyme, Australia) en 0,5 M de MES pH 6,5. Después de aproximadamente 30 mm de incubación a temperatura ambiente, el sustrato insoluble se retiró por centrifugado y se midió la absorbancia del sobrenadante a 590 nm. Fracciones que contienen actividad de galactanasa eluidas alrededor de 1 M de sulfato de amonio fueron agrupadas y dializadas contra 10 mM de citrato sódico pH 3,5. El dialisato (400 ml) se diluyó a 2000 ml con agua y se cargó sobre una columna de 50 ml de S-Sefarosa equilibrada con 10 mM de citrato sódico pH 3,5. La actividad de galactanasa no se enlazó con esta columna y se concentró a 80 ml en un dispositivo de ultrafiltración de Amicon con un 10 kDa de filtro de corte. El concentrado fue al menos 95% puro estimado a partir de SDS-PAGE.

[0096] El sobrenadante del cultivo de una fermentación de la cepa de Aspergillus oryzae que expresa la variante de galactanasa de Aspergillus aculeatus recombinante dirigida al sitio D181N+S90A+D91H fue filtrado como se ha descrito anteriormente. A 900 ml de filtrado se añadió sulfato de amonio a una concentración de 1,6 M, y se eluyó a partir de una columna de 50 ml de butilo como se ha descrito anteriormente. La actividad de galactanasa fue medida como se ha descrito anteriormente. Las fracciones que contenían actividad de galactanasa se eluyeron aproximadamente 0,35 M de sulfato de amonio y fueron agrupadas y dializadas contra 25 mM de acetato sódico pH 5,5. El dialisato (200 ml) se diluyó a 275 ml con agua, se cargó sobre una columna de 50 ml de Q-Sefarosa equilibrada con 25 mM de acetato sódico pH 5,5, y se eluyó con un gradiente lineal de 0 a 1 M de NaCl sobre 10 volúmenes de columna. Las fracciones que contenían actividad de galactanasa (alrededor de 0,8 M de NaCl) fueron agrupadas y concentradas a 10 ml en un dispositivo de ultrafiltración de Amicon con un filtro de corte de 10 kDa. El concentrado fue al menos 95% puro estimado a partir de SDS-PAGE.

Purificación de variantes de galactanasa de Myceliophthora thermophila

[0097] El sobrenadante del cultivo de una fermentación de la cepa de Aspergillus oryzae que expresa la variante de galactanasa de Myceliophthora thermophila recombinante dirigida al sitio A90S+H91D (descrito en el ejemplo 1) fue filtrado a través de un filtro de 0,22 µm para eliminar los micelios. Al filtrado de 1200 ml se añadió sulfato de amonio a una concentración de 1,6 M, se cargó sobre una columna de 50 ml de butilo equilibrada con 25 mM de acetato sódico, 1,6 M de sulfato de amonio pH 5,0 y se eluyó utilizando un sulfato de amonio lineal decreciente de 1,6 M a 0 M sobre 10 volúmenes de columna. La actividad de galactanasa fue medida mediante la mezcla de 40 µl de fracciones con 200 µl 10mg/ml AWL-galactano de altramuz (Megazyme, Australia) en 0,5 M de MES pH 6,5. Después de aproximadamente 30 mm de incubación a temperatura ambiente, el sustrato insoluble se eliminó por centrifugado, y la absorbancia del sobrenadante se midió en 590 nm. Fracciones que contienen actividad de galactanasa eluidas alrededor de 1 M de sulfato de amonio fueron agrupadas y dializadas contra 10 mM de citrato sódico pH 3,5. El dialisato (400 ml) fue diluido a 2000 ml con agua y cargado sobre una columna de 50 ml de S-Sefarosa equilibrada con 10 mM de citrato sódico pH 3,5. La actividad de galactanasa no enlazaba con esta columna y fue concentrada a 80 ml en un dispositivo de ultrafiltración de Amicon con un filtro de corte de 10 kDa. El concentrado fue al menos 95% puro estimado a partir de SDS-PAGE.

Caracterización de las variantes purificadas

[0098] Los perfiles de pH de las variantes purificadas anteriormente descritas fueron establecidos de la siguiente manera: la actividad de galactanasa en varios pH se midió mediante la mezcla 500 µl 4 mg/ml de AWL-galactano de altramuz (Megazyme, Australia) en agua con 500 µl de tampón (50 mM de acetato sódico, 50 mM de dihidrogenfosfato de potasio, 50 mM de ácido bórico, 1 mM de CaCl2, 0,01% de Tritón X100 ajustado a pH 2,5, 3,5, 4,5, 5,5, 6,5, 7,5, 8,5 o 9,5 con HCl/NaOH) y 25 µl de enzima purificada diluida a aproximadamente 0,5-2 µg/ml en agua. La mezcla fue incubada 15 mm a 37°C, el material insoluble se retiró por centrifugado, y la absorbancia en el sobrenadante se midió a 590 nm.

[0099] De los resultados mostrados en la tabla 1 por debajo, aparece que los perfiles de pH han cambiado (el perfil de las variantes de AAGAL D181N y D181N+S90A+D91H han sido desplazados al lado alcalino; y el perfil de pH de la variante MTGAL A9OS+H91D ha sido desplazado al lado ácido, en comparación con los tipos salvajes).

Tabla 1

Galactanasa/pH	2,5	3,5	4,5	5,5	6,5	7,5	8,5	9,5
AAGAL	73	100	83	47	32	0	2	0
AAGALD181N	74	99	100	87	74	35	7	0
AAGALD181N+S9OA+091H	55	59	71	83	100	90	21	0
MTGAL	0	12	41	63	90	100	54	7
MTGALA90S+H911D	0	8	51	75	100	95	35	4

Ejemplo comparativo 3: Actividad en galactooligosacáridos

Preparación de galactotriosa (Gal3), galactotetraosa (Gal4), metil-galactotriósido (MeGal3) y metil-galactotetraósido (MeGal4)

[0100] Galactano (altramuz) se compró de Megazyme. Todos los solventes, reactivos y placas de TLC (gel de sílice 60 F254) se compraron de Merck. Espectros de 1H-RMN fueron registrados en un Varian Mercury 400 MHz a 30°C. Como

valores de referencia CHCl3 en COCl3 (7,27 ppm) y HDO en D20 (4,67 ppm) fueron usados. Cromatografía en columna rápida fue realizada utilizando un módulo de cromatografía FLASH 40i de Biotage.

[0101] Undeca-O-acetil galactotriosa: galactano de altramuz tratado con arabinofuranosidasa (0,50 g) fue disuelto en 10 mM de tampón Bis-Tris pH 6,5 (50 mL) por agitación durante 1 h a 37°C. BLGAL se añadió (250 GalU/mL) y la solución se agitó durante 3 h a 37°C y luego 5 mm a 100°C. TLC (eluyente: propanol/etanol/H2O (7:1:2)) mostró un producto mayor (Gal3) y menor (Gal4) ambos eluyendo bajo galactobiosa comercial. Tras el enfriamiento, la solución se concentró, secó y acetiló y se elaboró por procedimientos estándar (Ac2O/piridina, 48 h a temperatura ambiente (rt)). El producto bruto fue purificado por cromatografía en columna rápida (eluyente: EtOAc/heptano 5:2) para dar 0,20 g de Gal3 peracetato puro (mezcla de alfa y beta-anómero (1:2)). 1H RMN (datos seleccionados, CDCl3): 6,29 ppm (d, J1,2 = 3,5 Hz, H-1alfa), 5,63 ppm (d, J1,2 = 8,4 Hz, H-1β).

[0102] Galactotriosa (Gal3): la desacetilación de la triosa acetilada se realizó por agitación durante toda la noche en metanol/NaOCH3 (1 mL 1M de NaOCH3 en 3 ml de metanol) y luego se neutralizó por adición de Dowex 50 Wx8. Se añadió agua (2 mL) y la resina se retiró por filtración. La solución limpia se concentró (liofilización) para dar 0,10 g de sólido G3. MS (MALDITOF): 527 (M+23, Na). 1H RMN (datos seleccionados, D2O): 5,20 ppm (d, J = 3,6 Hz, H-1alfa), 4,5-4,6 (3 x d, H-1β, H-1', H1").

[0103] Metil deca-O-acetil galactotriósido. La galactotriosa acetilada (0,24 g) se convirtió en bromuro por tratamiento (5 h) con 30% HBr en ácido acético (2,5 mL) y CH2Cl2 (2 mL) a 0°C →rt. La reacción se elaboró por procedimientos estándar y se concentró para dar un jarabe amarillento (194 mg) del compuesto de alfa-bromo, que se usó sin purificación adicional. 1H RMN (datos seleccionados, CDCl3): 6,57 ppm (d, 1 H, J1,2 = 3,8 Hz, H-1). El bromo-glicósido (0,19 g, 0,20 mmol) fue convertido en glicósido de metilo por tratamiento durante toda la noche con Ag2CO3 (60 mg, 22 mmol) en el metanol seco (10 mL) (bajo nitrógeno). Después de la elaboración, el glicósido de metilo fue purificado por cromatografía en columna rápida (eluyente: EtOAc/heptano (3:1)) para dar 30 mg de compuesto puro (aceite incoloro). 1H RMN (datos seleccionados, CDCl3): 4,48 ppm, 4,39 ppm y 4,35 ppm (3xd, 3H, J1,2 = 8,0 Hz, H-1; H-1' y H-1"), 3,47 ppm (3H, s, OCH3).

[0104] Metil galactotriósido (MeGal3). El glicósido de metilo acetilado (30 mg) fue desacetilado como se ha descrito anteriormente para dar 10 mg de material espeso.

[0105] Galactotetraosa (Gal4). Esta se preparó como se describe para Gal3 usando 100 GalU/mL. Rendimiento de producto desacetilado final: 17 mg.

[0106] Metil galactotetraósido (MeGal4). Este compuesto se preparó en la analogía con MeGal3 y 41 mg de MeGal4 se obtuvieron a partir de 1 g de galactano. MS (MALDITOF): 704 (M+23, Na).

Actividad de HIGAL, MTGAL, AAGAL y BLGAL en galactooligosacáridos

[0107] La actividad en los sustratos de galactooligosacárido preparada como se ha descrito anteriormente y en la galactobiosa disponible comercialmente (Gal2, Megazyme) fue estudiada para las cuatro galactanasas purificadas HIGAL, MTGAL, AAGAL y BLGAL. Los tampones y las temperaturas usados fueron: 25mM de acetato sódico, 0,5mM de CaCl2, 0,005% de Tritón X100, pH 6,5 a 37°C para HIGAL y MTGAL, 50 mM de acetato sódico, 1 mM de CaCl2, pH 4 a 30°C para AAGAL y 50 mM de Mes, 1 mM de CaCl2, pH 6,5 a 30°C para BLGAL. Las concentraciones enzimáticas usadas fueron 0,8 µg/ml para HIGAL, 0,2 µg/ml para MTGAL, y 10 µg/ml para AAGAL y BLGAL. Con HIGAL y MTGAL, las concentraciones de sustrato fueron todas 0,25 mg/ml, mientras que 0,34 mg/ml de Gal2, 0,050 mg/ml de Gal3 y 0,067 mg/ml de Gal4 fueron usados para AAGAL y BLGAL. La actividad enzimática en las muestras retiradas después de varios tiempos de incubación fue inactivada por calentamiento a 95°C durante 10 mm. Las composiciones de los productos reactivos fueron analizadas usando HPAE-PAD (Dionex) aplicando una columna PA100 y un gradiente lineal de acetato sódico (0-0,18 M) en 0,15 M de NaOH. Los factores de respuesta de los carbohidratos individuales fueron estimados a partir de las ejecuciones de referencia con MeGal3, MeGal4, Gal, Gal2, Gal3 y Gal4. Los resultados seleccionados se muestran en las tablas 2-8 más adelante (las figuras indican porcentaje en peso de galactooligosacáridos).

[0108] Ninguna de las enzimas HIGAL, MTGAL, AAGAL o BLGAL tuvo ninguna actividad detectable en Gal2 en 24 horas. HIGAL, MTGAL y AAGAL degradaron Gal3 a Gal2 y Gal, mientras que BLGAL no tuvo ninguna actividad visible en Gal3 después de 24 horas. La incubación de HIGAL y MTGAL con MeGal3 (véase tablas 2 y 3) dio una liberación mucho más alta de MeGal que de MeGal2, lo que indica que Gal se libera a partir del extremo reductor de Gal3 con ambas enzimas. HIGAL y MTGAL degradó Gal4 (también conteniendo aproximadamente 40% de Gal3) (tablas 4 y 5) principalmente a Gal y Gal2, mientras que Gal3 no se acumuló. Resultados para HIGAL y MTGAL con MeGal4 (tablas 6 y 7) dieron liberación inicial principalmente de MeGal, MeGal2 y Gal3 y algo de Gal2 pero poco Gal, nuevamente indicando que Gal se libera principalmente a partir del extremo reductor de Gal4. La producción de Gal a partir de MeGal4 en los últimos estadios de la hidrólisis se puede deber principalmente a la hidrólisis de productos de transglicosilación sin grupo metilo en el extremo reductor. BLGAL degrada galactotetraosa principalmente a galactosa y galactotriosa. Con MeGal4 los productos principales de BLGAL fueron MeGal y Gal3, indicando que Gal se libera a partir del extremo reductor de Gal4. Con AAGAL los productos iniciales de galactotetraosa son aproximadamente

cantidades equimolares de galactosa, galactobiosa y galactotriosa, pero posteriormente la galactotriosa se degrada a galactobiosa y galactosa.

Tabla 2: Degradación de MeGal3 con HIGAL

Tiempo de incubación (horas)	0,0	0,5	2,2	5,0	72,0
Gal	0,0	0,0	2,3	3,0	17,1
Gal2	0,0	3,9	12,5	20,2	36,2
Gal3	0,0	1,2	3,3	10,6	8,0
MeGal	0,0	11,4	18,4	36,8	34,6
MeGal2	0,0	3,3	3,7	5,2	4,2
MeGal3	100,0	80,3	59,7	24,2	0,0

Tabla 3: Degradación de MeGal3 con MTGAL

Tiempo de incubación (horas)	0,0	0,5	2,2	5,0	72,0
Gal	0,0	0,0	14,1	2,2	6,5
Gal2	0,0	0,0	8,5	10,9	37,2
Gal3	0,0	0,0	0,4	15,7	23,2
MeGal	0,0	10,1	27,6	17,4	28,3
MeGal2	0,0	2,7	1,9	3,2	3,5
MeGal3	100,0	87,2	47,5	50,6	1,3

Tabla 4: Degradación de Gal4 con HIGAL

Tiempo de incubación (horas)	0,0	0,5	2,2	5,0	72,0
Gal	0,0	5,8	16,7	35,6	65,2
Gal2	0,0	8,1	21,9	34,8	33,6
Gal3	42,0	43,2	39,8	23,9	0,9
Gal4	58,0	42,9	21,6	5,7	0,2

Tabla 5: Degradación de Gal4 con MTGAL

Tiempo de incubación (horas)	0,0	0,5	2,2	5,0	72,0
Gal	0,0	11,6	14,9	29,2	54,9
Gal2	0,0	9,9	17,4	29,1	43,5
Gal3	42,0	27,7	45,5	29,5	1,5
Gal4	58,0	50,8	22,3	12,1	0,0

Tabla 6: Degradación de MeGal4 con HIGAL

Tiempo de incubación (horas)	0,0	0,5	2,0	5,0	24,0
Gal	0,0	2,3	1,6	7,4	26,4
Gal2	0,0	6,3	5,0	13,8	25,3
Gal3	0,0	20,6	16,0	19,7	9,1
Gal4	0,0	3,3	3,2	3,2	1,7
MeGal	1,6	12,1	10,5	16,6	19,1
MeGal2	4,7	12,6	13,2	16,1	13,4
MeGal3	14,8	17,2	18,4	15,5	5,0
MeGal4	79,0	24,5	32,1	7,6	0,0

Tabla 7: Degradación de MeGal4 con MTGAL

Tiempo de incubación (horas)	0,0	0,5	2,0	5,0	24,0
Gal	0,0	0,9	4,8	12,4	24,2
Gal2	0,0	3,3	10,9	20,1	32,7
Gal3	0,0	13,7	23,9	17,9	3,4
Gal4	0,0	2,5	3,7	2,9	1,1
MeGal	1,6	8,9	16,2	19,3	20,1
MeGal2	4,7	9,6	13,6	13,9	13,3
MeGal3	14,8	17,1	16,0	9,9	2,3
MeGal4	79,0	43,9	10,9	3,5	2,9

Ejemplo comparativo 4: Actividad con o-nitrofenil-β-D-galactopiranósido (ONPG)

[0109] La actividad de HIGAL y MTGAL con ONPG se evaluó mediante la mezcla de 200 µl (normalmente 5,5 mg/ml) de ONPG en 50mM de acetato sódico, 1 mM de CaCl2, 0,01% de Tritón X1 00, pH 6,5 con 25 µl de galactanasa (normalmente 1 mg/ml) en el pocillo de una placa de microtitulación. La liberación de o-nitrofenol (ONP) se midió a temperatura ambiente a 405 nm cada 10 segundos normalmente durante 30 mm en un SpectraMaxPlus (Molecular Devices). Los efectos en la liberación observada de ONP se estudiaron con concentración enzimática variada, concentración de ONPG y con adición de galactosa (Gal), β-1,4-galactobiosa (Gal2) (Megazyme), β-1,4-galactotriosa (Gal3), β-1,4-galactotetraosa (Gal4), glucosa (Glu), arabinosa (Ara), ácido galacturónico (fiesta), maltosa (Mal) o maltotriosa (Mal3).

[0110] En las tablas 8-11 por debajo, se enumeran los tiempos de incubación requeridos para aumentar la absorbancia observada a 405 nm por cantidades dadas. Células marcadas 'n.a.' indican que el aumento en la absorbancia no se alcanzó en el experimento. En general, el aumento inicial en la absorbancia a 405 nm fue muy lento, pero después de que una fase de latencia el índice de liberación de ONP frecuentemente aumentó drásticamente frecuentemente aproximadamente exponencialmente. La explicación más probable para la cinética observada es que ONPG reacciona con la enzima para dar un intermedio de enzima-galactosil que hidroliza muy lentamente. En cambio, el Gal del intermedio se libera por transglicosilación, inicialmente con ONPG o azúcar añadido como aceptor. En casos donde el índice de liberación de ONP aumenta, estos productos de transglicosilación son aún mejores aceptadores que los iniciales. Como se ha visto en la tabla 8, el índice de liberación de ONP es aproximadamente proporcional a la cantidad de enzima añadida. HIGAL libera ONP más rápido que MTGAL a dosificación de enzima idéntica. La adición de Gal (5 mg/ml) se ve que ralentiza la liberación de ONP por aproximadamente un factor de dos para MTGAL y un factor de tres para HIGAL. Probablemente, Gal no ralentiza significativamente la formación del intermedio enzima-galactosil, que se acumularía incluso si Gal tuviera alta afinidad para el subsitio -1 o +1. Más posiblemente, Gal inhibe la transglicosilación posterior, que requiere la unión de ONFG a los subsitios +1 y +2, por ejemplo por unión al subsitio +2. Con 50 mg/ml de Gal añadido (resultados no mostrados) la liberación de ONP fue incluso más lenta con sólo aumento insignificante de absorbancia a 405 nm en 30 mm.

[0111] Los resultados en la tabla 9 muestran que el índice de liberación de ONP es similar con 5 y 10 mg/ml de ONPG pero más lento a 2,5 y especialmente 1,25 mg/ml de ONPG. Esto indica que el índice que limita la reacción de transglicosilación con ONPG como aceptor tiene un Km de aproximadamente 3 mg/ml.

[0112] En la tabla 10 se dan los efectos de adición de 0,5 o 0,05 mg/ml de Gal2, Gal3 o Gal4. A diferencia de Gal, cada uno de estos tres galactooligosacáridos aumenta el índice de liberación de ONP. Los índices de liberación de ONP iniciales indican que Gal4 es más eficaz que Gal3 como aceptor, y que Gal3 es más eficaz que Gal2. Con Gal2 y Gal3, el índice de liberación de ONP aumenta significativamente con el tiempo de incubación, indicando que los productos de transglicosilación (inicialmente Gal3 y Gal4, respectivamente) son aceptores más eficaces que los azúcares añadidos, mientras que el índice de liberación es relativamente constante con Gal4. Estos resultados indican que HIGAL posee cuatro subsitios significativos (+1,+2, +3, +4) en el lado de reducción del enlace dividido.

[0113] En la tabla 11 se dan los resultados sobre la adición de Glu, Ara, Mal, Mal3 y GalA. Como se llevaron a cabo experimentos en tres días diferentes, y el índice de liberación de ONP incluso en experimentos idénticos se vio que variaba ligeramente (posiblemente debido a variaciones en la temperatura), se muestran los resultados con solo ONPG e HIGAL añadido realizado en los mismos tres experimentos. Se puede observar que 5 mg/ml de Ara inhibe la transglicosilación, dando como resultado liberación de ONP aproximadamente tres veces más lenta. 5 mg/ml de Glu también tiene un ligero efecto inhibitorio, mientras que 50 mg/ml de Glu (resultados no mostrados) dio como resultado muy poca liberación de ONP (<0,02) en 30 mm. Como con Gal, esto indica unión de estos azúcares a subsitios en el intermedio enzima-galactosil, lo que impide que ONPG actúe como aceptor y donde los azúcares en sí también tienen función aceptora pequeña o ninguna. Con 5 mg/ml de Mal o Mal3 no se observan efectos significativos en la liberación ONP. 5 mg/ml de GalA tienen débil efecto inhibitorio, mientras que 50 mg/ml de GalA ralentiza la liberación de ONP en

aproximadamente un factor de dos. De estos resultados la clasificación del efecto inhibitorio de los azúcares evaluados es: Gal - Ara > Glu > GalA> Mal = Mal3 = 0.

[0114] Usando cromatografía HPAE-PAD (Dionex LC500 System, columna PA100, gradiente lineal de 0-0,6 M de acetato sódico en 100 mM de NaOH), la producción de oligosacáridos mayores a partir de transglicosilación con incubación de HIGAL (110 µg/ml) a temperatura ambiente (0,5 a 14 mm seguido de inactivación térmica durante 10 mm a 95°C da como resultado A405: 0,15-0,67) en 50 mM de acetato sódico, 1 mM de CaCl2, 0,01% de Tritón X100, pH 6,5 con ONPG (5 mg/ml) con y sin Gal2 (0,05 mg/ml) o Gal3 (0,05 mg/ml) como aceptor fue verificada.

Tabla 8: Índice de liberación de ONP MTGAL e HIGAL al variar las dosis y +1 azúcar

Enzima: µg/ml		MTGAL 110	MTGAL 55	MTGAL 28	MTGAL 110	MTGAL 55	HIGAL 110	HIGAL 55	HIGAL 28	HIGAL 110	HIGAL 55
ONPG (5 mg/ml)											
Azúcar: mg/ml					Gal: 5	Gal: 5				Gal: 5	Gal: 5
Tiempo (min) para aumentar A405 por:	0,025	14,0	29,9	40,4	26,9	40,2	9,0	20,4	41,4	32,0	57,0
	0,05	20,5	42,5	n.a.	44,5	n.a.	10,3	22,9	46,5	35,7	n.a.
	0,1	26,4	54,5	n.a.	n.a.	n.a.	11,5	25,4	51,0	41,5	n.a.
	0,2	31,4	n.a.	n.a.	n.a.	n.a.	12,7	28,0	56,5	46,7	n.a.
	0,4	34,5	n.a.	n.a.	n.a.	n.a.	13,8	30,9	n.a.	52,7	n.a.
	0,8	39,2	n.a.	n.a.	n.a.	n.a.	15,0	32,0	n.a.	59,0	n.a.
	1,6	43,9	n.a.	n.a.	n.a.	n.a.	15,0	35,0	n.a.	n.a.	n.a.
	3,2	46,7	n.a.	n.a.	n.a.	n.a.	17,7	37,9	n.a.	n.a.	n.a.

Tabla 9: Índice de liberación de ONP al variar concentraciones de ONPG

Enzima: µg/ml		HIGAL: 110	HIGAL: 110	HIGAL: 110	HIGAL: 110
ONPG (mg/ml)		10	5	2,5	1,25
Azúcar: mg/ml					
Tiempo (min) para aumentar A405 por:	0,025	6,3	6,0	9,7	28,7
	0,05	7,7	8,0	11,3	n.a.
	0,1	8,8	9,2	12,7	n.a.
	0,2	10,0	10,2	14,0	n.a.
	0,4	11,2	11,3	15,5	n.a.
	0,8	12,3	12,5	17,3	n.a.
	1,6	13,5	13,8	19,5	n.a.
	3,2	14,7	15,3	22,8	n.a.

Tabla 10: Índice de adición de liberación de ONP de varias cantidades de varios galactooligosacáridos

Enzima: μg/ml		HIGAL: 110	HIGAL: 100	HIGAL: 110	HIGAL: 110	HIGAL: 110	HIGAL: 110	HIGAL: 110
ONPG (mg/ml)		5	5	5	5	5	5	5
Azúcar: mg/ml			Gal2: 0,5	Gal2: 0,05	Gal3: 0,5	Gal3: 0,05	Gal4: 0,5	Ga14: 0,05
Índice inicial (modo/min)		0,9	6	2	200	40	700	80
Tiempo (mm) para aumentar A405 por:	0,025	10,0	2,7	5,5	0,0	0,5	0,0	0,2
	0,05	11,3	3,5	6,8	0,2	1,0	0,0	0,5
	0,1	12,8	4,8	8,2	0,3	1,7	0,0	0,8
	0,2	14,2	6,0	9,5	0,5	2,3	0,2	1,5
	0,4	15,7	7,2	10,7	0,8	3,3	0,5	2,5
	0,8	17,0	8,3	11,8	1,5	4,8	1,0	3,7
	1,6	18,5	9,7	13,3	2,5	6,3	2,2	5,2
	3,2	20,0	11,0	15,2	3,8	7,7	5,3	7,5

Tabla 11: Índice de inhibición de liberación de ONP por azúcares

Enzima: μg/ml		HIGAL: 110	HIGAL: 110	HIGAL: 110	HIGAL: 110	HIGAL: 110	HIGAL: 110	HIGAL: 110	HIGAL: 110	HIGAL: 110
ONPG(mg/ml)		5	5	5	5	5	5	5	5	5
Azúcar: mg/ml			Glu: 5	Ara: 5		Mal: 5	Ma13: 5		GalA: 50	GalA: 5
Tiempo (mm) para aumentar A405 por:	0,025	8,5	12,8	26,5	11,0	11,5	11,0	8,7	13,7	9,5
	0,05	9,5	14,8	n.a.	12,5	13,0	12,3	9,8	16,7	11,2
	0,1	10,8	17,0	n.a.	13,8	14,3	13,8	11,0	20,0	12,7
	0,2	12,0	19,3	n.a.	15,2	15,7	15,2	12,2	23,3	14,3
	0,4	13,3	21,8	n.a.	16,5	17,2	16,5	13,3	26,8	15,8
	0,8	14,5	24,3	n.a.	18,0	18,7	18,0	14,7	n.a.	17,5
	1,6	15,8	27,0	n.a.	19,5	20,2	19,3	16,0	n.a.	19,3
	3,2	17,3	n.a.	n.a.	21,3	22,0	21,3	17,3	n.a.	22,5

Ejemplo comparativo 5: Actividad en la lactosa

[0115] HIGAL (60 μg/ml) y MTGAL (750 μg/ml) fueron incubados a 50°C con lactosa (Lac) (100 mg/ml) a pH 4,8 (25 mM de citrato sódico), 6,45 (25 mM de acetato sódico, 0,5 mM de CaCl2, 0,005% de Tritón X100) y 8,6 (50 mM de Tris, 0,01% Brij 35). Muestras de 20 μl fueron retiradas después de 2, 23 y 120 horas, 980 de agua se añadió y la enzima se inactivó por calentamiento a 95°C durante 10 min. Después de otros 20 de tiempo de dilución con agua, las muestras fueron analizadas usando HPAE-PAD (Dionex LC500 System, columna PA100, 0-3 mm: 150mM de NaOH, 3-19 mm: gradiente lineal 0-0,18 M de acetato sódico en 150mM de NaOH). Los factores de respuesta para los picos individuales fueron estimados a partir de estándares de Gal, Glu, Lac, Gal2, Gal3 y Gal4.

[0116] Bajo estas condiciones solo MTGAL a pH 4,5 y 6,5 dio conversión significativa de Lac. En las tablas 12 y 13 se dan las fracciones de peso de los productos analizados con MTGAL a pH 4,5 y 6,45. Las figuras indican % en peso de los productos que resultan de la incubación. El término DP3 indica producto de transglicosilación que consiste en tres unidades de azúcar, y el término DP4+ productos de transglicosilación que consisten en cuatro o más unidades de azúcar. Desafortunadamente, el método de análisis usado no fue capaz de separar Glu y Gal.

[0117] Con transglicosilación ocurriendo según la reacción:

2 Lac -> DP3 (=Gal2Glu) + Glu

la fracción de peso de DP3 debería ser aproximadamente tres veces superior al peso del monómero. Después de 2 horas la proporción es aproximadamente 1.5 en ambos pH lo que indica que esta no es la única reacción que tiene lugar. La producción de oligosacáridos mayores (DP4+) es un resultado del producto de transglicosilación inicial que funciona como aceptor para transglicosilación adicional:

Lac + DP3 -> DP4 + Glu

[0118] También, de la creciente cantidad de Gal/Glu sin aumento correspondiente en los productos de transglicosilación (DP3 y DP4+) después de 23 y 120 horas, es evidente que la hidrólisis de productos de transglicosilación tiene lugar. Estas reacciones de hidrólisis parecen ser más lentas a pH 6,45 que a pH 4,5.

Tabla 12: Actividad de MTGAL en la lactosa (pH 4,5)

Tiempo de incubación (horas)	2	23	120
Glu/Gal	1,4	12,5	38,8
Lac/Ga12	96,0	78,7	51,2
DP3	2,0	7,0	8,9
DP4+	0,5	1,8	1,1

Tabla 13: Actividad de MTGAL en la lactosa (pH 6,45)

Tiempo de incubación (horas)	2	23	120
Glu/Gal	1,0	6,5	21,0
Lac/Ga12	95,7	85,3	62,6
DP3	1,4	6,3	11,7
DP4+	1,9	1,9	4,7

Ejemplo comparativo 6: Actividad en el galactano

[0119] Galactano de altramuz (Megazyme) se incubó con BLGAL (0,1-10 µg/ml) a pH 6,5 (50 mM de MES, 1mM de CaCl2) y con AAGAL (0,1-10 µg/ml) a pH 4,0 (50 mM de acetato sódico, 1 mM de CaCl2) a 30°C. Las muestras fueron retiradas después 45 mm a 24 horas y la enzima se inactivó por calentamiento a 95°C durante 10 mm. Los productos de reacción fueron analizados usando HPAEC-PAD en un sistema cromatográfico de Dionex utilizando una columna CarboPac PA100 y un gradiente lineal 0 a 0,3 M de acetato sódico en 0,15 M de NaOH. Galactooligosacáridos purificados se usaron para identificar productos.

[0120] Con BLGAL el producto principal inicial es galactotetraosa con ambos oligómeros menores y mayores también presentes. Con incubación más larga las fracciones de galactosa, galactobiosa y galactotriosa aumentan y después de incubación prolongada sólo estos tres oligómeros se ven en proporciones molares de aproximadamente 1:0,4:0,9.

[0121] AAGAL inicialmente produce una mezcla más homogénea de galactooligómeros. Degradación adicional produce principalmente galactosa, galactobiosa y galactotriosa, y finalmente casi exclusivamente galactosa y galactobiosa se ven en una proporción molar de aproximadamente 2:1. Pequeños picos probablemente correspondientes a galactobiosas y galactotriosas que resultan de reacciones de transglicosilación con enlaces glucosídicos diferente de β-1,4 están también presentes.

REIVINDICACIONES

1. Variante de una galactanasa de la familia glicósido hidrolasa 53 original que tiene un cambio en el perfil de la actividad de pH en comparación con la original; dicha variante comprende al menos una de las siguientes sustituciones: H91 N,L,D; A90S+H91D; D181N;
donde la variante tiene actividad de galactanasa;
donde la galactanasa original tiene cualquiera de las SEC ID nº: 1-4;
donde la variante tiene al menos 80% de identidad con la galactanasa original; y
donde la numeración se define por el alineamiento con SEC ID n: 1 utilizando el programa ClustalW con la opción alineamiento de perfil con alineamiento múltiple de la figura 5 como perfil 1, y cualquier secuencia no presente en la fig. 5 como perfil 2 para ser alineado con el primer perfil, usando los parámetros: Parámetros de alineamiento múltiple = Lento/Exacto; Penalización por apertura de espacio = 10,00; Penalización por extensión de espacio = 0,20; Secuencias divergentes de retraso = 30%; Peso de transiciones de ADN: 0,50; Matriz de peso de proteína =series Gonnet; Matriz de peso de ADN =IUB; Uso matriz negativa = OFF; Parámetros de espacio de proteína: Alternar sanciones específicas de residuos = ON; Alternar sanciones hidrofílicas = ON; Residuos hidrofílicos = GPSNDQEKR; Distancia de separación del espacio = 4; Alternar separación de espacio final = OFF.

2. Variante según la reivindicación 1, donde la variante comprende al menos una de las siguientes sustituciones: H91N,L,D.

3. Variante según cualquiera de las reivindicaciones 1-2, donde la variante comprende al menos las siguientes sustituciones: A90S+H91 D.

4. Variante según cualquiera de las reivindicaciones 1-3, donde la galactanasa original tiene cualquiera de SEC ID nº: 1-2.

5. Variante según cualquiera de las reivindicaciones 1-4, donde la galactanasa original tiene SEC ID nº: 1.

6. Variante según cualquiera de las reivindicaciones 1-5, que es una variante de una galactanasa de Myceliophfhora thermofila.

7. Variante según la reivindicación 1, donde la variante comprende al menos la siguiente sustitución: D181N.

8. Variante según la reivindicación 7, donde la galactanasa original tiene SEC ID nº: 3.

9. Secuencia de ácidos nucleicos aislada que comprende una secuencia de ácidos nucleicos que codifica la variante de galactanasa de cualquiera de las reivindicaciones 1-8.

10. Constructo de ácidos nucleicos que comprende la secuencia de ácidos nucleicos según la reivindicación 9 operativamente enlazada a una o más secuencias de control que dirigen la producción de la variante de galactanasa en un huésped de expresión adecuado.

11. Vector de expresión recombinante que comprende el constructo de ácidos nucleicos según la reivindicación 10.

12. Célula huésped recombinante que comprende el constructo de ácidos nucleicos de la reivindicación 10 o el vector de la reivindicación 11.

13. Método para producir una variante de galactanasa de cualquiera de las reivindicaciones 1-8, el método comprende (a) cultivo de una célula huésped recombinante según la reivindicación 1-2; y (b) recuperación del polipéptido.

14. Uso de al menos una variante de galactanasa de cualquiera de las reivindicaciones 1-8 en la industria láctea.

15. Uso de al menos una variante de galactanasa de cualquiera de las reivindicaciones 1-8 para preparar galactooligosacáridos y/o para la hidrólisis de lactosa.

```
HEADER                                                          MTGL
ATOM      1  CB  ALA     1      15.214  -2.789  18.265  1.00 29.91      MTGL
ATOM      2  C   ALA     1      17.670  -3.053  17.823  1.00 27.24      MTGL
ATOM      3  O   ALA     1      18.335  -2.394  17.026  1.00 27.44      MTGL
ATOM      4  N   ALA     1      16.132  -5.006  17.678  1.00 29.26      MTGL
ATOM      5  CA  ALA     1      16.268  -3.540  17.450  1.00 28.32      MTGL
ATOM      6  N   LEU     2      18.116  -3.378  19.034  1.00 25.13      MTGL
ATOM      7  CA  LEU     2      19.439  -2.955  19.486  1.00 23.17      MTGL
ATOM      8  CB  LEU     2      19.648  -3.322  20.957  1.00 23.07      MTGL
ATOM      9  CG  LEU     2      18.891  -2.507  22.005  1.00 23.57      MTGL
ATOM     10  CD1 LEU     2      19.156  -3.090  23.384  1.00 23.95      MTGL
ATOM     11  CD2 LEU     2      19.330  -1.057  21.940  1.00 23.31      MTGL
ATOM     12  C   LEU     2      20.560  -3.574  18.664  1.00 22.07      MTGL
ATOM     13  O   LEU     2      20.524  -4.757  18.340  1.00 21.83      MTGL
ATOM     14  N   THR     3      21.557  -2.767  18.329  1.00 20.29      MTGL
ATOM     15  CA  THR     3      22.699  -3.257  17.575  1.00 19.63      MTGL
ATOM     16  CB  THR     3      23.506  -2.100  16.978  1.00 20.33      MTGL
ATOM     17  OG1 THR     3      22.674  -1.360  16.083  1.00 20.92      MTGL
ATOM     18  CG2 THR     3      24.728  -2.626  16.227  1.00 20.96      MTGL
ATOM     19  C   THR     3      23.610  -4.038  18.515  1.00 19.16      MTGL
ATOM     20  O   THR     3      24.131  -5.092  18.156  1.00 19.29      MTGL
ATOM     21  N   TYR     4      23.796  -3.514  19.724  1.00 18.09      MTGL
ATOM     22  CA  TYR     4      24.652  -4.159  20.715  1.00 17.42      MTGL
ATOM     23  CB  TYR     4      25.724  -3.180  21.202  1.00 17.15      MTGL
ATOM     24  CG  TYR     4      26.514  -2.544  20.082  1.00 18.02      MTGL
ATOM     25  CD1 TYR     4      27.516  -3.251  19.412  1.00 17.43      MTGL
ATOM     26  CE1 TYR     4      28.210  -2.678  18.348  1.00 18.07      MTGL
ATOM     27  CD2 TYR     4      26.229  -1.246  19.661  1.00 17.07      MTGL
ATOM     28  CE2 TYR     4      26.916  -0.666  18.598  1.00 18.55      MTGL
ATOM     29  CZ  TYR     4      27.902  -1.386  17.948  1.00 17.59      MTGL
ATOM     30  OH  TYR     4      28.564  -0.814  16.891  1.00 18.07      MTGL
ATOM     31  C   TYR     4      23.858  -4.657  21.912  1.00 16.29      MTGL
ATOM     32  O   TYR     4      23.210  -3.876  22.615  1.00 16.95      MTGL
ATOM     33  N   ARG     5      23.907  -5.964  22.125  1.00 15.87      MTGL
ATOM     34  CA  ARG     5      23.232  -6.611  23.244  1.00 16.37      MTGL
ATOM     35  CB  ARG     5      22.281  -7.711  22.746  1.00 17.04      MTGL
ATOM     36  CG  ARG     5      21.203  -7.235  21.764  1.00 18.21      MTGL
ATOM     37  CD  ARG     5      20.189  -8.348  21.482  1.00 18.30      MTGL
ATOM     38  NE  ARG     5      20.839  -9.547  20.950  1.00 19.36      MTGL
ATOM     39  CZ  ARG     5      21.243  -9.681  19.692  1.00 20.62      MTGL
ATOM     40  NH1 ARG     5      21.054  -8.696  18.824  1.00 19.45      MTGL
ATOM     41  NH2 ARG     5      21.864 -10.790  19.307  1.00 21.29      MTGL
ATOM     42  C   ARG     5      24.390  -7.238  24.009  1.00 16.18      MTGL
ATOM     43  O   ARG     5      24.869  -8.311  23.642  1.00 16.58      MTGL
ATOM     44  N   GLY     6      24.853  -6.577  25.064  1.00 16.16      MTGL
ATOM     45  CA  GLY     6      25.991  -7.135  25.770  1.00 16.79      MTGL
ATOM     46  C   GLY     6      26.064  -7.065  27.275  1.00 15.64      MTGL
ATOM     47  O   GLY     6      25.129  -6.664  27.968  1.00 15.46      MTGL
ATOM     48  N   VAL     7      27.213  -7.497  27.775  1.00 15.87      MTGL
ATOM     49  CA  VAL     7      27.491  -7.500  29.199  1.00 15.12      MTGL
ATOM     50  CB  VAL     7      27.178  -8.877  29.846  1.00 14.43      MTGL
ATOM     51  CG1 VAL     7      25.750  -9.293  29.537  1.00 12.85      MTGL
ATOM     52  CG2 VAL     7      28.170  -9.931  29.348  1.00 13.29      MTGL
ATOM     53  C   VAL     7      28.977  -7.238  29.363  1.00 16.14      MTGL
ATOM     54  O   VAL     7      29.768  -7.469  28.440  1.00 17.27      MTGL
ATOM     55  N   ASP     8      29.354  -6.737  30.531  1.00 15.62      MTGL
ATOM     56  CA  ASP     8      30.755  -6.514  30.842  1.00 15.20      MTGL
ATOM     57  CB  ASP     8      30.920  -5.292  31.751  1.00 14.35      MTGL
```

Fig. 1

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ATOM     58  CG  ASP     8      32.373  -4.975  32.034  1.00 15.24      MTGL
ATOM     59  OD1 ASP     8      33.105  -5.881  32.486  1.00 14.12      MTGL
ATOM     60  OD2 ASP     8      32.784  -3.817  31.805  1.00 14.89      MTGL
ATOM     61  C   ASP     8      31.108  -7.793  31.602  1.00 14.33      MTGL
ATOM     62  O   ASP     8      30.573  -8.040  32.683  1.00 15.61      MTGL
ATOM     63  N   TRP     9      31.980  -8.614  31.027  1.00 13.27      MTGL
ATOM     64  CA  TRP     9      32.365  -9.872  31.653  1.00 13.40      MTGL
ATOM     65  CB  TRP     9      32.124 -11.020  30.663  1.00 12.58      MTGL
ATOM     66  CG  TRP     9      33.183 -11.146  29.585  1.00 13.96      MTGL
ATOM     67  CD2 TRP     9      33.682 -12.362  29.012  1.00 13.39      MTGL
ATOM     68  CE2 TRP     9      34.661 -12.008  28.057  1.00 13.29      MTGL
ATOM     69  CE3 TRP     9      33.396 -13.719  29.214  1.00 14.51      MTGL
ATOM     70  CD1 TRP     9      33.860 -10.128  28.964  1.00 14.11      MTGL
ATOM     71  NE1 TRP     9      34.752 -10.640  28.046  1.00 13.31      MTGL
ATOM     72  CZ2 TRP     9      35.357 -12.964  27.305  1.00 14.73      MTGL
ATOM     73  CZ3 TRP     9      34.093 -14.673  28.463  1.00 14.84      MTGL
ATOM     74  CH2 TRP     9      35.059 -14.287  27.523  1.00 14.12      MTGL
ATOM     75  C   TRP     9      33.832  -9.860  32.102  1.00 13.91      MTGL
ATOM     76  O   TRP     9      34.454 -10.915  32.272  1.00 13.71      MTGL
ATOM     77  N   SER    10      34.373  -8.660  32.295  1.00 13.08      MTGL
ATOM     78  CA  SER    10      35.770  -8.481  32.692  1.00 14.15      MTGL
ATOM     79  CB  SER    10      35.983  -7.052  33.193  1.00 13.75      MTGL
ATOM     80  OG  SER    10      35.691  -6.114  32.168  1.00 14.07      MTGL
ATOM     81  C   SER    10      36.321  -9.460  33.726  1.00 14.36      MTGL
ATOM     82  O   SER    10      37.414  -9.994  33.553  1.00 14.45      MTGL
ATOM     83  N   SER    11      35.561  -9.697  34.789  1.00 14.45      MTGL
ATOM     84  CA  SER    11      35.985 -10.588  35.870  1.00 15.55      MTGL
ATOM     85  CB  SER    11      35.053 -10.416  37.069  1.00 15.32      MTGL
ATOM     86  OG  SER    11      33.795 -11.014  36.792  1.00 13.85      MTGL
ATOM     87  C   SER    11      36.043 -12.080  35.544  1.00 16.02      MTGL
ATOM     88  O   SER    11      36.438 -12.870  36.401  1.00 16.91      MTGL
ATOM     89  N   VAL    12      35.656 -12.472  34.330  1.00 16.04      MTGL
ATOM     90  CA  VAL    12      35.640 -13.890  33.969  1.00 14.89      MTGL
ATOM     91  CB  VAL    12      35.367 -14.090  32.448  1.00 14.61      MTGL
ATOM     92  CG1 VAL    12      36.418 -13.371  31.604  1.00 13.79      MTGL
ATOM     93  CG2 VAL    12      35.336 -15.583  32.124  1.00 13.78      MTGL
ATOM     94  C   VAL    12      36.861 -14.726  34.373  1.00 15.76      MTGL
ATOM     95  O   VAL    12      36.709 -15.751  35.034  1.00 14.51      MTGL
ATOM     96  N   VAL    13      38.065 -14.312  33.990  1.00 16.87      MTGL
ATOM     97  CA  VAL    13      39.246 -15.100  34.343  1.00 17.35      MTGL
ATOM     98  CB  VAL    13      40.496 -14.656  33.534  1.00 17.20      MTGL
ATOM     99  CG1 VAL    13      41.775 -15.198  34.177  1.00 16.12      MTGL
ATOM    100  CG2 VAL    13      40.391 -15.193  32.109  1.00 15.88      MTGL
ATOM    101  C   VAL    13      39.534 -15.043  35.841  1.00 18.53      MTGL
ATOM    102  O   VAL    13      40.002 -16.024  36.430  1.00 19.44      MTGL
ATOM    103  N   VAL    14      39.242 -13.907  36.466  1.00 17.79      MTGL
ATOM    104  CA  VAL    14      39.463 -13.785  37.900  1.00 18.35      MTGL
ATOM    105  CB  VAL    14      39.106 -12.368  38.411  1.00 18.68      MTGL
ATOM    106  CG1 VAL    14      39.117 -12.347  39.939  1.00 19.58      MTGL
ATOM    107  CG2 VAL    14      40.113 -11.352  37.876  1.00 17.40      MTGL
ATOM    108  C   VAL    14      38.588 -14.816  38.620  1.00 17.85      MTGL
ATOM    109  O   VAL    14      39.034 -15.495  39.543  1.00 17.72      MTGL
ATOM    110  N   GLU    15      37.341 -14.941  38.181  1.00 17.47      MTGL
ATOM    111  CA  GLU    15      36.420 -15.889  38.800  1.00 18.52      MTGL
ATOM    112  CB  GLU    15      34.985 -15.585  38.373  1.00 19.09      MTGL
ATOM    113  CG  GLU    15      34.392 -14.361  39.056  1.00 20.86      MTGL
ATOM    114  CD  GLU    15      34.147 -14.579  40.542  1.00 22.32      MTGL
ATOM    115  OE1 GLU    15      35.113 -14.887  41.273  1.00 23.29      MTGL
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Fig. 1 cont.

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ATOM    116  OE2 GLU    15      32.984 -14.445  40.981  1.00 22.28      MTGL
ATOM    117  C   GLU    15      36.753 -17.346  38.502  1.00 18.21      MTGL
ATOM    118  O   GLU    15      36.640 -18.196  39.377  1.00 19.29      MTGL
ATOM    119  N   GLU    16      37.151 -17.639  37.272  1.00 18.79      MTGL
ATOM    120  CA  GLU    16      37.504 -19.006  36.921  1.00 19.07      MTGL
ATOM    121  CB  GLU    16      37.827 -19.103  35.424  1.00 19.33      MTGL
ATOM    122  CG  GLU    16      36.645 -18.735  34.530  1.00 19.54      MTGL
ATOM    123  CD  GLU    16      36.970 -18.798  33.049  1.00 19.73      MTGL
ATOM    124  OE1 GLU    16      38.143 -18.577  32.683  1.00 19.62      MTGL
ATOM    125  OE2 GLU    16      36.048 -19.048  32.244  1.00 20.12      MTGL
ATOM    126  C   GLU    16      38.706 -19.425  37.767  1.00 18.57      MTGL
ATOM    127  O   GLU    16      38.766 -20.557  38.250  1.00 17.78      MTGL
ATOM    128  N   ARG    17      39.640 -18.492  37.960  1.00 17.17      MTGL
ATOM    129  CA  ARG    17      40.842 -18.759  38.756  1.00 18.26      MTGL
ATOM    130  CB  ARG    17      41.872 -17.646  38.568  1.00 17.11      MTGL
ATOM    131  CG  ARG    17      42.593 -17.719  37.240  1.00 16.83      MTGL
ATOM    132  CD  ARG    17      43.446 -16.496  37.009  1.00 15.44      MTGL
ATOM    133  NE  ARG    17      44.246 -16.636  35.801  1.00 15.36      MTGL
ATOM    134  CZ  ARG    17      45.084 -15.708  35.357  1.00 15.76      MTGL
ATOM    135  NH1 ARG    17      45.225 -14.570  36.025  1.00 15.62      MTGL
ATOM    136  NH2 ARG    17      45.788 -15.922  34.254  1.00 15.66      MTGL
ATOM    137  C   ARG    17      40.502 -18.887  40.225  1.00 18.97      MTGL
ATOM    138  O   ARG    17      41.279 -19.407  41.017  1.00 19.60      MTGL
ATOM    139  N   ALA    18      39.330 -18.396  40.590  1.00 19.85      MTGL
ATOM    140  CA  ALA    18      38.890 -18.486  41.967  1.00 21.00      MTGL
ATOM    141  CB  ALA    18      38.071 -17.262  42.339  1.00 21.45      MTGL
ATOM    142  C   ALA    18      38.066 -19.756  42.154  1.00 21.18      MTGL
ATOM    143  O   ALA    18      37.495 -19.982  43.216  1.00 21.53      MTGL
ATOM    144  N   GLY    19      37.994 -20.577  41.110  1.00 20.78      MTGL
ATOM    145  CA  GLY    19      37.265 -21.827  41.218  1.00 21.14      MTGL
ATOM    146  C   GLY    19      35.833 -21.845  40.716  1.00 21.86      MTGL
ATOM    147  O   GLY    19      35.124 -22.833  40.901  1.00 20.92      MTGL
ATOM    148  N   VAL    20      35.386 -20.769  40.080  1.00 21.60      MTGL
ATOM    149  CA  VAL    20      34.021 -20.755  39.578  1.00 21.91      MTGL
ATOM    150  CB  VAL    20      33.533 -19.321  39.264  1.00 23.06      MTGL
ATOM    151  CG1 VAL    20      32.126 -19.370  38.674  1.00 22.39      MTGL
ATOM    152  CG2 VAL    20      33.530 -18.475  40.530  1.00 22.53      MTGL
ATOM    153  C   VAL    20      33.877 -21.589  38.305  1.00 21.53      MTGL
ATOM    154  O   VAL    20      34.673 -21.473  37.377  1.00 21.65      MTGL
ATOM    155  N   SER    21      32.864 -22.444  38.283  0.50 21.24      MTGL
ATOM    156  CA  SER    21      32.596 -23.272  37.116  0.50 21.35      MTGL
ATOM    157  CB  SER    21      32.602 -24.757  37.488  0.50 22.01      MTGL
ATOM    158  OG  SER    21      33.897 -25.165  37.901  0.50 22.69      MTGL
ATOM    159  C   SER    21      31.227 -22.857  36.605  0.50 20.74      MTGL
ATOM    160  O   SER    21      30.205 -23.167  37.214  0.50 20.32      MTGL
ATOM    161  N   TYR    22      31.216 -22.134  35.491  1.00 20.34      MTGL
ATOM    162  CA  TYR    22      29.972 -21.659  34.914  1.00 20.72      MTGL
ATOM    163  CB  TYR    22      30.270 -20.511  33.952  1.00 19.18      MTGL
ATOM    164  CG  TYR    22      30.765 -19.280  34.682  1.00 18.50      MTGL
ATOM    165  CD1 TYR    22      29.909 -18.548  35.503  1.00 17.85      MTGL
ATOM    166  CE1 TYR    22      30.357 -17.428  36.202  1.00 17.95      MTGL
ATOM    167  CD2 TYR    22      32.092 -18.865  34.578  1.00 17.87      MTGL
ATOM    168  CE2 TYR    22      32.552 -17.744  35.275  1.00 17.81      MTGL
ATOM    169  CZ  TYR    22      31.676 -17.031  36.083  1.00 17.46      MTGL
ATOM    170  OH  TYR    22      32.107 -15.915  36.767  1.00 17.47      MTGL
ATOM    171  C   TYR    22      29.152 -22.742  34.239  1.00 21.41      MTGL
ATOM    172  O   TYR    22      29.688 -23.634  33.588  1.00 21.91      MTGL
ATOM    173  N   LYS    23      27.839 -22.654  34.414  1.00 22.66      MTGL
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Fig. 1 cont.

ATOM	174	CA	LYS	23	26.918	-23.619	33.836	1.00 23.97	MTGL
ATOM	175	CB	LYS	23	26.387	-24.537	34.936	1.00 24.47	MTGL
ATOM	176	CG	LYS	23	27.479	-25.094	35.839	1.00 26.17	MTGL
ATOM	177	CD	LYS	23	26.894	-25.778	37.066	1.00 28.12	MTGL
ATOM	178	CE	LYS	23	27.985	-26.217	38.040	1.00 29.23	MTGL
ATOM	179	NZ	LYS	23	28.750	-25.069	38.615	1.00 28.37	MTGL
ATOM	180	C	LYS	23	25.748	-22.915	33.158	1.00 24.07	MTGL
ATOM	181	O	LYS	23	25.344	-21.823	33.570	1.00 23.42	MTGL
ATOM	182	N	ASN	24	25.210	-23.557	32.125	1.00 25.34	MTGL
ATOM	183	CA	ASN	24	24.074	-23.020	31.390	1.00 26.76	MTGL
ATOM	184	CB	ASN	24	23.907	-23.741	30.042	1.00 27.22	MTGL
ATOM	185	CG	ASN	24	23.925	-25.258	30.174	1.00 28.00	MTGL
ATOM	186	OD1	ASN	24	23.306	-25.825	31.075	1.00 28.00	MTGL
ATOM	187	ND2	ASN	24	24.626	-25.923	29.258	1.00 28.41	MTGL
ATOM	188	C	ASN	24	22.802	-23.171	32.216	1.00 27.53	MTGL
ATOM	189	O	ASN	24	22.830	-23.727	33.315	1.00 26.87	MTGL
ATOM	190	N	THR	25	21.691	-22.668	31.687	1.00 29.20	MTGL
ATOM	191	CA	THR	25	20.408	-22.754	32.378	1.00 31.61	MTGL
ATOM	192	CB	THR	25	19.299	-21.968	31.619	1.00 31.89	MTGL
ATOM	193	OG1	THR	25	19.269	-22.380	30.245	1.00 32.33	MTGL
ATOM	194	CG2	THR	25	19.558	-20.468	31.689	1.00 30.90	MTGL
ATOM	195	C	THR	25	19.968	-24.209	32.540	1.00 33.20	MTGL
ATOM	196	O	THR	25	19.107	-24.518	33.362	1.00 34.49	MTGL
ATOM	197	N	ASN	26	20.561	-25.101	31.754	1.00 33.98	MTGL
ATOM	198	CA	ASN	26	20.229	-26.521	31.831	1.00 34.91	MTGL
ATOM	199	CB	ASN	26	20.595	-27.233	30.529	1.00 37.07	MTGL
ATOM	200	CG	ASN	26	19.515	-27.114	29.479	1.00 38.98	MTGL
ATOM	201	OD1	ASN	26	19.743	-27.405	28.305	1.00 40.46	MTGL
ATOM	202	ND2	ASN	26	18.325	-26.696	29.898	1.00 39.01	MTGL
ATOM	203	C	ASN	26	21.000	-27.153	32.967	1.00 33.95	MTGL
ATOM	204	O	ASN	26	20.752	-28.294	33.356	1.00 34.07	MTGL
ATOM	205	N	GLY	27	21.952	-26.402	33.493	1.00 32.34	MTGL
ATOM	206	CA	GLY	27	22.739	-26.928	34.583	1.00 30.16	MTGL
ATOM	207	C	GLY	27	24.009	-27.629	34.140	1.00 29.51	MTGL
ATOM	208	O	GLY	27	24.692	-28.244	34.950	1.00 28.86	MTGL
ATOM	209	N	ASN	28	24.350	-27.547	32.864	1.00 29.22	MTGL
ATOM	210	CA	ASN	28	25.565	-28.205	32.419	1.00 28.62	MTGL
ATOM	211	CB	ASN	28	25.323	-28.945	31.108	1.00 30.49	MTGL
ATOM	212	CG	ASN	28	24.313	-30.063	31.258	1.00 31.94	MTGL
ATOM	213	OD1	ASN	28	24.453	-30.930	32.124	1.00 32.14	MTGL
ATOM	214	ND2	ASN	28	23.288	-30.049	30.417	1.00 32.11	MTGL
ATOM	215	C	ASN	28	26.714	-27.228	32.264	1.00 27.80	MTGL
ATOM	216	O	ASN	28	26.537	-26.085	31.831	1.00 26.86	MTGL
ATOM	217	N	ALA	29	27.897	-27.695	32.629	1.00 26.54	MTGL
ATOM	218	CA	ALA	29	29.103	-26.889	32.547	1.00 26.11	MTGL
ATOM	219	CB	ALA	29	30.290	-27.687	33.067	1.00 25.81	MTGL
ATOM	220	C	ALA	29	29.351	-26.456	31.110	1.00 25.11	MTGL
ATOM	221	O	ALA	29	29.232	-27.254	30.184	1.00 24.31	MTGL
ATOM	222	N	GLN	30	29.713	-25.192	30.932	1.00 23.82	MTGL
ATOM	223	CA	GLN	30	29.967	-24.655	29.603	1.00 23.10	MTGL
ATOM	224	CB	GLN	30	28.620	-24.424	28.901	1.00 23.68	MTGL
ATOM	225	CG	GLN	30	28.676	-23.687	27.578	1.00 26.45	MTGL
ATOM	226	CD	GLN	30	27.335	-23.695	26.858	1.00 27.43	MTGL
ATOM	227	OE1	GLN	30	26.282	-23.584	27.486	1.00 27.66	MTGL
ATOM	228	NE2	GLN	30	27.371	-23.815	25.537	1.00 27.00	MTGL
ATOM	229	C	GLN	30	30.748	-23.350	29.740	1.00 21.50	MTGL
ATOM	230	O	GLN	30	30.556	-22.609	30.700	1.00 21.61	MTGL
ATOM	231	N	PRO	31	31.661	-23.066	28.797	1.00 20.08	MTGL

Fig. 1 cont.

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ATOM    232  CD  PRO    31      32.110 -23.886  27.657  1.00 20.60      MTGL
ATOM    233  CA  PRO    31      32.432 -21.820  28.886  1.00 19.48      MTGL
ATOM    234  CB  PRO    31      33.262 -21.834  27.603  1.00 20.47      MTGL
ATOM    235  CG  PRO    31      33.489 -23.309  27.369  1.00 20.52      MTGL
ATOM    236  C   PRO    31      31.492 -20.617  28.960  1.00 18.32      MTGL
ATOM    237  O   PRO    31      30.491 -20.558  28.246  1.00 17.02      MTGL
ATOM    238  N   LEU    32      31.811 -19.664  29.828  1.00 18.30      MTGL
ATOM    239  CA  LEU    32      30.971 -18.477  29.987  1.00 18.52      MTGL
ATOM    240  CB  LEU    32      31.623 -17.476  30.954  1.00 17.22      MTGL
ATOM    241  CG  LEU    32      30.828 -16.190  31.227  1.00 17.71      MTGL
ATOM    242  CD1 LEU    32      29.443 -16.536  31.767  1.00 15.78      MTGL
ATOM    243  CD2 LEU    32      31.588 -15.319  32.235  1.00 15.40      MTGL
ATOM    244  C   LEU    32      30.655 -17.776  28.669  1.00 17.46      MTGL
ATOM    245  O   LEU    32      29.504 -17.413  28.429  1.00 18.85      MTGL
ATOM    246  N   GLU    33      31.660 -17.581  27.818  1.00 16.99      MTGL
ATOM    247  CA  GLU    33      31.421 -16.903  26.546  1.00 17.55      MTGL
ATOM    248  CB  GLU    33      32.716 -16.763  25.735  1.00 17.22      MTGL
ATOM    249  CG  GLU    33      33.426 -18.077  25.424  1.00 16.64      MTGL
ATOM    250  CD  GLU    33      34.496 -18.417  26.453  1.00 16.72      MTGL
ATOM    251  OE1 GLU    33      34.234 -18.270  27.667  1.00 14.95      MTGL
ATOM    252  OE2 GLU    33      35.597 -18.840  26.048  1.00 16.02      MTGL
ATOM    253  C   GLU    33      30.369 -17.630  25.712  1.00 18.39      MTGL
ATOM    254  O   GLU    33      29.576 -16.988  25.021  1.00 19.97      MTGL
ATOM    255  N   ASN    34      30.354 -18.959  25.779  1.00 18.00      MTGL
ATOM    256  CA  ASN    34      29.381 -19.739  25.019  1.00 19.90      MTGL
ATOM    257  CB  ASN    34      29.793 -21.214  24.955  1.00 21.66      MTGL
ATOM    258  CG  ASN    34      31.121 -21.420  24.251  1.00 24.08      MTGL
ATOM    259  OD1 ASN    34      31.355 -20.886  23.168  1.00 25.77      MTGL
ATOM    260  ND2 ASN    34      31.995 -22.207  24.861  1.00 26.27      MTGL
ATOM    261  C   ASN    34      27.991 -19.618  25.640  1.00 19.84      MTGL
ATOM    262  O   ASN    34      26.988 -19.598  24.931  1.00 19.75      MTGL
ATOM    263  N   ILE    35      27.932 -19.553  26.967  1.00 18.73      MTGL
ATOM    264  CA  ILE    35      26.656 -19.404  27.656  1.00 18.63      MTGL
ATOM    265  CB  ILE    35      26.845 -19.440  29.188  1.00 18.28      MTGL
ATOM    266  CG2 ILE    35      25.556 -19.028  29.890  1.00 17.35      MTGL
ATOM    267  CG1 ILE    35      27.270 -20.844  29.623  1.00 18.06      MTGL
ATOM    268  CD1 ILE    35      27.652 -20.946  31.091  1.00 19.14      MTGL
ATOM    269  C   ILE    35      26.048 -18.053  27.258  1.00 18.92      MTGL
ATOM    270  O   ILE    35      24.867 -17.966  26.907  1.00 18.51      MTGL
ATOM    271  N   LEU    36      26.866 -17.005  27.313  1.00 18.03      MTGL
ATOM    272  CA  LEU    36      26.416 -15.665  26.956  1.00 17.16      MTGL
ATOM    273  CB  LEU    36      27.563 -14.660  27.110  1.00 17.06      MTGL
ATOM    274  CG  LEU    36      28.076 -14.411  28.538  1.00 16.94      MTGL
ATOM    275  CD1 LEU    36      29.323 -13.516  28.504  1.00 14.36      MTGL
ATOM    276  CD2 LEU    36      26.969 -13.761  29.372  1.00 16.43      MTGL
ATOM    277  C   LEU    36      25.891 -15.636  25.522  1.00 17.26      MTGL
ATOM    278  O   LEU    36      24.795 -15.132  25.270  1.00 16.08      MTGL
ATOM    279  N   ALA    37      26.675 -16.174  24.589  1.00 17.12      MTGL
ATOM    280  CA  ALA    37      26.278 -16.203  23.187  1.00 17.86      MTGL
ATOM    281  CB  ALA    37      27.362 -16.863  22.338  1.00 16.93      MTGL
ATOM    282  C   ALA    37      24.961 -16.948  23.014  1.00 18.20      MTGL
ATOM    283  O   ALA    37      24.062 -16.480  22.314  1.00 19.46      MTGL
ATOM    284  N   ALA    38      24.850 -18.105  23.658  1.00 18.38      MTGL
ATOM    285  CA  ALA    38      23.643 -18.917  23.560  1.00 20.05      MTGL
ATOM    286  CB  ALA    38      23.809 -20.212  24.358  1.00 19.05      MTGL
ATOM    287  C   ALA    38      22.419 -18.154  24.049  1.00 20.48      MTGL
ATOM    288  O   ALA    38      21.294 -18.447  23.634  1.00 21.25      MTGL
ATOM    289  N   ASN    39      22.637 -17.173  24.923  1.00 20.10      MTGL
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Fig. 1 cont.

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ATOM    290  CA  ASN    39      21.531 -16.390  25.460  1.00 19.15      MTGL
ATOM    291  CB  ASN    39      21.717 -16.168  26.963  1.00 19.77      MTGL
ATOM    292  CG  ASN    39      21.416 -17.414  27.774  1.00 19.60      MTGL
ATOM    293  OD1 ASN    39      22.241 -18.327  27.872  1.00 22.00      MTGL
ATOM    294  ND2 ASN    39      20.224 -17.467  28.346  1.00 18.25      MTGL
ATOM    295  C   ASN    39      21.253 -15.056  24.768  1.00 18.64      MTGL
ATOM    296  O   ASN    39      20.544 -14.213  25.317  1.00 19.42      MTGL
ATOM    297  N   GLY    40      21.803 -14.862  23.572  1.00 17.47      MTGL
ATOM    298  CA  GLY    40      21.535 -13.635  22.837  1.00 17.26      MTGL
ATOM    299  C   GLY    40      22.585 -12.537  22.880  1.00 17.22      MTGL
ATOM    300  O   GLY    40      22.523 -11.594  22.095  1.00 17.12      MTGL
ATOM    301  N   VAL    41      23.544 -12.641  23.791  1.00 16.80      MTGL
ATOM    302  CA  VAL    41      24.589 -11.631  23.893  1.00 15.92      MTGL
ATOM    303  CB  VAL    41      25.510 -11.908  25.103  1.00 16.19      MTGL
ATOM    304  CG1 VAL    41      26.630 -10.888  25.144  1.00 14.75      MTGL
ATOM    305  CG2 VAL    41      24.707 -11.875  26.397  1.00 15.59      MTGL
ATOM    306  C   VAL    41      25.441 -11.645  22.626  1.00 15.77      MTGL
ATOM    307  O   VAL    41      25.832 -12.715  22.158  1.00 14.76      MTGL
ATOM    308  N   ASN    42      25.724 -10.469  22.064  1.00 16.34      MTGL
ATOM    309  CA  ASN    42      26.559 -10.406  20.864  1.00 16.57      MTGL
ATOM    310  CB  ASN    42      25.771  -9.889  19.646  1.00 17.06      MTGL
ATOM    311  CG  ASN    42      25.299  -8.443  19.798  1.00 18.15      MTGL
ATOM    312  OD1 ASN    42      25.727  -7.709  20.694  1.00 18.63      MTGL
ATOM    313  ND2 ASN    42      24.416  -8.028  18.898  1.00 16.75      MTGL
ATOM    314  C   ASN    42      27.812  -9.560  21.048  1.00 16.81      MTGL
ATOM    315  O   ASN    42      28.651  -9.478  20.147  1.00 17.52      MTGL
ATOM    316  N   THR    43      27.952  -8.951  22.221  1.00 16.55      MTGL
ATOM    317  CA  THR    43      29.108  -8.108  22.502  1.00 15.96      MTGL
ATOM    318  CB  THR    43      28.827  -6.634  22.136  1.00 16.50      MTGL
ATOM    319  OG1 THR    43      28.192  -6.565  20.850  1.00 17.26      MTGL
ATOM    320  CG2 THR    43      30.123  -5.840  22.102  1.00 15.22      MTGL
ATOM    321  C   THR    43      29.487  -8.144  23.976  1.00 15.93      MTGL
ATOM    322  O   THR    43      28.618  -8.180  24.849  1.00 16.10      MTGL
ATOM    323  N   VAL    44      30.786  -8.148  24.251  1.00 14.74      MTGL
ATOM    324  CA  VAL    44      31.251  -8.136  25.626  1.00 15.41      MTGL
ATOM    325  CB  VAL    44      32.038  -9.418  26.012  1.00 16.13      MTGL
ATOM    326  CG1 VAL    44      31.084 -10.603  26.096  1.00 16.11      MTGL
ATOM    327  CG2 VAL    44      33.146  -9.689  25.004  1.00 14.58      MTGL
ATOM    328  C   VAL    44      32.137  -6.922  25.849  1.00 15.69      MTGL
ATOM    329  O   VAL    44      32.974  -6.574  25.014  1.00 16.22      MTGL
ATOM    330  N   ARG    45      31.916  -6.271  26.981  1.00 14.86      MTGL
ATOM    331  CA  ARG    45      32.662  -5.091  27.383  1.00 15.51      MTGL
ATOM    332  CB  ARG    45      31.702  -4.129  28.087  1.00 16.51      MTGL
ATOM    333  CG  ARG    45      32.297  -2.828  28.597  1.00 17.41      MTGL
ATOM    334  CD  ARG    45      31.143  -1.971  29.107  1.00 18.63      MTGL
ATOM    335  NE  ARG    45      31.519  -0.636  29.554  1.00 19.44      MTGL
ATOM    336  CZ  ARG    45      31.756  -0.309  30.820  1.00 19.56      MTGL
ATOM    337  NH1 ARG    45      31.671  -1.225  31.777  1.00 18.15      MTGL
ATOM    338  NH2 ARG    45      32.032   0.949  31.130  1.00 19.68      MTGL
ATOM    339  C   ARG    45      33.752  -5.561  28.342  1.00 15.10      MTGL
ATOM    340  O   ARG    45      33.516  -6.446  29.168  1.00 13.85      MTGL
ATOM    341  N   GLN    46      34.938  -4.965  28.232  1.00 14.87      MTGL
ATOM    342  CA  GLN    46      36.071  -5.331  29.074  1.00 14.52      MTGL
ATOM    343  CB  GLN    46      37.030  -6.246  28.296  1.00 14.23      MTGL
ATOM    344  CG  GLN    46      36.376  -7.512  27.746  1.00 14.12      MTGL
ATOM    345  CD  GLN    46      37.310  -8.358  26.902  1.00 13.86      MTGL
ATOM    346  OE1 GLN    46      36.895  -9.363  26.335  1.00 15.22      MTGL
ATOM    347  NE2 GLN    46      38.575  -7.958  26.814  1.00 13.21      MTGL
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Fig. 1 cont.

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ATOM    348  C   GLN   46      36.831  -4.089  29.534  1.00 15.79      MTGL
ATOM    349  O   GLN   46      37.153  -3.211  28.728  1.00 15.74      MTGL
ATOM    350  N   ARG   47      37.111  -4.005  30.830  1.00 15.01      MTGL
ATOM    351  CA  ARG   47      37.851  -2.866  31.350  1.00 15.05      MTGL
ATOM    352  CB  ARG   47      37.524  -2.631  32.828  1.00 13.91      MTGL
ATOM    353  CG  ARG   47      37.649  -3.868  33.710  1.00 13.56      MTGL
ATOM    354  CD  ARG   47      37.391  -3.520  35.175  1.00 13.26      MTGL
ATOM    355  NE  ARG   47      37.207  -4.710  36.004  1.00 12.49      MTGL
ATOM    356  CZ  ARG   47      36.063  -5.382  36.117  1.00 13.71      MTGL
ATOM    357  NH1 ARG   47      34.983  -4.981  35.457  1.00 13.79      MTGL
ATOM    358  NH2 ARG   47      36.004  -6.477  36.876  1.00 12.61      MTGL
ATOM    359  C   ARG   47      39.347  -3.107  31.182  1.00 15.50      MTGL
ATOM    360  O   ARG   47      39.849  -4.209  31.433  1.00 15.21      MTGL
ATOM    361  N   VAL   48      40.056  -2.072  30.745  1.00 15.84      MTGL
ATOM    362  CA  VAL   48      41.496  -2.171  30.557  1.00 15.53      MTGL
ATOM    363  CB  VAL   48      41.899  -1.874  29.102  1.00 16.38      MTGL
ATOM    364  CG1 VAL   48      43.418  -1.906  28.975  1.00 15.45      MTGL
ATOM    365  CG2 VAL   48      41.258  -2.892  28.160  1.00 14.39      MTGL
ATOM    366  C   VAL   48      42.222  -1.185  31.459  1.00 16.31      MTGL
ATOM    367  O   VAL   48      41.941   0.013  31.433  1.00 14.76      MTGL
ATOM    368  N   TRP   49      43.139  -1.707  32.270  1.00 16.64      MTGL
ATOM    369  CA  TRP   49      43.938  -0.890  33.172  1.00 17.13      MTGL
ATOM    370  CB  TRP   49      43.893  -1.458  34.598  1.00 17.19      MTGL
ATOM    371  CG  TRP   49      42.525  -1.365  35.239  1.00 17.50      MTGL
ATOM    372  CD2 TRP   49      42.129  -1.903  36.510  1.00 17.36      MTGL
ATOM    373  CE2 TRP   49      40.773  -1.550  36.710  1.00 17.08      MTGL
ATOM    374  CE3 TRP   49      42.786  -2.651  37.497  1.00 16.24      MTGL
ATOM    375  CD1 TRP   49      41.426  -0.728  34.736  1.00 17.53      MTGL
ATOM    376  NE1 TRP   49      40.370  -0.832  35.614  1.00 17.76      MTGL
ATOM    377  CZ2 TRP   49      40.063  -1.915  37.860  1.00 16.34      MTGL
ATOM    378  CZ3 TRP   49      42.079  -3.014  38.642  1.00 17.30      MTGL
ATOM    379  CH2 TRP   49      40.729  -2.645  38.812  1.00 16.66      MTGL
ATOM    380  C   TRP   49      45.369  -0.870  32.632  1.00 17.96      MTGL
ATOM    381  O   TRP   49      45.819  -1.830  32.007  1.00 16.92      MTGL
ATOM    382  N   VAL   50      46.078   0.228  32.874  1.00 18.74      MTGL
ATOM    383  CA  VAL   50      47.438   0.408  32.373  1.00 18.43      MTGL
ATOM    384  CB  VAL   50      47.898   1.865  32.604  1.00 17.51      MTGL
ATOM    385  CG1 VAL   50      49.310   2.061  32.069  1.00 16.69      MTGL
ATOM    386  CG2 VAL   50      46.931   2.814  31.912  1.00 16.38      MTGL
ATOM    387  C   VAL   50      48.492  -0.568  32.910  1.00 20.17      MTGL
ATOM    388  O   VAL   50      49.035  -1.359  32.141  1.00 20.17      MTGL
ATOM    389  N   ASN   51      48.809  -0.513  34.203  1.00 20.54      MTGL
ATOM    390  CA  ASN   51      49.800  -1.438  34.780  1.00 22.14      MTGL
ATOM    391  CB  ASN   51      51.181  -0.778  34.894  1.00 22.82      MTGL
ATOM    392  CG  ASN   51      51.899  -0.671  33.564  1.00 24.64      MTGL
ATOM    393  OD1 ASN   51      52.211   0.430  33.102  1.00 25.29      MTGL
ATOM    394  ND2 ASN   51      52.180  -1.813  32.945  1.00 24.48      MTGL
ATOM    395  C   ASN   51      49.416  -1.943  36.173  1.00 22.18      MTGL
ATOM    396  O   ASN   51      50.177  -1.771  37.119  1.00 23.10      MTGL
ATOM    397  N   PRO   52      48.242  -2.584  36.317  1.00 21.49      MTGL
ATOM    398  CD  PRO   52      47.333  -3.089  35.273  1.00 20.91      MTGL
ATOM    399  CA  PRO   52      47.847  -3.079  37.642  1.00 20.88      MTGL
ATOM    400  CB  PRO   52      46.509  -3.769  37.370  1.00 20.37      MTGL
ATOM    401  CG  PRO   52      46.683  -4.283  35.963  1.00 20.56      MTGL
ATOM    402  C   PRO   52      48.905  -4.041  38.177  1.00 21.68      MTGL
ATOM    403  O   PRO   52      49.390  -4.902  37.449  1.00 20.78      MTGL
ATOM    404  N   ALA   53      49.261  -3.891  39.448  1.00 22.20      MTGL
ATOM    405  CA  ALA   53      50.278  -4.739  40.061  1.00 23.49      MTGL
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Fig. 1 cont.

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ATOM    406  CB  ALA    53      50.409  -4.407  41.549  1.00 23.83      MTGL
ATOM    407  C   ALA    53      50.037  -6.235  39.883  1.00 23.68      MTGL
ATOM    408  O   ALA    53      50.937  -6.960  39.466  1.00 23.33      MTGL
ATOM    409  N   ASP    54      48.831  -6.704  40.195  1.00 24.06      MTGL
ATOM    410  CA  ASP    54      48.539  -8.126  40.058  1.00 24.64      MTGL
ATOM    411  CB  ASP    54      47.400  -8.540  40.994  1.00 26.42      MTGL
ATOM    412  CG  ASP    54      46.109  -7.805  40.706  1.00 27.54      MTGL
ATOM    413  OD1 ASP    54      45.834  -7.515  39.522  1.00 29.32      MTGL
ATOM    414  OD2 ASP    54      45.360  -7.529  41.664  1.00 27.59      MTGL
ATOM    415  C   ASP    54      48.207  -8.560  38.631  1.00 24.00      MTGL
ATOM    416  O   ASP    54      47.878  -9.720  38.396  1.00 24.44      MTGL
ATOM    417  N   GLY    55      48.286  -7.630  37.686  1.00 22.74      MTGL
ATOM    418  CA  GLY    55      48.013  -7.959  36.296  1.00 21.74      MTGL
ATOM    419  C   GLY    55      46.566  -8.102  35.854  1.00 20.84      MTGL
ATOM    420  O   GLY    55      46.294  -8.150  34.652  1.00 20.70      MTGL
ATOM    421  N   ASN    56      45.627  -8.173  36.791  1.00 20.23      MTGL
ATOM    422  CA  ASN    56      44.229  -8.320  36.399  1.00 19.77      MTGL
ATOM    423  CB  ASN    56      43.329  -8.530  37.623  1.00 21.09      MTGL
ATOM    424  CG  ASN    56      43.569  -9.876  38.301  1.00 22.81      MTGL
ATOM    425  OD1 ASN    56      43.921 -10.859  37.647  1.00 20.74      MTGL
ATOM    426  ND2 ASN    56      43.359  -9.926  39.611  1.00 22.17      MTGL
ATOM    427  C   ASN    56      43.751  -7.108  35.612  1.00 18.30      MTGL
ATOM    428  O   ASN    56      43.972  -5.968  36.016  1.00 17.82      MTGL
ATOM    429  N   TYR    57      43.108  -7.376  34.480  1.00 16.29      MTGL
ATOM    430  CA  TYR    57      42.570  -6.353  33.591  1.00 15.51      MTGL
ATOM    431  CB  TYR    57      41.680  -5.376  34.368  1.00 15.50      MTGL
ATOM    432  CG  TYR    57      40.756  -6.062  35.348  1.00 16.25      MTGL
ATOM    433  CD1 TYR    57      39.969  -7.150  34.955  1.00 15.93      MTGL
ATOM    434  CE1 TYR    57      39.137  -7.799  35.859  1.00 16.29      MTGL
ATOM    435  CD2 TYR    57      40.681  -5.642  36.671  1.00 16.32      MTGL
ATOM    436  CE2 TYR    57      39.847  -6.288  37.585  1.00 17.00      MTGL
ATOM    437  CZ  TYR    57      39.080  -7.363  37.172  1.00 15.31      MTGL
ATOM    438  OH  TYR    57      38.254  -8.000  38.066  1.00 15.12      MTGL
ATOM    439  C   TYR    57      43.627  -5.579  32.807  1.00 15.53      MTGL
ATOM    440  O   TYR    57      43.315  -4.561  32.189  1.00 14.98      MTGL
ATOM    441  N   ASN    58      44.877  -6.033  32.825  1.00 14.46      MTGL
ATOM    442  CA  ASN    58      45.876  -5.327  32.032  1.00 15.65      MTGL
ATOM    443  CB  ASN    58      47.314  -5.594  32.522  1.00 15.44      MTGL
ATOM    444  CG  ASN    58      47.783  -7.030  32.319  1.00 16.49      MTGL
ATOM    445  OD1 ASN    58      48.869  -7.390  32.779  1.00 18.71      MTGL
ATOM    446  ND2 ASN    58      46.995  -7.844  31.640  1.00 13.70      MTGL
ATOM    447  C   ASN    58      45.660  -5.763  30.582  1.00 16.00      MTGL
ATOM    448  O   ASN    58      44.774  -6.579  30.317  1.00 14.12      MTGL
ATOM    449  N   LEU    59      46.447  -5.235  29.649  1.00 16.39      MTGL
ATOM    450  CA  LEU    59      46.241  -5.564  28.242  1.00 17.31      MTGL
ATOM    451  CB  LEU    59      47.192  -4.751  27.356  1.00 17.07      MTGL
ATOM    452  CG  LEU    59      46.797  -4.743  25.874  1.00 17.21      MTGL
ATOM    453  CD1 LEU    59      45.367  -4.208  25.722  1.00 16.29      MTGL
ATOM    454  CD2 LEU    59      47.769  -3.882  25.085  1.00 16.17      MTGL
ATOM    455  C   LEU    59      46.333  -7.046  27.880  1.00 17.51      MTGL
ATOM    456  O   LEU    59      45.517  -7.537  27.096  1.00 17.20      MTGL
ATOM    457  N   ASP    60      47.317  -7.754  28.432  1.00 17.48      MTGL
ATOM    458  CA  ASP    60      47.460  -9.183  28.152  1.00 18.05      MTGL
ATOM    459  CB  ASP    60      48.700  -9.768  28.837  1.00 20.82      MTGL
ATOM    460  CG  ASP    60      49.995  -9.286  28.217  1.00 23.01      MTGL
ATOM    461  OD1 ASP    60      50.012  -9.009  26.999  1.00 25.11      MTGL
ATOM    462  OD2 ASP    60      51.002  -9.204  28.946  1.00 25.50      MTGL
ATOM    463  C   ASP    60      46.237  -9.943  28.647  1.00 17.40      MTGL
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Fig. 1 cont.

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ATOM    464  O   ASP    60      45.749 -10.856  27.984  1.00 16.59      MTGL
ATOM    465  N   TYR    61      45.756  -9.573  29.827  1.00 15.42      MTGL
ATOM    466  CA  TYR    61      44.580 -10.215  30.398  1.00 15.67      MTGL
ATOM    467  CB  TYR    61      44.266  -9.581  31.759  1.00 15.24      MTGL
ATOM    468  CG  TYR    61      43.000 -10.071  32.427  1.00 15.21      MTGL
ATOM    469  CD1 TYR    61      41.746  -9.597  32.032  1.00 15.96      MTGL
ATOM    470  CE1 TYR    61      40.578 -10.025  32.670  1.00 14.87      MTGL
ATOM    471  CD2 TYR    61      43.058 -10.990  33.473  1.00 15.54      MTGL
ATOM    472  CE2 TYR    61      41.899 -11.428  34.120  1.00 14.46      MTGL
ATOM    473  CZ  TYR    61      40.662 -10.943  33.714  1.00 16.75      MTGL
ATOM    474  OH  TYR    61      39.511 -11.379  34.345  1.00 14.25      MTGL
ATOM    475  C   TYR    61      43.400 -10.042  29.434  1.00 15.36      MTGL
ATOM    476  O   TYR    61      42.651 -10.987  29.175  1.00 15.76      MTGL
ATOM    477  N   ASN    62      43.257  -8.834  28.897  1.00 14.42      MTGL
ATOM    478  CA  ASN    62      42.174  -8.509  27.971  1.00 16.00      MTGL
ATOM    479  CB  ASN    62      42.072  -6.990  27.811  1.00 15.99      MTGL
ATOM    480  CG  ASN    62      41.231  -6.354  28.895  1.00 18.27      MTGL
ATOM    481  OD1 ASN    62      39.998  -6.396  28.840  1.00 18.23      MTGL
ATOM    482  ND2 ASN    62      41.887  -5.780  29.901  1.00 16.02      MTGL
ATOM    483  C   ASN    62      42.306  -9.172  26.600  1.00 16.04      MTGL
ATOM    484  O   ASN    62      41.306  -9.546  25.990  1.00 15.56      MTGL
ATOM    485  N   ILE    63      43.534  -9.311  26.110  1.00 16.06      MTGL
ATOM    486  CA  ILE    63      43.732  -9.952  24.824  1.00 17.20      MTGL
ATOM    487  CB  ILE    63      45.202  -9.827  24.350  1.00 16.83      MTGL
ATOM    488  CG2 ILE    63      45.481 -10.814  23.214  1.00 17.67      MTGL
ATOM    489  CG1 ILE    63      45.463  -8.391  23.887  1.00 17.41      MTGL
ATOM    490  CD1 ILE    63      46.910  -8.105  23.521  1.00 18.09      MTGL
ATOM    491  C   ILE    63      43.333 -11.420  24.945  1.00 17.68      MTGL
ATOM    492  O   ILE    63      42.664 -11.964  24.068  1.00 18.06      MTGL
ATOM    493  N   ALA    64      43.722 -12.058  26.046  1.00 17.70      MTGL
ATOM    494  CA  ALA    64      43.379 -13.463  26.253  1.00 17.86      MTGL
ATOM    495  CB  ALA    64      44.000 -13.971  27.555  1.00 17.49      MTGL
ATOM    496  C   ALA    64      41.860 -13.703  26.262  1.00 17.48      MTGL
ATOM    497  O   ALA    64      41.370 -14.616  25.599  1.00 17.31      MTGL
ATOM    498  N   ILE    65      41.104 -12.895  27.002  1.00 16.55      MTGL
ATOM    499  CA  ILE    65      39.665 -13.117  27.030  1.00 16.75      MTGL
ATOM    500  CB  ILE    65      38.991 -12.503  28.289  1.00 16.00      MTGL
ATOM    501  CG2 ILE    65      39.574 -13.130  29.536  1.00 16.34      MTGL
ATOM    502  CG1 ILE    65      39.173 -10.984  28.322  1.00 18.05      MTGL
ATOM    503  CD1 ILE    65      38.423 -10.321  29.474  1.00 15.44      MTGL
ATOM    504  C   ILE    65      38.989 -12.598  25.760  1.00 16.71      MTGL
ATOM    505  O   ILE    65      37.938 -13.101  25.368  1.00 16.21      MTGL
ATOM    506  N   ALA    66      39.598 -11.609  25.107  1.00 16.15      MTGL
ATOM    507  CA  ALA    66      39.036 -11.087  23.866  1.00 16.93      MTGL
ATOM    508  CB  ALA    66      39.806  -9.854  23.404  1.00 15.85      MTGL
ATOM    509  C   ALA    66      39.106 -12.185  22.802  1.00 17.72      MTGL
ATOM    510  O   ALA    66      38.189 -12.330  21.989  1.00 16.94      MTGL
ATOM    511  N   LYS    67      40.188 -12.965  22.817  1.00 18.09      MTGL
ATOM    512  CA  LYS    67      40.340 -14.059  21.856  1.00 19.65      MTGL
ATOM    513  CB  LYS    67      41.700 -14.748  22.010  1.00 21.06      MTGL
ATOM    514  CG  LYS    67      42.892 -13.953  21.484  1.00 23.60      MTGL
ATOM    515  CD  LYS    67      44.159 -14.795  21.550  1.00 26.88      MTGL
ATOM    516  CE  LYS    67      45.365 -14.050  21.000  1.00 29.59      MTGL
ATOM    517  NZ  LYS    67      45.208 -13.714  19.551  1.00 32.62      MTGL
ATOM    518  C   LYS    67      39.229 -15.085  22.070  1.00 19.44      MTGL
ATOM    519  O   LYS    67      38.667 -15.616  21.109  1.00 19.17      MTGL
ATOM    520  N   ARG    68      38.921 -15.365  23.335  1.00 18.94      MTGL
ATOM    521  CA  ARG    68      37.866 -16.317  23.672  1.00 17.61      MTGL
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Fig. 1 cont.

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ATOM    522  CB  ARG    68      37.834 -16.567  25.181  1.00 16.99      MTGL
ATOM    523  CG  ARG    68      38.950 -17.488  25.679  1.00 18.79      MTGL
ATOM    524  CD  ARG    68      39.015 -17.515  27.199  1.00 17.89      MTGL
ATOM    525  NE  ARG    68      37.742 -17.892  27.809  1.00 18.08      MTGL
ATOM    526  CZ  ARG    68      37.555 -18.020  29.120  1.00 18.59      MTGL
ATOM    527  NH1 ARG    68      38.561 -17.798  29.961  1.00 18.68      MTGL
ATOM    528  NH2 ARG    68      36.371 -18.381  29.595  1.00 16.96      MTGL
ATOM    529  C   ARG    68      36.511 -15.799  23.209  1.00 17.25      MTGL
ATOM    530  O   ARG    68      35.679 -16.563  22.711  1.00 15.99      MTGL
ATOM    531  N   ALA    69      36.285 -14.503  23.395  1.00 16.95      MTGL
ATOM    532  CA  ALA    69      35.030 -13.886  22.982  1.00 18.21      MTGL
ATOM    533  CB  ALA    69      35.001 -12.411  23.393  1.00 18.02      MTGL
ATOM    534  C   ALA    69      34.907 -14.012  21.465  1.00 18.17      MTGL
ATOM    535  O   ALA    69      33.867 -14.407  20.945  1.00 16.83      MTGL
ATOM    536  N   LYS    70      35.984 -13.675  20.764  1.00 18.35      MTGL
ATOM    537  CA  LYS    70      36.011 -13.764  19.312  1.00 19.84      MTGL
ATOM    538  CB  LYS    70      37.402 -13.390  18.795  1.00 19.40      MTGL
ATOM    539  CG  LYS    70      37.548 -13.420  17.284  1.00 21.56      MTGL
ATOM    540  CD  LYS    70      38.992 -13.123  16.892  1.00 22.53      MTGL
ATOM    541  CE  LYS    70      39.180 -13.123  15.383  1.00 23.66      MTGL
ATOM    542  NZ  LYS    70      40.592 -12.852  15.015  1.00 21.95      MTGL
ATOM    543  C   LYS    70      35.648 -15.186  18.861  1.00 20.29      MTGL
ATOM    544  O   LYS    70      34.842 -15.365  17.948  1.00 19.93      MTGL
ATOM    545  N   ALA    71      36.235 -16.190  19.511  1.00 19.37      MTGL
ATOM    546  CA  ALA    71      35.970 -17.585  19.159  1.00 20.95      MTGL
ATOM    547  CB  ALA    71      36.896 -18.514  19.941  1.00 20.90      MTGL
ATOM    548  C   ALA    71      34.514 -17.975  19.405  1.00 21.38      MTGL
ATOM    549  O   ALA    71      34.010 -18.929  18.810  1.00 22.34      MTGL
ATOM    550  N   ALA    72      33.839 -17.244  20.282  1.00 20.63      MTGL
ATOM    551  CA  ALA    72      32.439 -17.529  20.574  1.00 20.92      MTGL
ATOM    552  CB  ALA    72      32.149 -17.284  22.050  1.00 20.20      MTGL
ATOM    553  C   ALA    72      31.523 -16.659  19.710  1.00 20.68      MTGL
ATOM    554  O   ALA    72      30.305 -16.644  19.899  1.00 20.23      MTGL
ATOM    555  N   GLY    73      32.116 -15.934  18.768  1.00 20.42      MTGL
ATOM    556  CA  GLY    73      31.339 -15.077  17.889  1.00 20.87      MTGL
ATOM    557  C   GLY    73      30.874 -13.774  18.523  1.00 21.42      MTGL
ATOM    558  O   GLY    73      29.946 -13.133  18.027  1.00 21.96      MTGL
ATOM    559  N   LEU    74      31.522 -13.373  19.612  1.00 20.70      MTGL
ATOM    560  CA  LEU    74      31.160 -12.146  20.315  1.00 19.98      MTGL
ATOM    561  CB  LEU    74      31.221 -12.372  21.830  1.00 19.61      MTGL
ATOM    562  CG  LEU    74      30.359 -13.491  22.420  1.00 19.97      MTGL
ATOM    563  CD1 LEU    74      30.692 -13.659  23.898  1.00 19.32      MTGL
ATOM    564  CD2 LEU    74      28.881 -13.162  22.232  1.00 18.79      MTGL
ATOM    565  C   LEU    74      32.071 -10.978  19.960  1.00 19.91      MTGL
ATOM    566  O   LEU    74      33.292 -11.133  19.882  1.00 20.26      MTGL
ATOM    567  N   GLY    75      31.473  -9.809  19.740  1.00 19.06      MTGL
ATOM    568  CA  GLY    75      32.261  -8.627  19.438  1.00 18.36      MTGL
ATOM    569  C   GLY    75      32.856  -8.106  20.738  1.00 17.17      MTGL
ATOM    570  O   GLY    75      32.380  -8.457  21.821  1.00 16.83      MTGL
ATOM    571  N   VAL    76      33.885  -7.271  20.648  1.00 16.99      MTGL
ATOM    572  CA  VAL    76      34.522  -6.748  21.853  1.00 17.15      MTGL
ATOM    573  CB  VAL    76      35.996  -7.202  21.947  1.00 18.28      MTGL
ATOM    574  CG1 VAL    76      36.626  -6.682  23.238  1.00 17.92      MTGL
ATOM    575  CG2 VAL    76      36.074  -8.726  21.896  1.00 17.32      MTGL
ATOM    576  C   VAL    76      34.476  -5.231  21.984  1.00 17.67      MTGL
ATOM    577  O   VAL    76      34.770  -4.491  21.039  1.00 18.33      MTGL
ATOM    578  N   TYR    77      34.108  -4.785  23.177  1.00 16.77      MTGL
ATOM    579  CA  TYR    77      34.013  -3.366  23.517  1.00 16.63      MTGL
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Fig. 1 cont.

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ATOM    580  CB  TYR    77      32.608  -3.102  24.097  1.00 15.27      MTGL
ATOM    581  CG  TYR    77      32.335  -1.799  24.840  1.00 15.55      MTGL
ATOM    582  CD1 TYR    77      33.343  -0.886  25.149  1.00 15.39      MTGL
ATOM    583  CE1 TYR    77      33.068   0.257  25.925  1.00 16.48      MTGL
ATOM    584  CD2 TYR    77      31.046  -1.532  25.312  1.00 16.02      MTGL
ATOM    585  CE2 TYR    77      30.766  -0.414  26.075  1.00 15.87      MTGL
ATOM    586  CZ  TYR    77      31.772   0.475  26.386  1.00 16.20      MTGL
ATOM    587  OH  TYR    77      31.471   1.541  27.200  1.00 15.93      MTGL
ATOM    588  C   TYR    77      35.114  -3.128  24.548  1.00 16.00      MTGL
ATOM    589  O   TYR    77      35.026  -3.604  25.683  1.00 16.53      MTGL
ATOM    590  N   ILE    78      36.163  -2.419  24.142  1.00 16.29      MTGL
ATOM    591  CA  ILE    78      37.280  -2.121  25.044  1.00 17.09      MTGL
ATOM    592  CB  ILE    78      38.611  -2.008  24.261  1.00 17.14      MTGL
ATOM    593  CG2 ILE    78      39.695  -1.387  25.140  1.00 16.04      MTGL
ATOM    594  CG1 ILE    78      39.049  -3.394  23.777  1.00 16.84      MTGL
ATOM    595  CD1 ILE    78      39.424  -4.364  24.905  1.00 17.38      MTGL
ATOM    596  C   ILE    78      37.031  -0.818  25.818  1.00 17.27      MTGL
ATOM    597  O   ILE    78      36.834   0.241  25.227  1.00 17.22      MTGL
ATOM    598  N   ASP    79      37.046  -0.912  27.142  1.00 16.43      MTGL
ATOM    599  CA  ASP    79      36.817   0.234  28.009  1.00 16.05      MTGL
ATOM    600  CB  ASP    79      35.738  -0.127  29.039  1.00 17.34      MTGL
ATOM    601  CG  ASP    79      35.577   0.920  30.133  1.00 19.18      MTGL
ATOM    602  OD1 ASP    79      36.023   2.072  29.952  1.00 19.88      MTGL
ATOM    603  OD2 ASP    79      34.986   0.583  31.181  1.00 20.19      MTGL
ATOM    604  C   ASP    79      38.113   0.657  28.699  1.00 16.01      MTGL
ATOM    605  O   ASP    79      38.479   0.102  29.732  1.00 15.54      MTGL
ATOM    606  N   PHE    80      38.810   1.626  28.105  1.00 15.57      MTGL
ATOM    607  CA  PHE    80      40.065   2.138  28.654  1.00 15.49      MTGL
ATOM    608  CB  PHE    80      40.811   3.005  27.627  1.00 14.72      MTGL
ATOM    609  CG  PHE    80      41.533   2.230  26.566  1.00 14.70      MTGL
ATOM    610  CD1 PHE    80      42.548   1.343  26.899  1.00 14.82      MTGL
ATOM    611  CD2 PHE    80      41.224   2.419  25.222  1.00 15.80      MTGL
ATOM    612  CE1 PHE    80      43.251   0.649  25.912  1.00 15.54      MTGL
ATOM    613  CE2 PHE    80      41.921   1.730  24.221  1.00 16.06      MTGL
ATOM    614  CZ  PHE    80      42.938   0.844  24.568  1.00 14.92      MTGL
ATOM    615  C   PHE    80      39.800   3.009  29.869  1.00 16.16      MTGL
ATOM    616  O   PHE    80      39.126   4.036  29.759  1.00 15.79      MTGL
ATOM    617  N   HIS    81      40.328   2.617  31.025  1.00 15.76      MTGL
ATOM    618  CA  HIS    81      40.140   3.419  32.234  1.00 15.04      MTGL
ATOM    619  CB  HIS    81      40.130   2.533  33.485  1.00 13.87      MTGL
ATOM    620  CG  HIS    81      38.846   1.790  33.686  1.00 14.70      MTGL
ATOM    621  CD2 HIS    81      37.971   1.263  32.795  1.00 13.78      MTGL
ATOM    622  ND1 HIS    81      38.312   1.554  34.933  1.00 13.45      MTGL
ATOM    623  CE1 HIS    81      37.161   0.918  34.804  1.00 15.90      MTGL
ATOM    624  NE2 HIS    81      36.931   0.730  33.516  1.00 14.78      MTGL
ATOM    625  C   HIS    81      41.244   4.466  32.357  1.00 15.46      MTGL
ATOM    626  O   HIS    81      41.113   5.439  33.102  1.00 14.94      MTGL
ATOM    627  N   TYR    82      42.326   4.273  31.609  1.00 15.09      MTGL
ATOM    628  CA  TYR    82      43.452   5.199  31.663  1.00 16.48      MTGL
ATOM    629  CB  TYR    82      43.092   6.520  30.974  1.00 15.74      MTGL
ATOM    630  CG  TYR    82      42.849   6.384  29.476  1.00 15.85      MTGL
ATOM    631  CD1 TYR    82      43.702   5.615  28.680  1.00 15.30      MTGL
ATOM    632  CE1 TYR    82      43.527   5.530  27.307  1.00 16.13      MTGL
ATOM    633  CD2 TYR    82      41.801   7.062  28.852  1.00 15.60      MTGL
ATOM    634  CE2 TYR    82      41.613   6.985  27.465  1.00 16.11      MTGL
ATOM    635  CZ  TYR    82      42.482   6.218  26.705  1.00 17.06      MTGL
ATOM    636  OH  TYR    82      42.331   6.148  25.345  1.00 18.86      MTGL
ATOM    637  C   TYR    82      43.866   5.437  33.122  1.00 17.11      MTGL
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Fig. 1 cont.

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ATOM    638  O   TYR   82      43.987   6.573  33.593  1.00 17.37      MTGL
ATOM    639  N   SER   83      44.077   4.329  33.822  1.00 17.17      MTGL
ATOM    640  CA  SER   83      44.482   4.328  35.223  1.00 17.21      MTGL
ATOM    641  CB  SER   83      43.288   4.679  36.115  1.00 16.41      MTGL
ATOM    642  OG  SER   83      43.639   4.651  37.487  1.00 16.64      MTGL
ATOM    643  C   SER   83      44.948   2.904  35.518  1.00 17.88      MTGL
ATOM    644  O   SER   83      44.689   1.993  34.732  1.00 17.59      MTGL
ATOM    645  N   ASP   84      45.646   2.706  36.630  1.00 18.00      MTGL
ATOM    646  CA  ASP   84      46.106   1.369  36.984  1.00 17.91      MTGL
ATOM    647  CB  ASP   84      47.378   1.415  37.840  1.00 18.31      MTGL
ATOM    648  CG  ASP   84      48.570   1.993  37.105  1.00 19.40      MTGL
ATOM    649  OD1 ASP   84      48.732   1.724  35.897  1.00 18.50      MTGL
ATOM    650  OD2 ASP   84      49.366   2.705  37.750  1.00 20.89      MTGL
ATOM    651  C   ASP   84      45.017   0.665  37.785  1.00 17.16      MTGL
ATOM    652  O   ASP   84      45.118  -0.525  38.061  1.00 16.64      MTGL
ATOM    653  N   THR   85      43.978   1.406  38.152  1.00 16.98      MTGL
ATOM    654  CA  THR   85      42.889   0.837  38.943  1.00 17.09      MTGL
ATOM    655  CB  THR   85      43.169   1.056  40.456  1.00 17.53      MTGL
ATOM    656  OG1 THR   85      42.211   0.337  41.239  1.00 20.04      MTGL
ATOM    657  CG2 THR   85      43.107   2.549  40.805  1.00 16.84      MTGL
ATOM    658  C   THR   85      41.543   1.460  38.546  1.00 16.53      MTGL
ATOM    659  O   THR   85      41.481   2.245  37.598  1.00 16.58      MTGL
ATOM    660  N   TRP   86      40.477   1.100  39.264  1.00 15.91      MTGL
ATOM    661  CA  TRP   86      39.130   1.597  38.982  1.00 16.71      MTGL
ATOM    662  CB  TRP   86      38.166   1.291  40.143  1.00 15.33      MTGL
ATOM    663  CG  TRP   86      38.079  -0.151  40.525  1.00 17.03      MTGL
ATOM    664  CD2 TRP   86      37.311  -1.165  39.871  1.00 16.85      MTGL
ATOM    665  CE2 TRP   86      37.548  -2.378  40.560  1.00 17.49      MTGL
ATOM    666  CE3 TRP   86      36.448  -1.170  38.767  1.00 16.06      MTGL
ATOM    667  CD1 TRP   86      38.731  -0.768  41.555  1.00 16.85      MTGL
ATOM    668  NE1 TRP   86      38.417  -2.104  41.583  1.00 17.28      MTGL
ATOM    669  CZ2 TRP   86      36.951  -3.588  40.180  1.00 16.23      MTGL
ATOM    670  CZ3 TRP   86      35.853  -2.373  38.388  1.00 17.14      MTGL
ATOM    671  CH2 TRP   86      36.110  -3.566  39.095  1.00 17.46      MTGL
ATOM    672  C   TRP   86      39.044   3.093  38.703  1.00 16.71      MTGL
ATOM    673  O   TRP   86      39.500   3.911  39.500  1.00 16.21      MTGL
ATOM    674  N   ALA   87      38.440   3.443  37.574  1.00 16.31      MTGL
ATOM    675  CA  ALA   87      38.249   4.845  37.223  1.00 17.57      MTGL
ATOM    676  CB  ALA   87      38.760   5.124  35.809  1.00 16.32      MTGL
ATOM    677  C   ALA   87      36.753   5.119  37.297  1.00 18.11      MTGL
ATOM    678  O   ALA   87      35.965   4.409  36.677  1.00 18.07      MTGL
ATOM    679  N   ASP   88      36.368   6.125  38.077  1.00 18.47      MTGL
ATOM    680  CA  ASP   88      34.965   6.512  38.213  1.00 18.85      MTGL
ATOM    681  CB  ASP   88      34.287   5.730  39.354  1.00 18.63      MTGL
ATOM    682  CG  ASP   88      35.047   5.816  40.661  1.00 19.12      MTGL
ATOM    683  OD1 ASP   88      35.352   6.940  41.109  1.00 18.34      MTGL
ATOM    684  OD2 ASP   88      35.331   4.749  41.248  1.00 19.72      MTGL
ATOM    685  C   ASP   88      34.932   8.021  38.460  1.00 18.13      MTGL
ATOM    686  O   ASP   88      35.980   8.656  38.505  1.00 17.65      MTGL
ATOM    687  N   PRO   89      33.737   8.616  38.615  1.00 18.93      MTGL
ATOM    688  CD  PRO   89      32.382   8.046  38.501  1.00 19.94      MTGL
ATOM    689  CA  PRO   89      33.672  10.066  38.842  1.00 19.49      MTGL
ATOM    690  CB  PRO   89      32.174  10.327  39.000  1.00 19.80      MTGL
ATOM    691  CG  PRO   89      31.555   9.263  38.125  1.00 19.69      MTGL
ATOM    692  C   PRO   89      34.476  10.600  40.025  1.00 19.90      MTGL
ATOM    693  O   PRO   89      34.833  11.778  40.048  1.00 20.62      MTGL
ATOM    694  N   ALA   90      34.760   9.743  40.999  1.00 18.70      MTGL
ATOM    695  CA  ALA   90      35.519  10.164  42.175  1.00 19.35      MTGL
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Fig. 1 cont.

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ATOM    696  CB  ALA    90      34.818   9.685  43.457  1.00 17.48      MTGL
ATOM    697  C   ALA    90      36.964   9.674  42.162  1.00 18.63      MTGL
ATOM    698  O   ALA    90      37.730   9.988  43.071  1.00 19.58      MTGL
ATOM    699  N   HIS    91      37.333   8.901  41.145  1.00 17.84      MTGL
ATOM    700  CA  HIS    91      38.698   8.391  41.039  1.00 17.68      MTGL
ATOM    701  CB  HIS    91      38.833   7.000  41.679  1.00 18.34      MTGL
ATOM    702  CG  HIS    91      38.298   6.910  43.072  1.00 20.31      MTGL
ATOM    703  CD2 HIS    91      38.927   6.936  44.272  1.00 19.87      MTGL
ATOM    704  ND1 HIS    91      36.953   6.784  43.344  1.00 18.50      MTGL
ATOM    705  CE1 HIS    91      36.775   6.736  44.653  1.00 20.43      MTGL
ATOM    706  NE2 HIS    91      37.956   6.826  45.238  1.00 21.64      MTGL
ATOM    707  C   HIS    91      39.177   8.280  39.597  1.00 16.55      MTGL
ATOM    708  O   HIS    91      38.661   7.478  38.823  1.00 16.39      MTGL
ATOM    709  N   GLN    92      40.169   9.087  39.246  1.00 15.52      MTGL
ATOM    710  CA  GLN    92      40.760   9.064  37.911  1.00 15.68      MTGL
ATOM    711  CB  GLN    92      40.281  10.255  37.072  1.00 14.49      MTGL
ATOM    712  CG  GLN    92      38.786  10.229  36.702  1.00 13.93      MTGL
ATOM    713  CD  GLN    92      38.413   9.127  35.699  1.00 14.84      MTGL
ATOM    714  OE1 GLN    92      39.173   8.814  34.779  1.00 15.41      MTGL
ATOM    715  NE2 GLN    92      37.221   8.559  35.861  1.00 14.23      MTGL
ATOM    716  C   GLN    92      42.254   9.166  38.190  1.00 15.81      MTGL
ATOM    717  O   GLN    92      42.925  10.108  37.782  1.00 16.26      MTGL
ATOM    718  N   THR    93      42.759   8.169  38.902  1.00 16.47      MTGL
ATOM    719  CA  THR    93      44.156   8.136  39.302  1.00 17.33      MTGL
ATOM    720  CB  THR    93      44.387   7.062  40.364  1.00 17.41      MTGL
ATOM    721  OG1 THR    93      43.433   7.239  41.417  1.00 19.90      MTGL
ATOM    722  CG2 THR    93      45.800   7.177  40.944  1.00 19.68      MTGL
ATOM    723  C   THR    93      45.136   7.925  38.165  1.00 17.55      MTGL
ATOM    724  O   THR    93      45.035   6.973  37.390  1.00 17.01      MTGL
ATOM    725  N   MET    94      46.093   8.839  38.089  1.00 17.63      MTGL
ATOM    726  CA  MET    94      47.131   8.820  37.079  1.00 18.68      MTGL
ATOM    727  CB  MET    94      48.144   9.926  37.383  1.00 21.10      MTGL
ATOM    728  CG  MET    94      49.195  10.133  36.315  1.00 23.55      MTGL
ATOM    729  SD  MET    94      48.474  10.956  34.894  1.00 27.41      MTGL
ATOM    730  CE  MET    94      48.342  12.657  35.533  1.00 25.13      MTGL
ATOM    731  C   MET    94      47.854   7.476  37.064  1.00 18.43      MTGL
ATOM    732  O   MET    94      48.179   6.925  38.113  1.00 18.13      MTGL
ATOM    733  N   PRO    95      48.088   6.914  35.871  1.00 17.41      MTGL
ATOM    734  CD  PRO    95      47.534   7.255  34.551  1.00 16.67      MTGL
ATOM    735  CA  PRO    95      48.797   5.631  35.834  1.00 17.83      MTGL
ATOM    736  CB  PRO    95      48.814   5.287  34.347  1.00 17.25      MTGL
ATOM    737  CG  PRO    95      47.544   5.914  33.843  1.00 17.35      MTGL
ATOM    738  C   PRO    95      50.202   5.903  36.371  1.00 18.71      MTGL
ATOM    739  O   PRO    95      50.784   6.952  36.084  1.00 17.30      MTGL
ATOM    740  N   ALA    96      50.746   4.978  37.152  1.00 18.59      MTGL
ATOM    741  CA  ALA    96      52.082   5.177  37.705  1.00 20.01      MTGL
ATOM    742  CB  ALA    96      52.470   3.983  38.587  1.00 19.66      MTGL
ATOM    743  C   ALA    96      53.095   5.357  36.577  1.00 20.37      MTGL
ATOM    744  O   ALA    96      53.081   4.617  35.595  1.00 20.80      MTGL
ATOM    745  N   GLY    97      53.959   6.356  36.710  1.00 20.53      MTGL
ATOM    746  CA  GLY    97      54.967   6.595  35.693  1.00 20.43      MTGL
ATOM    747  C   GLY    97      54.611   7.644  34.654  1.00 20.83      MTGL
ATOM    748  O   GLY    97      55.491   8.144  33.959  1.00 22.30      MTGL
ATOM    749  N   TRP    98      53.332   7.982  34.537  1.00 20.23      MTGL
ATOM    750  CA  TRP    98      52.902   8.978  33.561  1.00 19.86      MTGL
ATOM    751  CB  TRP    98      51.415   8.795  33.249  1.00 18.17      MTGL
ATOM    752  CG  TRP    98      51.106   7.576  32.421  1.00 17.34      MTGL
ATOM    753  CD2 TRP    98      49.987   7.397  31.543  1.00 16.19      MTGL
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Fig. 1 cont.

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ATOM    754  CE2 TRP    98      50.082   6.093  31.006  1.00 16.95      MTGL
ATOM    755  CE3 TRP    98      48.914   8.213  31.156  1.00 15.48      MTGL
ATOM    756  CD1 TRP    98      51.810   6.406  32.385  1.00 18.21      MTGL
ATOM    757  NE1 TRP    98      51.202   5.511  31.538  1.00 17.45      MTGL
ATOM    758  CZ2 TRP    98      49.140   5.580  30.103  1.00 17.12      MTGL
ATOM    759  CZ3 TRP    98      47.974   7.704  30.257  1.00 15.71      MTGL
ATOM    760  CH2 TRP    98      48.098   6.399  29.740  1.00 16.54      MTGL
ATOM    761  C   TRP    98      53.156  10.401  34.056  1.00 20.28      MTGL
ATOM    762  O   TRP    98      52.958  10.706  35.230  1.00 19.92      MTGL
ATOM    763  N   PRO    99      53.593  11.295  33.156  1.00 21.71      MTGL
ATOM    764  CD  PRO    99      53.852  11.048  31.725  1.00 22.15      MTGL
ATOM    765  CA  PRO    99      53.875  12.693  33.505  1.00 22.69      MTGL
ATOM    766  CB  PRO    99      54.610  13.205  32.269  1.00 22.58      MTGL
ATOM    767  CG  PRO    99      53.938  12.454  31.163  1.00 22.80      MTGL
ATOM    768  C   PRO    99      52.598  13.483  33.797  1.00 23.10      MTGL
ATOM    769  O   PRO    99      51.530  13.156  33.277  1.00 23.44      MTGL
ATOM    770  N   SER   100      52.716  14.522  34.621  1.00 22.96      MTGL
ATOM    771  CA  SER   100      51.572  15.353  34.995  1.00 23.06      MTGL
ATOM    772  CB  SER   100      51.714  15.831  36.445  1.00 24.32      MTGL
ATOM    773  OG  SER   100      51.658  14.746  37.353  1.00 26.38      MTGL
ATOM    774  C   SER   100      51.332  16.574  34.115  1.00 22.44      MTGL
ATOM    775  O   SER   100      50.202  17.051  34.032  1.00 22.25      MTGL
ATOM    776  N   ASP   101      52.379  17.098  33.480  1.00 22.38      MTGL
ATOM    777  CA  ASP   101      52.208  18.283  32.639  1.00 23.28      MTGL
ATOM    778  CB  ASP   101      53.565  18.890  32.254  1.00 24.51      MTGL
ATOM    779  CG  ASP   101      54.382  17.986  31.352  1.00 25.84      MTGL
ATOM    780  OD1 ASP   101      54.886  16.954  31.842  1.00 26.46      MTGL
ATOM    781  OD2 ASP   101      54.515  18.310  30.152  1.00 25.84      MTGL
ATOM    782  C   ASP   101      51.411  17.933  31.386  1.00 22.28      MTGL
ATOM    783  O   ASP   101      51.667  16.915  30.743  1.00 21.59      MTGL
ATOM    784  N   ILE   102      50.452  18.787  31.042  1.00 21.77      MTGL
ATOM    785  CA  ILE   102      49.584  18.548  29.890  1.00 21.42      MTGL
ATOM    786  CB  ILE   102      48.623  19.738  29.663  1.00 20.48      MTGL
ATOM    787  CG2 ILE   102      49.411  20.998  29.313  1.00 20.99      MTGL
ATOM    788  CG1 ILE   102      47.617  19.392  28.560  1.00 21.44      MTGL
ATOM    789  CD1 ILE   102      46.730  18.200  28.879  1.00 19.62      MTGL
ATOM    790  C   ILE   102      50.281  18.196  28.573  1.00 21.71      MTGL
ATOM    791  O   ILE   102      49.861  17.258  27.896  1.00 20.84      MTGL
ATOM    792  N   ASP   103      51.336  18.918  28.201  1.00 21.01      MTGL
ATOM    793  CA  ASP   103      52.012  18.608  26.945  1.00 22.44      MTGL
ATOM    794  CB  ASP   103      53.219  19.523  26.716  1.00 24.91      MTGL
ATOM    795  CG  ASP   103      52.821  20.942  26.370  1.00 27.06      MTGL
ATOM    796  OD1 ASP   103      51.633  21.178  26.070  1.00 27.99      MTGL
ATOM    797  OD2 ASP   103      53.703  21.823  26.385  1.00 28.69      MTGL
ATOM    798  C   ASP   103      52.478  17.160  26.886  1.00 22.61      MTGL
ATOM    799  O   ASP   103      52.144  16.435  25.948  1.00 23.39      MTGL
ATOM    800  N   ASN   104      53.244  16.734  27.885  1.00 21.79      MTGL
ATOM    801  CA  ASN   104      53.751  15.366  27.898  1.00 22.22      MTGL
ATOM    802  CB  ASN   104      54.912  15.244  28.884  1.00 23.92      MTGL
ATOM    803  CG  ASN   104      56.149  15.977  28.406  1.00 26.18      MTGL
ATOM    804  OD1 ASN   104      56.715  15.643  27.364  1.00 26.60      MTGL
ATOM    805  ND2 ASN   104      56.570  16.989  29.157  1.00 26.07      MTGL
ATOM    806  C   ASN   104      52.699  14.311  28.191  1.00 21.08      MTGL
ATOM    807  O   ASN   104      52.774  13.210  27.655  1.00 20.89      MTGL
ATOM    808  N   LEU   105      51.722  14.642  29.032  1.00 20.18      MTGL
ATOM    809  CA  LEU   105      50.663  13.693  29.361  1.00 19.91      MTGL
ATOM    810  CB  LEU   105      49.743  14.249  30.452  1.00 17.16      MTGL
ATOM    811  CG  LEU   105      48.568  13.339  30.842  1.00 18.64      MTGL
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Fig. 1 cont.

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ATOM    812  CD1 LEU   105      49.089  12.019  31.413  1.00 15.72      MTGL
ATOM    813  CD2 LEU   105      47.690  14.040  31.860  1.00 17.06      MTGL
ATOM    814  C   LEU   105      49.841  13.392  28.109  1.00 20.55      MTGL
ATOM    815  O   LEU   105      49.506  12.237  27.839  1.00 20.48      MTGL
ATOM    816  N   SER   106      49.521  14.435  27.346  1.00 20.24      MTGL
ATOM    817  CA  SER   106      48.746  14.264  26.124  1.00 21.47      MTGL
ATOM    818  CB  SER   106      48.514  15.610  25.437  1.00 22.23      MTGL
ATOM    819  OG  SER   106      47.695  16.447  26.235  1.00 27.30      MTGL
ATOM    820  C   SER   106      49.484  13.338  25.173  1.00 20.88      MTGL
ATOM    821  O   SER   106      48.884  12.487  24.527  1.00 19.42      MTGL
ATOM    822  N   TRP   107      50.795  13.513  25.096  1.00 22.85      MTGL
ATOM    823  CA  TRP   107      51.623  12.696  24.223  1.00 24.06      MTGL
ATOM    824  CB  TRP   107      53.033  13.282  24.164  1.00 27.94      MTGL
ATOM    825  CG  TRP   107      53.780  12.934  22.924  1.00 32.46      MTGL
ATOM    826  CD2 TRP   107      55.136  13.276  22.621  1.00 35.03      MTGL
ATOM    827  CE2 TRP   107      55.414  12.776  21.328  1.00 36.06      MTGL
ATOM    828  CE3 TRP   107      56.141  13.971  23.309  1.00 36.31      MTGL
ATOM    829  CD1 TRP   107      53.303  12.249  21.839  1.00 33.32      MTGL
ATOM    830  NE1 TRP   107      54.280  12.148  20.877  1.00 35.87      MTGL
ATOM    831  CZ2 TRP   107      56.662  12.934  20.715  1.00 36.87      MTGL
ATOM    832  CZ3 TRP   107      57.381  14.130  22.698  1.00 37.64      MTGL
ATOM    833  CH2 TRP   107      57.627  13.617  21.410  1.00 37.50      MTGL
ATOM    834  C   TRP   107      51.674  11.250  24.725  1.00 23.66      MTGL
ATOM    835  O   TRP   107      51.632  10.306  23.929  1.00 22.42      MTGL
ATOM    836  N   LYS   108      51.754  11.085  26.045  1.00 21.87      MTGL
ATOM    837  CA  LYS   108      51.810   9.758  26.654  1.00 21.77      MTGL
ATOM    838  CB  LYS   108      52.012   9.870  28.167  1.00 22.68      MTGL
ATOM    839  CG  LYS   108      52.928   8.818  28.787  1.00 25.44      MTGL
ATOM    840  CD  LYS   108      52.756   7.420  28.208  1.00 25.37      MTGL
ATOM    841  CE  LYS   108      53.657   6.436  28.948  1.00 26.82      MTGL
ATOM    842  NZ  LYS   108      53.912   5.168  28.202  1.00 25.16      MTGL
ATOM    843  C   LYS   108      50.502   9.016  26.400  1.00 21.11      MTGL
ATOM    844  O   LYS   108      50.499   7.825  26.082  1.00 20.02      MTGL
ATOM    845  N   LEU   109      49.394   9.733  26.569  1.00 20.01      MTGL
ATOM    846  CA  LEU   109      48.069   9.165  26.378  1.00 19.28      MTGL
ATOM    847  CB  LEU   109      46.998  10.210  26.701  1.00 17.83      MTGL
ATOM    848  CG  LEU   109      45.541   9.782  26.544  1.00 18.16      MTGL
ATOM    849  CD1 LEU   109      45.278   8.500  27.331  1.00 16.64      MTGL
ATOM    850  CD2 LEU   109      44.639  10.912  27.023  1.00 17.12      MTGL
ATOM    851  C   LEU   109      47.922   8.689  24.941  1.00 19.15      MTGL
ATOM    852  O   LEU   109      47.356   7.630  24.681  1.00 17.95      MTGL
ATOM    853  N   TYR   110      48.439   9.485  24.013  1.00 19.31      MTGL
ATOM    854  CA  TYR   110      48.390   9.141  22.602  1.00 20.23      MTGL
ATOM    855  CB  TYR   110      48.928  10.308  21.765  1.00 20.77      MTGL
ATOM    856  CG  TYR   110      49.112   9.988  20.301  1.00 22.28      MTGL
ATOM    857  CD1 TYR   110      50.324   9.483  19.827  1.00 22.42      MTGL
ATOM    858  CE1 TYR   110      50.500   9.174  18.478  1.00 23.01      MTGL
ATOM    859  CD2 TYR   110      48.072  10.179  19.388  1.00 21.90      MTGL
ATOM    860  CE2 TYR   110      48.236   9.873  18.033  1.00 22.98      MTGL
ATOM    861  CZ  TYR   110      49.453   9.373  17.589  1.00 22.70      MTGL
ATOM    862  OH  TYR   110      49.628   9.075  16.261  1.00 22.60      MTGL
ATOM    863  C   TYR   110      49.209   7.873  22.351  1.00 20.36      MTGL
ATOM    864  O   TYR   110      48.713   6.915  21.753  1.00 19.75      MTGL
ATOM    865  N   ASN   111      50.453   7.864  22.826  1.00 19.95      MTGL
ATOM    866  CA  ASN   111      51.333   6.712  22.650  1.00 20.79      MTGL
ATOM    867  CB  ASN   111      52.691   6.944  23.316  1.00 22.26      MTGL
ATOM    868  CG  ASN   111      53.496   8.030  22.642  1.00 26.38      MTGL
ATOM    869  OD1 ASN   111      53.175   8.463  21.534  1.00 25.33      MTGL
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Fig. 1 cont.

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ATOM    870  ND2 ASN   111      54.556   8.463  23.317  1.00 29.11      MTGL
ATOM    871  C   ASN   111      50.736   5.445  23.234  1.00 20.44      MTGL
ATOM    872  O   ASN   111      50.764   4.391  22.605  1.00 20.22      MTGL
ATOM    873  N   TYR   112      50.218   5.551  24.452  1.00 19.27      MTGL
ATOM    874  CA  TYR   112      49.622   4.406  25.123  1.00 18.94      MTGL
ATOM    875  CB  TYR   112      49.131   4.801  26.517  1.00 16.74      MTGL
ATOM    876  CG  TYR   112      48.211   3.770  27.137  1.00 17.22      MTGL
ATOM    877  CD1 TYR   112      48.723   2.632  27.766  1.00 15.42      MTGL
ATOM    878  CE1 TYR   112      47.876   1.671  28.311  1.00 17.32      MTGL
ATOM    879  CD2 TYR   112      46.827   3.916  27.065  1.00 15.87      MTGL
ATOM    880  CE2 TYR   112      45.971   2.960  27.604  1.00 17.72      MTGL
ATOM    881  CZ  TYR   112      46.500   1.844  28.225  1.00 16.39      MTGL
ATOM    882  OH  TYR   112      45.653   0.907  28.766  1.00 18.06      MTGL
ATOM    883  C   TYR   112      48.449   3.832  24.330  1.00 18.50      MTGL
ATOM    884  O   TYR   112      48.358   2.622  24.129  1.00 17.86      MTGL
ATOM    885  N   THR   113      47.545   4.709  23.903  1.00 18.56      MTGL
ATOM    886  CA  THR   113      46.372   4.288  23.152  1.00 18.24      MTGL
ATOM    887  CB  THR   113      45.408   5.474  22.930  1.00 17.98      MTGL
ATOM    888  OG1 THR   113      45.017   6.014  24.198  1.00 16.20      MTGL
ATOM    889  CG2 THR   113      44.158   5.021  22.184  1.00 17.01      MTGL
ATOM    890  C   THR   113      46.765   3.682  21.805  1.00 18.67      MTGL
ATOM    891  O   THR   113      46.272   2.619  21.423  1.00 18.43      MTGL
ATOM    892  N   LEU   114      47.655   4.360  21.090  1.00 19.14      MTGL
ATOM    893  CA  LEU   114      48.114   3.873  19.797  1.00 20.50      MTGL
ATOM    894  CB  LEU   114      49.133   4.848  19.197  1.00 20.12      MTGL
ATOM    895  CG  LEU   114      49.864   4.396  17.929  1.00 21.74      MTGL
ATOM    896  CD1 LEU   114      48.866   4.214  16.794  1.00 21.80      MTGL
ATOM    897  CD2 LEU   114      50.924   5.430  17.547  1.00 22.25      MTGL
ATOM    898  C   LEU   114      48.753   2.498  19.984  1.00 20.96      MTGL
ATOM    899  O   LEU   114      48.441   1.551  19.263  1.00 21.53      MTGL
ATOM    900  N   ASP   115      49.650   2.399  20.961  1.00 21.00      MTGL
ATOM    901  CA  ASP   115      50.335   1.148  21.252  1.00 21.18      MTGL
ATOM    902  CB  ASP   115      51.276   1.331  22.442  1.00 22.68      MTGL
ATOM    903  CG  ASP   115      51.957   0.041  22.843  1.00 24.76      MTGL
ATOM    904  OD1 ASP   115      52.826  -0.429  22.078  1.00 26.71      MTGL
ATOM    905  OD2 ASP   115      51.616  -0.509  23.917  1.00 25.94      MTGL
ATOM    906  C   ASP   115      49.351   0.018  21.561  1.00 21.01      MTGL
ATOM    907  O   ASP   115      49.461  -1.078  21.012  1.00 20.38      MTGL
ATOM    908  N   ALA   116      48.404   0.287  22.456  1.00 19.72      MTGL
ATOM    909  CA  ALA   116      47.410  -0.711  22.833  1.00 19.79      MTGL
ATOM    910  CB  ALA   116      46.501  -0.163  23.923  1.00 19.04      MTGL
ATOM    911  C   ALA   116      46.578  -1.140  21.627  1.00 18.78      MTGL
ATOM    912  O   ALA   116      46.302  -2.323  21.448  1.00 18.71      MTGL
ATOM    913  N   ALA   117      46.184  -0.172  20.806  1.00 18.51      MTGL
ATOM    914  CA  ALA   117      45.384  -0.456  19.616  1.00 19.07      MTGL
ATOM    915  CB  ALA   117      45.012   0.840  18.913  1.00 17.76      MTGL
ATOM    916  C   ALA   117      46.144  -1.372  18.662  1.00 19.00      MTGL
ATOM    917  O   ALA   117      45.588  -2.344  18.157  1.00 20.94      MTGL
ATOM    918  N   ASN   118      47.414  -1.064  18.421  1.00 19.11      MTGL
ATOM    919  CA  ASN   118      48.234  -1.880  17.530  1.00 20.09      MTGL
ATOM    920  CB  ASN   118      49.594  -1.214  17.280  1.00 19.53      MTGL
ATOM    921  CG  ASN   118      49.481   0.043  16.432  1.00 21.06      MTGL
ATOM    922  OD1 ASN   118      48.591   0.158  15.584  1.00 22.85      MTGL
ATOM    923  ND2 ASN   118      50.394   0.984  16.644  1.00 19.62      MTGL
ATOM    924  C   ASN   118      48.446  -3.294  18.069  1.00 20.53      MTGL
ATOM    925  O   ASN   118      48.509  -4.250  17.298  1.00 20.72      MTGL
ATOM    926  N   LYS   119      48.570  -3.427  19.389  1.00 20.26      MTGL
ATOM    927  CA  LYS   119      48.755  -4.745  19.992  1.00 19.69      MTGL
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Fig. 1 cont.

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ATOM    928  CB  LYS   119      49.134  -4.616  21.468  1.00 20.25      MTGL
ATOM    929  CG  LYS   119      50.589  -4.225  21.668  1.00 23.15      MTGL
ATOM    930  CD  LYS   119      50.933  -4.015  23.131  1.00 25.43      MTGL
ATOM    931  CE  LYS   119      52.378  -3.533  23.273  1.00 26.95      MTGL
ATOM    932  NZ  LYS   119      52.701  -3.126  24.666  1.00 26.48      MTGL
ATOM    933  C   LYS   119      47.482  -5.570  19.843  1.00 18.61      MTGL
ATOM    934  O   LYS   119      47.533  -6.777  19.615  1.00 16.84      MTGL
ATOM    935  N   LEU   120      46.339  -4.911  19.975  1.00 17.54      MTGL
ATOM    936  CA  LEU   120      45.064  -5.599  19.820  1.00 18.74      MTGL
ATOM    937  CB  LEU   120      43.909  -4.643  20.144  1.00 17.57      MTGL
ATOM    938  CG  LEU   120      43.736  -4.330  21.635  1.00 17.26      MTGL
ATOM    939  CD1 LEU   120      42.836  -3.117  21.830  1.00 17.85      MTGL
ATOM    940  CD2 LEU   120      43.152  -5.549  22.325  1.00 16.86      MTGL
ATOM    941  C   LEU   120      44.976  -6.086  18.372  1.00 18.39      MTGL
ATOM    942  O   LEU   120      44.660  -7.243  18.116  1.00 19.13      MTGL
ATOM    943  N   GLN   121      45.273  -5.193  17.434  1.00 19.05      MTGL
ATOM    944  CA  GLN   121      45.245  -5.524  16.013  1.00 20.51      MTGL
ATOM    945  CB  GLN   121      45.715  -4.324  15.182  1.00 20.27      MTGL
ATOM    946  CG  GLN   121      45.927  -4.606  13.694  1.00 19.88      MTGL
ATOM    947  CD  GLN   121      44.677  -5.116  12.998  1.00 20.20      MTGL
ATOM    948  OE1 GLN   121      43.565  -4.680  13.291  1.00 19.32      MTGL
ATOM    949  NE2 GLN   121      44.859  -6.035  12.055  1.00 20.98      MTGL
ATOM    950  C   GLN   121      46.142  -6.723  15.734  1.00 20.78      MTGL
ATOM    951  O   GLN   121      45.729  -7.672  15.078  1.00 21.20      MTGL
ATOM    952  N   ASN   122      47.369  -6.676  16.242  1.00 20.58      MTGL
ATOM    953  CA  ASN   122      48.322  -7.762  16.037  1.00 22.39      MTGL
ATOM    954  CB  ASN   122      49.685  -7.371  16.611  1.00 24.20      MTGL
ATOM    955  CG  ASN   122      50.350  -6.260  15.817  1.00 26.36      MTGL
ATOM    956  OD1 ASN   122      51.298  -5.630  16.285  1.00 29.40      MTGL
ATOM    957  ND2 ASN   122      49.863  -6.021  14.605  1.00 26.25      MTGL
ATOM    958  C   ASN   122      47.859  -9.082  16.646  1.00 22.40      MTGL
ATOM    959  O   ASN   122      48.312 -10.153  16.243  1.00 23.25      MTGL
ATOM    960  N   ALA   123      46.957  -9.005  17.616  1.00 21.34      MTGL
ATOM    961  CA  ALA   123      46.436 -10.209  18.252  1.00 21.19      MTGL
ATOM    962  CB  ALA   123      46.151  -9.939  19.730  1.00 21.28      MTGL
ATOM    963  C   ALA   123      45.163 -10.669  17.545  1.00 20.31      MTGL
ATOM    964  O   ALA   123      44.512 -11.621  17.981  1.00 21.19      MTGL
ATOM    965  N   GLY   124      44.813  -9.985  16.457  1.00 20.00      MTGL
ATOM    966  CA  GLY   124      43.621 -10.332  15.705  1.00 19.34      MTGL
ATOM    967  C   GLY   124      42.338  -9.853  16.367  1.00 20.32      MTGL
ATOM    968  O   GLY   124      41.255 -10.376  16.098  1.00 19.71      MTGL
ATOM    969  N   ILE   125      42.450  -8.855  17.239  1.00 18.85      MTGL
ATOM    970  CA  ILE   125      41.281  -8.327  17.928  1.00 17.97      MTGL
ATOM    971  CB  ILE   125      41.502  -8.279  19.465  1.00 18.21      MTGL
ATOM    972  CG2 ILE   125      40.264  -7.709  20.149  1.00 18.39      MTGL
ATOM    973  CG1 ILE   125      41.807  -9.681  20.013  1.00 16.78      MTGL
ATOM    974  CD1 ILE   125      40.682 -10.694  19.808  1.00 15.33      MTGL
ATOM    975  C   ILE   125      40.936  -6.908  17.460  1.00 18.72      MTGL
ATOM    976  O   ILE   125      41.682  -5.959  17.718  1.00 18.82      MTGL
ATOM    977  N   GLN   126      39.810  -6.771  16.769  1.00 17.38      MTGL
ATOM    978  CA  GLN   126      39.355  -5.463  16.310  1.00 17.54      MTGL
ATOM    979  CB  GLN   126      39.059  -5.459  14.810  1.00 17.95      MTGL
ATOM    980  CG  GLN   126      40.267  -5.634  13.905  1.00 18.48      MTGL
ATOM    981  CD  GLN   126      40.704  -7.082  13.784  1.00 19.41      MTGL
ATOM    982  OE1 GLN   126      39.874  -7.991  13.722  1.00 18.45      MTGL
ATOM    983  NE2 GLN   126      42.014  -7.302  13.731  1.00 18.37      MTGL
ATOM    984  C   GLN   126      38.078  -5.152  17.073  1.00 17.01      MTGL
ATOM    985  O   GLN   126      36.990  -5.578  16.686  1.00 17.42      MTGL
```

Fig. 1 cont.

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ATOM    986  N   PRO  127      38.196  -4.424  18.189  1.00 17.14      MTGL
ATOM    987  CD  PRO  127      39.397  -3.833  18.803  1.00 16.94      MTGL
ATOM    988  CA  PRO  127      36.990  -4.103  18.954  1.00 17.76      MTGL
ATOM    989  CB  PRO  127      37.534  -3.333  20.162  1.00 17.60      MTGL
ATOM    990  CG  PRO  127      38.806  -2.730  19.644  1.00 20.07      MTGL
ATOM    991  C   PRO  127      36.004  -3.290  18.130  1.00 17.06      MTGL
ATOM    992  O   PRO  127      36.400  -2.472  17.303  1.00 18.03      MTGL
ATOM    993  N   THR  128      34.719  -3.536  18.340  1.00 17.80      MTGL
ATOM    994  CA  THR  128      33.688  -2.803  17.620  1.00 17.59      MTGL
ATOM    995  CB  THR  128      32.357  -3.582  17.615  1.00 18.62      MTGL
ATOM    996  OG1 THR  128      32.035  -3.994  18.951  1.00 17.44      MTGL
ATOM    997  CG2 THR  128      32.467  -4.816  16.717  1.00 18.59      MTGL
ATOM    998  C   THR  128      33.499  -1.451  18.310  1.00 17.94      MTGL
ATOM    999  O   THR  128      33.086  -0.476  17.683  1.00 16.71      MTGL
ATOM   1000  N   ILE  129      33.834  -1.397  19.600  1.00 16.54      MTGL
ATOM   1001  CA  ILE  129      33.701  -0.161  20.373  1.00 16.74      MTGL
ATOM   1002  CB  ILE  129      32.426  -0.166  21.249  1.00 17.47      MTGL
ATOM   1003  CG2 ILE  129      32.323   1.138  22.032  1.00 16.90      MTGL
ATOM   1004  CG1 ILE  129      31.182  -0.340  20.380  1.00 18.59      MTGL
ATOM   1005  CD1 ILE  129      29.913  -0.501  21.189  1.00 18.26      MTGL
ATOM   1006  C   ILE  129      34.878   0.056  21.317  1.00 16.72      MTGL
ATOM   1007  O   ILE  129      35.361  -0.883  21.949  1.00 16.12      MTGL
ATOM   1008  N   VAL  130      35.329   1.303  21.410  1.00 16.38      MTGL
ATOM   1009  CA  VAL  130      36.413   1.666  22.313  1.00 16.43      MTGL
ATOM   1010  CB  VAL  130      37.738   1.891  21.568  1.00 16.85      MTGL
ATOM   1011  CG1 VAL  130      38.783   2.444  22.532  1.00 15.96      MTGL
ATOM   1012  CG2 VAL  130      38.224   0.581  20.958  1.00 16.65      MTGL
ATOM   1013  C   VAL  130      36.040   2.965  23.020  1.00 16.57      MTGL
ATOM   1014  O   VAL  130      35.807   3.981  22.369  1.00 17.33      MTGL
ATOM   1015  N   SER  131      35.955   2.931  24.347  1.00 15.26      MTGL
ATOM   1016  CA  SER  131      35.640   4.142  25.088  1.00 14.32      MTGL
ATOM   1017  CB  SER  131      34.741   3.840  26.296  1.00 13.74      MTGL
ATOM   1018  OG  SER  131      35.427   3.100  27.299  1.00 14.55      MTGL
ATOM   1019  C   SER  131      36.957   4.737  25.563  1.00 13.67      MTGL
ATOM   1020  O   SER  131      37.812   4.024  26.094  1.00 14.63      MTGL
ATOM   1021  N   ILE  132      37.140   6.033  25.349  1.00 12.98      MTGL
ATOM   1022  CA  ILE  132      38.362   6.684  25.791  1.00 13.07      MTGL
ATOM   1023  CB  ILE  132      38.793   7.796  24.811  1.00 13.05      MTGL
ATOM   1024  CG2 ILE  132      39.419   7.169  23.573  1.00 14.24      MTGL
ATOM   1025  CG1 ILE  132      37.591   8.649  24.397  1.00 13.32      MTGL
ATOM   1026  CD1 ILE  132      37.960   9.760  23.429  1.00 14.06      MTGL
ATOM   1027  C   ILE  132      38.103   7.234  27.188  1.00 13.33      MTGL
ATOM   1028  O   ILE  132      37.800   8.415  27.372  1.00 12.93      MTGL
ATOM   1029  N   GLY  133      38.206   6.339  28.170  1.00 12.78      MTGL
ATOM   1030  CA  GLY  133      37.957   6.703  29.552  1.00 13.26      MTGL
ATOM   1031  C   GLY  133      36.687   6.040  30.066  1.00 14.41      MTGL
ATOM   1032  O   GLY  133      35.821   5.638  29.279  1.00 14.45      MTGL
ATOM   1033  N   ASN  134      36.573   5.915  31.385  1.00 14.34      MTGL
ATOM   1034  CA  ASN  134      35.393   5.311  31.995  1.00 14.81      MTGL
ATOM   1035  CB  ASN  134      35.797   4.063  32.780  1.00 14.03      MTGL
ATOM   1036  CG  ASN  134      34.602   3.307  33.321  1.00 15.54      MTGL
ATOM   1037  OD1 ASN  134      33.932   2.558  32.596  1.00 14.69      MTGL
ATOM   1038  ND2 ASN  134      34.311   3.515  34.599  1.00 13.31      MTGL
ATOM   1039  C   ASN  134      34.727   6.328  32.929  1.00 15.45      MTGL
ATOM   1040  O   ASN  134      35.355   6.823  33.865  1.00 14.99      MTGL
ATOM   1041  N   GLU  135      33.458   6.632  32.672  1.00 15.32      MTGL
ATOM   1042  CA  GLU  135      32.708   7.600  33.480  1.00 16.19      MTGL
ATOM   1043  CB  GLU  135      32.225   6.948  34.780  1.00 16.84      MTGL
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Fig. 1 cont.

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ATOM   1044  CG  GLU   135      31.360   5.710  34.571  1.00 18.65      MTGL
ATOM   1045  CD  GLU   135      30.758   5.173  35.862  1.00 19.18      MTGL
ATOM   1046  OE1 GLU   135      31.449   5.200  36.905  1.00 20.99      MTGL
ATOM   1047  OE2 GLU   135      29.602   4.705  35.829  1.00 16.99      MTGL
ATOM   1048  C   GLU   135      33.553   8.834  33.806  1.00 16.49      MTGL
ATOM   1049  O   GLU   135      33.777   9.153  34.974  1.00 15.93      MTGL
ATOM   1050  N   ILE   136      34.004   9.536  32.770  1.00 15.57      MTGL
ATOM   1051  CA  ILE   136      34.846  10.712  32.957  1.00 16.13      MTGL
ATOM   1052  CB  ILE   136      35.802  10.887  31.756  1.00 16.05      MTGL
ATOM   1053  CG2 ILE   136      36.783   9.719  31.706  1.00 16.66      MTGL
ATOM   1054  CG1 ILE   136      35.001  10.956  30.451  1.00 16.40      MTGL
ATOM   1055  CD1 ILE   136      35.858  11.171  29.211  1.00 14.50      MTGL
ATOM   1056  C   ILE   136      34.060  12.006  33.168  1.00 16.79      MTGL
ATOM   1057  O   ILE   136      34.457  13.067  32.697  1.00 16.67      MTGL
ATOM   1058  N   ARG   137      32.949  11.909  33.890  1.00 17.28      MTGL
ATOM   1059  CA  ARG   137      32.099  13.057  34.170  1.00 18.25      MTGL
ATOM   1060  CB  ARG   137      30.884  12.612  34.976  1.00 20.33      MTGL
ATOM   1061  CG  ARG   137      29.879  13.712  35.248  1.00 22.61      MTGL
ATOM   1062  CD  ARG   137      29.087  13.370  36.487  1.00 26.40      MTGL
ATOM   1063  NE  ARG   137      29.837  13.668  37.696  1.00 28.06      MTGL
ATOM   1064  CZ  ARG   137      29.643  13.076  38.869  1.00 28.40      MTGL
ATOM   1065  NH1 ARG   137      28.726  12.132  39.006  1.00 27.39      MTGL
ATOM   1066  NH2 ARG   137      30.355  13.459  39.918  1.00 30.54      MTGL
ATOM   1067  C   ARG   137      32.849  14.145  34.937  1.00 19.12      MTGL
ATOM   1068  O   ARG   137      32.537  15.327  34.812  1.00 19.19      MTGL
ATOM   1069  N   ALA   138      33.832  13.744  35.738  1.00 17.89      MTGL
ATOM   1070  CA  ALA   138      34.626  14.708  36.487  1.00 18.61      MTGL
ATOM   1071  CB  ALA   138      34.679  14.320  37.965  1.00 18.89      MTGL
ATOM   1072  C   ALA   138      36.028  14.744  35.888  1.00 18.04      MTGL
ATOM   1073  O   ALA   138      37.003  15.050  36.573  1.00 18.75      MTGL
ATOM   1074  N   GLY   139      36.119  14.415  34.603  1.00 17.60      MTGL
ATOM   1075  CA  GLY   139      37.401  14.424  33.920  1.00 16.74      MTGL
ATOM   1076  C   GLY   139      38.141  13.103  33.979  1.00 17.00      MTGL
ATOM   1077  O   GLY   139      37.558  12.061  34.303  1.00 15.56      MTGL
ATOM   1078  N   LEU   140      39.430  13.150  33.653  1.00 16.36      MTGL
ATOM   1079  CA  LEU   140      40.288  11.965  33.666  1.00 16.91      MTGL
ATOM   1080  CB  LEU   140      40.254  11.255  32.308  1.00 16.55      MTGL
ATOM   1081  CG  LEU   140      40.965  11.954  31.137  1.00 17.14      MTGL
ATOM   1082  CD1 LEU   140      41.157  10.962  29.985  1.00 17.61      MTGL
ATOM   1083  CD2 LEU   140      40.158  13.157  30.673  1.00 16.51      MTGL
ATOM   1084  C   LEU   140      41.731  12.366  33.961  1.00 16.82      MTGL
ATOM   1085  O   LEU   140      42.078  13.549  33.919  1.00 16.86      MTGL
ATOM   1086  N   LEU   141      42.566  11.373  34.254  1.00 16.21      MTGL
ATOM   1087  CA  LEU   141      43.979  11.616  34.521  1.00 16.03      MTGL
ATOM   1088  CB  LEU   141      44.711  11.839  33.191  1.00 14.81      MTGL
ATOM   1089  CG  LEU   141      44.626  10.646  32.220  1.00 15.72      MTGL
ATOM   1090  CD1 LEU   141      45.076  11.054  30.818  1.00 14.73      MTGL
ATOM   1091  CD2 LEU   141      45.494   9.501  32.752  1.00 14.97      MTGL
ATOM   1092  C   LEU   141      44.166  12.822  35.444  1.00 16.13      MTGL
ATOM   1093  O   LEU   141      44.776  13.819  35.069  1.00 15.77      MTGL
ATOM   1094  N   TRP   142      43.631  12.715  36.655  1.00 16.15      MTGL
ATOM   1095  CA  TRP   142      43.718  13.789  37.635  1.00 16.13      MTGL
ATOM   1096  CB  TRP   142      42.854  13.446  38.845  1.00 16.04      MTGL
ATOM   1097  CG  TRP   142      41.387  13.408  38.559  1.00 16.68      MTGL
ATOM   1098  CD2 TRP   142      40.345  13.114  39.494  1.00 16.86      MTGL
ATOM   1099  CE2 TRP   142      39.117  13.217  38.800  1.00 16.85      MTGL
ATOM   1100  CE3 TRP   142      40.330  12.779  40.855  1.00 17.53      MTGL
ATOM   1101  CD1 TRP   142      40.769  13.669  37.365  1.00 16.02      MTGL
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Fig. 1 cont.

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ATOM   1102  NE1 TRP   142      39.404  13.557  37.503  1.00 16.14      MTGL
ATOM   1103  CZ2 TRP   142      37.884  12.993  39.421  1.00 16.71      MTGL
ATOM   1104  CZ3 TRP   142      39.097  12.557  41.475  1.00 17.85      MTGL
ATOM   1105  CH2 TRP   142      37.894  12.666  40.755  1.00 17.70      MTGL
ATOM   1106  C   TRP   142      45.151  14.036  38.092  1.00 16.70      MTGL
ATOM   1107  O   TRP   142      45.965  13.116  38.132  1.00 15.98      MTGL
ATOM   1108  N   PRO   143      45.476  15.289  38.452  1.00 18.10      MTGL
ATOM   1109  CD  PRO   143      46.716  15.597  39.183  1.00 18.05      MTGL
ATOM   1110  CA  PRO   143      44.586  16.458  38.444  1.00 17.24      MTGL
ATOM   1111  CB  PRO   143      45.170  17.362  39.539  1.00 17.56      MTGL
ATOM   1112  CG  PRO   143      46.199  16.496  40.260  1.00 19.44      MTGL
ATOM   1113  C   PRO   143      44.599  17.177  37.096  1.00 17.09      MTGL
ATOM   1114  O   PRO   143      43.804  18.092  36.864  1.00 16.74      MTGL
ATOM   1115  N   THR   144      45.509  16.767  36.219  1.00 16.23      MTGL
ATOM   1116  CA  THR   144      45.651  17.396  34.910  1.00 17.05      MTGL
ATOM   1117  CB  THR   144      46.677  16.640  34.048  1.00 17.49      MTGL
ATOM   1118  OG1 THR   144      47.864  16.413  34.817  1.00 18.41      MTGL
ATOM   1119  CG2 THR   144      47.040  17.453  32.811  1.00 17.61      MTGL
ATOM   1120  C   THR   144      44.346  17.510  34.129  1.00 16.98      MTGL
ATOM   1121  O   THR   144      44.027  18.579  33.610  1.00 17.37      MTGL
ATOM   1122  N   GLY   145      43.594  16.414  34.052  1.00 17.00      MTGL
ATOM   1123  CA  GLY   145      42.336  16.432  33.322  1.00 16.55      MTGL
ATOM   1124  C   GLY   145      41.111  16.472  34.219  1.00 17.19      MTGL
ATOM   1125  O   GLY   145      40.033  16.013  33.837  1.00 15.11      MTGL
ATOM   1126  N   ARG   146      41.269  17.009  35.423  1.00 16.86      MTGL
ATOM   1127  CA  ARG   146      40.153  17.118  36.361  1.00 18.80      MTGL
ATOM   1128  CB  ARG   146      40.707  17.308  37.784  1.00 20.43      MTGL
ATOM   1129  CG  ARG   146      39.671  17.572  38.870  1.00 24.77      MTGL
ATOM   1130  CD  ARG   146      38.729  16.394  39.052  1.00 27.03      MTGL
ATOM   1131  NE  ARG   146      37.715  16.623  40.081  1.00 30.10      MTGL
ATOM   1132  CZ  ARG   146      37.922  16.516  41.391  1.00 31.39      MTGL
ATOM   1133  NH1 ARG   146      39.122  16.182  41.861  1.00 31.38      MTGL
ATOM   1134  NH2 ARG   146      36.916  16.729  42.236  1.00 32.17      MTGL
ATOM   1135  C   ARG   146      39.261  18.308  35.961  1.00 18.91      MTGL
ATOM   1136  O   ARG   146      39.763  19.344  35.534  1.00 17.30      MTGL
ATOM   1137  N   THR   147      37.940  18.147  36.055  1.00 18.95      MTGL
ATOM   1138  CA  THR   147      37.037  19.255  35.732  1.00 19.02      MTGL
ATOM   1139  CB  THR   147      35.550  18.826  35.731  1.00 18.33      MTGL
ATOM   1140  OG1 THR   147      35.278  18.044  36.890  1.00 18.17      MTGL
ATOM   1141  CG2 THR   147      35.217  18.016  34.490  1.00 18.17      MTGL
ATOM   1142  C   THR   147      37.278  20.271  36.858  1.00 19.51      MTGL
ATOM   1143  O   THR   147      37.539  19.861  37.983  1.00 18.48      MTGL
ATOM   1144  N   GLU   148      37.158  21.574  36.598  1.00 19.44      MTGL
ATOM   1145  CA  GLU   148      36.771  22.124  35.317  1.00 20.37      MTGL
ATOM   1146  CB  GLU   148      35.829  23.309  35.551  1.00 22.32      MTGL
ATOM   1147  CG  GLU   148      34.576  22.960  36.356  1.00 26.58      MTGL
ATOM   1148  CD  GLU   148      34.081  24.123  37.217  1.00 29.48      MTGL
ATOM   1149  OE1 GLU   148      33.777  25.209  36.672  1.00 30.90      MTGL
ATOM   1150  OE2 GLU   148      33.988  23.929  38.448  1.00 30.75      MTGL
ATOM   1151  C   GLU   148      37.858  22.540  34.312  1.00 20.17      MTGL
ATOM   1152  O   GLU   148      37.649  23.550  33.633  1.00 20.26      MTGL
ATOM   1153  N   ASN   149      39.019  21.853  34.186  0.50 20.18      MTGL
ATOM   1154  CA  ASN   149      40.039  22.216  33.154  0.50 20.26      MTGL
ATOM   1155  CB  ASN   149      41.436  21.616  33.436  0.50 21.36      MTGL
ATOM   1156  CG  ASN   149      42.198  22.423  34.433  0.50 22.41      MTGL
ATOM   1157  OD1 ASN   149      42.651  23.520  34.132  0.50 23.31      MTGL
ATOM   1158  ND2 ASN   149      42.298  21.917  35.646  0.50 23.40      MTGL
ATOM   1159  C   ASN   149      39.555  21.656  31.811  0.50 19.48      MTGL
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Fig. 1 cont.

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ATOM   1160  O   ASN   149      40.152  20.702  31.289  0.50 17.94      MTGL
ATOM   1161  N   TRP   150      38.480  22.230  31.261  1.00 19.00      MTGL
ATOM   1162  CA  TRP   150      37.920  21.769  30.000  1.00 18.91      MTGL
ATOM   1163  CB  TRP   150      36.777  22.704  29.605  1.00 18.17      MTGL
ATOM   1164  CG  TRP   150      35.710  22.781  30.629  1.00 17.82      MTGL
ATOM   1165  CD2 TRP   150      34.895  21.702  31.094  1.00 18.44      MTGL
ATOM   1166  CE2 TRP   150      34.013  22.232  32.060  1.00 18.24      MTGL
ATOM   1167  CE3 TRP   150      34.824  20.335  30.787  1.00 18.25      MTGL
ATOM   1168  CD1 TRP   150      35.301  23.895  31.310  1.00 17.99      MTGL
ATOM   1169  NE1 TRP   150      34.282  23.571  32.170  1.00 19.19      MTGL
ATOM   1170  CZ2 TRP   150      33.066  21.443  32.725  1.00 19.86      MTGL
ATOM   1171  CZ3 TRP   150      33.879  19.547  31.448  1.00 19.02      MTGL
ATOM   1172  CH2 TRP   150      33.013  20.105  32.408  1.00 19.52      MTGL
ATOM   1173  C   TRP   150      38.990  21.744  28.904  1.00 19.25      MTGL
ATOM   1174  O   TRP   150      39.022  20.828  28.091  1.00 19.43      MTGL
ATOM   1175  N   ALA   151      39.851  22.759  28.880  1.00 17.86      MTGL
ATOM   1176  CA  ALA   151      40.897  22.822  27.864  1.00 18.96      MTGL
ATOM   1177  CB  ALA   151      41.753  24.090  28.047  1.00 19.41      MTGL
ATOM   1178  C   ALA   151      41.784  21.571  27.897  1.00 18.90      MTGL
ATOM   1179  O   ALA   151      42.098  20.994  26.857  1.00 19.89      MTGL
ATOM   1180  N   ASN   152      42.184  21.144  29.088  1.00 18.45      MTGL
ATOM   1181  CA  ASN   152      43.027  19.954  29.209  1.00 18.07      MTGL
ATOM   1182  CB  ASN   152      43.584  19.830  30.635  1.00 16.97      MTGL
ATOM   1183  CG  ASN   152      44.767  20.764  30.886  1.00 18.19      MTGL
ATOM   1184  OD1 ASN   152      45.095  21.603  30.054  1.00 17.89      MTGL
ATOM   1185  ND2 ASN   152      45.407  20.618  32.043  1.00 17.33      MTGL
ATOM   1186  C   ASN   152      42.250  18.686  28.848  1.00 17.48      MTGL
ATOM   1187  O   ASN   152      42.762  17.805  28.155  1.00 17.16      MTGL
ATOM   1188  N   ILE   153      41.016  18.598  29.325  1.00 17.57      MTGL
ATOM   1189  CA  ILE   153      40.177  17.437  29.048  1.00 18.34      MTGL
ATOM   1190  CB  ILE   153      38.801  17.573  29.741  1.00 17.84      MTGL
ATOM   1191  CG2 ILE   153      37.836  16.486  29.243  1.00 17.51      MTGL
ATOM   1192  CG1 ILE   153      38.987  17.468  31.255  1.00 17.49      MTGL
ATOM   1193  CD1 ILE   153      37.761  17.837  32.060  1.00 17.26      MTGL
ATOM   1194  C   ILE   153      39.974  17.246  27.548  1.00 17.82      MTGL
ATOM   1195  O   ILE   153      40.174  16.150  27.027  1.00 17.52      MTGL
ATOM   1196  N   ALA   154      39.596  18.318  26.858  1.00 17.93      MTGL
ATOM   1197  CA  ALA   154      39.359  18.255  25.416  1.00 18.68      MTGL
ATOM   1198  CB  ALA   154      38.884  19.620  24.896  1.00 17.82      MTGL
ATOM   1199  C   ALA   154      40.624  17.834  24.686  1.00 18.79      MTGL
ATOM   1200  O   ALA   154      40.584  17.037  23.744  1.00 17.95      MTGL
ATOM   1201  N   ARG   155      41.749  18.375  25.131  1.00 18.32      MTGL
ATOM   1202  CA  ARG   155      43.025  18.064  24.512  1.00 19.09      MTGL
ATOM   1203  CB  ARG   155      44.098  18.972  25.094  1.00 20.03      MTGL
ATOM   1204  CG  ARG   155      45.415  18.867  24.403  1.00 23.57      MTGL
ATOM   1205  CD  ARG   155      46.295  19.990  24.873  1.00 26.84      MTGL
ATOM   1206  NE  ARG   155      47.681  19.767  24.498  1.00 29.65      MTGL
ATOM   1207  CZ  ARG   155      48.686  20.513  24.931  1.00 28.58      MTGL
ATOM   1208  NH1 ARG   155      48.443  21.525  25.753  1.00 29.23      MTGL
ATOM   1209  NH2 ARG   155      49.922  20.244  24.540  1.00 29.12      MTGL
ATOM   1210  C   ARG   155      43.402  16.598  24.721  1.00 18.37      MTGL
ATOM   1211  O   ARG   155      43.848  15.916  23.792  1.00 17.92      MTGL
ATOM   1212  N   LEU   156      43.217  16.115  25.944  1.00 17.77      MTGL
ATOM   1213  CA  LEU   156      43.540  14.731  26.258  1.00 17.18      MTGL
ATOM   1214  CB  LEU   156      43.360  14.473  27.761  1.00 16.68      MTGL
ATOM   1215  CG  LEU   156      44.375  15.158  28.689  1.00 16.04      MTGL
ATOM   1216  CD1 LEU   156      43.921  15.032  30.139  1.00 17.64      MTGL
ATOM   1217  CD2 LEU   156      45.745  14.532  28.504  1.00 14.11      MTGL
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Fig. 1 cont.

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ATOM   1218  C   LEU  156      42.660  13.777  25.447  1.00 17.29      MTGL
ATOM   1219  O   LEU  156      43.152  12.794  24.886  1.00 16.71      MTGL
ATOM   1220  N   LEU  157      41.363  14.071  25.377  1.00 16.48      MTGL
ATOM   1221  CA  LEU  157      40.438  13.219  24.639  1.00 16.71      MTGL
ATOM   1222  CB  LEU  157      38.992  13.651  24.900  1.00 15.25      MTGL
ATOM   1223  CG  LEU  157      38.509  13.425  26.339  1.00 14.15      MTGL
ATOM   1224  CD1 LEU  157      37.080  13.903  26.505  1.00 13.65      MTGL
ATOM   1225  CD2 LEU  157      38.599  11.944  26.676  1.00 13.61      MTGL
ATOM   1226  C   LEU  157      40.744  13.230  23.146  1.00 18.12      MTGL
ATOM   1227  O   LEU  157      40.549  12.224  22.456  1.00 16.85      MTGL
ATOM   1228  N   HIS  158      41.231  14.366  22.652  1.00 19.80      MTGL
ATOM   1229  CA  HIS  158      41.600  14.498  21.244  1.00 20.98      MTGL
ATOM   1230  CB  HIS  158      42.001  15.946  20.938  1.00 22.94      MTGL
ATOM   1231  CG  HIS  158      42.458  16.170  19.528  1.00 24.32      MTGL
ATOM   1232  CD2 HIS  158      43.695  16.367  19.013  1.00 23.88      MTGL
ATOM   1233  ND1 HIS  158      41.586  16.230  18.460  1.00 24.92      MTGL
ATOM   1234  CE1 HIS  158      42.266  16.460  17.350  1.00 23.22      MTGL
ATOM   1235  NE2 HIS  158      43.548  16.547  17.658  1.00 24.57      MTGL
ATOM   1236  C   HIS  158      42.783  13.567  20.973  1.00 21.01      MTGL
ATOM   1237  O   HIS  158      42.809  12.851  19.971  1.00 21.78      MTGL
ATOM   1238  N   SER  159      43.762  13.578  21.874  1.00 20.28      MTGL
ATOM   1239  CA  SER  159      44.940  12.730  21.726  1.00 20.15      MTGL
ATOM   1240  CB  SER  159      45.961  13.021  22.829  1.00 21.81      MTGL
ATOM   1241  OG  SER  159      46.476  14.333  22.721  1.00 24.73      MTGL
ATOM   1242  C   SER  159      44.570  11.253  21.774  1.00 18.92      MTGL
ATOM   1243  O   SER  159      45.095  10.453  21.004  1.00 19.31      MTGL
ATOM   1244  N   ALA  160      43.675  10.894  22.687  1.00 17.87      MTGL
ATOM   1245  CA  ALA  160      43.249   9.504  22.824  1.00 17.96      MTGL
ATOM   1246  CB  ALA  160      42.322   9.352  24.026  1.00 18.26      MTGL
ATOM   1247  C   ALA  160      42.538   9.044  21.556  1.00 18.59      MTGL
ATOM   1248  O   ALA  160      42.844   7.982  21.013  1.00 17.77      MTGL
ATOM   1249  N   ALA  161      41.593   9.852  21.083  1.00 18.03      MTGL
ATOM   1250  CA  ALA  161      40.846   9.519  19.875  1.00 18.84      MTGL
ATOM   1251  CB  ALA  161      39.851  10.623  19.547  1.00 16.85      MTGL
ATOM   1252  C   ALA  161      41.778   9.294  18.695  1.00 18.82      MTGL
ATOM   1253  O   ALA  161      41.654   8.301  17.983  1.00 19.53      MTGL
ATOM   1254  N   TRP  162      42.715  10.211  18.485  1.00 18.98      MTGL
ATOM   1255  CA  TRP  162      43.636  10.057  17.371  1.00 19.92      MTGL
ATOM   1256  CB  TRP  162      44.330  11.386  17.064  1.00 21.12      MTGL
ATOM   1257  CG  TRP  162      43.420  12.264  16.268  1.00 24.00      MTGL
ATOM   1258  CD2 TRP  162      43.215  12.212  14.851  1.00 24.55      MTGL
ATOM   1259  CE2 TRP  162      42.158  13.102  14.546  1.00 24.96      MTGL
ATOM   1260  CE3 TRP  162      43.822  11.499  13.808  1.00 25.38      MTGL
ATOM   1261  CD1 TRP  162      42.509  13.160  16.752  1.00 24.55      MTGL
ATOM   1262  NE1 TRP  162      41.743  13.665  15.724  1.00 25.20      MTGL
ATOM   1263  CZ2 TRP  162      41.691  13.293  13.241  1.00 24.56      MTGL
ATOM   1264  CZ3 TRP  162      43.355  11.689  12.507  1.00 25.72      MTGL
ATOM   1265  CH2 TRP  162      42.302  12.581  12.238  1.00 24.73      MTGL
ATOM   1266  C   TRP  162      44.643   8.927  17.556  1.00 20.10      MTGL
ATOM   1267  O   TRP  162      45.263   8.483  16.596  1.00 19.99      MTGL
ATOM   1268  N   GLY  163      44.803   8.458  18.786  1.00 20.69      MTGL
ATOM   1269  CA  GLY  163      45.703   7.343  19.016  1.00 20.86      MTGL
ATOM   1270  C   GLY  163      45.051   6.124  18.375  1.00 20.81      MTGL
ATOM   1271  O   GLY  163      45.720   5.225  17.868  1.00 20.64      MTGL
ATOM   1272  N   ILE  164      43.724   6.109  18.395  1.00 20.00      MTGL
ATOM   1273  CA  ILE  164      42.956   5.020  17.810  1.00 19.28      MTGL
ATOM   1274  CB  ILE  164      41.515   5.020  18.347  1.00 18.69      MTGL
ATOM   1275  CG2 ILE  164      40.670   3.977  17.601  1.00 17.15      MTGL
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Fig. 1 cont.

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ATOM   1276  CG1 ILE   164      41.529   4.750  19.852  1.00 18.11      MTGL
ATOM   1277  CD1 ILE   164      40.155   4.779  20.489  1.00 18.52      MTGL
ATOM   1278  C   ILE   164      42.913   5.181  16.291  1.00 20.20      MTGL
ATOM   1279  O   ILE   164      43.125   4.219  15.548  1.00 18.00      MTGL
ATOM   1280  N   LYS   165      42.645   6.405  15.839  1.00 20.30      MTGL
ATOM   1281  CA  LYS   165      42.563   6.701  14.410  1.00 21.80      MTGL
ATOM   1282  CB  LYS   165      42.100   8.149  14.191  1.00 21.88      MTGL
ATOM   1283  CG  LYS   165      40.670   8.436  14.647  1.00 23.28      MTGL
ATOM   1284  CD  LYS   165      40.346   9.924  14.509  1.00 22.94      MTGL
ATOM   1285  CE  LYS   165      38.989  10.268  15.097  1.00 24.34      MTGL
ATOM   1286  NZ  LYS   165      37.857   9.632  14.363  1.00 25.77      MTGL
ATOM   1287  C   LYS   165      43.879   6.468  13.668  1.00 21.72      MTGL
ATOM   1288  O   LYS   165      43.868   6.086  12.501  1.00 21.82      MTGL
ATOM   1289  N   ASP   166      45.009   6.699  14.335  1.00 22.15      MTGL
ATOM   1290  CA  ASP   166      46.315   6.496  13.705  1.00 21.98      MTGL
ATOM   1291  CB  ASP   166      47.373   7.438  14.299  1.00 22.61      MTGL
ATOM   1292  CG  ASP   166      47.119   8.907  13.970  1.00 24.69      MTGL
ATOM   1293  OD1 ASP   166      46.345   9.197  13.032  1.00 25.51      MTGL
ATOM   1294  OD2 ASP   166      47.709   9.775  14.645  1.00 23.73      MTGL
ATOM   1295  C   ASP   166      46.818   5.063  13.853  1.00 21.80      MTGL
ATOM   1296  O   ASP   166      47.900   4.737  13.373  1.00 22.35      MTGL
ATOM   1297  N   SER   167      46.043   4.208  14.511  1.00 21.58      MTGL
ATOM   1298  CA  SER   167      46.460   2.822  14.722  1.00 21.57      MTGL
ATOM   1299  CB  SER   167      45.724   2.229  15.927  1.00 20.98      MTGL
ATOM   1300  OG  SER   167      44.368   1.952  15.620  1.00 20.07      MTGL
ATOM   1301  C   SER   167      46.235   1.920  13.508  1.00 21.73      MTGL
ATOM   1302  O   SER   167      45.669   2.347  12.503  1.00 21.01      MTGL
ATOM   1303  N   SER   168      46.676   0.668  13.619  1.00 21.44      MTGL
ATOM   1304  CA  SER   168      46.520  -0.304  12.539  1.00 20.71      MTGL
ATOM   1305  CB  SER   168      47.711  -1.264  12.519  1.00 21.31      MTGL
ATOM   1306  OG  SER   168      47.836  -1.921  13.768  1.00 23.08      MTGL
ATOM   1307  C   SER   168      45.229  -1.116  12.654  1.00 20.14      MTGL
ATOM   1308  O   SER   168      45.001  -2.033  11.869  1.00 19.79      MTGL
ATOM   1309  N   LEU   169      44.388  -0.792  13.630  1.00 19.27      MTGL
ATOM   1310  CA  LEU   169      43.132  -1.514  13.791  1.00 19.92      MTGL
ATOM   1311  CB  LEU   169      42.306  -0.921  14.935  1.00 19.48      MTGL
ATOM   1312  CG  LEU   169      42.758  -1.226  16.365  1.00 19.56      MTGL
ATOM   1313  CD1 LEU   169      41.918  -0.417  17.342  1.00 18.93      MTGL
ATOM   1314  CD2 LEU   169      42.612  -2.717  16.650  1.00 19.30      MTGL
ATOM   1315  C   LEU   169      42.323  -1.450  12.501  1.00 20.54      MTGL
ATOM   1316  O   LEU   169      42.053  -0.365  11.981  1.00 20.27      MTGL
ATOM   1317  N   SER   170      41.940  -2.614  11.987  1.00 20.36      MTGL
ATOM   1318  CA  SER   170      41.159  -2.678  10.760  1.00 21.47      MTGL
ATOM   1319  CB  SER   170      42.088  -2.784   9.545  1.00 22.54      MTGL
ATOM   1320  OG  SER   170      41.344  -2.749   8.341  1.00 22.78      MTGL
ATOM   1321  C   SER   170      40.216  -3.875  10.797  1.00 21.69      MTGL
ATOM   1322  O   SER   170      40.659  -5.024  10.819  1.00 21.79      MTGL
ATOM   1323  N   PRO   171      38.899  -3.621  10.800  1.00 21.30      MTGL
ATOM   1324  CD  PRO   171      37.874  -4.676  10.884  1.00 21.70      MTGL
ATOM   1325  CA  PRO   171      38.277  -2.294  10.764  1.00 21.48      MTGL
ATOM   1326  CB  PRO   171      36.806  -2.616  10.530  1.00 21.60      MTGL
ATOM   1327  CG  PRO   171      36.644  -3.901  11.285  1.00 22.67      MTGL
ATOM   1328  C   PRO   171      38.497  -1.472  12.039  1.00 21.36      MTGL
ATOM   1329  O   PRO   171      38.790  -2.009  13.109  1.00 20.24      MTGL
ATOM   1330  N   LYS   172      38.351  -0.161  11.908  1.00 20.37      MTGL
ATOM   1331  CA  LYS   172      38.525   0.749  13.032  1.00 21.42      MTGL
ATOM   1332  CB  LYS   172      38.670   2.183  12.501  1.00 22.43      MTGL
ATOM   1333  CG  LYS   172      39.602   3.071  13.310  1.00 25.68      MTGL
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Fig. 1 cont.

ATOM	1334	CD	LYS	172	41.052	2.616	13.220	1.00 24.85	MTGL
ATOM	1335	CE	LYS	172	41.659	2.946	11.878	1.00 25.80	MTGL
ATOM	1336	NZ	LYS	172	42.984	2.294	11.703	1.00 24.26	MTGL
ATOM	1337	C	LYS	172	37.295	0.626	13.940	1.00 20.16	MTGL
ATOM	1338	O	LYS	172	36.199	0.307	13.478	1.00 19.92	MTGL
ATOM	1339	N	PRO	173	37.465	0.848	15.248	1.00 19.30	MTGL
ATOM	1340	CD	PRO	173	38.722	1.088	15.980	1.00 19.67	MTGL
ATOM	1341	CA	PRO	173	36.335	0.751	16.177	1.00 19.05	MTGL
ATOM	1342	CB	PRO	173	37.018	0.437	17.497	1.00 19.14	MTGL
ATOM	1343	CG	PRO	173	38.237	1.321	17.412	1.00 18.48	MTGL
ATOM	1344	C	PRO	173	35.565	2.066	16.270	1.00 18.59	MTGL
ATOM	1345	O	PRO	173	36.049	3.110	15.832	1.00 16.92	MTGL
ATOM	1346	N	LYS	174	34.359	2.007	16.824	1.00 17.93	MTGL
ATOM	1347	CA	LYS	174	33.591	3.222	17.037	1.00 18.70	MTGL
ATOM	1348	CB	LYS	174	32.109	2.901	17.240	1.00 18.25	MTGL
ATOM	1349	CG	LYS	174	31.388	2.529	15.947	1.00 19.90	MTGL
ATOM	1350	CD	LYS	174	29.937	2.142	16.200	1.00 20.92	MTGL
ATOM	1351	CE	LYS	174	29.230	1.784	14.892	1.00 21.51	MTGL
ATOM	1352	NZ	LYS	174	27.839	1.317	15.135	1.00 20.89	MTGL
ATOM	1353	C	LYS	174	34.193	3.808	18.318	1.00 18.48	MTGL
ATOM	1354	O	LYS	174	34.452	3.076	19.281	1.00 18.00	MTGL
ATOM	1355	N	ILE	175	34.448	5.112	18.320	1.00 17.76	MTGL
ATOM	1356	CA	ILE	175	35.033	5.768	19.487	1.00 17.60	MTGL
ATOM	1357	CB	ILE	175	35.999	6.883	19.050	1.00 17.54	MTGL
ATOM	1358	CG2	ILE	175	36.564	7.610	20.271	1.00 17.48	MTGL
ATOM	1359	CG1	ILE	175	37.134	6.266	18.226	1.00 16.88	MTGL
ATOM	1360	CD1	ILE	175	38.083	7.263	17.618	1.00 15.96	MTGL
ATOM	1361	C	ILE	175	33.945	6.330	20.393	1.00 17.11	MTGL
ATOM	1362	O	ILE	175	33.102	7.122	19.962	1.00 17.92	MTGL
ATOM	1363	N	MET	176	33.966	5.914	21.653	1.00 16.13	MTGL
ATOM	1364	CA	MET	176	32.955	6.345	22.615	1.00 16.14	MTGL
ATOM	1365	CB	MET	176	32.223	5.120	23.171	1.00 16.50	MTGL
ATOM	1366	CG	MET	176	31.333	5.410	24.379	1.00 16.70	MTGL
ATOM	1367	SD	MET	176	30.643	3.896	25.097	1.00 19.61	MTGL
ATOM	1368	CE	MET	176	29.473	3.433	23.769	1.00 15.92	MTGL
ATOM	1369	C	MET	176	33.458	7.163	23.797	1.00 16.18	MTGL
ATOM	1370	O	MET	176	34.562	6.946	24.299	1.00 15.62	MTGL
ATOM	1371	N	ILE	177	32.628	8.109	24.227	1.00 16.05	MTGL
ATOM	1372	CA	ILE	177	32.915	8.927	25.402	1.00 16.22	MTGL
ATOM	1373	CB	ILE	177	32.786	10.436	25.117	1.00 15.59	MTGL
ATOM	1374	CG2	ILE	177	32.729	11.210	26.438	1.00 16.50	MTGL
ATOM	1375	CG1	ILE	177	33.985	10.900	24.273	1.00 16.91	MTGL
ATOM	1376	CD1	ILE	177	33.988	12.380	23.935	1.00 17.23	MTGL
ATOM	1377	C	ILE	177	31.847	8.467	26.383	1.00 15.72	MTGL
ATOM	1378	O	ILE	177	30.660	8.467	26.062	1.00 16.21	MTGL
ATOM	1379	N	HIS	178	32.278	8.061	27.571	1.00 16.15	MTGL
ATOM	1380	CA	HIS	178	31.376	7.518	28.581	1.00 16.02	MTGL
ATOM	1381	CB	HIS	178	31.866	6.112	28.949	1.00 14.76	MTGL
ATOM	1382	CG	HIS	178	31.099	5.461	30.057	1.00 14.66	MTGL
ATOM	1383	CD2	HIS	178	29.850	5.681	30.534	1.00 13.15	MTGL
ATOM	1384	ND1	HIS	178	31.612	4.415	30.793	1.00 13.39	MTGL
ATOM	1385	CE1	HIS	178	30.714	4.020	31.679	1.00 14.18	MTGL
ATOM	1386	NE2	HIS	178	29.636	4.770	31.543	1.00 13.19	MTGL
ATOM	1387	C	HIS	178	31.232	8.354	29.850	1.00 16.83	MTGL
ATOM	1388	O	HIS	178	32.210	8.605	30.553	1.00 16.59	MTGL
ATOM	1389	N	LEU	179	29.997	8.757	30.138	1.00 17.26	MTGL
ATOM	1390	CA	LEU	179	29.670	9.539	31.329	1.00 18.11	MTGL
ATOM	1391	CB	LEU	179	29.014	10.866	30.925	1.00 18.73	MTGL

Fig. 1 cont.

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ATOM   1392  CG  LEU   179      29.877  12.128  30.808  1.00 20.65      MTGL
ATOM   1393  CD1 LEU   179      31.265  11.812  30.272  1.00 19.45      MTGL
ATOM   1394  CD2 LEU   179      29.150  13.130  29.923  1.00 20.83      MTGL
ATOM   1395  C   LEU   179      28.693   8.732  32.186  1.00 18.96      MTGL
ATOM   1396  O   LEU   179      27.947   7.899  31.668  1.00 19.30      MTGL
ATOM   1397  N   ASP   180      28.693   8.974  33.493  1.00 18.24      MTGL
ATOM   1398  CA  ASP   180      27.780   8.267  34.385  1.00 18.02      MTGL
ATOM   1399  CB  ASP   180      28.377   8.171  35.795  1.00 17.69      MTGL
ATOM   1400  CG  ASP   180      28.398   9.505  36.518  1.00 19.25      MTGL
ATOM   1401  OD1 ASP   180      28.702  10.538  35.884  1.00 19.57      MTGL
ATOM   1402  OD2 ASP   180      28.117   9.512  37.734  1.00 20.92      MTGL
ATOM   1403  C   ASP   180      26.453   9.020  34.430  1.00 18.13      MTGL
ATOM   1404  O   ASP   180      26.268   9.995  33.708  1.00 17.92      MTGL
ATOM   1405  N   ASN   181      25.533   8.546  35.266  1.00 19.02      MTGL
ATOM   1406  CA  ASN   181      24.219   9.165  35.439  1.00 19.13      MTGL
ATOM   1407  CB  ASN   181      24.337  10.360  36.393  1.00 19.61      MTGL
ATOM   1408  CG  ASN   181      24.840   9.959  37.776  1.00 20.81      MTGL
ATOM   1409  OD1 ASN   181      24.561   8.857  38.259  1.00 20.36      MTGL
ATOM   1410  ND2 ASN   181      25.567  10.862  38.427  1.00 21.46      MTGL
ATOM   1411  C   ASN   181      23.541   9.604  34.135  1.00 19.21      MTGL
ATOM   1412  O   ASN   181      23.277  10.791  33.925  1.00 18.32      MTGL
ATOM   1413  N   GLY   182      23.238   8.635  33.276  1.00 18.94      MTGL
ATOM   1414  CA  GLY   182      22.610   8.937  32.003  1.00 18.55      MTGL
ATOM   1415  C   GLY   182      21.309   9.704  32.101  1.00 18.91      MTGL
ATOM   1416  O   GLY   182      20.952  10.428  31.179  1.00 18.95      MTGL
ATOM   1417  N   TRP   183      20.609   9.546  33.219  1.00 19.65      MTGL
ATOM   1418  CA  TRP   183      19.332  10.213  33.459  1.00 19.57      MTGL
ATOM   1419  CB  TRP   183      18.643   9.588  34.671  1.00 20.28      MTGL
ATOM   1420  CG  TRP   183      19.515   9.586  35.904  1.00 21.43      MTGL
ATOM   1421  CD2 TRP   183      19.671  10.653  36.856  1.00 21.48      MTGL
ATOM   1422  CE2 TRP   183      20.614  10.222  37.816  1.00 21.25      MTGL
ATOM   1423  CE3 TRP   183      19.103  11.931  36.989  1.00 21.53      MTGL
ATOM   1424  CD1 TRP   183      20.348   8.585  36.316  1.00 20.88      MTGL
ATOM   1425  NE1 TRP   183      21.011   8.959  37.463  1.00 21.48      MTGL
ATOM   1426  CZ2 TRP   183      21.010  11.024  38.896  1.00 22.46      MTGL
ATOM   1427  CZ3 TRP   183      19.497  12.732  38.065  1.00 21.36      MTGL
ATOM   1428  CH2 TRP   183      20.440  12.272  39.004  1.00 21.87      MTGL
ATOM   1429  C   TRP   183      19.477  11.705  33.724  1.00 20.04      MTGL
ATOM   1430  O   TRP   183      18.506  12.457  33.613  1.00 19.18      MTGL
ATOM   1431  N   ASP   184      20.686  12.126  34.083  1.00 20.76      MTGL
ATOM   1432  CA  ASP   184      20.957  13.522  34.417  1.00 20.14      MTGL
ATOM   1433  CB  ASP   184      22.085  13.581  35.455  1.00 21.31      MTGL
ATOM   1434  CG  ASP   184      22.327  14.986  35.988  1.00 24.62      MTGL
ATOM   1435  OD1 ASP   184      21.643  15.936  35.540  1.00 24.90      MTGL
ATOM   1436  OD2 ASP   184      23.210  15.138  36.859  1.00 25.79      MTGL
ATOM   1437  C   ASP   184      21.312  14.374  33.201  1.00 20.22      MTGL
ATOM   1438  O   ASP   184      22.487  14.584  32.899  1.00 19.35      MTGL
ATOM   1439  N   TRP   185      20.289  14.879  32.518  1.00 19.30      MTGL
ATOM   1440  CA  TRP   185      20.498  15.704  31.333  1.00 19.09      MTGL
ATOM   1441  CB  TRP   185      19.148  16.149  30.753  1.00 18.81      MTGL
ATOM   1442  CG  TRP   185      19.267  17.255  29.746  1.00 18.32      MTGL
ATOM   1443  CD2 TRP   185      20.044  17.245  28.541  1.00 18.10      MTGL
ATOM   1444  CE2 TRP   185      19.889  18.509  27.933  1.00 18.68      MTGL
ATOM   1445  CE3 TRP   185      20.856  16.290  27.917  1.00 18.54      MTGL
ATOM   1446  CD1 TRP   185      18.686  18.491  29.814  1.00 18.71      MTGL
ATOM   1447  NE1 TRP   185      19.057  19.250  28.730  1.00 18.49      MTGL
ATOM   1448  CZ2 TRP   185      20.518  18.845  26.732  1.00 19.18      MTGL
ATOM   1449  CZ3 TRP   185      21.484  16.626  26.722  1.00 18.13      MTGL
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Fig. 1 cont.

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ATOM   1450  CH2 TRP   185      21.311  17.891  26.144  1.00 19.60      MTGL
ATOM   1451  C   TRP   185      21.360  16.931  31.626  1.00 18.76      MTGL
ATOM   1452  O   TRP   185      22.271  17.256  30.866  1.00 17.61      MTGL
ATOM   1453  N   GLY   186      21.068  17.612  32.731  1.00 19.33      MTGL
ATOM   1454  CA  GLY   186      21.834  18.797  33.081  1.00 19.04      MTGL
ATOM   1455  C   GLY   186      23.336  18.565  33.066  1.00 19.17      MTGL
ATOM   1456  O   GLY   186      24.098  19.353  32.505  1.00 19.02      MTGL
ATOM   1457  N   THR   187      23.772  17.473  33.677  1.00 19.36      MTGL
ATOM   1458  CA  THR   187      25.192  17.172  33.718  1.00 20.31      MTGL
ATOM   1459  CB  THR   187      25.482  16.098  34.773  1.00 21.41      MTGL
ATOM   1460  OG1 THR   187      25.114  16.609  36.059  1.00 21.37      MTGL
ATOM   1461  CG2 THR   187      26.964  15.735  34.781  1.00 23.08      MTGL
ATOM   1462  C   THR   187      25.731  16.745  32.359  1.00 19.27      MTGL
ATOM   1463  O   THR   187      26.815  17.166  31.965  1.00 19.21      MTGL
ATOM   1464  N   GLN   188      24.980  15.916  31.637  1.00 19.95      MTGL
ATOM   1465  CA  GLN   188      25.420  15.479  30.312  1.00 19.24      MTGL
ATOM   1466  CB  GLN   188      24.356  14.602  29.638  1.00 19.13      MTGL
ATOM   1467  CG  GLN   188      24.033  13.278  30.329  1.00 18.75      MTGL
ATOM   1468  CD  GLN   188      25.203  12.299  30.339  1.00 18.38      MTGL
ATOM   1469  OE1 GLN   188      25.874  12.099  29.328  1.00 18.47      MTGL
ATOM   1470  NE2 GLN   188      25.435  11.675  31.483  1.00 16.34      MTGL
ATOM   1471  C   GLN   188      25.655  16.714  29.437  1.00 19.43      MTGL
ATOM   1472  O   GLN   188      26.695  16.850  28.792  1.00 18.38      MTGL
ATOM   1473  N   ASN   189      24.673  17.612  29.429  1.00 20.01      MTGL
ATOM   1474  CA  ASN   189      24.733  18.830  28.625  1.00 20.84      MTGL
ATOM   1475  CB  ASN   189      23.392  19.568  28.722  1.00 22.61      MTGL
ATOM   1476  CG  ASN   189      23.323  20.781  27.813  1.00 24.36      MTGL
ATOM   1477  OD1 ASN   189      23.788  20.744  26.674  1.00 24.74      MTGL
ATOM   1478  ND2 ASN   189      22.725  21.860  28.310  1.00 24.46      MTGL
ATOM   1479  C   ASN   189      25.878  19.746  29.050  1.00 21.20      MTGL
ATOM   1480  O   ASN   189      26.622  20.267  28.214  1.00 20.76      MTGL
ATOM   1481  N   TRP   190      26.015  19.935  30.356  1.00 21.74      MTGL
ATOM   1482  CA  TRP   190      27.073  20.770  30.917  1.00 22.16      MTGL
ATOM   1483  CB  TRP   190      26.959  20.758  32.442  1.00 23.20      MTGL
ATOM   1484  CG  TRP   190      28.143  21.315  33.192  1.00 25.19      MTGL
ATOM   1485  CD2 TRP   190      29.121  20.563  33.925  1.00 25.40      MTGL
ATOM   1486  CE2 TRP   190      30.015  21.491  34.505  1.00 25.48      MTGL
ATOM   1487  CE3 TRP   190      29.336  19.194  34.137  1.00 25.81      MTGL
ATOM   1488  CD1 TRP   190      28.474  22.632  33.355  1.00 24.81      MTGL
ATOM   1489  NE1 TRP   190      29.595  22.744  34.146  1.00 26.35      MTGL
ATOM   1490  CZ2 TRP   190      31.098  21.095  35.298  1.00 26.43      MTGL
ATOM   1491  CZ3 TRP   190      30.420  18.800  34.925  1.00 26.45      MTGL
ATOM   1492  CH2 TRP   190      31.288  19.750  35.490  1.00 25.29      MTGL
ATOM   1493  C   TRP   190      28.451  20.252  30.493  1.00 21.86      MTGL
ATOM   1494  O   TRP   190      29.322  21.023  30.081  1.00 21.57      MTGL
ATOM   1495  N   TRP   191      28.637  18.939  30.586  1.00 20.42      MTGL
ATOM   1496  CA  TRP   191      29.915  18.325  30.245  1.00 19.96      MTGL
ATOM   1497  CB  TRP   191      29.902  16.846  30.631  1.00 18.89      MTGL
ATOM   1498  CG  TRP   191      31.272  16.231  30.703  1.00 18.14      MTGL
ATOM   1499  CD2 TRP   191      32.017  15.658  29.621  1.00 17.74      MTGL
ATOM   1500  CE2 TRP   191      33.244  15.201  30.154  1.00 17.14      MTGL
ATOM   1501  CE3 TRP   191      31.767  15.481  28.253  1.00 17.05      MTGL
ATOM   1502  CD1 TRP   191      32.058  16.108  31.815  1.00 18.47      MTGL
ATOM   1503  NE1 TRP   191      33.241  15.489  31.494  1.00 16.67      MTGL
ATOM   1504  CZ2 TRP   191      34.221  14.583  29.366  1.00 16.52      MTGL
ATOM   1505  CZ3 TRP   191      32.739  14.862  27.468  1.00 15.97      MTGL
ATOM   1506  CH2 TRP   191      33.950  14.420  28.030  1.00 16.29      MTGL
ATOM   1507  C   TRP   191      30.293  18.455  28.770  1.00 19.44      MTGL
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Fig. 1 cont.

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ATOM   1508  O   TRP   191      31.342  19.019  28.436  1.00 18.48      MTGL
ATOM   1509  N   TYR   192      29.447  17.921  27.893  1.00 19.02      MTGL
ATOM   1510  CA  TYR   192      29.707  17.961  26.455  1.00 18.88      MTGL
ATOM   1511  CB  TYR   192      28.629  17.174  25.702  1.00 18.06      MTGL
ATOM   1512  CG  TYR   192      28.820  15.670  25.779  1.00 17.74      MTGL
ATOM   1513  CD1 TYR   192      29.890  15.048  25.126  1.00 17.96      MTGL
ATOM   1514  CE1 TYR   192      30.069  13.671  25.189  1.00 18.35      MTGL
ATOM   1515  CD2 TYR   192      27.935  14.870  26.502  1.00 16.89      MTGL
ATOM   1516  CE2 TYR   192      28.107  13.487  26.574  1.00 17.96      MTGL
ATOM   1517  CZ  TYR   192      29.172  12.895  25.917  1.00 18.14      MTGL
ATOM   1518  OH  TYR   192      29.340  11.530  25.986  1.00 19.50      MTGL
ATOM   1519  C   TYR   192      29.810  19.378  25.895  1.00 19.64      MTGL
ATOM   1520  O   TYR   192      30.661  19.651  25.047  1.00 17.67      MTGL
ATOM   1521  N   THR   193      28.956  20.280  26.373  1.00 20.13      MTGL
ATOM   1522  CA  THR   193      28.988  21.658  25.904  1.00 21.63      MTGL
ATOM   1523  CB  THR   193      27.884  22.504  26.569  1.00 21.95      MTGL
ATOM   1524  OG1 THR   193      26.600  21.990  26.195  1.00 23.39      MTGL
ATOM   1525  CG2 THR   193      27.978  23.956  26.114  1.00 23.15      MTGL
ATOM   1526  C   THR   193      30.346  22.306  26.189  1.00 21.54      MTGL
ATOM   1527  O   THR   193      30.978  22.863  25.291  1.00 21.18      MTGL
ATOM   1528  N   ASN   194      30.804  22.218  27.434  1.00 21.85      MTGL
ATOM   1529  CA  ASN   194      32.084  22.816  27.800  1.00 22.13      MTGL
ATOM   1530  CB  ASN   194      32.243  22.833  29.318  1.00 23.00      MTGL
ATOM   1531  CG  ASN   194      31.437  23.944  29.968  1.00 24.26      MTGL
ATOM   1532  OD1 ASN   194      31.675  25.123  29.709  1.00 25.08      MTGL
ATOM   1533  ND2 ASN   194      30.478  23.573  30.810  1.00 23.61      MTGL
ATOM   1534  C   ASN   194      33.292  22.146  27.156  1.00 21.45      MTGL
ATOM   1535  O   ASN   194      34.266  22.813  26.815  1.00 21.18      MTGL
ATOM   1536  N   VAL   195      33.236  20.831  26.986  1.00 21.36      MTGL
ATOM   1537  CA  VAL   195      34.346  20.123  26.362  1.00 20.65      MTGL
ATOM   1538  CB  VAL   195      34.187  18.590  26.503  1.00 20.76      MTGL
ATOM   1539  CG1 VAL   195      35.165  17.871  25.583  1.00 19.43      MTGL
ATOM   1540  CG2 VAL   195      34.429  18.179  27.947  1.00 20.62      MTGL
ATOM   1541  C   VAL   195      34.453  20.475  24.879  1.00 21.44      MTGL
ATOM   1542  O   VAL   195      35.540  20.792  24.385  1.00 20.78      MTGL
ATOM   1543  N   LEU   196      33.323  20.429  24.178  1.00 21.29      MTGL
ATOM   1544  CA  LEU   196      33.300  20.712  22.746  1.00 23.23      MTGL
ATOM   1545  CB  LEU   196      31.953  20.285  22.150  1.00 22.71      MTGL
ATOM   1546  CG  LEU   196      31.703  18.772  22.118  1.00 24.14      MTGL
ATOM   1547  CD1 LEU   196      30.276  18.477  21.657  1.00 22.72      MTGL
ATOM   1548  CD2 LEU   196      32.720  18.115  21.187  1.00 23.15      MTGL
ATOM   1549  C   LEU   196      33.589  22.158  22.354  1.00 24.05      MTGL
ATOM   1550  O   LEU   196      34.054  22.413  21.250  1.00 24.38      MTGL
ATOM   1551  N   LYS   197      33.326  23.104  23.248  1.00 25.84      MTGL
ATOM   1552  CA  LYS   197      33.562  24.506  22.919  1.00 27.64      MTGL
ATOM   1553  CB  LYS   197      32.753  25.413  23.850  1.00 29.58      MTGL
ATOM   1554  CG  LYS   197      33.282  25.505  25.268  1.00 32.86      MTGL
ATOM   1555  CD  LYS   197      32.239  26.101  26.207  1.00 35.16      MTGL
ATOM   1556  CE  LYS   197      31.742  27.456  25.726  1.00 37.48      MTGL
ATOM   1557  NZ  LYS   197      30.672  28.001  26.617  1.00 39.55      MTGL
ATOM   1558  C   LYS   197      35.038  24.897  22.956  1.00 27.59      MTGL
ATOM   1559  O   LYS   197      35.397  26.010  22.577  1.00 27.09      MTGL
ATOM   1560  N   GLN   198      35.896  23.980  23.395  1.00 27.10      MTGL
ATOM   1561  CA  GLN   198      37.323  24.271  23.459  1.00 26.85      MTGL
ATOM   1562  CB  GLN   198      38.053  23.202  24.274  1.00 26.22      MTGL
ATOM   1563  CG  GLN   198      37.608  23.127  25.718  1.00 24.93      MTGL
ATOM   1564  CD  GLN   198      37.637  24.480  26.400  1.00 25.72      MTGL
ATOM   1565  OE1 GLN   198      38.667  25.152  26.432  1.00 25.49      MTGL
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Fig. 1 cont.

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ATOM   1566  NE2 GLN   198      36.501  24.886  26.950  1.00 24.69      MTGL
ATOM   1567  C   GLN   198      37.953  24.381  22.071  1.00 27.46      MTGL
ATOM   1568  O   GLN   198      38.937  25.097  21.885  1.00 27.60      MTGL
ATOM   1569  N   GLY   199      37.401  23.664  21.101  1.00 27.40      MTGL
ATOM   1570  CA  GLY   199      37.941  23.738  19.757  1.00 28.72      MTGL
ATOM   1571  C   GLY   199      39.002  22.713  19.397  1.00 29.03      MTGL
ATOM   1572  O   GLY   199      39.487  22.711  18.269  1.00 30.82      MTGL
ATOM   1573  N   THR   200      39.382  21.852  20.337  1.00 27.35      MTGL
ATOM   1574  CA  THR   200      40.377  20.823  20.041  1.00 26.65      MTGL
ATOM   1575  CB  THR   200      41.335  20.596  21.230  1.00 26.55      MTGL
ATOM   1576  OG1 THR   200      40.579  20.447  22.438  1.00 27.05      MTGL
ATOM   1577  CG2 THR   200      42.297  21.780  21.366  1.00 26.96      MTGL
ATOM   1578  C   THR   200      39.633  19.532  19.705  1.00 25.68      MTGL
ATOM   1579  O   THR   200      39.665  19.072  18.569  1.00 25.00      MTGL
ATOM   1580  N   LEU   201      38.960  18.947  20.690  1.00 25.02      MTGL
ATOM   1581  CA  LEU   201      38.180  17.745  20.428  1.00 24.16      MTGL
ATOM   1582  CB  LEU   201      37.701  17.105  21.734  1.00 23.23      MTGL
ATOM   1583  CG  LEU   201      36.814  15.867  21.556  1.00 23.41      MTGL
ATOM   1584  CD1 LEU   201      37.674  14.680  21.136  1.00 22.70      MTGL
ATOM   1585  CD2 LEU   201      36.099  15.552  22.852  1.00 23.70      MTGL
ATOM   1586  C   LEU   201      36.967  18.221  19.628  1.00 23.81      MTGL
ATOM   1587  O   LEU   201      36.280  19.152  20.041  1.00 22.98      MTGL
ATOM   1588  N   GLU   202      36.710  17.608  18.480  1.00 23.89      MTGL
ATOM   1589  CA  GLU   202      35.554  18.002  17.672  1.00 25.20      MTGL
ATOM   1590  CB  GLU   202      35.962  18.281  16.227  1.00 26.99      MTGL
ATOM   1591  CG  GLU   202      37.142  19.208  16.054  1.00 30.89      MTGL
ATOM   1592  CD  GLU   202      37.380  19.539  14.596  1.00 33.28      MTGL
ATOM   1593  OE1 GLU   202      36.601  20.338  14.034  1.00 35.02      MTGL
ATOM   1594  OE2 GLU   202      38.333  18.989  14.004  1.00 34.29      MTGL
ATOM   1595  C   GLU   202      34.545  16.863  17.667  1.00 24.61      MTGL
ATOM   1596  O   GLU   202      34.886  15.725  17.990  1.00 23.46      MTGL
ATOM   1597  N   LEU   203      33.311  17.169  17.286  1.00 24.45      MTGL
ATOM   1598  CA  LEU   203      32.267  16.157  17.222  1.00 25.47      MTGL
ATOM   1599  CB  LEU   203      30.959  16.768  16.721  1.00 26.23      MTGL
ATOM   1600  CG  LEU   203      30.009  17.289  17.794  1.00 27.61      MTGL
ATOM   1601  CD1 LEU   203      28.830  17.970  17.126  1.00 28.79      MTGL
ATOM   1602  CD2 LEU   203      29.532  16.139  18.672  1.00 27.38      MTGL
ATOM   1603  C   LEU   203      32.666  15.007  16.305  1.00 25.18      MTGL
ATOM   1604  O   LEU   203      32.307  13.857  16.555  1.00 25.60      MTGL
ATOM   1605  N   SER   204      33.411  15.318  15.249  1.00 23.52      MTGL
ATOM   1606  CA  SER   204      33.841  14.295  14.305  1.00 23.46      MTGL
ATOM   1607  CB  SER   204      34.367  14.941  13.016  1.00 24.47      MTGL
ATOM   1608  OG  SER   204      35.559  15.677  13.253  1.00 23.17      MTGL
ATOM   1609  C   SER   204      34.918  13.379  14.877  1.00 22.84      MTGL
ATOM   1610  O   SER   204      35.235  12.353  14.278  1.00 22.80      MTGL
ATOM   1611  N   ASP   205      35.482  13.742  16.027  1.00 21.73      MTGL
ATOM   1612  CA  ASP   205      36.529  12.920  16.626  1.00 21.47      MTGL
ATOM   1613  CB  ASP   205      37.369  13.735  17.616  1.00 21.78      MTGL
ATOM   1614  CG  ASP   205      38.284  14.737  16.925  1.00 23.69      MTGL
ATOM   1615  OD1 ASP   205      38.859  14.388  15.870  1.00 23.46      MTGL
ATOM   1616  OD2 ASP   205      38.442  15.866  17.446  1.00 23.01      MTGL
ATOM   1617  C   ASP   205      36.020  11.653  17.310  1.00 20.42      MTGL
ATOM   1618  O   ASP   205      36.795  10.727  17.545  1.00 20.47      MTGL
ATOM   1619  N   PHE   206      34.736  11.609  17.650  1.00 19.52      MTGL
ATOM   1620  CA  PHE   206      34.183  10.408  18.275  1.00 20.33      MTGL
ATOM   1621  CB  PHE   206      34.060  10.565  19.801  1.00 18.69      MTGL
ATOM   1622  CG  PHE   206      33.098  11.626  20.244  1.00 18.95      MTGL
ATOM   1623  CD1 PHE   206      33.403  12.974  20.083  1.00 18.40      MTGL
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Fig. 1 cont.

ATOM	1624	CD2	PHE	206	31.899	11.275	20.861	1.00	18.16	MTGL
ATOM	1625	CE1	PHE	206	32.529	13.959	20.534	1.00	19.01	MTGL
ATOM	1626	CE2	PHE	206	31.015	12.253	21.316	1.00	19.53	MTGL
ATOM	1627	CZ	PHE	206	31.331	13.601	21.153	1.00	18.89	MTGL
ATOM	1628	C	PHE	206	32.850	10.031	17.642	1.00	20.83	MTGL
ATOM	1629	O	PHE	206	32.267	10.825	16.901	1.00	20.91	MTGL
ATOM	1630	N	ASP	207	32.365	8.827	17.937	1.00	20.94	MTGL
ATOM	1631	CA	ASP	207	31.134	8.331	17.322	1.00	21.05	MTGL
ATOM	1632	CB	ASP	207	31.470	7.084	16.500	1.00	21.79	MTGL
ATOM	1633	CG	ASP	207	32.766	7.235	15.730	1.00	22.83	MTGL
ATOM	1634	OD1	ASP	207	32.811	8.093	14.826	1.00	22.13	MTGL
ATOM	1635	OD2	ASP	207	33.739	6.506	16.036	1.00	21.38	MTGL
ATOM	1636	C	ASP	207	29.978	7.990	18.256	1.00	20.40	MTGL
ATOM	1637	O	ASP	207	28.813	8.022	17.847	1.00	20.09	MTGL
ATOM	1638	N	MET	208	30.286	7.660	19.502	1.00	19.17	MTGL
ATOM	1639	CA	MET	208	29.236	7.281	20.431	1.00	17.84	MTGL
ATOM	1640	CB	MET	208	29.282	5.771	20.688	1.00	17.36	MTGL
ATOM	1641	CG	MET	208	29.319	4.900	19.455	1.00	17.72	MTGL
ATOM	1642	SD	MET	208	29.434	3.141	19.906	1.00	19.72	MTGL
ATOM	1643	CE	MET	208	27.745	2.786	20.301	1.00	18.67	MTGL
ATOM	1644	C	MET	208	29.293	7.979	21.775	1.00	17.33	MTGL
ATOM	1645	O	MET	208	30.351	8.410	22.232	1.00	16.75	MTGL
ATOM	1646	N	MET	209	28.125	8.080	22.397	1.00	16.30	MTGL
ATOM	1647	CA	MET	209	27.991	8.653	23.722	1.00	17.25	MTGL
ATOM	1648	CB	MET	209	27.037	9.852	23.730	1.00	16.86	MTGL
ATOM	1649	CG	MET	209	27.525	11.048	22.926	1.00	17.20	MTGL
ATOM	1650	SD	MET	209	26.439	12.511	23.096	1.00	15.98	MTGL
ATOM	1651	CE	MET	209	27.636	13.808	22.762	1.00	17.32	MTGL
ATOM	1652	C	MET	209	27.405	7.529	24.557	1.00	16.92	MTGL
ATOM	1653	O	MET	209	26.311	7.033	24.273	1.00	16.52	MTGL
ATOM	1654	N	GLY	210	28.153	7.103	25.565	1.00	16.49	MTGL
ATOM	1655	CA	GLY	210	27.675	6.038	26.423	1.00	16.81	MTGL
ATOM	1656	C	GLY	210	27.361	6.585	27.797	1.00	16.14	MTGL
ATOM	1657	O	GLY	210	27.991	7.537	28.257	1.00	15.66	MTGL
ATOM	1658	N	VAL	211	26.370	5.998	28.450	1.00	16.46	MTGL
ATOM	1659	CA	VAL	211	25.999	6.431	29.784	1.00	15.55	MTGL
ATOM	1660	CB	VAL	211	24.691	7.247	29.773	1.00	15.54	MTGL
ATOM	1661	CG1	VAL	211	24.824	8.449	28.839	1.00	16.27	MTGL
ATOM	1662	CG2	VAL	211	23.525	6.354	29.353	1.00	14.06	MTGL
ATOM	1663	C	VAL	211	25.781	5.236	30.700	1.00	16.00	MTGL
ATOM	1664	O	VAL	211	25.418	4.148	30.243	1.00	15.69	MTGL
ATOM	1665	N	SER	212	26.013	5.445	31.991	1.00	15.22	MTGL
ATOM	1666	CA	SER	212	25.766	4.414	32.983	1.00	15.39	MTGL
ATOM	1667	CB	SER	212	26.741	4.537	34.158	1.00	15.48	MTGL
ATOM	1668	OG	SER	212	28.083	4.327	33.748	1.00	16.02	MTGL
ATOM	1669	C	SER	212	24.346	4.707	33.469	1.00	15.93	MTGL
ATOM	1670	O	SER	212	23.922	5.863	33.498	1.00	16.20	MTGL
ATOM	1671	N	PHE	213	23.599	3.670	33.821	1.00	15.04	MTGL
ATOM	1672	CA	PHE	213	22.248	3.866	34.323	1.00	15.18	MTGL
ATOM	1673	CB	PHE	213	21.218	3.762	33.191	1.00	14.75	MTGL
ATOM	1674	CG	PHE	213	19.801	3.982	33.647	1.00	14.40	MTGL
ATOM	1675	CD1	PHE	213	19.383	5.238	34.071	1.00	15.35	MTGL
ATOM	1676	CD2	PHE	213	18.897	2.924	33.694	1.00	14.80	MTGL
ATOM	1677	CE1	PHE	213	18.079	5.441	34.542	1.00	15.59	MTGL
ATOM	1678	CE2	PHE	213	17.594	3.113	34.160	1.00	15.14	MTGL
ATOM	1679	CZ	PHE	213	17.185	4.376	34.586	1.00	15.11	MTGL
ATOM	1680	C	PHE	213	21.956	2.821	35.388	1.00	16.01	MTGL
ATOM	1681	O	PHE	213	21.757	1.646	35.078	1.00	16.44	MTGL

Fig. 1 cont.

ATOM	1682	N	TYR	214	21.954	3.258	36.644	1.00	16.44	MTGL
ATOM	1683	CA	TYR	214	21.691	2.382	37.782	1.00	16.37	MTGL
ATOM	1684	CB	TYR	214	22.917	2.332	38.700	1.00	16.76	MTGL
ATOM	1685	CG	TYR	214	24.097	1.562	38.131	1.00	16.18	MTGL
ATOM	1686	CD1	TYR	214	24.114	0.168	38.139	1.00	16.62	MTGL
ATOM	1687	CE1	TYR	214	25.201	-0.544	37.637	1.00	17.99	MTGL
ATOM	1688	CD2	TYR	214	25.199	2.228	37.599	1.00	16.40	MTGL
ATOM	1689	CE2	TYR	214	26.295	1.524	37.093	1.00	16.27	MTGL
ATOM	1690	CZ	TYR	214	26.288	0.142	37.118	1.00	16.37	MTGL
ATOM	1691	OH	TYR	214	27.375	-0.556	36.648	1.00	17.15	MTGL
ATOM	1692	C	TYR	214	20.479	2.904	38.554	1.00	17.45	MTGL
ATOM	1693	O	TYR	214	20.246	4.111	38.632	1.00	17.08	MTGL
ATOM	1694	N	PRO	215	19.691	1.997	39.140	1.00	17.07	MTGL
ATOM	1695	CD	PRO	215	19.704	0.537	38.916	1.00	17.36	MTGL
ATOM	1696	CA	PRO	215	18.506	2.395	39.896	1.00	17.11	MTGL
ATOM	1697	CB	PRO	215	17.547	1.247	39.619	1.00	17.64	MTGL
ATOM	1698	CG	PRO	215	18.481	0.060	39.693	1.00	17.35	MTGL
ATOM	1699	C	PRO	215	18.728	2.576	41.395	1.00	18.08	MTGL
ATOM	1700	O	PRO	215	17.847	3.078	42.092	1.00	17.47	MTGL
ATOM	1701	N	PHE	216	19.896	2.180	41.891	1.00	18.78	MTGL
ATOM	1702	CA	PHE	216	20.152	2.251	43.328	1.00	19.20	MTGL
ATOM	1703	CB	PHE	216	20.530	0.851	43.836	1.00	17.80	MTGL
ATOM	1704	CG	PHE	216	21.456	0.095	42.915	1.00	18.00	MTGL
ATOM	1705	CD1	PHE	216	22.673	0.641	42.522	1.00	18.05	MTGL
ATOM	1706	CD2	PHE	216	21.117	-1.172	42.456	1.00	17.34	MTGL
ATOM	1707	CE1	PHE	216	23.543	-0.064	41.680	1.00	17.92	MTGL
ATOM	1708	CE2	PHE	216	21.981	-1.887	41.614	1.00	17.55	MTGL
ATOM	1709	CZ	PHE	216	23.194	-1.331	41.228	1.00	16.80	MTGL
ATOM	1710	C	PHE	216	21.145	3.276	43.872	1.00	19.84	MTGL
ATOM	1711	O	PHE	216	21.726	3.068	44.940	1.00	21.57	MTGL
ATOM	1712	N	TYR	217	21.346	4.379	43.161	1.00	19.60	MTGL
ATOM	1713	CA	TYR	217	22.251	5.419	43.647	1.00	20.50	MTGL
ATOM	1714	CB	TYR	217	23.468	5.575	42.732	1.00	20.09	MTGL
ATOM	1715	CG	TYR	217	24.398	4.382	42.724	1.00	21.44	MTGL
ATOM	1716	CD1	TYR	217	24.956	3.895	43.909	1.00	21.17	MTGL
ATOM	1717	CE1	TYR	217	25.815	2.797	43.902	1.00	21.86	MTGL
ATOM	1718	CD2	TYR	217	24.721	3.739	41.529	1.00	20.83	MTGL
ATOM	1719	CE2	TYR	217	25.577	2.642	41.511	1.00	21.46	MTGL
ATOM	1720	CZ	TYR	217	26.120	2.174	42.697	1.00	21.33	MTGL
ATOM	1721	OH	TYR	217	26.960	1.087	42.672	1.00	20.10	MTGL
ATOM	1722	C	TYR	217	21.520	6.752	43.727	1.00	21.29	MTGL
ATOM	1723	O	TYR	217	22.127	7.778	44.026	1.00	21.40	MTGL
ATOM	1724	N	SER	218	20.218	6.725	43.450	1.00	21.47	MTGL
ATOM	1725	CA	SER	218	19.387	7.926	43.475	1.00	22.44	MTGL
ATOM	1726	CB	SER	218	20.043	9.050	42.677	1.00	23.02	MTGL
ATOM	1727	OG	SER	218	19.128	10.108	42.463	1.00	23.85	MTGL
ATOM	1728	C	SER	218	18.012	7.661	42.888	1.00	22.12	MTGL
ATOM	1729	O	SER	218	17.888	7.058	41.821	1.00	22.86	MTGL
ATOM	1730	N	SER	219	16.980	8.128	43.577	1.00	21.77	MTGL
ATOM	1731	CA	SER	219	15.615	7.938	43.111	1.00	22.44	MTGL
ATOM	1732	CB	SER	219	14.624	8.308	44.216	1.00	22.46	MTGL
ATOM	1733	OG	SER	219	14.793	9.658	44.607	1.00	22.44	MTGL
ATOM	1734	C	SER	219	15.333	8.782	41.867	1.00	22.56	MTGL
ATOM	1735	O	SER	219	14.282	8.646	41.247	1.00	23.34	MTGL
ATOM	1736	N	SER	220	16.267	9.653	41.503	1.00	22.13	MTGL
ATOM	1737	CA	SER	220	16.088	10.488	40.319	1.00	22.61	MTGL
ATOM	1738	CB	SER	220	17.037	11.691	40.358	1.00	23.25	MTGL
ATOM	1739	OG	SER	220	16.688	12.584	41.403	1.00	25.72	MTGL

Fig. 1 cont.

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ATOM   1740  C   SER   220      16.330   9.704  39.032  1.00 22.26      MTGL
ATOM   1741  O   SER   220      16.025  10.187  37.942  1.00 22.75      MTGL
ATOM   1742  N   ALA   221      16.872   8.495  39.160  1.00 20.89      MTGL
ATOM   1743  CA  ALA   221      17.164   7.667  37.996  1.00 20.44      MTGL
ATOM   1744  CB  ALA   221      18.266   6.644  38.343  1.00 19.75      MTGL
ATOM   1745  C   ALA   221      15.933   6.949  37.439  1.00 20.80      MTGL
ATOM   1746  O   ALA   221      15.941   5.731  37.265  1.00 20.53      MTGL
ATOM   1747  N   THR   222      14.875   7.705  37.163  1.00 20.53      MTGL
ATOM   1748  CA  THR   222      13.651   7.134  36.607  1.00 20.82      MTGL
ATOM   1749  CB  THR   222      12.464   8.120  36.690  1.00 20.95      MTGL
ATOM   1750  OG1 THR   222      12.792   9.310  35.966  1.00 21.38      MTGL
ATOM   1751  CG2 THR   222      12.152   8.483  38.137  1.00 21.55      MTGL
ATOM   1752  C   THR   222      13.848   6.809  35.129  1.00 20.30      MTGL
ATOM   1753  O   THR   222      14.754   7.334  34.479  1.00 20.05      MTGL
ATOM   1754  N   LEU   223      12.990   5.947  34.598  1.00 20.97      MTGL
ATOM   1755  CA  LEU   223      13.060   5.583  33.190  1.00 20.57      MTGL
ATOM   1756  CB  LEU   223      12.116   4.412  32.894  1.00 21.05      MTGL
ATOM   1757  CG  LEU   223      12.455   3.097  33.612  1.00 22.20      MTGL
ATOM   1758  CD1 LEU   223      11.415   2.039  33.276  1.00 22.93      MTGL
ATOM   1759  CD2 LEU   223      13.841   2.629  33.195  1.00 21.13      MTGL
ATOM   1760  C   LEU   223      12.674   6.800  32.346  1.00 20.76      MTGL
ATOM   1761  O   LEU   223      13.214   7.009  31.258  1.00 19.94      MTGL
ATOM   1762  N   SER   224      11.741   7.607  32.852  1.00 20.13      MTGL
ATOM   1763  CA  SER   224      11.311   8.804  32.128  1.00 20.71      MTGL
ATOM   1764  CB  SER   224      10.096   9.448  32.812  1.00 21.29      MTGL
ATOM   1765  OG  SER   224      10.392   9.812  34.149  1.00 26.36      MTGL
ATOM   1766  C   SER   224      12.452   9.815  32.036  1.00 18.99      MTGL
ATOM   1767  O   SER   224      12.641  10.450  30.999  1.00 19.23      MTGL
ATOM   1768  N   ALA   225      13.214   9.967  33.115  1.00 18.09      MTGL
ATOM   1769  CA  ALA   225      14.333  10.901  33.093  1.00 17.82      MTGL
ATOM   1770  CB  ALA   225      14.928  11.057  34.492  1.00 17.28      MTGL
ATOM   1771  C   ALA   225      15.395  10.410  32.108  1.00 17.15      MTGL
ATOM   1772  O   ALA   225      16.018  11.208  31.410  1.00 18.25      MTGL
ATOM   1773  N   LEU   226      15.598   9.097  32.048  1.00 16.97      MTGL
ATOM   1774  CA  LEU   226      16.580   8.534  31.122  1.00 17.41      MTGL
ATOM   1775  CB  LEU   226      16.693   7.017  31.303  1.00 17.39      MTGL
ATOM   1776  CG  LEU   226      17.711   6.325  30.389  1.00 17.54      MTGL
ATOM   1777  CD1 LEU   226      19.109   6.852  30.679  1.00 17.23      MTGL
ATOM   1778  CD2 LEU   226      17.658   4.824  30.606  1.00 17.56      MTGL
ATOM   1779  C   LEU   226      16.126   8.839  29.696  1.00 17.60      MTGL
ATOM   1780  O   LEU   226      16.909   9.311  28.868  1.00 17.24      MTGL
ATOM   1781  N   LYS   227      14.854   8.566  29.423  1.00 17.18      MTGL
ATOM   1782  CA  LYS   227      14.277   8.811  28.105  1.00 18.16      MTGL
ATOM   1783  CB  LYS   227      12.780   8.488  28.120  1.00 18.24      MTGL
ATOM   1784  CG  LYS   227      12.007   8.984  26.890  1.00 18.81      MTGL
ATOM   1785  CD  LYS   227      12.540   8.394  25.590  1.00 17.63      MTGL
ATOM   1786  CE  LYS   227      11.629   8.737  24.411  1.00 18.20      MTGL
ATOM   1787  NZ  LYS   227      12.191   8.269  23.111  1.00 17.92      MTGL
ATOM   1788  C   LYS   227      14.476  10.258  27.668  1.00 18.40      MTGL
ATOM   1789  O   LYS   227      14.978  10.526  26.576  1.00 18.56      MTGL
ATOM   1790  N   SER   228      14.078  11.190  28.529  1.00 18.71      MTGL
ATOM   1791  CA  SER   228      14.209  12.610  28.225  1.00 18.63      MTGL
ATOM   1792  CB  SER   228      13.584  13.449  29.344  1.00 19.90      MTGL
ATOM   1793  OG  SER   228      13.763  14.835  29.096  1.00 20.80      MTGL
ATOM   1794  C   SER   228      15.662  13.022  28.024  1.00 18.30      MTGL
ATOM   1795  O   SER   228      15.973  13.778  27.106  1.00 18.71      MTGL
ATOM   1796  N   SER   229      16.553  12.525  28.880  1.00 17.99      MTGL
ATOM   1797  CA  SER   229      17.969  12.862  28.768  1.00 18.28      MTGL
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Fig. 1 cont.

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ATOM   1798  CB  SER   229      18.752  12.299  29.962  1.00 18.83      MTGL
ATOM   1799  OG  SER   229      20.127  12.641  29.867  1.00 17.92      MTGL
ATOM   1800  C   SER   229      18.577  12.339  27.463  1.00 18.05      MTGL
ATOM   1801  O   SER   229      19.251  13.076  26.744  1.00 18.70      MTGL
ATOM   1802  N   LEU   230      18.338  11.070  27.149  1.00 17.87      MTGL
ATOM   1803  CA  LEU   230      18.884  10.503  25.920  1.00 17.26      MTGL
ATOM   1804  CB  LEU   230      18.620   8.994  25.860  1.00 16.24      MTGL
ATOM   1805  CG  LEU   230      19.265   8.162  26.976  1.00 16.12      MTGL
ATOM   1806  CD1 LEU   230      19.069   6.676  26.671  1.00 16.29      MTGL
ATOM   1807  CD2 LEU   230      20.749   8.473  27.084  1.00 12.97      MTGL
ATOM   1808  C   LEU   230      18.299  11.204  24.689  1.00 17.08      MTGL
ATOM   1809  O   LEU   230      19.014  11.458  23.721  1.00 15.52      MTGL
ATOM   1810  N   ASP   231      17.006  11.525  24.728  1.00 18.20      MTGL
ATOM   1811  CA  ASP   231      16.380  12.223  23.604  1.00 18.97      MTGL
ATOM   1812  CB  ASP   231      14.896  12.494  23.878  1.00 20.35      MTGL
ATOM   1813  CG  ASP   231      13.985  11.337  23.455  1.00 20.69      MTGL
ATOM   1814  OD1 ASP   231      14.460  10.361  22.838  1.00 21.48      MTGL
ATOM   1815  OD2 ASP   231      12.775  11.418  23.738  1.00 20.71      MTGL
ATOM   1816  C   ASP   231      17.102  13.553  23.393  1.00 19.05      MTGL
ATOM   1817  O   ASP   231      17.423  13.927  22.265  1.00 20.05      MTGL
ATOM   1818  N   ASN   232      17.369  14.260  24.486  1.00 18.97      MTGL
ATOM   1819  CA  ASN   232      18.057  15.546  24.403  1.00 19.27      MTGL
ATOM   1820  CB  ASN   232      18.126  16.219  25.781  1.00 19.34      MTGL
ATOM   1821  CG  ASN   232      16.775  16.752  26.238  1.00 21.88      MTGL
ATOM   1822  OD1 ASN   232      15.911  17.054  25.420  1.00 23.78      MTGL
ATOM   1823  ND2 ASN   232      16.595  16.882  27.545  1.00 21.09      MTGL
ATOM   1824  C   ASN   232      19.459  15.397  23.834  1.00 19.42      MTGL
ATOM   1825  O   ASN   232      19.887  16.205  23.003  1.00 19.51      MTGL
ATOM   1826  N   MET   233      20.174  14.368  24.280  1.00 19.18      MTGL
ATOM   1827  CA  MET   233      21.533  14.124  23.803  1.00 19.15      MTGL
ATOM   1828  CB  MET   233      22.151  12.936  24.551  1.00 18.27      MTGL
ATOM   1829  CG  MET   233      22.433  13.191  26.029  1.00 19.33      MTGL
ATOM   1830  SD  MET   233      22.806  11.662  26.940  1.00 19.17      MTGL
ATOM   1831  CE  MET   233      24.330  11.165  26.125  1.00 17.20      MTGL
ATOM   1832  C   MET   233      21.510  13.833  22.305  1.00 19.80      MTGL
ATOM   1833  O   MET   233      22.356  14.314  21.547  1.00 19.41      MTGL
ATOM   1834  N   ALA   234      20.529  13.043  21.885  1.00 20.01      MTGL
ATOM   1835  CA  ALA   234      20.390  12.673  20.480  1.00 21.04      MTGL
ATOM   1836  CB  ALA   234      19.274  11.633  20.324  1.00 19.66      MTGL
ATOM   1837  C   ALA   234      20.111  13.879  19.583  1.00 21.48      MTGL
ATOM   1838  O   ALA   234      20.761  14.055  18.549  1.00 20.87      MTGL
ATOM   1839  N   LYS   235      19.156  14.715  19.985  1.00 22.48      MTGL
ATOM   1840  CA  LYS   235      18.804  15.881  19.176  1.00 24.12      MTGL
ATOM   1841  CB  LYS   235      17.507  16.515  19.681  1.00 26.52      MTGL
ATOM   1842  CG  LYS   235      17.053  17.695  18.835  1.00 33.00      MTGL
ATOM   1843  CD  LYS   235      15.744  18.274  19.331  1.00 36.39      MTGL
ATOM   1844  CE  LYS   235      15.288  19.436  18.451  1.00 40.33      MTGL
ATOM   1845  NZ  LYS   235      13.979  19.997  18.912  1.00 42.05      MTGL
ATOM   1846  C   LYS   235      19.900  16.937  19.145  1.00 22.78      MTGL
ATOM   1847  O   LYS   235      20.041  17.660  18.169  1.00 21.57      MTGL
ATOM   1848  N   THR   236      20.688  17.014  20.209  1.00 23.01      MTGL
ATOM   1849  CA  THR   236      21.753  18.004  20.280  1.00 22.42      MTGL
ATOM   1850  CB  THR   236      22.146  18.289  21.744  1.00 22.63      MTGL
ATOM   1851  OG1 THR   236      20.973  18.616  22.495  1.00 23.14      MTGL
ATOM   1852  CG2 THR   236      23.118  19.459  21.818  1.00 22.49      MTGL
ATOM   1853  C   THR   236      23.020  17.635  19.506  1.00 22.72      MTGL
ATOM   1854  O   THR   236      23.556  18.468  18.773  1.00 22.41      MTGL
ATOM   1855  N   TRP   237      23.495  16.398  19.655  1.00 21.45      MTGL
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Fig. 1 cont.

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ATOM   1856  CA  TRP   237      24.728  15.984  18.984  1.00 21.17      MTGL
ATOM   1857  CB  TRP   237      25.773  15.621  20.041  1.00 21.53      MTGL
ATOM   1858  CG  TRP   237      26.103  16.796  20.916  1.00 21.36      MTGL
ATOM   1859  CD2 TRP   237      25.684  17.004  22.270  1.00 20.90      MTGL
ATOM   1860  CE2 TRP   237      26.156  18.274  22.662  1.00 20.29      MTGL
ATOM   1861  CE3 TRP   237      24.957  16.237  23.191  1.00 20.64      MTGL
ATOM   1862  CD1 TRP   237      26.795  17.920  20.554  1.00 21.20      MTGL
ATOM   1863  NE1 TRP   237      26.827  18.811  21.595  1.00 19.36      MTGL
ATOM   1864  CZ2 TRP   237      25.919  18.799  23.935  1.00 20.39      MTGL
ATOM   1865  CZ3 TRP   237      24.724  16.760  24.458  1.00 20.25      MTGL
ATOM   1866  CH2 TRP   237      25.205  18.028  24.817  1.00 20.45      MTGL
ATOM   1867  C   TRP   237      24.600  14.868  17.941  1.00 21.19      MTGL
ATOM   1868  O   TRP   237      25.561  14.555  17.238  1.00 20.33      MTGL
ATOM   1869  N   ASN   238      23.414  14.274  17.865  0.50 21.58      MTGL
ATOM   1870  CA  ASN   238      23.119  13.212  16.908  0.50 21.97      MTGL
ATOM   1871  CB  ASN   238      22.847  13.829  15.534  0.50 23.20      MTGL
ATOM   1872  CG  ASN   238      21.696  14.822  15.560  0.50 24.82      MTGL
ATOM   1873  OD1 ASN   238      20.631  14.540  16.107  0.50 25.88      MTGL
ATOM   1874  ND2 ASN   238      21.904  15.989  14.960  0.50 26.50      MTGL
ATOM   1875  C   ASN   238      24.179  12.113  16.782  0.50 21.69      MTGL
ATOM   1876  O   ASN   238      24.564  11.730  15.678  0.50 21.51      MTGL
ATOM   1877  N   LYS   239      24.644  11.607  17.919  1.00 21.56      MTGL
ATOM   1878  CA  LYS   239      25.639  10.534  17.938  1.00 20.81      MTGL
ATOM   1879  CB  LYS   239      26.732  10.832  18.971  1.00 21.93      MTGL
ATOM   1880  CG  LYS   239      27.684  11.957  18.598  1.00 21.60      MTGL
ATOM   1881  CD  LYS   239      28.521  11.569  17.396  1.00 23.06      MTGL
ATOM   1882  CE  LYS   239      29.543  12.633  17.053  1.00 23.30      MTGL
ATOM   1883  NZ  LYS   239      30.266  12.280  15.800  1.00 22.03      MTGL
ATOM   1884  C   LYS   239      24.927   9.243  18.331  1.00 20.23      MTGL
ATOM   1885  O   LYS   239      23.814   9.287  18.856  1.00 19.43      MTGL
ATOM   1886  N   GLU   240      25.548   8.096  18.072  1.00 19.70      MTGL
ATOM   1887  CA  GLU   240      24.933   6.835  18.467  1.00 19.84      MTGL
ATOM   1888  CB  GLU   240      25.702   5.633  17.912  1.00 21.53      MTGL
ATOM   1889  CG  GLU   240      25.612   5.485  16.402  1.00 24.54      MTGL
ATOM   1890  CD  GLU   240      25.950   4.081  15.930  1.00 26.26      MTGL
ATOM   1891  OE1 GLU   240      26.984   3.532  16.366  1.00 27.61      MTGL
ATOM   1892  OE2 GLU   240      25.179   3.527  15.118  1.00 28.35      MTGL
ATOM   1893  C   GLU   240      24.972   6.823  19.985  1.00 18.12      MTGL
ATOM   1894  O   GLU   240      25.945   7.269  20.589  1.00 16.94      MTGL
ATOM   1895  N   ILE   241      23.910   6.320  20.598  1.00 17.17      MTGL
ATOM   1896  CA  ILE   241      23.816   6.290  22.049  1.00 17.75      MTGL
ATOM   1897  CB  ILE   241      22.639   7.161  22.509  1.00 18.47      MTGL
ATOM   1898  CG2 ILE   241      22.411   6.997  24.013  1.00 19.08      MTGL
ATOM   1899  CG1 ILE   241      22.918   8.617  22.126  1.00 17.74      MTGL
ATOM   1900  CD1 ILE   241      21.732   9.539  22.297  1.00 18.08      MTGL
ATOM   1901  C   ILE   241      23.651   4.894  22.625  1.00 17.68      MTGL
ATOM   1902  O   ILE   241      23.020   4.026  22.015  1.00 16.98      MTGL
ATOM   1903  N   ALA   242      24.219   4.683  23.809  1.00 17.80      MTGL
ATOM   1904  CA  ALA   242      24.115   3.389  24.465  1.00 17.48      MTGL
ATOM   1905  CB  ALA   242      25.170   2.433  23.906  1.00 16.79      MTGL
ATOM   1906  C   ALA   242      24.244   3.457  25.977  1.00 16.97      MTGL
ATOM   1907  O   ALA   242      24.966   4.291  26.520  1.00 16.47      MTGL
ATOM   1908  N   VAL   243      23.505   2.586  26.654  1.00 16.88      MTGL
ATOM   1909  CA  VAL   243      23.594   2.478  28.098  1.00 16.35      MTGL
ATOM   1910  CB  VAL   243      22.261   2.003  28.715  1.00 15.54      MTGL
ATOM   1911  CG1 VAL   243      22.470   1.580  30.159  1.00 16.43      MTGL
ATOM   1912  CG2 VAL   243      21.238   3.133  28.655  1.00 15.23      MTGL
ATOM   1913  C   VAL   243      24.667   1.396  28.212  1.00 16.01      MTGL
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Fig. 1 cont.

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ATOM   1914  O   VAL   243      24.424   0.243  27.856  1.00 16.07      MTGL
ATOM   1915  N   VAL   244      25.860   1.774  28.665  1.00 15.48      MTGL
ATOM   1916  CA  VAL   244      26.971   0.822  28.758  1.00 15.55      MTGL
ATOM   1917  CB  VAL   244      28.292   1.501  28.345  1.00 15.25      MTGL
ATOM   1918  CG1 VAL   244      28.167   2.024  26.922  1.00 15.71      MTGL
ATOM   1919  CG2 VAL   244      28.618   2.646  29.294  1.00 14.98      MTGL
ATOM   1920  C   VAL   244      27.163   0.125  30.097  1.00 15.27      MTGL
ATOM   1921  O   VAL   244      28.052  -0.710  30.244  1.00 16.53      MTGL
ATOM   1922  N   GLU   245      26.326  -0.464  31.068  1.00 15.31      MTGL
ATOM   1923  CA  GLU   245      26.387  -0.145  32.391  1.00 15.54      MTGL
ATOM   1924  CB  GLU   245      27.390   0.581  33.301  1.00 15.71      MTGL
ATOM   1925  CG  GLU   245      28.833   0.193  33.105  1.00 17.89      MTGL
ATOM   1926  CD  GLU   245      29.738   0.777  34.177  1.00 19.37      MTGL
ATOM   1927  OE1 GLU   245      29.322   0.824  35.359  1.00 18.55      MTGL
ATOM   1928  OE2 GLU   245      30.867   1.174  33.827  1.00 20.37      MTGL
ATOM   1929  C   GLU   245      25.024  -0.053  33.043  1.00 15.41      MTGL
ATOM   1930  O   GLU   245      24.421   1.014  33.060  1.00 16.55      MTGL
ATOM   1931  N   THR   246      24.533  -1.174  33.563  1.00 15.11      MTGL
ATOM   1932  CA  THR   246      23.266  -1.185  34.280  1.00 14.75      MTGL
ATOM   1933  CB  THR   246      22.053  -1.052  33.322  1.00 15.60      MTGL
ATOM   1934  OG1 THR   246      20.884  -0.721  34.085  1.00 14.95      MTGL
ATOM   1935  CG2 THR   246      21.809  -2.352  32.564  1.00 14.91      MTGL
ATOM   1936  C   THR   246      23.168  -2.467  35.100  1.00 14.67      MTGL
ATOM   1937  O   THR   246      23.853  -3.451  34.807  1.00 15.70      MTGL
ATOM   1938  N   ASN   247      22.331  -2.441  36.134  1.00 14.38      MTGL
ATOM   1939  CA  ASN   247      22.128  -3.579  37.035  1.00 14.91      MTGL
ATOM   1940  CB  ASN   247      23.012  -3.462  38.294  1.00 15.25      MTGL
ATOM   1941  CG  ASN   247      24.397  -4.085  38.150  1.00 16.92      MTGL
ATOM   1942  OD1 ASN   247      25.212  -3.972  39.068  1.00 16.53      MTGL
ATOM   1943  ND2 ASN   247      24.668  -4.746  37.024  1.00 14.82      MTGL
ATOM   1944  C   ASN   247      20.693  -3.554  37.560  1.00 15.99      MTGL
ATOM   1945  O   ASN   247      20.057  -2.496  37.609  1.00 15.64      MTGL
ATOM   1946  N   TRP   248      20.194  -4.723  37.946  1.00 15.53      MTGL
ATOM   1947  CA  TRP   248      18.893  -4.830  38.600  1.00 16.36      MTGL
ATOM   1948  CB  TRP   248      17.732  -5.127  37.657  1.00 14.84      MTGL
ATOM   1949  CG  TRP   248      16.455  -5.135  38.445  1.00 13.73      MTGL
ATOM   1950  CD2 TRP   248      15.743  -3.989  38.940  1.00 14.11      MTGL
ATOM   1951  CE2 TRP   248      14.684  -4.467  39.739  1.00 12.13      MTGL
ATOM   1952  CE3 TRP   248      15.902  -2.603  38.786  1.00 14.57      MTGL
ATOM   1953  CD1 TRP   248      15.812  -6.224  38.949  1.00 13.26      MTGL
ATOM   1954  NE1 TRP   248      14.751  -5.833  39.728  1.00 13.69      MTGL
ATOM   1955  CZ2 TRP   248      13.784  -3.613  40.384  1.00 14.00      MTGL
ATOM   1956  CZ3 TRP   248      15.008  -1.751  39.427  1.00 13.98      MTGL
ATOM   1957  CH2 TRP   248      13.962  -2.260  40.218  1.00 14.50      MTGL
ATOM   1958  C   TRP   248      19.080  -5.972  39.576  1.00 16.41      MTGL
ATOM   1959  O   TRP   248      19.507  -7.060  39.200  1.00 17.70      MTGL
ATOM   1960  N   PRO   249      18.765  -5.739  40.850  1.00 17.62      MTGL
ATOM   1961  CD  PRO   249      18.316  -4.468  41.449  1.00 17.41      MTGL
ATOM   1962  CA  PRO   249      18.933  -6.774  41.868  1.00 17.81      MTGL
ATOM   1963  CB  PRO   249      19.010  -5.961  43.156  1.00 18.08      MTGL
ATOM   1964  CG  PRO   249      18.056  -4.857  42.892  1.00 20.03      MTGL
ATOM   1965  C   PRO   249      17.922  -7.898  41.972  1.00 18.16      MTGL
ATOM   1966  O   PRO   249      16.729  -7.722  41.728  1.00 18.74      MTGL
ATOM   1967  N   ILE   250      18.426  -9.074  42.322  1.00 18.86      MTGL
ATOM   1968  CA  ILE   250      17.561 -10.215  42.549  1.00 20.06      MTGL
ATOM   1969  CB  ILE   250      18.189 -11.544  42.040  1.00 20.52      MTGL
ATOM   1970  CG2 ILE   250      18.230 -11.553  40.518  1.00 19.08      MTGL
ATOM   1971  CG1 ILE   250      19.590 -11.734  42.614  1.00 20.81      MTGL
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Fig. 1 cont.

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ATOM   1972  CD1 ILE   250      20.222 -13.061  42.216  1.00 21.09      MTGL
ATOM   1973  C   ILE   250      17.408 -10.234  44.075  1.00 19.97      MTGL
ATOM   1974  O   ILE   250      16.659 -11.028  44.637  1.00 20.48      MTGL
ATOM   1975  N   SER   251      18.127  -9.327  44.735  1.00 20.21      MTGL
ATOM   1976  CA  SER   251      18.072  -9.206  46.188  1.00 21.30      MTGL
ATOM   1977  CB  SER   251      18.878 -10.331  46.843  1.00 22.63      MTGL
ATOM   1978  OG  SER   251      18.757 -10.273  48.253  1.00 24.04      MTGL
ATOM   1979  C   SER   251      18.603  -7.855  46.658  1.00 21.50      MTGL
ATOM   1980  O   SER   251      19.735  -7.485  46.343  1.00 21.25      MTGL
ATOM   1981  N   CYS   252      17.784  -7.112  47.400  1.00 21.87      MTGL
ATOM   1982  CA  CYS   252      18.194  -5.806  47.918  1.00 23.27      MTGL
ATOM   1983  C   CYS   252      17.529  -5.505  49.263  1.00 24.17      MTGL
ATOM   1984  O   CYS   252      16.654  -4.647  49.340  1.00 24.61      MTGL
ATOM   1985  CB  CYS   252      17.840  -4.684  46.927  1.00 23.57      MTGL
ATOM   1986  SG  CYS   252      18.756  -3.154  47.311  1.00 23.83      MTGL
ATOM   1987  N   PRO   253      17.951  -6.199  50.340  1.00 25.34      MTGL
ATOM   1988  CD  PRO   253      18.950  -7.281  50.290  1.00 26.08      MTGL
ATOM   1989  CA  PRO   253      17.428  -6.052  51.707  1.00 25.93      MTGL
ATOM   1990  CB  PRO   253      18.308  -7.001  52.518  1.00 26.63      MTGL
ATOM   1991  CG  PRO   253      18.627  -8.068  51.539  1.00 27.12      MTGL
ATOM   1992  C   PRO   253      17.416  -4.645  52.294  1.00 26.16      MTGL
ATOM   1993  O   PRO   253      16.415  -4.223  52.865  1.00 26.46      MTGL
ATOM   1994  N   ASN   254      18.526  -3.922  52.178  1.00 26.96      MTGL
ATOM   1995  CA  ASN   254      18.574  -2.560  52.713  1.00 27.76      MTGL
ATOM   1996  CB  ASN   254      19.145  -2.538  54.137  1.00 29.54      MTGL
ATOM   1997  CG  ASN   254      20.541  -3.097  54.220  1.00 31.33      MTGL
ATOM   1998  OD1 ASN   254      20.854  -4.102  53.587  1.00 34.28      MTGL
ATOM   1999  ND2 ASN   254      21.388  -2.465  55.028  1.00 30.87      MTGL
ATOM   2000  C   ASN   254      19.329  -1.580  51.834  1.00 26.98      MTGL
ATOM   2001  O   ASN   254      20.525  -1.355  51.990  1.00 26.72      MTGL
ATOM   2002  N   PRO   255      18.623  -0.993  50.873  1.00 26.12      MTGL
ATOM   2003  CD  PRO   255      17.274  -1.385  50.443  1.00 25.65      MTGL
ATOM   2004  CA  PRO   255      19.222  -0.023  49.957  1.00 25.15      MTGL
ATOM   2005  CB  PRO   255      18.128   0.211  48.913  1.00 25.50      MTGL
ATOM   2006  CG  PRO   255      16.895  -0.262  49.550  1.00 25.88      MTGL
ATOM   2007  C   PRO   255      19.638   1.279  50.637  1.00 25.08      MTGL
ATOM   2008  O   PRO   255      18.993   1.735  51.586  1.00 24.66      MTGL
ATOM   2009  N   ARG   256      20.717   1.869  50.128  1.00 23.54      MTGL
ATOM   2010  CA  ARG   256      21.219   3.131  50.653  1.00 24.56      MTGL
ATOM   2011  CB  ARG   256      22.679   3.345  50.230  1.00 26.20      MTGL
ATOM   2012  CG  ARG   256      23.290   4.673  50.685  1.00 29.88      MTGL
ATOM   2013  CD  ARG   256      23.244   4.843  52.205  1.00 33.75      MTGL
ATOM   2014  NE  ARG   256      24.112   3.900  52.913  1.00 36.98      MTGL
ATOM   2015  CZ  ARG   256      24.215   3.826  54.241  1.00 38.13      MTGL
ATOM   2016  NH1 ARG   256      23.503   4.638  55.016  1.00 37.96      MTGL
ATOM   2017  NH2 ARG   256      25.034   2.942  54.796  1.00 38.27      MTGL
ATOM   2018  C   ARG   256      20.346   4.291  50.152  1.00 24.09      MTGL
ATOM   2019  O   ARG   256      20.223   5.312  50.820  1.00 22.82      MTGL
ATOM   2020  N   TYR   257      19.740   4.129  48.978  1.00 23.76      MTGL
ATOM   2021  CA  TYR   257      18.869   5.162  48.417  1.00 24.47      MTGL
ATOM   2022  CB  TYR   257      19.506   5.829  47.197  1.00 25.66      MTGL
ATOM   2023  CG  TYR   257      20.889   6.365  47.430  1.00 27.18      MTGL
ATOM   2024  CD1 TYR   257      22.003   5.538  47.316  1.00 27.30      MTGL
ATOM   2025  CE1 TYR   257      23.283   6.020  47.567  1.00 28.24      MTGL
ATOM   2026  CD2 TYR   257      21.086   7.693  47.802  1.00 28.37      MTGL
ATOM   2027  CE2 TYR   257      22.363   8.184  48.058  1.00 28.50      MTGL
ATOM   2028  CZ  TYR   257      23.455   7.341  47.940  1.00 29.46      MTGL
ATOM   2029  OH  TYR   257      24.720   7.814  48.215  1.00 30.61      MTGL
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Fig. 1 cont.

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ATOM   2030  C   TYR   257      17.539   4.578  47.986  1.00 24.30      MTGL
ATOM   2031  O   TYR   257      17.450   3.408  47.619  1.00 24.04      MTGL
ATOM   2032  N   SER   258      16.507   5.411  48.018  1.00 24.57      MTGL
ATOM   2033  CA  SER   258      15.178   4.984  47.607  1.00 24.95      MTGL
ATOM   2034  CB  SER   258      14.162   6.084  47.930  1.00 25.55      MTGL
ATOM   2035  OG  SER   258      14.261   6.471  49.292  1.00 27.69      MTGL
ATOM   2036  C   SER   258      15.230   4.746  46.102  1.00 23.31      MTGL
ATOM   2037  O   SER   258      15.949   5.449  45.392  1.00 23.48      MTGL
ATOM   2038  N   PHE   259      14.488   3.754  45.619  1.00 22.69      MTGL
ATOM   2039  CA  PHE   259      14.459   3.452  44.190  1.00 23.46      MTGL
ATOM   2040  CB  PHE   259      13.961   2.022  43.958  1.00 22.78      MTGL
ATOM   2041  CG  PHE   259      15.051   0.990  43.984  1.00 22.99      MTGL
ATOM   2042  CD1 PHE   259      15.923   0.904  45.066  1.00 24.03      MTGL
ATOM   2043  CD2 PHE   259      15.218   0.112  42.919  1.00 22.03      MTGL
ATOM   2044  CE1 PHE   259      16.945  -0.046  45.089  1.00 24.16      MTGL
ATOM   2045  CE2 PHE   259      16.233  -0.839  42.929  1.00 22.81      MTGL
ATOM   2046  CZ  PHE   259      17.103  -0.918  44.019  1.00 23.26      MTGL
ATOM   2047  C   PHE   259      13.580   4.429  43.411  1.00 23.33      MTGL
ATOM   2048  O   PHE   259      12.681   5.048  43.975  1.00 23.29      MTGL
ATOM   2049  N   PRO   260      13.840   4.581  42.100  1.00 23.87      MTGL
ATOM   2050  CD  PRO   260      14.959   4.002  41.338  1.00 23.34      MTGL
ATOM   2051  CA  PRO   260      13.057   5.492  41.259  1.00 23.83      MTGL
ATOM   2052  CB  PRO   260      13.711   5.346  39.888  1.00 23.96      MTGL
ATOM   2053  CG  PRO   260      15.138   5.012  40.229  1.00 23.75      MTGL
ATOM   2054  C   PRO   260      11.594   5.062  41.255  1.00 24.68      MTGL
ATOM   2055  O   PRO   260      11.287   3.867  41.233  1.00 22.71      MTGL
ATOM   2056  N   SER   261      10.700   6.042  41.274  1.00 24.81      MTGL
ATOM   2057  CA  SER   261       9.267   5.783  41.298  1.00 25.73      MTGL
ATOM   2058  CB  SER   261       8.494   7.107  41.254  1.00 26.69      MTGL
ATOM   2059  OG  SER   261       8.667   7.757  40.003  1.00 27.65      MTGL
ATOM   2060  C   SER   261       8.725   4.862  40.207  1.00 25.31      MTGL
ATOM   2061  O   SER   261       7.853   4.048  40.488  1.00 25.28      MTGL
ATOM   2062  N   ASP   262       9.214   4.979  38.973  1.00 26.49      MTGL
ATOM   2063  CA  ASP   262       8.678   4.131  37.909  1.00 27.78      MTGL
ATOM   2064  CB  ASP   262       8.762   4.824  36.535  1.00 27.44      MTGL
ATOM   2065  CG  ASP   262      10.166   5.267  36.170  1.00 29.75      MTGL
ATOM   2066  OD1 ASP   262      11.138   4.673  36.681  1.00 29.62      MTGL
ATOM   2067  OD2 ASP   262      10.289   6.207  35.349  1.00 29.82      MTGL
ATOM   2068  C   ASP   262       9.259   2.724  37.816  1.00 28.89      MTGL
ATOM   2069  O   ASP   262       9.063   2.037  36.812  1.00 29.03      MTGL
ATOM   2070  N   VAL   263       9.968   2.291  38.857  1.00 29.21      MTGL
ATOM   2071  CA  VAL   263      10.529   0.941  38.878  1.00 29.98      MTGL
ATOM   2072  CB  VAL   263      12.063   0.930  38.613  1.00 29.51      MTGL
ATOM   2073  CG1 VAL   263      12.355   1.468  37.226  1.00 28.86      MTGL
ATOM   2074  CG2 VAL   263      12.788   1.751  39.669  1.00 29.09      MTGL
ATOM   2075  C   VAL   263      10.254   0.257  40.218  1.00 30.76      MTGL
ATOM   2076  O   VAL   263      10.672  -0.879  40.434  1.00 30.49      MTGL
ATOM   2077  N   LYS   264       9.534   0.941  41.108  1.00 31.82      MTGL
ATOM   2078  CA  LYS   264       9.215   0.394  42.432  1.00 33.07      MTGL
ATOM   2079  CB  LYS   264       8.570   1.464  43.317  1.00 34.40      MTGL
ATOM   2080  CG  LYS   264       9.566   2.391  44.002  1.00 36.45      MTGL
ATOM   2081  CD  LYS   264       8.859   3.344  44.961  1.00 38.24      MTGL
ATOM   2082  CE  LYS   264       9.844   4.281  45.655  1.00 40.37      MTGL
ATOM   2083  NZ  LYS   264       9.148   5.291  46.508  1.00 40.59      MTGL
ATOM   2084  C   LYS   264       8.321  -0.842  42.415  1.00 33.40      MTGL
ATOM   2085  O   LYS   264       8.267  -1.595  43.394  1.00 33.28      MTGL
ATOM   2086  N   ASN   265       7.612  -1.049  41.313  1.00 32.77      MTGL
ATOM   2087  CA  ASN   265       6.738  -2.208  41.194  1.00 32.23      MTGL
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Fig. 1 cont.

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ATOM   2088  CB  ASN   265       5.587  -1.898  40.236  1.00 34.35      MTGL
ATOM   2089  CG  ASN   265       6.074  -1.544  38.845  1.00 36.81      MTGL
ATOM   2090  OD1 ASN   265       6.837  -0.593  38.667  1.00 37.33      MTGL
ATOM   2091  ND2 ASN   265       5.638  -2.311  37.848  1.00 38.71      MTGL
ATOM   2092  C   ASN   265       7.504  -3.436  40.689  1.00 30.70      MTGL
ATOM   2093  O   ASN   265       6.998  -4.555  40.744  1.00 30.83      MTGL
ATOM   2094  N   ILE   266       8.719  -3.226  40.192  1.00 28.28      MTGL
ATOM   2095  CA  ILE   266       9.517  -4.336  39.687  1.00 25.48      MTGL
ATOM   2096  CB  ILE   266      10.651  -3.848  38.767  1.00 23.96      MTGL
ATOM   2097  CG2 ILE   266      11.449  -5.046  38.257  1.00 23.40      MTGL
ATOM   2098  CG1 ILE   266      10.067  -3.054  37.594  1.00 23.38      MTGL
ATOM   2099  CD1 ILE   266      11.114  -2.516  36.627  1.00 22.30      MTGL
ATOM   2100  C   ILE   266      10.122  -5.094  40.867  1.00 24.88      MTGL
ATOM   2101  O   ILE   266      10.825  -4.520  41.691  1.00 22.68      MTGL
ATOM   2102  N   PRO   267       9.850  -6.404  40.960  1.00 24.25      MTGL
ATOM   2103  CD  PRO   267       9.012  -7.212  40.051  1.00 23.79      MTGL
ATOM   2104  CA  PRO   267      10.374  -7.225  42.052  1.00 23.72      MTGL
ATOM   2105  CB  PRO   267       9.542  -8.497  41.946  1.00 24.48      MTGL
ATOM   2106  CG  PRO   267       9.373  -8.633  40.455  1.00 24.22      MTGL
ATOM   2107  C   PRO   267      11.865  -7.526  41.943  1.00 23.20      MTGL
ATOM   2108  O   PRO   267      12.437  -7.515  40.851  1.00 22.29      MTGL
ATOM   2109  N   PHE   268      12.487  -7.781  43.090  1.00 22.29      MTGL
ATOM   2110  CA  PHE   268      13.898  -8.134  43.119  1.00 22.67      MTGL
ATOM   2111  CB  PHE   268      14.533  -7.757  44.462  1.00 22.68      MTGL
ATOM   2112  CG  PHE   268      14.493  -6.285  44.754  1.00 22.93      MTGL
ATOM   2113  CD1 PHE   268      14.838  -5.360  43.773  1.00 22.68      MTGL
ATOM   2114  CD2 PHE   268      14.115  -5.821  46.008  1.00 23.18      MTGL
ATOM   2115  CE1 PHE   268      14.806  -3.993  44.037  1.00 23.40      MTGL
ATOM   2116  CE2 PHE   268      14.079  -4.454  46.283  1.00 23.36      MTGL
ATOM   2117  CZ  PHE   268      14.425  -3.539  45.298  1.00 23.35      MTGL
ATOM   2118  C   PHE   268      13.925  -9.643  42.921  1.00 21.88      MTGL
ATOM   2119  O   PHE   268      13.780 -10.414  43.873  1.00 21.02      MTGL
ATOM   2120  N   SER   269      14.088 -10.049  41.667  1.00 21.08      MTGL
ATOM   2121  CA  SER   269      14.110 -11.457  41.294  1.00 20.72      MTGL
ATOM   2122  CB  SER   269      12.702 -12.052  41.417  1.00 19.79      MTGL
ATOM   2123  OG  SER   269      11.814 -11.416  40.509  1.00 19.06      MTGL
ATOM   2124  C   SER   269      14.554 -11.546  39.844  1.00 20.32      MTGL
ATOM   2125  O   SER   269      14.670 -10.530  39.161  1.00 19.97      MTGL
ATOM   2126  N   PRO   270      14.814 -12.767  39.354  1.00 21.15      MTGL
ATOM   2127  CD  PRO   270      14.896 -14.054  40.075  1.00 20.43      MTGL
ATOM   2128  CA  PRO   270      15.237 -12.915  37.958  1.00 20.91      MTGL
ATOM   2129  CB  PRO   270      15.407 -14.426  37.809  1.00 20.78      MTGL
ATOM   2130  CG  PRO   270      15.832 -14.852  39.196  1.00 20.58      MTGL
ATOM   2131  C   PRO   270      14.169 -12.348  37.016  1.00 20.97      MTGL
ATOM   2132  O   PRO   270      14.489 -11.688  36.028  1.00 20.64      MTGL
ATOM   2133  N   GLU   271      12.900 -12.605  37.331  1.00 21.15      MTGL
ATOM   2134  CA  GLU   271      11.797 -12.102  36.508  1.00 21.55      MTGL
ATOM   2135  CB  GLU   271      10.446 -12.538  37.082  1.00 22.38      MTGL
ATOM   2136  CG  GLU   271      10.155 -14.036  37.003  1.00 25.49      MTGL
ATOM   2137  CD  GLU   271      11.082 -14.873  37.870  1.00 26.37      MTGL
ATOM   2138  OE1 GLU   271      11.447 -14.415  38.970  1.00 26.39      MTGL
ATOM   2139  OE2 GLU   271      11.433 -15.997  37.457  1.00 27.82      MTGL
ATOM   2140  C   GLU   271      11.861 -10.577  36.476  1.00 20.84      MTGL
ATOM   2141  O   GLU   271      11.640  -9.949  35.434  1.00 20.80      MTGL
ATOM   2142  N   GLY   272      12.166  -9.993  37.631  1.00 19.71      MTGL
ATOM   2143  CA  GLY   272      12.271  -8.550  37.734  1.00 18.93      MTGL
ATOM   2144  C   GLY   272      13.415  -8.008  36.897  1.00 18.95      MTGL
ATOM   2145  O   GLY   272      13.284  -6.941  36.289  1.00 19.13      MTGL
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Fig. 1 cont.

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ATOM   2146  N   GLN   273      14.534  -8.734  36.859  1.00 17.61      MTGL
ATOM   2147  CA  GLN   273      15.687  -8.299  36.074  1.00 18.43      MTGL
ATOM   2148  CB  GLN   273      16.864  -9.260  36.230  1.00 17.76      MTGL
ATOM   2149  CG  GLN   273      17.467  -9.345  37.610  1.00 19.26      MTGL
ATOM   2150  CD  GLN   273      18.720 -10.190  37.607  1.00 19.87      MTGL
ATOM   2151  OE1 GLN   273      18.726 -11.304  37.073  1.00 18.60      MTGL
ATOM   2152  NE2 GLN   273      19.793  -9.667  38.198  1.00 19.12      MTGL
ATOM   2153  C   GLN   273      15.300  -8.270  34.607  1.00 18.09      MTGL
ATOM   2154  O   GLN   273      15.660  -7.353  33.869  1.00 17.98      MTGL
ATOM   2155  N   THR   274      14.579  -9.305  34.193  1.00 17.84      MTGL
ATOM   2156  CA  THR   274      14.131  -9.433  32.815  1.00 17.91      MTGL
ATOM   2157  CB  THR   274      13.293 -10.712  32.637  1.00 18.13      MTGL
ATOM   2158  OG1 THR   274      14.128 -11.857  32.859  1.00 19.81      MTGL
ATOM   2159  CG2 THR   274      12.695 -10.777  31.231  1.00 19.04      MTGL
ATOM   2160  C   THR   274      13.293  -8.219  32.428  1.00 17.34      MTGL
ATOM   2161  O   THR   274      13.504  -7.619  31.376  1.00 16.72      MTGL
ATOM   2162  N   THR   275      12.351  -7.859  33.294  1.00 16.98      MTGL
ATOM   2163  CA  THR   275      11.483  -6.712  33.056  1.00 17.24      MTGL
ATOM   2164  CB  THR   275      10.425  -6.574  34.169  1.00 17.29      MTGL
ATOM   2165  OG1 THR   275       9.587  -7.735  34.181  1.00 17.49      MTGL
ATOM   2166  CG2 THR   275       9.563  -5.331  33.937  1.00 16.88      MTGL
ATOM   2167  C   THR   275      12.270  -5.405  32.982  1.00 17.05      MTGL
ATOM   2168  O   THR   275      12.090  -4.618  32.052  1.00 17.86      MTGL
ATOM   2169  N   PHE   276      13.139  -5.174  33.963  1.00 16.71      MTGL
ATOM   2170  CA  PHE   276      13.937  -3.949  34.000  1.00 15.62      MTGL
ATOM   2171  CB  PHE   276      14.781  -3.890  35.278  1.00 15.45      MTGL
ATOM   2172  CG  PHE   276      15.621  -2.646  35.389  1.00 16.62      MTGL
ATOM   2173  CD1 PHE   276      15.048  -1.437  35.777  1.00 17.56      MTGL
ATOM   2174  CD2 PHE   276      16.976  -2.675  35.077  1.00 17.00      MTGL
ATOM   2175  CE1 PHE   276      15.817  -0.272  35.860  1.00 18.40      MTGL
ATOM   2176  CE2 PHE   276      17.757  -1.518  35.155  1.00 18.28      MTGL
ATOM   2177  CZ  PHE   276      17.176  -0.314  35.546  1.00 17.73      MTGL
ATOM   2178  C   PHE   276      14.866  -3.825  32.796  1.00 16.42      MTGL
ATOM   2179  O   PHE   276      14.907  -2.785  32.136  1.00 17.18      MTGL
ATOM   2180  N   ILE   277      15.627  -4.881  32.520  1.00 15.71      MTGL
ATOM   2181  CA  ILE   277      16.558  -4.864  31.399  1.00 14.72      MTGL
ATOM   2182  CB  ILE   277      17.364  -6.181  31.330  1.00 14.70      MTGL
ATOM   2183  CG2 ILE   277      18.227  -6.209  30.063  1.00 14.44      MTGL
ATOM   2184  CG1 ILE   277      18.238  -6.305  32.587  1.00 14.86      MTGL
ATOM   2185  CD1 ILE   277      18.945  -7.635  32.727  1.00 14.36      MTGL
ATOM   2186  C   ILE   277      15.832  -4.643  30.081  1.00 14.58      MTGL
ATOM   2187  O   ILE   277      16.286  -3.868  29.250  1.00 14.01      MTGL
ATOM   2188  N   THR   278      14.708  -5.330  29.890  1.00 14.56      MTGL
ATOM   2189  CA  THR   278      13.930  -5.182  28.663  1.00 15.56      MTGL
ATOM   2190  CB  THR   278      12.724  -6.159  28.635  1.00 15.82      MTGL
ATOM   2191  OG1 THR   278      13.203  -7.505  28.742  1.00 16.63      MTGL
ATOM   2192  CG2 THR   278      11.942  -6.017  27.329  1.00 15.47      MTGL
ATOM   2193  C   THR   278      13.411  -3.747  28.530  1.00 15.31      MTGL
ATOM   2194  O   THR   278      13.435  -3.168  27.446  1.00 16.65      MTGL
ATOM   2195  N   ASN   279      12.946  -3.174  29.634  1.00 15.85      MTGL
ATOM   2196  CA  ASN   279      12.430  -1.808  29.609  1.00 16.36      MTGL
ATOM   2197  CB  ASN   279      11.743  -1.475  30.939  1.00 15.56      MTGL
ATOM   2198  CG  ASN   279      10.388  -2.159  31.077  1.00 17.29      MTGL
ATOM   2199  OD1 ASN   279       9.939  -2.848  30.167  1.00 15.98      MTGL
ATOM   2200  ND2 ASN   279       9.736  -1.966  32.215  1.00 17.61      MTGL
ATOM   2201  C   ASN   279      13.520  -0.783  29.304  1.00 16.68      MTGL
ATOM   2202  O   ASN   279      13.300   0.155  28.533  1.00 16.98      MTGL
ATOM   2203  N   VAL   280      14.695  -0.950  29.904  1.00 16.27      MTGL
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Fig. 1 cont.

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ATOM   2204  CA  VAL   280      15.782  -0.013  29.641  1.00 15.63      MTGL
ATOM   2205  CB  VAL   280      17.005  -0.283  30.545  1.00 15.75      MTGL
ATOM   2206  CG1 VAL   280      18.171   0.623  30.126  1.00 14.59      MTGL
ATOM   2207  CG2 VAL   280      16.634  -0.023  32.007  1.00 14.29      MTGL
ATOM   2208  C   VAL   280      16.203  -0.144  28.183  1.00 15.42      MTGL
ATOM   2209  O   VAL   280      16.483   0.852  27.512  1.00 14.80      MTGL
ATOM   2210  N   ALA   281      16.236  -1.381  27.697  1.00 14.47      MTGL
ATOM   2211  CA  ALA   281      16.614  -1.645  26.315  1.00 15.95      MTGL
ATOM   2212  CB  ALA   281      16.573  -3.147  26.035  1.00 15.85      MTGL
ATOM   2213  C   ALA   281      15.662  -0.922  25.369  1.00 16.21      MTGL
ATOM   2214  O   ALA   281      16.087  -0.290  24.403  1.00 15.33      MTGL
ATOM   2215  N   ASN   282      14.369  -1.018  25.653  1.00 16.95      MTGL
ATOM   2216  CA  ASN   282      13.383  -0.386  24.792  1.00 17.84      MTGL
ATOM   2217  CB  ASN   282      12.015  -1.013  25.021  1.00 19.13      MTGL
ATOM   2218  CG  ASN   282      11.924  -2.398  24.400  1.00 20.19      MTGL
ATOM   2219  OD1 ASN   282      12.393  -2.605  23.289  1.00 23.04      MTGL
ATOM   2220  ND2 ASN   282      11.328  -3.341  25.108  1.00 19.74      MTGL
ATOM   2221  C   ASN   282      13.337   1.124  24.910  1.00 18.52      MTGL
ATOM   2222  O   ASN   282      12.841   1.806  24.011  1.00 17.57      MTGL
ATOM   2223  N   ILE   283      13.851   1.651  26.015  1.00 18.29      MTGL
ATOM   2224  CA  ILE   283      13.902   3.095  26.168  1.00 18.86      MTGL
ATOM   2225  CB  ILE   283      14.254   3.496  27.603  1.00 19.57      MTGL
ATOM   2226  CG2 ILE   283      14.818   4.917  27.636  1.00 20.74      MTGL
ATOM   2227  CG1 ILE   283      13.003   3.365  28.471  1.00 21.83      MTGL
ATOM   2228  CD1 ILE   283      13.214   3.728  29.909  1.00 25.75      MTGL
ATOM   2229  C   ILE   283      14.994   3.566  25.209  1.00 17.96      MTGL
ATOM   2230  O   ILE   283      14.816   4.543  24.483  1.00 17.19      MTGL
ATOM   2231  N   VAL   284      16.114   2.844  25.200  1.00 17.16      MTGL
ATOM   2232  CA  VAL   284      17.236   3.164  24.321  1.00 15.86      MTGL
ATOM   2233  CB  VAL   284      18.420   2.194  24.554  1.00 16.05      MTGL
ATOM   2234  CG1 VAL   284      19.491   2.409  23.491  1.00 14.09      MTGL
ATOM   2235  CG2 VAL   284      19.006   2.416  25.956  1.00 14.93      MTGL
ATOM   2236  C   VAL   284      16.797   3.075  22.861  1.00 16.21      MTGL
ATOM   2237  O   VAL   284      17.089   3.963  22.059  1.00 15.26      MTGL
ATOM   2238  N   SER   285      16.086   2.004  22.519  1.00 16.71      MTGL
ATOM   2239  CA  SER   285      15.618   1.813  21.145  1.00 18.87      MTGL
ATOM   2240  CB  SER   285      14.977   0.429  20.979  1.00 18.71      MTGL
ATOM   2241  OG  SER   285      15.954  -0.595  21.082  1.00 25.57      MTGL
ATOM   2242  C   SER   285      14.622   2.882  20.697  1.00 18.52      MTGL
ATOM   2243  O   SER   285      14.453   3.101  19.507  1.00 19.96      MTGL
ATOM   2244  N   SER   286      13.964   3.544  21.644  1.00 17.61      MTGL
ATOM   2245  CA  SER   286      12.993   4.574  21.295  1.00 18.49      MTGL
ATOM   2246  CB  SER   286      11.970   4.754  22.421  1.00 18.70      MTGL
ATOM   2247  OG  SER   286      12.505   5.533  23.483  1.00 18.21      MTGL
ATOM   2248  C   SER   286      13.686   5.909  21.040  1.00 18.76      MTGL
ATOM   2249  O   SER   286      13.043   6.892  20.676  1.00 17.84      MTGL
ATOM   2250  N   VAL   287      15.000   5.931  21.235  1.00 18.85      MTGL
ATOM   2251  CA  VAL   287      15.793   7.138  21.048  1.00 17.18      MTGL
ATOM   2252  CB  VAL   287      16.866   7.267  22.158  1.00 17.69      MTGL
ATOM   2253  CG1 VAL   287      17.764   8.477  21.890  1.00 17.29      MTGL
ATOM   2254  CG2 VAL   287      16.189   7.399  23.512  1.00 17.29      MTGL
ATOM   2255  C   VAL   287      16.493   7.144  19.702  1.00 17.44      MTGL
ATOM   2256  O   VAL   287      16.979   6.112  19.241  1.00 16.36      MTGL
ATOM   2257  N   SER   288      16.546   8.313  19.073  1.00 18.07      MTGL
ATOM   2258  CA  SER   288      17.215   8.442  17.787  1.00 18.93      MTGL
ATOM   2259  CB  SER   288      17.202   9.900  17.329  1.00 19.03      MTGL
ATOM   2260  OG  SER   288      17.858  10.045  16.082  1.00 21.05      MTGL
ATOM   2261  C   SER   288      18.657   7.950  17.911  1.00 18.73      MTGL
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Fig. 1 cont.

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ATOM   2262  O   SER  288      19.444   8.498  18.682  1.00 18.95      MTGL
ATOM   2263  N   ARG  289      18.984   6.915  17.145  1.00 17.81      MTGL
ATOM   2264  CA  ARG  289      20.313   6.311  17.137  1.00 18.49      MTGL
ATOM   2265  CB  ARG  289      21.387   7.347  16.760  1.00 20.78      MTGL
ATOM   2266  CG  ARG  289      21.128   8.067  15.429  1.00 24.72      MTGL
ATOM   2267  CD  ARG  289      22.378   8.761  14.890  1.00 26.86      MTGL
ATOM   2268  NE  ARG  289      23.269   7.812  14.225  1.00 31.29      MTGL
ATOM   2269  CZ  ARG  289      24.483   8.101  13.758  1.00 32.57      MTGL
ATOM   2270  NH1 ARG  289      24.981   9.327  13.880  1.00 33.06      MTGL
ATOM   2271  NH2 ARG  289      25.200   7.159  13.159  1.00 32.56      MTGL
ATOM   2272  C   ARG  289      20.687   5.616  18.456  1.00 17.41      MTGL
ATOM   2273  O   ARG  289      21.865   5.493  18.785  1.00 16.35      MTGL
ATOM   2274  N   GLY  290      19.681   5.173  19.207  1.00 16.31      MTGL
ATOM   2275  CA  GLY  290      19.944   4.449  20.442  1.00 16.82      MTGL
ATOM   2276  C   GLY  290      20.267   3.042  19.970  1.00 17.04      MTGL
ATOM   2277  O   GLY  290      19.393   2.353  19.450  1.00 16.17      MTGL
ATOM   2278  N   VAL  291      21.502   2.595  20.159  1.00 17.31      MTGL
ATOM   2279  CA  VAL  291      21.893   1.290  19.644  1.00 17.47      MTGL
ATOM   2280  CB  VAL  291      22.951   1.475  18.534  1.00 17.89      MTGL
ATOM   2281  CG1 VAL  291      22.387   2.347  17.419  1.00 18.32      MTGL
ATOM   2282  CG2 VAL  291      24.204   2.125  19.112  1.00 16.95      MTGL
ATOM   2283  C   VAL  291      22.403   0.194  20.581  1.00 18.18      MTGL
ATOM   2284  O   VAL  291      22.610  -0.933  20.133  1.00 17.39      MTGL
ATOM   2285  N   GLY  292      22.608   0.489  21.861  1.00 18.56      MTGL
ATOM   2286  CA  GLY  292      23.117  -0.559  22.730  1.00 17.86      MTGL
ATOM   2287  C   GLY  292      22.774  -0.538  24.205  1.00 18.08      MTGL
ATOM   2288  O   GLY  292      22.404   0.493  24.766  1.00 17.12      MTGL
ATOM   2289  N   LEU  293      22.913  -1.708  24.824  1.00 18.07      MTGL
ATOM   2290  CA  LEU  293      22.653  -1.902  26.246  1.00 18.28      MTGL
ATOM   2291  CB  LEU  293      21.223  -2.404  26.474  1.00 19.14      MTGL
ATOM   2292  CG  LEU  293      20.858  -2.808  27.910  1.00 22.33      MTGL
ATOM   2293  CD1 LEU  293      21.047  -1.625  28.842  1.00 23.17      MTGL
ATOM   2294  CD2 LEU  293      19.410  -3.278  27.965  1.00 23.54      MTGL
ATOM   2295  C   LEU  293      23.634  -2.952  26.744  1.00 17.77      MTGL
ATOM   2296  O   LEU  293      23.763  -4.009  26.130  1.00 17.95      MTGL
ATOM   2297  N   PHE  294      24.322  -2.658  27.847  1.00 16.70      MTGL
ATOM   2298  CA  PHE  294      25.288  -3.586  28.431  1.00 16.53      MTGL
ATOM   2299  CB  PHE  294      26.726  -3.097  28.229  1.00 16.07      MTGL
ATOM   2300  CG  PHE  294      27.199  -3.136  26.800  1.00 16.47      MTGL
ATOM   2301  CD1 PHE  294      26.792  -2.164  25.890  1.00 16.58      MTGL
ATOM   2302  CD2 PHE  294      28.069  -4.137  26.368  1.00 15.29      MTGL
ATOM   2303  CE1 PHE  294      27.241  -2.188  24.571  1.00 16.35      MTGL
ATOM   2304  CE2 PHE  294      28.523  -4.170  25.050  1.00 15.62      MTGL
ATOM   2305  CZ  PHE  294      28.110  -3.192  24.150  1.00 15.75      MTGL
ATOM   2306  C   PHE  294      25.046  -3.739  29.930  1.00 16.96      MTGL
ATOM   2307  O   PHE  294      25.032  -2.752  30.667  1.00 17.04      MTGL
ATOM   2308  N   TYR  295      24.855  -4.977  30.374  1.00 16.03      MTGL
ATOM   2309  CA  TYR  295      24.639  -5.253  31.789  1.00 15.26      MTGL
ATOM   2310  CB  TYR  295      23.905  -6.582  31.963  1.00 14.47      MTGL
ATOM   2311  CG  TYR  295      23.323  -6.755  33.344  1.00 14.21      MTGL
ATOM   2312  CD1 TYR  295      22.033  -6.312  33.637  1.00 12.09      MTGL
ATOM   2313  CE1 TYR  295      21.512  -6.421  34.918  1.00 13.83      MTGL
ATOM   2314  CD2 TYR  295      24.080  -7.316  34.372  1.00 13.69      MTGL
ATOM   2315  CE2 TYR  295      23.566  -7.431  35.662  1.00 13.74      MTGL
ATOM   2316  CZ  TYR  295      22.284  -6.979  35.930  1.00 14.39      MTGL
ATOM   2317  OH  TYR  295      21.784  -7.058  37.211  1.00 15.39      MTGL
ATOM   2318  C   TYR  295      26.033  -5.346  32.410  1.00 15.23      MTGL
ATOM   2319  O   TYR  295      26.932  -5.933  31.814  1.00 15.00      MTGL
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Fig. 1 cont.

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ATOM   2320  N   TRP   296      26.228  -4.778  33.594  1.00 14.56      MTGL
ATOM   2321  CA  TRP   296      27.559  -4.829  34.195  1.00 15.23      MTGL
ATOM   2322  CB  TRP   296      27.847  -3.541  34.984  1.00 14.28      MTGL
ATOM   2323  CG  TRP   296      29.306  -3.370  35.309  1.00 15.53      MTGL
ATOM   2324  CD2 TRP   296      29.918  -3.408  36.611  1.00 16.19      MTGL
ATOM   2325  CE2 TRP   296      31.309  -3.221  36.424  1.00 15.45      MTGL
ATOM   2326  CE3 TRP   296      29.428  -3.583  37.916  1.00 16.72      MTGL
ATOM   2327  CD1 TRP   296      30.321  -3.168  34.418  1.00 15.37      MTGL
ATOM   2328  NE1 TRP   296      31.526  -3.077  35.079  1.00 15.66      MTGL
ATOM   2329  CZ2 TRP   296      32.219  -3.201  37.495  1.00 15.21      MTGL
ATOM   2330  CZ3 TRP   296      30.334  -3.564  38.985  1.00 16.55      MTGL
ATOM   2331  CH2 TRP   296      31.715  -3.375  38.763  1.00 16.36      MTGL
ATOM   2332  C   TRP   296      27.842  -6.029  35.097  1.00 14.61      MTGL
ATOM   2333  O   TRP   296      27.174  -6.224  36.114  1.00 15.45      MTGL
ATOM   2334  N   GLU   297      28.835  -6.826  34.702  1.00 14.69      MTGL
ATOM   2335  CA  GLU   297      29.298  -7.977  35.479  1.00 14.59      MTGL
ATOM   2336  CB  GLU   297      30.125  -7.465  36.661  1.00 13.64      MTGL
ATOM   2337  CG  GLU   297      31.453  -6.849  36.261  1.00 14.27      MTGL
ATOM   2338  CD  GLU   297      32.506  -7.896  35.947  1.00 13.45      MTGL
ATOM   2339  OE1 GLU   297      32.176  -9.102  35.991  1.00 12.29      MTGL
ATOM   2340  OE2 GLU   297      33.661  -7.510  35.660  1.00 14.90      MTGL
ATOM   2341  C   GLU   297      28.245  -8.952  36.000  1.00 15.16      MTGL
ATOM   2342  O   GLU   297      28.177  -9.219  37.205  1.00 15.61      MTGL
ATOM   2343  N   PRO   298      27.436  -9.529  35.100  1.00 14.59      MTGL
ATOM   2344  CD  PRO   298      27.545  -9.487  33.631  1.00 12.84      MTGL
ATOM   2345  CA  PRO   298      26.395 -10.474  35.517  1.00 14.70      MTGL
ATOM   2346  CB  PRO   298      25.651 -10.750  34.217  1.00 13.52      MTGL
ATOM   2347  CG  PRO   298      26.765 -10.716  33.213  1.00 12.86      MTGL
ATOM   2348  C   PRO   298      26.897 -11.774  36.158  1.00 14.86      MTGL
ATOM   2349  O   PRO   298      26.159 -12.424  36.901  1.00 14.01      MTGL
ATOM   2350  N   ALA   299      28.143 -12.147  35.875  1.00 15.30      MTGL
ATOM   2351  CA  ALA   299      28.689 -13.397  36.396  1.00 16.12      MTGL
ATOM   2352  CB  ALA   299      29.321 -14.184  35.245  1.00 16.45      MTGL
ATOM   2353  C   ALA   299      29.684 -13.297  37.551  1.00 16.40      MTGL
ATOM   2354  O   ALA   299      30.281 -14.303  37.934  1.00 16.31      MTGL
ATOM   2355  N   TRP   300      29.861 -12.104  38.111  1.00 16.53      MTGL
ATOM   2356  CA  TRP   300      30.804 -11.911  39.218  1.00 16.99      MTGL
ATOM   2357  CB  TRP   300      31.205 -10.438  39.300  1.00 15.26      MTGL
ATOM   2358  CG  TRP   300      32.518 -10.195  39.960  1.00 16.30      MTGL
ATOM   2359  CD2 TRP   300      33.248  -8.960  39.982  1.00 14.96      MTGL
ATOM   2360  CE2 TRP   300      34.440  -9.195  40.697  1.00 14.93      MTGL
ATOM   2361  CE3 TRP   300      33.007  -7.679  39.463  1.00 15.40      MTGL
ATOM   2362  CD1 TRP   300      33.274 -11.099  40.648  1.00 14.90      MTGL
ATOM   2363  NE1 TRP   300      34.429 -10.508  41.092  1.00 16.48      MTGL
ATOM   2364  CZ2 TRP   300      35.398  -8.195  40.912  1.00 13.85      MTGL
ATOM   2365  CZ3 TRP   300      33.960  -6.678  39.678  1.00 13.88      MTGL
ATOM   2366  CH2 TRP   300      35.143  -6.949  40.398  1.00 15.26      MTGL
ATOM   2367  C   TRP   300      30.159 -12.347  40.536  1.00 17.14      MTGL
ATOM   2368  O   TRP   300      29.909 -11.522  41.423  1.00 16.66      MTGL
ATOM   2369  N   ILE   301      29.907 -13.645  40.670  1.00 17.69      MTGL
ATOM   2370  CA  ILE   301      29.255 -14.168  41.866  1.00 19.29      MTGL
ATOM   2371  CB  ILE   301      28.893 -15.655  41.695  1.00 20.95      MTGL
ATOM   2372  CG2 ILE   301      27.937 -15.812  40.517  1.00 19.88      MTGL
ATOM   2373  CG1 ILE   301      30.153 -16.496  41.479  1.00 22.04      MTGL
ATOM   2374  CD1 ILE   301      29.858 -17.985  41.366  1.00 23.83      MTGL
ATOM   2375  C   ILE   301      29.973 -13.980  43.205  1.00 19.82      MTGL
ATOM   2376  O   ILE   301      29.325 -14.022  44.249  1.00 19.53      MTGL
ATOM   2377  N   HIS   302      31.287 -13.768  43.189  1.00 19.79      MTGL
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Fig. 1 cont.

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ATOM   2378  CA  HIS   302      32.016 -13.555  44.441  1.00 21.73      MTGL
ATOM   2379  CB  HIS   302      33.464 -14.042  44.317  1.00 22.38      MTGL
ATOM   2380  CG  HIS   302      33.603 -15.529  44.396  1.00 24.09      MTGL
ATOM   2381  CD2 HIS   302      33.254 -16.405  45.368  1.00 25.41      MTGL
ATOM   2382  ND1 HIS   302      34.154 -16.282  43.382  1.00 25.82      MTGL
ATOM   2383  CE1 HIS   302      34.137 -17.558  43.724  1.00 26.05      MTGL
ATOM   2384  NE2 HIS   302      33.596 -17.659  44.924  1.00 26.28      MTGL
ATOM   2385  C   HIS   302      32.002 -12.085  44.857  1.00 21.31      MTGL
ATOM   2386  O   HIS   302      32.609 -11.707  45.854  1.00 22.67      MTGL
ATOM   2387  N   ASN   303      31.303 -11.265  44.079  1.00 20.90      MTGL
ATOM   2388  CA  ASN   303      31.183  -9.831  44.337  1.00 20.21      MTGL
ATOM   2389  CB  ASN   303      32.200  -9.074  43.473  1.00 20.27      MTGL
ATOM   2390  CG  ASN   303      32.170  -7.573  43.706  1.00 21.40      MTGL
ATOM   2391  OD1 ASN   303      31.977  -7.118  44.828  1.00 22.04      MTGL
ATOM   2392  ND2 ASN   303      32.380  -6.799  42.643  1.00 19.16      MTGL
ATOM   2393  C   ASN   303      29.752  -9.467  43.946  1.00 20.34      MTGL
ATOM   2394  O   ASN   303      29.508  -8.488  43.233  1.00 18.25      MTGL
ATOM   2395  N   ALA   304      28.820 -10.284  44.432  1.00 19.57      MTGL
ATOM   2396  CA  ALA   304      27.395 -10.180  44.134  1.00 19.48      MTGL
ATOM   2397  CB  ALA   304      26.612 -11.157  45.017  1.00 18.17      MTGL
ATOM   2398  C   ALA   304      26.731  -8.813  44.182  1.00 19.61      MTGL
ATOM   2399  O   ALA   304      25.909  -8.505  43.323  1.00 20.70      MTGL
ATOM   2400  N   ASN   305      27.050  -7.999  45.181  1.00 18.88      MTGL
ATOM   2401  CA  ASN   305      26.424  -6.685  45.271  1.00 19.31      MTGL
ATOM   2402  CB  ASN   305      26.580  -6.114  46.683  1.00 19.61      MTGL
ATOM   2403  CG  ASN   305      28.024  -5.847  47.048  1.00 20.60      MTGL
ATOM   2404  OD1 ASN   305      28.868  -6.747  47.014  1.00 21.53      MTGL
ATOM   2405  ND2 ASN   305      28.318  -4.606  47.403  1.00 21.29      MTGL
ATOM   2406  C   ASN   305      27.018  -5.723  44.240  1.00 19.61      MTGL
ATOM   2407  O   ASN   305      26.522  -4.611  44.041  1.00 19.33      MTGL
ATOM   2408  N   LEU   306      28.088  -6.160  43.587  1.00 18.26      MTGL
ATOM   2409  CA  LEU   306      28.747  -5.359  42.563  1.00 18.47      MTGL
ATOM   2410  CB  LEU   306      27.919  -5.384  41.270  1.00 17.67      MTGL
ATOM   2411  CG  LEU   306      27.771  -6.764  40.612  1.00 18.35      MTGL
ATOM   2412  CD1 LEU   306      26.888  -6.670  39.372  1.00 16.49      MTGL
ATOM   2413  CD2 LEU   306      29.144  -7.300  40.238  1.00 16.40      MTGL
ATOM   2414  C   LEU   306      28.994  -3.915  42.990  1.00 19.28      MTGL
ATOM   2415  O   LEU   306      28.698  -2.981  42.241  1.00 19.04      MTGL
ATOM   2416  N   GLY   307      29.529  -3.740  44.196  1.00 18.62      MTGL
ATOM   2417  CA  GLY   307      29.828  -2.414  44.700  1.00 18.44      MTGL
ATOM   2418  C   GLY   307      28.657  -1.530  45.092  1.00 18.36      MTGL
ATOM   2419  O   GLY   307      28.866  -0.379  45.466  1.00 18.04      MTGL
ATOM   2420  N   SER   308      27.435  -2.047  45.020  1.00 17.93      MTGL
ATOM   2421  CA  SER   308      26.256  -1.256  45.380  1.00 17.81      MTGL
ATOM   2422  CB  SER   308      25.134  -1.480  44.361  1.00 16.84      MTGL
ATOM   2423  OG  SER   308      24.555  -2.759  44.528  1.00 15.76      MTGL
ATOM   2424  C   SER   308      25.756  -1.651  46.762  1.00 18.10      MTGL
ATOM   2425  O   SER   308      26.282  -2.585  47.361  1.00 18.30      MTGL
ATOM   2426  N   SER   309      24.735  -0.947  47.250  1.00 18.76      MTGL
ATOM   2427  CA  SER   309      24.157  -1.220  48.560  1.00 20.76      MTGL
ATOM   2428  CB  SER   309      23.424   0.022  49.092  1.00 21.48      MTGL
ATOM   2429  OG  SER   309      22.304   0.358  48.283  1.00 22.88      MTGL
ATOM   2430  C   SER   309      23.193  -2.404  48.517  1.00 22.16      MTGL
ATOM   2431  O   SER   309      22.754  -2.899  49.560  1.00 23.34      MTGL
ATOM   2432  N   CYS   310      22.852  -2.846  47.312  1.00 22.36      MTGL
ATOM   2433  CA  CYS   310      21.954  -3.987  47.159  1.00 23.23      MTGL
ATOM   2434  C   CYS   310      22.784  -5.265  47.300  1.00 23.23      MTGL
ATOM   2435  O   CYS   310      23.935  -5.300  46.877  1.00 25.45      MTGL
```

Fig. 1 cont.

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ATOM   2436  CB  CYS   310      21.275  -3.945  45.793  1.00 23.30      MTGL
ATOM   2437  SG  CYS   310      19.871  -2.792  45.648  1.00 24.32      MTGL
ATOM   2438  N   ALA   311      22.197  -6.309  47.877  1.00 21.14      MTGL
ATOM   2439  CA  ALA   311      22.903  -7.564  48.110  1.00 20.13      MTGL
ATOM   2440  CB  ALA   311      22.076  -8.449  49.052  1.00 20.15      MTGL
ATOM   2441  C   ALA   311      23.335  -8.383  46.894  1.00 19.87      MTGL
ATOM   2442  O   ALA   311      24.442  -8.915  46.875  1.00 18.96      MTGL
ATOM   2443  N   ASP   312      22.482  -8.502  45.882  1.00 18.99      MTGL
ATOM   2444  CA  ASP   312      22.849  -9.313  44.723  1.00 19.21      MTGL
ATOM   2445  CB  ASP   312      22.346 -10.747  44.931  1.00 19.01      MTGL
ATOM   2446  CG  ASP   312      22.949 -11.733  43.946  1.00 19.92      MTGL
ATOM   2447  OD1 ASP   312      23.450 -11.305  42.884  1.00 19.68      MTGL
ATOM   2448  OD2 ASP   312      22.908 -12.948  44.230  1.00 20.69      MTGL
ATOM   2449  C   ASP   312      22.310  -8.772  43.403  1.00 18.27      MTGL
ATOM   2450  O   ASP   312      21.098  -8.692  43.205  1.00 18.94      MTGL
ATOM   2451  N   ASN   313      23.222  -8.418  42.500  1.00 17.28      MTGL
ATOM   2452  CA  ASN   313      22.855  -7.892  41.187  1.00 17.18      MTGL
ATOM   2453  CB  ASN   313      23.478  -6.507  40.962  1.00 16.90      MTGL
ATOM   2454  CG  ASN   313      22.860  -5.440  41.835  1.00 17.53      MTGL
ATOM   2455  OD1 ASN   313      21.636  -5.293  41.879  1.00 20.07      MTGL
ATOM   2456  ND2 ASN   313      23.704  -4.677  42.529  1.00 16.34      MTGL
ATOM   2457  C   ASN   313      23.305  -8.809  40.053  1.00 17.15      MTGL
ATOM   2458  O   ASN   313      23.190  -8.452  38.881  1.00 17.24      MTGL
ATOM   2459  N   THR   314      23.826  -9.982  40.391  1.00 15.74      MTGL
ATOM   2460  CA  THR   314      24.289 -10.903  39.365  1.00 15.54      MTGL
ATOM   2461  CB  THR   314      25.226 -11.977  39.953  1.00 15.83      MTGL
ATOM   2462  OG1 THR   314      24.502 -12.779  40.894  1.00 16.12      MTGL
ATOM   2463  CG2 THR   314      26.418 -11.322  40.651  1.00 14.76      MTGL
ATOM   2464  C   THR   314      23.130 -11.604  38.657  1.00 16.42      MTGL
ATOM   2465  O   THR   314      21.972 -11.525  39.087  1.00 15.23      MTGL
ATOM   2466  N   MET   315      23.453 -12.273  37.555  1.00 16.30      MTGL
ATOM   2467  CA  MET   315      22.458 -13.006  36.776  1.00 17.57      MTGL
ATOM   2468  CB  MET   315      22.390 -12.447  35.350  1.00 16.92      MTGL
ATOM   2469  CG  MET   315      21.934 -10.997  35.281  1.00 16.10      MTGL
ATOM   2470  SD  MET   315      21.871 -10.343  33.592  1.00 18.97      MTGL
ATOM   2471  CE  MET   315      20.232 -10.916  33.083  1.00 14.39      MTGL
ATOM   2472  C   MET   315      22.820 -14.492  36.753  1.00 17.49      MTGL
ATOM   2473  O   MET   315      22.404 -15.234  35.871  1.00 17.40      MTGL
ATOM   2474  N   PHE   316      23.614 -14.905  37.736  1.00 17.70      MTGL
ATOM   2475  CA  PHE   316      24.050 -16.291  37.879  1.00 18.51      MTGL
ATOM   2476  CB  PHE   316      25.521 -16.451  37.482  1.00 16.98      MTGL
ATOM   2477  CG  PHE   316      25.760 -16.485  35.995  1.00 17.56      MTGL
ATOM   2478  CD1 PHE   316      25.616 -15.337  35.220  1.00 17.13      MTGL
ATOM   2479  CD2 PHE   316      26.124 -17.671  35.370  1.00 16.95      MTGL
ATOM   2480  CE1 PHE   316      25.845 -15.370  33.845  1.00 17.76      MTGL
ATOM   2481  CE2 PHE   316      26.355 -17.717  33.993  1.00 17.39      MTGL
ATOM   2482  CZ  PHE   316      26.212 -16.566  33.227  1.00 16.28      MTGL
ATOM   2483  C   PHE   316      23.891 -16.679  39.344  1.00 19.70      MTGL
ATOM   2484  O   PHE   316      23.980 -15.825  40.229  1.00 19.34      MTGL
ATOM   2485  N   SER   317      23.659 -17.963  39.598  1.00 19.30      MTGL
ATOM   2486  CA  SER   317      23.495 -18.444  40.963  1.00 20.50      MTGL
ATOM   2487  CB  SER   317      22.894 -19.853  40.972  1.00 19.80      MTGL
ATOM   2488  OG  SER   317      23.832 -20.798  40.484  1.00 18.89      MTGL
ATOM   2489  C   SER   317      24.860 -18.479  41.633  1.00 20.89      MTGL
ATOM   2490  O   SER   317      25.895 -18.352  40.973  1.00 19.59      MTGL
ATOM   2491  N   GLN   318      24.857 -18.659  42.946  1.00 21.68      MTGL
ATOM   2492  CA  GLN   318      26.104 -18.711  43.685  1.00 22.69      MTGL
ATOM   2493  CB  GLN   318      25.813 -18.649  45.186  1.00 23.06      MTGL
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Fig. 1 cont.

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ATOM   2494  CG  GLN   318      25.363 -17.254  45.625  1.00 24.34      MTGL
ATOM   2495  CD  GLN   318      26.459 -16.209  45.445  1.00 25.12      MTGL
ATOM   2496  OE1 GLN   318      27.473 -16.241  46.142  1.00 27.51      MTGL
ATOM   2497  NE2 GLN   318      26.266 -15.287  44.503  1.00 23.16      MTGL
ATOM   2498  C   GLN   318      26.920 -19.947  43.315  1.00 22.71      MTGL
ATOM   2499  O   GLN   318      28.095 -20.052  43.662  1.00 24.10      MTGL
ATOM   2500  N   SER   319      26.307 -20.875  42.588  1.00 22.97      MTGL
ATOM   2501  CA  SER   319      27.022 -22.074  42.160  1.00 23.61      MTGL
ATOM   2502  CB  SER   319      26.112 -23.306  42.235  1.00 24.83      MTGL
ATOM   2503  OG  SER   319      24.914 -23.111  41.500  1.00 28.30      MTGL
ATOM   2504  C   SER   319      27.553 -21.900  40.737  1.00 23.21      MTGL
ATOM   2505  O   SER   319      28.158 -22.814  40.180  1.00 23.75      MTGL
ATOM   2506  N   GLY   320      27.315 -20.726  40.153  1.00 22.56      MTGL
ATOM   2507  CA  GLY   320      27.798 -20.439  38.811  1.00 22.10      MTGL
ATOM   2508  C   GLY   320      26.851 -20.771  37.670  1.00 22.30      MTGL
ATOM   2509  O   GLY   320      27.262 -20.809  36.504  1.00 22.30      MTGL
ATOM   2510  N   GLN   321      25.582 -21.009  37.984  1.00 21.21      MTGL
ATOM   2511  CA  GLN   321      24.618 -21.337  36.941  1.00 21.36      MTGL
ATOM   2512  CB  GLN   321      23.652 -22.415  37.426  1.00 23.27      MTGL
ATOM   2513  CG  GLN   321      22.649 -22.855  36.371  1.00 24.43      MTGL
ATOM   2514  CD  GLN   321      21.803 -24.021  36.833  1.00 26.48      MTGL
ATOM   2515  OE1 GLN   321      22.320 -25.009  37.347  1.00 27.39      MTGL
ATOM   2516  NE2 GLN   321      20.497 -23.920  36.641  1.00 27.02      MTGL
ATOM   2517  C   GLN   321      23.826 -20.121  36.483  1.00 20.04      MTGL
ATOM   2518  O   GLN   321      23.289 -19.371  37.291  1.00 19.56      MTGL
ATOM   2519  N   ALA   322      23.755 -19.939  35.172  1.00 20.60      MTGL
ATOM   2520  CA  ALA   322      23.028 -18.817  34.596  1.00 20.07      MTGL
ATOM   2521  CB  ALA   322      23.129 -18.864  33.079  1.00 18.41      MTGL
ATOM   2522  C   ALA   322      21.565 -18.855  35.017  1.00 20.05      MTGL
ATOM   2523  O   ALA   322      20.921 -19.901  34.945  1.00 19.07      MTGL
ATOM   2524  N   LEU   323      21.052 -17.713  35.464  0.50 19.28      MTGL
ATOM   2525  CA  LEU   323      19.658 -17.611  35.878  0.50 19.33      MTGL
ATOM   2526  CB  LEU   323      19.470 -16.426  36.830  0.50 18.12      MTGL
ATOM   2527  CG  LEU   323      20.241 -16.493  38.152  0.50 17.16      MTGL
ATOM   2528  CD1 LEU   323      19.944 -15.244  38.979  0.50 16.83      MTGL
ATOM   2529  CD2 LEU   323      19.844 -17.758  38.920  0.50 16.13      MTGL
ATOM   2530  C   LEU   323      18.779 -17.431  34.645  0.50 19.86      MTGL
ATOM   2531  O   LEU   323      19.270 -17.113  33.561  0.50 19.75      MTGL
ATOM   2532  N   SER   324      17.477 -17.630  34.817  1.00 21.01      MTGL
ATOM   2533  CA  SER   324      16.524 -17.511  33.719  1.00 21.34      MTGL
ATOM   2534  CB  SER   324      15.114 -17.827  34.220  1.00 21.65      MTGL
ATOM   2535  OG  SER   324      14.713 -16.887  35.202  1.00 22.41      MTGL
ATOM   2536  C   SER   324      16.529 -16.130  33.075  1.00 21.33      MTGL
ATOM   2537  O   SER   324      16.159 -15.980  31.913  1.00 20.59      MTGL
ATOM   2538  N   SER   325      16.955 -15.123  33.830  1.00 20.04      MTGL
ATOM   2539  CA  SER   325      16.984 -13.759  33.321  1.00 20.07      MTGL
ATOM   2540  CB  SER   325      17.227 -12.780  34.476  1.00 19.69      MTGL
ATOM   2541  OG  SER   325      18.417 -13.106  35.172  1.00 17.73      MTGL
ATOM   2542  C   SER   325      18.012 -13.515  32.213  1.00 20.16      MTGL
ATOM   2543  O   SER   325      17.892 -12.549  31.460  1.00 19.87      MTGL
ATOM   2544  N   LEU   326      19.010 -14.388  32.104  1.00 19.54      MTGL
ATOM   2545  CA  LEU   326      20.048 -14.230  31.085  1.00 19.73      MTGL
ATOM   2546  CB  LEU   326      21.126 -15.314  31.236  1.00 20.49      MTGL
ATOM   2547  CG  LEU   326      22.606 -14.910  31.307  1.00 22.10      MTGL
ATOM   2548  CD1 LEU   326      23.433 -15.966  30.587  1.00 21.95      MTGL
ATOM   2549  CD2 LEU   326      22.848 -13.551  30.678  1.00 22.81      MTGL
ATOM   2550  C   LEU   326      19.519 -14.274  29.646  1.00 19.72      MTGL
ATOM   2551  O   LEU   326      20.094 -13.655  28.754  1.00 19.08      MTGL
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Fig. 1 cont.

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ATOM   2552  N   SER   327      18.439 -15.015  29.412  1.00 18.98      MTGL
ATOM   2553  CA  SER   327      17.875 -15.133  28.067  1.00 18.71      MTGL
ATOM   2554  CB  SER   327      16.861 -16.271  28.023  1.00 17.52      MTGL
ATOM   2555  OG  SER   327      15.740 -15.947  28.825  1.00 16.77      MTGL
ATOM   2556  C   SER   327      17.191 -13.851  27.585  1.00 18.81      MTGL
ATOM   2557  O   SER   327      16.698 -13.795  26.459  1.00 18.63      MTGL
ATOM   2558  N   VAL   328      17.140 -12.836  28.440  1.00 18.22      MTGL
ATOM   2559  CA  VAL   328      16.517 -11.573  28.066  1.00 18.51      MTGL
ATOM   2560  CB  VAL   328      16.590 -10.545  29.223  1.00 19.11      MTGL
ATOM   2561  CG1 VAL   328      18.046 -10.177  29.509  1.00 17.14      MTGL
ATOM   2562  CG2 VAL   328      15.777  -9.304  28.868  1.00 19.04      MTGL
ATOM   2563  C   VAL   328      17.210 -10.983  26.839  1.00 19.25      MTGL
ATOM   2564  O   VAL   328      16.589 -10.285  26.039  1.00 18.81      MTGL
ATOM   2565  N   PHE   329      18.498 -11.273  26.685  1.00 20.22      MTGL
ATOM   2566  CA  PHE   329      19.258 -10.752  25.550  1.00 22.10      MTGL
ATOM   2567  CB  PHE   329      20.752 -10.989  25.774  1.00 21.20      MTGL
ATOM   2568  CG  PHE   329      21.307 -10.211  26.929  1.00 21.71      MTGL
ATOM   2569  CD1 PHE   329      21.525  -8.842  26.814  1.00 21.66      MTGL
ATOM   2570  CD2 PHE   329      21.551 -10.831  28.151  1.00 20.67      MTGL
ATOM   2571  CE1 PHE   329      21.979  -8.099  27.901  1.00 22.16      MTGL
ATOM   2572  CE2 PHE   329      22.003 -10.098  29.240  1.00 22.03      MTGL
ATOM   2573  CZ  PHE   329      22.215  -8.728  29.114  1.00 22.57      MTGL
ATOM   2574  C   PHE   329      18.815 -11.340  24.212  1.00 23.27      MTGL
ATOM   2575  O   PHE   329      19.267 -10.904  23.152  1.00 23.56      MTGL
ATOM   2576  N   GLN   330      17.927 -12.326  24.267  1.00 23.16      MTGL
ATOM   2577  CA  GLN   330      17.402 -12.950  23.058  1.00 24.83      MTGL
ATOM   2578  CB  GLN   330      16.994 -14.403  23.333  1.00 25.48      MTGL
ATOM   2579  CG  GLN   330      18.138 -15.371  23.573  1.00 25.89      MTGL
ATOM   2580  CD  GLN   330      17.648 -16.773  23.894  1.00 27.09      MTGL
ATOM   2581  OE1 GLN   330      18.390 -17.748  23.750  1.00 29.08      MTGL
ATOM   2582  NE2 GLN   330      16.400 -16.882  24.343  1.00 24.64      MTGL
ATOM   2583  C   GLN   330      16.157 -12.198  22.596  1.00 25.46      MTGL
ATOM   2584  O   GLN   330      15.651 -12.439  21.502  1.00 25.45      MTGL
ATOM   2585  N   ARG   331      15.669 -11.282  23.426  1.00 25.05      MTGL
ATOM   2586  CA  ARG   331      14.443 -10.573  23.094  1.00 25.37      MTGL
ATOM   2587  CB  ARG   331      13.356 -10.991  24.087  1.00 24.60      MTGL
ATOM   2588  CG  ARG   331      13.223 -12.507  24.246  1.00 25.96      MTGL
ATOM   2589  CD  ARG   331      12.110 -12.882  25.220  1.00 26.44      MTGL
ATOM   2590  NE  ARG   331      12.400 -12.493  26.600  1.00 27.25      MTGL
ATOM   2591  CZ  ARG   331      13.123 -13.218  27.451  1.00 27.98      MTGL
ATOM   2592  NH1 ARG   331      13.637 -14.383  27.073  1.00 26.83      MTGL
ATOM   2593  NH2 ARG   331      13.329 -12.777  28.683  1.00 26.92      MTGL
ATOM   2594  C   ARG   331      14.506  -9.049  23.017  1.00 25.38      MTGL
ATOM   2595  O   ARG   331      13.468  -8.391  23.085  1.00 25.25      MTGL
ATOM   2596  N   ILE   332      15.703  -8.487  22.863  1.00 25.52      MTGL
ATOM   2597  CA  ILE   332      15.847  -7.035  22.779  1.00 26.69      MTGL
ATOM   2598  CB  ILE   332      16.510  -6.459  24.049  1.00 26.08      MTGL
ATOM   2599  CG2 ILE   332      15.646  -6.765  25.269  1.00 25.81      MTGL
ATOM   2600  CG1 ILE   332      17.912  -7.047  24.224  1.00 25.06      MTGL
ATOM   2601  CD1 ILE   332      18.663  -6.506  25.425  1.00 23.51      MTGL
ATOM   2602  C   ILE   332      16.664  -6.599  21.567  1.00 27.88      MTGL
ATOM   2603  O   ILE   332      17.171  -7.485  20.855  1.00 28.65      MTGL
ATOM   2604  OXT ILE   332      16.787  -5.372  21.344  1.00 30.38      MTGL
END
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Fig. 1 cont.

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HEADER                                                          HIGL
ATOM      1  CB   ALA     1       6.247  74.348 114.849  1.00 27.43      HIGL
ATOM      2  C    ALA     1       7.283  72.458 113.617  1.00 26.21      HIGL
ATOM      3  O    ALA     1       6.683  72.007 112.638  1.00 26.69      HIGL
ATOM      4  N    ALA     1       7.237  74.771 112.633  1.00 26.59      HIGL
ATOM      5  CA   ALA     1       7.343  73.961 113.883  1.00 26.86      HIGL
ATOM      6  N    LEU     2       7.883  71.693 114.524  1.00 24.15      HIGL
ATOM      7  CA   LEU     2       7.971  70.244 114.405  1.00 22.16      HIGL
ATOM      8  CB   LEU     2       8.883  69.700 115.498  1.00 21.06      HIGL
ATOM      9  CG   LEU     2      10.274  70.334 115.565  1.00 20.32      HIGL
ATOM     10  CD1  LEU     2      10.966  69.921 116.848  1.00 19.78      HIGL
ATOM     11  CD2  LEU     2      11.076  69.921 114.346  1.00 20.05      HIGL
ATOM     12  C    LEU     2       6.663  69.471 114.429  1.00 22.53      HIGL
ATOM     13  O    LEU     2       5.748  69.767 115.202  1.00 23.10      HIGL
ATOM     14  N    GLN     3       6.597  68.456 113.576  1.00 21.51      HIGL
ATOM     15  CA   GLN     3       5.430  67.601 113.493  1.00 20.06      HIGL
ATOM     16  CB   GLN     3       5.435  66.837 112.175  1.00 18.80      HIGL
ATOM     17  CG   GLN     3       4.157  66.084 111.909  1.00 19.14      HIGL
ATOM     18  CD   GLN     3       4.246  65.213 110.680  1.00 19.73      HIGL
ATOM     19  OE1  GLN     3       4.884  65.577 109.689  1.00 21.27      HIGL
ATOM     20  NE2  GLN     3       3.594  64.062 110.728  1.00 18.71      HIGL
ATOM     21  C    GLN     3       5.504  66.609 114.644  1.00 19.78      HIGL
ATOM     22  O    GLN     3       4.513  66.342 115.324  1.00 20.14      HIGL
ATOM     23  N    TYR     4       6.696  66.060 114.849  1.00 19.50      HIGL
ATOM     24  CA   TYR     4       6.920  65.083 115.902  1.00 19.32      HIGL
ATOM     25  CB   TYR     4       7.614  63.849 115.328  1.00 18.96      HIGL
ATOM     26  CG   TYR     4       6.913  63.222 114.145  1.00 19.19      HIGL
ATOM     27  CD1  TYR     4       5.639  62.669 114.271  1.00 19.50      HIGL
ATOM     28  CE1  TYR     4       5.019  62.033 113.199  1.00 18.39      HIGL
ATOM     29  CD2  TYR     4       7.546  63.131 112.909  1.00 19.30      HIGL
ATOM     30  CE2  TYR     4       6.935  62.497 111.831  1.00 19.42      HIGL
ATOM     31  CZ   TYR     4       5.672  61.947 111.984  1.00 19.38      HIGL
ATOM     32  OH   TYR     4       5.083  61.288 110.922  1.00 18.91      HIGL
ATOM     33  C    TYR     4       7.790  65.686 117.000  1.00 19.57      HIGL
ATOM     34  O    TYR     4       8.954  66.022 116.776  1.00 19.37      HIGL
ATOM     35  N    LYS     5       7.220  65.845 118.185  1.00 19.13      HIGL
ATOM     36  CA   LYS     5       7.980  66.388 119.293  1.00 19.83      HIGL
ATOM     37  CB   LYS     5       7.666  67.874 119.495  1.00 21.28      HIGL
ATOM     38  CG   LYS     5       6.198  68.219 119.599  1.00 23.14      HIGL
ATOM     39  CD   LYS     5       6.031  69.730 119.695  1.00 25.10      HIGL
ATOM     40  CE   LYS     5       4.563  70.143 119.714  1.00 25.68      HIGL
ATOM     41  NZ   LYS     5       4.438  71.621 119.884  1.00 27.35      HIGL
ATOM     42  C    LYS     5       7.661  65.589 120.539  1.00 19.09      HIGL
ATOM     43  O    LYS     5       6.537  65.616 121.043  1.00 20.34      HIGL
ATOM     44  N    GLY     6       8.653  64.858 121.027  1.00 17.54      HIGL
ATOM     45  CA   GLY     6       8.428  64.050 122.203  1.00 16.41      HIGL
ATOM     46  C    GLY     6       9.685  63.574 122.897  1.00 15.75      HIGL
ATOM     47  O    GLY     6      10.779  64.112 122.698  1.00 15.49      HIGL
ATOM     48  N    VAL     7       9.518  62.548 123.721  1.00 14.73      HIGL
ATOM     49  CA   VAL     7      10.623  61.996 124.470  1.00 14.42      HIGL
ATOM     50  CB   VAL     7      10.518  62.373 125.963  1.00 15.12      HIGL
ATOM     51  CG1  VAL     7      10.337  63.879 126.121  1.00 15.55      HIGL
ATOM     52  CG2  VAL     7       9.361  61.620 126.605  1.00 14.47      HIGL
ATOM     53  C    VAL     7      10.629  60.481 124.392  1.00 13.95      HIGL
ATOM     54  O    VAL     7       9.650  59.863 123.979  1.00 13.25      HIGL
ATOM     55  N    ASP     8      11.753  59.895 124.784  1.00 13.51      HIGL
ATOM     56  CA   ASP     8      11.863  58.452 124.844  1.00 13.71      HIGL
ATOM     57  CB   ASP     8      13.263  57.981 124.473  1.00 13.57      HIGL
ATOM     58  CG   ASP     8      13.354  56.480 124.393  1.00 13.68      HIGL
ATOM     59  OD1  ASP     8      12.912  55.814 125.353  1.00 13.24      HIGL
ATOM     60  OD2  ASP     8      13.861  55.967 123.373  1.00 14.72      HIGL
ATOM     61  C    ASP     8      11.626  58.233 126.324  1.00 13.84      HIGL
ATOM     62  O    ASP     8      12.391  58.735 127.156  1.00 13.94      HIGL
ATOM     63  N    TRP     9      10.562  57.510 126.658  1.00 13.89      HIGL
ATOM     64  CA   TRP     9      10.207  57.280 128.059  1.00 13.87      HIGL
```

Fig. 2

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ATOM     65  CB  TRP     9       8.822  57.889 128.324  1.00 11.91      HIGL
ATOM     66  CG  TRP     9       7.684  57.044 127.823  1.00 12.26      HIGL
ATOM     67  CD2 TRP     9       6.406  56.867 128.448  1.00 12.11      HIGL
ATOM     68  CE2 TRP     9       5.670  55.963 127.647  1.00 12.19      HIGL
ATOM     69  CE3 TRP     9       5.809  57.383 129.609  1.00 11.70      HIGL
ATOM     70  CD1 TRP     9       7.668  56.268 126.696  1.00 11.92      HIGL
ATOM     71  NE1 TRP     9       6.466  55.614 126.586  1.00 11.76      HIGL
ATOM     72  CZ2 TRP     9       4.365  55.562 127.968  1.00 11.52      HIGL
ATOM     73  CZ3 TRP     9       4.510  56.986 129.930  1.00 11.57      HIGL
ATOM     74  CH2 TRP     9       3.804  56.085 129.111  1.00 11.64      HIGL
ATOM     75  C   TRP     9      10.212  55.798 128.440  1.00 14.10      HIGL
ATOM     76  O   TRP     9       9.551  55.392 129.392  1.00 15.49      HIGL
ATOM     77  N   SER    10      10.984  55.002 127.713  1.00 14.17      HIGL
ATOM     78  CA  SER    10      11.051  53.561 127.939  1.00 14.00      HIGL
ATOM     79  CB  SER    10      12.154  52.958 127.056  1.00 14.22      HIGL
ATOM     80  OG  SER    10      11.946  53.282 125.685  1.00 12.67      HIGL
ATOM     81  C   SER    10      11.232  53.095 129.385  1.00 13.46      HIGL
ATOM     82  O   SER    10      10.652  52.096 129.794  1.00 13.12      HIGL
ATOM     83  N   SER    11      12.021  53.821 130.162  1.00 13.49      HIGL
ATOM     84  CA  SER    11      12.281  53.437 131.542  1.00 13.65      HIGL
ATOM     85  CB  SER    11      13.490  54.200 132.051  1.00 12.96      HIGL
ATOM     86  OG  SER    11      13.175  55.576 132.142  1.00 11.73      HIGL
ATOM     87  C   SER    11      11.134  53.664 132.524  1.00 15.06      HIGL
ATOM     88  O   SER    11      11.192  53.198 133.667  1.00 15.59      HIGL
ATOM     89  N   VAL    12      10.090  54.357 132.089  1.00 15.52      HIGL
ATOM     90  CA  VAL    12       8.987  54.682 132.983  1.00 16.34      HIGL
ATOM     91  CB  VAL    12       7.793  55.248 132.197  1.00 16.01      HIGL
ATOM     92  CG1 VAL    12       7.264  54.205 131.248  1.00 16.29      HIGL
ATOM     93  CG2 VAL    12       6.714  55.720 133.159  1.00 15.28      HIGL
ATOM     94  C   VAL    12       8.485  53.594 133.945  1.00 17.29      HIGL
ATOM     95  O   VAL    12       8.361  53.855 135.143  1.00 18.04      HIGL
ATOM     96  N   MET    13       8.197  52.390 133.457  1.00 17.84      HIGL
ATOM     97  CA  MET    13       7.695  51.346 134.355  1.00 17.96      HIGL
ATOM     98  CB  MET    13       7.044  50.203 133.568  1.00 17.95      HIGL
ATOM     99  CG  MET    13       5.703  50.579 132.968  1.00 19.53      HIGL
ATOM    100  SD  MET    13       4.678  49.147 132.593  1.00 23.13      HIGL
ATOM    101  CE  MET    13       5.559  48.452 131.185  1.00 23.08      HIGL
ATOM    102  C   MET    13       8.756  50.788 135.290  1.00 17.76      HIGL
ATOM    103  O   MET    13       8.456  50.415 136.420  1.00 17.26      HIGL
ATOM    104  N   VAL    14       9.994  50.723 134.817  1.00 17.91      HIGL
ATOM    105  CA  VAL    14      11.082  50.225 135.640  1.00 17.21      HIGL
ATOM    106  CB  VAL    14      12.413  50.169 134.845  1.00 16.85      HIGL
ATOM    107  CG1 VAL    14      13.559  49.837 135.761  1.00 13.37      HIGL
ATOM    108  CG2 VAL    14      12.311  49.128 133.741  1.00 15.66      HIGL
ATOM    109  C   VAL    14      11.212  51.187 136.809  1.00 17.76      HIGL
ATOM    110  O   VAL    14      11.455  50.774 137.945  1.00 18.17      HIGL
ATOM    111  N   GLU    15      11.031  52.473 136.533  1.00 18.10      HIGL
ATOM    112  CA  GLU    15      11.120  53.476 137.586  1.00 19.10      HIGL
ATOM    113  CB  GLU    15      11.207  54.881 136.991  1.00 19.32      HIGL
ATOM    114  CG  GLU    15      12.554  55.178 136.365  1.00 20.08      HIGL
ATOM    115  CD  GLU    15      13.676  55.158 137.383  1.00 21.57      HIGL
ATOM    116  OE1 GLU    15      13.838  54.131 138.076  1.00 22.32      HIGL
ATOM    117  OE2 GLU    15      14.398  56.171 137.492  1.00 22.71      HIGL
ATOM    118  C   GLU    15       9.937  53.387 138.539  1.00 19.39      HIGL
ATOM    119  O   GLU    15      10.107  53.492 139.757  1.00 19.72      HIGL
ATOM    120  N   GLU    16       8.740  53.196 137.992  1.00 19.13      HIGL
ATOM    121  CA  GLU    16       7.562  53.084 138.839  1.00 19.39      HIGL
ATOM    122  CB  GLU    16       6.289  52.932 137.996  1.00 18.72      HIGL
ATOM    123  CG  GLU    16       5.945  54.180 137.193  1.00 19.94      HIGL
ATOM    124  CD  GLU    16       4.840  53.959 136.159  1.00 21.79      HIGL
ATOM    125  OE1 GLU    16       4.817  52.881 135.521  1.00 22.23      HIGL
ATOM    126  OE2 GLU    16       4.003  54.874 135.966  1.00 21.65      HIGL
ATOM    127  C   GLU    16       7.759  51.885 139.761  1.00 19.47      HIGL
ATOM    128  O   GLU    16       7.547  51.989 140.969  1.00 19.63      HIGL
ATOM    129  N   ARG    17       8.190  50.756 139.202  1.00 19.74      HIGL
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Fig. 2 cont.

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ATOM    130  CA  ARG    17       8.416  49.562 140.014  1.00 20.25       HIGL
ATOM    131  CB  ARG    17       8.911  48.392 139.164  1.00 21.03       HIGL
ATOM    132  CG  ARG    17       7.873  47.765 138.257  1.00 23.68       HIGL
ATOM    133  CD  ARG    17       8.178  46.286 138.053  1.00 27.08       HIGL
ATOM    134  NE  ARG    17       7.410  45.701 136.956  1.00 31.03       HIGL
ATOM    135  CZ  ARG    17       7.660  45.919 135.664  1.00 32.87       HIGL
ATOM    136  NH1 ARG    17       8.666  46.709 135.299  1.00 32.97       HIGL
ATOM    137  NH2 ARG    17       6.902  45.352 134.731  1.00 33.75       HIGL
ATOM    138  C   ARG    17       9.445  49.840 141.104  1.00 19.92       HIGL
ATOM    139  O   ARG    17       9.443  49.198 142.151  1.00 20.42       HIGL
ATOM    140  N   ALA    18      10.325  50.801 140.850  1.00 19.29       HIGL
ATOM    141  CA  ALA    18      11.357  51.153 141.811  1.00 17.90       HIGL
ATOM    142  CB  ALA    18      12.584  51.698 141.086  1.00 17.12       HIGL
ATOM    143  C   ALA    18      10.846  52.168 142.830  1.00 17.59       HIGL
ATOM    144  O   ALA    18      11.611  52.653 143.669  1.00 16.93       HIGL
ATOM    145  N   GLY    19       9.557  52.494 142.745  1.00 16.98       HIGL
ATOM    146  CA  GLY    19       8.963  53.424 143.687  1.00 16.15       HIGL
ATOM    147  C   GLY    19       8.935  54.890 143.298  1.00 16.93       HIGL
ATOM    148  O   GLY    19       8.543  55.734 144.104  1.00 17.33       HIGL
ATOM    149  N   VAL    20       9.333  55.209 142.072  1.00 17.17       HIGL
ATOM    150  CA  VAL    20       9.336  56.598 141.626  1.00 17.58       HIGL
ATOM    151  CB  VAL    20      10.148  56.764 140.330  1.00 17.22       HIGL
ATOM    152  CG1 VAL    20      10.013  58.190 139.814  1.00 16.00       HIGL
ATOM    153  CG2 VAL    20      11.609  56.419 140.584  1.00 17.68       HIGL
ATOM    154  C   VAL    20       7.945  57.167 141.370  1.00 17.79       HIGL
ATOM    155  O   VAL    20       7.084  56.490 140.826  1.00 18.75       HIGL
ATOM    156  N   ARG    21       7.740  58.420 141.760  1.00 17.99       HIGL
ATOM    157  CA  ARG    21       6.470  59.106 141.537  1.00 18.92       HIGL
ATOM    158  CB  ARG    21       5.775  59.399 142.862  1.00 19.66       HIGL
ATOM    159  CG  ARG    21       5.367  58.155 143.617  1.00 20.84       HIGL
ATOM    160  CD  ARG    21       4.245  57.425 142.917  1.00 21.60       HIGL
ATOM    161  NE  ARG    21       3.389  56.783 143.906  1.00 23.75       HIGL
ATOM    162  CZ  ARG    21       3.734  55.707 144.598  1.00 23.89       HIGL
ATOM    163  NH1 ARG    21       4.920  55.148 144.389  1.00 25.67       HIGL
ATOM    164  NH2 ARG    21       2.911  55.215 145.516  1.00 22.10       HIGL
ATOM    165  C   ARG    21       6.749  60.412 140.809  1.00 18.45       HIGL
ATOM    166  O   ARG    21       7.598  61.198 141.231  1.00 18.88       HIGL
ATOM    167  N   TYR    22       6.032  60.640 139.717  1.00 17.66       HIGL
ATOM    168  CA  TYR    22       6.221  61.846 138.920  1.00 16.70       HIGL
ATOM    169  CB  TYR    22       6.236  61.480 137.438  1.00 15.81       HIGL
ATOM    170  CG  TYR    22       7.402  60.608 137.038  1.00 16.16       HIGL
ATOM    171  CD1 TYR    22       8.706  61.124 136.998  1.00 14.69       HIGL
ATOM    172  CE1 TYR    22       9.790  60.322 136.647  1.00 14.60       HIGL
ATOM    173  CD2 TYR    22       7.211  59.260 136.715  1.00 15.58       HIGL
ATOM    174  CE2 TYR    22       8.294  58.442 136.361  1.00 16.20       HIGL
ATOM    175  CZ  TYR    22       9.582  58.980 136.330  1.00 15.43       HIGL
ATOM    176  OH  TYR    22      10.648  58.178 135.994  1.00 12.55       HIGL
ATOM    177  C   TYR    22       5.156  62.903 139.166  1.00 17.06       HIGL
ATOM    178  O   TYR    22       4.008  62.591 139.482  1.00 17.73       HIGL
ATOM    179  N   LYS    23       5.545  64.160 139.011  1.00 17.11       HIGL
ATOM    180  CA  LYS    23       4.631  65.279 139.191  1.00 17.49       HIGL
ATOM    181  CB  LYS    23       4.813  65.913 140.575  1.00 18.19       HIGL
ATOM    182  CG  LYS    23       4.800  64.938 141.748  1.00 19.57       HIGL
ATOM    183  CD  LYS    23       6.141  64.239 141.933  1.00 18.82       HIGL
ATOM    184  CE  LYS    23       6.061  63.255 143.085  1.00 18.77       HIGL
ATOM    185  NZ  LYS    23       7.366  62.602 143.352  1.00 19.04       HIGL
ATOM    186  C   LYS    23       4.975  66.318 138.137  1.00 17.45       HIGL
ATOM    187  O   LYS    23       6.098  66.342 137.640  1.00 17.10       HIGL
ATOM    188  N   ASN    24       4.021  67.171 137.786  1.00 17.71       HIGL
ATOM    189  CA  ASN    24       4.315  68.221 136.823  1.00 17.61       HIGL
ATOM    190  CB  ASN    24       3.029  68.792 136.210  1.00 17.78       HIGL
ATOM    191  CG  ASN    24       1.986  69.174 137.252  1.00 17.86       HIGL
ATOM    192  OD1 ASN    24       2.314  69.585 138.368  1.00 18.49       HIGL
ATOM    193  ND2 ASN    24       0.717  69.061 136.876  1.00 17.05       HIGL
ATOM    194  C   ASN    24       5.081  69.294 137.597  1.00 17.97       HIGL
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Fig. 2 cont.

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ATOM    195  O   ASN    24       5.481  69.060 138.739  1.00 16.84      HIGL
ATOM    196  N   VAL    25       5.285  70.462 136.994  1.00 19.12      HIGL
ATOM    197  CA  VAL    25       6.033  71.537 137.660  1.00 20.42      HIGL
ATOM    198  CB  VAL    25       6.164  72.813 136.789  1.00 20.47      HIGL
ATOM    199  CG1 VAL    25       7.591  73.345 136.856  1.00 18.59      HIGL
ATOM    200  CG2 VAL    25       5.749  72.534 135.377  1.00 21.79      HIGL
ATOM    201  C   VAL    25       5.399  72.009 138.957  1.00 20.49      HIGL
ATOM    202  O   VAL    25       6.071  72.577 139.812  1.00 19.69      HIGL
ATOM    203  N   ASN    26       4.101  71.782 139.094  1.00 21.96      HIGL
ATOM    204  CA  ASN    26       3.375  72.242 140.271  1.00 22.88      HIGL
ATOM    205  CB  ASN    26       1.979  72.686 139.841  1.00 23.37      HIGL
ATOM    206  CG  ASN    26       2.026  73.861 138.879  1.00 24.96      HIGL
ATOM    207  OD1 ASN    26       1.188  73.986 137.980  1.00 26.06      HIGL
ATOM    208  ND2 ASN    26       3.009  74.739 139.071  1.00 24.54      HIGL
ATOM    209  C   ASN    26       3.295  71.249 141.418  1.00 22.79      HIGL
ATOM    210  O   ASN    26       2.669  71.529 142.441  1.00 23.56      HIGL
ATOM    211  N   GLY    27       3.933  70.095 141.250  1.00 22.15      HIGL
ATOM    212  CA  GLY    27       3.932  69.094 142.299  1.00 20.67      HIGL
ATOM    213  C   GLY    27       2.743  68.157 142.290  1.00 19.93      HIGL
ATOM    214  O   GLY    27       2.574  67.357 143.214  1.00 20.18      HIGL
ATOM    215  N   GLN    28       1.912  68.247 141.258  1.00 19.35      HIGL
ATOM    216  CA  GLN    28       0.748  67.376 141.164  1.00 19.04      HIGL
ATOM    217  CB  GLN    28      -0.314  68.025 140.274  1.00 19.46      HIGL
ATOM    218  CG  GLN    28      -1.579  67.207 140.102  1.00 19.85      HIGL
ATOM    219  CD  GLN    28      -2.666  67.970 139.363  1.00 21.15      HIGL
ATOM    220  OE1 GLN    28      -2.425  68.547 138.299  1.00 21.73      HIGL
ATOM    221  NE2 GLN    28      -3.871  67.971 139.921  1.00 20.85      HIGL
ATOM    222  C   GLN    28       1.164  66.009 140.607  1.00 18.84      HIGL
ATOM    223  O   GLN    28       1.602  65.901 139.464  1.00 18.45      HIGL
ATOM    224  N   GLU    29       1.038  64.973 141.432  1.00 18.66      HIGL
ATOM    225  CA  GLU    29       1.402  63.619 141.042  1.00 18.76      HIGL
ATOM    226  CB  GLU    29       1.487  62.730 142.287  1.00 18.41      HIGL
ATOM    227  CG  GLU    29       1.966  61.316 141.998  1.00 19.70      HIGL
ATOM    228  CD  GLU    29       2.223  60.504 143.252  1.00 21.17      HIGL
ATOM    229  OE1 GLU    29       2.828  61.042 144.204  1.00 22.90      HIGL
ATOM    230  OE2 GLU    29       1.836  59.318 143.285  1.00 21.00      HIGL
ATOM    231  C   GLU    29       0.412  63.005 140.045  1.00 18.74      HIGL
ATOM    232  O   GLU    29      -0.793  63.133 140.205  1.00 20.35      HIGL
ATOM    233  N   LYS    30       0.929  62.357 139.007  1.00 18.03      HIGL
ATOM    234  CA  LYS    30       0.096  61.696 137.997  1.00 18.21      HIGL
ATOM    235  CB  LYS    30      -0.563  62.702 137.038  1.00 18.37      HIGL
ATOM    236  CG  LYS    30      -0.511  64.151 137.467  1.00 19.45      HIGL
ATOM    237  CD  LYS    30      -0.017  65.012 136.323  1.00 19.01      HIGL
ATOM    238  CE  LYS    30      -1.150  65.659 135.558  1.00 19.86      HIGL
ATOM    239  NZ  LYS    30      -1.471  67.014 136.095  1.00 19.22      HIGL
ATOM    240  C   LYS    30       0.999  60.777 137.179  1.00 17.33      HIGL
ATOM    241  O   LYS    30       2.227  60.837 137.297  1.00 18.02      HIGL
ATOM    242  N   PRO    31       0.404  59.905 136.353  1.00 16.17      HIGL
ATOM    243  CD  PRO    31      -1.032  59.580 136.274  1.00 16.56      HIGL
ATOM    244  CA  PRO    31       1.201  58.991 135.525  1.00 15.20      HIGL
ATOM    245  CB  PRO    31       0.147  58.122 134.854  1.00 15.51      HIGL
ATOM    246  CG  PRO    31      -1.001  58.135 135.843  1.00 16.29      HIGL
ATOM    247  C   PRO    31       1.992  59.830 134.521  1.00 15.68      HIGL
ATOM    248  O   PRO    31       1.455  60.782 133.943  1.00 16.00      HIGL
ATOM    249  N   LEU    32       3.258  59.478 134.313  1.00 14.62      HIGL
ATOM    250  CA  LEU    32       4.139  60.224 133.416  1.00 13.57      HIGL
ATOM    251  CB  LEU    32       5.433  59.437 133.198  1.00 12.66      HIGL
ATOM    252  CG  LEU    32       6.592  60.142 132.490  1.00 12.44      HIGL
ATOM    253  CD1 LEU    32       6.934  61.428 133.209  1.00 11.76      HIGL
ATOM    254  CD2 LEU    32       7.805  59.218 132.455  1.00 12.43      HIGL
ATOM    255  C   LEU    32       3.546  60.628 132.062  1.00 13.85      HIGL
ATOM    256  O   LEU    32       3.684  61.781 131.641  1.00 13.20      HIGL
ATOM    257  N   GLU    33       2.881  59.698 131.379  1.00 14.00      HIGL
ATOM    258  CA  GLU    33       2.316  60.020 130.073  1.00 14.95      HIGL
ATOM    259  CB  GLU    33       1.486  58.847 129.510  1.00 15.36      HIGL
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Fig. 2 cont.

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ATOM    260  CG  GLU    33       0.259  58.440 130.324  1.00 16.87      HIGL
ATOM    261  CD  GLU    33       0.560  57.350 131.339  1.00 18.43      HIGL
ATOM    262  OE1 GLU    33       1.586  57.459 132.049  1.00 19.77      HIGL
ATOM    263  OE2 GLU    33      -0.234  56.387 131.433  1.00 18.45      HIGL
ATOM    264  C   GLU    33       1.476  61.300 130.102  1.00 15.90      HIGL
ATOM    265  O   GLU    33       1.429  62.032 129.113  1.00 17.16      HIGL
ATOM    266  N   TYR    34       0.824  61.584 131.228  1.00 16.05      HIGL
ATOM    267  CA  TYR    34       0.005  62.787 131.325  1.00 15.44      HIGL
ATOM    268  CB  TYR    34      -1.104  62.593 132.358  1.00 16.32      HIGL
ATOM    269  CG  TYR    34      -2.087  61.551 131.901  1.00 16.99      HIGL
ATOM    270  CD1 TYR    34      -2.063  60.257 132.426  1.00 17.20      HIGL
ATOM    271  CE1 TYR    34      -2.915  59.267 131.937  1.00 17.14      HIGL
ATOM    272  CD2 TYR    34      -2.992  61.832 130.875  1.00 17.08      HIGL
ATOM    273  CE2 TYR    34      -3.845  60.851 130.378  1.00 17.17      HIGL
ATOM    274  CZ  TYR    34      -3.801  59.572 130.913  1.00 17.87      HIGL
ATOM    275  OH  TYR    34      -4.647  58.603 130.425  1.00 19.84      HIGL
ATOM    276  C   TYR    34       0.828  64.030 131.617  1.00 14.61      HIGL
ATOM    277  O   TYR    34       0.512  65.115 131.126  1.00 13.80      HIGL
ATOM    278  N   ILE    35       1.889  63.880 132.399  1.00 14.26      HIGL
ATOM    279  CA  ILE    35       2.763  65.014 132.672  1.00 14.92      HIGL
ATOM    280  CB  ILE    35       3.865  64.662 133.679  1.00 15.08      HIGL
ATOM    281  CG2 ILE    35       4.882  65.794 133.753  1.00 14.72      HIGL
ATOM    282  CG1 ILE    35       3.243  64.398 135.051  1.00 15.03      HIGL
ATOM    283  CD1 ILE    35       4.219  63.877 136.067  1.00 15.01      HIGL
ATOM    284  C   ILE    35       3.424  65.404 131.352  1.00 14.91      HIGL
ATOM    285  O   ILE    35       3.656  66.584 131.092  1.00 15.44      HIGL
ATOM    286  N   LEU    36       3.715  64.403 130.518  1.00 14.83      HIGL
ATOM    287  CA  LEU    36       4.332  64.649 129.215  1.00 14.44      HIGL
ATOM    288  CB  LEU    36       4.765  63.340 128.557  1.00 14.34      HIGL
ATOM    289  CG  LEU    36       5.806  62.491 129.280  1.00 15.12      HIGL
ATOM    290  CD1 LEU    36       6.153  61.306 128.385  1.00 15.81      HIGL
ATOM    291  CD2 LEU    36       7.050  63.320 129.595  1.00 13.46      HIGL
ATOM    292  C   LEU    36       3.385  65.375 128.267  1.00 14.40      HIGL
ATOM    293  O   LEU    36       3.761  66.376 127.659  1.00 13.88      HIGL
ATOM    294  N   ALA    37       2.162  64.864 128.131  1.00 14.45      HIGL
ATOM    295  CA  ALA    37       1.173  65.482 127.247  1.00 15.05      HIGL
ATOM    296  CB  ALA    37      -0.121  64.677 127.269  1.00 14.89      HIGL
ATOM    297  C   ALA    37       0.918  66.915 127.711  1.00 15.47      HIGL
ATOM    298  O   ALA    37       0.757  67.832 126.907  1.00 14.62      HIGL
ATOM    299  N   GLU    38       0.910  67.081 129.028  1.00 16.62      HIGL
ATOM    300  CA  GLU    38       0.693  68.362 129.689  1.00 17.33      HIGL
ATOM    301  CB  GLU    38       0.784  68.145 131.200  1.00 19.24      HIGL
ATOM    302  CG  GLU    38       0.365  69.311 132.054  1.00 21.29      HIGL
ATOM    303  CD  GLU    38       0.550  69.028 133.529  1.00 22.16      HIGL
ATOM    304  OE1 GLU    38       0.222  67.905 133.972  1.00 21.31      HIGL
ATOM    305  OE2 GLU    38       1.018  69.939 134.244  1.00 23.91      HIGL
ATOM    306  C   GLU    38       1.727  69.402 129.262  1.00 16.88      HIGL
ATOM    307  O   GLU    38       1.441  70.597 129.205  1.00 16.84      HIGL
ATOM    308  N   ASN    39       2.934  68.942 128.960  1.00 16.61      HIGL
ATOM    309  CA  ASN    39       4.010  69.841 128.569  1.00 16.17      HIGL
ATOM    310  CB  ASN    39       5.311  69.379 129.218  1.00 16.22      HIGL
ATOM    311  CG  ASN    39       5.441  69.846 130.650  1.00 16.62      HIGL
ATOM    312  OD1 ASN    39       5.928  70.948 130.907  1.00 16.26      HIGL
ATOM    313  ND2 ASN    39       4.991  69.017 131.594  1.00 15.54      HIGL
ATOM    314  C   ASN    39       4.218  70.024 127.067  1.00 16.04      HIGL
ATOM    315  O   ASN    39       5.226  70.597 126.649  1.00 16.85      HIGL
ATOM    316  N   GLY    40       3.279  69.535 126.259  1.00 15.42      HIGL
ATOM    317  CA  GLY    40       3.392  69.694 124.821  1.00 14.77      HIGL
ATOM    318  C   GLY    40       3.895  68.494 124.037  1.00 15.22      HIGL
ATOM    319  O   GLY    40       3.890  68.517 122.810  1.00 15.07      HIGL
ATOM    320  N   VAL    41       4.342  67.451 124.725  1.00 15.28      HIGL
ATOM    321  CA  VAL    41       4.822  66.257 124.038  1.00 15.01      HIGL
ATOM    322  CB  VAL    41       5.357  65.212 125.047  1.00 15.77      HIGL
ATOM    323  CG1 VAL    41       5.682  63.896 124.328  1.00 14.74      HIGL
ATOM    324  CG2 VAL    41       6.596  65.760 125.751  1.00 15.28      HIGL
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Fig. 2 cont.

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ATOM    325  C   VAL  41       3.668  65.643 123.259  1.00 14.29      HIGL
ATOM    326  O   VAL  41       2.560  65.558 123.776  1.00 14.34      HIGL
ATOM    327  N   ASN  42       3.913  65.230 122.017  1.00 14.20      HIGL
ATOM    328  CA  ASN  42       2.846  64.611 121.217  1.00 14.11      HIGL
ATOM    329  CB  ASN  42       2.451  65.488 120.008  1.00 13.09      HIGL
ATOM    330  CG  ASN  42       3.588  65.683 119.003  1.00 15.29      HIGL
ATOM    331  OD1 ASN  42       4.632  65.030 119.077  1.00 14.89      HIGL
ATOM    332  ND2 ASN  42       3.376  66.587 118.044  1.00 13.72      HIGL
ATOM    333  C   ASN  42       3.220  63.215 120.734  1.00 13.63      HIGL
ATOM    334  O   ASN  42       2.523  62.628 119.907  1.00 13.90      HIGL
ATOM    335  N   MET  43       4.319  62.683 121.259  1.00 13.09      HIGL
ATOM    336  CA  MET  43       4.776  61.355 120.865  1.00 12.43      HIGL
ATOM    337  CB  MET  43       5.290  61.373 119.421  1.00 12.54      HIGL
ATOM    338  CG  MET  43       5.833  60.029 118.943  1.00 13.16      HIGL
ATOM    339  SD  MET  43       6.153  59.988 117.164  1.00 15.39      HIGL
ATOM    340  CE  MET  43       4.461  60.024 116.523  1.00 14.86      HIGL
ATOM    341  C   MET  43       5.870  60.820 121.774  1.00 11.00      HIGL
ATOM    342  O   MET  43       6.730  61.563 122.229  1.00  9.98      HIGL
ATOM    343  N   VAL  44       5.824  59.522 122.041  1.00 10.40      HIGL
ATOM    344  CA  VAL  44       6.837  58.900 122.872  1.00 10.47      HIGL
ATOM    345  CB  VAL  44       6.218  58.213 124.113  1.00 10.16      HIGL
ATOM    346  CG1 VAL  44       5.663  59.259 125.057  1.00 10.97      HIGL
ATOM    347  CG2 VAL  44       5.120  57.251 123.696  1.00 10.36      HIGL
ATOM    348  C   VAL  44       7.607  57.868 122.051  1.00 10.89      HIGL
ATOM    349  O   VAL  44       7.060  57.241 121.140  1.00  9.61      HIGL
ATOM    350  N   ARG  45       8.889  57.721 122.368  1.00 11.52      HIGL
ATOM    351  CA  ARG  45       9.758  56.765 121.696  1.00 12.77      HIGL
ATOM    352  CB  ARG  45      11.085  57.442 121.351  1.00 14.01      HIGL
ATOM    353  CG  ARG  45      12.129  56.570 120.667  1.00 15.59      HIGL
ATOM    354  CD  ARG  45      13.326  57.430 120.305  1.00 16.97      HIGL
ATOM    355  NE  ARG  45      14.418  56.694 119.679  1.00 17.87      HIGL
ATOM    356  CZ  ARG  45      15.496  56.254 120.320  1.00 17.82      HIGL
ATOM    357  NH1 ARG  45      15.642  56.466 121.620  1.00 17.90      HIGL
ATOM    358  NH2 ARG  45      16.439  55.610 119.653  1.00 18.55      HIGL
ATOM    359  C   ARG  45       9.970  55.628 122.687  1.00 13.22      HIGL
ATOM    360  O   ARG  45      10.244  55.870 123.859  1.00 13.66      HIGL
ATOM    361  N   GLN  46       9.821  54.390 122.232  1.00 13.78      HIGL
ATOM    362  CA  GLN  46       9.996  53.243 123.118  1.00 14.54      HIGL
ATOM    363  CB  GLN  46       8.639  52.573 123.394  1.00 15.20      HIGL
ATOM    364  CG  GLN  46       7.582  53.492 124.043  1.00 16.94      HIGL
ATOM    365  CD  GLN  46       6.298  52.748 124.403  1.00 18.02      HIGL
ATOM    366  OE1 GLN  46       5.361  53.328 124.944  1.00 17.27      HIGL
ATOM    367  NE2 GLN  46       6.257  51.454 124.097  1.00 19.40      HIGL
ATOM    368  C   GLN  46      10.960  52.228 122.512  1.00 14.27      HIGL
ATOM    369  O   GLN  46      10.808  51.829 121.360  1.00 15.12      HIGL
ATOM    370  N   ARG  47      11.962  51.821 123.280  1.00 14.18      HIGL
ATOM    371  CA  ARG  47      12.923  50.847 122.787  1.00 14.34      HIGL
ATOM    372  CB  ARG  47      14.264  51.008 123.510  1.00 14.68      HIGL
ATOM    373  CG  ARG  47      14.172  51.059 125.026  1.00 14.19      HIGL
ATOM    374  CD  ARG  47      15.555  50.900 125.661  1.00 14.01      HIGL
ATOM    375  NE  ARG  47      15.530  51.133 127.101  1.00 13.64      HIGL
ATOM    376  CZ  ARG  47      15.463  52.341 127.651  1.00 13.65      HIGL
ATOM    377  NH1 ARG  47      15.422  53.415 126.872  1.00 12.61      HIGL
ATOM    378  NH2 ARG  47      15.436  52.479 128.969  1.00 12.29      HIGL
ATOM    379  C   ARG  47      12.375  49.434 122.979  1.00 14.38      HIGL
ATOM    380  O   ARG  47      11.742  49.139 123.990  1.00 14.26      HIGL
ATOM    381  N   VAL  48      12.616  48.567 121.999  1.00 14.13      HIGL
ATOM    382  CA  VAL  48      12.136  47.194 122.054  1.00 14.66      HIGL
ATOM    383  CB  VAL  48      11.108  46.931 120.946  1.00 14.30      HIGL
ATOM    384  CG1 VAL  48      10.497  45.549 121.109  1.00 12.51      HIGL
ATOM    385  CG2 VAL  48      10.044  48.001 120.977  1.00 14.44      HIGL
ATOM    386  C   VAL  48      13.266  46.185 121.901  1.00 15.87      HIGL
ATOM    387  O   VAL  48      13.987  46.200 120.903  1.00 16.88      HIGL
ATOM    388  N   TRP  49      13.420  45.319 122.901  1.00 16.25      HIGL
ATOM    389  CA  TRP  49      14.449  44.283 122.881  1.00 16.07      HIGL
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Fig. 2 cont.

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ATOM    390  CB  TRP  49      15.243  44.280 124.194  1.00 15.19      HIGL
ATOM    391  CG  TRP  49      16.039  45.533 124.422  1.00 15.37      HIGL
ATOM    392  CD2 TRP  49      16.745  45.898 125.613  1.00 15.05      HIGL
ATOM    393  CE2 TRP  49      17.359  47.146 125.370  1.00 14.69      HIGL
ATOM    394  CE3 TRP  49      16.922  45.290 126.864  1.00 15.17      HIGL
ATOM    395  CD1 TRP  49      16.247  46.550 123.529  1.00 15.47      HIGL
ATOM    396  NE1 TRP  49      17.037  47.521 124.093  1.00 14.49      HIGL
ATOM    397  CZ2 TRP  49      18.138  47.798 126.332  1.00 15.16      HIGL
ATOM    398  CZ3 TRP  49      17.696  45.939 127.819  1.00 14.43      HIGL
ATOM    399  CH2 TRP  49      18.294  47.179 127.547  1.00 14.14      HIGL
ATOM    400  C   TRP  49      13.793  42.924 122.665  1.00 16.51      HIGL
ATOM    401  O   TRP  49      12.657  42.695 123.100  1.00 16.05      HIGL
ATOM    402  N   VAL  50      14.517  42.031 121.990  1.00 16.88      HIGL
ATOM    403  CA  VAL  50      14.031  40.690 121.675  1.00 17.15      HIGL
ATOM    404  CB  VAL  50      15.039  39.953 120.754  1.00 17.71      HIGL
ATOM    405  CG1 VAL  50      14.449  38.639 120.260  1.00 17.30      HIGL
ATOM    406  CG2 VAL  50      15.402  40.841 119.571  1.00 17.23      HIGL
ATOM    407  C   VAL  50      13.763  39.843 122.923  1.00 17.92      HIGL
ATOM    408  O   VAL  50      12.617  39.724 123.362  1.00 18.11      HIGL
ATOM    409  N   ASN  51      14.812  39.258 123.495  1.00 18.58      HIGL
ATOM    410  CA  ASN  51      14.660  38.430 124.690  1.00 18.99      HIGL
ATOM    411  CB  ASN  51      15.126  37.010 124.410  1.00 21.64      HIGL
ATOM    412  CG  ASN  51      14.602  36.480 123.093  1.00 24.95      HIGL
ATOM    413  OD1 ASN  51      13.388  36.364 122.892  1.00 27.18      HIGL
ATOM    414  ND2 ASN  51      15.517  36.156 122.180  1.00 25.56      HIGL
ATOM    415  C   ASN  51      15.443  38.978 125.875  1.00 18.38      HIGL
ATOM    416  O   ASN  51      16.417  38.368 126.319  1.00 17.35      HIGL
ATOM    417  N   PRO  52      15.032  40.144 126.401  1.00 17.80      HIGL
ATOM    418  CD  PRO  52      13.867  40.972 126.053  1.00 17.12      HIGL
ATOM    419  CA  PRO  52      15.747  40.712 127.543  1.00 17.06      HIGL
ATOM    420  CB  PRO  52      14.949  41.971 127.861  1.00 16.91      HIGL
ATOM    421  CG  PRO  52      13.579  41.650 127.364  1.00 17.23      HIGL
ATOM    422  C   PRO  52      15.776  39.716 128.688  1.00 17.60      HIGL
ATOM    423  O   PRO  52      14.828  38.954 128.891  1.00 17.99      HIGL
ATOM    424  N   TRP  53      16.877  39.723 129.428  1.00 17.96      HIGL
ATOM    425  CA  TRP  53      17.068  38.801 130.536  1.00 17.77      HIGL
ATOM    426  CB  TRP  53      18.448  39.013 131.156  1.00 18.06      HIGL
ATOM    427  CG  TRP  53      18.543  40.298 131.917  1.00 18.50      HIGL
ATOM    428  CD2 TRP  53      18.389  40.459 133.328  1.00 18.71      HIGL
ATOM    429  CE2 TRP  53      18.452  41.844 133.600  1.00 17.92      HIGL
ATOM    430  CE3 TRP  53      18.198  39.565 134.390  1.00 18.46      HIGL
ATOM    431  CD1 TRP  53      18.698  41.553 131.404  1.00 18.32      HIGL
ATOM    432  NE1 TRP  53      18.642  42.489 132.409  1.00 17.61      HIGL
ATOM    433  CZ2 TRP  53      18.331  42.357 134.888  1.00 19.23      HIGL
ATOM    434  CZ3 TRP  53      18.077  40.074 135.674  1.00 19.45      HIGL
ATOM    435  CH2 TRP  53      18.143  41.460 135.912  1.00 19.83      HIGL
ATOM    436  C   TRP  53      16.017  38.919 131.631  1.00 17.78      HIGL
ATOM    437  O   TRP  53      15.726  37.944 132.324  1.00 18.33      HIGL
ATOM    438  N   ASP  54      15.447  40.106 131.793  1.00 17.42      HIGL
ATOM    439  CA  ASP  54      14.455  40.307 132.845  1.00 17.12      HIGL
ATOM    440  CB  ASP  54      14.976  41.352 133.830  1.00 16.85      HIGL
ATOM    441  CG  ASP  54      15.139  42.705 133.189  1.00 17.98      HIGL
ATOM    442  OD1 ASP  54      15.083  42.779 131.938  1.00 19.62      HIGL
ATOM    443  OD2 ASP  54      15.325  43.690 133.927  1.00 17.75      HIGL
ATOM    444  C   ASP  54      13.080  40.718 132.320  1.00 16.46      HIGL
ATOM    445  O   ASP  54      12.196  41.080 133.094  1.00 16.77      HIGL
ATOM    446  N   GLY  55      12.907  40.666 131.003  1.00 16.49      HIGL
ATOM    447  CA  GLY  55      11.629  41.019 130.406  1.00 15.10      HIGL
ATOM    448  C   GLY  55      11.396  42.494 130.120  1.00 14.82      HIGL
ATOM    449  O   GLY  55      10.461  42.844 129.401  1.00 14.82      HIGL
ATOM    450  N   ASN  56      12.225  43.375 130.667  1.00 14.46      HIGL
ATOM    451  CA  ASN  56      12.010  44.792 130.418  1.00 14.01      HIGL
ATOM    452  CB  ASN  56      12.784  45.649 131.417  1.00 14.38      HIGL
ATOM    453  CG  ASN  56      12.130  45.660 132.785  1.00 15.79      HIGL
ATOM    454  OD1 ASN  56      10.901  45.606 132.902  1.00 15.70      HIGL
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Fig. 2 cont.

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ATOM    455 ND2  ASN    56      12.941  45.743 133.826  1.00 16.95      HIGL
ATOM    456 C    ASN    56      12.341  45.204 128.999  1.00 13.31      HIGL
ATOM    457 O    ASN    56      13.366  44.817 128.442  1.00 12.12      HIGL
ATOM    458 N    TYR    57      11.439  45.991 128.424  1.00 13.34      HIGL
ATOM    459 CA   TYR    57      11.558  46.499 127.065  1.00 13.09      HIGL
ATOM    460 CB   TYR    57      12.968  47.049 126.789  1.00 12.20      HIGL
ATOM    461 CG   TYR    57      13.466  47.989 127.865  1.00 11.14      HIGL
ATOM    462 CD1  TYR    57      12.666  49.030 128.330  1.00 10.28      HIGL
ATOM    463 CE1  TYR    57      13.095  49.859 129.353  1.00  9.79      HIGL
ATOM    464 CD2  TYR    57      14.716  47.808 128.450  1.00 10.12      HIGL
ATOM    465 CE2  TYR    57      15.152  48.630 129.471  1.00  9.28      HIGL
ATOM    466 CZ   TYR    57      14.333  49.654 129.922  1.00  9.42      HIGL
ATOM    467 OH   TYR    57      14.737  50.450 130.973  1.00 10.17      HIGL
ATOM    468 C    TYR    57      11.214  45.426 126.052  1.00 13.71      HIGL
ATOM    469 O    TYR    57      11.460  45.591 124.854  1.00 13.96      HIGL
ATOM    470 N    ASN    58      10.657  44.313 126.515  1.00 13.75      HIGL
ATOM    471 CA   ASN    58      10.276  43.298 125.553  1.00 14.27      HIGL
ATOM    472 CB   ASN    58      10.325  41.874 126.147  1.00 12.09      HIGL
ATOM    473 CG   ASN    58       9.216  41.576 127.140  1.00  9.87      HIGL
ATOM    474 OD1  ASN    58       8.278  42.353 127.323  1.00 11.38      HIGL
ATOM    475 ND2  ASN    58       9.316  40.416 127.777  1.00  5.89      HIGL
ATOM    476 C    ASN    58       8.892  43.669 125.039  1.00 15.29      HIGL
ATOM    477 O    ASN    58       8.301  44.651 125.490  1.00 14.81      HIGL
ATOM    478 N    LEU    59       8.389  42.901 124.085  1.00 17.30      HIGL
ATOM    479 CA   LEU    59       7.096  43.188 123.482  1.00 19.48      HIGL
ATOM    480 CB   LEU    59       6.692  42.037 122.565  1.00 21.08      HIGL
ATOM    481 CG   LEU    59       5.709  42.447 121.470  1.00 23.34      HIGL
ATOM    482 CD1  LEU    59       6.296  43.624 120.673  1.00 23.05      HIGL
ATOM    483 CD2  LEU    59       5.436  41.247 120.561  1.00 23.47      HIGL
ATOM    484 C    LEU    59       5.970  43.488 124.471  1.00 19.90      HIGL
ATOM    485 O    LEU    59       5.367  44.557 124.415  1.00 21.04      HIGL
ATOM    486 N    ASP    60       5.683  42.555 125.372  1.00 20.10      HIGL
ATOM    487 CA   ASP    60       4.619  42.756 126.348  1.00 20.50      HIGL
ATOM    488 CB   ASP    60       4.599  41.613 127.369  1.00 21.74      HIGL
ATOM    489 CG   ASP    60       4.436  40.250 126.720  1.00 23.55      HIGL
ATOM    490 OD1  ASP    60       3.553  40.100 125.844  1.00 23.00      HIGL
ATOM    491 OD2  ASP    60       5.190  39.324 127.094  1.00 24.89      HIGL
ATOM    492 C    ASP    60       4.810  44.078 127.078  1.00 20.77      HIGL
ATOM    493 O    ASP    60       3.869  44.860 127.231  1.00 21.37      HIGL
ATOM    494 N    TYR    61       6.038  44.315 127.529  1.00 20.29      HIGL
ATOM    495 CA   TYR    61       6.393  45.533 128.241  1.00 19.19      HIGL
ATOM    496 CB   TYR    61       7.896  45.526 128.574  1.00 19.77      HIGL
ATOM    497 CG   TYR    61       8.400  46.776 129.274  1.00 19.20      HIGL
ATOM    498 CD1  TYR    61       8.572  47.975 128.580  1.00 19.12      HIGL
ATOM    499 CE1  TYR    61       8.998  49.132 129.229  1.00 19.60      HIGL
ATOM    500 CD2  TYR    61       8.675  46.766 130.638  1.00 19.18      HIGL
ATOM    501 CE2  TYR    61       9.101  47.916 131.297  1.00 20.13      HIGL
ATOM    502 CZ   TYR    61       9.259  49.096 130.589  1.00 20.45      HIGL
ATOM    503 OH   TYR    61       9.663  50.239 131.250  1.00 21.00      HIGL
ATOM    504 C    TYR    61       6.059  46.767 127.414  1.00 19.25      HIGL
ATOM    505 O    TYR    61       5.506  47.738 127.930  1.00 19.40      HIGL
ATOM    506 N    ASN    62       6.390  46.733 126.129  1.00 19.00      HIGL
ATOM    507 CA   ASN    62       6.128  47.878 125.271  1.00 19.77      HIGL
ATOM    508 CB   ASN    62       6.971  47.789 123.999  1.00 20.44      HIGL
ATOM    509 CG   ASN    62       8.403  48.223 124.229  1.00 21.08      HIGL
ATOM    510 OD1  ASN    62       8.685  49.415 124.376  1.00 21.94      HIGL
ATOM    511 ND2  ASN    62       9.315  47.259 124.284  1.00 20.37      HIGL
ATOM    512 C    ASN    62       4.664  48.053 124.925  1.00 19.75      HIGL
ATOM    513 O    ASN    62       4.235  49.156 124.588  1.00 20.46      HIGL
ATOM    514 N    ILE    63       3.892  46.977 125.009  1.00 19.62      HIGL
ATOM    515 CA   ILE    63       2.472  47.073 124.717  1.00 20.26      HIGL
ATOM    516 CB   ILE    63       1.856  45.693 124.478  1.00 20.11      HIGL
ATOM    517 CG2  ILE    63       0.336  45.761 124.598  1.00 19.41      HIGL
ATOM    518 CG1  ILE    63       2.293  45.198 123.101  1.00 20.67      HIGL
ATOM    519 CD1  ILE    63       1.599  43.952 122.648  1.00 23.84      HIGL
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Fig. 2 cont.

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ATOM    520  C   ILE   63       1.742  47.775 125.852  1.00 21.15      HIGL
ATOM    521  O   ILE   63       0.807  48.535 125.617  1.00 20.59      HIGL
ATOM    522  N   GLN   64       2.172  47.528 127.086  1.00 22.72      HIGL
ATOM    523  CA  GLN   64       1.547  48.177 128.235  1.00 23.28      HIGL
ATOM    524  CB  GLN   64       2.117  47.626 129.544  1.00 24.62      HIGL
ATOM    525  CG  GLN   64       1.064  47.428 130.630  1.00 27.22      HIGL
ATOM    526  CD  GLN   64       1.641  46.837 131.906  1.00 29.98      HIGL
ATOM    527  OE1 GLN   64       2.314  45.798 131.877  1.00 31.39      HIGL
ATOM    528  NE2 GLN   64       1.380  47.493 133.037  1.00 29.60      HIGL
ATOM    529  C   GLN   64       1.827  49.675 128.130  1.00 22.91      HIGL
ATOM    530  O   GLN   64       0.952  50.501 128.400  1.00 23.24      HIGL
ATOM    531  N   LEU   65       3.045  50.018 127.717  1.00 21.90      HIGL
ATOM    532  CA  LEU   65       3.436  51.415 127.559  1.00 21.80      HIGL
ATOM    533  CB  LEU   65       4.925  51.524 127.241  1.00 21.78      HIGL
ATOM    534  CG  LEU   65       5.863  51.436 128.439  1.00 22.02      HIGL
ATOM    535  CD1 LEU   65       7.300  51.702 128.006  1.00 21.72      HIGL
ATOM    536  CD2 LEU   65       5.424  52.459 129.459  1.00 22.32      HIGL
ATOM    537  C   LEU   65       2.650  52.104 126.458  1.00 21.48      HIGL
ATOM    538  O   LEU   65       2.107  53.191 126.651  1.00 20.27      HIGL
ATOM    539  N   ALA   66       2.604  51.467 125.297  1.00 21.88      HIGL
ATOM    540  CA  ALA   66       1.884  52.017 124.157  1.00 22.71      HIGL
ATOM    541  CB  ALA   66       1.908  51.026 123.006  1.00 21.67      HIGL
ATOM    542  C   ALA   66       0.447  52.340 124.546  1.00 22.91      HIGL
ATOM    543  O   ALA   66      -0.013  53.471 124.395  1.00 23.72      HIGL
ATOM    544  N   ARG   67      -0.256  51.340 125.059  1.00 23.00      HIGL
ATOM    545  CA  ARG   67      -1.635  51.517 125.457  1.00 22.83      HIGL
ATOM    546  CB  ARG   67      -2.121  50.260 126.173  1.00 24.13      HIGL
ATOM    547  CG  ARG   67      -3.621  50.147 126.305  1.00 26.38      HIGL
ATOM    548  CD  ARG   67      -3.993  48.774 126.824  1.00 29.10      HIGL
ATOM    549  NE  ARG   67      -3.810  47.732 125.815  1.00 30.83      HIGL
ATOM    550  CZ  ARG   67      -3.501  46.469 126.098  1.00 32.31      HIGL
ATOM    551  NH1 ARG   67      -3.333  46.096 127.361  1.00 33.65      HIGL
ATOM    552  NH2 ARG   67      -3.369  45.576 125.126  1.00 32.30      HIGL
ATOM    553  C   ARG   67      -1.747  52.749 126.351  1.00 22.02      HIGL
ATOM    554  O   ARG   67      -2.627  53.587 126.158  1.00 22.49      HIGL
ATOM    555  N   ARG   68      -0.843  52.876 127.313  1.00 21.00      HIGL
ATOM    556  CA  ARG   68      -0.860  54.031 128.207  1.00 20.10      HIGL
ATOM    557  CB  ARG   68       0.183  53.867 129.321  1.00 19.58      HIGL
ATOM    558  CG  ARG   68      -0.247  52.927 130.442  1.00 18.60      HIGL
ATOM    559  CD  ARG   68       0.858  52.723 131.475  1.00 17.98      HIGL
ATOM    560  NE  ARG   68       1.319  53.986 132.048  1.00 17.78      HIGL
ATOM    561  CZ  ARG   68       2.210  54.078 133.030  1.00 16.65      HIGL
ATOM    562  NH1 ARG   68       2.735  52.975 133.550  1.00 15.08      HIGL
ATOM    563  NH2 ARG   68       2.574  55.272 133.490  1.00 15.87      HIGL
ATOM    564  C   ARG   68      -0.588  55.322 127.441  1.00 20.06      HIGL
ATOM    565  O   ARG   68      -1.287  56.312 127.613  1.00 19.99      HIGL
ATOM    566  N   ALA   69       0.437  55.306 126.597  1.00 20.75      HIGL
ATOM    567  CA  ALA   69       0.800  56.477 125.808  1.00 21.00      HIGL
ATOM    568  CB  ALA   69       1.979  56.144 124.913  1.00 21.37      HIGL
ATOM    569  C   ALA   69      -0.379  56.960 124.965  1.00 21.40      HIGL
ATOM    570  O   ALA   69      -0.610  58.164 124.829  1.00 20.93      HIGL
ATOM    571  N   LYS   70      -1.114  56.007 124.402  1.00 21.23      HIGL
ATOM    572  CA  LYS   70      -2.273  56.295 123.574  1.00 22.04      HIGL
ATOM    573  CB  LYS   70      -2.770  54.991 122.941  1.00 24.06      HIGL
ATOM    574  CG  LYS   70      -4.006  55.118 122.060  1.00 26.72      HIGL
ATOM    575  CD  LYS   70      -4.553  53.734 121.710  1.00 29.26      HIGL
ATOM    576  CE  LYS   70      -5.785  53.811 120.813  1.00 30.47      HIGL
ATOM    577  NZ  LYS   70      -6.349  52.451 120.547  1.00 31.87      HIGL
ATOM    578  C   LYS   70      -3.394  56.946 124.403  1.00 21.81      HIGL
ATOM    579  O   LYS   70      -4.034  57.901 123.958  1.00 21.40      HIGL
ATOM    580  N   ALA   71      -3.631  56.439 125.609  1.00 20.36      HIGL
ATOM    581  CA  ALA   71      -4.682  57.000 126.448  1.00 19.90      HIGL
ATOM    582  CB  ALA   71      -4.770  56.242 127.767  1.00 19.16      HIGL
ATOM    583  C   ALA   71      -4.432  58.485 126.708  1.00 19.54      HIGL
ATOM    584  O   ALA   71      -5.371  59.259 126.862  1.00 20.19      HIGL
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Fig. 2 cont.

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ATOM    585  N   ALA  72      -3.166  58.881 126.754  1.00 18.45      HIGL
ATOM    586  CA  ALA  72      -2.822  60.276 126.987  1.00 17.24      HIGL
ATOM    587  CB  ALA  72      -1.507  60.374 127.753  1.00 16.31      HIGL
ATOM    588  C   ALA  72      -2.722  61.035 125.667  1.00 16.70      HIGL
ATOM    589  O   ALA  72      -2.210  62.147 125.628  1.00 17.88      HIGL
ATOM    590  N   GLY  73      -3.200  60.421 124.589  1.00 15.95      HIGL
ATOM    591  CA  GLY  73      -3.176  61.058 123.284  1.00 15.41      HIGL
ATOM    592  C   GLY  73      -1.809  61.236 122.647  1.00 16.92      HIGL
ATOM    593  O   GLY  73      -1.638  62.056 121.739  1.00 16.80      HIGL
ATOM    594  N   LEU  74      -0.826  60.470 123.107  1.00 16.80      HIGL
ATOM    595  CA  LEU  74       0.516  60.577 122.554  1.00 16.41      HIGL
ATOM    596  CB  LEU  74       1.545  60.366 123.663  1.00 15.23      HIGL
ATOM    597  CG  LEU  74       1.311  61.253 124.884  1.00 14.82      HIGL
ATOM    598  CD1 LEU  74       2.265  60.875 125.994  1.00 13.72      HIGL
ATOM    599  CD2 LEU  74       1.486  62.706 124.492  1.00 14.41      HIGL
ATOM    600  C   LEU  74       0.762  59.577 121.424  1.00 17.36      HIGL
ATOM    601  O   LEU  74       0.319  58.430 121.482  1.00 16.67      HIGL
ATOM    602  N   GLY  75       1.470  60.027 120.392  1.00 18.17      HIGL
ATOM    603  CA  GLY  75       1.785  59.155 119.278  1.00 17.81      HIGL
ATOM    604  C   GLY  75       2.846  58.153 119.695  1.00 18.44      HIGL
ATOM    605  O   GLY  75       3.486  58.299 120.748  1.00 18.86      HIGL
ATOM    606  N   LEU  76       3.058  57.147 118.858  1.00 17.36      HIGL
ATOM    607  CA  LEU  76       4.014  56.103 119.163  1.00 16.84      HIGL
ATOM    608  CB  LEU  76       3.262  54.777 119.306  1.00 16.53      HIGL
ATOM    609  CG  LEU  76       4.075  53.527 119.631  1.00 17.06      HIGL
ATOM    610  CD1 LEU  76       4.742  53.691 120.997  1.00 16.56      HIGL
ATOM    611  CD2 LEU  76       3.161  52.318 119.620  1.00 15.85      HIGL
ATOM    612  C   LEU  76       5.143  55.949 118.139  1.00 16.79      HIGL
ATOM    613  O   LEU  76       4.914  55.918 116.932  1.00 17.69      HIGL
ATOM    614  N   TYR  77       6.364  55.844 118.648  1.00 15.89      HIGL
ATOM    615  CA  TYR  77       7.560  55.664 117.835  1.00 15.08      HIGL
ATOM    616  CB  TYR  77       8.420  56.938 117.927  1.00 14.34      HIGL
ATOM    617  CG  TYR  77       9.866  56.872 117.435  1.00 14.79      HIGL
ATOM    618  CD1 TYR  77      10.428  55.695 116.925  1.00 13.89      HIGL
ATOM    619  CE1 TYR  77      11.774  55.644 116.552  1.00 14.56      HIGL
ATOM    620  CD2 TYR  77      10.693  57.994 117.547  1.00 15.32      HIGL
ATOM    621  CE2 TYR  77      12.039  57.955 117.179  1.00 14.67      HIGL
ATOM    622  CZ  TYR  77      12.577  56.783 116.688  1.00 15.26      HIGL
ATOM    623  OH  TYR  77      13.920  56.753 116.367  1.00 14.00      HIGL
ATOM    624  C   TYR  77       8.261  54.436 118.440  1.00 15.55      HIGL
ATOM    625  O   TYR  77       8.853  54.507 119.530  1.00 15.30      HIGL
ATOM    626  N   ILE  78       8.147  53.306 117.743  1.00 14.24      HIGL
ATOM    627  CA  ILE  78       8.751  52.051 118.183  1.00 14.13      HIGL
ATOM    628  CB  ILE  78       7.970  50.824 117.639  1.00 14.46      HIGL
ATOM    629  CG2 ILE  78       8.742  49.534 117.930  1.00 14.89      HIGL
ATOM    630  CG1 ILE  78       6.575  50.766 118.276  1.00 14.25      HIGL
ATOM    631  CD1 ILE  78       6.567  50.420 119.761  1.00 12.73      HIGL
ATOM    632  C   ILE  78      10.193  51.991 117.701  1.00 13.40      HIGL
ATOM    633  O   ILE  78      10.467  52.112 116.512  1.00 13.27      HIGL
ATOM    634  N   ASN  79      11.104  51.797 118.646  1.00 13.08      HIGL
ATOM    635  CA  ASN  79      12.533  51.753 118.378  1.00 12.27      HIGL
ATOM    636  CB  ASN  79      13.209  52.771 119.304  1.00 12.87      HIGL
ATOM    637  CG  ASN  79      14.714  52.607 119.393  1.00 12.44      HIGL
ATOM    638  OD1 ASN  79      15.291  52.886 120.435  1.00 12.93      HIGL
ATOM    639  ND2 ASN  79      15.353  52.175 118.311  1.00 12.14      HIGL
ATOM    640  C   ASN  79      13.111  50.354 118.587  1.00 12.54      HIGL
ATOM    641  O   ASN  79      13.453  49.979 119.708  1.00 12.54      HIGL
ATOM    642  N   PHE  80      13.209  49.590 117.501  1.00 12.76      HIGL
ATOM    643  CA  PHE  80      13.752  48.232 117.534  1.00 13.01      HIGL
ATOM    644  CB  PHE  80      13.453  47.486 116.228  1.00 12.75      HIGL
ATOM    645  CG  PHE  80      12.076  46.901 116.154  1.00 13.87      HIGL
ATOM    646  CD1 PHE  80      11.636  45.998 117.120  1.00 13.28      HIGL
ATOM    647  CD2 PHE  80      11.218  47.241 115.114  1.00 12.89      HIGL
ATOM    648  CE1 PHE  80      10.363  45.446 117.054  1.00 11.74      HIGL
ATOM    649  CE2 PHE  80       9.943  46.692 115.043  1.00 13.92      HIGL
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Fig. 2 cont.

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ATOM    650  CZ  PHE    80       9.517  45.792 116.019  1.00 13.02      HIGL
ATOM    651  C   PHE    80      15.259  48.253 117.690  1.00 13.33      HIGL
ATOM    652  O   PHE    80      15.937  48.944 116.940  1.00 14.29      HIGL
ATOM    653  N   HIS    81      15.784  47.499 118.649  1.00 12.98      HIGL
ATOM    654  CA  HIS    81      17.227  47.426 118.823  1.00 13.87      HIGL
ATOM    655  CB  HIS    81      17.626  47.425 120.304  1.00 13.89      HIGL
ATOM    656  CG  HIS    81      17.633  48.782 120.933  1.00 15.21      HIGL
ATOM    657  CD2 HIS    81      16.749  49.805 120.860  1.00 15.13      HIGL
ATOM    658  ND1 HIS    81      18.639  49.204 121.777  1.00 15.56      HIGL
ATOM    659  CE1 HIS    81      18.375  50.429 122.196  1.00 14.49      HIGL
ATOM    660  NE2 HIS    81      17.234  50.816 121.655  1.00 15.27      HIGL
ATOM    661  C   HIS    81      17.717  46.137 118.176  1.00 13.69      HIGL
ATOM    662  O   HIS    81      18.911  45.971 117.928  1.00 14.21      HIGL
ATOM    663  N   TYR    82      16.784  45.231 117.902  1.00 13.26      HIGL
ATOM    664  CA  TYR    82      17.105  43.939 117.299  1.00 13.09      HIGL
ATOM    665  CB  TYR    82      17.449  44.102 115.819  1.00 13.22      HIGL
ATOM    666  CG  TYR    82      16.277  44.556 114.986  1.00 13.70      HIGL
ATOM    667  CD1 TYR    82      15.014  43.977 115.161  1.00 13.38      HIGL
ATOM    668  CE1 TYR    82      13.939  44.348 114.378  1.00 12.96      HIGL
ATOM    669  CD2 TYR    82      16.429  45.529 114.002  1.00 12.39      HIGL
ATOM    670  CE2 TYR    82      15.359  45.908 113.209  1.00 13.19      HIGL
ATOM    671  CZ  TYR    82      14.114  45.310 113.400  1.00 14.02      HIGL
ATOM    672  OH  TYR    82      13.046  45.652 112.595  1.00 15.86      HIGL
ATOM    673  C   TYR    82      18.257  43.278 118.030  1.00 13.08      HIGL
ATOM    674  O   TYR    82      19.217  42.804 117.421  1.00 12.93      HIGL
ATOM    675  N   SER    83      18.137  43.256 119.352  1.00 13.03      HIGL
ATOM    676  CA  SER    83      19.132  42.668 120.227  1.00 13.56      HIGL
ATOM    677  CB  SER    83      20.266  43.671 120.439  1.00 13.70      HIGL
ATOM    678  OG  SER    83      21.309  43.114 121.210  1.00 15.51      HIGL
ATOM    679  C   SER    83      18.440  42.348 121.557  1.00 14.03      HIGL
ATOM    680  O   SER    83      17.332  42.827 121.805  1.00 13.59      HIGL
ATOM    681  N   ASP    84      19.066  41.532 122.405  1.00 14.12      HIGL
ATOM    682  CA  ASP    84      18.453  41.215 123.694  1.00 14.35      HIGL
ATOM    683  CB  ASP    84      19.025  39.927 124.294  1.00 15.38      HIGL
ATOM    684  CG  ASP    84      18.577  38.682 123.558  1.00 16.47      HIGL
ATOM    685  OD1 ASP    84      17.543  38.736 122.856  1.00 16.36      HIGL
ATOM    686  OD2 ASP    84      19.259  37.643 123.704  1.00 17.16      HIGL
ATOM    687  C   ASP    84      18.760  42.357 124.640  1.00 13.54      HIGL
ATOM    688  O   ASP    84      18.066  42.571 125.629  1.00 12.95      HIGL
ATOM    689  N   THR    85      19.806  43.100 124.308  1.00 12.90      HIGL
ATOM    690  CA  THR    85      20.240  44.199 125.141  1.00 12.85      HIGL
ATOM    691  CB  THR    85      21.471  43.771 125.920  1.00 12.51      HIGL
ATOM    692  OG1 THR    85      21.661  44.642 127.038  1.00 14.10      HIGL
ATOM    693  CG2 THR    85      22.685  43.810 125.013  1.00 12.87      HIGL
ATOM    694  C   THR    85      20.555  45.453 124.314  1.00 12.72      HIGL
ATOM    695  O   THR    85      20.377  45.463 123.095  1.00 12.75      HIGL
ATOM    696  N   TRP    86      21.038  46.495 124.989  1.00 11.76      HIGL
ATOM    697  CA  TRP    86      21.358  47.772 124.354  1.00 10.89      HIGL
ATOM    698  CB  TRP    86      22.198  48.651 125.276  1.00  9.89      HIGL
ATOM    699  CG  TRP    86      21.597  48.938 126.604  1.00 10.03      HIGL
ATOM    700  CD2 TRP    86      20.629  49.947 126.908  1.00  9.39      HIGL
ATOM    701  CE2 TRP    86      20.363  49.865 128.292  1.00  8.31      HIGL
ATOM    702  CE3 TRP    86      19.959  50.913 126.147  1.00  9.93      HIGL
ATOM    703  CD1 TRP    86      21.870  48.302 127.781  1.00  8.33      HIGL
ATOM    704  NE1 TRP    86      21.135  48.852 128.796  1.00  7.98      HIGL
ATOM    705  CZ2 TRP    86      19.457  50.711 128.932  1.00  7.91      HIGL
ATOM    706  CZ3 TRP    86      19.051  51.760 126.788  1.00  9.09      HIGL
ATOM    707  CH2 TRP    86      18.812  51.649 128.166  1.00  9.37      HIGL
ATOM    708  C   TRP    86      22.111  47.668 123.048  1.00 11.73      HIGL
ATOM    709  O   TRP    86      23.216  47.141 123.008  1.00 11.69      HIGL
ATOM    710  N   ALA    87      21.524  48.193 121.980  1.00 12.59      HIGL
ATOM    711  CA  ALA    87      22.189  48.180 120.685  1.00 12.82      HIGL
ATOM    712  CB  ALA    87      21.246  47.706 119.603  1.00 12.18      HIGL
ATOM    713  C   ALA    87      22.665  49.594 120.381  1.00 13.67      HIGL
ATOM    714  O   ALA    87      21.912  50.553 120.532  1.00 13.58      HIGL
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Fig. 2 cont.

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ATOM    715  N   ASP    88      23.929  49.710 119.984  1.00 14.42      HIGL
ATOM    716  CA  ASP    88      24.538  50.984 119.628  1.00 14.58      HIGL
ATOM    717  CB  ASP    88      24.990  51.744 120.889  1.00 14.68      HIGL
ATOM    718  CG  ASP    88      25.901  50.925 121.783  1.00 16.21      HIGL
ATOM    719  OD1 ASP    88      26.827  50.268 121.263  1.00 18.18      HIGL
ATOM    720  OD2 ASP    88      25.701  50.949 123.014  1.00 16.03      HIGL
ATOM    721  C   ASP    88      25.721  50.691 118.690  1.00 15.64      HIGL
ATOM    722  O   ASP    88      26.023  49.529 118.416  1.00 15.14      HIGL
ATOM    723  N   PRO    89      26.408  51.734 118.192  1.00 16.24      HIGL
ATOM    724  CD  PRO    89      26.232  53.163 118.505  1.00 16.14      HIGL
ATOM    725  CA  PRO    89      27.545  51.549 117.280  1.00 16.34      HIGL
ATOM    726  CB  PRO    89      28.119  52.954 117.159  1.00 16.73      HIGL
ATOM    727  CG  PRO    89      26.918  53.823 117.343  1.00 17.24      HIGL
ATOM    728  C   PRO    89      28.607  50.541 117.708  1.00 16.16      HIGL
ATOM    729  O   PRO    89      29.283  49.961 116.871  1.00 15.63      HIGL
ATOM    730  N   ALA    90      28.760  50.326 119.006  1.00 16.46      HIGL
ATOM    731  CA  ALA    90      29.773  49.387 119.462  1.00 16.48      HIGL
ATOM    732  CB  ALA    90      30.596  50.003 120.598  1.00 14.72      HIGL
ATOM    733  C   ALA    90      29.191  48.054 119.899  1.00 16.00      HIGL
ATOM    734  O   ALA    90      29.939  47.143 120.241  1.00 17.19      HIGL
ATOM    735  N   HIS    91      27.867  47.933 119.889  1.00 15.05      HIGL
ATOM    736  CA  HIS    91      27.230  46.680 120.288  1.00 14.58      HIGL
ATOM    737  CB  HIS    91      26.897  46.673 121.785  1.00 15.34      HIGL
ATOM    738  CG  HIS    91      27.967  47.242 122.662  1.00 14.94      HIGL
ATOM    739  CD2 HIS    91      28.755  46.663 123.599  1.00 15.42      HIGL
ATOM    740  ND1 HIS    91      28.296  48.582 122.660  1.00 15.37      HIGL
ATOM    741  CE1 HIS    91      29.237  48.803 123.561  1.00 16.41      HIGL
ATOM    742  NE2 HIS    91      29.534  47.654 124.146  1.00 15.75      HIGL
ATOM    743  C   HIS    91      25.939  46.414 119.518  1.00 14.68      HIGL
ATOM    744  O   HIS    91      24.944  47.123 119.679  1.00 14.01      HIGL
ATOM    745  N   GLN    92      25.968  45.385 118.680  1.00 14.89      HIGL
ATOM    746  CA  GLN    92      24.818  44.974 117.885  1.00 14.67      HIGL
ATOM    747  CB  GLN    92      25.000  45.394 116.421  1.00 13.95      HIGL
ATOM    748  CG  GLN    92      24.928  46.904 116.159  1.00 13.75      HIGL
ATOM    749  CD  GLN    92      23.529  47.497 116.368  1.00 13.63      HIGL
ATOM    750  OE1 GLN    92      22.517  46.899 115.985  1.00 12.06      HIGL
ATOM    751  NE2 GLN    92      23.475  48.685 116.958  1.00 11.96      HIGL
ATOM    752  C   GLN    92      24.786  43.451 118.005  1.00 15.14      HIGL
ATOM    753  O   GLN    92      24.994  42.721 117.033  1.00 14.92      HIGL
ATOM    754  N   THR    93      24.530  42.984 119.222  1.00 15.07      HIGL
ATOM    755  CA  THR    93      24.510  41.561 119.520  1.00 14.27      HIGL
ATOM    756  CB  THR    93      24.672  41.329 121.023  1.00 14.39      HIGL
ATOM    757  OG1 THR    93      25.783  42.100 121.497  1.00 13.20      HIGL
ATOM    758  CG2 THR    93      24.906  39.842 121.315  1.00 12.37      HIGL
ATOM    759  C   THR    93      23.259  40.838 119.070  1.00 15.03      HIGL
ATOM    760  O   THR    93      22.169  41.066 119.600  1.00 15.53      HIGL
ATOM    761  N   THR    94      23.428  39.951 118.097  1.00 14.94      HIGL
ATOM    762  CA  THR    94      22.323  39.162 117.576  1.00 15.30      HIGL
ATOM    763  CB  THR    94      22.818  38.169 116.503  1.00 15.55      HIGL
ATOM    764  OG1 THR    94      23.376  38.893 115.399  1.00 15.22      HIGL
ATOM    765  CG2 THR    94      21.677  37.302 116.013  1.00 15.52      HIGL
ATOM    766  C   THR    94      21.720  38.373 118.732  1.00 15.67      HIGL
ATOM    767  O   THR    94      22.447  37.830 119.563  1.00 15.25      HIGL
ATOM    768  N   PRO    95      20.381  38.309 118.806  1.00 16.47      HIGL
ATOM    769  CD  PRO    95      19.409  38.946 117.901  1.00 16.88      HIGL
ATOM    770  CA  PRO    95      19.695  37.573 119.878  1.00 16.79      HIGL
ATOM    771  CB  PRO    95      18.220  37.690 119.490  1.00 16.02      HIGL
ATOM    772  CG  PRO    95      18.161  38.991 118.754  1.00 16.42      HIGL
ATOM    773  C   PRO    95      20.156  36.119 119.896  1.00 17.32      HIGL
ATOM    774  O   PRO    95      20.230  35.480 118.845  1.00 18.48      HIGL
ATOM    775  N   ALA    96      20.472  35.590 121.073  1.00 17.31      HIGL
ATOM    776  CA  ALA    96      20.903  34.196 121.149  1.00 17.43      HIGL
ATOM    777  CB  ALA    96      21.086  33.769 122.598  1.00 17.13      HIGL
ATOM    778  C   ALA    96      19.821  33.356 120.495  1.00 16.72      HIGL
ATOM    779  O   ALA    96      18.636  33.612 120.693  1.00 15.96      HIGL
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Fig. 2 cont.

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ATOM    780  N   GLY    97      20.229  32.371 119.700  1.00 17.32      HIGL
ATOM    781  CA  GLY    97      19.263  31.515 119.031  1.00 17.04      HIGL
ATOM    782  C   GLY    97      19.001  31.856 117.573  1.00 17.23      HIGL
ATOM    783  O   GLY    97      18.675  30.976 116.783  1.00 17.90      HIGL
ATOM    784  N   TRP    98      19.135  33.124 117.205  1.00 16.99      HIGL
ATOM    785  CA  TRP    98      18.907  33.524 115.820  1.00 17.97      HIGL
ATOM    786  CB  TRP    98      18.901  35.051 115.726  1.00 18.18      HIGL
ATOM    787  CG  TRP    98      17.627  35.621 116.258  1.00 18.37      HIGL
ATOM    788  CD2 TRP    98      17.022  36.870 115.907  1.00 18.66      HIGL
ATOM    789  CE2 TRP    98      15.824  36.978 116.650  1.00 18.98      HIGL
ATOM    790  CE3 TRP    98      17.372  37.909 115.036  1.00 18.95      HIGL
ATOM    791  CD1 TRP    98      16.798  35.041 117.175  1.00 18.96      HIGL
ATOM    792  NE1 TRP    98      15.714  35.846 117.415  1.00 19.48      HIGL
ATOM    793  CZ2 TRP    98      14.973  38.083 116.550  1.00 18.24      HIGL
ATOM    794  CZ3 TRP    98      16.521  39.011 114.936  1.00 18.88      HIGL
ATOM    795  CH2 TRP    98      15.336  39.085 115.690  1.00 18.43      HIGL
ATOM    796  C   TRP    98      19.939  32.897 114.877  1.00 17.57      HIGL
ATOM    797  O   TRP    98      21.042  32.569 115.285  1.00 17.56      HIGL
ATOM    798  N   PRO    99      19.577  32.707 113.601  1.00 17.79      HIGL
ATOM    799  CD  PRO    99      18.219  32.889 113.063  1.00 17.38      HIGL
ATOM    800  CA  PRO    99      20.459  32.106 112.594  1.00 17.62      HIGL
ATOM    801  CB  PRO    99      19.578  32.055 111.342  1.00 17.40      HIGL
ATOM    802  CG  PRO    99      18.491  33.041 111.616  1.00 18.07      HIGL
ATOM    803  C   PRO    99      21.842  32.693 112.326  1.00 17.38      HIGL
ATOM    804  O   PRO    99      22.147  33.820 112.709  1.00 17.86      HIGL
ATOM    805  N   SER   100      22.670  31.887 111.660  1.00 17.52      HIGL
ATOM    806  CA  SER   100      24.045  32.240 111.323  1.00 16.92      HIGL
ATOM    807  CB  SER   100      24.992  31.142 111.793  1.00 16.67      HIGL
ATOM    808  OG  SER   100      24.564  30.601 113.025  1.00 20.79      HIGL
ATOM    809  C   SER   100      24.283  32.452 109.833  1.00 16.73      HIGL
ATOM    810  O   SER   100      25.419  32.675 109.423  1.00 17.27      HIGL
ATOM    811  N   ASP   101      23.247  32.336 109.012  1.00 16.22      HIGL
ATOM    812  CA  ASP   101      23.422  32.564 107.579  1.00 16.38      HIGL
ATOM    813  CB  ASP   101      23.121  31.303 106.751  1.00 16.22      HIGL
ATOM    814  CG  ASP   101      21.708  30.805 106.929  1.00 15.46      HIGL
ATOM    815  OD1 ASP   101      21.423  30.151 107.950  1.00 16.82      HIGL
ATOM    816  OD2 ASP   101      20.877  31.073 106.047  1.00 16.15      HIGL
ATOM    817  C   ASP   101      22.494  33.707 107.201  1.00 16.52      HIGL
ATOM    818  O   ASP   101      21.387  33.825 107.736  1.00 16.54      HIGL
ATOM    819  N   ILE   102      22.957  34.545 106.280  1.00 15.85      HIGL
ATOM    820  CA  ILE   102      22.220  35.727 105.871  1.00 15.30      HIGL
ATOM    821  CB  ILE   102      22.958  36.484 104.746  1.00 14.62      HIGL
ATOM    822  CG2 ILE   102      22.862  35.709 103.433  1.00 14.59      HIGL
ATOM    823  CG1 ILE   102      22.361  37.884 104.594  1.00 13.26      HIGL
ATOM    824  CD1 ILE   102      22.438  38.731 105.856  1.00 10.57      HIGL
ATOM    825  C   ILE   102      20.779  35.519 105.452  1.00 16.31      HIGL
ATOM    826  O   ILE   102      19.929  36.365 105.739  1.00 17.53      HIGL
ATOM    827  N   ASN   103      20.486  34.409 104.784  1.00 15.84      HIGL
ATOM    828  CA  ASN   103      19.118  34.174 104.347  1.00 15.26      HIGL
ATOM    829  CB  ASN   103      19.056  33.026 103.345  1.00 16.44      HIGL
ATOM    830  CG  ASN   103      17.643  32.754 102.881  1.00 17.90      HIGL
ATOM    831  OD1 ASN   103      17.012  33.606 102.251  1.00 17.31      HIGL
ATOM    832  ND2 ASN   103      17.128  31.568 103.207  1.00 18.73      HIGL
ATOM    833  C   ASN   103      18.195  33.872 105.520  1.00 14.76      HIGL
ATOM    834  O   ASN   103      17.081  34.390 105.592  1.00 14.43      HIGL
ATOM    835  N   ASN   104      18.655  33.029 106.437  1.00 14.10      HIGL
ATOM    836  CA  ASN   104      17.849  32.684 107.598  1.00 13.79      HIGL
ATOM    837  CB  ASN   104      18.391  31.424 108.277  1.00 13.76      HIGL
ATOM    838  CG  ASN   104      17.923  30.149 107.594  1.00 14.35      HIGL
ATOM    839  OD1 ASN   104      16.738  30.006 107.264  1.00 13.83      HIGL
ATOM    840  ND2 ASN   104      18.843  29.212 107.392  1.00 11.49      HIGL
ATOM    841  C   ASN   104      17.766  33.822 108.603  1.00 13.46      HIGL
ATOM    842  O   ASN   104      16.706  34.066 109.169  1.00 13.67      HIGL
ATOM    843  N   LEU   105      18.875  34.522 108.824  1.00 13.84      HIGL
ATOM    844  CA  LEU   105      18.885  35.640 109.762  1.00 14.45      HIGL
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Fig. 2 cont.

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ATOM    845  CB  LEU   105      20.282  36.256 109.855  1.00 14.35      HIGL
ATOM    846  CG  LEU   105      20.373  37.492 110.754  1.00 15.28      HIGL
ATOM    847  CD1 LEU   105      19.941  37.133 112.168  1.00 14.98      HIGL
ATOM    848  CD2 LEU   105      21.791  38.025 110.756  1.00 15.43      HIGL
ATOM    849  C   LEU   105      17.891  36.694 109.291  1.00 15.25      HIGL
ATOM    850  O   LEU   105      17.087  37.204 110.074  1.00 14.19      HIGL
ATOM    851  N   ALA   106      17.956  37.009 108.000  1.00 15.85      HIGL
ATOM    852  CA  ALA   106      17.067  37.990 107.399  1.00 17.40      HIGL
ATOM    853  CB  ALA   106      17.417  38.177 105.916  1.00 15.61      HIGL
ATOM    854  C   ALA   106      15.618  37.532 107.548  1.00 18.34      HIGL
ATOM    855  O   ALA   106      14.730  38.326 107.859  1.00 19.25      HIGL
ATOM    856  N   TRP   107      15.390  36.245 107.320  1.00 19.52      HIGL
ATOM    857  CA  TRP   107      14.060  35.663 107.430  1.00 20.70      HIGL
ATOM    858  CB  TRP   107      14.140  34.177 107.104  1.00 22.69      HIGL
ATOM    859  CG  TRP   107      12.847  33.566 106.709  1.00 26.10      HIGL
ATOM    860  CD2 TRP   107      12.607  32.179 106.453  1.00 27.36      HIGL
ATOM    861  CE2 TRP   107      11.256  32.056 106.055  1.00 28.11      HIGL
ATOM    862  CE3 TRP   107      13.404  31.028 106.517  1.00 27.84      HIGL
ATOM    863  CD1 TRP   107      11.665  34.212 106.466  1.00 26.98      HIGL
ATOM    864  NE1 TRP   107      10.705  33.310 106.072  1.00 27.36      HIGL
ATOM    865  CZ2 TRP   107      10.683  30.821 105.720  1.00 28.94      HIGL
ATOM    866  CZ3 TRP   107      12.836  29.804 106.184  1.00 28.94      HIGL
ATOM    867  CH2 TRP   107      11.487  29.711 105.790  1.00 28.79      HIGL
ATOM    868  C   TRP   107      13.567  35.862 108.862  1.00 20.80      HIGL
ATOM    869  O   TRP   107      12.428  36.280 109.097  1.00 19.49      HIGL
ATOM    870  N   LYS   108      14.453  35.567 109.812  1.00 20.81      HIGL
ATOM    871  CA  LYS   108      14.158  35.707 111.231  1.00 20.77      HIGL
ATOM    872  CB  LYS   108      15.358  35.255 112.070  1.00 21.15      HIGL
ATOM    873  CG  LYS   108      15.018  34.250 113.161  1.00 22.88      HIGL
ATOM    874  CD  LYS   108      13.942  34.770 114.100  1.00 23.37      HIGL
ATOM    875  CE  LYS   108      13.525  33.698 115.088  1.00 23.83      HIGL
ATOM    876  NZ  LYS   108      12.322  34.107 115.853  1.00 24.90      HIGL
ATOM    877  C   LYS   108      13.830  37.161 111.554  1.00 19.90      HIGL
ATOM    878  O   LYS   108      12.836  37.450 112.214  1.00 20.08      HIGL
ATOM    879  N   LEU   109      14.674  38.074 111.094  1.00 19.75      HIGL
ATOM    880  CA  LEU   109      14.445  39.488 111.344  1.00 19.93      HIGL
ATOM    881  CB  LEU   109      15.508  40.337 110.654  1.00 17.82      HIGL
ATOM    882  CG  LEU   109      15.390  41.827 110.968  1.00 17.82      HIGL
ATOM    883  CD1 LEU   109      15.672  42.054 112.449  1.00 16.38      HIGL
ATOM    884  CD2 LEU   109      16.368  42.620 110.103  1.00 16.81      HIGL
ATOM    885  C   LEU   109      13.063  39.861 110.822  1.00 20.34      HIGL
ATOM    886  O   LEU   109      12.362  40.679 111.423  1.00 20.28      HIGL
ATOM    887  N   TYR   110      12.679  39.247 109.704  1.00 20.51      HIGL
ATOM    888  CA  TYR   110      11.377  39.489 109.100  1.00 20.92      HIGL
ATOM    889  CB  TYR   110      11.309  38.862 107.704  1.00 21.24      HIGL
ATOM    890  CG  TYR   110       9.918  38.842 107.101  1.00 21.40      HIGL
ATOM    891  CD1 TYR   110       9.064  37.757 107.292  1.00 22.61      HIGL
ATOM    892  CE1 TYR   110       7.771  37.748 106.754  1.00 22.76      HIGL
ATOM    893  CD2 TYR   110       9.445  39.922 106.358  1.00 23.16      HIGL
ATOM    894  CE2 TYR   110       8.155  39.926 105.817  1.00 22.90      HIGL
ATOM    895  CZ  TYR   110       7.325  38.838 106.018  1.00 23.09      HIGL
ATOM    896  OH  TYR   110       6.056  38.849 105.482  1.00 22.70      HIGL
ATOM    897  C   TYR   110      10.249  38.938 109.972  1.00 21.45      HIGL
ATOM    898  O   TYR   110       9.312  39.671 110.303  1.00 22.10      HIGL
ATOM    899  N   ASN   111      10.326  37.659 110.344  1.00 20.73      HIGL
ATOM    900  CA  ASN   111       9.281  37.073 111.182  1.00 20.87      HIGL
ATOM    901  CB  ASN   111       9.589  35.619 111.546  1.00 23.22      HIGL
ATOM    902  CG  ASN   111       9.612  34.699 110.348  1.00 26.49      HIGL
ATOM    903  OD1 ASN   111       9.040  35.005 109.301  1.00 27.21      HIGL
ATOM    904  ND2 ASN   111      10.265  33.552 110.516  1.00 29.16      HIGL
ATOM    905  C   ASN   111       9.147  37.864 112.474  1.00 19.60      HIGL
ATOM    906  O   ASN   111       8.039  38.190 112.905  1.00 19.02      HIGL
ATOM    907  N   TYR   112      10.288  38.169 113.084  1.00 18.21      HIGL
ATOM    908  CA  TYR   112      10.310  38.905 114.337  1.00 16.83      HIGL
ATOM    909  CB  TYR   112      11.751  39.129 114.810  1.00 16.36      HIGL
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Fig. 2 cont.

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ATOM    910  CG  TYR  112      11.839  40.071 115.991  1.00 14.95      HIGL
ATOM    911  CD1 TYR  112      11.369  39.691 117.245  1.00 15.11      HIGL
ATOM    912  CE1 TYR  112      11.369  40.581 118.316  1.00 14.94      HIGL
ATOM    913  CD2 TYR  112      12.319  41.366 115.836  1.00 14.45      HIGL
ATOM    914  CE2 TYR  112      12.323  42.264 116.897  1.00 14.83      HIGL
ATOM    915  CZ  TYR  112      11.847  41.866 118.133  1.00 14.96      HIGL
ATOM    916  OH  TYR  112      11.848  42.754 119.182  1.00 15.27      HIGL
ATOM    917  C   TYR  112       9.601  40.243 114.224  1.00 16.36      HIGL
ATOM    918  O   TYR  112       8.686  40.534 114.999  1.00 15.41      HIGL
ATOM    919  N   THR  113      10.034  41.056 113.265  1.00 16.21      HIGL
ATOM    920  CA  THR  113       9.443  42.369 113.058  1.00 15.87      HIGL
ATOM    921  CB  THR  113      10.142  43.125 111.922  1.00 16.16      HIGL
ATOM    922  OG1 THR  113      11.537  43.252 112.221  1.00 15.12      HIGL
ATOM    923  CG2 THR  113       9.537  44.515 111.758  1.00 15.98      HIGL
ATOM    924  C   THR  113       7.973  42.216 112.717  1.00 16.24      HIGL
ATOM    925  O   THR  113       7.124  42.896 113.290  1.00 16.57      HIGL
ATOM    926  N   LEU  114       7.678  41.307 111.790  1.00 16.92      HIGL
ATOM    927  CA  LEU  114       6.304  41.043 111.366  1.00 16.65      HIGL
ATOM    928  CB  LEU  114       6.264  39.849 110.411  1.00 15.97      HIGL
ATOM    929  CG  LEU  114       4.861  39.423 109.964  1.00 16.54      HIGL
ATOM    930  CD1 LEU  114       4.220  40.543 109.154  1.00 15.93      HIGL
ATOM    931  CD2 LEU  114       4.948  38.144 109.146  1.00 14.91      HIGL
ATOM    932  C   LEU  114       5.404  40.754 112.565  1.00 16.56      HIGL
ATOM    933  O   LEU  114       4.420  41.450 112.799  1.00 16.01      HIGL
ATOM    934  N   ASP  115       5.749  39.720 113.320  1.00 16.95      HIGL
ATOM    935  CA  ASP  115       4.967  39.347 114.484  1.00 17.44      HIGL
ATOM    936  CB  ASP  115       5.562  38.104 115.139  1.00 18.68      HIGL
ATOM    937  CG  ASP  115       5.489  36.884 114.235  1.00 20.91      HIGL
ATOM    938  OD1 ASP  115       4.994  37.019 113.095  1.00 20.18      HIGL
ATOM    939  OD2 ASP  115       5.928  35.789 114.658  1.00 22.87      HIGL
ATOM    940  C   ASP  115       4.879  40.481 115.491  1.00 17.05      HIGL
ATOM    941  O   ASP  115       3.813  40.732 116.048  1.00 16.42      HIGL
ATOM    942  N   SER  116       5.990  41.174 115.713  1.00 16.71      HIGL
ATOM    943  CA  SER  116       6.005  42.279 116.660  1.00 17.19      HIGL
ATOM    944  CB  SER  116       7.409  42.869 116.774  1.00 17.37      HIGL
ATOM    945  OG  SER  116       8.307  41.969 117.391  1.00 17.53      HIGL
ATOM    946  C   SER  116       5.023  43.381 116.262  1.00 18.12      HIGL
ATOM    947  O   SER  116       4.231  43.847 117.084  1.00 17.59      HIGL
ATOM    948  N   MET  117       5.080  43.812 115.008  1.00 18.86      HIGL
ATOM    949  CA  MET  117       4.176  44.856 114.552  1.00 19.77      HIGL
ATOM    950  CB  MET  117       4.525  45.262 113.125  1.00 19.25      HIGL
ATOM    951  CG  MET  117       5.862  45.989 113.006  1.00 18.96      HIGL
ATOM    952  SD  MET  117       5.846  47.687 113.654  1.00 20.56      HIGL
ATOM    953  CE  MET  117       6.173  47.395 115.398  1.00 20.80      HIGL
ATOM    954  C   MET  117       2.729  44.384 114.641  1.00 20.69      HIGL
ATOM    955  O   MET  117       1.843  45.134 115.056  1.00 19.86      HIGL
ATOM    956  N   ASN  118       2.488  43.132 114.266  1.00 22.17      HIGL
ATOM    957  CA  ASN  118       1.137  42.589 114.327  1.00 23.55      HIGL
ATOM    958  CB  ASN  118       1.081  41.192 113.704  1.00 22.99      HIGL
ATOM    959  CG  ASN  118       0.966  41.236 112.197  1.00 24.24      HIGL
ATOM    960  OD1 ASN  118       0.231  42.054 111.648  1.00 24.38      HIGL
ATOM    961  ND2 ASN  118       1.680  40.345 111.516  1.00 25.71      HIGL
ATOM    962  C   ASN  118       0.665  42.536 115.772  1.00 24.12      HIGL
ATOM    963  O   ASN  118      -0.532  42.535 116.054  1.00 24.65      HIGL
ATOM    964  N   ARG  119       1.617  42.501 116.691  1.00 25.04      HIGL
ATOM    965  CA  ARG  119       1.289  42.457 118.104  1.00 25.97      HIGL
ATOM    966  CB  ARG  119       2.564  42.289 118.916  1.00 27.25      HIGL
ATOM    967  CG  ARG  119       2.324  41.905 120.343  1.00 30.86      HIGL
ATOM    968  CD  ARG  119       1.727  40.518 120.464  1.00 32.19      HIGL
ATOM    969  NE  ARG  119       1.381  40.252 121.856  1.00 35.20      HIGL
ATOM    970  CZ  ARG  119       2.266  40.036 122.826  1.00 35.79      HIGL
ATOM    971  NH1 ARG  119       3.566  40.038 122.564  1.00 35.68      HIGL
ATOM    972  NH2 ARG  119       1.845  39.846 124.070  1.00 37.32      HIGL
ATOM    973  C   ARG  119       0.572  43.755 118.483  1.00 26.06      HIGL
ATOM    974  O   ARG  119      -0.406  43.744 119.234  1.00 26.17      HIGL
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Fig. 2 cont.

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ATOM    975 N    PHE 120      1.058  44.874 117.952  1.00 25.97      HIGL
ATOM    976 CA   PHE 120      0.438  46.166 118.218  1.00 25.91      HIGL
ATOM    977 CB   PHE 120      1.369  47.312 117.811  1.00 24.71      HIGL
ATOM    978 CG   PHE 120      2.516  47.519 118.748  1.00 23.82      HIGL
ATOM    979 CD1  PHE 120      3.748  46.923 118.508  1.00 24.05      HIGL
ATOM    980 CD2  PHE 120      2.356  48.289 119.892  1.00 23.49      HIGL
ATOM    981 CE1  PHE 120      4.806  47.088 119.396  1.00 23.14      HIGL
ATOM    982 CE2  PHE 120      3.407  48.461 120.788  1.00 23.31      HIGL
ATOM    983 CZ   PHE 120      4.632  47.860 120.540  1.00 23.49      HIGL
ATOM    984 C    PHE 120     -0.879  46.283 117.452  1.00 26.35      HIGL
ATOM    985 O    PHE 120     -1.879  46.758 117.988  1.00 26.78      HIGL
ATOM    986 N    ALA 121     -0.870  45.844 116.198  1.00 26.40      HIGL
ATOM    987 CA   ALA 121     -2.058  45.891 115.357  1.00 26.80      HIGL
ATOM    988 CB   ALA 121     -1.755  45.280 114.003  1.00 27.18      HIGL
ATOM    989 C    ALA 121     -3.211  45.143 116.016  1.00 27.34      HIGL
ATOM    990 O    ALA 121     -4.314  45.674 116.152  1.00 27.77      HIGL
ATOM    991 N    ASP 122     -2.948  43.905 116.423  1.00 26.89      HIGL
ATOM    992 CA   ASP 122     -3.965  43.084 117.063  1.00 26.21      HIGL
ATOM    993 CB   ASP 122     -3.436  41.665 117.303  1.00 25.67      HIGL
ATOM    994 CG   ASP 122     -3.074  40.950 116.012  1.00 25.38      HIGL
ATOM    995 OD1  ASP 122     -3.544  41.379 114.929  1.00 24.57      HIGL
ATOM    996 OD2  ASP 122     -2.328  39.950 116.089  1.00 24.15      HIGL
ATOM    997 C    ASP 122     -4.414  43.686 118.389  1.00 26.13      HIGL
ATOM    998 O    ASP 122     -5.549  43.478 118.822  1.00 26.95      HIGL
ATOM    999 N    ALA 123     -3.517  44.427 119.033  1.00 24.90      HIGL
ATOM   1000 CA   ALA 123     -3.821  45.053 120.308  1.00 22.75      HIGL
ATOM   1001 CB   ALA 123     -2.548  45.330 121.058  1.00 23.23      HIGL
ATOM   1002 C    ALA 123     -4.595  46.344 120.102  1.00 22.12      HIGL
ATOM   1003 O    ALA 123     -5.085  46.935 121.058  1.00 22.33      HIGL
ATOM   1004 N    GLY 124     -4.704  46.778 118.850  1.00 21.85      HIGL
ATOM   1005 CA   GLY 124     -5.424  48.002 118.548  1.00 21.93      HIGL
ATOM   1006 C    GLY 124     -4.604  49.253 118.809  1.00 22.90      HIGL
ATOM   1007 O    GLY 124     -5.150  50.350 118.957  1.00 22.21      HIGL
ATOM   1008 N    ILE 125     -3.286  49.078 118.876  1.00 23.51      HIGL
ATOM   1009 CA   ILE 125     -2.352  50.174 119.113  1.00 23.71      HIGL
ATOM   1010 CB   ILE 125     -1.132  49.706 119.949  1.00 24.28      HIGL
ATOM   1011 CG2  ILE 125     -0.171  50.871 120.153  1.00 22.68      HIGL
ATOM   1012 CG1  ILE 125     -1.587  49.094 121.283  1.00 24.08      HIGL
ATOM   1013 CD1  ILE 125     -2.168  50.078 122.258  1.00 24.75      HIGL
ATOM   1014 C    ILE 125     -1.817  50.648 117.765  1.00 24.07      HIGL
ATOM   1015 O    ILE 125     -1.416  49.837 116.939  1.00 24.23      HIGL
ATOM   1016 N    GLN 126     -1.805  51.952 117.533  1.00 24.42      HIGL
ATOM   1017 CA   GLN 126     -1.282  52.451 116.274  1.00 25.40      HIGL
ATOM   1018 CB   GLN 126     -2.112  53.631 115.766  1.00 26.92      HIGL
ATOM   1019 CG   GLN 126     -1.591  54.243 114.464  1.00 29.76      HIGL
ATOM   1020 CD   GLN 126     -1.473  53.223 113.329  1.00 32.33      HIGL
ATOM   1021 OE1  GLN 126     -2.456  52.570 112.953  1.00 33.86      HIGL
ATOM   1022 NE2  GLN 126     -0.267  53.086 112.777  1.00 31.82      HIGL
ATOM   1023 C    GLN 126      0.174  52.883 116.424  1.00 25.09      HIGL
ATOM   1024 O    GLN 126      0.494  53.731 117.260  1.00 25.29      HIGL
ATOM   1025 N    VAL 127      1.046  52.280 115.617  1.00 23.64      HIGL
ATOM   1026 CA   VAL 127      2.465  52.605 115.614  1.00 21.87      HIGL
ATOM   1027 CB   VAL 127      3.329  51.373 115.255  1.00 21.30      HIGL
ATOM   1028 CG1  VAL 127      4.800  51.730 115.338  1.00 20.09      HIGL
ATOM   1029 CG2  VAL 127      3.010  50.217 116.184  1.00 20.69      HIGL
ATOM   1030 C    VAL 127      2.635  53.658 114.526  1.00 21.93      HIGL
ATOM   1031 O    VAL 127      2.268  53.427 113.378  1.00 22.89      HIGL
ATOM   1032 N    ASP 128      3.192  54.809 114.882  1.00 21.66      HIGL
ATOM   1033 CA   ASP 128      3.378  55.896 113.927  1.00 21.09      HIGL
ATOM   1034 CB   ASP 128      3.080  57.211 114.628  1.00 21.65      HIGL
ATOM   1035 CG   ASP 128      1.662  57.260 115.145  1.00 22.08      HIGL
ATOM   1036 OD1  ASP 128      0.744  57.299 114.301  1.00 23.35      HIGL
ATOM   1037 OD2  ASP 128      1.458  57.231 116.380  1.00 22.69      HIGL
ATOM   1038 C    ASP 128      4.746  55.932 113.256  1.00 21.00      HIGL
ATOM   1039 O    ASP 128      4.854  56.276 112.077  1.00 20.64      HIGL
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Fig. 2 cont.

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ATOM   1040  N   ILE  129       5.786  55.587 114.010  1.00 19.93      HIGL
ATOM   1041  CA  ILE  129       7.139  55.535 113.472  1.00 18.94      HIGL
ATOM   1042  CB  ILE  129       7.999  56.721 113.927  1.00 17.89      HIGL
ATOM   1043  CG2 ILE  129       9.425  56.533 113.444  1.00 16.07      HIGL
ATOM   1044  CG1 ILE  129       7.440  58.027 113.375  1.00 17.25      HIGL
ATOM   1045  CD1 ILE  129       8.207  59.241 113.843  1.00 16.76      HIGL
ATOM   1046  C   ILE  129       7.808  54.267 113.985  1.00 19.57      HIGL
ATOM   1047  O   ILE  129       7.591  53.867 115.130  1.00 20.12      HIGL
ATOM   1048  N   VAL  130       8.614  53.640 113.133  1.00 19.09      HIGL
ATOM   1049  CA  VAL  130       9.343  52.430 113.497  1.00 18.61      HIGL
ATOM   1050  CB  VAL  130       8.734  51.154 112.868  1.00 19.46      HIGL
ATOM   1051  CG1 VAL  130       9.424  49.923 113.431  1.00 18.88      HIGL
ATOM   1052  CG2 VAL  130       7.255  51.087 113.133  1.00 21.50      HIGL
ATOM   1053  C   VAL  130      10.762  52.531 112.962  1.00 17.57      HIGL
ATOM   1054  O   VAL  130      10.962  52.707 111.759  1.00 17.98      HIGL
ATOM   1055  N   SER  131      11.749  52.439 113.843  1.00 15.84      HIGL
ATOM   1056  CA  SER  131      13.127  52.470 113.377  1.00 14.70      HIGL
ATOM   1057  CB  SER  131      14.038  53.282 114.314  1.00 15.28      HIGL
ATOM   1058  OG  SER  131      14.319  52.589 115.514  1.00 18.11      HIGL
ATOM   1059  C   SER  131      13.565  51.018 113.345  1.00 12.96      HIGL
ATOM   1060  O   SER  131      13.436  50.299 114.335  1.00 11.68      HIGL
ATOM   1061  N   ILE  132      14.039  50.572 112.191  1.00 10.75      HIGL
ATOM   1062  CA  ILE  132      14.492  49.207 112.073  1.00 10.19      HIGL
ATOM   1063  CB  ILE  132      14.319  48.707 110.632  1.00 10.00      HIGL
ATOM   1064  CG2 ILE  132      12.858  48.371 110.380  1.00  9.71      HIGL
ATOM   1065  CG1 ILE  132      14.785  49.781 109.646  1.00 10.09      HIGL
ATOM   1066  CD1 ILE  132      14.716  49.350 108.198  1.00 10.00      HIGL
ATOM   1067  C   ILE  132      15.954  49.155 112.508  1.00 10.16      HIGL
ATOM   1068  O   ILE  132      16.869  49.045 111.693  1.00  9.89      HIGL
ATOM   1069  N   GLY  133      16.160  49.253 113.814  1.00  9.99      HIGL
ATOM   1070  CA  GLY  133      17.500  49.230 114.364  1.00 10.91      HIGL
ATOM   1071  C   GLY  133      17.711  50.461 115.220  1.00 11.73      HIGL
ATOM   1072  O   GLY  133      16.885  51.378 115.193  1.00 11.22      HIGL
ATOM   1073  N   ASN  134      18.804  50.482 115.983  1.00 11.81      HIGL
ATOM   1074  CA  ASN  134      19.119  51.621 116.843  1.00 11.67      HIGL
ATOM   1075  CB  ASN  134      18.878  51.271 118.307  1.00 11.03      HIGL
ATOM   1076  CG  ASN  134      19.010  52.481 119.217  1.00 11.61      HIGL
ATOM   1077  OD1 ASN  134      18.116  53.328 119.269  1.00  9.26      HIGL
ATOM   1078  ND2 ASN  134      20.140  52.579 119.923  1.00 10.03      HIGL
ATOM   1079  C   ASN  134      20.578  52.041 116.673  1.00 12.23      HIGL
ATOM   1080  O   ASN  134      21.488  51.299 117.047  1.00 12.50      HIGL
ATOM   1081  N   GLU  135      20.796  53.237 116.130  1.00 12.34      HIGL
ATOM   1082  CA  GLU  135      22.148  53.745 115.905  1.00 12.34      HIGL
ATOM   1083  CB  GLU  135      22.819  54.137 117.233  1.00 12.86      HIGL
ATOM   1084  CG  GLU  135      22.107  55.229 118.021  1.00 13.57      HIGL
ATOM   1085  CD  GLU  135      22.988  55.855 119.109  1.00 14.70      HIGL
ATOM   1086  OE1 GLU  135      23.605  55.107 119.895  1.00 13.98      HIGL
ATOM   1087  OE2 GLU  135      23.059  57.100 119.186  1.00 14.17      HIGL
ATOM   1088  C   GLU  135      22.980  52.662 115.217  1.00 11.83      HIGL
ATOM   1089  O   GLU  135      24.062  52.307 115.689  1.00 11.40      HIGL
ATOM   1090  N   ILE  136      22.464  52.139 114.107  1.00 11.55      HIGL
ATOM   1091  CA  ILE  136      23.145  51.086 113.366  1.00 12.33      HIGL
ATOM   1092  CB  ILE  136      22.134  50.255 112.537  1.00 11.21      HIGL
ATOM   1093  CG2 ILE  136      21.187  49.523 113.478  1.00 11.90      HIGL
ATOM   1094  CG1 ILE  136      21.346  51.166 111.583  1.00 10.88      HIGL
ATOM   1095  CD1 ILE  136      20.307  50.439 110.712  1.00  5.41      HIGL
ATOM   1096  C   ILE  136      24.272  51.570 112.446  1.00 13.31      HIGL
ATOM   1097  O   ILE  136      24.512  50.981 111.397  1.00 13.57      HIGL
ATOM   1098  N   THR  137      24.978  52.621 112.860  1.00 14.02      HIGL
ATOM   1099  CA  THR  137      26.076  53.177 112.073  1.00 15.42      HIGL
ATOM   1100  CB  THR  137      26.796  54.290 112.828  1.00 15.31      HIGL
ATOM   1101  OG1 THR  137      25.835  55.190 113.390  1.00 15.48      HIGL
ATOM   1102  CG2 THR  137      27.705  55.043 111.887  1.00 13.55      HIGL
ATOM   1103  C   THR  137      27.128  52.139 111.688  1.00 16.83      HIGL
ATOM   1104  O   THR  137      27.690  52.197 110.595  1.00 17.91      HIGL
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Fig. 2 cont.

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ATOM   1105  N   GLN   138      27.421  51.214 112.596  1.00 17.23      HIGL
ATOM   1106  CA  GLN   138      28.396  50.166 112.308  1.00 17.23      HIGL
ATOM   1107  CB  GLN   138      29.328  49.926 113.503  1.00 18.55      HIGL
ATOM   1108  CG  GLN   138      30.240  51.101 113.856  1.00 22.06      HIGL
ATOM   1109  CD  GLN   138      30.963  51.687 112.642  1.00 24.27      HIGL
ATOM   1110  OE1 GLN   138      31.641  50.975 111.897  1.00 24.26      HIGL
ATOM   1111  NE2 GLN   138      30.821  52.997 112.445  1.00 24.87      HIGL
ATOM   1112  C   GLN   138      27.633  48.886 111.985  1.00 16.30      HIGL
ATOM   1113  O   GLN   138      28.133  47.774 112.187  1.00 15.80      HIGL
ATOM   1114  N   GLY   139      26.411  49.059 111.490  1.00 14.43      HIGL
ATOM   1115  CA  GLY   139      25.590  47.917 111.138  1.00 14.15      HIGL
ATOM   1116  C   GLY   139      24.778  47.376 112.304  1.00 13.48      HIGL
ATOM   1117  O   GLY   139      24.703  48.001 113.363  1.00 11.76      HIGL
ATOM   1118  N   LEU   140      24.175  46.207 112.098  1.00 12.77      HIGL
ATOM   1119  CA  LEU   140      23.353  45.562 113.114  1.00 12.79      HIGL
ATOM   1120  CB  LEU   140      21.878  45.922 112.917  1.00 12.46      HIGL
ATOM   1121  CG  LEU   140      21.162  45.335 111.695  1.00 12.85      HIGL
ATOM   1122  CD1 LEU   140      19.672  45.582 111.817  1.00 13.35      HIGL
ATOM   1123  CD2 LEU   140      21.687  45.954 110.416  1.00 12.87      HIGL
ATOM   1124  C   LEU   140      23.504  44.055 113.010  1.00 13.36      HIGL
ATOM   1125  O   LEU   140      24.120  43.554 112.072  1.00 13.25      HIGL
ATOM   1126  N   LEU   141      22.937  43.342 113.980  1.00 13.28      HIGL
ATOM   1127  CA  LEU   141      22.975  41.883 114.008  1.00 12.60      HIGL
ATOM   1128  CB  LEU   141      21.895  41.340 113.069  1.00 10.91      HIGL
ATOM   1129  CG  LEU   141      20.481  41.627 113.587  1.00 10.89      HIGL
ATOM   1130  CD1 LEU   141      19.432  41.270 112.543  1.00  9.50      HIGL
ATOM   1131  CD2 LEU   141      20.264  40.846 114.880  1.00  8.29      HIGL
ATOM   1132  C   LEU   141      24.337  41.284 113.656  1.00 13.21      HIGL
ATOM   1133  O   LEU   141      24.462  40.504 112.708  1.00 14.64      HIGL
ATOM   1134  N   TRP   142      25.353  41.644 114.432  1.00 13.26      HIGL
ATOM   1135  CA  TRP   142      26.705  41.149 114.204  1.00 13.14      HIGL
ATOM   1136  CB  TRP   142      27.686  41.859 115.130  1.00 11.33      HIGL
ATOM   1137  CG  TRP   142      27.757  43.330 114.910  1.00 10.90      HIGL
ATOM   1138  CD2 TRP   142      28.488  44.272 115.695  1.00 11.10      HIGL
ATOM   1139  CE2 TRP   142      28.289  45.545 115.113  1.00 11.19      HIGL
ATOM   1140  CE3 TRP   142      29.290  44.167 116.835  1.00 10.40      HIGL
ATOM   1141  CD1 TRP   142      27.158  44.046 113.911  1.00 10.69      HIGL
ATOM   1142  NE1 TRP   142      27.474  45.379 114.025  1.00 10.00      HIGL
ATOM   1143  CZ2 TRP   142      28.869  46.705 115.635  1.00 11.44      HIGL
ATOM   1144  CZ3 TRP   142      29.863  45.319 117.353  1.00 11.67      HIGL
ATOM   1145  CH2 TRP   142      29.650  46.573 116.750  1.00 11.55      HIGL
ATOM   1146  C   TRP   142      26.768  39.652 114.442  1.00 13.84      HIGL
ATOM   1147  O   TRP   142      26.046  39.126 115.286  1.00 14.95      HIGL
ATOM   1148  N   PRO   143      27.680  38.952 113.751  1.00 13.87      HIGL
ATOM   1149  CD  PRO   143      27.900  37.534 114.052  1.00 13.74      HIGL
ATOM   1150  CA  PRO   143      28.675  39.417 112.776  1.00 14.76      HIGL
ATOM   1151  CB  PRO   143      29.669  38.253 112.701  1.00 13.49      HIGL
ATOM   1152  CG  PRO   143      29.386  37.438 113.918  1.00 13.80      HIGL
ATOM   1153  C   PRO   143      28.174  39.778 111.381  1.00 15.67      HIGL
ATOM   1154  O   PRO   143      28.703  40.693 110.755  1.00 16.90      HIGL
ATOM   1155  N   LEU   144      27.182  39.044 110.887  1.00 15.74      HIGL
ATOM   1156  CA  LEU   144      26.648  39.272 109.549  1.00 16.05      HIGL
ATOM   1157  CB  LEU   144      25.366  38.459 109.358  1.00 15.16      HIGL
ATOM   1158  CG  LEU   144      25.558  36.942 109.467  1.00 14.79      HIGL
ATOM   1159  CD1 LEU   144      24.214  36.248 109.414  1.00 14.16      HIGL
ATOM   1160  CD2 LEU   144      26.455  36.449 108.331  1.00 14.04      HIGL
ATOM   1161  C   LEU   144      26.397  40.727 109.159  1.00 17.32      HIGL
ATOM   1162  O   LEU   144      26.911  41.191 108.144  1.00 17.71      HIGL
ATOM   1163  N   GLY   145      25.617  41.451 109.956  1.00 17.84      HIGL
ATOM   1164  CA  GLY   145      25.325  42.835 109.617  1.00 17.98      HIGL
ATOM   1165  C   GLY   145      26.335  43.888 110.051  1.00 18.71      HIGL
ATOM   1166  O   GLY   145      26.008  45.077 110.123  1.00 19.15      HIGL
ATOM   1167  N   LYS   146      27.560  43.477 110.341  1.00 18.29      HIGL
ATOM   1168  CA  LYS   146      28.575  44.428 110.762  1.00 19.30      HIGL
ATOM   1169  CB  LYS   146      29.733  43.687 111.423  1.00 18.95      HIGL
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Fig. 2 cont.

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ATOM   1170  CG  LYS   146      30.533  44.508 112.414  1.00 18.69      HIGL
ATOM   1171  CD  LYS   146      31.624  43.643 113.039  1.00 20.37      HIGL
ATOM   1172  CE  LYS   146      32.528  44.430 113.984  1.00 20.86      HIGL
ATOM   1173  NZ  LYS   146      31.799  44.955 115.162  1.00 21.63      HIGL
ATOM   1174  C   LYS   146      29.062  45.228 109.550  1.00 20.47      HIGL
ATOM   1175  O   LYS   146      29.211  44.685 108.453  1.00 19.27      HIGL
ATOM   1176  N   THR   147      29.312  46.519 109.752  1.00 21.74      HIGL
ATOM   1177  CA  THR   147      29.746  47.374 108.659  1.00 23.27      HIGL
ATOM   1178  CB  THR   147      30.212  48.734 109.130  1.00 22.61      HIGL
ATOM   1179  OG1 THR   147      30.794  48.619 110.430  1.00 23.56      HIGL
ATOM   1180  CG2 THR   147      29.050  49.703 109.127  1.00 23.05      HIGL
ATOM   1181  C   THR   147      30.817  46.833 107.747  1.00 24.76      HIGL
ATOM   1182  O   THR   147      31.763  46.161 108.173  1.00 24.27      HIGL
ATOM   1183  N   ASN   148      30.631  47.193 106.478  1.00 26.25      HIGL
ATOM   1184  CA  ASN   148      31.456  46.818 105.346  1.00 26.20      HIGL
ATOM   1185  CB  ASN   148      32.917  46.692 105.763  1.00 26.56      HIGL
ATOM   1186  CG  ASN   148      33.560  48.057 105.998  1.00 26.62      HIGL
ATOM   1187  OD1 ASN   148      32.903  48.985 106.472  1.00 26.28      HIGL
ATOM   1188  ND2 ASN   148      34.842  48.183 105.670  1.00 25.69      HIGL
ATOM   1189  C   ASN   148      30.865  45.542 104.762  1.00 26.28      HIGL
ATOM   1190  O   ASN   148      31.279  45.076 103.707  1.00 28.00      HIGL
ATOM   1191  N   ASN   149      29.873  44.998 105.464  1.00 25.38      HIGL
ATOM   1192  CA  ASN   149      29.127  43.826 105.007  1.00 24.20      HIGL
ATOM   1193  CB  ASN   149      28.733  42.927 106.177  1.00 24.04      HIGL
ATOM   1194  CG  ASN   149      29.858  42.016 106.615  1.00 24.57      HIGL
ATOM   1195  OD1 ASN   149      31.033  42.309 106.391  1.00 25.70      HIGL
ATOM   1196  ND2 ASN   149      29.505  40.910 107.260  1.00 23.86      HIGL
ATOM   1197  C   ASN   149      27.877  44.466 104.421  1.00 23.50      HIGL
ATOM   1198  O   ASN   149      26.753  44.012 104.637  1.00 24.05      HIGL
ATOM   1199  N   TRP   150      28.101  45.554 103.698  1.00 21.67      HIGL
ATOM   1200  CA  TRP   150      27.039  46.323 103.079  1.00 20.87      HIGL
ATOM   1201  CB  TRP   150      27.649  47.265 102.045  1.00 19.65      HIGL
ATOM   1202  CG  TRP   150      28.654  48.200 102.653  1.00 19.10      HIGL
ATOM   1203  CD2 TRP   150      28.411  49.153 103.697  1.00 19.28      HIGL
ATOM   1204  CE2 TRP   150      29.631  49.828 103.938  1.00 18.98      HIGL
ATOM   1205  CE3 TRP   150      27.278  49.506 104.452  1.00 18.67      HIGL
ATOM   1206  CD1 TRP   150      29.976  48.329 102.315  1.00 18.26      HIGL
ATOM   1207  NE1 TRP   150      30.567  49.306 103.080  1.00 17.94      HIGL
ATOM   1208  CZ2 TRP   150      29.751  50.837 104.902  1.00 19.36      HIGL
ATOM   1209  CZ3 TRP   150      27.395  50.506 105.409  1.00 19.12      HIGL
ATOM   1210  CH2 TRP   150      28.627  51.162 105.626  1.00 19.64      HIGL
ATOM   1211  C   TRP   150      25.939  45.479 102.451  1.00 20.95      HIGL
ATOM   1212  O   TRP   150      24.757  45.801 102.583  1.00 21.08      HIGL
ATOM   1213  N   TYR   151      26.315  44.400 101.769  1.00 20.56      HIGL
ATOM   1214  CA  TYR   151      25.312  43.551 101.146  1.00 19.67      HIGL
ATOM   1215  CB  TYR   151      25.949  42.403 100.362  1.00 19.65      HIGL
ATOM   1216  CG  TYR   151      24.910  41.515  99.711  1.00 20.60      HIGL
ATOM   1217  CD1 TYR   151      24.183  41.962  98.610  1.00 20.83      HIGL
ATOM   1218  CE1 TYR   151      23.180  41.179  98.036  1.00 20.50      HIGL
ATOM   1219  CD2 TYR   151      24.609  40.249 100.228  1.00 20.51      HIGL
ATOM   1220  CE2 TYR   151      23.601  39.457  99.656  1.00 20.06      HIGL
ATOM   1221  CZ  TYR   151      22.894  39.933  98.559  1.00 20.06      HIGL
ATOM   1222  OH  TYR   151      21.904  39.171  97.972  1.00 19.92      HIGL
ATOM   1223  C   TYR   151      24.389  42.972 102.204  1.00 19.26      HIGL
ATOM   1224  O   TYR   151      23.176  43.114 102.113  1.00 18.33      HIGL
ATOM   1225  N   ASN   152      24.966  42.317 103.209  1.00 19.42      HIGL
ATOM   1226  CA  ASN   152      24.158  41.722 104.267  1.00 19.11      HIGL
ATOM   1227  CB  ASN   152      25.040  41.046 105.326  1.00 19.23      HIGL
ATOM   1228  CG  ASN   152      25.663  39.739 104.835  1.00 20.56      HIGL
ATOM   1229  OD1 ASN   152      25.221  39.154 103.839  1.00 19.15      HIGL
ATOM   1230  ND2 ASN   152      26.687  39.267 105.549  1.00 19.90      HIGL
ATOM   1231  C   ASN   152      23.265  42.756 104.937  1.00 18.86      HIGL
ATOM   1232  O   ASN   152      22.111  42.469 105.248  1.00 19.25      HIGL
ATOM   1233  N   ILE   153      23.792  43.958 105.154  1.00 18.55      HIGL
ATOM   1234  CA  ILE   153      23.024  45.020 105.804  1.00 18.75      HIGL
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Fig. 2 cont.

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ATOM   1235  CB  ILE   153      23.891  46.283 106.033  1.00 17.77      HIGL
ATOM   1236  CG2 ILE   153      23.053  47.395 106.623  1.00 16.52      HIGL
ATOM   1237  CG1 ILE   153      25.046  45.949 106.982  1.00 17.36      HIGL
ATOM   1238  CD1 ILE   153      26.068  47.050 107.128  1.00 16.15      HIGL
ATOM   1239  C   ILE   153      21.770  45.414 105.021  1.00 19.29      HIGL
ATOM   1240  O   ILE   153      20.653  45.369 105.557  1.00 18.88      HIGL
ATOM   1241  N   ALA   154      21.950  45.791 103.758  1.00 18.63      HIGL
ATOM   1242  CA  ALA   154      20.814  46.198 102.936  1.00 19.02      HIGL
ATOM   1243  CB  ALA   154      21.280  46.567 101.536  1.00 17.23      HIGL
ATOM   1244  C   ALA   154      19.828  45.043 102.880  1.00 19.18      HIGL
ATOM   1245  O   ALA   154      18.609  45.227 102.823  1.00 19.09      HIGL
ATOM   1246  N   ARG   155      20.393  43.846 102.908  1.00 19.15      HIGL
ATOM   1247  CA  ARG   155      19.646  42.602 102.864  1.00 18.74      HIGL
ATOM   1248  CB  ARG   155      20.661  41.461 102.775  1.00 18.99      HIGL
ATOM   1249  CG  ARG   155      20.110  40.111 102.485  1.00 19.95      HIGL
ATOM   1250  CD  ARG   155      19.495  39.997 101.104  1.00 20.00      HIGL
ATOM   1251  NE  ARG   155      18.768  38.740 101.065  1.00 21.33      HIGL
ATOM   1252  CZ  ARG   155      19.341  37.554 100.901  1.00 22.66      HIGL
ATOM   1253  NH1 ARG   155      20.655  37.462 100.728  1.00 22.62      HIGL
ATOM   1254  NH2 ARG   155      18.607  36.454 100.981  1.00 24.41      HIGL
ATOM   1255  C   ARG   155      18.798  42.509 104.142  1.00 18.62      HIGL
ATOM   1256  O   ARG   155      17.593  42.257 104.105  1.00 18.01      HIGL
ATOM   1257  N   LEU   156      19.432  42.748 105.280  1.00 18.71      HIGL
ATOM   1258  CA  LEU   156      18.725  42.688 106.548  1.00 17.91      HIGL
ATOM   1259  CB  LEU   156      19.720  42.796 107.707  1.00 16.34      HIGL
ATOM   1260  CG  LEU   156      20.507  41.507 107.927  1.00 16.27      HIGL
ATOM   1261  CD1 LEU   156      21.555  41.716 109.000  1.00 15.19      HIGL
ATOM   1262  CD2 LEU   156      19.547  40.384 108.310  1.00 15.70      HIGL
ATOM   1263  C   LEU   156      17.651  43.757 106.680  1.00 17.08      HIGL
ATOM   1264  O   LEU   156      16.531  43.472 107.097  1.00 18.08      HIGL
ATOM   1265  N   LEU   157      17.984  44.987 106.323  1.00 16.61      HIGL
ATOM   1266  CA  LEU   157      17.025  46.069 106.448  1.00 16.27      HIGL
ATOM   1267  CB  LEU   157      17.710  47.405 106.169  1.00 15.39      HIGL
ATOM   1268  CG  LEU   157      18.901  47.674 107.103  1.00 15.27      HIGL
ATOM   1269  CD1 LEU   157      19.582  48.989 106.730  1.00 14.68      HIGL
ATOM   1270  CD2 LEU   157      18.425  47.688 108.546  1.00 13.43      HIGL
ATOM   1271  C   LEU   157      15.819  45.870 105.543  1.00 16.79      HIGL
ATOM   1272  O   LEU   157      14.686  46.120 105.950  1.00 17.48      HIGL
ATOM   1273  N   HIS   158      16.050  45.403 104.321  1.00 17.58      HIGL
ATOM   1274  CA  HIS   158      14.944  45.174 103.401  1.00 17.25      HIGL
ATOM   1275  CB  HIS   158      15.439  44.552 102.099  1.00 17.36      HIGL
ATOM   1276  CG  HIS   158      14.335  44.187 101.159  1.00 18.88      HIGL
ATOM   1277  CD2 HIS   158      13.798  42.986 100.834  1.00 18.45      HIGL
ATOM   1278  ND1 HIS   158      13.587  45.133 100.484  1.00 19.56      HIGL
ATOM   1279  CE1 HIS   158      12.641  44.530  99.790  1.00 18.81      HIGL
ATOM   1280  NE2 HIS   158      12.746  43.225  99.985  1.00 19.02      HIGL
ATOM   1281  C   HIS   158      13.920  44.242 104.051  1.00 17.47      HIGL
ATOM   1282  O   HIS   158      12.723  44.531 104.066  1.00 16.46      HIGL
ATOM   1283  N   SER   159      14.402  43.127 104.592  1.00 17.53      HIGL
ATOM   1284  CA  SER   159      13.535  42.157 105.244  1.00 17.96      HIGL
ATOM   1285  CB  SER   159      14.353  40.973 105.753  1.00 18.70      HIGL
ATOM   1286  OG  SER   159      14.963  40.280 104.684  1.00 20.45      HIGL
ATOM   1287  C   SER   159      12.778  42.782 106.409  1.00 18.11      HIGL
ATOM   1288  O   SER   159      11.577  42.549 106.577  1.00 17.79      HIGL
ATOM   1289  N   ALA   160      13.483  43.573 107.214  1.00 17.67      HIGL
ATOM   1290  CA  ALA   160      12.871  44.231 108.363  1.00 17.44      HIGL
ATOM   1291  CB  ALA   160      13.929  44.922 109.187  1.00 16.81      HIGL
ATOM   1292  C   ALA   160      11.824  45.239 107.918  1.00 17.59      HIGL
ATOM   1293  O   ALA   160      10.737  45.322 108.492  1.00 17.41      HIGL
ATOM   1294  N   ALA   161      12.157  46.012 106.892  1.00 18.14      HIGL
ATOM   1295  CA  ALA   161      11.230  47.011 106.377  1.00 18.38      HIGL
ATOM   1296  CB  ALA   161      11.831  47.714 105.189  1.00 16.08      HIGL
ATOM   1297  C   ALA   161       9.931  46.337 105.974  1.00 19.43      HIGL
ATOM   1298  O   ALA   161       8.844  46.848 106.244  1.00 20.06      HIGL
ATOM   1299  N   TRP   162      10.045  45.176 105.335  1.00 19.98      HIGL
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Fig. 2 cont.

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ATOM   1300  CA  TRP   162       8.864  44.463 104.889  1.00 20.45      HIGL
ATOM   1301  CB  TRP   162       9.215  43.511 103.746  1.00 21.00      HIGL
ATOM   1302  CG  TRP   162       9.298  44.267 102.482  1.00 21.58      HIGL
ATOM   1303  CD2 TRP   162       8.222  44.516 101.575  1.00 21.96      HIGL
ATOM   1304  CE2 TRP   162       8.691  45.440 100.612  1.00 21.86      HIGL
ATOM   1305  CE3 TRP   162       6.902  44.056 101.487  1.00 22.03      HIGL
ATOM   1306  CD1 TRP   162      10.354  45.019 102.040  1.00 21.86      HIGL
ATOM   1307  NE1 TRP   162       9.995  45.729 100.919  1.00 21.88      HIGL
ATOM   1308  CZ2 TRP   162       7.884  45.913  99.572  1.00 21.45      HIGL
ATOM   1309  CZ3 TRP   162       6.096  44.530 100.448  1.00 22.27      HIGL
ATOM   1310  CH2 TRP   162       6.594  45.449  99.506  1.00 21.62      HIGL
ATOM   1311  C   TRP   162       8.108  43.746 105.982  1.00 20.46      HIGL
ATOM   1312  O   TRP   162       6.919  43.463 105.829  1.00 21.30      HIGL
ATOM   1313  N   GLY   163       8.783  43.453 107.085  1.00 19.69      HIGL
ATOM   1314  CA  GLY   163       8.089  42.816 108.182  1.00 19.99      HIGL
ATOM   1315  C   GLY   163       7.048  43.833 108.622  1.00 20.35      HIGL
ATOM   1316  O   GLY   163       5.954  43.491 109.075  1.00 20.66      HIGL
ATOM   1317  N   VAL   164       7.398  45.106 108.469  1.00 19.87      HIGL
ATOM   1318  CA  VAL   164       6.504  46.194 108.832  1.00 18.68      HIGL
ATOM   1319  CB  VAL   164       7.266  47.534 108.946  1.00 18.24      HIGL
ATOM   1320  CG1 VAL   164       6.305  48.650 109.336  1.00 17.70      HIGL
ATOM   1321  CG2 VAL   164       8.391  47.409 109.959  1.00 17.30      HIGL
ATOM   1322  C   VAL   164       5.447  46.336 107.748  1.00 18.61      HIGL
ATOM   1323  O   VAL   164       4.254  46.415 108.027  1.00 18.31      HIGL
ATOM   1324  N   LYS   165       5.891  46.356 106.502  1.00 18.63      HIGL
ATOM   1325  CA  LYS   165       4.965  46.516 105.403  1.00 19.93      HIGL
ATOM   1326  CB  LYS   165       5.728  46.615 104.087  1.00 19.36      HIGL
ATOM   1327  CG  LYS   165       6.589  47.869 103.981  1.00 18.36      HIGL
ATOM   1328  CD  LYS   165       7.335  47.923 102.644  1.00 18.25      HIGL
ATOM   1329  CE  LYS   165       8.175  49.182 102.534  1.00 17.76      HIGL
ATOM   1330  NZ  LYS   165       7.317  50.401 102.629  1.00 18.31      HIGL
ATOM   1331  C   LYS   165       3.904  45.428 105.325  1.00 20.82      HIGL
ATOM   1332  O   LYS   165       2.746  45.727 105.049  1.00 21.60      HIGL
ATOM   1333  N   ASP   166       4.283  44.179 105.581  1.00 21.39      HIGL
ATOM   1334  CA  ASP   166       3.327  43.073 105.522  1.00 22.03      HIGL
ATOM   1335  CB  ASP   166       4.039  41.749 105.219  1.00 22.56      HIGL
ATOM   1336  CG  ASP   166       4.642  41.702 103.833  1.00 23.22      HIGL
ATOM   1337  OD1 ASP   166       4.195  42.463 102.951  1.00 23.72      HIGL
ATOM   1338  OD2 ASP   166       5.560  40.879 103.623  1.00 23.83      HIGL
ATOM   1339  C   ASP   166       2.481  42.860 106.782  1.00 22.48      HIGL
ATOM   1340  O   ASP   166       1.724  41.896 106.852  1.00 22.92      HIGL
ATOM   1341  N   SER   167       2.596  43.732 107.777  1.00 22.71      HIGL
ATOM   1342  CA  SER   167       1.825  43.554 109.006  1.00 22.64      HIGL
ATOM   1343  CB  SER   167       2.519  44.259 110.169  1.00 22.61      HIGL
ATOM   1344  OG  SER   167       2.442  45.667 110.023  1.00 23.18      HIGL
ATOM   1345  C   SER   167       0.396  44.081 108.886  1.00 23.16      HIGL
ATOM   1346  O   SER   167       0.040  44.722 107.903  1.00 22.85      HIGL
ATOM   1347  N   ARG   168      -0.418  43.798 109.898  1.00 23.80      HIGL
ATOM   1348  CA  ARG   168      -1.805  44.250 109.933  1.00 23.78      HIGL
ATOM   1349  CB  ARG   168      -2.601  43.465 110.978  1.00 23.09      HIGL
ATOM   1350  CG  ARG   168      -3.597  42.463 110.420  1.00 22.15      HIGL
ATOM   1351  CD  ARG   168      -3.088  41.049 110.571  1.00 21.65      HIGL
ATOM   1352  NE  ARG   168      -2.910  40.664 111.971  1.00 18.91      HIGL
ATOM   1353  CZ  ARG   168      -2.272  39.564 112.348  1.00 18.78      HIGL
ATOM   1354  NH1 ARG   168      -1.763  38.753 111.430  1.00 18.16      HIGL
ATOM   1355  NH2 ARG   168      -2.127  39.278 113.633  1.00 19.17      HIGL
ATOM   1356  C   ARG   168      -1.890  45.734 110.284  1.00 24.65      HIGL
ATOM   1357  O   ARG   168      -2.980  46.299 110.348  1.00 25.72      HIGL
ATOM   1358  N   LEU   169      -0.751  46.366 110.534  1.00 24.93      HIGL
ATOM   1359  CA  LEU   169      -0.767  47.779 110.873  1.00 25.57      HIGL
ATOM   1360  CB  LEU   169       0.642  48.300 111.135  1.00 24.39      HIGL
ATOM   1361  CG  LEU   169       1.239  47.981 112.501  1.00 23.91      HIGL
ATOM   1362  CD1 LEU   169       2.643  48.570 112.579  1.00 23.28      HIGL
ATOM   1363  CD2 LEU   169       0.350  48.545 113.595  1.00 21.07      HIGL
ATOM   1364  C   LEU   169      -1.395  48.596 109.768  1.00 26.78      HIGL
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Fig. 2 cont.

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ATOM   1365  O   LEU   169      -1.086  48.421 108.591  1.00 26.61      HIGL
ATOM   1366  N   ASN   170      -2.292  49.485 110.160  1.00 28.98      HIGL
ATOM   1367  CA  ASN   170      -2.962  50.356 109.216  1.00 31.16      HIGL
ATOM   1368  CB  ASN   170      -4.126  49.638 108.536  1.00 34.31      HIGL
ATOM   1369  CG  ASN   170      -4.532  50.301 107.223  1.00 37.73      HIGL
ATOM   1370  OD1 ASN   170      -5.637  50.087 106.717  1.00 39.55      HIGL
ATOM   1371  ND2 ASN   170      -3.628  51.098 106.657  1.00 38.83      HIGL
ATOM   1372  C   ASN   170      -3.482  51.560 109.989  1.00 31.18      HIGL
ATOM   1373  O   ASN   170      -4.227  51.411 110.965  1.00 31.87      HIGL
ATOM   1374  N   PRO   171      -3.044  52.767 109.599  1.00 29.94      HIGL
ATOM   1375  CD  PRO   171      -3.373  54.060 110.227  1.00 29.80      HIGL
ATOM   1376  CA  PRO   171      -2.101  52.949 108.492  1.00 28.18      HIGL
ATOM   1377  CB  PRO   171      -2.094  54.459 108.295  1.00 28.38      HIGL
ATOM   1378  CG  PRO   171      -2.269  54.960 109.698  1.00 29.83      HIGL
ATOM   1379  C   PRO   171      -0.728  52.413 108.889  1.00 26.71      HIGL
ATOM   1380  O   PRO   171      -0.472  52.183 110.068  1.00 25.16      HIGL
ATOM   1381  N   LYS   172       0.139  52.204 107.900  1.00 25.19      HIGL
ATOM   1382  CA  LYS   172       1.482  51.709 108.155  1.00 24.35      HIGL
ATOM   1383  CB  LYS   172       2.119  51.187 106.867  1.00 25.60      HIGL
ATOM   1384  CG  LYS   172       1.274  50.201 106.093  1.00 27.94      HIGL
ATOM   1385  CD  LYS   172       1.253  48.826 106.725  1.00 29.37      HIGL
ATOM   1386  CE  LYS   172       0.451  47.875 105.848  1.00 30.03      HIGL
ATOM   1387  NZ  LYS   172       0.492  46.469 106.329  1.00 30.93      HIGL
ATOM   1388  C   LYS   172       2.332  52.858 108.686  1.00 22.94      HIGL
ATOM   1389  O   LYS   172       2.212  53.992 108.220  1.00 22.83      HIGL
ATOM   1390  N   PRO   173       3.200  52.580 109.671  1.00 21.18      HIGL
ATOM   1391  CD  PRO   173       3.396  51.290 110.354  1.00 21.36      HIGL
ATOM   1392  CA  PRO   173       4.069  53.599 110.254  1.00 20.28      HIGL
ATOM   1393  CB  PRO   173       4.595  52.915 111.508  1.00 20.26      HIGL
ATOM   1394  CG  PRO   173       4.718  51.502 111.059  1.00 20.58      HIGL
ATOM   1395  C   PRO   173       5.197  53.947 109.297  1.00 19.51      HIGL
ATOM   1396  O   PRO   173       5.525  53.172 108.407  1.00 19.40      HIGL
ATOM   1397  N   LYS   174       5.778  55.123 109.482  1.00 18.84      HIGL
ATOM   1398  CA  LYS   174       6.887  55.548 108.655  1.00 18.05      HIGL
ATOM   1399  CB  LYS   174       7.168  57.032 108.875  1.00 18.15      HIGL
ATOM   1400  CG  LYS   174       5.984  57.905 108.527  1.00 18.80      HIGL
ATOM   1401  CD  LYS   174       6.308  59.380 108.602  1.00 19.52      HIGL
ATOM   1402  CE  LYS   174       5.140  60.200 108.085  1.00 18.38      HIGL
ATOM   1403  NZ  LYS   174       5.521  61.622 107.893  1.00 19.70      HIGL
ATOM   1404  C   LYS   174       8.073  54.712 109.097  1.00 17.68      HIGL
ATOM   1405  O   LYS   174       8.348  54.586 110.288  1.00 18.33      HIGL
ATOM   1406  N   ILE   175       8.764  54.119 108.139  1.00 17.03      HIGL
ATOM   1407  CA  ILE   175       9.909  53.291 108.461  1.00 16.37      HIGL
ATOM   1408  CB  ILE   175      10.071  52.178 107.420  1.00 15.88      HIGL
ATOM   1409  CG2 ILE   175      11.276  51.317 107.767  1.00 14.85      HIGL
ATOM   1410  CG1 ILE   175       8.785  51.342 107.387  1.00 14.92      HIGL
ATOM   1411  CD1 ILE   175       8.694  50.358 106.232  1.00 16.47      HIGL
ATOM   1412  C   ILE   175      11.142  54.176 108.517  1.00 15.73      HIGL
ATOM   1413  O   ILE   175      11.417  54.933 107.588  1.00 15.78      HIGL
ATOM   1414  N   MET   176      11.874  54.075 109.620  1.00 14.73      HIGL
ATOM   1415  CA  MET   176      13.054  54.896 109.836  1.00 14.35      HIGL
ATOM   1416  CB  MET   176      12.830  55.786 111.070  1.00 13.52      HIGL
ATOM   1417  CG  MET   176      14.060  56.557 111.518  1.00 13.16      HIGL
ATOM   1418  SD  MET   176      13.928  57.167 113.201  1.00 14.72      HIGL
ATOM   1419  CE  MET   176      12.695  58.477 112.999  1.00 14.08      HIGL
ATOM   1420  C   MET   176      14.358  54.122 110.024  1.00 14.18      HIGL
ATOM   1421  O   MET   176      14.376  53.040 110.603  1.00 14.19      HIGL
ATOM   1422  N   VAL   177      15.444  54.693 109.511  1.00 14.60      HIGL
ATOM   1423  CA  VAL   177      16.777  54.123 109.664  1.00 13.89      HIGL
ATOM   1424  CB  VAL   177      17.532  54.024 108.319  1.00 13.58      HIGL
ATOM   1425  CG1 VAL   177      19.004  53.680 108.573  1.00 12.32      HIGL
ATOM   1426  CG2 VAL   177      16.892  52.940 107.454  1.00 12.15      HIGL
ATOM   1427  C   VAL   177      17.461  55.113 110.597  1.00 13.92      HIGL
ATOM   1428  O   VAL   177      17.503  56.314 110.326  1.00 13.57      HIGL
ATOM   1429  N   HIS   178      17.966  54.595 111.710  1.00 14.28      HIGL
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Fig. 2 cont.

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ATOM   1430 CA   HIS   178      18.591  55.407 112.743  1.00 14.37      HIGL
ATOM   1431 CB   HIS   178      17.910  55.083 114.083  1.00 14.38      HIGL
ATOM   1432 CG   HIS   178      18.522  55.762 115.268  1.00 14.85      HIGL
ATOM   1433 CD2  HIS   178      18.456  55.471 116.589  1.00 14.94      HIGL
ATOM   1434 ND1  HIS   178      19.287  56.903 115.163  1.00 15.06      HIGL
ATOM   1435 CE1  HIS   178      19.670  57.285 116.369  1.00 14.39      HIGL
ATOM   1436 NE2  HIS   178      19.179  56.434 117.251  1.00 15.19      HIGL
ATOM   1437 C    HIS   178      20.102  55.235 112.850  1.00 14.74      HIGL
ATOM   1438 O    HIS   178      20.605  54.132 113.072  1.00 14.60      HIGL
ATOM   1439 N    LEU   179      20.812  56.346 112.685  1.00 14.68      HIGL
ATOM   1440 CA   LEU   179      22.269  56.381 112.769  1.00 14.88      HIGL
ATOM   1441 CB   LEU   179      22.866  56.817 111.430  1.00 14.85      HIGL
ATOM   1442 CG   LEU   179      23.217  55.794 110.349  1.00 15.01      HIGL
ATOM   1443 CD1  LEU   179      22.120  54.786 110.177  1.00 15.16      HIGL
ATOM   1444 CD2  LEU   179      23.476  56.536 109.049  1.00 14.52      HIGL
ATOM   1445 C    LEU   179      22.632  57.406 113.830  1.00 14.77      HIGL
ATOM   1446 O    LEU   179      21.867  58.336 114.070  1.00 16.15      HIGL
ATOM   1447 N    ASP   180      23.786  57.244 114.468  1.00 14.56      HIGL
ATOM   1448 CA   ASP   180      24.217  58.200 115.483  1.00 15.13      HIGL
ATOM   1449 CB   ASP   180      25.040  57.491 116.576  1.00 15.21      HIGL
ATOM   1450 CG   ASP   180      26.496  57.238 116.171  1.00 16.64      HIGL
ATOM   1451 OD1  ASP   180      26.744  56.712 115.060  1.00 15.02      HIGL
ATOM   1452 OD2  ASP   180      27.393  57.560 116.987  1.00 16.16      HIGL
ATOM   1453 C    ASP   180      25.039  59.279 114.776  1.00 15.95      HIGL
ATOM   1454 O    ASP   180      25.185  59.233 113.555  1.00 17.25      HIGL
ATOM   1455 N    ASN   181      25.556  60.249 115.525  1.00 15.91      HIGL
ATOM   1456 CA   ASN   181      26.362  61.334 114.960  1.00 15.67      HIGL
ATOM   1457 CB   ASN   181      27.754  60.824 114.594  1.00 16.57      HIGL
ATOM   1458 CG   ASN   181      28.573  60.449 115.807  1.00 17.66      HIGL
ATOM   1459 OD1  ASN   181      28.418  61.031 116.881  1.00 19.18      HIGL
ATOM   1460 ND2  ASN   181      29.464  59.487 115.641  1.00 18.44      HIGL
ATOM   1461 C    ASN   181      25.763  62.034 113.742  1.00 15.63      HIGL
ATOM   1462 O    ASN   181      26.433  62.200 112.731  1.00 15.55      HIGL
ATOM   1463 N    GLY   182      24.508  62.455 113.847  1.00 15.79      HIGL
ATOM   1464 CA   GLY   182      23.853  63.129 112.744  1.00 15.12      HIGL
ATOM   1465 C    GLY   182      24.575  64.373 112.287  1.00 15.79      HIGL
ATOM   1466 O    GLY   182      24.331  64.857 111.184  1.00 16.16      HIGL
ATOM   1467 N    TRP   183      25.459  64.902 113.130  1.00 16.94      HIGL
ATOM   1468 CA   TRP   183      26.227  66.100 112.784  1.00 16.80      HIGL
ATOM   1469 CB   TRP   183      26.854  66.746 114.034  1.00 16.19      HIGL
ATOM   1470 CG   TRP   183      27.735  65.829 114.837  1.00 14.99      HIGL
ATOM   1471 CD2  TRP   183      29.108  65.506 114.577  1.00 14.85      HIGL
ATOM   1472 CE2  TRP   183      29.505  64.558 115.547  1.00 14.72      HIGL
ATOM   1473 CE3  TRP   183      30.041  65.922 113.616  1.00 15.26      HIGL
ATOM   1474 CD1  TRP   183      27.369  65.091 115.919  1.00 15.04      HIGL
ATOM   1475 NE1  TRP   183      28.424  64.324 116.353  1.00 14.56      HIGL
ATOM   1476 CZ2  TRP   183      30.798  64.015 115.586  1.00 13.96      HIGL
ATOM   1477 CZ3  TRP   183      31.332  65.379 113.654  1.00 14.45      HIGL
ATOM   1478 CH2  TRP   183      31.693  64.436 114.634  1.00 13.99      HIGL
ATOM   1479 C    TRP   183      27.333  65.755 111.797  1.00 17.18      HIGL
ATOM   1480 O    TRP   183      27.780  66.606 111.040  1.00 18.90      HIGL
ATOM   1481 N    ASN   184      27.780  64.508 111.807  1.00 17.37      HIGL
ATOM   1482 CA   ASN   184      28.838  64.087 110.901  1.00 18.52      HIGL
ATOM   1483 CB   ASN   184      29.623  62.936 111.514  1.00 18.43      HIGL
ATOM   1484 CG   ASN   184      30.892  62.651 110.760  1.00 18.15      HIGL
ATOM   1485 OD1  ASN   184      30.904  62.652 109.528  1.00 17.65      HIGL
ATOM   1486 ND2  ASN   184      31.972  62.403 111.490  1.00 16.66      HIGL
ATOM   1487 C    ASN   184      28.265  63.647 109.551  1.00 19.20      HIGL
ATOM   1488 O    ASN   184      27.800  62.515 109.406  1.00 19.59      HIGL
ATOM   1489 N    TRP   185      28.318  64.536 108.563  1.00 18.87      HIGL
ATOM   1490 CA   TRP   185      27.780  64.239 107.246  1.00 18.50      HIGL
ATOM   1491 CB   TRP   185      27.752  65.517 106.404  1.00 19.66      HIGL
ATOM   1492 CG   TRP   185      27.658  65.269 104.923  1.00 20.74      HIGL
ATOM   1493 CD2  TRP   185      26.584  64.623 104.224  1.00 21.65      HIGL
ATOM   1494 CE2  TRP   185      26.952  64.564 102.857  1.00 21.97      HIGL
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Fig. 2 cont.

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ATOM   1495 CE3  TRP   185      25.349  64.085 104.618  1.00 21.22      HIGL
ATOM   1496 CD1  TRP   185      28.601  65.570 103.982  1.00 20.45      HIGL
ATOM   1497 NE1  TRP   185      28.184  65.151 102.740  1.00 21.70      HIGL
ATOM   1498 CZ2  TRP   185      26.127  63.985 101.880  1.00 21.82      HIGL
ATOM   1499 CZ3  TRP   185      24.526  63.509 103.645  1.00 21.31      HIGL
ATOM   1500 CH2  TRP   185      24.921  63.465 102.292  1.00 21.28      HIGL
ATOM   1501 C    TRP   185      28.510  63.126 106.489  1.00 18.87      HIGL
ATOM   1502 O    TRP   185      27.873  62.328 105.796  1.00 18.21      HIGL
ATOM   1503 N    ASP   186      29.835  63.074 106.606  1.00 18.26      HIGL
ATOM   1504 CA   ASP   186      30.595  62.042 105.918  1.00 18.41      HIGL
ATOM   1505 CB   ASP   186      32.094  62.185 106.181  1.00 19.07      HIGL
ATOM   1506 CG   ASP   186      32.662  63.492 105.644  1.00 19.86      HIGL
ATOM   1507 OD1  ASP   186      32.235  63.922 104.546  1.00 18.31      HIGL
ATOM   1508 OD2  ASP   186      33.539  64.082 106.321  1.00 20.67      HIGL
ATOM   1509 C    ASP   186      30.127  60.669 106.375  1.00 18.79      HIGL
ATOM   1510 O    ASP   186      30.057  59.738 105.569  1.00 19.44      HIGL
ATOM   1511 N    THR   187      29.804  60.541 107.662  1.00 18.54      HIGL
ATOM   1512 CA   THR   187      29.326  59.267 108.185  1.00 18.36      HIGL
ATOM   1513 CB   THR   187      29.144  59.303 109.717  1.00 18.81      HIGL
ATOM   1514 OG1  THR   187      30.334  59.779 110.359  1.00 17.18      HIGL
ATOM   1515 CG2  THR   187      28.841  57.898 110.229  1.00 17.29      HIGL
ATOM   1516 C    THR   187      27.955  58.970 107.554  1.00 18.81      HIGL
ATOM   1517 O    THR   187      27.749  57.924 106.953  1.00 18.82      HIGL
ATOM   1518 N    GLN   188      27.028  59.912 107.690  1.00 18.92      HIGL
ATOM   1519 CA   GLN   188      25.678  59.756 107.123  1.00 18.70      HIGL
ATOM   1520 CB   GLN   188      24.868  61.025 107.278  1.00 18.92      HIGL
ATOM   1521 CG   GLN   188      24.691  61.548 108.719  1.00 20.75      HIGL
ATOM   1522 CD   GLN   188      24.217  60.494 109.715  1.00 21.45      HIGL
ATOM   1523 OE1  GLN   188      23.340  59.658 109.425  1.00 21.55      HIGL
ATOM   1524 NE2  GLN   188      24.775  60.558 110.916  1.00 20.88      HIGL
ATOM   1525 C    GLN   188      25.693  59.419 105.628  1.00 18.27      HIGL
ATOM   1526 O    GLN   188      24.854  58.643 105.144  1.00 19.06      HIGL
ATOM   1527 N    ASN   189      26.652  60.019 104.912  1.00 18.01      HIGL
ATOM   1528 CA   ASN   189      26.837  59.855 103.466  1.00 17.83      HIGL
ATOM   1529 CB   ASN   189      27.713  61.007 102.897  1.00 18.12      HIGL
ATOM   1530 CG   ASN   189      27.816  60.975 101.367  1.00 18.97      HIGL
ATOM   1531 OD1  ASN   189      27.022  60.302 100.708  1.00 18.06      HIGL
ATOM   1532 ND2  ASN   189      28.776  61.718 100.800  1.00 19.12      HIGL
ATOM   1533 C    ASN   189      27.460  58.493 103.165  1.00 17.73      HIGL
ATOM   1534 O    ASN   189      26.935  57.760 102.331  1.00 17.69      HIGL
ATOM   1535 N    TRP   190      28.583  58.180 103.812  1.00 17.17      HIGL
ATOM   1536 CA   TRP   190      29.272  56.895 103.656  1.00 16.53      HIGL
ATOM   1537 CB   TRP   190      30.409  56.855 104.679  1.00 16.92      HIGL
ATOM   1538 CG   TRP   190      30.943  55.516 105.033  1.00 17.78      HIGL
ATOM   1539 CD2  TRP   190      30.714  54.794 106.253  1.00 17.06      HIGL
ATOM   1540 CE2  TRP   190      31.490  53.620 106.192  1.00 18.29      HIGL
ATOM   1541 CE3  TRP   190      29.931  55.028 107.392  1.00 17.68      HIGL
ATOM   1542 CD1  TRP   190      31.811  54.770 104.303  1.00 18.04      HIGL
ATOM   1543 NE1  TRP   190      32.150  53.630 104.991  1.00 18.09      HIGL
ATOM   1544 CZ2  TRP   190      31.511  52.675 107.230  1.00 18.43      HIGL
ATOM   1545 CZ3  TRP   190      29.951  54.083 108.431  1.00 18.02      HIGL
ATOM   1546 CH2  TRP   190      30.738  52.925 108.336  1.00 17.37      HIGL
ATOM   1547 C    TRP   190      28.307  55.715 103.874  1.00 15.60      HIGL
ATOM   1548 O    TRP   190      28.193  54.800 103.053  1.00 16.16      HIGL
ATOM   1549 N    TRP   191      27.609  55.744 104.997  1.00 14.48      HIGL
ATOM   1550 CA   TRP   191      26.674  54.686 105.327  1.00 14.21      HIGL
ATOM   1551 CB   TRP   191      26.028  54.956 106.681  1.00 12.41      HIGL
ATOM   1552 CG   TRP   191      25.437  53.729 107.273  1.00 11.51      HIGL
ATOM   1553 CD2  TRP   191      24.101  53.250 107.097  1.00 10.28      HIGL
ATOM   1554 CE2  TRP   191      23.990  52.044 107.827  1.00 10.64      HIGL
ATOM   1555 CE3  TRP   191      22.986  53.720 106.393  1.00  7.88      HIGL
ATOM   1556 CD1  TRP   191      26.068  52.820 108.074  1.00 12.10      HIGL
ATOM   1557 NE1  TRP   191      25.208  51.805 108.413  1.00 10.86      HIGL
ATOM   1558 CZ2  TRP   191      22.808  51.304 107.876  1.00  9.13      HIGL
ATOM   1559 CZ3  TRP   191      21.818  52.988 106.440  1.00  8.78      HIGL
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Fig. 2 cont.

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ATOM   1560 CH2  TRP   191      21.735  51.790 107.178  1.00  9.52      HIGL
ATOM   1561 C    TRP   191      25.566  54.471 104.292  1.00 14.99      HIGL
ATOM   1562 O    TRP   191      25.485  53.409 103.664  1.00 14.62      HIGL
ATOM   1563 N    TYR   192      24.703  55.468 104.121  1.00 15.56      HIGL
ATOM   1564 CA   TYR   192      23.595  55.341 103.178  1.00 16.00      HIGL
ATOM   1565 CB   TYR   192      22.739  56.615 103.195  1.00 15.03      HIGL
ATOM   1566 CG   TYR   192      21.859  56.737 104.428  1.00 14.42      HIGL
ATOM   1567 CD1  TYR   192      20.759  55.886 104.617  1.00 14.00      HIGL
ATOM   1568 CE1  TYR   192      19.954  55.987 105.746  1.00 13.21      HIGL
ATOM   1569 CD2  TYR   192      22.128  57.691 105.408  1.00 13.33      HIGL
ATOM   1570 CE2  TYR   192      21.332  57.804 106.544  1.00 13.35      HIGL
ATOM   1571 CZ   TYR   192      20.244  56.950 106.709  1.00 13.89      HIGL
ATOM   1572 OH   TYR   192      19.442  57.073 107.826  1.00 12.40      HIGL
ATOM   1573 C    TYR   192      24.052  55.015 101.760  1.00 17.04      HIGL
ATOM   1574 O    TYR   192      23.433  54.199 101.071  1.00 17.52      HIGL
ATOM   1575 N    THR   193      25.137  55.643 101.325  1.00 17.90      HIGL
ATOM   1576 CA   THR   193      25.654  55.388  99.993  1.00 18.57      HIGL
ATOM   1577 CB   THR   193      26.949  56.186  99.738  1.00 19.70      HIGL
ATOM   1578 OG1  THR   193      26.634  57.582  99.645  1.00 20.25      HIGL
ATOM   1579 CG2  THR   193      27.629  55.716  98.441  1.00 17.66      HIGL
ATOM   1580 C    THR   193      25.950  53.897  99.842  1.00 18.55      HIGL
ATOM   1581 O    THR   193      25.442  53.230  98.937  1.00 18.73      HIGL
ATOM   1582 N    ASN   194      26.772  53.377 100.742  1.00 17.82      HIGL
ATOM   1583 CA   ASN   194      27.127  51.972 100.693  1.00 18.02      HIGL
ATOM   1584 CB   ASN   194      28.166  51.663 101.762  1.00 17.18      HIGL
ATOM   1585 CG   ASN   194      29.546  52.148 101.381  1.00 16.79      HIGL
ATOM   1586 OD1  ASN   194      30.135  51.668 100.411  1.00 17.28      HIGL
ATOM   1587 ND2  ASN   194      30.073  53.102 102.137  1.00 16.49      HIGL
ATOM   1588 C    ASN   194      25.934  51.031 100.830  1.00 18.35      HIGL
ATOM   1589 O    ASN   194      25.860  50.029 100.123  1.00 20.21      HIGL
ATOM   1590 N    VAL   195      25.003  51.345 101.724  1.00 17.31      HIGL
ATOM   1591 CA   VAL   195      23.838  50.495 101.908  1.00 17.12      HIGL
ATOM   1592 CB   VAL   195      23.052  50.887 103.185  1.00 17.17      HIGL
ATOM   1593 CG1  VAL   195      21.789  50.062 103.290  1.00 16.39      HIGL
ATOM   1594 CG2  VAL   195      23.906  50.675 104.411  1.00 16.35      HIGL
ATOM   1595 C    VAL   195      22.882  50.550 100.711  1.00 17.84      HIGL
ATOM   1596 O    VAL   195      22.414  49.514 100.223  1.00 17.57      HIGL
ATOM   1597 N    LEU   196      22.591  51.755 100.234  1.00 17.80      HIGL
ATOM   1598 CA   LEU   196      21.672  51.906  99.114  1.00 18.71      HIGL
ATOM   1599 CB   LEU   196      21.164  53.346  99.049  1.00 19.05      HIGL
ATOM   1600 CG   LEU   196      20.389  53.814 100.284  1.00 19.84      HIGL
ATOM   1601 CD1  LEU   196      19.935  55.255 100.071  1.00 19.18      HIGL
ATOM   1602 CD2  LEU   196      19.188  52.901 100.532  1.00 18.91      HIGL
ATOM   1603 C    LEU   196      22.219  51.490  97.745  1.00 18.86      HIGL
ATOM   1604 O    LEU   196      21.446  51.326  96.798  1.00 18.34      HIGL
ATOM   1605 N    SER   197      23.537  51.316  97.631  1.00 18.55      HIGL
ATOM   1606 CA   SER   197      24.126  50.913  96.355  1.00 18.26      HIGL
ATOM   1607 CB   SER   197      25.561  51.426  96.232  1.00 17.73      HIGL
ATOM   1608 OG   SER   197      26.436  50.722  97.091  1.00 18.32      HIGL
ATOM   1609 C    SER   197      24.113  49.397  96.184  1.00 18.38      HIGL
ATOM   1610 O    SER   197      24.322  48.884  95.088  1.00 18.24      HIGL
ATOM   1611 N    GLN   198      23.859  48.677  97.269  1.00 18.80      HIGL
ATOM   1612 CA   GLN   198      23.822  47.223  97.212  1.00 18.22      HIGL
ATOM   1613 CB   GLN   198      23.686  46.653  98.620  1.00 19.28      HIGL
ATOM   1614 CG   GLN   198      24.836  46.994  99.518  1.00 19.81      HIGL
ATOM   1615 CD   GLN   198      26.161  46.734  98.847  1.00 21.32      HIGL
ATOM   1616 OE1  GLN   198      26.353  45.693  98.210  1.00 21.68      HIGL
ATOM   1617 NE2  GLN   198      27.091  47.679  98.984  1.00 21.99      HIGL
ATOM   1618 C    GLN   198      22.682  46.707  96.340  1.00 17.65      HIGL
ATOM   1619 O    GLN   198      22.877  45.821  95.514  1.00 17.50      HIGL
ATOM   1620 N    GLY   199      21.486  47.253  96.536  1.00 17.03      HIGL
ATOM   1621 CA   GLY   199      20.347  46.821  95.745  1.00 15.62      HIGL
ATOM   1622 C    GLY   199      19.181  46.278  96.560  1.00 15.72      HIGL
ATOM   1623 O    GLY   199      18.045  46.710  96.364  1.00 15.60      HIGL
ATOM   1624 N    PRO   200      19.422  45.336  97.488  1.00 15.34      HIGL
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Fig. 2 cont.

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ATOM   1625  CD  PRO   200      20.704  44.672  97.783  1.00 14.88      HIGL
ATOM   1626  CA  PRO   200      18.350  44.764  98.306  1.00 14.92      HIGL
ATOM   1627  CB  PRO   200      19.104  43.814  99.225  1.00 16.05      HIGL
ATOM   1628  CG  PRO   200      20.245  43.367  98.366  1.00 14.92      HIGL
ATOM   1629  C   PRO   200      17.518  45.794  99.076  1.00 15.90      HIGL
ATOM   1630  O   PRO   200      16.288  45.699  99.112  1.00 14.94      HIGL
ATOM   1631  N   PHE   201      18.178  46.771  99.698  1.00 16.66      HIGL
ATOM   1632  CA  PHE   201      17.457  47.806 100.439  1.00 17.91      HIGL
ATOM   1633  CB  PHE   201      18.296  48.317 101.607  1.00 17.39      HIGL
ATOM   1634  CG  PHE   201      17.523  49.154 102.585  1.00 16.03      HIGL
ATOM   1635  CD1 PHE   201      16.320  48.696 103.108  1.00 15.39      HIGL
ATOM   1636  CD2 PHE   201      18.019  50.376 103.019  1.00 16.33      HIGL
ATOM   1637  CE1 PHE   201      15.627  49.436 104.049  1.00 16.04      HIGL
ATOM   1638  CE2 PHE   201      17.331  51.130 103.967  1.00 16.47      HIGL
ATOM   1639  CZ  PHE   201      16.133  50.658 104.484  1.00 16.02      HIGL
ATOM   1640  C   PHE   201      17.160  48.947  99.481  1.00 19.32      HIGL
ATOM   1641  O   PHE   201      18.052  49.707  99.113  1.00 19.83      HIGL
ATOM   1642  N   GLU   202      15.899  49.066  99.088  1.00 20.88      HIGL
ATOM   1643  CA  GLU   202      15.492  50.079  98.130  1.00 22.59      HIGL
ATOM   1644  CB  GLU   202      14.381  49.527  97.248  1.00 25.23      HIGL
ATOM   1645  CG  GLU   202      14.646  48.127  96.733  1.00 29.70      HIGL
ATOM   1646  CD  GLU   202      13.649  47.709  95.670  1.00 31.92      HIGL
ATOM   1647  OE1 GLU   202      13.642  48.342  94.588  1.00 33.85      HIGL
ATOM   1648  OE2 GLU   202      12.876  46.758  95.916  1.00 32.65      HIGL
ATOM   1649  C   GLU   202      15.033  51.394  98.724  1.00 22.89      HIGL
ATOM   1650  O   GLU   202      14.660  51.473  99.892  1.00 23.53      HIGL
ATOM   1651  N   MET   203      15.046  52.426  97.891  1.00 23.12      HIGL
ATOM   1652  CA  MET   203      14.624  53.748  98.309  1.00 23.40      HIGL
ATOM   1653  CB  MET   203      14.768  54.734  97.153  1.00 24.47      HIGL
ATOM   1654  CG  MET   203      16.202  55.007  96.767  1.00 27.52      HIGL
ATOM   1655  SD  MET   203      17.161  55.583  98.175  1.00 30.04      HIGL
ATOM   1656  CE  MET   203      16.411  57.199  98.411  1.00 29.30      HIGL
ATOM   1657  C   MET   203      13.185  53.748  98.808  1.00 22.78      HIGL
ATOM   1658  O   MET   203      12.835  54.522  99.696  1.00 22.95      HIGL
ATOM   1659  N   SER   204      12.352  52.878  98.251  1.00 21.87      HIGL
ATOM   1660  CA  SER   204      10.956  52.823  98.668  1.00 21.55      HIGL
ATOM   1661  CB  SER   204      10.077  52.307  97.521  1.00 21.02      HIGL
ATOM   1662  OG  SER   204      10.458  51.006  97.107  1.00 20.98      HIGL
ATOM   1663  C   SER   204      10.741  51.961  99.913  1.00 21.58      HIGL
ATOM   1664  O   SER   204       9.610  51.822 100.379  1.00 21.09      HIGL
ATOM   1665  N   ASP   205      11.821  51.388 100.448  1.00 20.89      HIGL
ATOM   1666  CA  ASP   205      11.723  50.545 101.640  1.00 20.32      HIGL
ATOM   1667  CB  ASP   205      12.882  49.539 101.716  1.00 20.48      HIGL
ATOM   1668  CG  ASP   205      12.750  48.411 100.710  1.00 19.95      HIGL
ATOM   1669  OD1 ASP   205      11.607  47.992 100.424  1.00 20.12      HIGL
ATOM   1670  OD2 ASP   205      13.792  47.933 100.220  1.00 19.93      HIGL
ATOM   1671  C   ASP   205      11.681  51.325 102.944  1.00 19.69      HIGL
ATOM   1672  O   ASP   205      11.284  50.780 103.971  1.00 19.83      HIGL
ATOM   1673  N   PHE   206      12.109  52.584 102.927  1.00 19.32      HIGL
ATOM   1674  CA  PHE   206      12.062  53.377 104.149  1.00 19.43      HIGL
ATOM   1675  CB  PHE   206      13.413  53.376 104.877  1.00 19.75      HIGL
ATOM   1676  CG  PHE   206      14.492  54.155 104.194  1.00 20.11      HIGL
ATOM   1677  CD1 PHE   206      14.975  53.768 102.951  1.00 20.98      HIGL
ATOM   1678  CD2 PHE   206      15.090  55.233 104.839  1.00 19.93      HIGL
ATOM   1679  CE1 PHE   206      16.048  54.442 102.364  1.00 20.58      HIGL
ATOM   1680  CE2 PHE   206      16.154  55.908 104.264  1.00 19.23      HIGL
ATOM   1681  CZ  PHE   206      16.636  55.509 103.025  1.00 19.95      HIGL
ATOM   1682  C   PHE   206      11.588  54.791 103.900  1.00 19.04      HIGL
ATOM   1683  O   PHE   206      11.597  55.267 102.773  1.00 19.32      HIGL
ATOM   1684  N   ASP   207      11.173  55.462 104.965  1.00 19.22      HIGL
ATOM   1685  CA  ASP   207      10.636  56.810 104.841  1.00 19.23      HIGL
ATOM   1686  CB  ASP   207       9.175  56.802 105.286  1.00 19.16      HIGL
ATOM   1687  CG  ASP   207       8.407  55.625 104.718  1.00 19.38      HIGL
ATOM   1688  OD1 ASP   207       8.277  55.543 103.480  1.00 20.06      HIGL
ATOM   1689  OD2 ASP   207       7.942  54.778 105.507  1.00 18.36      HIGL
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Fig. 2 cont.

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ATOM   1690  C   ASP   207      11.381  57.871 105.629  1.00 18.86      HIGL
ATOM   1691  O   ASP   207      11.381  59.045 105.260  1.00 19.26      HIGL
ATOM   1692  N   MET   208      12.015  57.466 106.716  1.00 18.21      HIGL
ATOM   1693  CA  MET   208      12.714  58.433 107.540  1.00 18.11      HIGL
ATOM   1694  CB  MET   208      12.006  58.596 108.894  1.00 18.41      HIGL
ATOM   1695  CG  MET   208      10.534  58.987 108.820  1.00 20.52      HIGL
ATOM   1696  SD  MET   208       9.808  59.310 110.452  1.00 22.01      HIGL
ATOM   1697  CE  MET   208      10.379  60.977 110.731  1.00 20.87      HIGL
ATOM   1698  C   MET   208      14.161  58.083 107.804  1.00 17.69      HIGL
ATOM   1699  O   MET   208      14.579  56.928 107.707  1.00 17.61      HIGL
ATOM   1700  N   MET   209      14.918  59.119 108.129  1.00 16.92      HIGL
ATOM   1701  CA  MET   209      16.308  58.994 108.488  1.00 16.07      HIGL
ATOM   1702  CB  MET   209      17.213  59.645 107.443  1.00 16.00      HIGL
ATOM   1703  CG  MET   209      17.373  58.828 106.170  1.00 16.81      HIGL
ATOM   1704  SD  MET   209      18.554  59.575 105.009  1.00 19.85      HIGL
ATOM   1705  CE  MET   209      18.496  58.407 103.621  1.00 17.63      HIGL
ATOM   1706  C   MET   209      16.374  59.747 109.809  1.00 16.16      HIGL
ATOM   1707  O   MET   209      16.174  60.969 109.850  1.00 15.45      HIGL
ATOM   1708  N   GLY   210      16.600  59.001 110.891  1.00 15.65      HIGL
ATOM   1709  CA  GLY   210      16.695  59.603 112.210  1.00 14.42      HIGL
ATOM   1710  C   GLY   210      18.150  59.686 112.629  1.00 14.08      HIGL
ATOM   1711  O   GLY   210      18.961  58.883 112.175  1.00 13.68      HIGL
ATOM   1712  N   VAL   211      18.490  60.651 113.484  1.00 13.61      HIGL
ATOM   1713  CA  VAL   211      19.869  60.802 113.936  1.00 13.15      HIGL
ATOM   1714  CB  VAL   211      20.627  61.892 113.141  1.00 12.33      HIGL
ATOM   1715  CG1 VAL   211      20.537  61.611 111.663  1.00 13.18      HIGL
ATOM   1716  CG2 VAL   211      20.067  63.271 113.465  1.00 11.20      HIGL
ATOM   1717  C   VAL   211      19.984  61.175 115.400  1.00 13.77      HIGL
ATOM   1718  O   VAL   211      19.118  61.837 115.958  1.00 13.69      HIGL
ATOM   1719  N   SER   212      21.069  60.741 116.022  1.00 15.09      HIGL
ATOM   1720  CA  SER   212      21.313  61.079 117.411  1.00 15.93      HIGL
ATOM   1721  CB  SER   212      22.016  59.929 118.130  1.00 16.46      HIGL
ATOM   1722  OG  SER   212      21.185  58.781 118.176  1.00 17.21      HIGL
ATOM   1723  C   SER   212      22.208  62.315 117.376  1.00 16.32      HIGL
ATOM   1724  O   SER   212      23.149  62.395 116.582  1.00 16.25      HIGL
ATOM   1725  N   PHE   213      21.890  63.289 118.214  1.00 15.47      HIGL
ATOM   1726  CA  PHE   213      22.666  64.512 118.267  1.00 15.45      HIGL
ATOM   1727  CB  PHE   213      21.923  65.634 117.528  1.00 15.73      HIGL
ATOM   1728  CG  PHE   213      22.673  66.936 117.484  1.00 16.40      HIGL
ATOM   1729  CD1 PHE   213      23.883  67.036 116.799  1.00 16.45      HIGL
ATOM   1730  CD2 PHE   213      22.183  68.057 118.146  1.00 16.56      HIGL
ATOM   1731  CE1 PHE   213      24.596  68.231 116.777  1.00 15.36      HIGL
ATOM   1732  CE2 PHE   213      22.889  69.257 118.130  1.00 16.74      HIGL
ATOM   1733  CZ  PHE   213      24.100  69.340 117.443  1.00 16.06      HIGL
ATOM   1734  C   PHE   213      22.849  64.850 119.738  1.00 14.96      HIGL
ATOM   1735  O   PHE   213      21.888  65.175 120.436  1.00 15.30      HIGL
ATOM   1736  N   TYR   214      24.085  64.742 120.208  1.00 14.20      HIGL
ATOM   1737  CA  TYR   214      24.420  65.016 121.600  1.00 13.58      HIGL
ATOM   1738  CB  TYR   214      24.875  63.736 122.298  1.00 12.69      HIGL
ATOM   1739  CG  TYR   214      23.775  62.742 122.558  1.00 11.90      HIGL
ATOM   1740  CD1 TYR   214      22.902  62.906 123.631  1.00 11.71      HIGL
ATOM   1741  CE1 TYR   214      21.885  61.989 123.874  1.00 11.65      HIGL
ATOM   1742  CD2 TYR   214      23.602  61.635 121.731  1.00 10.99      HIGL
ATOM   1743  CE2 TYR   214      22.591  60.717 121.962  1.00 11.61      HIGL
ATOM   1744  CZ  TYR   214      21.735  60.899 123.035  1.00 11.76      HIGL
ATOM   1745  OH  TYR   214      20.722  59.997 123.259  1.00 12.70      HIGL
ATOM   1746  C   TYR   214      25.541  66.035 121.660  1.00 14.26      HIGL
ATOM   1747  O   TYR   214      26.346  66.141 120.742  1.00 15.11      HIGL
ATOM   1748  N   PRO   215      25.619  66.794 122.755  1.00 14.63      HIGL
ATOM   1749  CD  PRO   215      24.581  67.036 123.775  1.00 14.17      HIGL
ATOM   1750  CA  PRO   215      26.682  67.790 122.847  1.00 14.95      HIGL
ATOM   1751  CB  PRO   215      25.990  68.930 123.572  1.00 14.94      HIGL
ATOM   1752  CG  PRO   215      25.175  68.176 124.596  1.00 14.41      HIGL
ATOM   1753  C   PRO   215      27.924  67.322 123.598  1.00 15.93      HIGL
ATOM   1754  O   PRO   215      28.999  67.898 123.437  1.00 16.94      HIGL
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Fig. 2 cont.

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ATOM   1755  N   PHE   216      27.778  66.276 124.405  1.00 16.00      HIGL
ATOM   1756  CA  PHE   216      28.878  65.791 125.231  1.00 16.24      HIGL
ATOM   1757  CB  PHE   216      28.350  65.520 126.644  1.00 16.24      HIGL
ATOM   1758  CG  PHE   216      27.018  64.792 126.677  1.00 16.08      HIGL
ATOM   1759  CD1 PHE   216      26.861  63.555 126.055  1.00 15.04      HIGL
ATOM   1760  CD2 PHE   216      25.924  65.347 127.343  1.00 15.16      HIGL
ATOM   1761  CE1 PHE   216      25.638  62.889 126.095  1.00 15.26      HIGL
ATOM   1762  CE2 PHE   216      24.703  64.686 127.386  1.00 14.85      HIGL
ATOM   1763  CZ  PHE   216      24.560  63.453 126.759  1.00 14.72      HIGL
ATOM   1764  C   PHE   216      29.709  64.595 124.763  1.00 16.64      HIGL
ATOM   1765  O   PHE   216      30.291  63.882 125.580  1.00 16.43      HIGL
ATOM   1766  N   TYR   217      29.789  64.377 123.459  1.00 17.14      HIGL
ATOM   1767  CA  TYR   217      30.582  63.260 122.947  1.00 17.62      HIGL
ATOM   1768  CB  TYR   217      29.675  62.193 122.323  1.00 16.27      HIGL
ATOM   1769  CG  TYR   217      28.847  61.399 123.315  1.00 16.34      HIGL
ATOM   1770  CD1 TYR   217      29.440  60.785 124.421  1.00 16.29      HIGL
ATOM   1771  CE1 TYR   217      28.687  60.024 125.312  1.00 15.97      HIGL
ATOM   1772  CD2 TYR   217      27.477  61.232 123.131  1.00 15.38      HIGL
ATOM   1773  CE2 TYR   217      26.717  60.477 124.016  1.00 14.99      HIGL
ATOM   1774  CZ  TYR   217      27.324  59.875 125.102  1.00 16.23      HIGL
ATOM   1775  OH  TYR   217      26.566  59.120 125.977  1.00 17.30      HIGL
ATOM   1776  C   TYR   217      31.605  63.723 121.909  1.00 18.43      HIGL
ATOM   1777  O   TYR   217      32.308  62.908 121.317  1.00 19.53      HIGL
ATOM   1778  N   SER   218      31.693  65.034 121.703  1.00 18.33      HIGL
ATOM   1779  CA  SER   218      32.616  65.598 120.724  1.00 17.79      HIGL
ATOM   1780  CB  SER   218      32.501  64.839 119.403  1.00 17.69      HIGL
ATOM   1781  OG  SER   218      33.128  65.542 118.347  1.00 18.59      HIGL
ATOM   1782  C   SER   218      32.298  67.070 120.485  1.00 17.69      HIGL
ATOM   1783  O   SER   218      31.141  67.438 120.306  1.00 18.71      HIGL
ATOM   1784  N   ALA   219      33.321  67.912 120.476  1.00 17.22      HIGL
ATOM   1785  CA  ALA   219      33.104  69.337 120.252  1.00 17.23      HIGL
ATOM   1786  CB  ALA   219      34.382  70.118 120.554  1.00 16.44      HIGL
ATOM   1787  C   ALA   219      32.661  69.589 118.816  1.00 16.60      HIGL
ATOM   1788  O   ALA   219      32.258  70.696 118.467  1.00 17.34      HIGL
ATOM   1789  N   SER   220      32.730  68.550 117.991  1.00 16.51      HIGL
ATOM   1790  CA  SER   220      32.355  68.641 116.581  1.00 16.08      HIGL
ATOM   1791  CB  SER   220      32.954  67.466 115.809  1.00 15.86      HIGL
ATOM   1792  OG  SER   220      34.364  67.460 115.917  1.00 16.86      HIGL
ATOM   1793  C   SER   220      30.857  68.682 116.317  1.00 15.46      HIGL
ATOM   1794  O   SER   220      30.432  69.049 115.229  1.00 14.91      HIGL
ATOM   1795  N   ALA   221      30.061  68.300 117.309  1.00 15.99      HIGL
ATOM   1796  CA  ALA   221      28.606  68.279 117.164  1.00 16.78      HIGL
ATOM   1797  CB  ALA   221      27.995  67.427 118.271  1.00 16.23      HIGL
ATOM   1798  C   ALA   221      27.969  69.673 117.164  1.00 17.33      HIGL
ATOM   1799  O   ALA   221      27.074  69.959 117.963  1.00 17.73      HIGL
ATOM   1800  N   THR   222      28.422  70.534 116.260  1.00 17.34      HIGL
ATOM   1801  CA  THR   222      27.889  71.888 116.168  1.00 17.44      HIGL
ATOM   1802  CB  THR   222      28.805  72.788 115.326  1.00 16.76      HIGL
ATOM   1803  OG1 THR   222      28.859  72.290 113.988  1.00 16.54      HIGL
ATOM   1804  CG2 THR   222      30.211  72.801 115.899  1.00 17.46      HIGL
ATOM   1805  C   THR   222      26.505  71.891 115.531  1.00 18.33      HIGL
ATOM   1806  O   THR   222      26.189  71.044 114.692  1.00 19.58      HIGL
ATOM   1807  N   LEU   223      25.675  72.842 115.933  1.00 18.21      HIGL
ATOM   1808  CA  LEU   223      24.338  72.949 115.374  1.00 18.34      HIGL
ATOM   1809  CB  LEU   223      23.611  74.143 115.991  1.00 18.27      HIGL
ATOM   1810  CG  LEU   223      23.370  74.045 117.500  1.00 19.89      HIGL
ATOM   1811  CD1 LEU   223      22.888  75.388 118.034  1.00 19.53      HIGL
ATOM   1812  CD2 LEU   223      22.340  72.943 117.786  1.00 19.06      HIGL
ATOM   1813  C   LEU   223      24.437  73.122 113.860  1.00 18.82      HIGL
ATOM   1814  O   LEU   223      23.605  72.608 113.120  1.00 20.15      HIGL
ATOM   1815  N   ASP   224      25.457  73.846 113.406  1.00 18.59      HIGL
ATOM   1816  CA  ASP   224      25.669  74.086 111.982  1.00 19.10      HIGL
ATOM   1817  CB  ASP   224      26.858  75.026 111.769  1.00 18.84      HIGL
ATOM   1818  CG  ASP   224      26.468  76.494 111.816  1.00 18.91      HIGL
ATOM   1819  OD1 ASP   224      25.286  76.812 112.069  1.00 19.14      HIGL
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Fig. 2 cont.

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ATOM   1820 OD2  ASP   224      27.355  77.341 111.593  1.00 19.90      HIGL
ATOM   1821 C    ASP   224      25.915  72.793 111.214  1.00 19.58      HIGL
ATOM   1822 O    ASP   224      25.341  72.583 110.146  1.00 20.23      HIGL
ATOM   1823 N    SER   225      26.785  71.939 111.750  1.00 19.67      HIGL
ATOM   1824 CA   SER   225      27.095  70.664 111.112  1.00 19.06      HIGL
ATOM   1825 CB   SER   225      28.155  69.908 111.907  1.00 18.84      HIGL
ATOM   1826 OG   SER   225      29.403  70.567 111.840  1.00 18.91      HIGL
ATOM   1827 C    SER   225      25.838  69.811 110.997  1.00 19.40      HIGL
ATOM   1828 O    SER   225      25.601  69.186 109.968  1.00 19.64      HIGL
ATOM   1829 N    LEU   226      25.039  69.774 112.058  1.00 19.24      HIGL
ATOM   1830 CA   LEU   226      23.799  69.009 112.026  1.00 19.90      HIGL
ATOM   1831 CB   LEU   226      23.069  69.103 113.372  1.00 18.41      HIGL
ATOM   1832 CG   LEU   226      21.655  68.517 113.419  1.00 18.06      HIGL
ATOM   1833 CD1  LEU   226      21.698  67.027 113.124  1.00 17.29      HIGL
ATOM   1834 CD2  LEU   226      21.042  68.768 114.786  1.00 18.51      HIGL
ATOM   1835 C    LEU   226      22.943  69.628 110.925  1.00 20.05      HIGL
ATOM   1836 O    LEU   226      22.369  68.932 110.086  1.00 19.89      HIGL
ATOM   1837 N    ARG   227      22.883  70.951 110.941  1.00 20.56      HIGL
ATOM   1838 CA   ARG   227      22.127  71.717 109.965  1.00 22.15      HIGL
ATOM   1839 CB   ARG   227      22.374  73.203 110.200  1.00 23.23      HIGL
ATOM   1840 CG   ARG   227      21.847  74.113 109.125  1.00 23.67      HIGL
ATOM   1841 CD   ARG   227      20.585  74.801 109.561  1.00 25.35      HIGL
ATOM   1842 NE   ARG   227      20.264  75.881 108.636  1.00 27.51      HIGL
ATOM   1843 CZ   ARG   227      20.963  77.007 108.534  1.00 27.97      HIGL
ATOM   1844 NH1  ARG   227      22.025  77.213 109.308  1.00 27.24      HIGL
ATOM   1845 NH2  ARG   227      20.609  77.919 107.639  1.00 28.04      HIGL
ATOM   1846 C    ARG   227      22.532  71.349 108.541  1.00 22.77      HIGL
ATOM   1847 O    ARG   227      21.682  71.091 107.685  1.00 23.17      HIGL
ATOM   1848 N    ARG   228      23.835  71.337 108.292  1.00 22.62      HIGL
ATOM   1849 CA   ARG   228      24.351  71.005 106.974  1.00 23.23      HIGL
ATOM   1850 CB   ARG   228      25.854  71.275 106.907  1.00 25.19      HIGL
ATOM   1851 CG   ARG   228      26.497  70.808 105.611  1.00 27.85      HIGL
ATOM   1852 CD   ARG   228      27.951  71.218 105.576  1.00 31.64      HIGL
ATOM   1853 NE   ARG   228      28.217  72.426 104.784  1.00 34.16      HIGL
ATOM   1854 CZ   ARG   228      27.482  73.539 104.787  1.00 34.92      HIGL
ATOM   1855 NH1  ARG   228      26.385  73.644 105.537  1.00 34.00      HIGL
ATOM   1856 NH2  ARG   228      27.869  74.572 104.049  1.00 34.79      HIGL
ATOM   1857 C    ARG   228      24.106  69.553 106.623  1.00 21.71      HIGL
ATOM   1858 O    ARG   228      23.697  69.233 105.511  1.00 21.40      HIGL
ATOM   1859 N    SER   229      24.372  68.677 107.583  1.00 20.74      HIGL
ATOM   1860 CA   SER   229      24.209  67.248 107.385  1.00 19.19      HIGL
ATOM   1861 CB   SER   229      24.596  66.499 108.657  1.00 17.46      HIGL
ATOM   1862 OG   SER   229      24.667  65.112 108.415  1.00 16.03      HIGL
ATOM   1863 C    SER   229      22.778  66.920 106.985  1.00 19.19      HIGL
ATOM   1864 O    SER   229      22.551  66.215 106.001  1.00 19.76      HIGL
ATOM   1865 N    LEU   230      21.816  67.443 107.738  1.00 18.51      HIGL
ATOM   1866 CA   LEU   230      20.414  67.200 107.437  1.00 18.83      HIGL
ATOM   1867 CB   LEU   230      19.513  67.904 108.459  1.00 18.57      HIGL
ATOM   1868 CG   LEU   230      19.748  67.471 109.906  1.00 18.99      HIGL
ATOM   1869 CD1  LEU   230      18.765  68.159 110.830  1.00 18.90      HIGL
ATOM   1870 CD2  LEU   230      19.611  65.966 110.011  1.00 19.09      HIGL
ATOM   1871 C    LEU   230      20.072  67.673 106.025  1.00 18.43      HIGL
ATOM   1872 O    LEU   230      19.440  66.944 105.261  1.00 18.80      HIGL
ATOM   1873 N    ASN   231      20.492  68.887 105.678  1.00 17.99      HIGL
ATOM   1874 CA   ASN   231      20.222  69.418 104.348  1.00 18.50      HIGL
ATOM   1875 CB   ASN   231      20.775  70.832 104.203  1.00 20.27      HIGL
ATOM   1876 CG   ASN   231      19.831  71.884 104.755  1.00 21.88      HIGL
ATOM   1877 OD1  ASN   231      18.703  72.029 104.276  1.00 23.81      HIGL
ATOM   1878 ND2  ASN   231      20.284  72.624 105.763  1.00 21.50      HIGL
ATOM   1879 C    ASN   231      20.815  68.529 103.271  1.00 18.28      HIGL
ATOM   1880 O    ASN   231      20.164  68.262 102.256  1.00 17.76      HIGL
ATOM   1881 N    ASN   232      22.042  68.064 103.497  1.00 17.66      HIGL
ATOM   1882 CA   ASN   232      22.703  67.190 102.534  1.00 17.99      HIGL
ATOM   1883 CB   ASN   232      24.141  66.893 102.963  1.00 17.29      HIGL
ATOM   1884 CG   ASN   232      25.037  68.116 102.915  1.00 16.38      HIGL
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Fig. 2 cont.

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ATOM   1885 OD1  ASN   232      24.686  69.141 102.334  1.00 15.50      HIGL
ATOM   1886 ND2  ASN   232      26.213  68.005 103.521  1.00 16.64      HIGL
ATOM   1887 C    ASN   232      21.948  65.872 102.375  1.00 18.25      HIGL
ATOM   1888 O    ASN   232      21.748  65.387 101.259  1.00 17.98      HIGL
ATOM   1889 N    MET   233      21.536  65.298 103.501  1.00 18.52      HIGL
ATOM   1890 CA   MET   233      20.805  64.033 103.507  1.00 18.43      HIGL
ATOM   1891 CB   MET   233      20.538  63.589 104.951  1.00 18.18      HIGL
ATOM   1892 CG   MET   233      21.795  63.269 105.754  1.00 18.25      HIGL
ATOM   1893 SD   MET   233      21.474  63.063 107.531  1.00 19.43      HIGL
ATOM   1894 CE   MET   233      20.199  61.766 107.504  1.00 17.54      HIGL
ATOM   1895 C    MET   233      19.485  64.177 102.758  1.00 18.12      HIGL
ATOM   1896 O    MET   233      19.183  63.394 101.851  1.00 18.23      HIGL
ATOM   1897 N    VAL   234      18.707  65.186 103.146  1.00 17.24      HIGL
ATOM   1898 CA   VAL   234      17.411  65.455 102.530  1.00 16.91      HIGL
ATOM   1899 CB   VAL   234      16.744  66.687 103.179  1.00 15.88      HIGL
ATOM   1900 CG1  VAL   234      15.486  67.056 102.420  1.00 15.35      HIGL
ATOM   1901 CG2  VAL   234      16.413  66.390 104.638  1.00 15.47      HIGL
ATOM   1902 C    VAL   234      17.502  65.678 101.017  1.00 16.63      HIGL
ATOM   1903 O    VAL   234      16.784  65.045 100.245  1.00 16.27      HIGL
ATOM   1904 N    SER   235      18.391  66.575 100.603  1.00 16.80      HIGL
ATOM   1905 CA   SER   235      18.573  66.882  99.190  1.00 17.13      HIGL
ATOM   1906 CB   SER   235      19.578  68.023  99.024  1.00 17.78      HIGL
ATOM   1907 OG   SER   235      19.784  68.317  97.656  1.00 17.56      HIGL
ATOM   1908 C    SER   235      19.049  65.677  98.384  1.00 16.92      HIGL
ATOM   1909 O    SER   235      18.768  65.562  97.190  1.00 17.15      HIGL
ATOM   1910 N    ARG   236      19.759  64.774  99.045  1.00 16.40      HIGL
ATOM   1911 CA   ARG   236      20.290  63.595  98.384  1.00 16.55      HIGL
ATOM   1912 CB   ARG   236      21.568  63.161  99.084  1.00 17.11      HIGL
ATOM   1913 CG   ARG   236      22.156  61.872  98.562  1.00 18.73      HIGL
ATOM   1914 CD   ARG   236      22.995  62.074  97.321  1.00 19.62      HIGL
ATOM   1915 NE   ARG   236      23.973  60.997  97.231  1.00 24.11      HIGL
ATOM   1916 CZ   ARG   236      23.732  59.794  96.710  1.00 25.92      HIGL
ATOM   1917 NH1  ARG   236      22.532  59.505  96.205  1.00 24.62      HIGL
ATOM   1918 NH2  ARG   236      24.691  58.867  96.725  1.00 25.67      HIGL
ATOM   1919 C    ARG   236      19.343  62.400  98.298  1.00 16.75      HIGL
ATOM   1920 O    ARG   236      19.259  61.740  97.259  1.00 15.62      HIGL
ATOM   1921 N    TRP   237      18.637  62.111  99.385  1.00 16.82      HIGL
ATOM   1922 CA   TRP   237      17.745  60.961  99.390  1.00 16.41      HIGL
ATOM   1923 CB   TRP   237      18.224  59.966 100.453  1.00 16.05      HIGL
ATOM   1924 CG   TRP   237      19.505  59.294 100.040  1.00 14.89      HIGL
ATOM   1925 CD2  TRP   237      20.817  59.526 100.571  1.00 14.04      HIGL
ATOM   1926 CE2  TRP   237      21.717  58.738  99.817  1.00 14.30      HIGL
ATOM   1927 CE3  TRP   237      21.322  60.327 101.604  1.00 13.86      HIGL
ATOM   1928 CD1  TRP   237      19.659  58.398  99.023  1.00 15.03      HIGL
ATOM   1929 NE1  TRP   237      20.983  58.060  98.882  1.00 14.90      HIGL
ATOM   1930 CZ2  TRP   237      23.097  58.727 100.061  1.00 13.70      HIGL
ATOM   1931 CZ3  TRP   237      22.695  60.319 101.847  1.00 13.61      HIGL
ATOM   1932 CH2  TRP   237      23.566  59.522 101.074  1.00 14.26      HIGL
ATOM   1933 C    TRP   237      16.266  61.281  99.557  1.00 16.86      HIGL
ATOM   1934 O    TRP   237      15.430  60.383  99.522  1.00 18.12      HIGL
ATOM   1935 N    GLY   238      15.953  62.562  99.732  1.00 16.74      HIGL
ATOM   1936 CA   GLY   238      14.574  62.995  99.869  1.00 16.56      HIGL
ATOM   1937 C    GLY   238      13.714  62.388 100.966  1.00 17.47      HIGL
ATOM   1938 O    GLY   238      12.486  62.346 100.836  1.00 17.51      HIGL
ATOM   1939 N    LYS   239      14.330  61.933 102.053  1.00 16.96      HIGL
ATOM   1940 CA   LYS   239      13.564  61.339 103.146  1.00 16.74      HIGL
ATOM   1941 CB   LYS   239      14.327  60.152 103.724  1.00 16.66      HIGL
ATOM   1942 CG   LYS   239      14.606  59.053 102.730  1.00 17.05      HIGL
ATOM   1943 CD   LYS   239      13.312  58.511 102.175  1.00 15.57      HIGL
ATOM   1944 CE   LYS   239      13.561  57.342 101.262  1.00 14.83      HIGL
ATOM   1945 NZ   LYS   239      12.275  56.925 100.661  1.00 14.06      HIGL
ATOM   1946 C    LYS   239      13.302  62.344 104.261  1.00 16.96      HIGL
ATOM   1947 O    LYS   239      14.036  63.323 104.398  1.00 17.61      HIGL
ATOM   1948 N    GLU   240      12.257  62.118 105.056  1.00 17.26      HIGL
ATOM   1949 CA   GLU   240      11.985  63.016 106.181  1.00 16.82      HIGL
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Fig. 2 cont.

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ATOM   1950  CB  GLU   240      10.615  62.743 106.808  1.00 17.65      HIGL
ATOM   1951  CG  GLU   240       9.430  63.085 105.923  1.00 18.86      HIGL
ATOM   1952  CD  GLU   240       8.116  63.080 106.690  1.00 20.65      HIGL
ATOM   1953  OE1 GLU   240       7.818  62.067 107.353  1.00 21.31      HIGL
ATOM   1954  OE2 GLU   240       7.381  64.091 106.634  1.00 21.43      HIGL
ATOM   1955  C   GLU   240      13.088  62.751 107.209  1.00 16.31      HIGL
ATOM   1956  O   GLU   240      13.562  61.621 107.360  1.00 15.76      HIGL
ATOM   1957  N   VAL   241      13.493  63.793 107.917  1.00 15.69      HIGL
ATOM   1958  CA  VAL   241      14.571  63.666 108.883  1.00 15.54      HIGL
ATOM   1959  CB  VAL   241      15.754  64.547 108.432  1.00 14.72      HIGL
ATOM   1960  CG1 VAL   241      16.789  64.623 109.501  1.00 17.13      HIGL
ATOM   1961  CG2 VAL   241      16.361  63.974 107.178  1.00 15.36      HIGL
ATOM   1962  C   VAL   241      14.149  64.045 110.299  1.00 15.60      HIGL
ATOM   1963  O   VAL   241      13.161  64.758 110.495  1.00 16.76      HIGL
ATOM   1964  N   ALA   242      14.900  63.573 111.290  1.00 14.40      HIGL
ATOM   1965  CA  ALA   242      14.577  63.888 112.673  1.00 13.72      HIGL
ATOM   1966  CB  ALA   242      13.286  63.177 113.082  1.00 12.95      HIGL
ATOM   1967  C   ALA   242      15.681  63.519 113.645  1.00 13.47      HIGL
ATOM   1968  O   ALA   242      16.428  62.561 113.429  1.00 13.51      HIGL
ATOM   1969  N   VAL   243      15.791  64.303 114.711  1.00 13.04      HIGL
ATOM   1970  CA  VAL   243      16.760  64.023 115.758  1.00 13.08      HIGL
ATOM   1971  CB  VAL   243      17.192  65.294 116.497  1.00 12.64      HIGL
ATOM   1972  CG1 VAL   243      17.918  64.924 117.771  1.00 12.23      HIGL
ATOM   1973  CG2 VAL   243      18.088  66.125 115.604  1.00 12.08      HIGL
ATOM   1974  C   VAL   243      15.964  63.139 116.701  1.00 13.56      HIGL
ATOM   1975  O   VAL   243      15.014  63.593 117.346  1.00 13.37      HIGL
ATOM   1976  N   VAL   244      16.328  61.866 116.754  1.00 14.00      HIGL
ATOM   1977  CA  VAL   244      15.608  60.927 117.593  1.00 14.42      HIGL
ATOM   1978  CB  VAL   244      15.476  59.569 116.877  1.00 13.73      HIGL
ATOM   1979  CG1 VAL   244      14.782  59.774 115.548  1.00 13.75      HIGL
ATOM   1980  CG2 VAL   244      16.831  58.955 116.653  1.00 12.09      HIGL
ATOM   1981  C   VAL   244      16.242  60.742 118.965  1.00 15.18      HIGL
ATOM   1982  O   VAL   244      15.748  59.965 119.783  1.00 14.93      HIGL
ATOM   1983  N   GLU   245      17.320  61.479 119.218  1.00 15.57      HIGL
ATOM   1984  CA  GLU   245      18.023  61.397 120.490  1.00 16.66      HIGL
ATOM   1985  CB  GLU   245      18.933  60.176 120.517  1.00 17.90      HIGL
ATOM   1986  CG  GLU   245      18.295  58.883 120.921  1.00 19.86      HIGL
ATOM   1987  CD  GLU   245      19.325  57.778 121.021  1.00 21.19      HIGL
ATOM   1988  OE1 GLU   245      20.395  58.018 121.624  1.00 22.19      HIGL
ATOM   1989  OE2 GLU   245      19.071  56.673 120.502  1.00 22.22      HIGL
ATOM   1990  C   GLU   245      18.892  62.616 120.780  1.00 17.25      HIGL
ATOM   1991  O   GLU   245      19.756  62.984 119.979  1.00 17.63      HIGL
ATOM   1992  N   THR   246      18.675  63.226 121.938  1.00 16.70      HIGL
ATOM   1993  CA  THR   246      19.468  64.372 122.350  1.00 16.24      HIGL
ATOM   1994  CB  THR   246      19.133  65.632 121.534  1.00 16.24      HIGL
ATOM   1995  OG1 THR   246      20.097  66.649 121.831  1.00 16.02      HIGL
ATOM   1996  CG2 THR   246      17.737  66.146 121.872  1.00 14.97      HIGL
ATOM   1997  C   THR   246      19.221  64.650 123.824  1.00 16.42      HIGL
ATOM   1998  O   THR   246      18.165  64.315 124.356  1.00 16.91      HIGL
ATOM   1999  N   ASN   247      20.206  65.256 124.475  1.00 16.16      HIGL
ATOM   2000  CA  ASN   247      20.125  65.586 125.891  1.00 16.42      HIGL
ATOM   2001  CB  ASN   247      20.753  64.482 126.754  1.00 18.32      HIGL
ATOM   2002  CG  ASN   247      19.876  63.247 126.900  1.00 19.99      HIGL
ATOM   2003  OD1 ASN   247      20.357  62.190 127.311  1.00 20.70      HIGL
ATOM   2004  ND2 ASN   247      18.593  63.374 126.587  1.00 19.85      HIGL
ATOM   2005  C   ASN   247      20.931  66.850 126.139  1.00 16.21      HIGL
ATOM   2006  O   ASN   247      21.769  67.235 125.329  1.00 16.56      HIGL
ATOM   2007  N   TRP   248      20.664  67.491 127.267  1.00 15.12      HIGL
ATOM   2008  CA  TRP   248      21.407  68.666 127.680  1.00 14.40      HIGL
ATOM   2009  CB  TRP   248      20.750  69.965 127.235  1.00 14.05      HIGL
ATOM   2010  CG  TRP   248      21.582  71.144 127.642  1.00 13.41      HIGL
ATOM   2011  CD2 TRP   248      22.789  71.592 127.020  1.00 12.55      HIGL
ATOM   2012  CE2 TRP   248      23.279  72.674 127.787  1.00 13.08      HIGL
ATOM   2013  CE3 TRP   248      23.508  71.183 125.890  1.00 12.85      HIGL
ATOM   2014  CD1 TRP   248      21.391  71.950 128.728  1.00 13.60      HIGL
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Fig. 2 cont.

ATOM	2015	NE1	TRP	248	22.408	72.870	128.824	1.00	12.73	HIGL
ATOM	2016	CZ2	TRP	248	24.457	73.352	127.458	1.00	12.54	HIGL
ATOM	2017	CZ3	TRP	248	24.679	71.857	125.564	1.00	11.70	HIGL
ATOM	2018	CH2	TRP	248	25.141	72.929	126.347	1.00	12.92	HIGL
ATOM	2019	C	TRP	248	21.404	68.570	129.188	1.00	14.62	HIGL
ATOM	2020	O	TRP	248	20.351	68.434	129.802	1.00	15.22	HIGL
ATOM	2021	N	PRO	249	22.585	68.633	129.808	1.00	14.33	HIGL
ATOM	2022	CD	PRO	249	23.925	68.623	129.197	1.00	14.04	HIGL
ATOM	2023	CA	PRO	249	22.673	68.532	131.260	1.00	14.94	HIGL
ATOM	2024	CB	PRO	249	24.099	68.041	131.468	1.00	14.74	HIGL
ATOM	2025	CG	PRO	249	24.836	68.752	130.390	1.00	13.70	HIGL
ATOM	2026	C	PRO	249	22.381	69.783	132.066	1.00	15.82	HIGL
ATOM	2027	O	PRO	249	22.594	70.895	131.604	1.00	16.63	HIGL
ATOM	2028	N	THR	250	21.882	69.578	133.282	1.00	17.24	HIGL
ATOM	2029	CA	THR	250	21.603	70.672	134.207	1.00	17.83	HIGL
ATOM	2030	CB	THR	250	20.308	70.451	134.975	1.00	16.40	HIGL
ATOM	2031	OG1	THR	250	20.478	69.353	135.875	1.00	16.53	HIGL
ATOM	2032	CG2	THR	250	19.174	70.153	134.014	1.00	17.51	HIGL
ATOM	2033	C	THR	250	22.758	70.645	135.206	1.00	18.49	HIGL
ATOM	2034	O	THR	250	22.875	71.509	136.078	1.00	19.82	HIGL
ATOM	2035	N	SER	251	23.601	69.627	135.057	1.00	18.20	HIGL
ATOM	2036	CA	SER	251	24.769	69.426	135.897	1.00	17.27	HIGL
ATOM	2037	CB	SER	251	24.373	68.700	137.181	1.00	16.80	HIGL
ATOM	2038	OG	SER	251	25.486	68.537	138.046	1.00	16.67	HIGL
ATOM	2039	C	SER	251	25.769	68.579	135.122	1.00	17.65	HIGL
ATOM	2040	O	SER	251	25.444	67.476	134.682	1.00	17.82	HIGL
ATOM	2041	N	CYS	252	26.975	69.099	134.936	1.00	17.77	HIGL
ATOM	2042	CA	CYS	252	28.012	68.359	134.218	1.00	19.00	HIGL
ATOM	2043	C	CYS	252	29.375	68.791	134.751	1.00	18.46	HIGL
ATOM	2044	O	CYS	252	30.142	69.460	134.069	1.00	18.37	HIGL
ATOM	2045	CB	CYS	252	27.940	68.611	132.703	1.00	19.48	HIGL
ATOM	2046	SG	CYS	252	28.860	67.349	131.755	1.00	21.91	HIGL
ATOM	2047	N	PRO	253	29.687	68.402	135.992	1.00	18.43	HIGL
ATOM	2048	CD	PRO	253	28.822	67.630	136.898	1.00	17.81	HIGL
ATOM	2049	CA	PRO	253	30.950	68.739	136.650	1.00	18.32	HIGL
ATOM	2050	CB	PRO	253	30.789	68.130	138.038	1.00	17.88	HIGL
ATOM	2051	CG	PRO	253	29.313	68.078	138.228	1.00	18.40	HIGL
ATOM	2052	C	PRO	253	32.191	68.204	135.952	1.00	18.83	HIGL
ATOM	2053	O	PRO	253	33.213	68.887	135.900	1.00	18.49	HIGL
ATOM	2054	N	TYR	254	32.102	66.989	135.414	1.00	19.26	HIGL
ATOM	2055	CA	TYR	254	33.256	66.378	134.766	1.00	19.93	HIGL
ATOM	2056	CB	TYR	254	33.782	65.223	135.616	1.00	19.85	HIGL
ATOM	2057	CG	TYR	254	33.909	65.574	137.076	1.00	19.85	HIGL
ATOM	2058	CD1	TYR	254	32.816	65.468	137.934	1.00	18.49	HIGL
ATOM	2059	CE1	TYR	254	32.915	65.836	139.268	1.00	18.20	HIGL
ATOM	2060	CD2	TYR	254	35.112	66.060	137.594	1.00	19.80	HIGL
ATOM	2061	CE2	TYR	254	35.218	66.434	138.930	1.00	18.50	HIGL
ATOM	2062	CZ	TYR	254	34.115	66.319	139.755	1.00	18.08	HIGL
ATOM	2063	OH	TYR	254	34.207	66.697	141.065	1.00	18.79	HIGL
ATOM	2064	C	TYR	254	33.031	65.873	133.357	1.00	21.05	HIGL
ATOM	2065	O	TYR	254	32.995	64.667	133.128	1.00	22.11	HIGL
ATOM	2066	N	PRO	255	32.898	66.789	132.387	1.00	21.11	HIGL
ATOM	2067	CD	PRO	255	33.042	68.251	132.488	1.00	20.35	HIGL
ATOM	2068	CA	PRO	255	32.684	66.391	130.999	1.00	21.28	HIGL
ATOM	2069	CB	PRO	255	32.472	67.724	130.299	1.00	21.29	HIGL
ATOM	2070	CG	PRO	255	33.369	68.632	131.075	1.00	20.00	HIGL
ATOM	2071	C	PRO	255	33.910	65.667	130.469	1.00	22.18	HIGL
ATOM	2072	O	PRO	255	35.034	66.059	130.767	1.00	22.28	HIGL
ATOM	2073	N	ARG	256	33.698	64.613	129.686	1.00	23.41	HIGL
ATOM	2074	CA	ARG	256	34.817	63.872	129.118	1.00	24.09	HIGL
ATOM	2075	CB	ARG	256	34.386	62.462	128.702	1.00	25.18	HIGL
ATOM	2076	CG	ARG	256	35.537	61.602	128.198	1.00	28.36	HIGL
ATOM	2077	CD	ARG	256	35.062	60.254	127.676	1.00	31.88	HIGL
ATOM	2078	NE	ARG	256	36.176	59.403	127.254	1.00	35.40	HIGL
ATOM	2079	CZ	ARG	256	36.043	58.228	126.636	1.00	36.69	HIGL

Fig. 2 cont.

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ATOM   2080 NH1  ARG   256      34.837  57.744 126.353  1.00 36.99      HIGL
ATOM   2081 NH2  ARG   256      37.122  57.528 126.305  1.00 37.44      HIGL
ATOM   2082 C    ARG   256      35.354  64.625 127.905  1.00 23.61      HIGL
ATOM   2083 O    ARG   256      36.538  64.553 127.593  1.00 23.73      HIGL
ATOM   2084 N    TYR   257      34.481  65.357 127.226  1.00 22.94      HIGL
ATOM   2085 CA   TYR   257      34.893  66.107 126.054  1.00 23.27      HIGL
ATOM   2086 CB   TYR   257      34.287  65.502 124.788  1.00 23.86      HIGL
ATOM   2087 CG   TYR   257      34.485  64.018 124.653  1.00 24.59      HIGL
ATOM   2088 CD1  TYR   257      33.570  63.124 125.204  1.00 25.20      HIGL
ATOM   2089 CE1  TYR   257      33.742  61.747 125.077  1.00 26.62      HIGL
ATOM   2090 CD2  TYR   257      35.585  63.502 123.970  1.00 24.88      HIGL
ATOM   2091 CE2  TYR   257      35.771  62.128 123.838  1.00 26.37      HIGL
ATOM   2092 CZ   TYR   257      34.843  61.255 124.395  1.00 27.15      HIGL
ATOM   2093 OH   TYR   257      35.018  59.895 124.276  1.00 27.95      HIGL
ATOM   2094 C    TYR   257      34.480  67.567 126.127  1.00 23.40      HIGL
ATOM   2095 O    TYR   257      33.530  67.929 126.813  1.00 23.44      HIGL
ATOM   2096 N    GLN   258      35.204  68.406 125.404  1.00 23.33      HIGL
ATOM   2097 CA   GLN   258      34.886  69.816 125.367  1.00 23.32      HIGL
ATOM   2098 CB   GLN   258      35.998  70.566 124.641  1.00 25.30      HIGL
ATOM   2099 CG   GLN   258      35.814  72.063 124.549  1.00 29.69      HIGL
ATOM   2100 CD   GLN   258      37.146  72.781 124.380  1.00 33.22      HIGL
ATOM   2101 OE1  GLN   258      37.199  73.936 123.943  1.00 34.85      HIGL
ATOM   2102 NE2  GLN   258      38.234  72.099 124.741  1.00 33.71      HIGL
ATOM   2103 C    GLN   258      33.573  69.922 124.608  1.00 21.85      HIGL
ATOM   2104 O    GLN   258      33.359  69.209 123.632  1.00 21.62      HIGL
ATOM   2105 N    PHE   259      32.680  70.784 125.067  1.00 20.74      HIGL
ATOM   2106 CA   PHE   259      31.405  70.954 124.390  1.00 20.36      HIGL
ATOM   2107 CB   PHE   259      30.415  71.652 125.318  1.00 20.17      HIGL
ATOM   2108 CG   PHE   259      29.691  70.718 126.243  1.00 20.50      HIGL
ATOM   2109 CD1  PHE   259      30.383  69.756 126.969  1.00 20.48      HIGL
ATOM   2110 CD2  PHE   259      28.310  70.803 126.391  1.00 19.48      HIGL
ATOM   2111 CE1  PHE   259      29.707  68.887 127.830  1.00 21.21      HIGL
ATOM   2112 CE2  PHE   259      27.629  69.943 127.246  1.00 19.74      HIGL
ATOM   2113 CZ   PHE   259      28.328  68.982 127.968  1.00 20.03      HIGL
ATOM   2114 C    PHE   259      31.578  71.769 123.110  1.00 20.28      HIGL
ATOM   2115 O    PHE   259      32.557  72.486 122.953  1.00 19.93      HIGL
ATOM   2116 N    PRO   260      30.637  71.651 122.165  1.00 20.85      HIGL
ATOM   2117 CD   PRO   260      29.527  70.687 122.073  1.00 20.21      HIGL
ATOM   2118 CA   PRO   260      30.766  72.427 120.924  1.00 21.17      HIGL
ATOM   2119 CB   PRO   260      29.506  72.048 120.156  1.00 21.01      HIGL
ATOM   2120 CG   PRO   260      29.291  70.617 120.584  1.00 20.56      HIGL
ATOM   2121 C    PRO   260      30.837  73.928 121.239  1.00 21.74      HIGL
ATOM   2122 O    PRO   260      30.163  74.414 122.150  1.00 21.19      HIGL
ATOM   2123 N    ALA   261      31.657  74.654 120.487  1.00 21.93      HIGL
ATOM   2124 CA   ALA   261      31.830  76.089 120.697  1.00 22.38      HIGL
ATOM   2125 CB   ALA   261      32.836  76.636 119.697  1.00 21.76      HIGL
ATOM   2126 C    ALA   261      30.540  76.901 120.621  1.00 22.55      HIGL
ATOM   2127 O    ALA   261      30.411  77.929 121.290  1.00 23.31      HIGL
ATOM   2128 N    ASP   262      29.586  76.449 119.814  1.00 22.59      HIGL
ATOM   2129 CA   ASP   262      28.331  77.173 119.674  1.00 23.66      HIGL
ATOM   2130 CB   ASP   262      27.570  76.715 118.426  1.00 24.06      HIGL
ATOM   2131 CG   ASP   262      27.368  75.206 118.369  1.00 25.82      HIGL
ATOM   2132 OD1  ASP   262      27.333  74.550 119.435  1.00 26.18      HIGL
ATOM   2133 OD2  ASP   262      27.224  74.677 117.243  1.00 26.76      HIGL
ATOM   2134 C    ASP   262      27.401  77.095 120.878  1.00 24.22      HIGL
ATOM   2135 O    ASP   262      26.449  77.866 120.965  1.00 24.88      HIGL
ATOM   2136 N    VAL   263      27.661  76.174 121.802  1.00 25.01      HIGL
ATOM   2137 CA   VAL   263      26.803  76.042 122.976  1.00 26.27      HIGL
ATOM   2138 CB   VAL   263      26.062  74.680 122.990  1.00 25.93      HIGL
ATOM   2139 CG1  VAL   263      25.179  74.554 121.757  1.00 24.73      HIGL
ATOM   2140 CG2  VAL   263      27.056  73.540 123.063  1.00 25.19      HIGL
ATOM   2141 C    VAL   263      27.525  76.211 124.309  1.00 27.53      HIGL
ATOM   2142 O    VAL   263      26.931  76.014 125.365  1.00 27.35      HIGL
ATOM   2143 N    ARG   264      28.799  76.590 124.257  1.00 29.44      HIGL
ATOM   2144 CA   ARG   264      29.595  76.782 125.466  1.00 31.50      HIGL
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Fig. 2 cont.

ATOM	2145	CB	ARG	264	31.066	76.969	125.092	1.00	32.75	HIGL
ATOM	2146	CG	ARG	264	31.645	75.755	124.389	1.00	35.35	HIGL
ATOM	2147	CD	ARG	264	33.075	75.968	123.917	1.00	37.11	HIGL
ATOM	2148	NE	ARG	264	33.550	74.810	123.161	1.00	38.51	HIGL
ATOM	2149	CZ	ARG	264	34.738	74.727	122.571	1.00	38.26	HIGL
ATOM	2150	NH1	ARG	264	35.590	75.742	122.646	1.00	38.84	HIGL
ATOM	2151	NH2	ARG	264	35.072	73.629	121.903	1.00	37.21	HIGL
ATOM	2152	C	ARG	264	29.110	77.968	126.294	1.00	31.82	HIGL
ATOM	2153	O	ARG	264	29.649	78.256	127.360	1.00	32.57	HIGL
ATOM	2154	N	ASN	265	28.086	78.648	125.796	1.00	31.94	HIGL
ATOM	2155	CA	ASN	265	27.508	79.801	126.480	1.00	31.74	HIGL
ATOM	2156	CB	ASN	265	27.189	80.893	125.464	1.00	33.87	HIGL
ATOM	2157	CG	ASN	265	26.419	80.357	124.264	1.00	35.62	HIGL
ATOM	2158	OD1	ASN	265	25.213	80.600	124.115	1.00	36.81	HIGL
ATOM	2159	ND2	ASN	265	27.113	79.608	123.407	1.00	35.24	HIGL
ATOM	2160	C	ASN	265	26.227	79.376	127.175	1.00	30.26	HIGL
ATOM	2161	O	ASN	265	25.738	80.064	128.067	1.00	31.10	HIGL
ATOM	2162	N	VAL	266	25.685	78.240	126.746	1.00	28.31	HIGL
ATOM	2163	CA	VAL	266	24.455	77.701	127.307	1.00	25.56	HIGL
ATOM	2164	CB	VAL	266	23.844	76.635	126.374	1.00	25.88	HIGL
ATOM	2165	CG1	VAL	266	22.547	76.096	126.970	1.00	25.25	HIGL
ATOM	2166	CG2	VAL	266	23.594	77.241	124.992	1.00	24.06	HIGL
ATOM	2167	C	VAL	266	24.755	77.087	128.668	1.00	23.91	HIGL
ATOM	2168	O	VAL	266	25.624	76.228	128.798	1.00	23.76	HIGL
ATOM	2169	N	PRO	267	24.038	77.534	129.706	1.00	21.98	HIGL
ATOM	2170	CD	PRO	267	23.034	78.615	129.662	1.00	20.37	HIGL
ATOM	2171	CA	PRO	267	24.216	77.047	131.075	1.00	20.98	HIGL
ATOM	2172	CB	PRO	267	23.483	78.099	131.899	1.00	20.76	HIGL
ATOM	2173	CG	PRO	267	22.349	78.475	130.996	1.00	20.01	HIGL
ATOM	2174	C	PRO	267	23.670	75.655	131.340	1.00	20.67	HIGL
ATOM	2175	O	PRO	267	22.759	75.190	130.652	1.00	20.51	HIGL
ATOM	2176	N	PHE	268	24.239	74.985	132.338	1.00	20.18	HIGL
ATOM	2177	CA	PHE	268	23.755	73.668	132.713	1.00	19.81	HIGL
ATOM	2178	CB	PHE	268	24.863	72.819	133.338	1.00	19.33	HIGL
ATOM	2179	CG	PHE	268	26.001	72.540	132.405	1.00	18.57	HIGL
ATOM	2180	CD1	PHE	268	25.755	72.175	131.079	1.00	18.00	HIGL
ATOM	2181	CD2	PHE	268	27.320	72.663	132.837	1.00	17.98	HIGL
ATOM	2182	CE1	PHE	268	26.802	71.941	130.196	1.00	17.94	HIGL
ATOM	2183	CE2	PHE	268	28.382	72.431	131.961	1.00	17.83	HIGL
ATOM	2184	CZ	PHE	268	28.121	72.070	130.635	1.00	18.17	HIGL
ATOM	2185	C	PHE	268	22.667	73.953	133.727	1.00	19.80	HIGL
ATOM	2186	O	PHE	268	22.942	74.140	134.916	1.00	19.98	HIGL
ATOM	2187	N	SER	269	21.434	74.020	133.234	1.00	18.90	HIGL
ATOM	2188	CA	SER	269	20.281	74.310	134.066	1.00	18.82	HIGL
ATOM	2189	CB	SER	269	20.339	75.752	134.567	1.00	19.28	HIGL
ATOM	2190	OG	SER	269	20.163	76.667	133.494	1.00	20.35	HIGL
ATOM	2191	C	SER	269	19.021	74.133	133.243	1.00	18.90	HIGL
ATOM	2192	O	SER	269	19.080	73.972	132.022	1.00	19.79	HIGL
ATOM	2193	N	ALA	270	17.880	74.169	133.917	1.00	17.92	HIGL
ATOM	2194	CA	ALA	270	16.604	74.030	133.245	1.00	17.69	HIGL
ATOM	2195	CB	ALA	270	15.478	74.256	134.230	1.00	17.34	HIGL
ATOM	2196	C	ALA	270	16.526	75.050	132.111	1.00	18.21	HIGL
ATOM	2197	O	ALA	270	16.018	74.752	131.028	1.00	19.17	HIGL
ATOM	2198	N	ALA	271	17.033	76.254	132.359	1.00	17.66	HIGL
ATOM	2199	CA	ALA	271	17.008	77.307	131.346	1.00	16.71	HIGL
ATOM	2200	CB	ALA	271	17.545	78.605	131.926	1.00	16.21	HIGL
ATOM	2201	C	ALA	271	17.838	76.886	130.145	1.00	16.17	HIGL
ATOM	2202	O	ALA	271	17.407	77.035	129.006	1.00	15.94	HIGL
ATOM	2203	N	GLY	272	19.024	76.348	130.415	1.00	16.09	HIGL
ATOM	2204	CA	GLY	272	19.906	75.900	129.353	1.00	16.02	HIGL
ATOM	2205	C	GLY	272	19.321	74.768	128.528	1.00	16.50	HIGL
ATOM	2206	O	GLY	272	19.527	74.700	127.316	1.00	16.42	HIGL
ATOM	2207	N	GLN	273	18.593	73.867	129.177	1.00	16.88	HIGL
ATOM	2208	CA	GLN	273	17.985	72.762	128.454	1.00	17.26	HIGL
ATOM	2209	CB	GLN	273	17.267	71.809	129.414	1.00	16.57	HIGL

Fig. 2 cont.

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ATOM   2210  CG  GLN   273      18.186  71.041 130.354  1.00 16.40      HIGL
ATOM   2211  CD  GLN   273      17.438  70.007 131.175  1.00 15.47      HIGL
ATOM   2212  OE1 GLN   273      16.479  70.330 131.868  1.00 15.89      HIGL
ATOM   2213  NE2 GLN   273      17.877  68.758 131.101  1.00 15.09      HIGL
ATOM   2214  C   GLN   273      16.986  73.323 127.452  1.00 18.10      HIGL
ATOM   2215  O   GLN   273      16.955  72.903 126.297  1.00 19.02      HIGL
ATOM   2216  N   THR   274      16.172  74.275 127.901  1.00 18.71      HIGL
ATOM   2217  CA  THR   274      15.161  74.899 127.058  1.00 19.11      HIGL
ATOM   2218  CB  THR   274      14.419  76.016 127.826  1.00 20.20      HIGL
ATOM   2219  OG1 THR   274      13.856  75.469 129.026  1.00 21.70      HIGL
ATOM   2220  CG2 THR   274      13.293  76.603 126.978  1.00 20.14      HIGL
ATOM   2221  C   THR   274      15.840  75.498 125.842  1.00 19.34      HIGL
ATOM   2222  O   THR   274      15.485  75.213 124.700  1.00 18.39      HIGL
ATOM   2223  N   GLN   275      16.838  76.325 126.115  1.00 20.37      HIGL
ATOM   2224  CA  GLN   275      17.613  76.999 125.087  1.00 21.17      HIGL
ATOM   2225  CB  GLN   275      18.747  77.761 125.766  1.00 22.42      HIGL
ATOM   2226  CG  GLN   275      19.418  78.828 124.942  1.00 25.01      HIGL
ATOM   2227  CD  GLN   275      20.454  79.578 125.759  1.00 28.13      HIGL
ATOM   2228  OE1 GLN   275      20.205  79.943 126.918  1.00 28.91      HIGL
ATOM   2229  NE2 GLN   275      21.621  79.817 125.166  1.00 29.71      HIGL
ATOM   2230  C   GLN   275      18.180  75.997 124.077  1.00 21.54      HIGL
ATOM   2231  O   GLN   275      18.022  76.167 122.866  1.00 21.25      HIGL
ATOM   2232  N   TYR   276      18.831  74.948 124.579  1.00 20.83      HIGL
ATOM   2233  CA  TYR   276      19.431  73.941 123.712  1.00 20.67      HIGL
ATOM   2234  CB  TYR   276      20.283  72.961 124.528  1.00 19.62      HIGL
ATOM   2235  CG  TYR   276      20.995  71.923 123.681  1.00 18.90      HIGL
ATOM   2236  CD1 TYR   276      22.193  72.222 123.020  1.00 18.90      HIGL
ATOM   2237  CE1 TYR   276      22.854  71.260 122.245  1.00 18.33      HIGL
ATOM   2238  CD2 TYR   276      20.471  70.641 123.540  1.00 18.85      HIGL
ATOM   2239  CE2 TYR   276      21.114  69.677 122.769  1.00 18.77      HIGL
ATOM   2240  CZ  TYR   276      22.304  69.986 122.127  1.00 19.64      HIGL
ATOM   2241  OH  TYR   276      22.938  69.006 121.391  1.00 19.63      HIGL
ATOM   2242  C   TYR   276      18.406  73.150 122.907  1.00 20.77      HIGL
ATOM   2243  O   TYR   276      18.547  72.992 121.695  1.00 20.48      HIGL
ATOM   2244  N   ILE   277      17.386  72.639 123.584  1.00 21.04      HIGL
ATOM   2245  CA  ILE   277      16.361  71.857 122.912  1.00 21.46      HIGL
ATOM   2246  CB  ILE   277      15.303  71.345 123.913  1.00 21.68      HIGL
ATOM   2247  CG2 ILE   277      14.172  70.635 123.167  1.00 21.01      HIGL
ATOM   2248  CG1 ILE   277      15.965  70.393 124.912  1.00 20.42      HIGL
ATOM   2249  CD1 ILE   277      15.058  69.950 126.033  1.00 21.50      HIGL
ATOM   2250  C   ILE   277      15.685  72.690 121.841  1.00 21.85      HIGL
ATOM   2251  O   ILE   277      15.334  72.185 120.780  1.00 21.88      HIGL
ATOM   2252  N   GLN   278      15.520  73.975 122.114  1.00 22.68      HIGL
ATOM   2253  CA  GLN   278      14.881  74.863 121.159  1.00 23.40      HIGL
ATOM   2254  CB  GLN   278      14.468  76.164 121.856  1.00 25.27      HIGL
ATOM   2255  CG  GLN   278      13.664  77.127 120.993  1.00 28.71      HIGL
ATOM   2256  CD  GLN   278      12.524  77.786 121.759  1.00 31.37      HIGL
ATOM   2257  OE1 GLN   278      12.699  78.244 122.900  1.00 32.36      HIGL
ATOM   2258  NE2 GLN   278      11.347  77.845 121.132  1.00 31.74      HIGL
ATOM   2259  C   GLN   278      15.789  75.145 119.963  1.00 22.37      HIGL
ATOM   2260  O   GLN   278      15.319  75.205 118.829  1.00 22.41      HIGL
ATOM   2261  N   SER   279      17.085  75.311 120.213  1.00 21.36      HIGL
ATOM   2262  CA  SER   279      18.042  75.563 119.137  1.00 20.77      HIGL
ATOM   2263  CB  SER   279      19.445  75.775 119.697  1.00 20.20      HIGL
ATOM   2264  OG  SER   279      19.492  76.892 120.554  1.00 21.57      HIGL
ATOM   2265  C   SER   279      18.083  74.372 118.185  1.00 20.98      HIGL
ATOM   2266  O   SER   279      18.103  74.536 116.962  1.00 21.23      HIGL
ATOM   2267  N   VAL   280      18.102  73.172 118.762  1.00 20.27      HIGL
ATOM   2268  CA  VAL   280      18.141  71.945 117.983  1.00 19.59      HIGL
ATOM   2269  CB  VAL   280      18.294  70.721 118.905  1.00 18.93      HIGL
ATOM   2270  CG1 VAL   280      18.277  69.436 118.088  1.00 18.16      HIGL
ATOM   2271  CG2 VAL   280      19.586  70.837 119.686  1.00 17.85      HIGL
ATOM   2272  C   VAL   280      16.865  71.821 117.161  1.00 19.71      HIGL
ATOM   2273  O   VAL   280      16.895  71.371 116.015  1.00 19.74      HIGL
ATOM   2274  N   ALA   281      15.744  72.229 117.746  1.00 19.63      HIGL
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Fig. 2 cont.

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ATOM   2275 CA   ALA   281      14.467  72.176 117.044  1.00 19.86      HIGL
ATOM   2276 CB   ALA   281      13.324  72.570 117.982  1.00 19.49      HIGL
ATOM   2277 C    ALA   281      14.519  73.123 115.847  1.00 19.99      HIGL
ATOM   2278 O    ALA   281      14.070  72.782 114.751  1.00 19.99      HIGL
ATOM   2279 N    ASN   282      15.080  74.309 116.056  1.00 20.40      HIGL
ATOM   2280 CA   ASN   282      15.189  75.283 114.979  1.00 21.01      HIGL
ATOM   2281 CB   ASN   282      15.867  76.562 115.463  1.00 22.58      HIGL
ATOM   2282 CG   ASN   282      15.081  77.253 116.555  1.00 25.95      HIGL
ATOM   2283 OD1  ASN   282      13.850  77.335 116.489  1.00 27.58      HIGL
ATOM   2284 ND2  ASN   282      15.786  77.765 117.567  1.00 25.99      HIGL
ATOM   2285 C    ASN   282      15.976  74.709 113.818  1.00 20.44      HIGL
ATOM   2286 O    ASN   282      15.608  74.915 112.662  1.00 21.36      HIGL
ATOM   2287 N    VAL   283      17.058  73.995 114.118  1.00 18.69      HIGL
ATOM   2288 CA   VAL   283      17.868  73.396 113.064  1.00 18.11      HIGL
ATOM   2289 CB   VAL   283      19.105  72.668 113.639  1.00 17.40      HIGL
ATOM   2290 CG1  VAL   283      19.738  71.771 112.581  1.00 15.51      HIGL
ATOM   2291 CG2  VAL   283      20.117  73.692 114.128  1.00 15.34      HIGL
ATOM   2292 C    VAL   283      17.028  72.418 112.256  1.00 18.82      HIGL
ATOM   2293 O    VAL   283      16.972  72.504 111.034  1.00 19.69      HIGL
ATOM   2294 N    VAL   284      16.365  71.497 112.942  1.00 19.82      HIGL
ATOM   2295 CA   VAL   284      15.518  70.514 112.277  1.00 20.48      HIGL
ATOM   2296 CB   VAL   284      14.874  69.570 113.304  1.00 19.52      HIGL
ATOM   2297 CG1  VAL   284      14.015  68.549 112.595  1.00 17.63      HIGL
ATOM   2298 CG2  VAL   284      15.956  68.896 114.132  1.00 18.42      HIGL
ATOM   2299 C    VAL   284      14.405  71.185 111.452  1.00 21.90      HIGL
ATOM   2300 O    VAL   284      14.205  70.863 110.279  1.00 22.17      HIGL
ATOM   2301 N    SER   285      13.685  72.117 112.068  1.00 22.19      HIGL
ATOM   2302 CA   SER   285      12.609  72.820 111.380  1.00 22.67      HIGL
ATOM   2303 CB   SER   285      11.936  73.817 112.317  1.00 22.73      HIGL
ATOM   2304 OG   SER   285      11.369  73.153 113.426  1.00 26.28      HIGL
ATOM   2305 C    SER   285      13.112  73.571 110.160  1.00 23.02      HIGL
ATOM   2306 O    SER   285      12.447  73.585 109.126  1.00 23.75      HIGL
ATOM   2307 N    SER   286      14.279  74.203 110.282  1.00 23.31      HIGL
ATOM   2308 CA   SER   286      14.848  74.975 109.177  1.00 23.26      HIGL
ATOM   2309 CB   SER   286      16.231  75.524 109.545  1.00 22.79      HIGL
ATOM   2310 OG   SER   286      17.224  74.513 109.479  1.00 22.57      HIGL
ATOM   2311 C    SER   286      14.969  74.104 107.937  1.00 23.61      HIGL
ATOM   2312 O    SER   286      14.824  74.586 106.812  1.00 24.61      HIGL
ATOM   2313 N    VAL   287      15.227  72.817 108.150  1.00 22.94      HIGL
ATOM   2314 CA   VAL   287      15.371  71.876 107.051  1.00 22.39      HIGL
ATOM   2315 CB   VAL   287      16.126  70.596 107.494  1.00 21.12      HIGL
ATOM   2316 CG1  VAL   287      16.217  69.617 106.341  1.00 19.58      HIGL
ATOM   2317 CG2  VAL   287      17.500  70.952 107.989  1.00 19.96      HIGL
ATOM   2318 C    VAL   287      14.020  71.452 106.510  1.00 22.70      HIGL
ATOM   2319 O    VAL   287      13.129  71.075 107.266  1.00 22.82      HIGL
ATOM   2320 N    SER   288      13.857  71.530 105.197  1.00 23.99      HIGL
ATOM   2321 CA   SER   288      12.609  71.083 104.598  1.00 25.42      HIGL
ATOM   2322 CB   SER   288      12.661  71.204 103.077  1.00 25.83      HIGL
ATOM   2323 OG   SER   288      13.511  70.204 102.537  1.00 26.10      HIGL
ATOM   2324 C    SER   288      12.606  69.606 104.969  1.00 25.73      HIGL
ATOM   2325 O    SER   288      13.655  68.951 104.917  1.00 27.44      HIGL
ATOM   2326 N    LYS   289      11.456  69.073 105.342  1.00 24.12      HIGL
ATOM   2327 CA   LYS   289      11.400  67.668 105.716  1.00 23.58      HIGL
ATOM   2328 CB   LYS   289      12.074  66.790 104.657  1.00 23.46      HIGL
ATOM   2329 CG   LYS   289      11.229  66.659 103.407  1.00 24.42      HIGL
ATOM   2330 CD   LYS   289      11.870  65.809 102.341  1.00 24.82      HIGL
ATOM   2331 CE   LYS   289      10.907  65.640 101.180  1.00 25.59      HIGL
ATOM   2332 NZ   LYS   289       9.680  64.915 101.624  1.00 27.30      HIGL
ATOM   2333 C    LYS   289      12.010  67.422 107.085  1.00 22.49      HIGL
ATOM   2334 O    LYS   289      12.135  66.281 107.524  1.00 22.48      HIGL
ATOM   2335 N    GLY   290      12.415  68.498 107.749  1.00 21.72      HIGL
ATOM   2336 CA   GLY   290      12.913  68.353 109.102  1.00 21.35      HIGL
ATOM   2337 C    GLY   290      11.587  68.203 109.830  1.00 20.86      HIGL
ATOM   2338 O    GLY   290      10.805  69.154 109.888  1.00 21.50      HIGL
ATOM   2339 N    VAL   291      11.305  67.029 110.379  1.00 19.98      HIGL
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Fig. 2 cont.

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ATOM   2340  CA  VAL  291      10.008  66.845 111.013  1.00 19.00      HIGL
ATOM   2341  CB  VAL  291       9.168  65.836 110.206  1.00 18.98      HIGL
ATOM   2342  CG1 VAL  291       9.040  66.301 108.764  1.00 18.95      HIGL
ATOM   2343  CG2 VAL  291       9.816  64.471 110.258  1.00 19.17      HIGL
ATOM   2344  C   VAL  291       9.927  66.441 112.479  1.00 18.36      HIGL
ATOM   2345  O   VAL  291       8.834  66.482 113.055  1.00 18.16      HIGL
ATOM   2346  N   GLY  292      11.043  66.061 113.098  1.00 16.75      HIGL
ATOM   2347  CA  GLY  292      10.943  65.657 114.489  1.00 15.82      HIGL
ATOM   2348  C   GLY  292      12.114  65.858 115.421  1.00 15.38      HIGL
ATOM   2349  O   GLY  292      13.248  66.043 114.990  1.00 15.70      HIGL
ATOM   2350  N   LEU  293      11.822  65.825 116.719  1.00 15.28      HIGL
ATOM   2351  CA  LEU  293      12.842  65.963 117.757  1.00 14.98      HIGL
ATOM   2352  CB  LEU  293      13.059  67.436 118.131  1.00 14.38      HIGL
ATOM   2353  CG  LEU  293      14.200  67.697 119.131  1.00 14.97      HIGL
ATOM   2354  CD1 LEU  293      14.507  69.175 119.180  1.00 16.01      HIGL
ATOM   2355  CD2 LEU  293      13.824  67.197 120.524  1.00 15.85      HIGL
ATOM   2356  C   LEU  293      12.450  65.168 119.006  1.00 14.59      HIGL
ATOM   2357  O   LEU  293      11.367  65.356 119.559  1.00 14.50      HIGL
ATOM   2358  N   PHE  294      13.334  64.281 119.454  1.00 14.69      HIGL
ATOM   2359  CA  PHE  294      13.047  63.487 120.644  1.00 14.76      HIGL
ATOM   2360  CB  PHE  294      12.807  62.023 120.288  1.00 13.63      HIGL
ATOM   2361  CG  PHE  294      11.566  61.788 119.496  1.00 14.32      HIGL
ATOM   2362  CD1 PHE  294      11.557  61.983 118.116  1.00 14.42      HIGL
ATOM   2363  CD2 PHE  294      10.394  61.372 120.127  1.00 14.49      HIGL
ATOM   2364  CE1 PHE  294      10.395  61.763 117.372  1.00 14.13      HIGL
ATOM   2365  CE2 PHE  294       9.225  61.149 119.397  1.00 14.10      HIGL
ATOM   2366  CZ  PHE  294       9.224  61.344 118.017  1.00 14.44      HIGL
ATOM   2367  C   PHE  294      14.152  63.552 121.684  1.00 14.75      HIGL
ATOM   2368  O   PHE  294      15.312  63.249 121.394  1.00 15.47      HIGL
ATOM   2369  N   TYR  295      13.778  63.947 122.897  1.00 14.13      HIGL
ATOM   2370  CA  TYR  295      14.716  64.024 124.006  1.00 13.77      HIGL
ATOM   2371  CB  TYR  295      14.199  64.993 125.065  1.00 13.42      HIGL
ATOM   2372  CG  TYR  295      15.267  65.439 126.031  1.00 12.18      HIGL
ATOM   2373  CD1 TYR  295      15.972  66.628 125.825  1.00 11.42      HIGL
ATOM   2374  CE1 TYR  295      16.991  67.020 126.696  1.00 11.09      HIGL
ATOM   2375  CD2 TYR  295      15.602  64.656 127.131  1.00 10.29      HIGL
ATOM   2376  CE2 TYR  295      16.612  65.040 128.004  1.00 10.79      HIGL
ATOM   2377  CZ  TYR  295      17.304  66.217 127.782  1.00 10.57      HIGL
ATOM   2378  OH  TYR  295      18.317  66.569 128.640  1.00  9.73      HIGL
ATOM   2379  C   TYR  295      14.783  62.609 124.586  1.00 13.63      HIGL
ATOM   2380  O   TYR  295      13.747  61.970 124.793  1.00 13.59      HIGL
ATOM   2381  N   TRP  296      15.990  62.120 124.854  1.00 12.80      HIGL
ATOM   2382  CA  TRP  296      16.138  60.764 125.369  1.00 12.83      HIGL
ATOM   2383  CB  TRP  296      17.412  60.119 124.809  1.00 13.03      HIGL
ATOM   2384  CG  TRP  296      17.448  58.640 125.023  1.00 13.14      HIGL
ATOM   2385  CD2 TRP  296      18.316  57.918 125.900  1.00 13.55      HIGL
ATOM   2386  CE2 TRP  296      17.949  56.555 125.825  1.00 13.63      HIGL
ATOM   2387  CE3 TRP  296      19.369  58.289 126.747  1.00 14.63      HIGL
ATOM   2388  CD1 TRP  296      16.615  57.711 124.460  1.00 14.08      HIGL
ATOM   2389  NE1 TRP  296      16.909  56.456 124.939  1.00 13.47      HIGL
ATOM   2390  CZ2 TRP  296      18.596  55.562 126.567  1.00 13.78      HIGL
ATOM   2391  CZ3 TRP  296      20.017  57.297 127.487  1.00 13.79      HIGL
ATOM   2392  CH2 TRP  296      19.624  55.953 127.390  1.00 14.10      HIGL
ATOM   2393  C   TRP  296      16.135  60.615 126.887  1.00 12.44      HIGL
ATOM   2394  O   TRP  296      16.964  61.202 127.582  1.00 11.79      HIGL
ATOM   2395  N   GLU  297      15.190  59.811 127.376  1.00 12.90      HIGL
ATOM   2396  CA  GLU  297      15.029  59.502 128.797  1.00 12.94      HIGL
ATOM   2397  CB  GLU  297      16.061  58.455 129.199  1.00 13.78      HIGL
ATOM   2398  CG  GLU  297      15.780  57.087 128.595  1.00 14.60      HIGL
ATOM   2399  CD  GLU  297      14.616  56.394 129.271  1.00 14.61      HIGL
ATOM   2400  OE1 GLU  297      13.947  57.031 130.112  1.00 13.68      HIGL
ATOM   2401  OE2 GLU  297      14.370  55.211 128.962  1.00 15.38      HIGL
ATOM   2402  C   GLU  297      15.089  60.687 129.749  1.00 13.20      HIGL
ATOM   2403  O   GLU  297      15.911  60.728 130.665  1.00 11.51      HIGL
ATOM   2404  N   PRO  298      14.185  61.659 129.563  1.00 14.35      HIGL
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Fig. 2 cont.

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ATOM   2535  N   PHE  316      13.844  66.195 135.108  1.00 18.72      HIGL
ATOM   2536  CA  PHE  316      13.075  66.002 136.316  1.00 19.71      HIGL
ATOM   2537  CB  PHE  316      12.431  64.619 136.349  1.00 20.13      HIGL
ATOM   2538  CG  PHE  316      11.179  64.517 135.541  1.00 20.75      HIGL
ATOM   2539  CD1 PHE  316      11.232  64.450 134.153  1.00 21.09      HIGL
ATOM   2540  CD2 PHE  316       9.942  64.492 136.167  1.00 19.49      HIGL
ATOM   2541  CE1 PHE  316      10.065  64.359 133.402  1.00 20.74      HIGL
ATOM   2542  CE2 PHE  316       8.776  64.401 135.429  1.00 19.68      HIGL
ATOM   2543  CZ  PHE  316       8.836  64.335 134.041  1.00 20.74      HIGL
ATOM   2544  C   PHE  316      13.926  66.175 137.561  1.00 20.14      HIGL
ATOM   2545  O   PHE  316      15.155  66.134 137.528  1.00 21.09      HIGL
ATOM   2546  N   THR  317      13.232  66.386 138.662  1.00 20.18      HIGL
ATOM   2547  CA  THR  317      13.836  66.550 139.960  1.00 20.01      HIGL
ATOM   2548  CB  THR  317      12.783  67.140 140.933  1.00 19.47      HIGL
ATOM   2549  OG1 THR  317      13.102  68.508 141.196  1.00 20.10      HIGL
ATOM   2550  CG2 THR  317      12.710  66.363 142.215  1.00 18.19      HIGL
ATOM   2551  C   THR  317      14.271  65.161 140.408  1.00 20.33      HIGL
ATOM   2552  O   THR  317      13.739  64.155 139.939  1.00 20.58      HIGL
ATOM   2553  N   PRO  318      15.265  65.087 141.299  1.00 20.32      HIGL
ATOM   2554  CD  PRO  318      16.162  66.175 141.728  1.00 20.23      HIGL
ATOM   2555  CA  PRO  318      15.740  63.793 141.791  1.00 19.64      HIGL
ATOM   2556  CB  PRO  318      16.859  64.187 142.743  1.00 19.58      HIGL
ATOM   2557  CG  PRO  318      17.416  65.425 142.093  1.00 19.55      HIGL
ATOM   2558  C   PRO  318      14.615  63.044 142.498  1.00 19.76      HIGL
ATOM   2559  O   PRO  318      14.709  61.841 142.739  1.00 19.67      HIGL
ATOM   2560  N   SER  319      13.551  63.772 142.827  1.00 19.98      HIGL
ATOM   2561  CA  SER  319      12.403  63.195 143.504  1.00 20.20      HIGL
ATOM   2562  CB  SER  319      11.887  64.147 144.578  1.00 20.64      HIGL
ATOM   2563  OG  SER  319      11.025  65.119 144.016  1.00 23.02      HIGL
ATOM   2564  C   SER  319      11.291  62.889 142.504  1.00 20.42      HIGL
ATOM   2565  O   SER  319      10.263  62.305 142.861  1.00 20.64      HIGL
ATOM   2566  N   GLY  320      11.489  63.298 141.254  1.00 20.38      HIGL
ATOM   2567  CA  GLY  320      10.505  63.006 140.225  1.00 19.64      HIGL
ATOM   2568  C   GLY  320       9.585  64.119 139.765  1.00 19.52      HIGL
ATOM   2569  O   GLY  320       8.657  63.862 138.996  1.00 19.02      HIGL
ATOM   2570  N   GLN  321       9.833  65.347 140.213  1.00 18.90      HIGL
ATOM   2571  CA  GLN  321       8.991  66.475 139.824  1.00 19.06      HIGL
ATOM   2572  CB  GLN  321       8.940  67.520 140.948  1.00 20.13      HIGL
ATOM   2573  CG  GLN  321       8.219  68.811 140.564  1.00 22.26      HIGL
ATOM   2574  CD  GLN  321       7.946  69.703 141.762  1.00 23.01      HIGL
ATOM   2575  OE1 GLN  321       7.346  69.264 142.748  1.00 25.05      HIGL
ATOM   2576  NE2 GLN  321       8.377  70.958 141.682  1.00 20.98      HIGL
ATOM   2577  C   GLN  321       9.477  67.129 138.540  1.00 18.11      HIGL
ATOM   2578  O   GLN  321      10.639  67.520 138.428  1.00 17.69      HIGL
ATOM   2579  N   ALA  322       8.578  67.263 137.574  1.00 17.71      HIGL
ATOM   2580  CA  ALA  322       8.938  67.857 136.293  1.00 17.37      HIGL
ATOM   2581  CB  ALA  322       7.725  67.942 135.387  1.00 16.48      HIGL
ATOM   2582  C   ALA  322       9.546  69.231 136.466  1.00 17.45      HIGL
ATOM   2583  O   ALA  322       9.078  70.041 137.268  1.00 19.09      HIGL
ATOM   2584  N   LEU  323      10.601  69.476 135.706  1.00 17.15      HIGL
ATOM   2585  CA  LEU  323      11.305  70.743 135.720  1.00 16.94      HIGL
ATOM   2586  CB  LEU  323      12.755  70.512 135.299  1.00 16.28      HIGL
ATOM   2587  CG  LEU  323      13.901  70.773 136.279  1.00 15.82      HIGL
ATOM   2588  CD1 LEU  323      13.500  70.423 137.707  1.00 14.61      HIGL
ATOM   2589  CD2 LEU  323      15.113  69.964 135.823  1.00 14.44      HIGL
ATOM   2590  C   LEU  323      10.603  71.677 134.731  1.00 17.93      HIGL
ATOM   2591  O   LEU  323       9.883  71.225 133.838  1.00 16.70      HIGL
ATOM   2592  N   SER  324      10.811  72.980 134.893  1.00 18.92      HIGL
ATOM   2593  CA  SER  324      10.186  73.966 134.018  1.00 19.03      HIGL
ATOM   2594  CB  SER  324      10.663  75.370 134.383  1.00 19.54      HIGL
ATOM   2595  OG  SER  324      12.069  75.478 134.241  1.00 20.56      HIGL
ATOM   2596  C   SER  324      10.496  73.707 132.555  1.00 19.19      HIGL
ATOM   2597  O   SER  324       9.628  73.843 131.697  1.00 20.39      HIGL
ATOM   2598  N   SER  325      11.743  73.338 132.282  1.00 19.12      HIGL
ATOM   2599  CA  SER  325      12.217  73.073 130.927  1.00 18.61      HIGL
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Fig. 2 cont.

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ATOM   2470 CA   LEU   306      22.035  58.657 131.080  1.00 17.26      HIGL
ATOM   2471 CB   LEU   306      21.217  59.670 130.270  1.00 16.18      HIGL
ATOM   2472 CG   LEU   306      19.907  60.128 130.937  1.00 16.97      HIGL
ATOM   2473 CD1  LEU   306      19.284  61.278 130.161  1.00 15.17      HIGL
ATOM   2474 CD2  LEU   306      18.937  58.954 131.024  1.00 16.01      HIGL
ATOM   2475 C    LEU   306      23.156  58.076 130.216  1.00 17.50      HIGL
ATOM   2476 O    LEU   306      23.137  58.195 128.988  1.00 17.52      HIGL
ATOM   2477 N    GLY   307      24.131  57.450 130.870  1.00 17.26      HIGL
ATOM   2478 CA   GLY   307      25.235  56.836 130.159  1.00 16.70      HIGL
ATOM   2479 C    GLY   307      26.294  57.773 129.616  1.00 16.64      HIGL
ATOM   2480 O    GLY   307      27.191  57.333 128.901  1.00 16.25      HIGL
ATOM   2481 N    SER   308      26.204  59.056 129.950  1.00 16.62      HIGL
ATOM   2482 CA   SER   308      27.181  60.032 129.471  1.00 17.50      HIGL
ATOM   2483 CB   SER   308      26.477  61.300 128.987  1.00 17.40      HIGL
ATOM   2484 OG   SER   308      26.026  62.065 130.091  1.00 18.14      HIGL
ATOM   2485 C    SER   308      28.159  60.402 130.582  1.00 17.77      HIGL
ATOM   2486 O    SER   308      28.059  59.905 131.712  1.00 18.46      HIGL
ATOM   2487 N    SER   309      29.104  61.278 130.265  1.00 17.09      HIGL
ATOM   2488 CA   SER   309      30.074  61.693 131.263  1.00 17.48      HIGL
ATOM   2489 CB   SER   309      31.384  62.138 130.599  1.00 15.98      HIGL
ATOM   2490 OG   SER   309      31.196  63.287 129.794  1.00 15.84      HIGL
ATOM   2491 C    SER   309      29.485  62.818 132.118  1.00 17.77      HIGL
ATOM   2492 O    SER   309      30.100  63.268 133.084  1.00 17.93      HIGL
ATOM   2493 N    CYS   310      28.289  63.273 131.763  1.00 18.10      HIGL
ATOM   2494 CA   CYS   310      27.641  64.323 132.541  1.00 18.95      HIGL
ATOM   2495 C    CYS   310      26.881  63.668 133.695  1.00 18.10      HIGL
ATOM   2496 O    CYS   310      26.437  62.528 133.583  1.00 18.94      HIGL
ATOM   2497 CB   CYS   310      26.686  65.139 131.670  1.00 19.41      HIGL
ATOM   2498 SG   CYS   310      27.452  66.412 130.600  1.00 24.23      HIGL
ATOM   2499 N    ALA   311      26.733  64.392 134.798  1.00 16.72      HIGL
ATOM   2500 CA   ALA   311      26.061  63.873 135.986  1.00 15.09      HIGL
ATOM   2501 CB   ALA   311      26.451  64.713 137.187  1.00 13.34      HIGL
ATOM   2502 C    ALA   311      24.539  63.768 135.917  1.00 14.53      HIGL
ATOM   2503 O    ALA   311      23.959  62.805 136.416  1.00 14.36      HIGL
ATOM   2504 N    ASP   312      23.893  64.755 135.308  1.00 14.02      HIGL
ATOM   2505 CA   ASP   312      22.437  64.767 135.233  1.00 14.14      HIGL
ATOM   2506 CB   ASP   312      21.888  65.569 136.414  1.00 13.88      HIGL
ATOM   2507 CG   ASP   312      20.417  65.338 136.647  1.00 15.05      HIGL
ATOM   2508 OD1  ASP   312      19.703  64.943 135.692  1.00 16.00      HIGL
ATOM   2509 OD2  ASP   312      19.973  65.562 137.795  1.00 14.74      HIGL
ATOM   2510 C    ASP   312      21.910  65.376 133.932  1.00 14.14      HIGL
ATOM   2511 O    ASP   312      22.085  66.571 133.690  1.00 13.77      HIGL
ATOM   2512 N    ASN   313      21.260  64.555 133.108  1.00 14.50      HIGL
ATOM   2513 CA   ASN   313      20.684  65.016 131.845  1.00 15.03      HIGL
ATOM   2514 CB   ASN   313      21.177  64.160 130.672  1.00 16.08      HIGL
ATOM   2515 CG   ASN   313      22.633  64.403 130.337  1.00 18.13      HIGL
ATOM   2516 OD1  ASN   313      23.069  65.544 130.228  1.00 19.71      HIGL
ATOM   2517 ND2  ASN   313      23.391  63.326 130.159  1.00 17.96      HIGL
ATOM   2518 C    ASN   313      19.159  64.947 131.889  1.00 14.73      HIGL
ATOM   2519 O    ASN   313      18.491  65.155 130.881  1.00 14.78      HIGL
ATOM   2520 N    THR   314      18.608  64.649 133.057  1.00 15.17      HIGL
ATOM   2521 CA   THR   314      17.160  64.535 133.207  1.00 16.32      HIGL
ATOM   2522 CB   THR   314      16.794  63.799 134.499  1.00 16.08      HIGL
ATOM   2523 OG1  THR   314      17.198  64.596 135.619  1.00 16.57      HIGL
ATOM   2524 CG2  THR   314      17.497  62.452 134.563  1.00 15.34      HIGL
ATOM   2525 C    THR   314      16.444  65.878 133.237  1.00 16.22      HIGL
ATOM   2526 O    THR   314      17.033  66.908 133.551  1.00 17.07      HIGL
ATOM   2527 N    MET   315      15.161  65.851 132.911  1.00 16.05      HIGL
ATOM   2528 CA   MET   315      14.352  67.055 132.929  1.00 17.30      HIGL
ATOM   2529 CB   MET   315      13.588  67.205 131.613  1.00 17.97      HIGL
ATOM   2530 CG   MET   315      14.505  67.282 130.405  1.00 18.13      HIGL
ATOM   2531 SD   MET   315      13.637  67.606 128.894  1.00 18.76      HIGL
ATOM   2532 CE   MET   315      13.387  69.339 129.091  1.00 19.34      HIGL
ATOM   2533 C    MET   315      13.393  66.933 134.104  1.00 18.03      HIGL
ATOM   2534 O    MET   315      12.283  67.467 134.103  1.00 17.72      HIGL
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Fig. 2 cont.

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ATOM   2535  N   PHE  316      13.844  66.195 135.108  1.00 18.72      HIGL
ATOM   2536  CA  PHE  316      13.075  66.002 136.316  1.00 19.71      HIGL
ATOM   2537  CB  PHE  316      12.431  64.619 136.349  1.00 20.13      HIGL
ATOM   2538  CG  PHE  316      11.179  64.517 135.541  1.00 20.75      HIGL
ATOM   2539  CD1 PHE  316      11.232  64.450 134.153  1.00 21.09      HIGL
ATOM   2540  CD2 PHE  316       9.942  64.492 136.167  1.00 19.49      HIGL
ATOM   2541  CE1 PHE  316      10.065  64.359 133.402  1.00 20.74      HIGL
ATOM   2542  CE2 PHE  316       8.776  64.401 135.429  1.00 19.68      HIGL
ATOM   2543  CZ  PHE  316       8.836  64.335 134.041  1.00 20.74      HIGL
ATOM   2544  C   PHE  316      13.926  66.175 137.561  1.00 20.14      HIGL
ATOM   2545  O   PHE  316      15.155  66.134 137.528  1.00 21.09      HIGL
ATOM   2546  N   THR  317      13.232  66.386 138.662  1.00 20.18      HIGL
ATOM   2547  CA  THR  317      13.836  66.550 139.960  1.00 20.01      HIGL
ATOM   2548  CB  THR  317      12.783  67.140 140.933  1.00 19.47      HIGL
ATOM   2549  OG1 THR  317      13.102  68.508 141.196  1.00 20.10      HIGL
ATOM   2550  CG2 THR  317      12.710  66.363 142.215  1.00 18.19      HIGL
ATOM   2551  C   THR  317      14.271  65.161 140.408  1.00 20.33      HIGL
ATOM   2552  O   THR  317      13.739  64.155 139.939  1.00 20.58      HIGL
ATOM   2553  N   PRO  318      15.265  65.087 141.299  1.00 20.32      HIGL
ATOM   2554  CD  PRO  318      16.162  66.175 141.728  1.00 20.23      HIGL
ATOM   2555  CA  PRO  318      15.740  63.793 141.791  1.00 19.64      HIGL
ATOM   2556  CB  PRO  318      16.859  64.187 142.743  1.00 19.58      HIGL
ATOM   2557  CG  PRO  318      17.416  65.425 142.093  1.00 19.55      HIGL
ATOM   2558  C   PRO  318      14.615  63.044 142.498  1.00 19.76      HIGL
ATOM   2559  O   PRO  318      14.709  61.841 142.739  1.00 19.67      HIGL
ATOM   2560  N   SER  319      13.551  63.772 142.827  1.00 19.98      HIGL
ATOM   2561  CA  SER  319      12.403  63.195 143.504  1.00 20.20      HIGL
ATOM   2562  CB  SER  319      11.887  64.147 144.578  1.00 20.64      HIGL
ATOM   2563  OG  SER  319      11.025  65.119 144.016  1.00 23.02      HIGL
ATOM   2564  C   SER  319      11.291  62.889 142.504  1.00 20.42      HIGL
ATOM   2565  O   SER  319      10.263  62.305 142.861  1.00 20.64      HIGL
ATOM   2566  N   GLY  320      11.489  63.298 141.254  1.00 20.38      HIGL
ATOM   2567  CA  GLY  320      10.505  63.006 140.225  1.00 19.64      HIGL
ATOM   2568  C   GLY  320       9.585  64.119 139.765  1.00 19.52      HIGL
ATOM   2569  O   GLY  320       8.657  63.862 138.996  1.00 19.02      HIGL
ATOM   2570  N   GLN  321       9.833  65.347 140.213  1.00 18.90      HIGL
ATOM   2571  CA  GLN  321       8.991  66.475 139.824  1.00 19.06      HIGL
ATOM   2572  CB  GLN  321       8.940  67.520 140.948  1.00 20.13      HIGL
ATOM   2573  CG  GLN  321       8.219  68.811 140.564  1.00 22.26      HIGL
ATOM   2574  CD  GLN  321       7.946  69.703 141.762  1.00 23.01      HIGL
ATOM   2575  OE1 GLN  321       7.346  69.264 142.748  1.00 25.05      HIGL
ATOM   2576  NE2 GLN  321       8.377  70.958 141.682  1.00 20.98      HIGL
ATOM   2577  C   GLN  321       9.477  67.129 138.540  1.00 18.11      HIGL
ATOM   2578  O   GLN  321      10.639  67.520 138.428  1.00 17.69      HIGL
ATOM   2579  N   ALA  322       8.578  67.263 137.574  1.00 17.71      HIGL
ATOM   2580  CA  ALA  322       8.938  67.857 136.293  1.00 17.37      HIGL
ATOM   2581  CB  ALA  322       7.725  67.942 135.387  1.00 16.48      HIGL
ATOM   2582  C   ALA  322       9.546  69.231 136.466  1.00 17.45      HIGL
ATOM   2583  O   ALA  322       9.078  70.041 137.268  1.00 19.09      HIGL
ATOM   2584  N   LEU  323      10.601  69.476 135.706  1.00 17.15      HIGL
ATOM   2585  CA  LEU  323      11.305  70.743 135.720  1.00 16.94      HIGL
ATOM   2586  CB  LEU  323      12.755  70.512 135.299  1.00 16.28      HIGL
ATOM   2587  CG  LEU  323      13.901  70.773 136.279  1.00 15.82      HIGL
ATOM   2588  CD1 LEU  323      13.500  70.423 137.707  1.00 14.61      HIGL
ATOM   2589  CD2 LEU  323      15.113  69.964 135.823  1.00 14.44      HIGL
ATOM   2590  C   LEU  323      10.603  71.677 134.731  1.00 17.93      HIGL
ATOM   2591  O   LEU  323       9.883  71.225 133.838  1.00 16.70      HIGL
ATOM   2592  N   SER  324      10.811  72.980 134.893  1.00 18.92      HIGL
ATOM   2593  CA  SER  324      10.186  73.966 134.018  1.00 19.03      HIGL
ATOM   2594  CB  SER  324      10.663  75.370 134.383  1.00 19.54      HIGL
ATOM   2595  OG  SER  324      12.069  75.478 134.241  1.00 20.56      HIGL
ATOM   2596  C   SER  324      10.496  73.707 132.555  1.00 19.19      HIGL
ATOM   2597  O   SER  324       9.628  73.843 131.697  1.00 20.39      HIGL
ATOM   2598  N   SER  325      11.743  73.338 132.282  1.00 19.12      HIGL
ATOM   2599  CA  SER  325      12.217  73.073 130.927  1.00 18.61      HIGL
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Fig. 2 cont.

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ATOM   2600  CB  SER   325      13.681  72.639 130.980  1.00 18.82      HIGL
ATOM   2601  OG  SER   325      13.838  71.516 131.828  1.00 18.06      HIGL
ATOM   2602  C   SER   325      11.414  72.047 130.132  1.00 18.61      HIGL
ATOM   2603  O   SER   325      11.458  72.036 128.905  1.00 18.45      HIGL
ATOM   2604  N   LEU   326      10.680  71.184 130.820  1.00 19.28      HIGL
ATOM   2605  CA  LEU   326       9.893  70.167 130.132  1.00 19.85      HIGL
ATOM   2606  CB  LEU   326       9.212  69.243 131.145  1.00 20.13      HIGL
ATOM   2607  CG  LEU   326       9.112  67.733 130.862  1.00 22.13      HIGL
ATOM   2608  CD1 LEU   326       7.849  67.179 131.542  1.00 20.56      HIGL
ATOM   2609  CD2 LEU   326       9.063  67.453 129.364  1.00 21.71      HIGL
ATOM   2610  C   LEU   326       8.822  70.787 129.230  1.00 20.36      HIGL
ATOM   2611  O   LEU   326       8.415  70.187 128.233  1.00 19.41      HIGL
ATOM   2612  N   SER   327       8.363  71.986 129.580  1.00 20.97      HIGL
ATOM   2613  CA  SER   327       7.317  72.642 128.803  1.00 21.71      HIGL
ATOM   2614  CB  SER   327       6.595  73.684 129.653  1.00 21.54      HIGL
ATOM   2615  OG  SER   327       7.439  74.785 129.921  1.00 23.10      HIGL
ATOM   2616  C   SER   327       7.829  73.301 127.533  1.00 22.18      HIGL
ATOM   2617  O   SER   327       7.100  74.056 126.887  1.00 23.13      HIGL
ATOM   2618  N   VAL   328       9.080  73.032 127.180  1.00 21.90      HIGL
ATOM   2619  CA  VAL   328       9.651  73.588 125.959  1.00 22.31      HIGL
ATOM   2620  CB  VAL   328      11.188  73.333 125.873  1.00 22.21      HIGL
ATOM   2621  CG1 VAL   328      11.483  71.843 125.809  1.00 21.74      HIGL
ATOM   2622  CG2 VAL   328      11.759  74.026 124.657  1.00 21.78      HIGL
ATOM   2623  C   VAL   328       8.958  72.917 124.764  1.00 22.65      HIGL
ATOM   2624  O   VAL   328       8.973  73.429 123.645  1.00 22.63      HIGL
ATOM   2625  N   PHE   329       8.338  71.771 125.013  1.00 22.73      HIGL
ATOM   2626  CA  PHE   329       7.654  71.048 123.959  1.00 23.91      HIGL
ATOM   2627  CB  PHE   329       7.268  69.658 124.454  1.00 23.67      HIGL
ATOM   2628  CG  PHE   329       8.440  68.723 124.557  1.00 24.39      HIGL
ATOM   2629  CD1 PHE   329       9.067  68.252 123.409  1.00 24.10      HIGL
ATOM   2630  CD2 PHE   329       8.949  68.349 125.796  1.00 23.95      HIGL
ATOM   2631  CE1 PHE   329      10.185  67.424 123.491  1.00 24.86      HIGL
ATOM   2632  CE2 PHE   329      10.063  67.524 125.887  1.00 24.79      HIGL
ATOM   2633  CZ  PHE   329      10.686  67.060 124.729  1.00 24.99      HIGL
ATOM   2634  C   PHE   329       6.446  71.806 123.420  1.00 24.94      HIGL
ATOM   2635  O   PHE   329       5.885  71.438 122.384  1.00 24.54      HIGL
ATOM   2636  N   HIS   330       6.053  72.867 124.123  1.00 25.53      HIGL
ATOM   2637  CA  HIS   330       4.944  73.706 123.677  1.00 25.92      HIGL
ATOM   2638  CB  HIS   330       4.376  74.554 124.828  1.00 25.05      HIGL
ATOM   2639  CG  HIS   330       3.507  73.795 125.786  1.00 23.98      HIGL
ATOM   2640  CD2 HIS   330       3.511  73.739 127.139  1.00 23.72      HIGL
ATOM   2641  ND1 HIS   330       2.451  73.010 125.377  1.00 23.63      HIGL
ATOM   2642  CE1 HIS   330       1.843  72.503 126.434  1.00 22.96      HIGL
ATOM   2643  NE2 HIS   330       2.467  72.931 127.517  1.00 23.30      HIGL
ATOM   2644  C   HIS   330       5.488  74.650 122.601  1.00 26.65      HIGL
ATOM   2645  O   HIS   330       4.891  74.806 121.540  1.00 27.30      HIGL
ATOM   2646  N   ARG   331       6.632  75.267 122.888  1.00 27.80      HIGL
ATOM   2647  CA  ARG   331       7.273  76.214 121.976  1.00 28.68      HIGL
ATOM   2648  CB  ARG   331       8.405  76.953 122.698  1.00 31.32      HIGL
ATOM   2649  CG  ARG   331       7.935  78.120 123.555  1.00 35.13      HIGL
ATOM   2650  CD  ARG   331       9.101  78.976 124.057  1.00 37.60      HIGL
ATOM   2651  NE  ARG   331       9.862  78.322 125.116  1.00 39.32      HIGL
ATOM   2652  CZ  ARG   331       9.311  77.800 126.208  1.00 41.08      HIGL
ATOM   2653  NH1 ARG   331       7.994  77.854 126.382  1.00 41.70      HIGL
ATOM   2654  NH2 ARG   331      10.075  77.233 127.133  1.00 41.35      HIGL
ATOM   2655  C   ARG   331       7.821  75.668 120.661  1.00 28.01      HIGL
ATOM   2656  O   ARG   331       8.119  76.440 119.753  1.00 28.33      HIGL
ATOM   2657  N   ILE   332       7.966  74.355 120.545  1.00 27.15      HIGL
ATOM   2658  CA  ILE   332       8.503  73.790 119.313  1.00 25.82      HIGL
ATOM   2659  CB  ILE   332       9.717  72.876 119.596  1.00 24.07      HIGL
ATOM   2660  CG2 ILE   332      10.747  73.636 120.419  1.00 22.61      HIGL
ATOM   2661  CG1 ILE   332       9.262  71.611 120.331  1.00 23.55      HIGL
ATOM   2662  CD1 ILE   332      10.328  70.559 120.487  1.00 21.73      HIGL
ATOM   2663  C   ILE   332       7.463  72.999 118.534  1.00 26.35      HIGL
ATOM   2664  O   ILE   332       7.659  72.716 117.351  1.00 27.46      HIGL
END
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Fig. 2 cont.

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HEADER                                                          AAGL
ATOM      1  CB  ALA     1      30.233  36.166 100.975  1.00 33.89      AAGL
ATOM      2  C   ALA     1      30.173  35.826 103.455  1.00 33.23      AAGL
ATOM      3  O   ALA     1      30.978  35.045 103.960  1.00 32.69      AAGL
ATOM      4  N   ALA     1      32.066  36.993 102.404  1.00 32.99      AAGL
ATOM      5  CA  ALA     1      30.595  36.767 102.330  1.00 33.73      AAGL
ATOM      6  N   LEU     2      28.909  35.906 103.856  1.00 31.18      AAGL
ATOM      7  CA  LEU     2      28.412  35.052 104.926  1.00 29.30      AAGL
ATOM      8  CB  LEU     2      27.023  35.510 105.362  1.00 29.79      AAGL
ATOM      9  CG  LEU     2      26.868  36.944 105.864  1.00 30.10      AAGL
ATOM     10  CD1 LEU     2      25.382  37.292 105.912  1.00 32.47      AAGL
ATOM     11  CD2 LEU     2      27.511  37.098 107.236  1.00 30.25      AAGL
ATOM     12  C   LEU     2      28.340  33.612 104.451  1.00 28.19      AAGL
ATOM     13  O   LEU     2      28.258  33.351 103.250  1.00 28.93      AAGL
ATOM     14  N   THR     3      28.370  32.679 105.396  1.00 27.70      AAGL
ATOM     15  CA  THR     3      28.304  31.267 105.071  1.00 27.25      AAGL
ATOM     16  CB  THR     3      28.401  30.410 106.349  1.00 28.42      AAGL
ATOM     17  OG1 THR     3      29.650  30.681 107.001  1.00 28.17      AAGL
ATOM     18  CG2 THR     3      28.327  28.920 106.010  1.00 27.90      AAGL
ATOM     19  C   THR     3      27.000  30.971 104.343  1.00 26.98      AAGL
ATOM     20  O   THR     3      26.965  30.159 103.416  1.00 26.10      AAGL
ATOM     21  N   TYR     4      25.931  31.650 104.756  1.00 26.84      AAGL
ATOM     22  CA  TYR     4      24.623  31.465 104.137  1.00 24.81      AAGL
ATOM     23  CB  TYR     4      23.665  30.721 105.079  1.00 25.74      AAGL
ATOM     24  CG  TYR     4      24.137  29.377 105.602  1.00 25.74      AAGL
ATOM     25  CD1 TYR     4      24.318  28.288 104.746  1.00 26.33      AAGL
ATOM     26  CE1 TYR     4      24.692  27.034 105.247  1.00 27.71      AAGL
ATOM     27  CD2 TYR     4      24.349  29.182 106.965  1.00 25.74      AAGL
ATOM     28  CE2 TYR     4      24.724  27.940 107.473  1.00 26.87      AAGL
ATOM     29  CZ  TYR     4      24.891  26.870 106.609  1.00 26.22      AAGL
ATOM     30  OH  TYR     4      25.248  25.646 107.118  1.00 29.24      AAGL
ATOM     31  C   TYR     4      23.977  32.803 103.787  1.00 24.69      AAGL
ATOM     32  O   TYR     4      23.914  33.712 104.619  1.00 24.65      AAGL
ATOM     33  N   ARG     5      23.515  32.919 102.549  1.00 23.45      AAGL
ATOM     34  CA  ARG     5      22.801  34.103 102.069  1.00 25.24      AAGL
ATOM     35  CB  ARG     5      23.551  34.823 100.939  1.00 29.22      AAGL
ATOM     36  CG  ARG     5      24.781  35.609 101.366  1.00 29.88      AAGL
ATOM     37  CD  ARG     5      26.042  34.797 101.168  1.00 29.48      AAGL
ATOM     38  NE  ARG     5      26.159  34.336  99.792  1.00 29.78      AAGL
ATOM     39  CZ  ARG     5      27.061  33.454  99.373  1.00 27.81      AAGL
ATOM     40  NH1 ARG     5      27.934  32.940 100.225  1.00 27.49      AAGL
ATOM     41  NH2 ARG     5      27.068  33.068  98.104  1.00 29.30      AAGL
ATOM     42  C   ARG     5      21.554  33.439 101.507  1.00 25.34      AAGL
ATOM     43  O   ARG     5      21.547  32.962 100.371  1.00 23.77      AAGL
ATOM     44  N   GLY     6      20.502  33.381 102.308  1.00 24.34      AAGL
ATOM     45  CA  GLY     6      19.321  32.694 101.837  1.00 21.41      AAGL
ATOM     46  C   GLY     6      18.031  33.457 101.755  1.00 22.93      AAGL
ATOM     47  O   GLY     6      17.957  34.649 102.053  1.00 21.36      AAGL
ATOM     48  N   ALA     7      17.008  32.727 101.330  1.00 21.72      AAGL
ATOM     49  CA  ALA     7      15.669  33.248 101.182  1.00 22.02      AAGL
ATOM     50  CB  ALA     7      15.481  33.797  99.780  1.00 22.89      AAGL
ATOM     51  C   ALA     7      14.689  32.110 101.422  1.00 21.79      AAGL
ATOM     52  O   ALA     7      14.973  30.956 101.101  1.00 23.27      AAGL
ATOM     53  N   ASP     8      13.548  32.435 102.014  1.00 20.87      AAGL
ATOM     54  CA  ASP     8      12.501  31.448 102.247  1.00 21.47      AAGL
ATOM     55  CB  ASP     8      11.854  31.650 103.625  1.00 20.38      AAGL
ATOM     56  CG  ASP     8      10.772  30.617 103.923  1.00 20.93      AAGL
ATOM     57  OD1 ASP     8       9.920  30.363 103.044  1.00 20.43      AAGL
ATOM     58  OD2 ASP     8      10.768  30.069 105.048  1.00 19.51      AAGL
ATOM     59  C   ASP     8      11.482  31.736 101.153  1.00 19.96      AAGL
ATOM     60  O   ASP     8      10.773  32.738 101.205  1.00 21.04      AAGL
ATOM     61  N   ILE     9      11.424  30.870 100.149  1.00 20.91      AAGL
ATOM     62  CA  ILE     9      10.490  31.065  99.049  1.00 21.73      AAGL
ATOM     63  CB  ILE     9      11.234  31.102  97.689  1.00 21.80      AAGL
ATOM     64  CG2 ILE     9      12.174  32.300  97.648  1.00 23.18      AAGL
ATOM     65  CG1 ILE     9      12.015  29.807  97.479  1.00 22.70      AAGL
```

Fig. 3

ATOM	66	CD1	ILE	9	12.626	29.683	96.085	1.00	25.10	AAGL
ATOM	67	C	ILE	9	9.452	29.945	99.038	1.00	23.69	AAGL
ATOM	68	O	ILE	9	9.018	29.490	97.984	1.00	22.97	AAGL
ATOM	69	N	SER	10	9.059	29.511	100.232	1.00	22.26	AAGL
ATOM	70	CA	SER	10	8.080	28.441	100.377	1.00	22.83	AAGL
ATOM	71	CB	SER	10	7.658	28.325	101.840	1.00	20.03	AAGL
ATOM	72	OG	SER	10	8.782	28.078	102.658	1.00	21.43	AAGL
ATOM	73	C	SER	10	6.833	28.617	99.508	1.00	22.20	AAGL
ATOM	74	O	SER	10	6.286	27.649	98.995	1.00	24.50	AAGL
ATOM	75	N	SER	11	6.388	29.855	99.347	1.00	23.05	AAGL
ATOM	76	CA	SER	11	5.198	30.148	98.563	1.00	24.59	AAGL
ATOM	77	CB	SER	11	4.784	31.598	98.792	1.00	26.58	AAGL
ATOM	78	OG	SER	11	5.775	32.473	98.275	1.00	26.05	AAGL
ATOM	79	C	SER	11	5.347	29.935	97.057	1.00	25.49	AAGL
ATOM	80	O	SER	11	4.351	29.913	96.338	1.00	25.69	AAGL
ATOM	81	N	LEU	12	6.578	29.781	96.583	1.00	26.51	AAGL
ATOM	82	CA	LEU	12	6.817	29.637	95.149	1.00	25.87	AAGL
ATOM	83	CB	LEU	12	8.237	29.143	94.884	1.00	26.84	AAGL
ATOM	84	CG	LEU	12	8.609	29.025	93.398	1.00	26.26	AAGL
ATOM	85	CD1	LEU	12	8.307	30.324	92.665	1.00	26.19	AAGL
ATOM	86	CD2	LEU	12	10.078	28.685	93.273	1.00	28.47	AAGL
ATOM	87	C	LEU	12	5.844	28.768	94.362	1.00	28.42	AAGL
ATOM	88	O	LEU	12	5.181	29.257	93.447	1.00	28.84	AAGL
ATOM	89	N	LEU	13	5.758	27.487	94.701	1.00	28.60	AAGL
ATOM	90	CA	LEU	13	4.879	26.590	93.963	1.00	30.83	AAGL
ATOM	91	CB	LEU	13	4.997	25.164	94.514	1.00	30.59	AAGL
ATOM	92	CG	LEU	13	6.443	24.657	94.640	1.00	29.90	AAGL
ATOM	93	CD1	LEU	13	6.441	23.200	95.044	1.00	30.84	AAGL
ATOM	94	CD2	LEU	13	7.179	24.821	93.315	1.00	31.95	AAGL
ATOM	95	C	LEU	13	3.430	27.062	93.967	1.00	31.99	AAGL
ATOM	96	O	LEU	13	2.703	26.844	93.001	1.00	33.62	AAGL
ATOM	97	N	LEU	14	3.008	27.725	95.038	1.00	33.18	AAGL
ATOM	98	CA	LEU	14	1.639	28.226	95.106	1.00	33.64	AAGL
ATOM	99	CB	LEU	14	1.289	28.683	96.523	1.00	34.87	AAGL
ATOM	100	CG	LEU	14	0.959	27.561	97.502	1.00	35.78	AAGL
ATOM	101	CD1	LEU	14	0.492	28.145	98.828	1.00	36.41	AAGL
ATOM	102	CD2	LEU	14	-0.137	26.693	96.895	1.00	37.20	AAGL
ATOM	103	C	LEU	14	1.423	29.385	94.141	1.00	34.86	AAGL
ATOM	104	O	LEU	14	0.352	29.522	93.551	1.00	33.97	AAGL
ATOM	105	N	LEU	15	2.443	30.218	93.978	1.00	34.48	AAGL
ATOM	106	CA	LEU	15	2.344	31.359	93.080	1.00	35.10	AAGL
ATOM	107	CB	LEU	15	3.428	32.390	93.415	1.00	35.52	AAGL
ATOM	108	CG	LEU	15	3.232	33.227	94.696	1.00	37.21	AAGL
ATOM	109	CD1	LEU	15	2.912	32.357	95.879	1.00	37.69	AAGL
ATOM	110	CD2	LEU	15	4.496	34.018	94.975	1.00	35.91	AAGL
ATOM	111	C	LEU	15	2.458	30.904	91.624	1.00	35.48	AAGL
ATOM	112	O	LEU	15	1.647	31.306	90.782	1.00	35.67	AAGL
ATOM	113	N	GLU	16	3.449	30.065	91.329	1.00	35.68	AAGL
ATOM	114	CA	GLU	16	3.619	29.561	89.966	1.00	37.14	AAGL
ATOM	115	CB	GLU	16	4.747	28.527	89.890	1.00	35.01	AAGL
ATOM	116	CG	GLU	16	6.159	29.083	90.020	1.00	34.68	AAGL
ATOM	117	CD	GLU	16	7.214	27.993	89.905	1.00	35.45	AAGL
ATOM	118	OE1	GLU	16	6.928	26.849	90.317	1.00	35.57	AAGL
ATOM	119	OE2	GLU	16	8.336	28.271	89.419	1.00	35.12	AAGL
ATOM	120	C	GLU	16	2.317	28.913	89.527	1.00	39.70	AAGL
ATOM	121	O	GLU	16	1.846	29.139	88.411	1.00	40.81	AAGL
ATOM	122	N	ASP	17	1.727	28.112	90.411	1.00	41.41	AAGL
ATOM	123	CA	ASP	17	0.470	27.444	90.099	1.00	44.13	AAGL
ATOM	124	CB	ASP	17	0.029	26.557	91.262	1.00	44.94	AAGL
ATOM	125	CG	ASP	17	0.510	25.127	91.117	1.00	47.20	AAGL
ATOM	126	OD1	ASP	17	0.423	24.359	92.103	1.00	47.97	AAGL
ATOM	127	OD2	ASP	17	0.959	24.757	90.006	1.00	50.11	AAGL
ATOM	128	C	ASP	17	-0.625	28.447	89.771	1.00	45.54	AAGL
ATOM	129	O	ASP	17	-1.458	28.195	88.896	1.00	47.39	AAGL
ATOM	130	N	GLU	18	-0.629	29.581	90.471	1.00	45.43	AAGL
ATOM	131	CA	GLU	18	-1.625	30.617	90.234	1.00	47.08	AAGL

Fig. 3 cont.

ATOM	132	CB	GLU	18	-1.762	31.537	91.458	1.00 49.00	AAGL
ATOM	133	CG	GLU	18	-2.526	30.900	92.622	1.00 52.65	AAGL
ATOM	134	CD	GLU	18	-2.530	31.755	93.890	1.00 55.02	AAGL
ATOM	135	OE1	GLU	18	-3.112	31.305	94.911	1.00 55.65	AAGL
ATOM	136	OE2	GLU	18	-1.953	32.870	93.870	1.00 56.34	AAGL
ATOM	137	C	GLU	18	-1.267	31.432	88.994	1.00 46.48	AAGL
ATOM	138	O	GLU	18	-1.845	32.492	88.743	1.00 46.57	AAGL
ATOM	139	N	GLY	19	-0.307	30.929	88.223	1.00 45.75	AAGL
ATOM	140	CA	GLY	19	0.091	31.609	87.006	1.00 45.53	AAGL
ATOM	141	C	GLY	19	1.245	32.588	87.113	1.00 45.29	AAGL
ATOM	142	O	GLY	19	1.636	33.185	86.113	1.00 44.87	AAGL
ATOM	143	N	TYR	20	1.802	32.758	88.309	1.00 44.55	AAGL
ATOM	144	CA	TYR	20	2.911	33.685	88.497	1.00 44.04	AAGL
ATOM	145	CB	TYR	20	3.098	33.987	89.985	1.00 46.33	AAGL
ATOM	146	CG	TYR	20	2.199	35.092	90.475	1.00 46.92	AAGL
ATOM	147	CD1	TYR	20	1.174	34.837	91.384	1.00 47.92	AAGL
ATOM	148	CE1	TYR	20	0.317	35.856	91.804	1.00 48.81	AAGL
ATOM	149	CD2	TYR	20	2.351	36.388	89.995	1.00 48.25	AAGL
ATOM	150	CE2	TYR	20	1.509	37.406	90.399	1.00 48.75	AAGL
ATOM	151	CZ	TYR	20	0.494	37.135	91.301	1.00 49.08	AAGL
ATOM	152	OH	TYR	20	-0.350	38.146	91.676	1.00 50.05	AAGL
ATOM	153	C	TYR	20	4.243	33.232	87.916	1.00 42.70	AAGL
ATOM	154	O	TYR	20	4.541	32.043	87.857	1.00 41.19	AAGL
ATOM	155	N	SER	21	5.040	34.211	87.494	1.00 42.54	AAGL
ATOM	156	CA	SER	21	6.360	33.981	86.918	1.00 42.59	AAGL
ATOM	157	CB	SER	21	6.255	33.775	85.402	1.00 43.78	AAGL
ATOM	158	OG	SER	21	5.527	34.835	84.790	1.00 44.41	AAGL
ATOM	159	C	SER	21	7.191	35.224	87.221	1.00 41.81	AAGL
ATOM	160	O	SER	21	6.639	36.307	87.421	1.00 42.15	AAGL
ATOM	161	N	TYR	22	8.510	35.075	87.260	1.00 40.81	AAGL
ATOM	162	CA	TYR	22	9.382	36.205	87.558	1.00 40.63	AAGL
ATOM	163	CB	TYR	22	10.143	35.955	88.855	1.00 39.48	AAGL
ATOM	164	CG	TYR	22	9.248	35.579	90.010	1.00 37.92	AAGL
ATOM	165	CD1	TYR	22	8.820	34.261	90.186	1.00 35.93	AAGL
ATOM	166	CE1	TYR	22	7.987	33.913	91.246	1.00 35.62	AAGL
ATOM	167	CD2	TYR	22	8.820	36.540	90.921	1.00 37.21	AAGL
ATOM	168	CE2	TYR	22	7.982	36.204	91.982	1.00 35.75	AAGL
ATOM	169	CZ	TYR	22	7.574	34.897	92.140	1.00 36.41	AAGL
ATOM	170	OH	TYR	22	6.761	34.573	93.196	1.00 34.78	AAGL
ATOM	171	C	TYR	22	10.385	36.498	86.455	1.00 41.14	AAGL
ATOM	172	O	TYR	22	10.607	35.672	85.568	1.00 40.90	AAGL
ATOM	173	N	LYS	23	10.990	37.684	86.532	1.00 40.98	AAGL
ATOM	174	CA	LYS	23	11.987	38.131	85.565	1.00 41.42	AAGL
ATOM	175	CB	LYS	23	11.430	39.257	84.690	1.00 44.58	AAGL
ATOM	176	CG	LYS	23	10.779	38.781	83.398	1.00 49.11	AAGL
ATOM	177	CD	LYS	23	9.379	38.262	83.633	1.00 51.49	AAGL
ATOM	178	CE	LYS	23	8.453	39.401	84.042	1.00 52.49	AAGL
ATOM	179	NZ	LYS	23	8.461	40.487	83.021	1.00 51.35	AAGL
ATOM	180	C	LYS	23	13.248	38.634	86.243	1.00 40.33	AAGL
ATOM	181	O	LYS	23	13.184	39.363	87.241	1.00 39.11	AAGL
ATOM	182	N	ASN	24	14.396	38.246	85.693	1.00 38.79	AAGL
ATOM	183	CA	ASN	24	15.682	38.672	86.226	1.00 40.03	AAGL
ATOM	184	CB	ASN	24	16.807	37.935	85.509	1.00 42.29	AAGL
ATOM	185	CG	ASN	24	16.738	38.104	84.004	1.00 42.84	AAGL
ATOM	186	OD1	ASN	24	16.732	39.224	83.497	1.00 43.55	AAGL
ATOM	187	ND2	ASN	24	16.675	36.993	83.282	1.00 45.13	AAGL
ATOM	188	C	ASN	24	15.840	40.178	86.018	1.00 40.98	AAGL
ATOM	189	O	ASN	24	14.938	40.837	85.494	1.00 38.96	AAGL
ATOM	190	N	LEU	25	16.987	40.720	86.423	1.00 42.28	AAGL
ATOM	191	CA	LEU	25	17.246	42.149	86.283	1.00 44.49	AAGL
ATOM	192	CB	LEU	25	18.528	42.543	87.032	1.00 44.66	AAGL
ATOM	193	CG	LEU	25	18.549	42.643	88.563	1.00 45.79	AAGL
ATOM	194	CD1	LEU	25	17.376	43.494	89.037	1.00 45.23	AAGL
ATOM	195	CD2	LEU	25	18.493	41.252	89.189	1.00 46.13	AAGL
ATOM	196	C	LEU	25	17.345	42.614	84.824	1.00 45.76	AAGL
ATOM	197	O	LEU	25	17.454	43.814	84.562	1.00 46.23	AAGL

Fig. 3 cont.

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ATOM    198  N   ASN    26      17.311  41.675  83.880  1.00 46.41      AAGL
ATOM    199  CA  ASN    26      17.365  42.021  82.455  1.00 47.05      AAGL
ATOM    200  CB  ASN    26      18.288  41.066  81.676  1.00 47.42      AAGL
ATOM    201  CG  ASN    26      19.747  41.198  82.074  1.00 49.18      AAGL
ATOM    202  OD1 ASN    26      20.207  42.276  82.459  1.00 49.93      AAGL
ATOM    203  ND2 ASN    26      20.492  40.100  81.961  1.00 49.97      AAGL
ATOM    204  C   ASN    26      15.966  41.947  81.848  1.00 47.00      AAGL
ATOM    205  O   ASN    26      15.796  42.082  80.634  1.00 47.34      AAGL
ATOM    206  N   GLY    27      14.961  41.712  82.684  1.00 45.83      AAGL
ATOM    207  CA  GLY    27      13.602  41.628  82.176  1.00 45.48      AAGL
ATOM    208  C   GLY    27      13.343  40.327  81.436  1.00 45.43      AAGL
ATOM    209  O   GLY    27      12.388  40.225  80.669  1.00 46.84      AAGL
ATOM    210  N   GLN    28      14.198  39.332  81.648  1.00 45.03      AAGL
ATOM    211  CA  GLN    28      14.023  38.037  81.002  1.00 44.89      AAGL
ATOM    212  CB  GLN    28      15.385  37.428  80.633  1.00 46.09      AAGL
ATOM    213  CG  GLN    28      16.346  38.371  79.909  1.00 48.72      AAGL
ATOM    214  CD  GLN    28      17.649  37.684  79.531  1.00 49.91      AAGL
ATOM    215  OE1 GLN    28      17.674  36.802  78.668  1.00 51.23      AAGL
ATOM    216  NE2 GLN    28      18.740  38.075  80.187  1.00 51.05      AAGL
ATOM    217  C   GLN    28      13.312  37.093  81.980  1.00 43.57      AAGL
ATOM    218  O   GLN    28      13.800  36.871  83.088  1.00 40.72      AAGL
ATOM    219  N   THR    29      12.166  36.542  81.580  1.00 42.64      AAGL
ATOM    220  CA  THR    29      11.441  35.610  82.445  1.00 42.01      AAGL
ATOM    221  CB  THR    29      10.201  35.022  81.746  1.00 42.12      AAGL
ATOM    222  OG1 THR    29       9.191  36.030  81.626  1.00 42.02      AAGL
ATOM    223  CG2 THR    29       9.639  33.857  82.552  1.00 41.97      AAGL
ATOM    224  C   THR    29      12.393  34.472  82.787  1.00 41.90      AAGL
ATOM    225  O   THR    29      13.233  34.095  81.966  1.00 41.33      AAGL
ATOM    226  N   GLN    30      12.261  33.909  83.984  1.00 40.58      AAGL
ATOM    227  CA  GLN    30      13.158  32.835  84.392  1.00 39.49      AAGL
ATOM    228  CB  GLN    30      14.585  33.383  84.396  1.00 40.50      AAGL
ATOM    229  CG  GLN    30      15.604  32.528  85.100  1.00 43.69      AAGL
ATOM    230  CD  GLN    30      17.014  33.031  84.892  1.00 46.36      AAGL
ATOM    231  OE1 GLN    30      17.325  34.200  85.159  1.00 45.16      AAGL
ATOM    232  NE2 GLN    30      17.888  32.145  84.409  1.00 47.79      AAGL
ATOM    233  C   GLN    30      12.790  32.268  85.763  1.00 38.44      AAGL
ATOM    234  O   GLN    30      12.368  33.004  86.656  1.00 38.87      AAGL
ATOM    235  N   ALA    31      12.946  30.958  85.929  1.00 36.80      AAGL
ATOM    236  CA  ALA    31      12.617  30.314  87.202  1.00 34.49      AAGL
ATOM    237  CB  ALA    31      13.079  28.855  87.186  1.00 34.38      AAGL
ATOM    238  C   ALA    31      13.261  31.059  88.371  1.00 32.91      AAGL
ATOM    239  O   ALA    31      14.474  31.278  88.392  1.00 32.07      AAGL
ATOM    240  N   LEU    32      12.441  31.432  89.352  1.00 33.31      AAGL
ATOM    241  CA  LEU    32      12.914  32.180  90.522  1.00 29.54      AAGL
ATOM    242  CB  LEU    32      11.809  32.294  91.574  1.00 28.70      AAGL
ATOM    243  CG  LEU    32      12.229  33.100  92.815  1.00 26.84      AAGL
ATOM    244  CD1 LEU    32      12.430  34.545  92.422  1.00 26.55      AAGL
ATOM    245  CD2 LEU    32      11.173  32.985  93.916  1.00 26.84      AAGL
ATOM    246  C   LEU    32      14.160  31.618  91.192  1.00 30.30      AAGL
ATOM    247  O   LEU    32      15.068  32.375  91.545  1.00 29.24      AAGL
ATOM    248  N   GLU    33      14.205  30.304  91.387  1.00 29.20      AAGL
ATOM    249  CA  GLU    33      15.360  29.698  92.036  1.00 29.33      AAGL
ATOM    250  CB  GLU    33      15.164  28.184  92.223  1.00 30.11      AAGL
ATOM    251  CG  GLU    33      15.225  27.380  90.934  1.00 32.96      AAGL
ATOM    252  CD  GLU    33      13.872  27.167  90.294  1.00 32.82      AAGL
ATOM    253  OE1 GLU    33      12.979  28.030  90.451  1.00 32.32      AAGL
ATOM    254  OE2 GLU    33      13.706  26.126  89.609  1.00 34.46      AAGL
ATOM    255  C   GLU    33      16.641  29.949  91.242  1.00 30.20      AAGL
ATOM    256  O   GLU    33      17.708  30.125  91.828  1.00 30.32      AAGL
ATOM    257  N   THR    34      16.544  29.967  89.912  1.00 31.16      AAGL
ATOM    258  CA  THR    34      17.734  30.197  89.102  1.00 32.16      AAGL
ATOM    259  CB  THR    34      17.545  29.703  87.636  1.00 34.39      AAGL
ATOM    260  OG1 THR    34      16.690  30.598  86.916  1.00 39.01      AAGL
ATOM    261  CG2 THR    34      16.915  28.315  87.628  1.00 33.29      AAGL
ATOM    262  C   THR    34      18.100  31.677  89.120  1.00 30.19      AAGL
ATOM    263  O   THR    34      19.269  32.027  89.031  1.00 32.36      AAGL
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Fig. 3 cont.

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ATOM    264  N   ILE    35      17.101  32.542  89.254  1.00 29.48      AAGL
ATOM    265  CA  ILE    35      17.343  33.982  89.318  1.00 29.20      AAGL
ATOM    266  CB  ILE    35      16.030  34.783  89.364  1.00 29.36      AAGL
ATOM    267  CG2 ILE    35      16.329  36.253  89.647  1.00 32.47      AAGL
ATOM    268  CG1 ILE    35      15.265  34.620  88.052  1.00 30.39      AAGL
ATOM    269  CD1 ILE    35      13.998  35.456  87.981  1.00 32.09      AAGL
ATOM    270  C   ILE    35      18.103  34.276  90.605  1.00 29.48      AAGL
ATOM    271  O   ILE    35      19.039  35.068  90.627  1.00 28.30      AAGL
ATOM    272  N   LEU    36      17.676  33.631  91.684  1.00 28.93      AAGL
ATOM    273  CA  LEU    36      18.297  33.809  92.989  1.00 27.40      AAGL
ATOM    274  CB  LEU    36      17.420  33.142  94.050  1.00 29.01      AAGL
ATOM    275  CG  LEU    36      16.067  33.824  94.220  1.00 29.41      AAGL
ATOM    276  CD1 LEU    36      15.139  32.993  95.105  1.00 32.23      AAGL
ATOM    277  CD2 LEU    36      16.318  35.198  94.831  1.00 29.88      AAGL
ATOM    278  C   LEU    36      19.693  33.220  93.036  1.00 26.84      AAGL
ATOM    279  O   LEU    36      20.630  33.840  93.542  1.00 26.88      AAGL
ATOM    280  N   ALA    37      19.829  32.005  92.515  1.00 28.77      AAGL
ATOM    281  CA  ALA    37      21.118  31.325  92.509  1.00 30.25      AAGL
ATOM    282  CB  ALA    37      20.988  29.971  91.805  1.00 29.94      AAGL
ATOM    283  C   ALA    37      22.185  32.180  91.827  1.00 29.84      AAGL
ATOM    284  O   ALA    37      23.274  32.373  92.365  1.00 30.61      AAGL
ATOM    285  N   ASP    38      21.856  32.706  90.652  1.00 30.68      AAGL
ATOM    286  CA  ASP    38      22.798  33.524  89.894  1.00 31.88      AAGL
ATOM    287  CB  ASP    38      22.240  33.843  88.508  1.00 32.57      AAGL
ATOM    288  CG  ASP    38      22.007  32.603  87.673  1.00 36.25      AAGL
ATOM    289  OD1 ASP    38      22.749  31.610  87.859  1.00 36.97      AAGL
ATOM    290  OD2 ASP    38      21.085  32.621  86.830  1.00 37.38      AAGL
ATOM    291  C   ASP    38      23.127  34.824  90.601  1.00 31.89      AAGL
ATOM    292  O   ASP    38      24.174  35.423  90.353  1.00 33.41      AAGL
ATOM    293  N   ALA    39      22.226  35.265  91.476  1.00 31.50      AAGL
ATOM    294  CA  ALA    39      22.433  36.503  92.207  1.00 29.58      AAGL
ATOM    295  CB  ALA    39      21.088  37.099  92.626  1.00 29.62      AAGL
ATOM    296  C   ALA    39      23.319  36.300  93.423  1.00 29.11      AAGL
ATOM    297  O   ALA    39      23.739  37.268  94.053  1.00 28.08      AAGL
ATOM    298  N   GLY    40      23.603  35.047  93.769  1.00 28.38      AAGL
ATOM    299  CA  GLY    40      24.462  34.804  94.915  1.00 28.68      AAGL
ATOM    300  C   GLY    40      23.804  34.079  96.077  1.00 27.30      AAGL
ATOM    301  O   GLY    40      24.489  33.628  96.994  1.00 28.21      AAGL
ATOM    302  N   ILE    41      22.480  33.973  96.046  1.00 27.82      AAGL
ATOM    303  CA  ILE    41      21.754  33.271  97.105  1.00 28.31      AAGL
ATOM    304  CB  ILE    41      20.231  33.267  96.841  1.00 28.86      AAGL
ATOM    305  CG2 ILE    41      19.502  32.678  98.047  1.00 26.11      AAGL
ATOM    306  CG1 ILE    41      19.741  34.680  96.490  1.00 32.71      AAGL
ATOM    307  CD1 ILE    41      20.041  35.739  97.526  1.00 34.86      AAGL
ATOM    308  C   ILE    41      22.262  31.830  97.055  1.00 29.05      AAGL
ATOM    309  O   ILE    41      22.275  31.223  95.982  1.00 28.58      AAGL
ATOM    310  N   ASN    42      22.694  31.283  98.192  1.00 27.24      AAGL
ATOM    311  CA  ASN    42      23.209  29.921  98.192  1.00 27.38      AAGL
ATOM    312  CB  ASN    42      24.715  29.897  98.547  1.00 26.67      AAGL
ATOM    313  CG  ASN    42      25.014  30.267  99.999  1.00 29.27      AAGL
ATOM    314  OD1 ASN    42      26.177  30.238 100.422  1.00 30.70      AAGL
ATOM    315  ND2 ASN    42      23.984  30.620 100.767  1.00 28.35      AAGL
ATOM    316  C   ASN    42      22.449  28.945  99.077  1.00 27.09      AAGL
ATOM    317  O   ASN    42      22.873  27.801  99.244  1.00 25.65      AAGL
ATOM    318  N   SER    43      21.324  29.390  99.633  1.00 25.87      AAGL
ATOM    319  CA  SER    43      20.525  28.520 100.481  1.00 25.56      AAGL
ATOM    320  CB  SER    43      21.049  28.551 101.913  1.00 26.01      AAGL
ATOM    321  OG  SER    43      20.497  27.483 102.665  1.00 25.97      AAGL
ATOM    322  C   SER    43      19.051  28.914 100.462  1.00 25.21      AAGL
ATOM    323  O   SER    43      18.714  30.096 100.411  1.00 22.67      AAGL
ATOM    324  N   ILE    44      18.177  27.910 100.494  1.00 24.04      AAGL
ATOM    325  CA  ILE    44      16.737  28.146 100.475  1.00 23.25      AAGL
ATOM    326  CB  ILE    44      16.105  27.603  99.166  1.00 25.17      AAGL
ATOM    327  CG2 ILE    44      14.599  27.796  99.185  1.00 23.06      AAGL
ATOM    328  CG1 ILE    44      16.698  28.333  97.953  1.00 25.29      AAGL
ATOM    329  CD1 ILE    44      16.327  29.795  97.867  1.00 26.67      AAGL
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Fig. 3 cont.

ATOM	330	C	ILE	44	16.057	27.481	101.677	1.00	23.88	AAGL
ATOM	331	O	ILE	44	16.273	26.305	101.953	1.00	22.19	AAGL
ATOM	332	N	ARG	45	15.244	28.262	102.384	1.00	21.15	AAGL
ATOM	333	CA	ARG	45	14.512	27.796	103.558	1.00	20.84	AAGL
ATOM	334	CB	ARG	45	14.497	28.905	104.607	1.00	19.60	AAGL
ATOM	335	CG	ARG	45	13.815	28.594	105.927	1.00	22.30	AAGL
ATOM	336	CD	ARG	45	13.941	29.840	106.803	1.00	22.44	AAGL
ATOM	337	NE	ARG	45	13.442	29.713	108.172	1.00	21.57	AAGL
ATOM	338	CZ	ARG	45	12.253	30.147	108.580	1.00	21.21	AAGL
ATOM	339	NH1	ARG	45	11.420	30.721	107.726	1.00	19.38	AAGL
ATOM	340	NH2	ARG	45	11.924	30.071	109.864	1.00	18.87	AAGL
ATOM	341	C	ARG	45	13.091	27.456	103.120	1.00	18.60	AAGL
ATOM	342	O	ARG	45	12.471	28.214	102.376	1.00	19.88	AAGL
ATOM	343	N	GLN	46	12.582	26.314	103.574	1.00	19.69	AAGL
ATOM	344	CA	GLN	46	11.235	25.881	103.212	1.00	18.26	AAGL
ATOM	345	CB	GLN	46	11.311	24.701	102.234	1.00	19.90	AAGL
ATOM	346	CG	GLN	46	12.070	25.027	100.949	1.00	19.68	AAGL
ATOM	347	CD	GLN	46	12.093	23.880	99.946	1.00	23.43	AAGL
ATOM	348	OE1	GLN	46	12.705	23.992	98.882	1.00	26.77	AAGL
ATOM	349	NE2	GLN	46	11.429	22.777	100.278	1.00	21.73	AAGL
ATOM	350	C	GLN	46	10.432	25.467	104.445	1.00	17.71	AAGL
ATOM	351	O	GLN	46	10.896	24.649	105.238	1.00	18.22	AAGL
ATOM	352	N	ARG	47	9.233	26.023	104.601	1.00	18.28	AAGL
ATOM	353	CA	ARG	47	8.409	25.670	105.751	1.00	18.38	AAGL
ATOM	354	CB	ARG	47	7.414	26.792	106.095	1.00	18.50	AAGL
ATOM	355	CG	ARG	47	6.542	27.319	104.954	1.00	21.41	AAGL
ATOM	356	CD	ARG	47	5.455	28.254	105.503	1.00	20.07	AAGL
ATOM	357	NE	ARG	47	4.735	28.978	104.453	1.00	18.68	AAGL
ATOM	358	CZ	ARG	47	5.228	30.016	103.783	1.00	19.34	AAGL
ATOM	359	NH1	ARG	47	6.448	30.472	104.054	1.00	20.84	AAGL
ATOM	360	NH2	ARG	47	4.513	30.582	102.819	1.00	19.53	AAGL
ATOM	361	C	ARG	47	7.677	24.365	105.472	1.00	18.74	AAGL
ATOM	362	O	ARG	47	7.101	24.183	104.403	1.00	18.19	AAGL
ATOM	363	N	VAL	48	7.710	23.458	106.445	1.00	19.24	AAGL
ATOM	364	CA	VAL	48	7.074	22.155	106.301	1.00	20.17	AAGL
ATOM	365	CB	VAL	48	8.109	21.023	106.490	1.00	20.89	AAGL
ATOM	366	CG1	VAL	48	7.488	19.677	106.130	1.00	20.76	AAGL
ATOM	367	CG2	VAL	48	9.350	21.301	105.644	1.00	21.80	AAGL
ATOM	368	C	VAL	48	5.947	21.932	107.311	1.00	20.72	AAGL
ATOM	369	O	VAL	48	6.166	22.027	108.517	1.00	19.48	AAGL
ATOM	370	N	TRP	49	4.748	21.647	106.805	1.00	18.93	AAGL
ATOM	371	CA	TRP	49	3.590	21.371	107.646	1.00	19.06	AAGL
ATOM	372	CB	TRP	49	2.382	22.168	107.167	1.00	19.85	AAGL
ATOM	373	CG	TRP	49	2.525	23.645	107.414	1.00	19.05	AAGL
ATOM	374	CD2	TRP	49	1.608	24.673	107.024	1.00	18.82	AAGL
ATOM	375	CE2	TRP	49	2.125	25.897	107.504	1.00	19.73	AAGL
ATOM	376	CE3	TRP	49	0.396	24.678	106.316	1.00	20.02	AAGL
ATOM	377	CD1	TRP	49	3.535	24.271	108.090	1.00	17.67	AAGL
ATOM	378	NE1	TRP	49	3.300	25.620	108.149	1.00	18.03	AAGL
ATOM	379	CZ2	TRP	49	1.475	27.117	107.301	1.00	20.25	AAGL
ATOM	380	CZ3	TRP	49	-0.253	25.899	106.112	1.00	22.82	AAGL
ATOM	381	CH2	TRP	49	0.291	27.100	106.606	1.00	22.06	AAGL
ATOM	382	C	TRP	49	3.306	19.873	107.587	1.00	19.52	AAGL
ATOM	383	O	TRP	49	3.553	19.231	106.563	1.00	19.96	AAGL
ATOM	384	N	VAL	50	2.778	19.322	108.677	1.00	18.80	AAGL
ATOM	385	CA	VAL	50	2.522	17.886	108.756	1.00	20.11	AAGL
ATOM	386	CB	VAL	50	2.398	17.443	110.231	1.00	18.82	AAGL
ATOM	387	CG1	VAL	50	2.120	15.954	110.316	1.00	21.34	AAGL
ATOM	388	CG2	VAL	50	3.695	17.768	110.966	1.00	21.13	AAGL
ATOM	389	C	VAL	50	1.340	17.362	107.947	1.00	22.22	AAGL
ATOM	390	O	VAL	50	1.538	16.629	106.973	1.00	23.75	AAGL
ATOM	391	N	ASN	51	0.119	17.721	108.329	1.00	22.74	AAGL
ATOM	392	CA	ASN	51	-1.044	17.251	107.585	1.00	25.51	AAGL
ATOM	393	CB	ASN	51	-1.765	16.133	108.354	1.00	26.96	AAGL
ATOM	394	CG	ASN	51	-0.879	14.932	108.619	0.50	27.07	AAGL
ATOM	395	OD1	ASN	51	-0.265	14.387	107.707	0.50	29.27	AAGL

Fig. 3 cont.

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ATOM    396  ND2 ASN    51      -0.821  14.505 109.878  0.50 28.87      AAGL
ATOM    397  C   ASN    51      -2.055  18.350 107.238  1.00 26.72      AAGL
ATOM    398  O   ASN    51      -3.204  18.305 107.668  1.00 27.90      AAGL
ATOM    399  N   PRO    52      -1.638  19.358 106.459  1.00 26.25      AAGL
ATOM    400  CD  PRO    52      -0.337  19.594 105.814  1.00 25.34      AAGL
ATOM    401  CA  PRO    52      -2.599  20.410 106.113  1.00 26.62      AAGL
ATOM    402  CB  PRO    52      -1.735  21.431 105.389  1.00 25.68      AAGL
ATOM    403  CG  PRO    52      -0.697  20.582 104.735  1.00 25.47      AAGL
ATOM    404  C   PRO    52      -3.690  19.816 105.215  1.00 28.63      AAGL
ATOM    405  O   PRO    52      -3.391  19.112 104.254  1.00 27.01      AAGL
ATOM    406  N   SER    53      -4.949  20.086 105.543  1.00 29.82      AAGL
ATOM    407  CA  SER    53      -6.062  19.554 104.760  1.00 33.18      AAGL
ATOM    408  CB  SER    53      -7.394  20.100 105.281  1.00 35.65      AAGL
ATOM    409  OG  SER    53      -7.728  19.496 106.515  1.00 38.67      AAGL
ATOM    410  C   SER    53      -5.948  19.859 103.274  1.00 32.30      AAGL
ATOM    411  O   SER    53      -6.284  19.019 102.434  1.00 32.67      AAGL
ATOM    412  N   ASP    54      -5.469  21.053 102.949  1.00 31.58      AAGL
ATOM    413  CA  ASP    54      -5.343  21.444 101.555  1.00 31.37      AAGL
ATOM    414  CB  ASP    54      -5.736  22.922 101.389  1.00 33.51      AAGL
ATOM    415  CG  ASP    54      -4.616  23.878 101.754  1.00 35.96      AAGL
ATOM    416  OD1 ASP    54      -3.796  23.537 102.630  1.00 35.79      AAGL
ATOM    417  OD2 ASP    54      -4.569  24.986 101.166  1.00 38.48      AAGL
ATOM    418  C   ASP    54      -3.974  21.164 100.937  1.00 30.51      AAGL
ATOM    419  O   ASP    54      -3.715  21.572  99.812  1.00 30.89      AAGL
ATOM    420  N   GLY    55      -3.110  20.460 101.670  1.00 31.08      AAGL
ATOM    421  CA  GLY    55      -1.790  20.102 101.161  1.00 29.00      AAGL
ATOM    422  C   GLY    55      -0.684  21.149 101.119  1.00 28.85      AAGL
ATOM    423  O   GLY    55       0.475  20.829 100.834  1.00 27.57      AAGL
ATOM    424  N   SER    56      -1.028  22.399 101.398  1.00 29.06      AAGL
ATOM    425  CA  SER    56      -0.036  23.468 101.362  1.00 29.25      AAGL
ATOM    426  CB  SER    56      -0.685  24.799 101.747  1.00 33.01      AAGL
ATOM    427  OG  SER    56      -1.603  25.222 100.746  1.00 35.28      AAGL
ATOM    428  C   SER    56       1.163  23.211 102.266  1.00 27.16      AAGL
ATOM    429  O   SER    56       1.013  22.944 103.462  1.00 26.75      AAGL
ATOM    430  N   TYR    57       2.350  23.282 101.673  1.00 24.25      AAGL
ATOM    431  CA  TYR    57       3.611  23.102 102.379  1.00 23.39      AAGL
ATOM    432  CB  TYR    57       3.773  24.192 103.455  1.00 21.44      AAGL
ATOM    433  CG  TYR    57       3.411  25.586 102.983  1.00 18.93      AAGL
ATOM    434  CD1 TYR    57       4.090  26.183 101.927  1.00 20.85      AAGL
ATOM    435  CE1 TYR    57       3.733  27.448 101.457  1.00 20.55      AAGL
ATOM    436  CD2 TYR    57       2.363  26.291 103.575  1.00 20.42      AAGL
ATOM    437  CE2 TYR    57       1.992  27.555 103.119  1.00 23.25      AAGL
ATOM    438  CZ  TYR    57       2.687  28.130 102.049  1.00 22.03      AAGL
ATOM    439  OH  TYR    57       2.323  29.367 101.572  1.00 24.57      AAGL
ATOM    440  C   TYR    57       3.809  21.736 103.024  1.00 24.63      AAGL
ATOM    441  O   TYR    57       4.583  21.619 103.972  1.00 22.67      AAGL
ATOM    442  N   ASP    58       3.121  20.701 102.540  1.00 25.81      AAGL
ATOM    443  CA  ASP    58       3.319  19.376 103.128  1.00 27.04      AAGL
ATOM    444  CB  ASP    58       2.084  18.473 102.946  1.00 27.80      AAGL
ATOM    445  CG  ASP    58       1.763  18.160 101.491  1.00 32.21      AAGL
ATOM    446  OD1 ASP    58       2.652  18.279 100.623  1.00 30.26      AAGL
ATOM    447  OD2 ASP    58       0.597  17.768 101.228  1.00 32.38      AAGL
ATOM    448  C   ASP    58       4.574  18.724 102.542  1.00 28.05      AAGL
ATOM    449  O   ASP    58       5.320  19.367 101.793  1.00 27.53      AAGL
ATOM    450  N   LEU    59       4.820  17.462 102.883  1.00 26.92      AAGL
ATOM    451  CA  LEU    59       6.018  16.786 102.403  1.00 28.31      AAGL
ATOM    452  CB  LEU    59       6.116  15.377 103.001  1.00 30.14      AAGL
ATOM    453  CG  LEU    59       7.435  14.620 102.784  1.00 29.84      AAGL
ATOM    454  CD1 LEU    59       8.609  15.430 103.323  1.00 31.61      AAGL
ATOM    455  CD2 LEU    59       7.355  13.265 103.479  1.00 31.80      AAGL
ATOM    456  C   LEU    59       6.145  16.714 100.885  1.00 26.89      AAGL
ATOM    457  O   LEU    59       7.220  16.952 100.342  1.00 24.30      AAGL
ATOM    458  N   ASP    60       5.061  16.401 100.188  1.00 28.43      AAGL
ATOM    459  CA  ASP    60       5.145  16.315  98.736  1.00 29.43      AAGL
ATOM    460  CB  ASP    60       3.850  15.740  98.149  1.00 32.44      AAGL
ATOM    461  CG  ASP    60       3.557  14.332  98.651  1.00 37.53      AAGL
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Fig. 3 cont.

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ATOM    462  OD1 ASP    60       4.518  13.547  98.833  1.00 40.66      AAGL
ATOM    463  OD2 ASP    60       2.365  14.000  98.858  1.00 42.65      AAGL
ATOM    464  C   ASP    60       5.439  17.689  98.137  1.00 30.40      AAGL
ATOM    465  O   ASP    60       6.266  17.816  97.237  1.00 28.80      AAGL
ATOM    466  N   TYR    61       4.761  18.710  98.651  1.00 28.48      AAGL
ATOM    467  CA  TYR    61       4.944  20.088  98.203  1.00 25.60      AAGL
ATOM    468  CB  TYR    61       4.100  21.031  99.080  1.00 25.21      AAGL
ATOM    469  CG  TYR    61       4.182  22.508  98.723  1.00 25.14      AAGL
ATOM    470  CD1 TYR    61       5.283  23.286  99.095  1.00 23.80      AAGL
ATOM    471  CE1 TYR    61       5.360  24.639  98.759  1.00 24.64      AAGL
ATOM    472  CD2 TYR    61       3.154  23.125  98.006  1.00 25.32      AAGL
ATOM    473  CE2 TYR    61       3.220  24.481  97.664  1.00 26.31      AAGL
ATOM    474  CZ  TYR    61       4.327  25.231  98.043  1.00 25.45      AAGL
ATOM    475  OH  TYR    61       4.403  26.565  97.687  1.00 24.80      AAGL
ATOM    476  C   TYR    61       6.422  20.444  98.330  1.00 26.83      AAGL
ATOM    477  O   TYR    61       7.039  20.948  97.393  1.00 25.72      AAGL
ATOM    478  N   ASN    62       6.992  20.159  99.493  1.00 24.55      AAGL
ATOM    479  CA  ASN    62       8.388  20.458  99.733  1.00 25.46      AAGL
ATOM    480  CB  ASN    62       8.695  20.315 101.225  1.00 25.35      AAGL
ATOM    481  CG  ASN    62       8.316  21.568 102.009  1.00 25.66      AAGL
ATOM    482  OD1 ASN    62       9.047  22.556 101.998  1.00 23.45      AAGL
ATOM    483  ND2 ASN    62       7.159  21.539 102.666  1.00 21.77      AAGL
ATOM    484  C   ASN    62       9.355  19.629  98.899  1.00 25.81      AAGL
ATOM    485  O   ASN    62      10.450  20.090  98.596  1.00 23.79      AAGL
ATOM    486  N   LEU    63       8.969  18.411  98.528  1.00 25.79      AAGL
ATOM    487  CA  LEU    63       9.856  17.589  97.708  1.00 27.44      AAGL
ATOM    488  CB  LEU    63       9.320  16.153  97.581  1.00 29.01      AAGL
ATOM    489  CG  LEU    63       9.673  15.225  98.743  1.00 31.95      AAGL
ATOM    490  CD1 LEU    63       9.041  13.851  98.508  1.00 32.91      AAGL
ATOM    491  CD2 LEU    63      11.199  15.114  98.872  1.00 32.19      AAGL
ATOM    492  C   LEU    63      10.001  18.207  96.322  1.00 27.90      AAGL
ATOM    493  O   LEU    63      11.102  18.275  95.772  1.00 29.37      AAGL
ATOM    494  N   GLU    64       8.882  18.662  95.768  1.00 28.38      AAGL
ATOM    495  CA  GLU    64       8.859  19.280  94.447  1.00 30.60      AAGL
ATOM    496  CB  GLU    64       7.414  19.642  94.078  1.00 32.03      AAGL
ATOM    497  CG  GLU    64       7.198  20.124  92.639  1.00 36.66      AAGL
ATOM    498  CD  GLU    64       5.747  20.468  92.364  1.00 38.83      AAGL
ATOM    499  OE1 GLU    64       4.874  19.637  92.688  1.00 41.75      AAGL
ATOM    500  OE2 GLU    64       5.464  21.565  91.822  1.00 41.60      AAGL
ATOM    501  C   GLU    64       9.727  20.536  94.454  1.00 29.58      AAGL
ATOM    502  O   GLU    64      10.525  20.769  93.541  1.00 27.18      AAGL
ATOM    503  N   LEU    65       9.578  21.343  95.497  1.00 27.01      AAGL
ATOM    504  CA  LEU    65      10.344  22.576  95.611  1.00 25.95      AAGL
ATOM    505  CB  LEU    65       9.754  23.455  96.721  1.00 27.05      AAGL
ATOM    506  CG  LEU    65      10.420  24.806  97.018  1.00 25.59      AAGL
ATOM    507  CD1 LEU    65      10.528  25.628  95.760  1.00 24.36      AAGL
ATOM    508  CD2 LEU    65       9.600  25.544  98.074  1.00 25.15      AAGL
ATOM    509  C   LEU    65      11.824  22.329  95.877  1.00 26.00      AAGL
ATOM    510  O   LEU    65      12.677  23.029  95.329  1.00 27.12      AAGL
ATOM    511  N   ALA    66      12.131  21.330  96.699  1.00 23.38      AAGL
ATOM    512  CA  ALA    66      13.517  21.025  97.038  1.00 25.19      AAGL
ATOM    513  CB  ALA    66      13.572  20.017  98.203  1.00 25.90      AAGL
ATOM    514  C   ALA    66      14.278  20.481  95.833  1.00 27.46      AAGL
ATOM    515  O   ALA    66      15.479  20.714  95.697  1.00 28.22      AAGL
ATOM    516  N   LYS    67      13.578  19.752  94.969  1.00 28.70      AAGL
ATOM    517  CA  LYS    67      14.201  19.188  93.768  1.00 32.17      AAGL
ATOM    518  CB  LYS    67      13.164  18.444  92.924  1.00 32.68      AAGL
ATOM    519  CG  LYS    67      12.902  17.003  93.358  1.00 36.34      AAGL
ATOM    520  CD  LYS    67      11.676  16.443  92.655  1.00 38.14      AAGL
ATOM    521  CE  LYS    67      11.447  14.989  93.012  1.00 41.38      AAGL
ATOM    522  NZ  LYS    67      10.184  14.468  92.407  1.00 43.11      AAGL
ATOM    523  C   LYS    67      14.813  20.303  92.931  1.00 32.63      AAGL
ATOM    524  O   LYS    67      15.943  20.192  92.453  1.00 32.89      AAGL
ATOM    525  N   ARG    68      14.053  21.376  92.763  1.00 31.49      AAGL
ATOM    526  CA  ARG    68      14.497  22.523  91.988  1.00 31.44      AAGL
ATOM    527  CB  ARG    68      13.300  23.419  91.683  1.00 31.14      AAGL
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Fig. 3 cont.

ATOM	528	CG	ARG	68	12.313	22.760	90.730	1.00	33.54	AAGL
ATOM	529	CD	ARG	68	11.016	23.518	90.619	1.00	32.13	AAGL
ATOM	530	NE	ARG	68	11.222	24.924	90.303	1.00	31.17	AAGL
ATOM	531	CZ	ARG	68	10.238	25.763	90.002	1.00	32.92	AAGL
ATOM	532	NH1	ARG	68	8.985	25.327	89.970	1.00	33.31	AAGL
ATOM	533	NH2	ARG	68	10.498	27.040	89.755	1.00	31.47	AAGL
ATOM	534	C	ARG	68	15.595	23.311	92.691	1.00	31.54	AAGL
ATOM	535	O	ARG	68	16.459	23.905	92.040	1.00	31.76	AAGL
ATOM	536	N	VAL	69	15.570	23.319	94.021	1.00	28.62	AAGL
ATOM	537	CA	VAL	69	16.584	24.025	94.794	1.00	27.79	AAGL
ATOM	538	CB	VAL	69	16.204	24.061	96.281	1.00	24.83	AAGL
ATOM	539	CG1	VAL	69	17.294	24.735	97.092	1.00	27.63	AAGL
ATOM	540	CG2	VAL	69	14.886	24.781	96.442	1.00	26.08	AAGL
ATOM	541	C	VAL	69	17.934	23.325	94.635	1.00	29.09	AAGL
ATOM	542	O	VAL	69	18.968	23.970	94.458	1.00	28.64	AAGL
ATOM	543	N	LYS	70	17.908	21.998	94.711	1.00	29.15	AAGL
ATOM	544	CA	LYS	70	19.108	21.187	94.561	1.00	31.30	AAGL
ATOM	545	CB	LYS	70	18.756	19.707	94.743	1.00	34.31	AAGL
ATOM	546	CG	LYS	70	19.889	18.752	94.422	1.00	36.20	AAGL
ATOM	547	CD	LYS	70	19.399	17.319	94.271	1.00	40.57	AAGL
ATOM	548	CE	LYS	70	18.290	17.224	93.229	1.00	41.78	AAGL
ATOM	549	NZ	LYS	70	18.666	17.932	91.966	1.00	42.36	AAGL
ATOM	550	C	LYS	70	19.693	21.403	93.159	1.00	31.39	AAGL
ATOM	551	O	LYS	70	20.903	21.592	92.997	1.00	31.53	AAGL
ATOM	552	N	ALA	71	18.813	21.386	92.165	1.00	30.10	AAGL
ATOM	553	CA	ALA	71	19.196	21.564	90.771	1.00	31.78	AAGL
ATOM	554	CB	ALA	71	17.957	21.525	89.879	1.00	30.31	AAGL
ATOM	555	C	ALA	71	19.949	22.870	90.570	1.00	33.02	AAGL
ATOM	556	O	ALA	71	20.975	22.900	89.888	1.00	32.79	AAGL
ATOM	557	N	ALA	72	19.442	23.940	91.179	1.00	32.06	AAGL
ATOM	558	CA	ALA	72	20.054	25.257	91.071	1.00	30.23	AAGL
ATOM	559	CB	ALA	72	19.048	26.323	91.463	1.00	31.29	AAGL
ATOM	560	C	ALA	72	21.316	25.389	91.915	1.00	29.83	AAGL
ATOM	561	O	ALA	72	21.908	26.463	91.990	1.00	29.82	AAGL
ATOM	562	N	GLY	73	21.714	24.298	92.561	1.00	28.89	AAGL
ATOM	563	CA	GLY	73	22.926	24.304	93.360	1.00	30.91	AAGL
ATOM	564	C	GLY	73	22.909	25.064	94.675	1.00	32.00	AAGL
ATOM	565	O	GLY	73	23.939	25.589	95.111	1.00	30.50	AAGL
ATOM	566	N	MET	74	21.748	25.121	95.316	1.00	31.23	AAGL
ATOM	567	CA	MET	74	21.641	25.814	96.593	1.00	31.02	AAGL
ATOM	568	CB	MET	74	20.500	26.840	96.537	1.00	29.51	AAGL
ATOM	569	CG	MET	74	20.676	27.893	95.434	1.00	29.42	AAGL
ATOM	570	SD	MET	74	19.481	29.259	95.503	1.00	28.77	AAGL
ATOM	571	CE	MET	74	18.129	28.654	94.532	1.00	26.24	AAGL
ATOM	572	C	MET	74	21.388	24.768	97.681	1.00	29.72	AAGL
ATOM	573	O	MET	74	20.893	23.682	97.385	1.00	30.60	AAGL
ATOM	574	N	SER	75	21.750	25.075	98.925	1.00	28.06	AAGL
ATOM	575	CA	SER	75	21.534	24.125	100.011	1.00	25.93	AAGL
ATOM	576	CB	SER	75	22.454	24.426	101.202	1.00	25.27	AAGL
ATOM	577	OG	SER	75	22.281	25.752	101.671	1.00	24.77	AAGL
ATOM	578	C	SER	75	20.075	24.203	100.439	1.00	27.57	AAGL
ATOM	579	O	SER	75	19.343	25.089	99.997	1.00	26.04	AAGL
ATOM	580	N	LEU	76	19.655	23.268	101.286	1.00	25.74	AAGL
ATOM	581	CA	LEU	76	18.273	23.227	101.747	1.00	27.05	AAGL
ATOM	582	CB	LEU	76	17.602	21.941	101.268	1.00	28.62	AAGL
ATOM	583	CG	LEU	76	16.130	21.726	101.615	1.00	31.64	AAGL
ATOM	584	CD1	LEU	76	15.268	22.677	100.772	1.00	29.51	AAGL
ATOM	585	CD2	LEU	76	15.748	20.268	101.346	1.00	32.16	AAGL
ATOM	586	C	LEU	76	18.177	23.309	103.264	1.00	24.07	AAGL
ATOM	587	O	LEU	76	18.890	22.619	103.985	1.00	24.81	AAGL
ATOM	588	N	TYR	77	17.293	24.179	103.732	1.00	24.59	AAGL
ATOM	589	CA	TYR	77	17.044	24.375	105.162	1.00	21.21	AAGL
ATOM	590	CB	TYR	77	17.441	25.812	105.550	1.00	21.04	AAGL
ATOM	591	CG	TYR	77	16.903	26.417	106.849	1.00	22.71	AAGL
ATOM	592	CD1	TYR	77	16.207	25.664	107.800	1.00	20.07	AAGL
ATOM	593	CE1	TYR	77	15.681	26.276	108.959	1.00	21.30	AAGL

Fig. 3 cont.

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ATOM    594  CD2 TYR    77      17.069  27.784 107.091  1.00 20.07      AAGL
ATOM    595  CE2 TYR    77      16.558  28.394 108.232  1.00 22.16      AAGL
ATOM    596  CZ  TYR    77      15.863  27.646 109.159  1.00 22.47      AAGL
ATOM    597  OH  TYR    77      15.331  28.312 110.248  1.00 21.22      AAGL
ATOM    598  C   TYR    77      15.553  24.121 105.318  1.00 19.67      AAGL
ATOM    599  O   TYR    77      14.730  24.875 104.804  1.00 21.16      AAGL
ATOM    600  N   LEU    78      15.217  23.021 105.989  1.00 19.73      AAGL
ATOM    601  CA  LEU    78      13.826  22.662 106.216  1.00 20.07      AAGL
ATOM    602  CB  LEU    78      13.645  21.140 106.164  1.00 20.48      AAGL
ATOM    603  CG  LEU    78      13.793  20.485 104.784  1.00 24.57      AAGL
ATOM    604  CD1 LEU    78      13.633  18.969 104.898  1.00 25.27      AAGL
ATOM    605  CD2 LEU    78      12.750  21.067 103.833  1.00 23.90      AAGL
ATOM    606  C   LEU    78      13.379  23.199 107.568  1.00 17.57      AAGL
ATOM    607  O   LEU    78      13.980  22.891 108.599  1.00 18.99      AAGL
ATOM    608  N   ASP    79      12.332  24.018 107.534  1.00 18.03      AAGL
ATOM    609  CA  ASP    79      11.754  24.642 108.721  1.00 18.85      AAGL
ATOM    610  CB  ASP    79      11.386  26.098 108.389  1.00 19.55      AAGL
ATOM    611  CG  ASP    79      10.593  26.785 109.493  1.00 25.39      AAGL
ATOM    612  OD1 ASP    79      10.682  26.370 110.662  1.00 22.47      AAGL
ATOM    613  OD2 ASP    79       9.885  27.761 109.180  1.00 27.84      AAGL
ATOM    614  C   ASP    79      10.514  23.848 109.116  1.00 16.61      AAGL
ATOM    615  O   ASP    79       9.427  24.105 108.608  1.00 16.77      AAGL
ATOM    616  N   LEU    80      10.686  22.881 110.014  1.00 16.76      AAGL
ATOM    617  CA  LEU    80       9.573  22.051 110.452  1.00 17.99      AAGL
ATOM    618  CB  LEU    80      10.077  20.777 111.132  1.00 18.64      AAGL
ATOM    619  CG  LEU    80      11.103  19.918 110.385  1.00 19.36      AAGL
ATOM    620  CD1 LEU    80      11.345  18.636 111.166  1.00 20.62      AAGL
ATOM    621  CD2 LEU    80      10.603  19.605 108.986  1.00 18.29      AAGL
ATOM    622  C   LEU    80       8.708  22.802 111.441  1.00 18.46      AAGL
ATOM    623  O   LEU    80       9.162  23.121 112.529  1.00 20.06      AAGL
ATOM    624  N   HIS    81       7.464  23.086 111.071  1.00 17.32      AAGL
ATOM    625  CA  HIS    81       6.572  23.780 111.987  1.00 16.30      AAGL
ATOM    626  CB  HIS    81       5.475  24.525 111.223  1.00 15.62      AAGL
ATOM    627  CG  HIS    81       5.939  25.810 110.612  1.00 19.94      AAGL
ATOM    628  CD2 HIS    81       7.137  26.167 110.093  1.00 19.51      AAGL
ATOM    629  ND1 HIS    81       5.129  26.921 110.507  1.00 20.10      AAGL
ATOM    630  CE1 HIS    81       5.811  27.909 109.952  1.00 20.61      AAGL
ATOM    631  NE2 HIS    81       7.031  27.477 109.693  1.00 20.38      AAGL
ATOM    632  C   HIS    81       5.939  22.811 112.984  1.00 17.32      AAGL
ATOM    633  O   HIS    81       5.368  23.240 113.987  1.00 18.88      AAGL
ATOM    634  N   LEU    82       6.045  21.513 112.709  1.00 16.02      AAGL
ATOM    635  CA  LEU    82       5.484  20.480 113.588  1.00 17.14      AAGL
ATOM    636  CB  LEU    82       6.339  20.342 114.850  1.00 16.85      AAGL
ATOM    637  CG  LEU    82       7.813  20.007 114.595  1.00 20.75      AAGL
ATOM    638  CD1 LEU    82       8.537  19.890 115.923  1.00 18.12      AAGL
ATOM    639  CD2 LEU    82       7.935  18.712 113.812  1.00 18.95      AAGL
ATOM    640  C   LEU    82       4.048  20.826 113.965  1.00 18.59      AAGL
ATOM    641  O   LEU    82       3.664  20.829 115.146  1.00 18.40      AAGL
ATOM    642  N   SER    83       3.268  21.109 112.930  1.00 16.93      AAGL
ATOM    643  CA  SER    83       1.868  21.475 113.052  1.00 16.95      AAGL
ATOM    644  CB  SER    83       1.757  22.914 113.569  1.00 17.01      AAGL
ATOM    645  OG  SER    83       0.415  23.351 113.629  1.00 17.93      AAGL
ATOM    646  C   SER    83       1.276  21.367 111.649  1.00 18.89      AAGL
ATOM    647  O   SER    83       2.011  21.239 110.664  1.00 19.84      AAGL
ATOM    648  N   ASP    84      -0.046  21.404 111.561  1.00 19.63      AAGL
ATOM    649  CA  ASP    84      -0.715  21.317 110.275  1.00 20.59      AAGL
ATOM    650  CB  ASP    84      -2.107  20.695 110.421  1.00 22.19      AAGL
ATOM    651  CG  ASP    84      -2.062  19.246 110.817  1.00 21.52      AAGL
ATOM    652  OD1 ASP    84      -1.025  18.597 110.572  1.00 23.10      AAGL
ATOM    653  OD2 ASP    84      -3.079  18.755 111.360  1.00 23.55      AAGL
ATOM    654  C   ASP    84      -0.866  22.706 109.689  1.00 21.71      AAGL
ATOM    655  O   ASP    84      -1.340  22.854 108.563  1.00 21.81      AAGL
ATOM    656  N   THR    85      -0.461  23.717 110.453  1.00 21.01      AAGL
ATOM    657  CA  THR    85      -0.573  25.102 110.012  1.00 19.92      AAGL
ATOM    658  CB  THR    85      -1.971  25.670 110.370  1.00 22.17      AAGL
ATOM    659  OG1 THR    85      -2.144  26.952 109.763  1.00 22.62      AAGL
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Fig. 3 cont.

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ATOM    660  CG2 THR    85      -2.134  25.800 111.874  1.00 23.94      AAGL
ATOM    661  C   THR    85       0.527  25.958 110.646  1.00 19.33      AAGL
ATOM    662  O   THR    85       1.429  25.425 111.298  1.00 18.85      AAGL
ATOM    663  N   TRP    86       0.454  27.276 110.450  1.00 18.81      AAGL
ATOM    664  CA  TRP    86       1.455  28.199 110.988  1.00 17.88      AAGL
ATOM    665  CB  TRP    86       1.011  29.654 110.800  1.00 17.85      AAGL
ATOM    666  CG  TRP    86       0.672  30.016 109.399  1.00 18.75      AAGL
ATOM    667  CD2 TRP    86       1.587  30.427 108.382  1.00 18.96      AAGL
ATOM    668  CE2 TRP    86       0.832  30.649 107.209  1.00 21.98      AAGL
ATOM    669  CE3 TRP    86       2.975  30.628 108.345  1.00 18.78      AAGL
ATOM    670  CD1 TRP    86      -0.563  30.004 108.826  1.00 21.00      AAGL
ATOM    671  NE1 TRP    86      -0.478  30.386 107.508  1.00 21.68      AAGL
ATOM    672  CZ2 TRP    86       1.418  31.065 106.007  1.00 19.73      AAGL
ATOM    673  CZ3 TRP    86       3.556  31.041 107.151  1.00 20.30      AAGL
ATOM    674  CH2 TRP    86       2.775  31.255 105.998  1.00 18.40      AAGL
ATOM    675  C   TRP    86       1.757  27.994 112.467  1.00 18.54      AAGL
ATOM    676  O   TRP    86       0.847  27.998 113.302  1.00 17.68      AAGL
ATOM    677  N   ALA    87       3.035  27.830 112.793  1.00 15.65      AAGL
ATOM    678  CA  ALA    87       3.440  27.669 114.182  1.00 19.55      AAGL
ATOM    679  CB  ALA    87       4.263  26.393 114.355  1.00 17.55      AAGL
ATOM    680  C   ALA    87       4.266  28.880 114.613  1.00 17.89      AAGL
ATOM    681  O   ALA    87       5.179  29.303 113.896  1.00 18.09      AAGL
ATOM    682  N   ASP    88       3.933  29.441 115.772  1.00 18.18      AAGL
ATOM    683  CA  ASP    88       4.655  30.585 116.325  1.00 18.94      AAGL
ATOM    684  CB  ASP    88       4.276  31.885 115.604  1.00 21.76      AAGL
ATOM    685  CG  ASP    88       2.798  32.205 115.699  1.00 26.60      AAGL
ATOM    686  OD1 ASP    88       2.221  32.074 116.789  1.00 24.49      AAGL
ATOM    687  OD2 ASP    88       2.216  32.599 114.673  1.00 30.64      AAGL
ATOM    688  C   ASP    88       4.349  30.674 117.826  1.00 20.25      AAGL
ATOM    689  O   ASP    88       3.617  29.838 118.354  1.00 18.36      AAGL
ATOM    690  N   PRO    89       4.900  31.681 118.528  1.00 19.03      AAGL
ATOM    691  CD  PRO    89       5.879  32.685 118.078  1.00 20.41      AAGL
ATOM    692  CA  PRO    89       4.656  31.813 119.969  1.00 19.78      AAGL
ATOM    693  CB  PRO    89       5.435  33.071 120.339  1.00 22.34      AAGL
ATOM    694  CG  PRO    89       6.561  33.059 119.354  1.00 20.37      AAGL
ATOM    695  C   PRO    89       3.206  31.882 120.421  1.00 21.51      AAGL
ATOM    696  O   PRO    89       2.909  31.593 121.578  1.00 22.07      AAGL
ATOM    697  N   SER    90       2.297  32.251 119.527  1.00 20.56      AAGL
ATOM    698  CA  SER    90       0.904  32.335 119.924  1.00 21.51      AAGL
ATOM    699  CB  SER    90       0.283  33.644 119.425  1.00 24.67      AAGL
ATOM    700  OG  SER    90       0.139  33.643 118.023  1.00 29.17      AAGL
ATOM    701  C   SER    90       0.086  31.138 119.451  1.00 21.66      AAGL
ATOM    702  O   SER    90      -1.094  31.018 119.792  1.00 18.80      AAGL
ATOM    703  N   ASP    91       0.710  30.249 118.674  1.00 19.99      AAGL
ATOM    704  CA  ASP    91       0.025  29.052 118.188  1.00 21.82      AAGL
ATOM    705  CB  ASP    91      -0.839  29.374 116.961  1.00 26.37      AAGL
ATOM    706  CG  ASP    91      -2.057  30.208 117.305  0.50 27.60      AAGL
ATOM    707  OD1 ASP    91      -2.904  29.743 118.104  0.50 29.99      AAGL
ATOM    708  OD2 ASP    91      -2.168  31.328 116.770  0.50 29.72      AAGL
ATOM    709  C   ASP    91       0.974  27.912 117.816  1.00 19.33      AAGL
ATOM    710  O   ASP    91       1.713  27.997 116.834  1.00 20.80      AAGL
ATOM    711  N   GLN    92       0.945  26.851 118.614  1.00 16.40      AAGL
ATOM    712  CA  GLN    92       1.751  25.653 118.369  1.00 17.43      AAGL
ATOM    713  CB  GLN    92       2.820  25.482 119.449  1.00 16.72      AAGL
ATOM    714  CG  GLN    92       3.897  26.562 119.457  1.00 15.88      AAGL
ATOM    715  CD  GLN    92       4.894  26.427 118.319  1.00 16.69      AAGL
ATOM    716  OE1 GLN    92       5.078  25.345 117.770  1.00 18.84      AAGL
ATOM    717  NE2 GLN    92       5.550  27.524 117.970  1.00 15.00      AAGL
ATOM    718  C   GLN    92       0.782  24.472 118.403  1.00 17.98      AAGL
ATOM    719  O   GLN    92       0.855  23.615 119.284  1.00 18.87      AAGL
ATOM    720  N   THR    93      -0.140  24.444 117.450  1.00 18.32      AAGL
ATOM    721  CA  THR    93      -1.137  23.378 117.396  1.00 19.90      AAGL
ATOM    722  CB  THR    93      -2.303  23.732 116.451  1.00 21.83      AAGL
ATOM    723  OG1 THR    93      -2.845  25.001 116.824  1.00 23.30      AAGL
ATOM    724  CG2 THR    93      -3.415  22.691 116.564  1.00 23.34      AAGL
ATOM    725  C   THR    93      -0.553  22.052 116.946  1.00 19.51      AAGL
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Fig. 3 cont.

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ATOM    726  O   THR    93       0.000  21.935 115.856  1.00 19.99      AAGL
ATOM    727  N   THR    94      -0.685  21.050 117.802  1.00 19.55      AAGL
ATOM    728  CA  THR    94      -0.181  19.716 117.510  1.00 20.32      AAGL
ATOM    729  CB  THR    94      -0.463  18.775 118.699  1.00 20.34      AAGL
ATOM    730  OG1 THR    94       0.320  19.190 119.824  1.00 20.72      AAGL
ATOM    731  CG2 THR    94      -0.141  17.334 118.348  1.00 20.41      AAGL
ATOM    732  C   THR    94      -0.866  19.171 116.261  1.00 19.20      AAGL
ATOM    733  O   THR    94      -2.060  19.367 116.071  1.00 19.04      AAGL
ATOM    734  N   PRO    95      -0.111  18.495 115.381  1.00 19.53      AAGL
ATOM    735  CD  PRO    95       1.352  18.315 115.386  1.00 17.38      AAGL
ATOM    736  CA  PRO    95      -0.703  17.937 114.160  1.00 20.73      AAGL
ATOM    737  CB  PRO    95       0.424  17.086 113.590  1.00 16.98      AAGL
ATOM    738  CG  PRO    95       1.638  17.872 113.952  1.00 20.07      AAGL
ATOM    739  C   PRO    95      -1.939  17.091 114.452  1.00 22.21      AAGL
ATOM    740  O   PRO    95      -2.002  16.399 115.468  1.00 19.37      AAGL
ATOM    741  N   SER    96      -2.926  17.163 113.569  1.00 23.26      AAGL
ATOM    742  CA  SER    96      -4.125  16.353 113.740  1.00 27.34      AAGL
ATOM    743  CB  SER    96      -5.153  16.695 112.656  1.00 29.38      AAGL
ATOM    744  OG  SER    96      -4.577  16.561 111.365  1.00 34.62      AAGL
ATOM    745  C   SER    96      -3.635  14.911 113.590  1.00 28.07      AAGL
ATOM    746  O   SER    96      -2.863  14.602 112.685  1.00 29.54      AAGL
ATOM    747  N   GLY    97      -4.064  14.029 114.482  1.00 28.91      AAGL
ATOM    748  CA  GLY    97      -3.607  12.655 114.390  1.00 28.58      AAGL
ATOM    749  C   GLY    97      -2.478  12.365 115.365  1.00 27.25      AAGL
ATOM    750  O   GLY    97      -2.214  11.202 115.679  1.00 28.56      AAGL
ATOM    751  N   TRP    98      -1.786  13.408 115.819  1.00 23.62      AAGL
ATOM    752  CA  TRP    98      -0.715  13.227 116.801  1.00 20.63      AAGL
ATOM    753  CB  TRP    98       0.396  14.250 116.590  1.00 20.68      AAGL
ATOM    754  CG  TRP    98       1.253  13.995 115.382  1.00 20.26      AAGL
ATOM    755  CD2 TRP    98       2.561  14.517 115.148  1.00 19.57      AAGL
ATOM    756  CE2 TRP    98       2.945  14.123 113.845  1.00 20.94      AAGL
ATOM    757  CE3 TRP    98       3.449  15.288 115.913  1.00 19.61      AAGL
ATOM    758  CD1 TRP    98       0.905  13.311 114.246  1.00 21.24      AAGL
ATOM    759  NE1 TRP    98       1.918  13.386 113.318  1.00 21.31      AAGL
ATOM    760  CZ2 TRP    98       4.178  14.475 113.290  1.00 20.47      AAGL
ATOM    761  CZ3 TRP    98       4.675  15.638 115.362  1.00 20.55      AAGL
ATOM    762  CH2 TRP    98       5.028  15.230 114.058  1.00 21.24      AAGL
ATOM    763  C   TRP    98      -1.348  13.397 118.190  1.00 21.31      AAGL
ATOM    764  O   TRP    98      -2.422  13.973 118.312  1.00 21.68      AAGL
ATOM    765  N   SER    99      -0.675  12.910 119.227  1.00 22.27      AAGL
ATOM    766  CA  SER    99      -1.210  12.951 120.591  1.00 20.04      AAGL
ATOM    767  CB  SER    99      -0.531  11.870 121.446  1.00 21.78      AAGL
ATOM    768  OG  SER    99      -1.115  11.794 122.746  1.00 19.99      AAGL
ATOM    769  C   SER    99      -1.172  14.262 121.377  1.00 20.81      AAGL
ATOM    770  O   SER    99      -0.174  14.974 121.391  1.00 20.17      AAGL
ATOM    771  N   THR   100      -2.284  14.555 122.039  1.00 21.47      AAGL
ATOM    772  CA  THR   100      -2.401  15.730 122.896  1.00 22.60      AAGL
ATOM    773  CB  THR   100      -3.564  16.655 122.455  1.00 22.41      AAGL
ATOM    774  OG1 THR   100      -4.759  15.882 122.308  1.00 23.06      AAGL
ATOM    775  CG2 THR   100      -3.248  17.339 121.128  1.00 22.11      AAGL
ATOM    776  C   THR   100      -2.706  15.190 124.294  1.00 23.80      AAGL
ATOM    777  O   THR   100      -3.150  15.930 125.174  1.00 23.03      AAGL
ATOM    778  N   THR   101      -2.448  13.895 124.488  1.00 24.54      AAGL
ATOM    779  CA  THR   101      -2.737  13.228 125.755  1.00 23.47      AAGL
ATOM    780  CB  THR   101      -4.055  12.440 125.638  1.00 24.48      AAGL
ATOM    781  OG1 THR   101      -3.897  11.412 124.652  1.00 25.27      AAGL
ATOM    782  CG2 THR   101      -5.198  13.356 125.213  1.00 25.93      AAGL
ATOM    783  C   THR   101      -1.679  12.256 126.301  1.00 25.35      AAGL
ATOM    784  O   THR   101      -1.794  11.802 127.437  1.00 25.05      AAGL
ATOM    785  N   ASP   102      -0.657  11.932 125.513  1.00 23.02      AAGL
ATOM    786  CA  ASP   102       0.366  10.989 125.968  1.00 24.03      AAGL
ATOM    787  CB  ASP   102       0.013   9.579 125.488  1.00 25.87      AAGL
ATOM    788  CG  ASP   102       0.934   8.515 126.052  1.00 29.80      AAGL
ATOM    789  OD1 ASP   102       2.163   8.600 125.864  1.00 30.75      AAGL
ATOM    790  OD2 ASP   102       0.425   7.571 126.683  1.00 35.27      AAGL
ATOM    791  C   ASP   102       1.746  11.370 125.446  1.00 24.10      AAGL
ATOM    792  O   ASP   102       2.005  11.269 124.245  1.00 24.23      AAGL
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Fig. 3 cont.

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ATOM    793  N   LEU  103       2.640  11.791 126.338  1.00 23.33      AAGL
ATOM    794  CA  LEU  103       3.974  12.189 125.898  1.00 23.77      AAGL
ATOM    795  CB  LEU  103       4.801  12.749 127.056  1.00 24.26      AAGL
ATOM    796  CG  LEU  103       6.113  13.383 126.579  1.00 23.41      AAGL
ATOM    797  CD1 LEU  103       5.800  14.627 125.765  1.00 23.25      AAGL
ATOM    798  CD2 LEU  103       7.005  13.729 127.764  1.00 24.01      AAGL
ATOM    799  C   LEU  103       4.744  11.046 125.257  1.00 24.93      AAGL
ATOM    800  O   LEU  103       5.522  11.259 124.326  1.00 22.87      AAGL
ATOM    801  N   GLY  104       4.535   9.837 125.765  1.00 24.55      AAGL
ATOM    802  CA  GLY  104       5.229   8.689 125.213  1.00 25.67      AAGL
ATOM    803  C   GLY  104       4.863   8.514 123.757  1.00 24.34      AAGL
ATOM    804  O   GLY  104       5.727   8.334 122.899  1.00 25.72      AAGL
ATOM    805  N   THR  105       3.571   8.571 123.475  1.00 23.33      AAGL
ATOM    806  CA  THR  105       3.084   8.425 122.115  1.00 24.93      AAGL
ATOM    807  CB  THR  105       1.546   8.360 122.095  1.00 25.14      AAGL
ATOM    808  OG1 THR  105       1.109   7.236 122.870  1.00 28.55      AAGL
ATOM    809  CG2 THR  105       1.029   8.211 120.684  1.00 27.78      AAGL
ATOM    810  C   THR  105       3.561   9.596 121.260  1.00 23.97      AAGL
ATOM    811  O   THR  105       4.008   9.412 120.132  1.00 24.40      AAGL
ATOM    812  N   LEU  106       3.485  10.802 121.812  1.00 22.92      AAGL
ATOM    813  CA  LEU  106       3.898  12.000 121.085  1.00 21.38      AAGL
ATOM    814  CB  LEU  106       3.568  13.254 121.896  1.00 19.99      AAGL
ATOM    815  CG  LEU  106       3.895  14.579 121.196  1.00 18.13      AAGL
ATOM    816  CD1 LEU  106       3.066  14.714 119.923  1.00 16.54      AAGL
ATOM    817  CD2 LEU  106       3.613  15.735 122.141  1.00 15.43      AAGL
ATOM    818  C   LEU  106       5.382  11.995 120.729  1.00 23.00      AAGL
ATOM    819  O   LEU  106       5.755  12.330 119.601  1.00 22.17      AAGL
ATOM    820  N   LYS  107       6.230  11.627 121.684  1.00 23.39      AAGL
ATOM    821  CA  LYS  107       7.662  11.578 121.420  1.00 24.69      AAGL
ATOM    822  CB  LYS  107       8.446  11.129 122.660  1.00 25.78      AAGL
ATOM    823  CG  LYS  107       8.496  12.144 123.789  1.00 27.94      AAGL
ATOM    824  CD  LYS  107       9.574  11.781 124.801  1.00 31.83      AAGL
ATOM    825  CE  LYS  107       9.360  10.393 125.384  1.00 36.44      AAGL
ATOM    826  NZ  LYS  107      10.431  10.009 126.355  1.00 39.34      AAGL
ATOM    827  C   LYS  107       7.942  10.609 120.278  1.00 24.60      AAGL
ATOM    828  O   LYS  107       8.829  10.852 119.461  1.00 24.29      AAGL
ATOM    829  N   TRP  108       7.183   9.518 120.220  1.00 24.58      AAGL
ATOM    830  CA  TRP  108       7.372   8.526 119.165  1.00 26.57      AAGL
ATOM    831  CB  TRP  108       6.616   7.231 119.487  1.00 30.79      AAGL
ATOM    832  CG  TRP  108       7.429   6.243 120.257  1.00 37.55      AAGL
ATOM    833  CD2 TRP  108       8.617   5.579 119.806  1.00 41.19      AAGL
ATOM    834  CE2 TRP  108       9.055   4.744 120.861  1.00 41.70      AAGL
ATOM    835  CE3 TRP  108       9.356   5.610 118.611  1.00 40.79      AAGL
ATOM    836  CD1 TRP  108       7.199   5.797 121.530  1.00 39.67      AAGL
ATOM    837  NE1 TRP  108       8.173   4.898 121.899  1.00 41.76      AAGL
ATOM    838  CZ2 TRP  108      10.202   3.942 120.760  1.00 42.41      AAGL
ATOM    839  CZ3 TRP  108      10.498   4.814 118.510  1.00 42.96      AAGL
ATOM    840  CH2 TRP  108      10.908   3.992 119.582  1.00 43.14      AAGL
ATOM    841  C   TRP  108       6.925   9.040 117.807  1.00 25.36      AAGL
ATOM    842  O   TRP  108       7.585   8.785 116.801  1.00 25.01      AAGL
ATOM    843  N   GLN  109       5.808   9.763 117.782  1.00 22.63      AAGL
ATOM    844  CA  GLN  109       5.277  10.304 116.539  1.00 22.94      AAGL
ATOM    845  CB  GLN  109       3.884  10.886 116.784  1.00 22.73      AAGL
ATOM    846  CG  GLN  109       2.863   9.838 117.229  1.00 24.36      AAGL
ATOM    847  CD  GLN  109       1.555  10.447 117.706  1.00 25.79      AAGL
ATOM    848  OE1 GLN  109       1.551  11.462 118.410  1.00 25.25      AAGL
ATOM    849  NE2 GLN  109       0.434   9.821 117.340  1.00 24.06      AAGL
ATOM    850  C   GLN  109       6.212  11.362 115.958  1.00 22.81      AAGL
ATOM    851  O   GLN  109       6.416  11.418 114.747  1.00 23.48      AAGL
ATOM    852  N   LEU  110       6.796  12.181 116.826  1.00 23.23      AAGL
ATOM    853  CA  LEU  110       7.716  13.223 116.389  1.00 23.80      AAGL
ATOM    854  CB  LEU  110       8.031  14.188 117.539  1.00 24.37      AAGL
ATOM    855  CG  LEU  110       9.119  15.231 117.255  1.00 22.16      AAGL
ATOM    856  CD1 LEU  110       8.792  15.973 115.960  1.00 22.25      AAGL
ATOM    857  CD2 LEU  110       9.230  16.199 118.420  1.00 23.11      AAGL
ATOM    858  C   LEU  110       9.005  12.596 115.870  1.00 25.82      AAGL
ATOM    859  O   LEU  110       9.523  13.010 114.835  1.00 24.35      AAGL
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Fig. 3 cont.

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ATOM    860  N   TYR  111       9.524  11.608 116.594  1.00 25.68      AAGL
ATOM    861  CA  TYR  111      10.746  10.915 116.179  1.00 24.78      AAGL
ATOM    862  CB  TYR  111      11.151   9.869 117.230  1.00 25.83      AAGL
ATOM    863  CG  TYR  111      12.199   8.874 116.767  1.00 27.35      AAGL
ATOM    864  CD1 TYR  111      11.848   7.774 115.986  1.00 29.55      AAGL
ATOM    865  CE1 TYR  111      12.810   6.866 115.544  1.00 31.93      AAGL
ATOM    866  CD2 TYR  111      13.541   9.043 117.099  1.00 28.41      AAGL
ATOM    867  CE2 TYR  111      14.514   8.143 116.661  1.00 32.12      AAGL
ATOM    868  CZ  TYR  111      14.143   7.060 115.882  1.00 31.55      AAGL
ATOM    869  OH  TYR  111      15.104   6.183 115.423  1.00 34.00      AAGL
ATOM    870  C   TYR  111      10.505  10.246 114.832  1.00 24.33      AAGL
ATOM    871  O   TYR  111      11.307  10.383 113.901  1.00 26.25      AAGL
ATOM    872  N   ASN  112       9.398   9.521 114.731  1.00 23.20      AAGL
ATOM    873  CA  ASN  112       9.042   8.842 113.492  1.00 24.57      AAGL
ATOM    874  CB  ASN  112       7.750   8.041 113.688  1.00 27.15      AAGL
ATOM    875  CG  ASN  112       7.963   6.757 114.473  0.50 25.91      AAGL
ATOM    876  OD1 ASN  112       7.010   6.023 114.752  0.50 29.07      AAGL
ATOM    877  ND2 ASN  112       9.209   6.475 114.825  0.50 26.44      AAGL
ATOM    878  C   ASN  112       8.865   9.865 112.364  1.00 26.29      AAGL
ATOM    879  O   ASN  112       9.227   9.607 111.211  1.00 23.16      AAGL
ATOM    880  N   TYR  113       8.317  11.028 112.702  1.00 23.87      AAGL
ATOM    881  CA  TYR  113       8.097  12.075 111.711  1.00 23.73      AAGL
ATOM    882  CB  TYR  113       7.328  13.239 112.315  1.00 23.08      AAGL
ATOM    883  CG  TYR  113       7.148  14.387 111.341  1.00 22.30      AAGL
ATOM    884  CD1 TYR  113       6.290  14.271 110.243  1.00 20.43      AAGL
ATOM    885  CE1 TYR  113       6.134  15.327 109.335  1.00 21.15      AAGL
ATOM    886  CD2 TYR  113       7.847  15.584 111.510  1.00 20.85      AAGL
ATOM    887  CE2 TYR  113       7.699  16.642 110.612  1.00 18.32      AAGL
ATOM    888  CZ  TYR  113       6.846  16.512 109.533  1.00 19.02      AAGL
ATOM    889  OH  TYR  113       6.706  17.562 108.654  1.00 18.05      AAGL
ATOM    890  C   TYR  113       9.391  12.613 111.111  1.00 23.40      AAGL
ATOM    891  O   TYR  113       9.561  12.611 109.891  1.00 24.13      AAGL
ATOM    892  N   THR  114      10.300  13.085 111.957  1.00 22.35      AAGL
ATOM    893  CA  THR  114      11.552  13.623 111.441  1.00 23.52      AAGL
ATOM    894  CB  THR  114      12.413  14.260 112.569  1.00 22.78      AAGL
ATOM    895  OG1 THR  114      12.714  13.292 113.578  1.00 23.02      AAGL
ATOM    896  CG2 THR  114      11.662  15.433 113.210  1.00 22.56      AAGL
ATOM    897  C   THR  114      12.339  12.530 110.711  1.00 24.38      AAGL
ATOM    898  O   THR  114      12.954  12.783 109.673  1.00 23.70      AAGL
ATOM    899  N   LEU  115      12.309  11.315 111.250  1.00 26.01      AAGL
ATOM    900  CA  LEU  115      12.995  10.189 110.618  1.00 26.48      AAGL
ATOM    901  CB  LEU  115      12.785   8.909 111.443  1.00 27.61      AAGL
ATOM    902  CG  LEU  115      13.278   7.573 110.853  1.00 28.64      AAGL
ATOM    903  CD1 LEU  115      14.787   7.644 110.546  1.00 29.41      AAGL
ATOM    904  CD2 LEU  115      12.991   6.434 111.836  1.00 31.02      AAGL
ATOM    905  C   LEU  115      12.432  10.002 109.208  1.00 27.33      AAGL
ATOM    906  O   LEU  115      13.180   9.902 108.236  1.00 29.69      AAGL
ATOM    907  N   GLU  116      11.106   9.979 109.102  1.00 27.14      AAGL
ATOM    908  CA  GLU  116      10.428   9.800 107.825  1.00 28.85      AAGL
ATOM    909  CB  GLU  116       8.919   9.674 108.057  1.00 33.11      AAGL
ATOM    910  CG  GLU  116       8.111   9.374 106.803  1.00 40.59      AAGL
ATOM    911  CD  GLU  116       8.196   7.914 106.368  1.00 44.26      AAGL
ATOM    912  OE1 GLU  116       7.696   7.603 105.266  1.00 47.23      AAGL
ATOM    913  OE2 GLU  116       8.744   7.073 107.118  1.00 47.05      AAGL
ATOM    914  C   GLU  116      10.707  10.952 106.853  1.00 28.50      AAGL
ATOM    915  O   GLU  116      10.936  10.730 105.667  1.00 28.60      AAGL
ATOM    916  N   VAL  117      10.671  12.184 107.354  1.00 25.75      AAGL
ATOM    917  CA  VAL  117      10.933  13.345 106.507  1.00 25.01      AAGL
ATOM    918  CB  VAL  117      10.841  14.657 107.303  1.00 25.08      AAGL
ATOM    919  CG1 VAL  117      11.393  15.810 106.473  1.00 24.84      AAGL
ATOM    920  CG2 VAL  117       9.390  14.924 107.685  1.00 25.17      AAGL
ATOM    921  C   VAL  117      12.321  13.256 105.894  1.00 25.14      AAGL
ATOM    922  O   VAL  117      12.488  13.445 104.684  1.00 26.07      AAGL
ATOM    923  N   CYS  118      13.313  12.982 106.734  1.00 22.94      AAGL
ATOM    924  CA  CYS  118      14.684  12.868 106.261  1.00 24.56      AAGL
ATOM    925  CB  CYS  118      15.644  12.710 107.446  1.00 24.73      AAGL
ATOM    926  SG  CYS  118      15.852  14.220 108.485  1.00 26.92      AAGL
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Fig. 3 cont.

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ATOM    927  C   CYS  118      14.810  11.682 105.289  1.00 25.33      AAGL
ATOM    928  O   CYS  118      15.417  11.813 104.228  1.00 25.49      AAGL
ATOM    929  N   ASN  119      14.224  10.537 105.638  1.00 25.35      AAGL
ATOM    930  CA  ASN  119      14.296   9.372 104.753  1.00 28.13      AAGL
ATOM    931  CB  ASN  119      13.618   8.156 105.382  1.00 28.39      AAGL
ATOM    932  CG  ASN  119      14.446   7.539 106.477  1.00 28.84      AAGL
ATOM    933  OD1 ASN  119      15.607   7.906 106.681  1.00 28.82      AAGL
ATOM    934  ND2 ASN  119      13.858   6.592 107.191  1.00 31.56      AAGL
ATOM    935  C   ASN  119      13.685   9.618 103.381  1.00 28.08      AAGL
ATOM    936  O   ASN  119      14.199   9.129 102.376  1.00 31.49      AAGL
ATOM    937  N   THR  120      12.594  10.372 103.326  1.00 28.01      AAGL
ATOM    938  CA  THR  120      11.952  10.641 102.046  1.00 27.89      AAGL
ATOM    939  CB  THR  120      10.596  11.321 102.231  1.00 30.29      AAGL
ATOM    940  OG1 THR  120       9.752  10.480 103.034  1.00 31.43      AAGL
ATOM    941  CG2 THR  120       9.926  11.536 100.873  1.00 30.28      AAGL
ATOM    942  C   THR  120      12.838  11.495 101.147  1.00 28.78      AAGL
ATOM    943  O   THR  120      12.869  11.290  99.933  1.00 29.09      AAGL
ATOM    944  N   PHE  121      13.557  12.452 101.728  1.00 28.45      AAGL
ATOM    945  CA  PHE  121      14.463  13.269 100.930  1.00 28.19      AAGL
ATOM    946  CB  PHE  121      14.985  14.461 101.741  1.00 29.04      AAGL
ATOM    947  CG  PHE  121      14.023  15.616 101.789  1.00 27.88      AAGL
ATOM    948  CD1 PHE  121      12.847  15.529 102.530  1.00 28.91      AAGL
ATOM    949  CD2 PHE  121      14.242  16.753 101.018  1.00 28.77      AAGL
ATOM    950  CE1 PHE  121      11.905  16.549 102.496  1.00 26.83      AAGL
ATOM    951  CE2 PHE  121      13.301  17.780 100.979  1.00 29.21      AAGL
ATOM    952  CZ  PHE  121      12.130  17.676 101.719  1.00 29.40      AAGL
ATOM    953  C   PHE  121      15.622  12.391 100.454  1.00 28.62      AAGL
ATOM    954  O   PHE  121      16.064  12.485  99.308  1.00 29.15      AAGL
ATOM    955  N   ALA  122      16.102  11.519 101.332  1.00 28.34      AAGL
ATOM    956  CA  ALA  122      17.187  10.622 100.964  1.00 29.64      AAGL
ATOM    957  CB  ALA  122      17.599   9.768 102.158  1.00 27.49      AAGL
ATOM    958  C   ALA  122      16.748   9.731  99.795  1.00 29.44      AAGL
ATOM    959  O   ALA  122      17.538   9.447  98.890  1.00 30.54      AAGL
ATOM    960  N   GLU  123      15.492   9.295  99.801  1.00 27.94      AAGL
ATOM    961  CA  GLU  123      15.004   8.448  98.720  1.00 28.60      AAGL
ATOM    962  CB  GLU  123      13.654   7.837  99.085  1.00 30.65      AAGL
ATOM    963  CG  GLU  123      13.693   7.161 100.439  1.00 35.94      AAGL
ATOM    964  CD  GLU  123      12.401   6.467 100.813  1.00 38.73      AAGL
ATOM    965  OE1 GLU  123      11.315   6.915 100.376  1.00 39.11      AAGL
ATOM    966  OE2 GLU  123      12.485   5.476 101.570  1.00 39.90      AAGL
ATOM    967  C   GLU  123      14.899   9.237  97.420  1.00 28.83      AAGL
ATOM    968  O   GLU  123      14.826   8.658  96.338  1.00 25.94      AAGL
ATOM    969  N   ASN  124      14.893  10.561  97.535  1.00 27.22      AAGL
ATOM    970  CA  ASN  124      14.825  11.434  96.366  1.00 26.84      AAGL
ATOM    971  CB  ASN  124      13.786  12.537  96.579  1.00 27.25      AAGL
ATOM    972  CG  ASN  124      12.367  12.067  96.302  1.00 28.47      AAGL
ATOM    973  OD1 ASN  124      11.888  12.130  95.168  1.00 28.23      AAGL
ATOM    974  ND2 ASN  124      11.691  11.580  97.336  1.00 30.75      AAGL
ATOM    975  C   ASN  124      16.186  12.063  96.085  1.00 26.40      AAGL
ATOM    976  O   ASN  124      16.290  13.015  95.315  1.00 25.52      AAGL
ATOM    977  N   ASP  125      17.223  11.538  96.726  1.00 26.35      AAGL
ATOM    978  CA  ASP  125      18.580  12.039  96.532  1.00 29.66      AAGL
ATOM    979  CB  ASP  125      19.066  11.654  95.131  1.00 31.58      AAGL
ATOM    980  CG  ASP  125      20.550  11.898  94.939  1.00 34.86      AAGL
ATOM    981  OD1 ASP  125      21.314  11.723  95.912  1.00 36.55      AAGL
ATOM    982  OD2 ASP  125      20.958  12.254  93.813  1.00 35.76      AAGL
ATOM    983  C   ASP  125      18.715  13.555  96.738  1.00 30.52      AAGL
ATOM    984  O   ASP  125      19.286  14.265  95.906  1.00 28.80      AAGL
ATOM    985  N   ILE  126      18.181  14.042  97.853  1.00 30.01      AAGL
ATOM    986  CA  ILE  126      18.270  15.458  98.200  1.00 30.54      AAGL
ATOM    987  CB  ILE  126      16.886  16.127  98.234  1.00 30.36      AAGL
ATOM    988  CG2 ILE  126      17.014  17.532  98.817  1.00 31.24      AAGL
ATOM    989  CG1 ILE  126      16.294  16.182  96.823  1.00 29.46      AAGL
ATOM    990  CD1 ILE  126      14.803  16.480  96.798  1.00 32.42      AAGL
ATOM    991  C   ILE  126      18.894  15.566  99.590  1.00 32.08      AAGL
ATOM    992  O   ILE  126      18.381  14.988 100.550  1.00 33.29      AAGL
ATOM    993  N   ASP  127      20.004  16.292  99.689  1.00 30.97      AAGL
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Fig. 3 cont.

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ATOM    994  CA  ASP  127      20.701  16.475 100.960  1.00 32.32      AAGL
ATOM    995  CB  ASP  127      22.181  16.777 100.719  1.00 36.39      AAGL
ATOM    996  CG  ASP  127      22.849  15.758  99.822  1.00 40.70      AAGL
ATOM    997  OD1 ASP  127      23.019  14.591 100.244  1.00 43.54      AAGL
ATOM    998  OD2 ASP  127      23.201  16.126  98.680  1.00 45.38      AAGL
ATOM    999  C   ASP  127      20.082  17.655 101.687  1.00 31.14      AAGL
ATOM   1000  O   ASP  127      19.643  18.616 101.053  1.00 30.94      AAGL
ATOM   1001  N   ILE  128      20.063  17.587 103.012  1.00 29.03      AAGL
ATOM   1002  CA  ILE  128      19.505  18.659 103.825  1.00 27.70      AAGL
ATOM   1003  CB  ILE  128      18.442  18.112 104.806  1.00 27.94      AAGL
ATOM   1004  CG2 ILE  128      17.866  19.250 105.645  1.00 25.95      AAGL
ATOM   1005  CG1 ILE  128      17.333  17.408 104.017  1.00 27.55      AAGL
ATOM   1006  CD1 ILE  128      16.289  16.716 104.883  1.00 29.46      AAGL
ATOM   1007  C   ILE  128      20.630  19.317 104.611  1.00 25.60      AAGL
ATOM   1008  O   ILE  128      21.370  18.645 105.328  1.00 28.07      AAGL
ATOM   1009  N   GLU  129      20.766  20.632 104.465  1.00 24.98      AAGL
ATOM   1010  CA  GLU  129      21.818  21.380 105.156  1.00 24.49      AAGL
ATOM   1011  CB  GLU  129      22.107  22.671 104.382  1.00 27.35      AAGL
ATOM   1012  CG  GLU  129      23.218  23.552 104.946  1.00 30.16      AAGL
ATOM   1013  CD  GLU  129      24.601  22.996 104.682  1.00 32.15      AAGL
ATOM   1014  OE1 GLU  129      24.720  22.097 103.821  1.00 32.40      AAGL
ATOM   1015  OE2 GLU  129      25.563  23.469 105.326  1.00 31.39      AAGL
ATOM   1016  C   GLU  129      21.418  21.713 106.593  1.00 24.14      AAGL
ATOM   1017  O   GLU  129      22.210  21.561 107.531  1.00 23.23      AAGL
ATOM   1018  N   ILE  130      20.184  22.174 106.761  1.00 22.11      AAGL
ATOM   1019  CA  ILE  130      19.696  22.535 108.083  1.00 20.15      AAGL
ATOM   1020  CB  ILE  130      19.719  24.065 108.301  1.00 21.07      AAGL
ATOM   1021  CG2 ILE  130      19.096  24.406 109.636  1.00 22.31      AAGL
ATOM   1022  CG1 ILE  130      21.147  24.601 108.233  1.00 20.04      AAGL
ATOM   1023  CD1 ILE  130      21.215  26.109 108.266  1.00 21.74      AAGL
ATOM   1024  C   ILE  130      18.256  22.091 108.265  1.00 20.32      AAGL
ATOM   1025  O   ILE  130      17.464  22.096 107.328  1.00 18.94      AAGL
ATOM   1026  N   ILE  131      17.920  21.696 109.480  1.00 21.44      AAGL
ATOM   1027  CA  ILE  131      16.551  21.316 109.759  1.00 22.36      AAGL
ATOM   1028  CB  ILE  131      16.324  19.791 109.544  1.00 23.90      AAGL
ATOM   1029  CG2 ILE  131      17.138  18.979 110.541  1.00 28.54      AAGL
ATOM   1030  CG1 ILE  131      14.826  19.488 109.629  1.00 26.48      AAGL
ATOM   1031  CD1 ILE  131      14.427  18.156 109.005  1.00 28.03      AAGL
ATOM   1032  C   ILE  131      16.253  21.765 111.185  1.00 21.53      AAGL
ATOM   1033  O   ILE  131      16.978  21.430 112.119  1.00 20.84      AAGL
ATOM   1034  N   SER  132      15.217  22.587 111.335  1.00 20.93      AAGL
ATOM   1035  CA  SER  132      14.859  23.089 112.654  1.00 19.31      AAGL
ATOM   1036  CB  SER  132      14.444  24.562 112.578  1.00 18.01      AAGL
ATOM   1037  OG  SER  132      13.232  24.709 111.869  1.00 21.72      AAGL
ATOM   1038  C   SER  132      13.720  22.261 113.221  1.00 19.27      AAGL
ATOM   1039  O   SER  132      12.766  21.930 112.520  1.00 19.32      AAGL
ATOM   1040  N   ILE  133      13.842  21.901 114.491  1.00 19.77      AAGL
ATOM   1041  CA  ILE  133      12.806  21.122 115.143  1.00 20.58      AAGL
ATOM   1042  CB  ILE  133      13.367  20.295 116.317  1.00 21.64      AAGL
ATOM   1043  CG2 ILE  133      12.297  19.334 116.823  1.00 18.97      AAGL
ATOM   1044  CG1 ILE  133      14.644  19.559 115.890  1.00 21.37      AAGL
ATOM   1045  CD1 ILE  133      14.515  18.774 114.605  1.00 25.39      AAGL
ATOM   1046  C   ILE  133      11.815  22.142 115.689  1.00 20.75      AAGL
ATOM   1047  O   ILE  133      11.890  22.529 116.850  1.00 21.44      AAGL
ATOM   1048  N   GLY  134      10.904  22.581 114.833  1.00 19.14      AAGL
ATOM   1049  CA  GLY  134       9.919  23.560 115.241  1.00 18.88      AAGL
ATOM   1050  C   GLY  134      10.240  24.936 114.690  1.00 18.31      AAGL
ATOM   1051  O   GLY  134      11.344  25.181 114.199  1.00 19.16      AAGL
ATOM   1052  N   ASN  135       9.268  25.835 114.769  1.00 16.66      AAGL
ATOM   1053  CA  ASN  135       9.427  27.201 114.289  1.00 16.54      AAGL
ATOM   1054  CB  ASN  135       8.507  27.457 113.097  1.00 15.67      AAGL
ATOM   1055  CG  ASN  135       8.666  28.854 112.532  1.00 20.06      AAGL
ATOM   1056  OD1 ASN  135       9.590  29.120 111.759  1.00 19.47      AAGL
ATOM   1057  ND2 ASN  135       7.773  29.762 112.932  1.00 14.55      AAGL
ATOM   1058  C   ASN  135       9.044  28.146 115.420  1.00 17.93      AAGL
ATOM   1059  O   ASN  135       7.940  28.063 115.935  1.00 16.64      AAGL
ATOM   1060  N   GLU  136       9.967  29.030 115.793  1.00 16.85      AAGL
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Fig. 3 cont.

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ATOM   1061  CA  GLU   136       9.760  30.001 116.865  1.00 17.43      AAGL
ATOM   1062  CB  GLU   136       8.892  31.169 116.371  1.00 18.10      AAGL
ATOM   1063  CG  GLU   136       9.517  31.970 115.228  1.00 17.17      AAGL
ATOM   1064  CD  GLU   136       8.747  33.240 114.867  1.00 18.85      AAGL
ATOM   1065  OE1 GLU   136       7.592  33.416 115.314  1.00 19.27      AAGL
ATOM   1066  OE2 GLU   136       9.305  34.071 114.120  1.00 18.05      AAGL
ATOM   1067  C   GLU   136       9.116  29.338 118.080  1.00 17.00      AAGL
ATOM   1068  O   GLU   136       8.013  29.697 118.478  1.00 18.88      AAGL
ATOM   1069  N   ILE   137       9.819  28.379 118.674  1.00 16.48      AAGL
ATOM   1070  CA  ILE   137       9.283  27.657 119.828  1.00 16.33      AAGL
ATOM   1071  CB  ILE   137       9.753  26.185 119.830  1.00 17.11      AAGL
ATOM   1072  CG2 ILE   137       9.204  25.457 118.615  1.00 18.25      AAGL
ATOM   1073  CG1 ILE   137      11.276  26.119 119.848  1.00 18.08      AAGL
ATOM   1074  CD1 ILE   137      11.822  24.717 120.029  1.00 19.03      AAGL
ATOM   1075  C   ILE   137       9.600  28.266 121.200  1.00 16.65      AAGL
ATOM   1076  O   ILE   137       9.770  27.540 122.178  1.00 18.23      AAGL
ATOM   1077  N   ARG   138       9.668  29.591 121.271  1.00 15.75      AAGL
ATOM   1078  CA  ARG   138       9.948  30.265 122.537  1.00 19.97      AAGL
ATOM   1079  CB  ARG   138      10.069  31.776 122.327  1.00 21.48      AAGL
ATOM   1080  CG  ARG   138      10.434  32.559 123.586  1.00 23.19      AAGL
ATOM   1081  CD  ARG   138      10.971  33.946 123.230  1.00 25.82      AAGL
ATOM   1082  NE  ARG   138      10.007  34.726 122.454  1.00 29.47      AAGL
ATOM   1083  CZ  ARG   138       8.900  35.263 122.956  1.00 29.69      AAGL
ATOM   1084  NH1 ARG   138       8.610  35.110 124.243  1.00 32.98      AAGL
ATOM   1085  NH2 ARG   138       8.075  35.939 122.168  1.00 29.53      AAGL
ATOM   1086  C   ARG   138       8.852  29.971 123.557  1.00 20.72      AAGL
ATOM   1087  O   ARG   138       9.112  29.926 124.755  1.00 22.83      AAGL
ATOM   1088  N   ALA   139       7.624  29.788 123.081  1.00 19.30      AAGL
ATOM   1089  CA  ALA   139       6.513  29.470 123.969  1.00 19.27      AAGL
ATOM   1090  CB  ALA   139       5.268  30.275 123.586  1.00 21.29      AAGL
ATOM   1091  C   ALA   139       6.227  27.971 123.893  1.00 20.13      AAGL
ATOM   1092  O   ALA   139       5.102  27.517 124.135  1.00 19.76      AAGL
ATOM   1093  N   GLY   140       7.264  27.207 123.565  1.00 16.96      AAGL
ATOM   1094  CA  GLY   140       7.124  25.769 123.465  1.00 17.78      AAGL
ATOM   1095  C   GLY   140       6.640  25.305 122.102  1.00 18.69      AAGL
ATOM   1096  O   GLY   140       6.669  26.058 121.119  1.00 15.87      AAGL
ATOM   1097  N   LEU   141       6.185  24.058 122.051  1.00 18.79      AAGL
ATOM   1098  CA  LEU   141       5.689  23.458 120.815  1.00 18.06      AAGL
ATOM   1099  CB  LEU   141       6.855  22.900 119.999  1.00 17.19      AAGL
ATOM   1100  CG  LEU   141       7.477  21.595 120.523  1.00 18.49      AAGL
ATOM   1101  CD1 LEU   141       8.404  21.018 119.457  1.00 17.04      AAGL
ATOM   1102  CD2 LEU   141       8.231  21.842 121.827  1.00 17.24      AAGL
ATOM   1103  C   LEU   141       4.741  22.310 121.145  1.00 17.11      AAGL
ATOM   1104  O   LEU   141       4.632  21.901 122.295  1.00 19.24      AAGL
ATOM   1105  N   LEU   142       4.063  21.795 120.126  1.00 15.85      AAGL
ATOM   1106  CA  LEU   142       3.162  20.664 120.293  1.00 16.79      AAGL
ATOM   1107  CB  LEU   142       3.981  19.370 120.301  1.00 17.91      AAGL
ATOM   1108  CG  LEU   142       4.783  19.127 119.017  1.00 18.45      AAGL
ATOM   1109  CD1 LEU   142       5.725  17.947 119.195  1.00 16.19      AAGL
ATOM   1110  CD2 LEU   142       3.827  18.888 117.861  1.00 18.62      AAGL
ATOM   1111  C   LEU   142       2.319  20.766 121.562  1.00 18.08      AAGL
ATOM   1112  O   LEU   142       2.374  19.909 122.440  1.00 18.47      AAGL
ATOM   1113  N   TRP   143       1.539  21.830 121.652  1.00 18.54      AAGL
ATOM   1114  CA  TRP   143       0.684  22.038 122.810  1.00 18.96      AAGL
ATOM   1115  CB  TRP   143       0.063  23.431 122.763  1.00 17.05      AAGL
ATOM   1116  CG  TRP   143       1.061  24.544 122.780  1.00 15.57      AAGL
ATOM   1117  CD2 TRP   143       0.807  25.920 122.475  1.00 16.04      AAGL
ATOM   1118  CE2 TRP   143       2.014  26.621 122.675  1.00 15.69      AAGL
ATOM   1119  CE3 TRP   143      -0.324  26.629 122.053  1.00 17.45      AAGL
ATOM   1120  CD1 TRP   143       2.375  24.468 123.139  1.00 15.44      AAGL
ATOM   1121  NE1 TRP   143       2.954  25.711 123.081  1.00 14.73      AAGL
ATOM   1122  CZ2 TRP   143       2.120  27.998 122.467  1.00 18.72      AAGL
ATOM   1123  CZ3 TRP   143      -0.215  28.000 121.848  1.00 20.29      AAGL
ATOM   1124  CH2 TRP   143       0.995  28.666 122.055  1.00 18.09      AAGL
ATOM   1125  C   TRP   143      -0.420  20.989 122.830  1.00 17.60      AAGL
ATOM   1126  O   TRP   143      -0.860  20.526 121.787  1.00 19.46      AAGL
ATOM   1127  N   PRO   144      -0.928  20.646 124.022  1.00 19.35      AAGL
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Fig. 3 cont.

ATOM	1128	CD	PRO	144	-2.116	19.777	124.132	1.00	18.54	AAGL
ATOM	1129	CA	PRO	144	-0.549	21.167	125.340	1.00	18.49	AAGL
ATOM	1130	CB	PRO	144	-1.796	20.898	126.169	1.00	18.97	AAGL
ATOM	1131	CG	PRO	144	-2.228	19.560	125.628	1.00	20.05	AAGL
ATOM	1132	C	PRO	144	0.687	20.546	125.990	1.00	17.18	AAGL
ATOM	1133	O	PRO	144	1.303	21.162	126.855	1.00	17.80	AAGL
ATOM	1134	N	LEU	145	1.043	19.329	125.592	1.00	16.38	AAGL
ATOM	1135	CA	LEU	145	2.184	18.655	126.206	1.00	18.03	AAGL
ATOM	1136	CB	LEU	145	2.401	17.277	125.567	1.00	19.70	AAGL
ATOM	1137	CG	LEU	145	1.382	16.208	125.988	1.00	21.47	AAGL
ATOM	1138	CD1	LEU	145	1.529	14.966	125.133	1.00	24.17	AAGL
ATOM	1139	CD2	LEU	145	1.584	15.871	127.450	1.00	22.76	AAGL
ATOM	1140	C	LEU	145	3.482	19.449	126.189	1.00	18.55	AAGL
ATOM	1141	O	LEU	145	4.291	19.335	127.113	1.00	18.42	AAGL
ATOM	1142	N	GLY	146	3.671	20.262	125.152	1.00	18.88	AAGL
ATOM	1143	CA	GLY	146	4.884	21.050	125.045	1.00	18.53	AAGL
ATOM	1144	C	GLY	146	4.759	22.511	125.444	1.00	19.09	AAGL
ATOM	1145	O	GLY	146	5.509	23.351	124.948	1.00	17.40	AAGL
ATOM	1146	N	GLU	147	3.811	22.827	126.326	1.00	18.92	AAGL
ATOM	1147	CA	GLU	147	3.647	24.207	126.792	1.00	18.48	AAGL
ATOM	1148	CB	GLU	147	2.298	24.382	127.499	1.00	17.73	AAGL
ATOM	1149	CG	GLU	147	1.111	24.296	126.565	1.00	18.17	AAGL
ATOM	1150	CD	GLU	147	0.452	25.642	126.328	1.00	21.87	AAGL
ATOM	1151	OE1	GLU	147	1.137	26.684	126.464	1.00	24.40	AAGL
ATOM	1152	OE2	GLU	147	-0.751	25.655	125.997	1.00	22.11	AAGL
ATOM	1153	C	GLU	147	4.789	24.512	127.759	1.00	19.00	AAGL
ATOM	1154	O	GLU	147	5.421	23.589	128.287	1.00	20.89	AAGL
ATOM	1155	N	THR	148	5.046	25.797	128.003	1.00	18.85	AAGL
ATOM	1156	CA	THR	148	6.137	26.194	128.887	1.00	21.19	AAGL
ATOM	1157	CB	THR	148	6.486	27.705	128.746	1.00	21.41	AAGL
ATOM	1158	OG1	THR	148	5.307	28.498	128.908	1.00	23.59	AAGL
ATOM	1159	CG2	THR	148	7.095	27.987	127.379	1.00	21.18	AAGL
ATOM	1160	C	THR	148	5.889	25.868	130.354	1.00	21.42	AAGL
ATOM	1161	O	THR	148	6.711	26.180	131.207	1.00	21.58	AAGL
ATOM	1162	N	SER	149	4.753	25.251	130.656	1.00	20.92	AAGL
ATOM	1163	CA	SER	149	4.487	24.852	132.027	1.00	22.49	AAGL
ATOM	1164	CB	SER	149	2.990	24.593	132.228	1.00	20.24	AAGL
ATOM	1165	OG	SER	149	2.442	23.871	131.142	1.00	21.26	AAGL
ATOM	1166	C	SER	149	5.314	23.582	132.275	1.00	23.11	AAGL
ATOM	1167	O	SER	149	5.420	23.093	133.397	1.00	23.52	AAGL
ATOM	1168	N	SER	150	5.914	23.062	131.205	1.00	22.32	AAGL
ATOM	1169	CA	SER	150	6.749	21.868	131.299	1.00	22.70	AAGL
ATOM	1170	CB	SER	150	5.925	20.609	131.003	1.00	23.28	AAGL
ATOM	1171	OG	SER	150	6.735	19.445	131.058	1.00	24.36	AAGL
ATOM	1172	C	SER	150	7.946	21.937	130.345	1.00	22.43	AAGL
ATOM	1173	O	SER	150	7.909	21.386	129.246	1.00	22.55	AAGL
ATOM	1174	N	TYR	151	9.007	22.619	130.766	1.00	22.50	AAGL
ATOM	1175	CA	TYR	151	10.195	22.714	129.932	1.00	23.76	AAGL
ATOM	1176	CB	TYR	151	11.192	23.730	130.511	1.00	23.66	AAGL
ATOM	1177	CG	TYR	151	10.861	25.169	130.153	1.00	25.07	AAGL
ATOM	1178	CD1	TYR	151	10.054	25.950	130.978	1.00	22.33	AAGL
ATOM	1179	CE1	TYR	151	9.719	27.270	130.628	1.00	22.71	AAGL
ATOM	1180	CD2	TYR	151	11.329	25.740	128.965	1.00	24.38	AAGL
ATOM	1181	CE2	TYR	151	10.997	27.057	128.610	1.00	23.11	AAGL
ATOM	1182	CZ	TYR	151	10.195	27.812	129.446	1.00	22.47	AAGL
ATOM	1183	OH	TYR	151	9.881	29.113	129.116	1.00	23.02	AAGL
ATOM	1184	C	TYR	151	10.827	21.327	129.804	1.00	24.63	AAGL
ATOM	1185	O	TYR	151	11.627	21.070	128.903	1.00	23.36	AAGL
ATOM	1186	N	SER	152	10.441	20.427	130.703	1.00	25.50	AAGL
ATOM	1187	CA	SER	152	10.942	19.064	130.670	1.00	24.95	AAGL
ATOM	1188	CB	SER	152	10.539	18.325	131.945	1.00	25.80	AAGL
ATOM	1189	OG	SER	152	11.051	17.010	131.928	1.00	31.90	AAGL
ATOM	1190	C	SER	152	10.364	18.358	129.442	1.00	23.88	AAGL
ATOM	1191	O	SER	152	11.081	17.695	128.696	1.00	24.71	AAGL
ATOM	1192	N	ASN	153	9.059	18.502	129.229	1.00	24.00	AAGL
ATOM	1193	CA	ASN	153	8.414	17.885	128.075	1.00	22.02	AAGL
ATOM	1194	CB	ASN	153	6.901	18.108	128.132	1.00	21.03	AAGL

Fig. 3 cont.

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ATOM   1195  CG  ASN   153       6.225  17.239 129.168  1.00 22.68      AAGL
ATOM   1196  OD1 ASN   153       6.888  16.579 129.971  1.00 21.72      AAGL
ATOM   1197  ND2 ASN   153       4.897  17.235 129.159  1.00 19.51      AAGL
ATOM   1198  C   ASN   153       8.970  18.486 126.782  1.00 21.57      AAGL
ATOM   1199  O   ASN   153       9.178  17.782 125.792  1.00 19.66      AAGL
ATOM   1200  N   ILE   154       9.192  19.797 126.798  1.00 20.58      AAGL
ATOM   1201  CA  ILE   154       9.733  20.490 125.636  1.00 21.12      AAGL
ATOM   1202  CB  ILE   154       9.922  21.988 125.909  1.00 21.27      AAGL
ATOM   1203  CG2 ILE   154      10.721  22.626 124.771  1.00 20.30      AAGL
ATOM   1204  CG1 ILE   154       8.563  22.666 126.092  1.00 20.35      AAGL
ATOM   1205  CD1 ILE   154       8.664  24.125 126.509  1.00 21.33      AAGL
ATOM   1206  C   ILE   154      11.097  19.901 125.304  1.00 22.17      AAGL
ATOM   1207  O   ILE   154      11.395  19.610 124.147  1.00 19.83      AAGL
ATOM   1208  N   GLY   155      11.920  19.735 126.337  1.00 23.65      AAGL
ATOM   1209  CA  GLY   155      13.246  19.181 126.147  1.00 24.02      AAGL
ATOM   1210  C   GLY   155      13.201  17.756 125.635  1.00 23.51      AAGL
ATOM   1211  O   GLY   155      13.968  17.384 124.745  1.00 23.80      AAGL
ATOM   1212  N   ALA   156      12.300  16.952 126.191  1.00 24.34      AAGL
ATOM   1213  CA  ALA   156      12.169  15.560 125.774  1.00 23.36      AAGL
ATOM   1214  CB  ALA   156      11.203  14.826 126.700  1.00 25.00      AAGL
ATOM   1215  C   ALA   156      11.701  15.457 124.324  1.00 23.25      AAGL
ATOM   1216  O   ALA   156      12.121  14.571 123.589  1.00 22.33      AAGL
ATOM   1217  N   LEU   157      10.831  16.371 123.911  1.00 22.39      AAGL
ATOM   1218  CA  LEU   157      10.340  16.376 122.538  1.00 21.31      AAGL
ATOM   1219  CB  LEU   157       9.161  17.343 122.408  1.00 20.00      AAGL
ATOM   1220  CG  LEU   157       7.868  16.843 123.059  1.00 22.93      AAGL
ATOM   1221  CD1 LEU   157       6.894  17.994 123.274  1.00 22.57      AAGL
ATOM   1222  CD2 LEU   157       7.260  15.751 122.164  1.00 21.07      AAGL
ATOM   1223  C   LEU   157      11.443  16.772 121.564  1.00 21.89      AAGL
ATOM   1224  O   LEU   157      11.616  16.146 120.518  1.00 20.81      AAGL
ATOM   1225  N   LEU   158      12.195  17.813 121.905  1.00 21.14      AAGL
ATOM   1226  CA  LEU   158      13.267  18.257 121.021  1.00 22.43      AAGL
ATOM   1227  CB  LEU   158      13.903  19.540 121.569  1.00 22.22      AAGL
ATOM   1228  CG  LEU   158      12.982  20.775 121.562  1.00 21.62      AAGL
ATOM   1229  CD1 LEU   158      13.640  21.917 122.316  1.00 21.34      AAGL
ATOM   1230  CD2 LEU   158      12.683  21.193 120.131  1.00 21.57      AAGL
ATOM   1231  C   LEU   158      14.299  17.133 120.880  1.00 24.78      AAGL
ATOM   1232  O   LEU   158      14.807  16.880 119.794  1.00 23.68      AAGL
ATOM   1233  N   HIS   159      14.584  16.457 121.990  1.00 24.81      AAGL
ATOM   1234  CA  HIS   159      15.518  15.332 122.009  1.00 26.46      AAGL
ATOM   1235  CB  HIS   159      15.566  14.738 123.423  1.00 27.84      AAGL
ATOM   1236  CG  HIS   159      16.473  13.553 123.563  1.00 30.73      AAGL
ATOM   1237  CD2 HIS   159      16.204  12.248 123.812  1.00 32.59      AAGL
ATOM   1238  ND1 HIS   159      17.845  13.651 123.482  1.00 31.02      AAGL
ATOM   1239  CE1 HIS   159      18.383  12.460 123.676  1.00 32.44      AAGL
ATOM   1240  NE2 HIS   159      17.409  11.592 123.880  1.00 33.23      AAGL
ATOM   1241  C   HIS   159      15.029  14.270 121.017  1.00 26.31      AAGL
ATOM   1242  O   HIS   159      15.796  13.772 120.190  1.00 26.14      AAGL
ATOM   1243  N   SER   160      13.749  13.922 121.110  1.00 25.57      AAGL
ATOM   1244  CA  SER   160      13.149  12.927 120.220  1.00 26.09      AAGL
ATOM   1245  CB  SER   160      11.679  12.695 120.590  1.00 26.91      AAGL
ATOM   1246  OG  SER   160      11.555  12.082 121.857  1.00 28.98      AAGL
ATOM   1247  C   SER   160      13.225  13.333 118.745  1.00 25.22      AAGL
ATOM   1248  O   SER   160      13.564  12.516 117.885  1.00 26.49      AAGL
ATOM   1249  N   GLY   161      12.890  14.586 118.452  1.00 22.94      AAGL
ATOM   1250  CA  GLY   161      12.934  15.051 117.078  1.00 22.94      AAGL
ATOM   1251  C   GLY   161      14.359  15.017 116.556  1.00 23.15      AAGL
ATOM   1252  O   GLY   161      14.631  14.541 115.450  1.00 23.15      AAGL
ATOM   1253  N   ALA   162      15.277  15.519 117.368  1.00 24.30      AAGL
ATOM   1254  CA  ALA   162      16.683  15.548 117.002  1.00 26.37      AAGL
ATOM   1255  CB  ALA   162      17.510  16.073 118.164  1.00 24.96      AAGL
ATOM   1256  C   ALA   162      17.172  14.160 116.598  1.00 27.69      AAGL
ATOM   1257  O   ALA   162      17.801  13.995 115.546  1.00 27.54      AAGL
ATOM   1258  N   TRP   163      16.876  13.159 117.423  1.00 27.38      AAGL
ATOM   1259  CA  TRP   163      17.320  11.806 117.124  1.00 26.93      AAGL
ATOM   1260  CB  TRP   163      17.222  10.929 118.368  1.00 28.85      AAGL
ATOM   1261  CG  TRP   163      18.386  11.181 119.245  1.00 31.71      AAGL
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Fig. 3 cont.

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ATOM   1262  CD2 TRP   163      19.668  10.565 119.134  1.00 32.43      AAGL
ATOM   1263  CE2 TRP   163      20.516  11.194 120.068  1.00 31.66      AAGL
ATOM   1264  CE3 TRP   163      20.185   9.541 118.329  1.00 32.40      AAGL
ATOM   1265  CD1 TRP   163      18.497  12.130 120.217  1.00 31.49      AAGL
ATOM   1266  NE1 TRP   163      19.776  12.149 120.715  1.00 32.86      AAGL
ATOM   1267  CZ2 TRP   163      21.858  10.836 120.223  1.00 32.68      AAGL
ATOM   1268  CZ3 TRP   163      21.522   9.184 118.479  1.00 32.50      AAGL
ATOM   1269  CH2 TRP   163      22.342   9.832 119.421  1.00 32.64      AAGL
ATOM   1270  C   TRP   163      16.636  11.144 115.952  1.00 27.25      AAGL
ATOM   1271  O   TRP   163      17.177  10.205 115.372  1.00 28.73      AAGL
ATOM   1272  N   GLY   164      15.448  11.613 115.598  1.00 25.57      AAGL
ATOM   1273  CA  GLY   164      14.782  11.045 114.445  1.00 24.90      AAGL
ATOM   1274  C   GLY   164      15.651  11.409 113.253  1.00 26.22      AAGL
ATOM   1275  O   GLY   164      15.831  10.618 112.326  1.00 26.72      AAGL
ATOM   1276  N   VAL   165      16.206  12.618 113.290  1.00 25.62      AAGL
ATOM   1277  CA  VAL   165      17.078  13.087 112.219  1.00 26.48      AAGL
ATOM   1278  CB  VAL   165      17.379  14.598 112.356  1.00 26.61      AAGL
ATOM   1279  CG1 VAL   165      18.398  15.026 111.293  1.00 23.67      AAGL
ATOM   1280  CG2 VAL   165      16.090  15.397 112.216  1.00 25.11      AAGL
ATOM   1281  C   VAL   165      18.406  12.328 112.251  1.00 27.69      AAGL
ATOM   1282  O   VAL   165      18.850  11.788 111.233  1.00 29.75      AAGL
ATOM   1283  N   LYS   166      19.037  12.295 113.420  1.00 27.66      AAGL
ATOM   1284  CA  LYS   166      20.313  11.607 113.581  1.00 29.81      AAGL
ATOM   1285  CB  LYS   166      20.770  11.661 115.045  1.00 29.36      AAGL
ATOM   1286  CG  LYS   166      21.062  13.060 115.590  1.00 30.72      AAGL
ATOM   1287  CD  LYS   166      21.442  12.982 117.065  1.00 33.25      AAGL
ATOM   1288  CE  LYS   166      21.674  14.358 117.677  1.00 33.72      AAGL
ATOM   1289  NZ  LYS   166      22.883  15.036 117.122  1.00 33.70      AAGL
ATOM   1290  C   LYS   166      20.229  10.144 113.136  1.00 31.30      AAGL
ATOM   1291  O   LYS   166      21.206   9.594 112.622  1.00 31.56      AAGL
ATOM   1292  N   ASP   167      19.065   9.519 113.319  1.00 30.83      AAGL
ATOM   1293  CA  ASP   167      18.893   8.116 112.944  1.00 32.56      AAGL
ATOM   1294  CB  ASP   167      17.863   7.442 113.854  1.00 31.71      AAGL
ATOM   1295  CG  ASP   167      18.387   7.187 115.245  1.00 33.01      AAGL
ATOM   1296  OD1 ASP   167      19.620   7.148 115.425  1.00 33.60      AAGL
ATOM   1297  OD2 ASP   167      17.558   7.006 116.160  1.00 32.14      AAGL
ATOM   1298  C   ASP   167      18.481   7.858 111.494  1.00 33.63      AAGL
ATOM   1299  O   ASP   167      18.347   6.696 111.082  1.00 32.89      AAGL
ATOM   1300  N   SER   168      18.280   8.925 110.724  1.00 31.74      AAGL
ATOM   1301  CA  SER   168      17.846   8.786 109.341  1.00 31.90      AAGL
ATOM   1302  CB  SER   168      17.279  10.111 108.823  1.00 29.91      AAGL
ATOM   1303  OG  SER   168      18.301  11.074 108.654  1.00 30.10      AAGL
ATOM   1304  C   SER   168      18.922   8.294 108.378  1.00 32.86      AAGL
ATOM   1305  O   SER   168      20.114   8.248 108.704  1.00 31.48      AAGL
ATOM   1306  N   ASN   169      18.470   7.950 107.179  1.00 34.44      AAGL
ATOM   1307  CA  ASN   169      19.328   7.430 106.123  1.00 37.26      AAGL
ATOM   1308  CB  ASN   169      18.493   6.545 105.195  1.00 38.60      AAGL
ATOM   1309  CG  ASN   169      17.848   5.377 105.925  1.00 37.67      AAGL
ATOM   1310  OD1 ASN   169      16.833   4.841 105.482  1.00 40.60      AAGL
ATOM   1311  ND2 ASN   169      18.440   4.971 107.044  1.00 39.67      AAGL
ATOM   1312  C   ASN   169      20.043   8.508 105.308  1.00 38.79      AAGL
ATOM   1313  O   ASN   169      20.725   8.194 104.324  1.00 39.86      AAGL
ATOM   1314  N   LEU   170      19.891   9.773 105.695  1.00 38.43      AAGL
ATOM   1315  CA  LEU   170      20.562  10.849 104.966  1.00 39.07      AAGL
ATOM   1316  CB  LEU   170      20.133  12.222 105.502  1.00 36.50      AAGL
ATOM   1317  CG  LEU   170      18.784  12.783 105.053  1.00 35.65      AAGL
ATOM   1318  CD1 LEU   170      18.533  14.122 105.733  1.00 36.42      AAGL
ATOM   1319  CD2 LEU   170      18.775  12.960 103.548  1.00 35.41      AAGL
ATOM   1320  C   LEU   170      22.068  10.672 105.146  1.00 40.51      AAGL
ATOM   1321  O   LEU   170      22.580  10.787 106.257  1.00 41.18      AAGL
ATOM   1322  N   ALA   171      22.770  10.392 104.050  1.00 43.25      AAGL
ATOM   1323  CA  ALA   171      24.219  10.180 104.078  1.00 44.92      AAGL
ATOM   1324  CB  ALA   171      24.796  10.430 102.700  1.00 45.32      AAGL
ATOM   1325  C   ALA   171      24.913  11.063 105.117  1.00 45.99      AAGL
ATOM   1326  O   ALA   171      25.671  10.568 105.962  1.00 47.05      AAGL
ATOM   1327  N   THR   172      24.668  12.370 105.044  1.00 46.11      AAGL
ATOM   1328  CA  THR   172      25.246  13.316 105.998  1.00 45.78      AAGL
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Fig. 3 cont.

ATOM	1329	CB	THR	172	25.856	14.549	105.320	1.00	46.89	AAGL
ATOM	1330	OG1	THR	172	26.551	14.167	104.132	1.00	48.14	AAGL
ATOM	1331	CG2	THR	172	26.822	15.224	106.269	1.00	46.74	AAGL
ATOM	1332	C	THR	172	24.117	13.844	106.868	1.00	44.10	AAGL
ATOM	1333	O	THR	172	23.086	14.272	106.351	1.00	44.98	AAGL
ATOM	1334	N	THR	173	24.311	13.835	108.179	1.00	42.61	AAGL
ATOM	1335	CA	THR	173	23.283	14.319	109.088	1.00	39.37	AAGL
ATOM	1336	CB	THR	173	23.621	13.926	110.530	1.00	39.69	AAGL
ATOM	1337	OG1	THR	173	23.691	12.497	110.620	1.00	40.97	AAGL
ATOM	1338	CG2	THR	173	22.555	14.436	111.494	1.00	40.31	AAGL
ATOM	1339	C	THR	173	23.140	15.837	108.969	1.00	36.34	AAGL
ATOM	1340	O	THR	173	24.118	16.581	109.083	1.00	35.72	AAGL
ATOM	1341	N	PRO	174	21.916	16.319	108.702	1.00	33.51	AAGL
ATOM	1342	CD	PRO	174	20.709	15.592	108.274	1.00	33.11	AAGL
ATOM	1343	CA	PRO	174	21.728	17.766	108.580	1.00	30.76	AAGL
ATOM	1344	CB	PRO	174	20.252	17.891	108.223	1.00	31.41	AAGL
ATOM	1345	CG	PRO	174	19.989	16.624	107.452	1.00	33.06	AAGL
ATOM	1346	C	PRO	174	22.056	18.475	109.883	1.00	27.61	AAGL
ATOM	1347	O	PRO	174	22.074	17.865	110.945	1.00	26.79	AAGL
ATOM	1348	N	LYS	175	22.332	19.767	109.800	1.00	28.61	AAGL
ATOM	1349	CA	LYS	175	22.614	20.541	111.001	1.00	27.46	AAGL
ATOM	1350	CB	LYS	175	23.167	21.917	110.636	1.00	30.67	AAGL
ATOM	1351	CG	LYS	175	24.679	22.002	110.611	1.00	35.14	AAGL
ATOM	1352	CD	LYS	175	25.286	20.926	109.751	1.00	39.94	AAGL
ATOM	1353	CE	LYS	175	26.804	21.046	109.733	1.00	42.54	AAGL
ATOM	1354	NZ	LYS	175	27.396	20.867	111.091	1.00	43.56	AAGL
ATOM	1355	C	LYS	175	21.267	20.693	111.695	1.00	26.21	AAGL
ATOM	1356	O	LYS	175	20.297	21.096	111.068	1.00	25.54	AAGL
ATOM	1357	N	ILE	176	21.209	20.350	112.975	1.00	24.86	AAGL
ATOM	1358	CA	ILE	176	19.968	20.443	113.728	1.00	24.97	AAGL
ATOM	1359	CB	ILE	176	19.899	19.320	114.779	1.00	25.45	AAGL
ATOM	1360	CG2	ILE	176	18.689	19.515	115.676	1.00	25.15	AAGL
ATOM	1361	CG1	ILE	176	19.847	17.964	114.061	1.00	25.46	AAGL
ATOM	1362	CD1	ILE	176	20.148	16.775	114.941	1.00	26.04	AAGL
ATOM	1363	C	ILE	176	19.866	21.807	114.395	1.00	23.30	AAGL
ATOM	1364	O	ILE	176	20.752	22.208	115.136	1.00	24.10	AAGL
ATOM	1365	N	MET	177	18.769	22.507	114.127	1.00	23.38	AAGL
ATOM	1366	CA	MET	177	18.557	23.847	114.656	1.00	22.20	AAGL
ATOM	1367	CB	MET	177	18.401	24.837	113.488	1.00	20.47	AAGL
ATOM	1368	CG	MET	177	17.934	26.249	113.903	1.00	21.58	AAGL
ATOM	1369	SD	MET	177	17.586	27.336	112.488	1.00	22.93	AAGL
ATOM	1370	CE	MET	177	19.288	27.706	111.969	1.00	22.76	AAGL
ATOM	1371	C	MET	177	17.352	24.013	115.576	1.00	21.82	AAGL
ATOM	1372	O	MET	177	16.343	23.326	115.425	1.00	21.31	AAGL
ATOM	1373	N	ILE	178	17.485	24.927	116.534	1.00	20.60	AAGL
ATOM	1374	CA	ILE	178	16.395	25.294	117.433	1.00	21.53	AAGL
ATOM	1375	CB	ILE	178	16.750	25.134	118.932	1.00	22.17	AAGL
ATOM	1376	CG2	ILE	178	15.678	25.810	119.798	1.00	22.88	AAGL
ATOM	1377	CG1	ILE	178	16.830	23.647	119.286	1.00	23.39	AAGL
ATOM	1378	CD1	ILE	178	17.014	23.363	120.767	1.00	25.76	AAGL
ATOM	1379	C	ILE	178	16.204	26.766	117.088	1.00	19.40	AAGL
ATOM	1380	O	ILE	178	17.156	27.555	117.127	1.00	19.88	AAGL
ATOM	1381	N	HIS	179	14.971	27.125	116.751	1.00	18.62	AAGL
ATOM	1382	CA	HIS	179	14.632	28.475	116.312	1.00	18.14	AAGL
ATOM	1383	CB	HIS	179	14.054	28.356	114.899	1.00	17.60	AAGL
ATOM	1384	CG	HIS	179	13.454	29.617	114.363	1.00	18.42	AAGL
ATOM	1385	CD2	HIS	179	13.731	30.919	114.609	1.00	17.14	AAGL
ATOM	1386	ND1	HIS	179	12.438	29.611	113.432	1.00	18.37	AAGL
ATOM	1387	CE1	HIS	179	12.114	30.855	113.129	1.00	16.27	AAGL
ATOM	1388	NE2	HIS	179	12.883	31.668	113.830	1.00	17.92	AAGL
ATOM	1389	C	HIS	179	13.658	29.235	117.227	1.00	20.10	AAGL
ATOM	1390	O	HIS	179	12.541	28.780	117.470	1.00	20.46	AAGL
ATOM	1391	N	LEU	180	14.090	30.394	117.716	1.00	18.07	AAGL
ATOM	1392	CA	LEU	180	13.258	31.237	118.574	1.00	19.85	AAGL
ATOM	1393	CB	LEU	180	13.930	31.480	119.928	1.00	20.54	AAGL
ATOM	1394	CG	LEU	180	14.253	30.306	120.854	1.00	24.61	AAGL
ATOM	1395	CD1	LEU	180	14.701	30.866	122.208	1.00	23.57	AAGL

Fig. 3 cont.

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ATOM   1396  CD2 LEU   180      13.038  29.405 121.029  1.00 22.59      AAGL
ATOM   1397  C   LEU   180      13.027  32.588 117.905  1.00 20.35      AAGL
ATOM   1398  O   LEU   180      13.838  33.032 117.099  1.00 20.34      AAGL
ATOM   1399  N   ASP   181      11.918  33.237 118.240  1.00 19.30      AAGL
ATOM   1400  CA  ASP   181      11.623  34.548 117.688  1.00 19.90      AAGL
ATOM   1401  CB  ASP   181      10.112  34.796 117.680  1.00 21.15      AAGL
ATOM   1402  CG  ASP   181       9.522  34.825 119.070  1.00 22.95      AAGL
ATOM   1403  OD1 ASP   181       9.910  33.973 119.900  1.00 22.67      AAGL
ATOM   1404  OD2 ASP   181       8.664  35.697 119.336  1.00 25.18      AAGL
ATOM   1405  C   ASP   181      12.315  35.580 118.576  1.00 21.86      AAGL
ATOM   1406  O   ASP   181      13.020  35.218 119.524  1.00 23.76      AAGL
ATOM   1407  N   ASP   182      12.107  36.856 118.271  1.00 22.19      AAGL
ATOM   1408  CA  ASP   182      12.718  37.948 119.034  1.00 22.68      AAGL
ATOM   1409  CB  ASP   182      12.013  38.129 120.381  1.00 24.73      AAGL
ATOM   1410  CG  ASP   182      10.589  38.605 120.234  1.00 26.20      AAGL
ATOM   1411  OD1 ASP   182      10.226  39.052 119.134  1.00 30.46      AAGL
ATOM   1412  OD2 ASP   182       9.829  38.539 121.226  1.00 30.54      AAGL
ATOM   1413  C   ASP   182      14.205  37.719 119.282  1.00 21.94      AAGL
ATOM   1414  O   ASP   182      14.645  37.656 120.432  1.00 22.68      AAGL
ATOM   1415  N   GLY   183      14.975  37.610 118.203  1.00 21.90      AAGL
ATOM   1416  CA  GLY   183      16.403  37.388 118.334  1.00 20.97      AAGL
ATOM   1417  C   GLY   183      17.158  38.524 119.003  1.00 21.01      AAGL
ATOM   1418  O   GLY   183      18.279  38.340 119.478  1.00 24.20      AAGL
ATOM   1419  N   TRP   184      16.550  39.701 119.045  1.00 23.43      AAGL
ATOM   1420  CA  TRP   184      17.191  40.859 119.655  1.00 25.63      AAGL
ATOM   1421  CB  TRP   184      16.514  42.141 119.173  1.00 24.89      AAGL
ATOM   1422  CG  TRP   184      15.045  42.120 119.376  1.00 27.09      AAGL
ATOM   1423  CD2 TRP   184      14.346  42.467 120.576  1.00 28.81      AAGL
ATOM   1424  CE2 TRP   184      12.971  42.248 120.336  1.00 28.20      AAGL
ATOM   1425  CE3 TRP   184      14.750  42.944 121.833  1.00 30.34      AAGL
ATOM   1426  CD1 TRP   184      14.098  41.717 118.481  1.00 27.72      AAGL
ATOM   1427  NE1 TRP   184      12.847  41.792 119.049  1.00 27.27      AAGL
ATOM   1428  CZ2 TRP   184      11.994  42.487 121.308  1.00 32.25      AAGL
ATOM   1429  CZ3 TRP   184      13.776  43.184 122.802  1.00 33.25      AAGL
ATOM   1430  CH2 TRP   184      12.414  42.954 122.533  1.00 30.56      AAGL
ATOM   1431  C   TRP   184      17.155  40.816 121.184  1.00 27.12      AAGL
ATOM   1432  O   TRP   184      17.869  41.563 121.850  1.00 26.68      AAGL
ATOM   1433  N   SER   185      16.332  39.935 121.742  1.00 26.77      AAGL
ATOM   1434  CA  SER   185      16.207  39.846 123.190  1.00 28.56      AAGL
ATOM   1435  CB  SER   185      14.739  39.648 123.558  1.00 28.06      AAGL
ATOM   1436  OG  SER   185      14.594  39.465 124.949  1.00 31.97      AAGL
ATOM   1437  C   SER   185      17.055  38.761 123.858  1.00 27.96      AAGL
ATOM   1438  O   SER   185      16.660  37.600 123.919  1.00 29.29      AAGL
ATOM   1439  N   TRP   186      18.218  39.142 124.374  1.00 27.87      AAGL
ATOM   1440  CA  TRP   186      19.091  38.176 125.032  1.00 27.87      AAGL
ATOM   1441  CB  TRP   186      20.380  38.853 125.511  1.00 29.10      AAGL
ATOM   1442  CG  TRP   186      21.165  38.036 126.509  1.00 27.39      AAGL
ATOM   1443  CD2 TRP   186      21.670  36.705 126.335  1.00 29.36      AAGL
ATOM   1444  CE2 TRP   186      22.338  36.352 127.531  1.00 30.06      AAGL
ATOM   1445  CE3 TRP   186      21.625  35.774 125.285  1.00 30.04      AAGL
ATOM   1446  CD1 TRP   186      21.534  38.422 127.765  1.00 29.38      AAGL
ATOM   1447  NE1 TRP   186      22.239  37.417 128.386  1.00 28.39      AAGL
ATOM   1448  CZ2 TRP   186      22.957  35.108 127.705  1.00 30.53      AAGL
ATOM   1449  CZ3 TRP   186      22.240  34.540 125.459  1.00 30.87      AAGL
ATOM   1450  CH2 TRP   186      22.898  34.218 126.662  1.00 31.05      AAGL
ATOM   1451  C   TRP   186      18.418  37.486 126.217  1.00 28.13      AAGL
ATOM   1452  O   TRP   186      18.620  36.291 126.445  1.00 27.04      AAGL
ATOM   1453  N   ASP   187      17.628  38.232 126.979  1.00 28.09      AAGL
ATOM   1454  CA  ASP   187      16.961  37.643 128.131  1.00 29.42      AAGL
ATOM   1455  CB  ASP   187      16.156  38.704 128.887  1.00 32.15      AAGL
ATOM   1456  CG  ASP   187      17.028  39.817 129.450  1.00 37.52      AAGL
ATOM   1457  OD1 ASP   187      18.255  39.612 129.611  1.00 39.29      AAGL
ATOM   1458  OD2 ASP   187      16.476  40.896 129.748  1.00 41.44      AAGL
ATOM   1459  C   ASP   187      16.035  36.488 127.724  1.00 28.91      AAGL
ATOM   1460  O   ASP   187      16.033  35.431 128.357  1.00 27.77      AAGL
ATOM   1461  N   GLN   188      15.250  36.691 126.668  1.00 27.43      AAGL
ATOM   1462  CA  GLN   188      14.326  35.657 126.215  1.00 27.67      AAGL
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Fig. 3 cont.

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ATOM   1463  CB  GLN   188      13.357  36.220 125.170  1.00 28.11      AAGL
ATOM   1464  CG  GLN   188      12.222  37.066 125.735  1.00 31.74      AAGL
ATOM   1465  CD  GLN   188      11.247  36.258 126.588  1.00 36.22      AAGL
ATOM   1466  OE1 GLN   188      10.921  35.103 126.274  1.00 36.68      AAGL
ATOM   1467  NE2 GLN   188      10.760  36.867 127.660  1.00 37.18      AAGL
ATOM   1468  C   GLN   188      15.061  34.456 125.641  1.00 26.39      AAGL
ATOM   1469  O   GLN   188      14.710  33.318 125.934  1.00 26.19      AAGL
ATOM   1470  N   GLN   189      16.086  34.712 124.829  1.00 25.52      AAGL
ATOM   1471  CA  GLN   189      16.864  33.633 124.225  1.00 24.65      AAGL
ATOM   1472  CB  GLN   189      17.997  34.191 123.351  1.00 24.63      AAGL
ATOM   1473  CG  GLN   189      17.576  34.991 122.126  1.00 24.46      AAGL
ATOM   1474  CD  GLN   189      16.736  34.191 121.149  1.00 21.93      AAGL
ATOM   1475  OE1 GLN   189      17.097  33.084 120.760  1.00 20.15      AAGL
ATOM   1476  NE2 GLN   189      15.613  34.759 120.739  1.00 23.53      AAGL
ATOM   1477  C   GLN   189      17.484  32.759 125.308  1.00 25.42      AAGL
ATOM   1478  O   GLN   189      17.314  31.544 125.324  1.00 23.58      AAGL
ATOM   1479  N   ASN   190      18.199  33.405 126.219  1.00 25.59      AAGL
ATOM   1480  CA  ASN   190      18.892  32.725 127.293  1.00 26.28      AAGL
ATOM   1481  CB  ASN   190      19.745  33.736 128.056  1.00 28.08      AAGL
ATOM   1482  CG  ASN   190      20.593  33.091 129.135  1.00 29.88      AAGL
ATOM   1483  OD1 ASN   190      21.204  32.041 128.922  1.00 29.87      AAGL
ATOM   1484  ND2 ASN   190      20.649  33.727 130.295  1.00 33.02      AAGL
ATOM   1485  C   ASN   190      17.978  31.970 128.250  1.00 26.80      AAGL
ATOM   1486  O   ASN   190      18.300  30.866 128.675  1.00 27.29      AAGL
ATOM   1487  N   TYR   191      16.838  32.554 128.590  1.00 27.59      AAGL
ATOM   1488  CA  TYR   191      15.931  31.878 129.504  1.00 27.82      AAGL
ATOM   1489  CB  TYR   191      14.735  32.767 129.832  1.00 28.23      AAGL
ATOM   1490  CG  TYR   191      13.815  32.132 130.844  1.00 30.08      AAGL
ATOM   1491  CD1 TYR   191      12.775  31.294 130.446  1.00 32.24      AAGL
ATOM   1492  CE1 TYR   191      11.975  30.641 131.385  1.00 33.28      AAGL
ATOM   1493  CD2 TYR   191      14.032  32.308 132.210  1.00 31.47      AAGL
ATOM   1494  CE2 TYR   191      13.240  31.662 133.157  1.00 31.82      AAGL
ATOM   1495  CZ  TYR   191      12.219  30.830 132.739  1.00 34.47      AAGL
ATOM   1496  OH  TYR   191      11.458  30.168 133.679  1.00 36.38      AAGL
ATOM   1497  C   TYR   191      15.443  30.551 128.929  1.00 27.27      AAGL
ATOM   1498  O   TYR   191      15.392  29.537 129.631  1.00 25.68      AAGL
ATOM   1499  N   PHE   192      15.079  30.557 127.651  1.00 25.48      AAGL
ATOM   1500  CA  PHE   192      14.605  29.341 127.016  1.00 26.24      AAGL
ATOM   1501  CB  PHE   192      14.260  29.593 125.541  1.00 24.60      AAGL
ATOM   1502  CG  PHE   192      13.854  28.351 124.799  1.00 22.89      AAGL
ATOM   1503  CD1 PHE   192      12.541  27.893 124.848  1.00 23.14      AAGL
ATOM   1504  CD2 PHE   192      14.795  27.607 124.098  1.00 22.70      AAGL
ATOM   1505  CE1 PHE   192      12.169  26.706 124.208  1.00 22.64      AAGL
ATOM   1506  CE2 PHE   192      14.439  26.417 123.455  1.00 22.68      AAGL
ATOM   1507  CZ  PHE   192      13.125  25.965 123.510  1.00 23.16      AAGL
ATOM   1508  C   PHE   192      15.651  28.237 127.095  1.00 26.50      AAGL
ATOM   1509  O   PHE   192      15.386  27.154 127.612  1.00 25.06      AAGL
ATOM   1510  N   TYR   193      16.847  28.513 126.577  1.00 26.97      AAGL
ATOM   1511  CA  TYR   193      17.898  27.510 126.570  1.00 28.47      AAGL
ATOM   1512  CB  TYR   193      19.066  27.991 125.704  1.00 25.93      AAGL
ATOM   1513  CG  TYR   193      18.675  28.113 124.243  1.00 26.36      AAGL
ATOM   1514  CD1 TYR   193      18.344  26.979 123.498  1.00 24.37      AAGL
ATOM   1515  CE1 TYR   193      17.905  27.084 122.178  1.00 23.29      AAGL
ATOM   1516  CD2 TYR   193      18.561  29.357 123.632  1.00 26.34      AAGL
ATOM   1517  CE2 TYR   193      18.121  29.474 122.307  1.00 24.57      AAGL
ATOM   1518  CZ  TYR   193      17.797  28.331 121.592  1.00 23.44      AAGL
ATOM   1519  OH  TYR   193      17.370  28.431 120.290  1.00 24.47      AAGL
ATOM   1520  C   TYR   193      18.384  27.087 127.952  1.00 28.72      AAGL
ATOM   1521  O   TYR   193      18.542  25.892 128.212  1.00 29.46      AAGL
ATOM   1522  N   GLU   194      18.610  28.046 128.844  1.00 30.56      AAGL
ATOM   1523  CA  GLU   194      19.081  27.684 130.177  1.00 32.74      AAGL
ATOM   1524  CB  GLU   194      19.344  28.921 131.048  1.00 36.66      AAGL
ATOM   1525  CG  GLU   194      20.119  28.543 132.325  1.00 42.88      AAGL
ATOM   1526  CD  GLU   194      20.271  29.668 133.327  1.00 46.55      AAGL
ATOM   1527  OE1 GLU   194      21.086  29.502 134.275  1.00 48.27      AAGL
ATOM   1528  OE2 GLU   194      19.580  30.704 133.194  1.00 47.67      AAGL
ATOM   1529  C   GLU   194      18.056  26.802 130.875  1.00 31.54      AAGL
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Fig. 3 cont.

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ATOM   1530  O   GLU   194      18.396  25.764 131.445  1.00 31.58      AAGL
ATOM   1531  N   THR   195      16.795  27.212 130.823  1.00 30.56      AAGL
ATOM   1532  CA  THR   195      15.731  26.453 131.468  1.00 28.40      AAGL
ATOM   1533  CB  THR   195      14.408  27.226 131.402  1.00 27.94      AAGL
ATOM   1534  OG1 THR   195      14.611  28.545 131.929  1.00 25.50      AAGL
ATOM   1535  CG2 THR   195      13.330  26.516 132.211  1.00 26.24      AAGL
ATOM   1536  C   THR   195      15.535  25.054 130.868  1.00 28.06      AAGL
ATOM   1537  O   THR   195      15.427  24.071 131.599  1.00 26.71      AAGL
ATOM   1538  N   VAL   196      15.486  24.961 129.545  1.00 27.08      AAGL
ATOM   1539  CA  VAL   196      15.301  23.666 128.902  1.00 27.16      AAGL
ATOM   1540  CB  VAL   196      15.035  23.838 127.369  1.00 29.10      AAGL
ATOM   1541  CG1 VAL   196      16.227  24.510 126.700  1.00 30.65      AAGL
ATOM   1542  CG2 VAL   196      14.748  22.487 126.727  1.00 31.18      AAGL
ATOM   1543  C   VAL   196      16.502  22.736 129.137  1.00 26.59      AAGL
ATOM   1544  O   VAL   196      16.330  21.563 129.449  1.00 25.06      AAGL
ATOM   1545  N   LEU   197      17.716  23.266 129.015  1.00 26.11      AAGL
ATOM   1546  CA  LEU   197      18.911  22.451 129.214  1.00 28.97      AAGL
ATOM   1547  CB  LEU   197      20.161  23.207 128.735  1.00 29.84      AAGL
ATOM   1548  CG  LEU   197      20.233  23.474 127.220  1.00 30.49      AAGL
ATOM   1549  CD1 LEU   197      21.377  24.445 126.927  1.00 32.56      AAGL
ATOM   1550  CD2 LEU   197      20.413  22.176 126.464  1.00 30.05      AAGL
ATOM   1551  C   LEU   197      19.069  22.032 130.674  1.00 28.89      AAGL
ATOM   1552  O   LEU   197      19.632  20.976 130.971  1.00 30.68      AAGL
ATOM   1553  N   ALA   198      18.550  22.844 131.586  1.00 29.81      AAGL
ATOM   1554  CA  ALA   198      18.646  22.530 133.008  1.00 30.14      AAGL
ATOM   1555  CB  ALA   198      18.110  23.688 133.831  1.00 29.46      AAGL
ATOM   1556  C   ALA   198      17.913  21.237 133.387  1.00 31.06      AAGL
ATOM   1557  O   ALA   198      18.223  20.624 134.411  1.00 30.62      AAGL
ATOM   1558  N   THR   199      16.951  20.814 132.569  1.00 30.12      AAGL
ATOM   1559  CA  THR   199      16.192  19.599 132.868  1.00 29.04      AAGL
ATOM   1560  CB  THR   199      14.831  19.569 132.137  1.00 30.14      AAGL
ATOM   1561  OG1 THR   199      15.051  19.375 130.735  1.00 28.92      AAGL
ATOM   1562  CG2 THR   199      14.058  20.876 132.351  1.00 28.52      AAGL
ATOM   1563  C   THR   199      16.926  18.308 132.497  1.00 30.21      AAGL
ATOM   1564  O   THR   199      16.602  17.237 133.006  1.00 31.94      AAGL
ATOM   1565  N   GLY   200      17.907  18.406 131.613  1.00 29.95      AAGL
ATOM   1566  CA  GLY   200      18.626  17.219 131.194  1.00 30.95      AAGL
ATOM   1567  C   GLY   200      17.868  16.428 130.143  1.00 31.30      AAGL
ATOM   1568  O   GLY   200      18.376  15.436 129.625  1.00 31.90      AAGL
ATOM   1569  N   GLU   201      16.647  16.850 129.823  1.00 31.18      AAGL
ATOM   1570  CA  GLU   201      15.856  16.145 128.813  1.00 30.31      AAGL
ATOM   1571  CB  GLU   201      14.385  16.557 128.881  1.00 29.74      AAGL
ATOM   1572  CG  GLU   201      13.640  16.062 130.110  1.00 32.87      AAGL
ATOM   1573  CD  GLU   201      13.710  14.555 130.285  1.00 33.76      AAGL
ATOM   1574  OE1 GLU   201      13.838  13.833 129.274  1.00 34.18      AAGL
ATOM   1575  OE2 GLU   201      13.617  14.086 131.443  1.00 34.63      AAGL
ATOM   1576  C   GLU   201      16.399  16.440 127.423  1.00 28.94      AAGL
ATOM   1577  O   GLU   201      16.271  15.625 126.511  1.00 27.79      AAGL
ATOM   1578  N   LEU   202      16.988  17.623 127.272  1.00 28.10      AAGL
ATOM   1579  CA  LEU   202      17.587  18.033 126.009  1.00 28.10      AAGL
ATOM   1580  CB  LEU   202      17.029  19.376 125.548  1.00 28.75      AAGL
ATOM   1581  CG  LEU   202      17.766  19.987 124.350  1.00 27.26      AAGL
ATOM   1582  CD1 LEU   202      17.461  19.196 123.090  1.00 27.62      AAGL
ATOM   1583  CD2 LEU   202      17.337  21.430 124.178  1.00 29.02      AAGL
ATOM   1584  C   LEU   202      19.088  18.170 126.240  1.00 28.79      AAGL
ATOM   1585  O   LEU   202      19.518  18.888 127.141  1.00 29.33      AAGL
ATOM   1586  N   LEU   203      19.875  17.473 125.433  1.00 29.74      AAGL
ATOM   1587  CA  LEU   203      21.326  17.524 125.557  1.00 32.35      AAGL
ATOM   1588  CB  LEU   203      21.920  16.146 125.271  1.00 33.32      AAGL
ATOM   1589  CG  LEU   203      21.643  15.084 126.328  1.00 33.68      AAGL
ATOM   1590  CD1 LEU   203      22.436  13.828 125.998  1.00 38.12      AAGL
ATOM   1591  CD2 LEU   203      22.053  15.615 127.694  1.00 37.93      AAGL
ATOM   1592  C   LEU   203      21.934  18.541 124.603  1.00 32.26      AAGL
ATOM   1593  O   LEU   203      21.475  18.694 123.474  1.00 33.19      AAGL
ATOM   1594  N   SER   204      22.975  19.231 125.055  1.00 33.40      AAGL
ATOM   1595  CA  SER   204      23.634  20.215 124.213  1.00 34.27      AAGL
ATOM   1596  CB  SER   204      24.824  20.826 124.947  1.00 34.70      AAGL
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Fig. 3 cont.

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ATOM   1597  OG  SER   204      25.380  21.894 124.194  1.00 36.69      AAGL
ATOM   1598  C   SER   204      24.103  19.529 122.934  1.00 34.03      AAGL
ATOM   1599  O   SER   204      24.163  20.145 121.871  1.00 35.28      AAGL
ATOM   1600  N   THR   205      24.438  18.248 123.043  1.00 32.63      AAGL
ATOM   1601  CA  THR   205      24.890  17.491 121.880  1.00 33.11      AAGL
ATOM   1602  CB  THR   205      25.650  16.204 122.302  1.00 33.97      AAGL
ATOM   1603  OG1 THR   205      24.875  15.458 123.256  1.00 35.21      AAGL
ATOM   1604  CG2 THR   205      26.989  16.572 122.919  1.00 34.51      AAGL
ATOM   1605  C   THR   205      23.737  17.111 120.951  1.00 32.07      AAGL
ATOM   1606  O   THR   205      23.960  16.584 119.865  1.00 32.54      AAGL
ATOM   1607  N   ASP   206      22.504  17.389 121.367  1.00 30.83      AAGL
ATOM   1608  CA  ASP   206      21.352  17.054 120.536  1.00 29.51      AAGL
ATOM   1609  CB  ASP   206      20.060  17.033 121.351  1.00 28.56      AAGL
ATOM   1610  CG  ASP   206      19.996  15.871 122.315  1.00 31.99      AAGL
ATOM   1611  OD1 ASP   206      20.539  14.791 121.990  1.00 30.07      AAGL
ATOM   1612  OD2 ASP   206      19.385  16.037 123.390  1.00 30.30      AAGL
ATOM   1613  C   ASP   206      21.151  17.986 119.352  1.00 28.75      AAGL
ATOM   1614  O   ASP   206      20.514  17.597 118.376  1.00 29.56      AAGL
ATOM   1615  N   PHE   207      21.653  19.217 119.437  1.00 27.57      AAGL
ATOM   1616  CA  PHE   207      21.496  20.147 118.321  1.00 27.18      AAGL
ATOM   1617  CB  PHE   207      20.315  21.106 118.567  1.00 24.79      AAGL
ATOM   1618  CG  PHE   207      20.541  22.115 119.651  1.00 24.63      AAGL
ATOM   1619  CD1 PHE   207      20.643  21.728 120.981  1.00 26.07      AAGL
ATOM   1620  CD2 PHE   207      20.613  23.473 119.341  1.00 26.18      AAGL
ATOM   1621  CE1 PHE   207      20.811  22.677 121.986  1.00 23.87      AAGL
ATOM   1622  CE2 PHE   207      20.782  24.433 120.340  1.00 24.35      AAGL
ATOM   1623  CZ  PHE   207      20.880  24.032 121.661  1.00 26.22      AAGL
ATOM   1624  C   PHE   207      22.767  20.917 117.974  1.00 27.60      AAGL
ATOM   1625  O   PHE   207      23.700  20.987 118.772  1.00 28.27      AAGL
ATOM   1626  N   ASP   208      22.784  21.503 116.780  1.00 28.39      AAGL
ATOM   1627  CA  ASP   208      23.958  22.209 116.278  1.00 28.84      AAGL
ATOM   1628  CB  ASP   208      24.329  21.618 114.918  1.00 28.97      AAGL
ATOM   1629  CG  ASP   208      24.337  20.102 114.930  1.00 29.39      AAGL
ATOM   1630  OD1 ASP   208      25.139  19.521 115.686  1.00 30.72      AAGL
ATOM   1631  OD2 ASP   208      23.537  19.494 114.187  1.00 30.15      AAGL
ATOM   1632  C   ASP   208      23.910  23.737 116.143  1.00 28.85      AAGL
ATOM   1633  O   ASP   208      24.866  24.418 116.520  1.00 28.49      AAGL
ATOM   1634  N   TYR   209      22.817  24.263 115.595  1.00 26.19      AAGL
ATOM   1635  CA  TYR   209      22.674  25.704 115.368  1.00 25.08      AAGL
ATOM   1636  CB  TYR   209      22.353  26.001 113.896  1.00 26.01      AAGL
ATOM   1637  CG  TYR   209      23.397  25.677 112.854  1.00 23.51      AAGL
ATOM   1638  CD1 TYR   209      24.728  25.427 113.191  1.00 27.73      AAGL
ATOM   1639  CE1 TYR   209      25.693  25.222 112.194  1.00 27.06      AAGL
ATOM   1640  CD2 TYR   209      23.056  25.705 111.506  1.00 26.41      AAGL
ATOM   1641  CE2 TYR   209      24.007  25.503 110.505  1.00 29.44      AAGL
ATOM   1642  CZ  TYR   209      25.318  25.267 110.856  1.00 25.86      AAGL
ATOM   1643  OH  TYR   209      26.244  25.103 109.853  1.00 26.38      AAGL
ATOM   1644  C   TYR   209      21.578  26.398 116.163  1.00 23.78      AAGL
ATOM   1645  O   TYR   209      20.611  25.774 116.589  1.00 23.59      AAGL
ATOM   1646  N   PHE   210      21.745  27.711 116.315  1.00 25.60      AAGL
ATOM   1647  CA  PHE   210      20.775  28.584 116.969  1.00 24.58      AAGL
ATOM   1648  CB  PHE   210      21.441  29.576 117.918  1.00 25.18      AAGL
ATOM   1649  CG  PHE   210      21.826  29.004 119.234  1.00 26.35      AAGL
ATOM   1650  CD1 PHE   210      20.895  28.309 120.004  1.00 26.01      AAGL
ATOM   1651  CD2 PHE   210      23.104  29.214 119.741  1.00 26.73      AAGL
ATOM   1652  CE1 PHE   210      21.234  27.836 121.269  1.00 28.08      AAGL
ATOM   1653  CE2 PHE   210      23.453  28.746 121.000  1.00 29.00      AAGL
ATOM   1654  CZ  PHE   210      22.519  28.057 121.768  1.00 28.84      AAGL
ATOM   1655  C   PHE   210      20.167  29.402 115.842  1.00 25.37      AAGL
ATOM   1656  O   PHE   210      20.894  29.932 115.005  1.00 26.01      AAGL
ATOM   1657  N   GLY   211      18.845  29.514 115.817  1.00 22.48      AAGL
ATOM   1658  CA  GLY   211      18.214  30.313 114.784  1.00 21.15      AAGL
ATOM   1659  C   GLY   211      17.305  31.333 115.441  1.00 20.32      AAGL
ATOM   1660  O   GLY   211      16.631  31.007 116.412  1.00 22.35      AAGL
ATOM   1661  N   VAL   212      17.285  32.560 114.931  1.00 20.60      AAGL
ATOM   1662  CA  VAL   212      16.428  33.595 115.501  1.00 19.19      AAGL
ATOM   1663  CB  VAL   212      17.206  34.592 116.400  1.00 20.57      AAGL
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Fig. 3 cont.

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ATOM   1664  CG1 VAL   212      17.920  33.859 117.512  1.00 21.04      AAGL
ATOM   1665  CG2 VAL   212      18.169  35.419 115.554  1.00 22.31      AAGL
ATOM   1666  C   VAL   212      15.781  34.426 114.410  1.00 19.78      AAGL
ATOM   1667  O   VAL   212      16.358  34.616 113.339  1.00 19.10      AAGL
ATOM   1668  N   SER   213      14.581  34.914 114.692  1.00 18.35      AAGL
ATOM   1669  CA  SER   213      13.869  35.775 113.758  1.00 19.01      AAGL
ATOM   1670  CB  SER   213      12.353  35.630 113.933  1.00 18.11      AAGL
ATOM   1671  OG  SER   213      11.934  34.305 113.696  1.00 17.61      AAGL
ATOM   1672  C   SER   213      14.277  37.187 114.148  1.00 18.11      AAGL
ATOM   1673  O   SER   213      14.506  37.461 115.323  1.00 21.77      AAGL
ATOM   1674  N   TYR   214      14.384  38.081 113.174  1.00 17.30      AAGL
ATOM   1675  CA  TYR   214      14.744  39.458 113.478  1.00 17.43      AAGL
ATOM   1676  CB  TYR   214      16.252  39.688 113.352  1.00 19.55      AAGL
ATOM   1677  CG  TYR   214      16.647  41.122 113.624  1.00 18.83      AAGL
ATOM   1678  CD1 TYR   214      16.558  41.661 114.911  1.00 22.19      AAGL
ATOM   1679  CE1 TYR   214      16.872  43.004 115.158  1.00 22.03      AAGL
ATOM   1680  CD2 TYR   214      17.063  41.959 112.590  1.00 23.69      AAGL
ATOM   1681  CE2 TYR   214      17.381  43.307 112.828  1.00 22.60      AAGL
ATOM   1682  CZ  TYR   214      17.279  43.816 114.113  1.00 22.17      AAGL
ATOM   1683  OH  TYR   214      17.561  45.141 114.346  1.00 24.19      AAGL
ATOM   1684  C   TYR   214      14.013  40.386 112.534  1.00 18.48      AAGL
ATOM   1685  O   TYR   214      14.361  40.488 111.358  1.00 18.33      AAGL
ATOM   1686  N   TYR   215      12.990  41.048 113.067  1.00 18.28      AAGL
ATOM   1687  CA  TYR   215      12.171  41.979 112.311  1.00 16.96      AAGL
ATOM   1688  CB  TYR   215      10.717  41.506 112.321  1.00 16.58      AAGL
ATOM   1689  CG  TYR   215      10.497  40.277 111.465  1.00 16.72      AAGL
ATOM   1690  CD1 TYR   215      10.456  40.377 110.075  1.00 19.62      AAGL
ATOM   1691  CE1 TYR   215      10.264  39.252 109.274  1.00 18.54      AAGL
ATOM   1692  CD2 TYR   215      10.346  39.013 112.038  1.00 16.88      AAGL
ATOM   1693  CE2 TYR   215      10.156  37.875 111.245  1.00 17.19      AAGL
ATOM   1694  CZ  TYR   215      10.111  38.007 109.862  1.00 16.90      AAGL
ATOM   1695  OH  TYR   215       9.868  36.910 109.064  1.00 17.46      AAGL
ATOM   1696  C   TYR   215      12.297  43.374 112.920  1.00 19.56      AAGL
ATOM   1697  O   TYR   215      12.487  43.523 114.124  1.00 19.95      AAGL
ATOM   1698  N   PRO   216      12.184  44.418 112.087  1.00 20.63      AAGL
ATOM   1699  CD  PRO   216      12.160  44.396 110.613  1.00 20.25      AAGL
ATOM   1700  CA  PRO   216      12.308  45.788 112.589  1.00 20.50      AAGL
ATOM   1701  CB  PRO   216      13.033  46.476 111.450  1.00 22.26      AAGL
ATOM   1702  CG  PRO   216      12.318  45.881 110.243  1.00 20.29      AAGL
ATOM   1703  C   PRO   216      11.005  46.503 112.922  1.00 21.80      AAGL
ATOM   1704  O   PRO   216      11.021  47.552 113.569  1.00 23.06      AAGL
ATOM   1705  N   PHE   217       9.885  45.934 112.495  1.00 20.15      AAGL
ATOM   1706  CA  PHE   217       8.599  46.580 112.682  1.00 19.12      AAGL
ATOM   1707  CB  PHE   217       7.940  46.729 111.308  1.00 21.27      AAGL
ATOM   1708  CG  PHE   217       8.166  45.548 110.390  1.00 22.97      AAGL
ATOM   1709  CD1 PHE   217       7.783  44.263 110.773  1.00 22.42      AAGL
ATOM   1710  CD2 PHE   217       8.733  45.730 109.129  1.00 24.02      AAGL
ATOM   1711  CE1 PHE   217       7.953  43.177 109.912  1.00 22.58      AAGL
ATOM   1712  CE2 PHE   217       8.910  44.651 108.260  1.00 22.45      AAGL
ATOM   1713  CZ  PHE   217       8.518  43.372 108.652  1.00 22.51      AAGL
ATOM   1714  C   PHE   217       7.586  46.016 113.671  1.00 20.44      AAGL
ATOM   1715  O   PHE   217       6.391  46.271 113.523  1.00 21.67      AAGL
ATOM   1716  N   TYR   218       8.040  45.270 114.676  1.00 22.47      AAGL
ATOM   1717  CA  TYR   218       7.130  44.715 115.688  1.00 23.80      AAGL
ATOM   1718  CB  TYR   218       7.155  43.177 115.681  1.00 24.44      AAGL
ATOM   1719  CG  TYR   218       6.583  42.525 114.439  1.00 21.12      AAGL
ATOM   1720  CD1 TYR   218       5.331  42.891 113.952  1.00 22.80      AAGL
ATOM   1721  CE1 TYR   218       4.789  42.281 112.815  1.00 25.22      AAGL
ATOM   1722  CD2 TYR   218       7.286  41.528 113.763  1.00 23.62      AAGL
ATOM   1723  CE2 TYR   218       6.753  40.910 112.625  1.00 23.28      AAGL
ATOM   1724  CZ  TYR   218       5.504  41.294 112.159  1.00 24.22      AAGL
ATOM   1725  OH  TYR   218       4.970  40.698 111.038  1.00 24.13      AAGL
ATOM   1726  C   TYR   218       7.493  45.201 117.089  1.00 26.28      AAGL
ATOM   1727  O   TYR   218       6.956  44.707 118.087  1.00 28.68      AAGL
ATOM   1728  N   SER   219       8.407  46.163 117.165  1.00 27.77      AAGL
ATOM   1729  CA  SER   219       8.854  46.712 118.447  1.00 28.32      AAGL
ATOM   1730  CB  SER   219       9.124  45.592 119.457  1.00 29.25      AAGL
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Fig. 3 cont.

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ATOM   1731  OG  SER   219       9.908  46.078 120.538  1.00 31.84      AAGL
ATOM   1732  C   SER   219      10.119  47.549 118.303  1.00 28.53      AAGL
ATOM   1733  O   SER   219      11.107  47.110 117.716  1.00 26.20      AAGL
ATOM   1734  N   ALA   220      10.090  48.750 118.870  1.00 29.00      AAGL
ATOM   1735  CA  ALA   220      11.235  49.647 118.816  1.00 28.92      AAGL
ATOM   1736  CB  ALA   220      10.851  51.003 119.371  1.00 28.98      AAGL
ATOM   1737  C   ALA   220      12.440  49.104 119.572  1.00 29.06      AAGL
ATOM   1738  O   ALA   220      13.520  49.683 119.507  1.00 30.49      AAGL
ATOM   1739  N   SER   221      12.260  48.003 120.293  1.00 29.58      AAGL
ATOM   1740  CA  SER   221      13.358  47.404 121.046  1.00 29.31      AAGL
ATOM   1741  CB  SER   221      12.815  46.522 122.169  1.00 29.65      AAGL
ATOM   1742  OG  SER   221      12.148  47.295 123.152  1.00 33.54      AAGL
ATOM   1743  C   SER   221      14.278  46.565 120.160  1.00 27.63      AAGL
ATOM   1744  O   SER   221      15.375  46.201 120.570  1.00 27.79      AAGL
ATOM   1745  N   ALA   222      13.828  46.264 118.948  1.00 26.73      AAGL
ATOM   1746  CA  ALA   222      14.598  45.445 118.017  1.00 25.72      AAGL
ATOM   1747  CB  ALA   222      13.662  44.864 116.953  1.00 24.78      AAGL
ATOM   1748  C   ALA   222      15.764  46.187 117.347  1.00 26.39      AAGL
ATOM   1749  O   ALA   222      15.889  46.189 116.117  1.00 24.72      AAGL
ATOM   1750  N   THR   223      16.619  46.809 118.157  1.00 25.12      AAGL
ATOM   1751  CA  THR   223      17.771  47.536 117.632  1.00 26.47      AAGL
ATOM   1752  CB  THR   223      18.360  48.498 118.678  1.00 26.69      AAGL
ATOM   1753  OG1 THR   223      18.793  47.749 119.822  1.00 28.21      AAGL
ATOM   1754  CG2 THR   223      17.321  49.520 119.104  1.00 25.83      AAGL
ATOM   1755  C   THR   223      18.877  46.573 117.223  1.00 25.83      AAGL
ATOM   1756  O   THR   223      18.982  45.465 117.751  1.00 28.38      AAGL
ATOM   1757  N   LEU   224      19.703  47.000 116.278  1.00 26.34      AAGL
ATOM   1758  CA  LEU   224      20.807  46.177 115.817  1.00 27.64      AAGL
ATOM   1759  CB  LEU   224      21.516  46.857 114.647  1.00 30.65      AAGL
ATOM   1760  CG  LEU   224      20.769  46.842 113.311  1.00 31.90      AAGL
ATOM   1761  CD1 LEU   224      21.565  47.603 112.257  1.00 32.52      AAGL
ATOM   1762  CD2 LEU   224      20.558  45.406 112.873  1.00 32.19      AAGL
ATOM   1763  C   LEU   224      21.781  45.958 116.967  1.00 28.76      AAGL
ATOM   1764  O   LEU   224      22.495  44.956 117.011  1.00 30.90      AAGL
ATOM   1765  N   ALA   225      21.796  46.902 117.903  1.00 29.40      AAGL
ATOM   1766  CA  ALA   225      22.663  46.833 119.070  1.00 29.81      AAGL
ATOM   1767  CB  ALA   225      22.632  48.163 119.812  1.00 31.20      AAGL
ATOM   1768  C   ALA   225      22.252  45.701 120.013  1.00 30.35      AAGL
ATOM   1769  O   ALA   225      23.105  45.003 120.560  1.00 29.58      AAGL
ATOM   1770  N   SER   226      20.948  45.526 120.215  1.00 30.66      AAGL
ATOM   1771  CA  SER   226      20.472  44.454 121.090  1.00 30.00      AAGL
ATOM   1772  CB  SER   226      18.995  44.642 121.423  1.00 30.27      AAGL
ATOM   1773  OG  SER   226      18.851  45.426 122.592  1.00 34.03      AAGL
ATOM   1774  C   SER   226      20.685  43.096 120.437  1.00 27.61      AAGL
ATOM   1775  O   SER   226      21.003  42.114 121.113  1.00 27.38      AAGL
ATOM   1776  N   LEU   227      20.510  43.053 119.119  1.00 26.75      AAGL
ATOM   1777  CA  LEU   227      20.691  41.828 118.359  1.00 27.51      AAGL
ATOM   1778  CB  LEU   227      20.337  42.060 116.884  1.00 25.07      AAGL
ATOM   1779  CG  LEU   227      20.555  40.857 115.967  1.00 24.78      AAGL
ATOM   1780  CD1 LEU   227      19.578  39.755 116.340  1.00 24.45      AAGL
ATOM   1781  CD2 LEU   227      20.374  41.268 114.514  1.00 23.51      AAGL
ATOM   1782  C   LEU   227      22.148  41.407 118.465  1.00 28.41      AAGL
ATOM   1783  O   LEU   227      22.456  40.253 118.726  1.00 28.87      AAGL
ATOM   1784  N   LYS   228      23.037  42.372 118.256  1.00 30.45      AAGL
ATOM   1785  CA  LYS   228      24.474  42.132 118.316  1.00 31.96      AAGL
ATOM   1786  CB  LYS   228      25.201  43.469 118.150  1.00 36.24      AAGL
ATOM   1787  CG  LYS   228      26.700  43.390 117.906  1.00 41.65      AAGL
ATOM   1788  CD  LYS   228      27.242  44.757 117.477  1.00 43.74      AAGL
ATOM   1789  CE  LYS   228      26.876  45.827 118.489  1.00 46.64      AAGL
ATOM   1790  NZ  LYS   228      27.322  47.191 118.075  1.00 47.80      AAGL
ATOM   1791  C   LYS   228      24.820  41.485 119.653  1.00 30.16      AAGL
ATOM   1792  O   LYS   228      25.538  40.484 119.710  1.00 31.36      AAGL
ATOM   1793  N   THR   229      24.299  42.056 120.732  1.00 29.71      AAGL
ATOM   1794  CA  THR   229      24.553  41.532 122.063  1.00 30.66      AAGL
ATOM   1795  CB  THR   229      23.981  42.452 123.142  1.00 31.91      AAGL
ATOM   1796  OG1 THR   229      24.783  43.637 123.232  1.00 35.38      AAGL
ATOM   1797  CG2 THR   229      23.978  41.748 124.483  1.00 34.76      AAGL
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Fig. 3 cont.

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ATOM   1798  C   THR   229      23.973  40.145 122.282  1.00 30.52      AAGL
ATOM   1799  O   THR   229      24.615  39.290 122.883  1.00 30.20      AAGL
ATOM   1800  N   SER   230      22.753  39.932 121.795  1.00 29.88      AAGL
ATOM   1801  CA  SER   230      22.077  38.646 121.948  1.00 27.75      AAGL
ATOM   1802  CB  SER   230      20.626  38.766 121.470  1.00 27.43      AAGL
ATOM   1803  OG  SER   230      19.947  37.532 121.612  1.00 28.20      AAGL
ATOM   1804  C   SER   230      22.790  37.534 121.178  1.00 27.11      AAGL
ATOM   1805  O   SER   230      22.994  36.436 121.698  1.00 27.65      AAGL
ATOM   1806  N   LEU   231      23.157  37.814 119.935  1.00 27.30      AAGL
ATOM   1807  CA  LEU   231      23.859  36.829 119.122  1.00 28.25      AAGL
ATOM   1808  CB  LEU   231      24.037  37.341 117.687  1.00 28.04      AAGL
ATOM   1809  CG  LEU   231      22.767  37.430 116.832  1.00 28.82      AAGL
ATOM   1810  CD1 LEU   231      23.091  38.027 115.468  1.00 29.62      AAGL
ATOM   1811  CD2 LEU   231      22.171  36.034 116.670  1.00 25.68      AAGL
ATOM   1812  C   LEU   231      25.228  36.541 119.733  1.00 29.07      AAGL
ATOM   1813  O   LEU   231      25.685  35.399 119.743  1.00 27.21      AAGL
ATOM   1814  N   ALA   232      25.874  37.585 120.244  1.00 30.00      AAGL
ATOM   1815  CA  ALA   232      27.198  37.449 120.849  1.00 31.64      AAGL
ATOM   1816  CB  ALA   232      27.733  38.828 121.257  1.00 30.69      AAGL
ATOM   1817  C   ALA   232      27.142  36.535 122.063  1.00 31.96      AAGL
ATOM   1818  O   ALA   232      27.980  35.645 122.229  1.00 32.99      AAGL
ATOM   1819  N   ASN   233      26.146  36.757 122.913  1.00 31.75      AAGL
ATOM   1820  CA  ASN   233      25.989  35.960 124.118  1.00 33.65      AAGL
ATOM   1821  CB  ASN   233      25.010  36.646 125.071  1.00 33.95      AAGL
ATOM   1822  CG  ASN   233      25.507  38.010 125.528  1.00 37.26      AAGL
ATOM   1823  OD1 ASN   233      26.712  38.267 125.547  1.00 37.11      AAGL
ATOM   1824  ND2 ASN   233      24.582  38.884 125.912  1.00 37.35      AAGL
ATOM   1825  C   ASN   233      25.558  34.513 123.866  1.00 33.38      AAGL
ATOM   1826  O   ASN   233      25.932  33.616 124.621  1.00 34.08      AAGL
ATOM   1827  N   LEU   234      24.780  34.280 122.812  1.00 32.11      AAGL
ATOM   1828  CA  LEU   234      24.331  32.927 122.498  1.00 31.75      AAGL
ATOM   1829  CB  LEU   234      23.387  32.935 121.286  1.00 29.34      AAGL
ATOM   1830  CG  LEU   234      21.875  33.038 121.527  1.00 28.94      AAGL
ATOM   1831  CD1 LEU   234      21.151  33.301 120.209  1.00 28.45      AAGL
ATOM   1832  CD2 LEU   234      21.373  31.739 122.157  1.00 29.20      AAGL
ATOM   1833  C   LEU   234      25.529  32.036 122.200  1.00 31.64      AAGL
ATOM   1834  O   LEU   234      25.651  30.937 122.737  1.00 31.64      AAGL
ATOM   1835  N   GLN   235      26.413  32.530 121.340  1.00 31.31      AAGL
ATOM   1836  CA  GLN   235      27.601  31.797 120.944  1.00 34.83      AAGL
ATOM   1837  CB  GLN   235      28.302  32.560 119.810  1.00 34.48      AAGL
ATOM   1838  CG  GLN   235      29.283  31.756 118.991  1.00 36.34      AAGL
ATOM   1839  CD  GLN   235      30.545  31.410 119.747  1.00 38.22      AAGL
ATOM   1840  OE1 GLN   235      31.065  32.224 120.511  1.00 38.29      AAGL
ATOM   1841  NE2 GLN   235      31.059  30.204 119.521  1.00 38.94      AAGL
ATOM   1842  C   GLN   235      28.557  31.597 122.122  1.00 35.64      AAGL
ATOM   1843  O   GLN   235      29.063  30.500 122.335  1.00 34.97      AAGL
ATOM   1844  N   SER   236      28.776  32.659 122.894  1.00 36.91      AAGL
ATOM   1845  CA  SER   236      29.694  32.626 124.034  1.00 39.04      AAGL
ATOM   1846  CB  SER   236      29.942  34.056 124.552  1.00 39.04      AAGL
ATOM   1847  OG  SER   236      28.764  34.620 125.122  1.00 40.94      AAGL
ATOM   1848  C   SER   236      29.221  31.750 125.191  1.00 39.31      AAGL
ATOM   1849  O   SER   236      30.027  31.118 125.885  1.00 40.12      AAGL
ATOM   1850  N   THR   237      27.913  31.703 125.394  1.00 38.31      AAGL
ATOM   1851  CA  THR   237      27.353  30.930 126.489  1.00 37.56      AAGL
ATOM   1852  CB  THR   237      26.002  31.514 126.918  1.00 36.05      AAGL
ATOM   1853  OG1 THR   237      26.183  32.883 127.291  1.00 35.25      AAGL
ATOM   1854  CG2 THR   237      25.432  30.738 128.101  1.00 36.50      AAGL
ATOM   1855  C   THR   237      27.169  29.459 126.181  1.00 36.88      AAGL
ATOM   1856  O   THR   237      27.503  28.606 127.003  1.00 37.95      AAGL
ATOM   1857  N   TYR   238      26.653  29.158 124.992  1.00 35.86      AAGL
ATOM   1858  CA  TYR   238      26.391  27.777 124.594  1.00 34.18      AAGL
ATOM   1859  CB  TYR   238      24.955  27.684 124.059  1.00 33.21      AAGL
ATOM   1860  CG  TYR   238      23.924  28.178 125.056  1.00 32.37      AAGL
ATOM   1861  CD1 TYR   238      23.513  27.376 126.125  1.00 31.26      AAGL
ATOM   1862  CE1 TYR   238      22.630  27.860 127.093  1.00 32.64      AAGL
ATOM   1863  CD2 TYR   238      23.416  29.473 124.976  1.00 31.04      AAGL
ATOM   1864  CE2 TYR   238      22.531  29.961 125.935  1.00 32.31      AAGL
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Fig. 3 cont.

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ATOM   1865  CZ  TYR  238      22.146  29.150 126.992  1.00 32.31      AAGL
ATOM   1866  OH  TYR  238      21.291  29.646 127.951  1.00 34.51      AAGL
ATOM   1867  C   TYR  238      27.377  27.210 123.570  1.00 34.17      AAGL
ATOM   1868  O   TYR  238      27.327  26.023 123.245  1.00 32.44      AAGL
ATOM   1869  N   ASP  239      28.263  28.060 123.060  1.00 34.59      AAGL
ATOM   1870  CA  ASP  239      29.267  27.645 122.080  1.00 35.46      AAGL
ATOM   1871  CB  ASP  239      30.292  26.716 122.754  1.00 38.30      AAGL
ATOM   1872  CG  ASP  239      31.412  26.290 121.819  1.00 39.89      AAGL
ATOM   1873  OD1 ASP  239      31.811  27.088 120.939  1.00 40.54      AAGL
ATOM   1874  OD2 ASP  239      31.911  25.155 121.975  1.00 41.25      AAGL
ATOM   1875  C   ASP  239      28.688  26.982 120.829  1.00 34.34      AAGL
ATOM   1876  O   ASP  239      29.098  25.885 120.451  1.00 34.85      AAGL
ATOM   1877  N   LYS  240      27.735  27.656 120.190  1.00 32.57      AAGL
ATOM   1878  CA  LYS  240      27.121  27.155 118.963  1.00 31.63      AAGL
ATOM   1879  CB  LYS  240      25.746  26.525 119.234  1.00 30.18      AAGL
ATOM   1880  CG  LYS  240      25.764  25.264 120.104  1.00 33.39      AAGL
ATOM   1881  CD  LYS  240      24.367  24.648 120.218  1.00 31.95      AAGL
ATOM   1882  CE  LYS  240      24.318  23.502 121.247  1.00 32.26      AAGL
ATOM   1883  NZ  LYS  240      25.241  22.379 120.930  1.00 29.98      AAGL
ATOM   1884  C   LYS  240      26.953  28.315 117.990  1.00 29.66      AAGL
ATOM   1885  O   LYS  240      26.779  29.460 118.400  1.00 30.38      AAGL
ATOM   1886  N   PRO  241      27.010  28.036 116.679  1.00 29.06      AAGL
ATOM   1887  CD  PRO  241      27.422  26.781 116.028  1.00 29.36      AAGL
ATOM   1888  CA  PRO  241      26.850  29.106 115.691  1.00 27.35      AAGL
ATOM   1889  CB  PRO  241      27.136  28.403 114.371  1.00 27.28      AAGL
ATOM   1890  CG  PRO  241      28.058  27.285 114.768  1.00 29.28      AAGL
ATOM   1891  C   PRO  241      25.434  29.693 115.732  1.00 28.09      AAGL
ATOM   1892  O   PRO  241      24.491  29.048 116.201  1.00 27.43      AAGL
ATOM   1893  N   VAL  242      25.294  30.911 115.225  1.00 27.44      AAGL
ATOM   1894  CA  VAL  242      24.005  31.588 115.192  1.00 27.37      AAGL
ATOM   1895  CB  VAL  242      24.047  32.871 116.015  1.00 24.62      AAGL
ATOM   1896  CG1 VAL  242      24.156  32.531 117.479  1.00 27.77      AAGL
ATOM   1897  CG2 VAL  242      25.242  33.719 115.588  1.00 27.66      AAGL
ATOM   1898  C   VAL  242      23.614  31.929 113.763  1.00 26.08      AAGL
ATOM   1899  O   VAL  242      24.468  32.140 112.903  1.00 27.26      AAGL
ATOM   1900  N   VAL  243      22.313  31.990 113.512  1.00 25.38      AAGL
ATOM   1901  CA  VAL  243      21.806  32.287 112.179  1.00 22.94      AAGL
ATOM   1902  CB  VAL  243      21.431  30.973 111.419  1.00 24.38      AAGL
ATOM   1903  CG1 VAL  243      20.994  31.285 109.996  1.00 23.02      AAGL
ATOM   1904  CG2 VAL  243      22.612  30.009 111.409  1.00 25.53      AAGL
ATOM   1905  C   VAL  243      20.541  33.129 112.289  1.00 22.55      AAGL
ATOM   1906  O   VAL  243      19.691  32.836 113.115  1.00 21.01      AAGL
ATOM   1907  N   VAL  244      20.432  34.188 111.487  1.00 21.40      AAGL
ATOM   1908  CA  VAL  244      19.213  34.995 111.483  1.00 21.25      AAGL
ATOM   1909  CB  VAL  244      19.469  36.463 111.094  1.00 21.49      AAGL
ATOM   1910  CG1 VAL  244      18.139  37.170 110.884  1.00 22.74      AAGL
ATOM   1911  CG2 VAL  244      20.263  37.163 112.188  1.00 20.20      AAGL
ATOM   1912  C   VAL  244      18.414  34.309 110.387  1.00 19.60      AAGL
ATOM   1913  O   VAL  244      18.720  34.446 109.205  1.00 20.42      AAGL
ATOM   1914  N   VAL  245      17.395  33.557 110.780  1.00 17.97      AAGL
ATOM   1915  CA  VAL  245      16.635  32.788 109.807  1.00 17.90      AAGL
ATOM   1916  CB  VAL  245      16.234  31.431 110.413  1.00 18.93      AAGL
ATOM   1917  CG1 VAL  245      17.485  30.699 110.871  1.00 18.12      AAGL
ATOM   1918  CG2 VAL  245      15.274  31.637 111.578  1.00 17.48      AAGL
ATOM   1919  C   VAL  245      15.415  33.450 109.192  1.00 17.32      AAGL
ATOM   1920  O   VAL  245      14.783  32.882 108.308  1.00 17.57      AAGL
ATOM   1921  N   GLU  246      15.085  34.644 109.666  1.00 17.88      AAGL
ATOM   1922  CA  GLU  246      13.949  35.392 109.143  1.00 18.02      AAGL
ATOM   1923  CB  GLU  246      12.657  35.023 109.875  1.00 22.04      AAGL
ATOM   1924  CG  GLU  246      11.917  33.816 109.352  1.00 22.72      AAGL
ATOM   1925  CD  GLU  246      10.611  33.589 110.102  1.00 24.03      AAGL
ATOM   1926  OE1 GLU  246       9.882  34.579 110.340  1.00 20.71      AAGL
ATOM   1927  OE2 GLU  246      10.311  32.422 110.438  1.00 22.70      AAGL
ATOM   1928  C   GLU  246      14.163  36.882 109.327  1.00 18.20      AAGL
ATOM   1929  O   GLU  246      14.547  37.316 110.404  1.00 19.12      AAGL
ATOM   1930  N   THR  247      13.912  37.658 108.281  1.00 17.83      AAGL
ATOM   1931  CA  THR  247      14.024  39.114 108.372  1.00 19.34      AAGL
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Fig. 3 cont.

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ATOM   1932  CB  THR   247      15.505  39.584 108.487  1.00 21.29      AAGL
ATOM   1933  OG1 THR   247      15.532  40.968 108.857  1.00 22.65      AAGL
ATOM   1934  CG2 THR   247      16.238  39.409 107.172  1.00 20.07      AAGL
ATOM   1935  C   THR   247      13.356  39.774 107.167  1.00 18.87      AAGL
ATOM   1936  O   THR   247      13.167  39.141 106.134  1.00 19.64      AAGL
ATOM   1937  N   ASN   248      12.980  41.039 107.326  1.00 17.13      AAGL
ATOM   1938  CA  ASN   248      12.312  41.816 106.281  1.00 18.39      AAGL
ATOM   1939  CB  ASN   248      10.793  41.800 106.466  1.00 19.04      AAGL
ATOM   1940  CG  ASN   248      10.095  40.616 105.836  1.00 20.07      AAGL
ATOM   1941  OD1 ASN   248       8.889  40.475 106.007  1.00 23.76      AAGL
ATOM   1942  ND2 ASN   248      10.820  39.775 105.113  1.00 20.10      AAGL
ATOM   1943  C   ASN   248      12.685  43.291 106.427  1.00 18.69      AAGL
ATOM   1944  O   ASN   248      13.135  43.725 107.483  1.00 17.33      AAGL
ATOM   1945  N   TRP   249      12.466  44.046 105.355  1.00 19.91      AAGL
ATOM   1946  CA  TRP   249      12.630  45.503 105.355  1.00 21.18      AAGL
ATOM   1947  CB  TRP   249      14.065  45.981 105.129  1.00 21.42      AAGL
ATOM   1948  CG  TRP   249      14.117  47.491 105.288  1.00 19.99      AAGL
ATOM   1949  CD2 TRP   249      14.261  48.225 106.517  1.00 19.73      AAGL
ATOM   1950  CE2 TRP   249      14.108  49.599 106.208  1.00 19.65      AAGL
ATOM   1951  CE3 TRP   249      14.499  47.853 107.847  1.00 19.37      AAGL
ATOM   1952  CD1 TRP   249      13.895  48.431 104.313  1.00 20.84      AAGL
ATOM   1953  NE1 TRP   249      13.887  49.693 104.861  1.00 19.99      AAGL
ATOM   1954  CZ2 TRP   249      14.185  50.604 107.187  1.00 20.08      AAGL
ATOM   1955  CZ3 TRP   249      14.575  48.853 108.820  1.00 21.35      AAGL
ATOM   1956  CH2 TRP   249      14.418  50.214 108.481  1.00 21.66      AAGL
ATOM   1957  C   TRP   249      11.722  46.003 104.241  1.00 20.70      AAGL
ATOM   1958  O   TRP   249      11.800  45.539 103.102  1.00 22.36      AAGL
ATOM   1959  N   PRO   250      10.838  46.957 104.559  1.00 22.00      AAGL
ATOM   1960  CD  PRO   250      10.686  47.625 105.865  1.00 21.04      AAGL
ATOM   1961  CA  PRO   250       9.894  47.508 103.587  1.00 21.27      AAGL
ATOM   1962  CB  PRO   250       8.876  48.210 104.477  1.00 22.31      AAGL
ATOM   1963  CG  PRO   250       9.744  48.783 105.538  1.00 22.64      AAGL
ATOM   1964  C   PRO   250      10.402  48.435 102.507  1.00 23.33      AAGL
ATOM   1965  O   PRO   250      11.270  49.268 102.743  1.00 21.79      AAGL
ATOM   1966  N   VAL   251       9.844  48.282 101.311  1.00 23.27      AAGL
ATOM   1967  CA  VAL   251      10.185  49.165 100.212  1.00 24.85      AAGL
ATOM   1968  CB  VAL   251      10.171  48.437  98.854  1.00 24.44      AAGL
ATOM   1969  CG1 VAL   251      11.335  47.476  98.787  1.00 24.31      AAGL
ATOM   1970  CG2 VAL   251       8.865  47.699  98.657  1.00 28.76      AAGL
ATOM   1971  C   VAL   251       9.095  50.227 100.278  1.00 26.42      AAGL
ATOM   1972  O   VAL   251       9.177  51.281  99.646  1.00 24.68      AAGL
ATOM   1973  N   SER   252       8.075  49.934 101.083  1.00 27.57      AAGL
ATOM   1974  CA  SER   252       6.962  50.851 101.298  1.00 27.22      AAGL
ATOM   1975  CB  SER   252       5.942  50.722 100.164  1.00 28.72      AAGL
ATOM   1976  OG  SER   252       4.895  51.662 100.327  1.00 28.82      AAGL
ATOM   1977  C   SER   252       6.289  50.558 102.642  1.00 28.31      AAGL
ATOM   1978  O   SER   252       5.858  49.434 102.886  1.00 26.39      AAGL
ATOM   1979  N   CYS   253       6.232  51.559 103.518  1.00 27.82      AAGL
ATOM   1980  CA  CYS   253       5.594  51.413 104.824  1.00 27.19      AAGL
ATOM   1981  C   CYS   253       4.932  52.738 105.201  1.00 28.86      AAGL
ATOM   1982  O   CYS   253       5.411  53.436 106.091  1.00 27.40      AAGL
ATOM   1983  CB  CYS   253       6.611  51.031 105.913  1.00 27.78      AAGL
ATOM   1984  SG  CYS   253       5.803  50.369 107.406  1.00 28.15      AAGL
ATOM   1985  N   PRO   254       3.812  53.089 104.528  1.00 30.47      AAGL
ATOM   1986  CD  PRO   254       3.166  52.222 103.525  1.00 30.66      AAGL
ATOM   1987  CA  PRO   254       3.022  54.314 104.725  1.00 32.44      AAGL
ATOM   1988  CB  PRO   254       1.739  54.023 103.951  1.00 32.43      AAGL
ATOM   1989  CG  PRO   254       2.206  53.171 102.837  1.00 33.11      AAGL
ATOM   1990  C   PRO   254       2.739  54.660 106.181  1.00 34.76      AAGL
ATOM   1991  O   PRO   254       2.780  55.828 106.570  1.00 35.87      AAGL
ATOM   1992  N   ASN   255       2.429  53.653 106.987  1.00 35.37      AAGL
ATOM   1993  CA  ASN   255       2.161  53.912 108.392  1.00 36.89      AAGL
ATOM   1994  CB  ASN   255       0.755  54.457 108.575  1.00 37.41      AAGL
ATOM   1995  CG  ASN   255       0.410  54.682 110.030  1.00 38.46      AAGL
ATOM   1996  OD1 ASN   255       1.254  55.124 110.832  1.00 35.39      AAGL
ATOM   1997  ND2 ASN   255      -0.833  54.389 110.387  1.00 34.81      AAGL
ATOM   1998  C   ASN   255       2.354  52.691 109.263  1.00 35.87      AAGL
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Fig. 3 cont.

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ATOM   1999  O   ASN  255       1.471  51.841 109.375  1.00 36.70      AAGL
ATOM   2000  N   PRO  256       3.520  52.601 109.910  1.00 35.76      AAGL
ATOM   2001  CD  PRO  256       4.640  53.550 109.780  1.00 35.85      AAGL
ATOM   2002  CA  PRO  256       3.878  51.493 110.791  1.00 34.93      AAGL
ATOM   2003  CB  PRO  256       5.387  51.654 110.927  1.00 35.60      AAGL
ATOM   2004  CG  PRO  256       5.558  53.122 110.901  1.00 36.37      AAGL
ATOM   2005  C   PRO  256       3.158  51.543 112.140  1.00 34.50      AAGL
ATOM   2006  O   PRO  256       3.041  52.604 112.752  1.00 33.71      AAGL
ATOM   2007  N   ALA  257       2.683  50.393 112.603  1.00 32.93      AAGL
ATOM   2008  CA  ALA  257       1.988  50.327 113.880  1.00 31.85      AAGL
ATOM   2009  CB  ALA  257       1.371  48.946 114.079  1.00 31.01      AAGL
ATOM   2010  C   ALA  257       2.970  50.621 115.000  1.00 32.12      AAGL
ATOM   2011  O   ALA  257       2.591  51.139 116.046  1.00 31.82      AAGL
ATOM   2012  N   TYR  258       4.237  50.291 114.771  1.00 31.15      AAGL
ATOM   2013  CA  TYR  258       5.279  50.504 115.761  1.00 32.72      AAGL
ATOM   2014  CB  TYR  258       5.892  49.168 116.169  1.00 35.88      AAGL
ATOM   2015  CG  TYR  258       4.954  48.226 116.880  1.00 38.05      AAGL
ATOM   2016  CD1 TYR  258       4.136  47.341 116.170  1.00 37.62      AAGL
ATOM   2017  CE1 TYR  258       3.276  46.468 116.840  1.00 40.53      AAGL
ATOM   2018  CD2 TYR  258       4.889  48.216 118.267  1.00 39.82      AAGL
ATOM   2019  CE2 TYR  258       4.039  47.357 118.943  1.00 41.64      AAGL
ATOM   2020  CZ  TYR  258       3.236  46.489 118.232  1.00 42.48      AAGL
ATOM   2021  OH  TYR  258       2.386  45.659 118.934  1.00 45.83      AAGL
ATOM   2022  C   TYR  258       6.414  51.411 115.293  1.00 32.44      AAGL
ATOM   2023  O   TYR  258       6.736  51.468 114.108  1.00 31.27      AAGL
ATOM   2024  N   ALA  259       7.021  52.121 116.237  1.00 30.79      AAGL
ATOM   2025  CA  ALA  259       8.147  52.983 115.919  1.00 31.35      AAGL
ATOM   2026  CB  ALA  259       8.479  53.864 117.118  1.00 33.39      AAGL
ATOM   2027  C   ALA  259       9.315  52.046 115.607  1.00 29.93      AAGL
ATOM   2028  O   ALA  259       9.458  51.004 116.242  1.00 29.16      AAGL
ATOM   2029  N   PHE  260      10.137  52.392 114.623  1.00 29.81      AAGL
ATOM   2030  CA  PHE  260      11.281  51.548 114.285  1.00 29.03      AAGL
ATOM   2031  CB  PHE  260      11.772  51.871 112.867  1.00 28.71      AAGL
ATOM   2032  CG  PHE  260      11.007  51.157 111.776  1.00 29.00      AAGL
ATOM   2033  CD1 PHE  260       9.622  51.242 111.704  1.00 29.61      AAGL
ATOM   2034  CD2 PHE  260      11.676  50.379 110.840  1.00 28.02      AAGL
ATOM   2035  CE1 PHE  260       8.915  50.558 110.720  1.00 30.59      AAGL
ATOM   2036  CE2 PHE  260      10.979  49.694 109.854  1.00 29.46      AAGL
ATOM   2037  CZ  PHE  260       9.594  49.783 109.796  1.00 29.30      AAGL
ATOM   2038  C   PHE  260      12.409  51.765 115.300  1.00 29.23      AAGL
ATOM   2039  O   PHE  260      12.464  52.806 115.957  1.00 29.38      AAGL
ATOM   2040  N   PRO  261      13.302  50.771 115.466  1.00 29.34      AAGL
ATOM   2041  CD  PRO  261      13.247  49.414 114.891  1.00 29.47      AAGL
ATOM   2042  CA  PRO  261      14.418  50.891 116.409  1.00 29.63      AAGL
ATOM   2043  CB  PRO  261      15.194  49.599 116.186  1.00 28.18      AAGL
ATOM   2044  CG  PRO  261      14.096  48.617 115.852  1.00 28.51      AAGL
ATOM   2045  C   PRO  261      15.240  52.137 116.063  1.00 29.95      AAGL
ATOM   2046  O   PRO  261      15.312  52.539 114.897  1.00 30.37      AAGL
ATOM   2047  N   SER  262      15.846  52.736 117.082  1.00 32.41      AAGL
ATOM   2048  CA  SER  262      16.637  53.951 116.922  1.00 31.88      AAGL
ATOM   2049  CB  SER  262      17.167  54.396 118.291  1.00 33.67      AAGL
ATOM   2050  OG  SER  262      17.708  53.295 119.003  1.00 37.49      AAGL
ATOM   2051  C   SER  262      17.785  53.858 115.918  1.00 32.30      AAGL
ATOM   2052  O   SER  262      17.967  54.773 115.107  1.00 32.95      AAGL
ATOM   2053  N   ASP  263      18.565  52.778 115.955  1.00 31.17      AAGL
ATOM   2054  CA  ASP  263      19.660  52.663 115.000  1.00 31.60      AAGL
ATOM   2055  CB  ASP  263      20.768  51.724 115.512  1.00 31.48      AAGL
ATOM   2056  CG  ASP  263      20.241  50.418 116.090  1.00 31.74      AAGL
ATOM   2057  OD1 ASP  263      19.111  49.994 115.748  1.00 30.33      AAGL
ATOM   2058  OD2 ASP  263      20.987  49.796 116.887  1.00 30.41      AAGL
ATOM   2059  C   ASP  263      19.210  52.227 113.604  1.00 31.45      AAGL
ATOM   2060  O   ASP  263      20.036  51.858 112.768  1.00 32.04      AAGL
ATOM   2061  N   LEU  264      17.905  52.296 113.344  1.00 30.59      AAGL
ATOM   2062  CA  LEU  264      17.363  51.920 112.038  1.00 28.75      AAGL
ATOM   2063  CB  LEU  264      16.621  50.575 112.123  1.00 27.83      AAGL
ATOM   2064  CG  LEU  264      17.375  49.323 112.570  1.00 24.26      AAGL
ATOM   2065  CD1 LEU  264      16.389  48.179 112.752  1.00 25.96      AAGL
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Fig. 3 cont.

ATOM	2066	CD2	LEU	264	18.429	48.955	111.552	1.00 27.53	AAGL
ATOM	2067	C	LEU	264	16.391	52.971	111.512	1.00 28.95	AAGL
ATOM	2068	O	LEU	264	15.941	52.893	110.374	1.00 27.43	AAGL
ATOM	2069	N	SER	265	16.074	53.965	112.331	1.00 30.75	AAGL
ATOM	2070	CA	SER	265	15.120	54.986	111.925	1.00 32.24	AAGL
ATOM	2071	CB	SER	265	14.662	55.779	113.154	1.00 33.67	AAGL
ATOM	2072	OG	SER	265	15.763	56.287	113.892	1.00 34.70	AAGL
ATOM	2073	C	SER	265	15.572	55.941	110.815	1.00 33.25	AAGL
ATOM	2074	O	SER	265	14.776	56.742	110.328	1.00 34.94	AAGL
ATOM	2075	N	SER	266	16.832	55.859	110.399	1.00 33.96	AAGL
ATOM	2076	CA	SER	266	17.305	56.745	109.339	1.00 33.28	AAGL
ATOM	2077	CB	SER	266	18.765	57.133	109.576	1.00 34.74	AAGL
ATOM	2078	OG	SER	266	19.652	56.107	109.142	1.00 40.32	AAGL
ATOM	2079	C	SER	266	17.176	56.085	107.964	1.00 31.87	AAGL
ATOM	2080	O	SER	266	17.236	56.754	106.931	1.00 30.82	AAGL
ATOM	2081	N	ILE	267	16.982	54.773	107.956	1.00 28.10	AAGL
ATOM	2082	CA	ILE	267	16.874	54.025	106.713	1.00 26.55	AAGL
ATOM	2083	CB	ILE	267	17.067	52.523	106.983	1.00 25.69	AAGL
ATOM	2084	CG2	ILE	267	17.120	51.757	105.666	1.00 26.74	AAGL
ATOM	2085	CG1	ILE	267	18.349	52.323	107.801	1.00 28.70	AAGL
ATOM	2086	CD1	ILE	267	18.606	50.889	108.250	1.00 27.91	AAGL
ATOM	2087	C	ILE	267	15.537	54.267	106.024	1.00 25.54	AAGL
ATOM	2088	O	ILE	267	14.482	54.060	106.604	1.00 24.26	AAGL
ATOM	2089	N	PRO	268	15.567	54.734	104.767	1.00 25.09	AAGL
ATOM	2090	CD	PRO	268	16.725	55.097	103.932	1.00 26.35	AAGL
ATOM	2091	CA	PRO	268	14.312	54.986	104.058	1.00 25.07	AAGL
ATOM	2092	CB	PRO	268	14.767	55.792	102.844	1.00 26.89	AAGL
ATOM	2093	CG	PRO	268	16.108	55.205	102.560	1.00 26.87	AAGL
ATOM	2094	C	PRO	268	13.602	53.694	103.662	1.00 24.21	AAGL
ATOM	2095	O	PRO	268	14.208	52.622	103.644	1.00 23.10	AAGL
ATOM	2096	N	PHE	269	12.313	53.806	103.362	1.00 23.20	AAGL
ATOM	2097	CA	PHE	269	11.525	52.664	102.931	1.00 23.46	AAGL
ATOM	2098	CB	PHE	269	10.091	52.765	103.446	1.00 24.32	AAGL
ATOM	2099	CG	PHE	269	9.994	52.861	104.942	1.00 24.64	AAGL
ATOM	2100	CD1	PHE	269	10.819	52.093	105.758	1.00 25.88	AAGL
ATOM	2101	CD2	PHE	269	9.070	53.706	105.535	1.00 25.95	AAGL
ATOM	2102	CE1	PHE	269	10.722	52.168	107.151	1.00 26.08	AAGL
ATOM	2103	CE2	PHE	269	8.965	53.788	106.925	1.00 23.79	AAGL
ATOM	2104	CZ	PHE	269	9.793	53.016	107.732	1.00 23.02	AAGL
ATOM	2105	C	PHE	269	11.548	52.698	101.413	1.00 23.22	AAGL
ATOM	2106	O	PHE	269	10.778	53.420	100.774	1.00 23.95	AAGL
ATOM	2107	N	SER	270	12.462	51.916	100.848	1.00 23.29	AAGL
ATOM	2108	CA	SER	270	12.649	51.848	99.410	1.00 24.41	AAGL
ATOM	2109	CB	SER	270	13.282	53.140	98.924	1.00 24.90	AAGL
ATOM	2110	OG	SER	270	14.547	53.300	99.540	1.00 25.23	AAGL
ATOM	2111	C	SER	270	13.596	50.702	99.125	1.00 22.81	AAGL
ATOM	2112	O	SER	270	14.147	50.105	100.055	1.00 25.01	AAGL
ATOM	2113	N	VAL	271	13.791	50.392	97.845	1.00 23.71	AAGL
ATOM	2114	CA	VAL	271	14.702	49.316	97.477	1.00 22.85	AAGL
ATOM	2115	CB	VAL	271	14.846	49.170	95.948	1.00 24.85	AAGL
ATOM	2116	CG1	VAL	271	15.953	48.172	95.630	1.00 23.46	AAGL
ATOM	2117	CG2	VAL	271	13.534	48.698	95.338	1.00 22.67	AAGL
ATOM	2118	C	VAL	271	16.065	49.649	98.056	1.00 24.60	AAGL
ATOM	2119	O	VAL	271	16.744	48.787	98.613	1.00 24.45	AAGL
ATOM	2120	N	ALA	272	16.453	50.914	97.932	1.00 25.33	AAGL
ATOM	2121	CA	ALA	272	17.740	51.373	98.442	1.00 24.59	AAGL
ATOM	2122	CB	ALA	272	17.946	52.858	98.104	1.00 26.33	AAGL
ATOM	2123	C	ALA	272	17.814	51.162	99.951	1.00 21.83	AAGL
ATOM	2124	O	ALA	272	18.839	50.732	100.479	1.00 21.37	AAGL
ATOM	2125	N	GLY	273	16.722	51.463	100.646	1.00 22.29	AAGL
ATOM	2126	CA	GLY	273	16.710	51.284	102.086	1.00 22.02	AAGL
ATOM	2127	C	GLY	273	16.808	49.814	102.448	1.00 21.98	AAGL
ATOM	2128	O	GLY	273	17.427	49.442	103.443	1.00 22.94	AAGL
ATOM	2129	N	GLN	274	16.192	48.973	101.623	1.00 23.13	AAGL
ATOM	2130	CA	GLN	274	16.210	47.534	101.837	1.00 23.82	AAGL
ATOM	2131	CB	GLN	274	15.354	46.862	100.770	1.00 26.47	AAGL
ATOM	2132	CG	GLN	274	14.976	45.429	101.049	1.00 28.49	AAGL

Fig. 3 cont.

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ATOM   2133  CD  GLN   274      13.969  44.926 100.034  1.00 29.11      AAGL
ATOM   2134  OE1 GLN   274      14.273  44.819  98.846  1.00 26.58      AAGL
ATOM   2135  NE2 GLN   274      12.760  44.630 100.491  1.00 22.87      AAGL
ATOM   2136  C   GLN   274      17.655  47.047 101.741  1.00 24.42      AAGL
ATOM   2137  O   GLN   274      18.090  46.184 102.500  1.00 23.54      AAGL
ATOM   2138  N   GLN   275      18.405  47.621 100.807  1.00 22.92      AAGL
ATOM   2139  CA  GLN   275      19.802  47.240 100.627  1.00 22.23      AAGL
ATOM   2140  CB  GLN   275      20.347  47.863  99.349  1.00 25.17      AAGL
ATOM   2141  CG  GLN   275      19.668  47.370  98.089  1.00 25.16      AAGL
ATOM   2142  CD  GLN   275      20.162  48.099  96.862  1.00 29.65      AAGL
ATOM   2143  OE1 GLN   275      19.879  49.283  96.677  1.00 33.06      AAGL
ATOM   2144  NE2 GLN   275      20.915  47.403  96.021  1.00 30.34      AAGL
ATOM   2145  C   GLN   275      20.658  47.679 101.807  1.00 22.46      AAGL
ATOM   2146  O   GLN   275      21.492  46.924 102.289  1.00 23.14      AAGL
ATOM   2147  N   GLU   276      20.444  48.906 102.268  1.00 23.39      AAGL
ATOM   2148  CA  GLU   276      21.203  49.448 103.386  1.00 22.93      AAGL
ATOM   2149  CB  GLU   276      20.821  50.917 103.615  1.00 26.77      AAGL
ATOM   2150  CG  GLU   276      21.393  51.518 104.891  1.00 31.09      AAGL
ATOM   2151  CD  GLU   276      21.007  52.982 105.081  1.00 33.52      AAGL
ATOM   2152  OE1 GLU   276      19.968  53.402 104.533  1.00 35.95      AAGL
ATOM   2153  OE2 GLU   276      21.734  53.704 105.791  1.00 34.45      AAGL
ATOM   2154  C   GLU   276      20.948  48.620 104.643  1.00 23.86      AAGL
ATOM   2155  O   GLU   276      21.870  48.302 105.385  1.00 22.86      AAGL
ATOM   2156  N   PHE   277      19.692  48.261 104.876  1.00 22.41      AAGL
ATOM   2157  CA  PHE   277      19.355  47.458 106.042  1.00 21.05      AAGL
ATOM   2158  CB  PHE   277      17.844  47.222 106.120  1.00 20.89      AAGL
ATOM   2159  CG  PHE   277      17.447  46.219 107.171  1.00 19.02      AAGL
ATOM   2160  CD1 PHE   277      17.541  46.533 108.518  1.00 21.55      AAGL
ATOM   2161  CD2 PHE   277      17.003  44.946 106.805  1.00 22.72      AAGL
ATOM   2162  CE1 PHE   277      17.200  45.594 109.498  1.00 23.87      AAGL
ATOM   2163  CE2 PHE   277      16.660  43.998 107.781  1.00 21.01      AAGL
ATOM   2164  CZ  PHE   277      16.759  44.323 109.122  1.00 22.10      AAGL
ATOM   2165  C   PHE   277      20.051  46.102 105.989  1.00 20.46      AAGL
ATOM   2166  O   PHE   277      20.676  45.674 106.952  1.00 20.12      AAGL
ATOM   2167  N   LEU   278      19.928  45.421 104.856  1.00 20.92      AAGL
ATOM   2168  CA  LEU   278      20.541  44.107 104.716  1.00 23.04      AAGL
ATOM   2169  CB  LEU   278      20.225  43.512 103.340  1.00 24.67      AAGL
ATOM   2170  CG  LEU   278      18.764  43.076 103.160  1.00 24.46      AAGL
ATOM   2171  CD1 LEU   278      18.548  42.589 101.741  1.00 26.14      AAGL
ATOM   2172  CD2 LEU   278      18.427  41.964 104.161  1.00 26.55      AAGL
ATOM   2173  C   LEU   278      22.040  44.144 104.947  1.00 23.23      AAGL
ATOM   2174  O   LEU   278      22.593  43.273 105.615  1.00 20.93      AAGL
ATOM   2175  N   GLU   279      22.707  45.155 104.404  1.00 24.22      AAGL
ATOM   2176  CA  GLU   279      24.141  45.244 104.601  1.00 25.09      AAGL
ATOM   2177  CB  GLU   279      24.735  46.309 103.682  1.00 26.59      AAGL
ATOM   2178  CG  GLU   279      24.418  46.045 102.213  1.00 32.07      AAGL
ATOM   2179  CD  GLU   279      25.419  46.691 101.274  1.00 37.00      AAGL
ATOM   2180  OE1 GLU   279      25.859  47.815 101.576  1.00 39.68      AAGL
ATOM   2181  OE2 GLU   279      25.756  46.078 100.235  1.00 40.09      AAGL
ATOM   2182  C   GLU   279      24.460  45.537 106.062  1.00 23.19      AAGL
ATOM   2183  O   GLU   279      25.409  44.984 106.614  1.00 23.97      AAGL
ATOM   2184  N   LYS   280      23.669  46.391 106.701  1.00 24.51      AAGL
ATOM   2185  CA  LYS   280      23.922  46.688 108.105  1.00 24.24      AAGL
ATOM   2186  CB  LYS   280      23.076  47.879 108.566  1.00 25.42      AAGL
ATOM   2187  CG  LYS   280      23.535  49.186 107.912  1.00 30.50      AAGL
ATOM   2188  CD  LYS   280      22.847  50.429 108.463  1.00 35.06      AAGL
ATOM   2189  CE  LYS   280      23.561  51.683 107.932  1.00 38.33      AAGL
ATOM   2190  NZ  LYS   280      23.003  52.962 108.460  1.00 39.58      AAGL
ATOM   2191  C   LYS   280      23.665  45.458 108.975  1.00 24.77      AAGL
ATOM   2192  O   LYS   280      24.382  45.219 109.949  1.00 21.68      AAGL
ATOM   2193  N   LEU   281      22.655  44.669 108.614  1.00 23.74      AAGL
ATOM   2194  CA  LEU   281      22.351  43.449 109.365  1.00 23.71      AAGL
ATOM   2195  CB  LEU   281      21.023  42.844 108.891  1.00 21.53      AAGL
ATOM   2196  CG  LEU   281      20.603  41.484 109.478  1.00 21.28      AAGL
ATOM   2197  CD1 LEU   281      20.583  41.533 110.996  1.00 19.24      AAGL
ATOM   2198  CD2 LEU   281      19.226  41.109 108.937  1.00 19.79      AAGL
ATOM   2199  C   LEU   281      23.482  42.429 109.172  1.00 22.36      AAGL
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Fig. 3 cont.

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ATOM   2200  O   LEU   281      23.940  41.803 110.125  1.00 24.16      AAGL
ATOM   2201  N   ALA   282      23.921  42.267 107.928  1.00 23.73      AAGL
ATOM   2202  CA  ALA   282      24.998  41.339 107.611  1.00 23.94      AAGL
ATOM   2203  CB  ALA   282      25.272  41.356 106.120  1.00 23.77      AAGL
ATOM   2204  C   ALA   282      26.264  41.713 108.382  1.00 24.05      AAGL
ATOM   2205  O   ALA   282      27.060  40.848 108.741  1.00 25.21      AAGL
ATOM   2206  N   ALA   283      26.441  43.005 108.643  1.00 25.21      AAGL
ATOM   2207  CA  ALA   283      27.614  43.477 109.372  1.00 25.75      AAGL
ATOM   2208  CB  ALA   283      27.616  45.005 109.424  1.00 26.48      AAGL
ATOM   2209  C   ALA   283      27.635  42.898 110.786  1.00 26.18      AAGL
ATOM   2210  O   ALA   283      28.658  42.387 111.248  1.00 25.57      AAGL
ATOM   2211  N   VAL   284      26.493  42.963 111.466  1.00 25.74      AAGL
ATOM   2212  CA  VAL   284      26.383  42.438 112.824  1.00 25.11      AAGL
ATOM   2213  CB  VAL   284      24.972  42.711 113.414  1.00 24.63      AAGL
ATOM   2214  CG1 VAL   284      24.806  41.992 114.744  1.00 24.88      AAGL
ATOM   2215  CG2 VAL   284      24.779  44.220 113.606  1.00 27.53      AAGL
ATOM   2216  C   VAL   284      26.658  40.941 112.857  1.00 23.65      AAGL
ATOM   2217  O   VAL   284      27.416  40.456 113.694  1.00 23.12      AAGL
ATOM   2218  N   VAL   285      26.052  40.209 111.930  1.00 25.11      AAGL
ATOM   2219  CA  VAL   285      26.236  38.769 111.881  1.00 23.69      AAGL
ATOM   2220  CB  VAL   285      25.302  38.135 110.839  1.00 24.54      AAGL
ATOM   2221  CG1 VAL   285      25.490  36.626 110.822  1.00 25.86      AAGL
ATOM   2222  CG2 VAL   285      23.855  38.490 111.171  1.00 26.53      AAGL
ATOM   2223  C   VAL   285      27.679  38.406 111.559  1.00 26.05      AAGL
ATOM   2224  O   VAL   285      28.256  37.514 112.179  1.00 25.09      AAGL
ATOM   2225  N   GLU   286      28.259  39.101 110.587  1.00 24.87      AAGL
ATOM   2226  CA  GLU   286      29.639  38.847 110.201  1.00 26.91      AAGL
ATOM   2227  CB  GLU   286      30.041  39.737 109.025  1.00 29.06      AAGL
ATOM   2228  CG  GLU   286      31.518  39.586 108.629  1.00 32.60      AAGL
ATOM   2229  CD  GLU   286      31.812  38.250 107.971  1.00 35.44      AAGL
ATOM   2230  OE1 GLU   286      31.578  38.120 106.751  1.00 36.64      AAGL
ATOM   2231  OE2 GLU   286      32.264  37.322 108.672  1.00 35.13      AAGL
ATOM   2232  C   GLU   286      30.587  39.110 111.367  1.00 26.68      AAGL
ATOM   2233  O   GLU   286      31.528  38.354 111.590  1.00 27.24      AAGL
ATOM   2234  N   ALA   287      30.343  40.181 112.111  1.00 25.24      AAGL
ATOM   2235  CA  ALA   287      31.211  40.522 113.230  1.00 27.43      AAGL
ATOM   2236  CB  ALA   287      31.032  41.990 113.600  1.00 27.81      AAGL
ATOM   2237  C   ALA   287      31.003  39.650 114.465  1.00 29.71      AAGL
ATOM   2238  O   ALA   287      31.726  39.795 115.451  1.00 31.32      AAGL
ATOM   2239  N   THR   288      30.024  38.749 114.415  1.00 28.83      AAGL
ATOM   2240  CA  THR   288      29.744  37.871 115.549  1.00 29.55      AAGL
ATOM   2241  CB  THR   288      28.242  37.499 115.618  1.00 28.36      AAGL
ATOM   2242  OG1 THR   288      27.444  38.680 115.459  1.00 29.45      AAGL
ATOM   2243  CG2 THR   288      27.921  36.854 116.962  1.00 31.36      AAGL
ATOM   2244  C   THR   288      30.533  36.577 115.393  1.00 27.55      AAGL
ATOM   2245  O   THR   288      30.708  36.094 114.280  1.00 27.21      AAGL
ATOM   2246  N   THR   289      31.006  36.015 116.504  1.00 30.08      AAGL
ATOM   2247  CA  THR   289      31.757  34.770 116.437  1.00 31.68      AAGL
ATOM   2248  CB  THR   289      32.352  34.384 117.806  1.00 34.06      AAGL
ATOM   2249  OG1 THR   289      33.186  35.449 118.291  1.00 35.86      AAGL
ATOM   2250  CG2 THR   289      33.186  33.128 117.673  1.00 34.89      AAGL
ATOM   2251  C   THR   289      30.817  33.659 115.964  1.00 33.04      AAGL
ATOM   2252  O   THR   289      29.842  33.332 116.632  1.00 34.14      AAGL
ATOM   2253  N   ASP   290      31.120  33.085 114.807  1.00 33.28      AAGL
ATOM   2254  CA  ASP   290      30.298  32.030 114.211  1.00 32.82      AAGL
ATOM   2255  CB  ASP   290      30.183  30.812 115.137  1.00 33.97      AAGL
ATOM   2256  CG  ASP   290      31.397  29.900 115.054  1.00 38.26      AAGL
ATOM   2257  OD1 ASP   290      32.093  29.921 114.006  1.00 38.79      AAGL
ATOM   2258  OD2 ASP   290      31.651  29.152 116.024  1.00 38.34      AAGL
ATOM   2259  C   ASP   290      28.903  32.495 113.793  1.00 30.86      AAGL
ATOM   2260  O   ASP   290      27.909  31.781 113.979  1.00 31.04      AAGL
ATOM   2261  N   GLY   291      28.841  33.705 113.246  1.00 30.92      AAGL
ATOM   2262  CA  GLY   291      27.590  34.240 112.740  1.00 28.36      AAGL
ATOM   2263  C   GLY   291      27.579  33.689 111.331  1.00 28.69      AAGL
ATOM   2264  O   GLY   291      28.358  34.133 110.487  1.00 29.95      AAGL
ATOM   2265  N   LEU   292      26.702  32.726 111.065  1.00 25.52      AAGL
ATOM   2266  CA  LEU   292      26.662  32.072 109.767  1.00 25.89      AAGL
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Fig. 3 cont.

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ATOM   2267  CB  LEU   292      26.184  30.632 109.940  1.00 25.46      AAGL
ATOM   2268  CG  LEU   292      27.072  29.798 110.858  1.00 26.52      AAGL
ATOM   2269  CD1 LEU   292      26.632  28.354 110.807  1.00 26.92      AAGL
ATOM   2270  CD2 LEU   292      28.526  29.929 110.418  1.00 27.08      AAGL
ATOM   2271  C   LEU   292      25.908  32.700 108.613  1.00 25.35      AAGL
ATOM   2272  O   LEU   292      26.298  32.528 107.459  1.00 25.52      AAGL
ATOM   2273  N   GLY   293      24.824  33.413 108.887  1.00 25.75      AAGL
ATOM   2274  CA  GLY   293      24.118  33.990 107.769  1.00 22.89      AAGL
ATOM   2275  C   GLY   293      22.785  34.642 108.043  1.00 23.42      AAGL
ATOM   2276  O   GLY   293      22.366  34.828 109.187  1.00 21.61      AAGL
ATOM   2277  N   VAL   294      22.123  34.984 106.950  1.00 21.14      AAGL
ATOM   2278  CA  VAL   294      20.841  35.647 107.003  1.00 22.60      AAGL
ATOM   2279  CB  VAL   294      21.013  37.164 106.775  1.00 24.33      AAGL
ATOM   2280  CG1 VAL   294      19.657  37.818 106.538  1.00 25.68      AAGL
ATOM   2281  CG2 VAL   294      21.719  37.789 107.969  1.00 23.35      AAGL
ATOM   2282  C   VAL   294      19.926  35.094 105.932  1.00 23.50      AAGL
ATOM   2283  O   VAL   294      20.351  34.867 104.799  1.00 22.80      AAGL
ATOM   2284  N   TYR   295      18.668  34.871 106.293  1.00 21.62      AAGL
ATOM   2285  CA  TYR   295      17.684  34.387 105.338  1.00 20.32      AAGL
ATOM   2286  CB  TYR   295      17.105  33.035 105.761  1.00 20.96      AAGL
ATOM   2287  CG  TYR   295      18.040  31.862 105.606  1.00 21.66      AAGL
ATOM   2288  CD1 TYR   295      19.124  31.692 106.461  1.00 20.77      AAGL
ATOM   2289  CE1 TYR   295      19.974  30.584 106.337  1.00 22.52      AAGL
ATOM   2290  CD2 TYR   295      17.820  30.904 104.617  1.00 21.20      AAGL
ATOM   2291  CE2 TYR   295      18.658  29.798 104.481  1.00 22.01      AAGL
ATOM   2292  CZ  TYR   295      19.732  29.640 105.341  1.00 22.76      AAGL
ATOM   2293  OH  TYR   295      20.564  28.543 105.211  1.00 23.00      AAGL
ATOM   2294  C   TYR   295      16.554  35.399 105.295  1.00 21.79      AAGL
ATOM   2295  O   TYR   295      15.933  35.672 106.325  1.00 20.79      AAGL
ATOM   2296  N   TYR   296      16.296  35.966 104.118  1.00 20.08      AAGL
ATOM   2297  CA  TYR   296      15.212  36.927 103.975  1.00 19.64      AAGL
ATOM   2298  CB  TYR   296      15.328  37.704 102.666  1.00 20.69      AAGL
ATOM   2299  CG  TYR   296      14.503  38.972 102.656  1.00 19.70      AAGL
ATOM   2300  CD1 TYR   296      15.005  40.152 103.194  1.00 21.48      AAGL
ATOM   2301  CE1 TYR   296      14.236  41.310 103.232  1.00 21.48      AAGL
ATOM   2302  CD2 TYR   296      13.203  38.980 102.147  1.00 19.37      AAGL
ATOM   2303  CE2 TYR   296      12.423  40.138 102.182  1.00 21.23      AAGL
ATOM   2304  CZ  TYR   296      12.948  41.295 102.729  1.00 20.28      AAGL
ATOM   2305  OH  TYR   296      12.177  42.427 102.797  1.00 19.16      AAGL
ATOM   2306  C   TYR   296      13.947  36.090 103.939  1.00 20.23      AAGL
ATOM   2307  O   TYR   296      13.945  35.010 103.359  1.00 22.11      AAGL
ATOM   2308  N   TRP   297      12.868  36.578 104.538  1.00 17.43      AAGL
ATOM   2309  CA  TRP   297      11.641  35.795 104.553  1.00 17.69      AAGL
ATOM   2310  CB  TRP   297      10.942  35.894 105.920  1.00 19.08      AAGL
ATOM   2311  CG  TRP   297       9.854  34.864 106.075  1.00 19.30      AAGL
ATOM   2312  CD2 TRP   297       8.440  35.098 106.104  1.00 19.62      AAGL
ATOM   2313  CE2 TRP   297       7.808  33.837 106.201  1.00 20.98      AAGL
ATOM   2314  CE3 TRP   297       7.644  36.250 106.057  1.00 21.65      AAGL
ATOM   2315  CD1 TRP   297      10.018  33.511 106.155  1.00 21.34      AAGL
ATOM   2316  NE1 TRP   297       8.793  32.885 106.231  1.00 21.42      AAGL
ATOM   2317  CZ2 TRP   297       6.418  33.696 106.251  1.00 19.44      AAGL
ATOM   2318  CZ3 TRP   297       6.257  36.109 106.106  1.00 24.11      AAGL
ATOM   2319  CH2 TRP   297       5.661  34.836 106.201  1.00 22.67      AAGL
ATOM   2320  C   TRP   297      10.647  36.175 103.464  1.00 18.74      AAGL
ATOM   2321  O   TRP   297      10.158  37.305 103.428  1.00 17.76      AAGL
ATOM   2322  N   GLU   298      10.357  35.214 102.584  1.00 18.51      AAGL
ATOM   2323  CA  GLU   298       9.391  35.390 101.505  1.00 18.03      AAGL
ATOM   2324  CB  GLU   298       7.976  35.340 102.084  1.00 19.76      AAGL
ATOM   2325  CG  GLU   298       7.562  33.964 102.582  1.00 19.56      AAGL
ATOM   2326  CD  GLU   298       7.283  32.996 101.447  1.00 20.53      AAGL
ATOM   2327  OE1 GLU   298       7.320  33.422 100.274  1.00 21.41      AAGL
ATOM   2328  OE2 GLU   298       7.016  31.811 101.733  1.00 22.59      AAGL
ATOM   2329  C   GLU   298       9.553  36.664 100.668  1.00 20.54      AAGL
ATOM   2330  O   GLU   298       8.636  37.482 100.569  1.00 21.31      AAGL
ATOM   2331  N   PRO   299      10.715  36.832 100.025  1.00 21.16      AAGL
ATOM   2332  CD  PRO   299      11.893  35.949 100.046  1.00 20.70      AAGL
ATOM   2333  CA  PRO   299      10.964  38.022  99.203  1.00 21.46      AAGL
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Fig. 3 cont.

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ATOM   2334  CB  PRO   299      12.455  37.913  98.897  1.00 22.49      AAGL
ATOM   2335  CG  PRO   299      12.658  36.429  98.826  1.00 23.37      AAGL
ATOM   2336  C   PRO   299      10.133  38.131  97.924  1.00 21.34      AAGL
ATOM   2337  O   PRO   299      10.051  39.203  97.329  1.00 25.08      AAGL
ATOM   2338  N   ALA   300       9.515  37.031  97.507  1.00 21.73      AAGL
ATOM   2339  CA  ALA   300       8.751  37.021  96.264  1.00 23.94      AAGL
ATOM   2340  CB  ALA   300       9.418  36.071  95.272  1.00 23.80      AAGL
ATOM   2341  C   ALA   300       7.280  36.663  96.386  1.00 23.97      AAGL
ATOM   2342  O   ALA   300       6.663  36.277  95.394  1.00 24.57      AAGL
ATOM   2343  N   TRP   301       6.707  36.802  97.579  1.00 25.04      AAGL
ATOM   2344  CA  TRP   301       5.301  36.454  97.775  1.00 24.04      AAGL
ATOM   2345  CB  TRP   301       5.007  36.244  99.266  1.00 25.15      AAGL
ATOM   2346  CG  TRP   301       3.744  35.459  99.531  1.00 23.59      AAGL
ATOM   2347  CD2 TRP   301       3.394  34.781 100.744  1.00 23.73      AAGL
ATOM   2348  CE2 TRP   301       2.119  34.200 100.548  1.00 23.63      AAGL
ATOM   2349  CE3 TRP   301       4.033  34.607 101.980  1.00 24.03      AAGL
ATOM   2350  CD1 TRP   301       2.697  35.267  98.673  1.00 23.60      AAGL
ATOM   2351  NE1 TRP   301       1.717  34.513  99.278  1.00 24.88      AAGL
ATOM   2352  CZ2 TRP   301       1.470  33.458 101.544  1.00 22.63      AAGL
ATOM   2353  CZ3 TRP   301       3.387  33.871 102.969  1.00 22.92      AAGL
ATOM   2354  CH2 TRP   301       2.119  33.306 102.741  1.00 21.62      AAGL
ATOM   2355  C   TRP   301       4.322  37.485  97.213  1.00 25.72      AAGL
ATOM   2356  O   TRP   301       3.682  38.220  97.968  1.00 24.12      AAGL
ATOM   2357  N   ILE   302       4.192  37.532  95.889  1.00 26.27      AAGL
ATOM   2358  CA  ILE   302       3.273  38.475  95.256  1.00 26.33      AAGL
ATOM   2359  CB  ILE   302       3.257  38.317  93.722  1.00 28.94      AAGL
ATOM   2360  CG2 ILE   302       2.804  39.615  93.081  1.00 30.12      AAGL
ATOM   2361  CG1 ILE   302       4.653  37.963  93.215  1.00 32.05      AAGL
ATOM   2362  CD1 ILE   302       5.671  39.038  93.462  1.00 33.22      AAGL
ATOM   2363  C   ILE   302       1.872  38.180  95.770  1.00 24.91      AAGL
ATOM   2364  O   ILE   302       1.467  37.017  95.840  1.00 26.39      AAGL
ATOM   2365  N   GLY   303       1.134  39.223  96.133  1.00 25.25      AAGL
ATOM   2366  CA  GLY   303      -0.210  39.018  96.646  1.00 27.25      AAGL
ATOM   2367  C   GLY   303      -0.298  39.086  98.159  1.00 26.83      AAGL
ATOM   2368  O   GLY   303      -1.394  39.110  98.728  1.00 27.53      AAGL
ATOM   2369  N   ASN   304       0.861  39.090  98.812  1.00 25.82      AAGL
ATOM   2370  CA  ASN   304       0.958  39.182 100.267  1.00 23.80      AAGL
ATOM   2371  CB  ASN   304       1.113  37.783 100.887  1.00 22.97      AAGL
ATOM   2372  CG  ASN   304       1.131  37.811 102.413  1.00 23.62      AAGL
ATOM   2373  OD1 ASN   304       0.494  38.663 103.038  1.00 25.26      AAGL
ATOM   2374  ND2 ASN   304       1.841  36.864 103.017  1.00 20.66      AAGL
ATOM   2375  C   ASN   304       2.200  40.031 100.539  1.00 22.75      AAGL
ATOM   2376  O   ASN   304       3.030  39.704 101.382  1.00 21.47      AAGL
ATOM   2377  N   ALA   305       2.306  41.139  99.812  1.00 23.77      AAGL
ATOM   2378  CA  ALA   305       3.454  42.028  99.926  1.00 23.13      AAGL
ATOM   2379  CB  ALA   305       3.281  43.211  98.980  1.00 25.11      AAGL
ATOM   2380  C   ALA   305       3.770  42.520 101.335  1.00 22.70      AAGL
ATOM   2381  O   ALA   305       4.928  42.784 101.650  1.00 23.39      AAGL
ATOM   2382  N   GLY   306       2.753  42.632 102.182  1.00 23.04      AAGL
ATOM   2383  CA  GLY   306       2.970  43.093 103.543  1.00 21.61      AAGL
ATOM   2384  C   GLY   306       3.592  42.023 104.421  1.00 20.83      AAGL
ATOM   2385  O   GLY   306       4.185  42.323 105.461  1.00 20.31      AAGL
ATOM   2386  N   LEU   307       3.445  40.771 103.997  1.00 20.88      AAGL
ATOM   2387  CA  LEU   307       3.980  39.615 104.710  1.00 19.63      AAGL
ATOM   2388  CB  LEU   307       5.511  39.575 104.599  1.00 19.26      AAGL
ATOM   2389  CG  LEU   307       6.089  39.333 103.198  1.00 17.07      AAGL
ATOM   2390  CD1 LEU   307       7.602  39.293 103.292  1.00 21.74      AAGL
ATOM   2391  CD2 LEU   307       5.568  38.012 102.625  1.00 18.50      AAGL
ATOM   2392  C   LEU   307       3.580  39.543 106.178  1.00 20.69      AAGL
ATOM   2393  O   LEU   307       4.377  39.131 107.018  1.00 20.75      AAGL
ATOM   2394  N   GLY   308       2.352  39.955 106.484  1.00 19.76      AAGL
ATOM   2395  CA  GLY   308       1.870  39.898 107.854  1.00 22.38      AAGL
ATOM   2396  C   GLY   308       2.188  41.068 108.769  1.00 23.64      AAGL
ATOM   2397  O   GLY   308       1.785  41.072 109.938  1.00 23.65      AAGL
ATOM   2398  N   SER   309       2.907  42.060 108.252  1.00 23.88      AAGL
ATOM   2399  CA  SER   309       3.275  43.227 109.045  1.00 22.50      AAGL
ATOM   2400  CB  SER   309       4.693  43.684 108.695  1.00 22.00      AAGL
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Fig. 3 cont.

ATOM	2401	OG	SER	309	4.719	44.264	107.407	1.00 20.09	AAGL
ATOM	2402	C	SER	309	2.312	44.385	108.790	1.00 23.02	AAGL
ATOM	2403	O	SER	309	1.388	44.271	107.983	1.00 23.42	AAGL
ATOM	2404	N	SER	310	2.539	45.494	109.486	1.00 20.79	AAGL
ATOM	2405	CA	SER	310	1.707	46.684	109.316	1.00 23.22	AAGL
ATOM	2406	CB	SER	310	1.715	47.535	110.592	1.00 22.59	AAGL
ATOM	2407	OG	SER	310	3.022	48.003	110.903	1.00 24.03	AAGL
ATOM	2408	C	SER	310	2.234	47.512	108.138	1.00 23.44	AAGL
ATOM	2409	O	SER	310	1.658	48.545	107.773	1.00 23.68	AAGL
ATOM	2410	N	CYS	311	3.340	47.069	107.548	1.00 21.68	AAGL
ATOM	2411	CA	CYS	311	3.892	47.788	106.413	1.00 23.63	AAGL
ATOM	2412	C	CYS	311	3.210	47.381	105.123	1.00 24.17	AAGL
ATOM	2413	O	CYS	311	2.591	46.321	105.044	1.00 26.98	AAGL
ATOM	2414	CB	CYS	311	5.387	47.545	106.289	1.00 25.30	AAGL
ATOM	2415	SG	CYS	311	6.407	48.425	107.501	1.00 27.01	AAGL
ATOM	2416	N	ALA	312	3.343	48.219	104.104	1.00 23.57	AAGL
ATOM	2417	CA	ALA	312	2.707	47.954	102.821	1.00 25.20	AAGL
ATOM	2418	CB	ALA	312	2.516	49.266	102.053	1.00 25.76	AAGL
ATOM	2419	C	ALA	312	3.400	46.950	101.919	1.00 25.50	AAGL
ATOM	2420	O	ALA	312	2.741	46.128	101.288	1.00 24.61	AAGL
ATOM	2421	N	ASP	313	4.726	47.003	101.858	1.00 25.50	AAGL
ATOM	2422	CA	ASP	313	5.444	46.122	100.949	1.00 25.55	AAGL
ATOM	2423	CB	ASP	313	5.560	46.827	99.596	1.00 28.83	AAGL
ATOM	2424	CG	ASP	313	5.870	45.886	98.471	1.00 31.63	AAGL
ATOM	2425	OD1	ASP	313	6.652	44.940	98.680	1.00 29.42	AAGL
ATOM	2426	OD2	ASP	313	5.337	46.107	97.358	1.00 37.09	AAGL
ATOM	2427	C	ASP	313	6.836	45.752	101.440	1.00 25.26	AAGL
ATOM	2428	O	ASP	313	7.698	46.620	101.575	1.00 25.34	AAGL
ATOM	2429	N	ASN	314	7.049	44.460	101.685	1.00 22.30	AAGL
ATOM	2430	CA	ASN	314	8.335	43.956	102.157	1.00 21.78	AAGL
ATOM	2431	CB	ASN	314	8.156	43.167	103.458	1.00 23.69	AAGL
ATOM	2432	CG	ASN	314	7.832	44.056	104.640	1.00 25.29	AAGL
ATOM	2433	OD1	ASN	314	8.520	45.039	104.883	1.00 28.43	AAGL
ATOM	2434	ND2	ASN	314	6.787	43.710	105.382	1.00 24.92	AAGL
ATOM	2435	C	ASN	314	8.999	43.053	101.127	1.00 22.83	AAGL
ATOM	2436	O	ASN	314	10.043	42.469	101.393	1.00 21.72	AAGL
ATOM	2437	N	LEU	315	8.388	42.942	99.955	1.00 22.78	AAGL
ATOM	2438	CA	LEU	315	8.919	42.086	98.907	1.00 22.99	AAGL
ATOM	2439	CB	LEU	315	7.879	41.913	97.796	1.00 22.49	AAGL
ATOM	2440	CG	LEU	315	6.491	41.421	98.219	1.00 22.62	AAGL
ATOM	2441	CD1	LEU	315	5.599	41.214	96.991	1.00 25.48	AAGL
ATOM	2442	CD2	LEU	315	6.638	40.117	98.978	1.00 23.90	AAGL
ATOM	2443	C	LEU	315	10.219	42.604	98.310	1.00 24.65	AAGL
ATOM	2444	O	LEU	315	10.608	43.756	98.523	1.00 24.23	AAGL
ATOM	2445	N	MET	316	10.898	41.728	97.576	1.00 25.62	AAGL
ATOM	2446	CA	MET	316	12.135	42.088	96.901	1.00 28.28	AAGL
ATOM	2447	CB	MET	316	13.280	41.159	97.321	1.00 26.81	AAGL
ATOM	2448	CG	MET	316	13.718	41.299	98.777	1.00 27.89	AAGL
ATOM	2449	SD	MET	316	15.182	40.302	99.187	1.00 29.46	AAGL
ATOM	2450	CE	MET	316	16.470	41.485	98.890	1.00 29.41	AAGL
ATOM	2451	C	MET	316	11.889	41.977	95.393	1.00 29.33	AAGL
ATOM	2452	O	MET	316	12.824	41.939	94.599	1.00 29.21	AAGL
ATOM	2453	N	VAL	317	10.616	41.910	95.015	1.00 30.78	AAGL
ATOM	2454	CA	VAL	317	10.217	41.820	93.614	1.00 32.20	AAGL
ATOM	2455	CB	VAL	317	9.681	40.416	93.263	1.00 31.88	AAGL
ATOM	2456	CG1	VAL	317	10.763	39.374	93.477	1.00 33.90	AAGL
ATOM	2457	CG2	VAL	317	8.479	40.100	94.128	1.00 36.43	AAGL
ATOM	2458	C	VAL	317	9.113	42.836	93.346	1.00 33.46	AAGL
ATOM	2459	O	VAL	317	8.342	43.169	94.246	1.00 30.98	AAGL
ATOM	2460	N	ASP	318	9.041	43.333	92.113	1.00 33.99	AAGL
ATOM	2461	CA	ASP	318	8.015	44.309	91.760	1.00 38.16	AAGL
ATOM	2462	CB	ASP	318	8.405	45.073	90.493	1.00 39.54	AAGL
ATOM	2463	CG	ASP	318	7.502	46.252	90.240	1.00 38.96	AAGL
ATOM	2464	OD1	ASP	318	6.267	46.066	90.216	1.00 40.93	AAGL
ATOM	2465	OD2	ASP	318	8.022	47.370	90.058	1.00 42.03	AAGL
ATOM	2466	C	ASP	318	6.671	43.621	91.547	1.00 41.03	AAGL
ATOM	2467	O	ASP	318	6.512	42.800	90.642	1.00 41.02	AAGL

Fig. 3 cont.

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ATOM   2468  N   TYR  319       5.695  43.985  92.373  1.00 43.91      AAGL
ATOM   2469  CA  TYR  319       4.370  43.388  92.312  1.00 46.99      AAGL
ATOM   2470  CB  TYR  319       3.555  43.811  93.548  1.00 48.59      AAGL
ATOM   2471  CG  TYR  319       3.003  45.224  93.516  1.00 48.66      AAGL
ATOM   2472  CD1 TYR  319       1.702  45.475  93.080  1.00 49.01      AAGL
ATOM   2473  CE1 TYR  319       1.180  46.778  93.066  1.00 49.49      AAGL
ATOM   2474  CD2 TYR  319       3.772  46.305  93.937  1.00 49.12      AAGL
ATOM   2475  CE2 TYR  319       3.264  47.610  93.929  1.00 49.13      AAGL
ATOM   2476  CZ  TYR  319       1.967  47.836  93.493  1.00 49.15      AAGL
ATOM   2477  OH  TYR  319       1.457  49.115  93.495  1.00 48.83      AAGL
ATOM   2478  C   TYR  319       3.602  43.705  91.034  1.00 49.01      AAGL
ATOM   2479  O   TYR  319       2.479  43.221  90.840  1.00 51.46      AAGL
ATOM   2480  N   THR  320       4.178  44.522  90.158  1.00 48.98      AAGL
ATOM   2481  CA  THR  320       3.491  44.827  88.909  1.00 48.98      AAGL
ATOM   2482  CB  THR  320       3.383  46.349  88.642  1.00 48.87      AAGL
ATOM   2483  OG1 THR  320       4.681  46.899  88.371  1.00 48.24      AAGL
ATOM   2484  CG2 THR  320       2.770  47.054  89.829  1.00 48.99      AAGL
ATOM   2485  C   THR  320       4.206  44.184  87.730  1.00 49.75      AAGL
ATOM   2486  O   THR  320       3.572  43.536  86.896  1.00 50.61      AAGL
ATOM   2487  N   THR  321       5.524  44.349  87.671  1.00 49.77      AAGL
ATOM   2488  CA  THR  321       6.316  43.798  86.575  1.00 50.22      AAGL
ATOM   2489  CB  THR  321       7.561  44.673  86.297  1.00 50.80      AAGL
ATOM   2490  OG1 THR  321       8.505  44.522  87.368  1.00 51.66      AAGL
ATOM   2491  CG2 THR  321       7.168  46.144  86.193  1.00 51.57      AAGL
ATOM   2492  C   THR  321       6.805  42.371  86.807  1.00 50.00      AAGL
ATOM   2493  O   THR  321       7.360  41.743  85.905  1.00 50.77      AAGL
ATOM   2494  N   ASP  322       6.617  41.859  88.016  1.00 49.25      AAGL
ATOM   2495  CA  ASP  322       7.082  40.515  88.345  1.00 47.20      AAGL
ATOM   2496  CB  ASP  322       6.534  39.471  87.354  1.00 50.64      AAGL
ATOM   2497  CG  ASP  322       5.010  39.462  87.262  1.00 52.01      AAGL
ATOM   2498  OD1 ASP  322       4.313  39.445  88.309  1.00 52.82      AAGL
ATOM   2499  OD2 ASP  322       4.502  39.442  86.113  1.00 55.12      AAGL
ATOM   2500  C   ASP  322       8.616  40.486  88.288  1.00 44.47      AAGL
ATOM   2501  O   ASP  322       9.231  39.416  88.385  1.00 44.83      AAGL
ATOM   2502  N   GLU  323       9.236  41.652  88.124  1.00 41.39      AAGL
ATOM   2503  CA  GLU  323      10.696  41.745  88.049  1.00 39.30      AAGL
ATOM   2504  CB  GLU  323      11.093  42.894  87.127  1.00 41.31      AAGL
ATOM   2505  CG  GLU  323      12.586  43.108  86.977  1.00 44.75      AAGL
ATOM   2506  CD  GLU  323      12.911  44.040  85.812  1.00 47.16      AAGL
ATOM   2507  OE1 GLU  323      14.099  44.371  85.612  1.00 47.71      AAGL
ATOM   2508  OE2 GLU  323      11.971  44.438  85.091  1.00 47.99      AAGL
ATOM   2509  C   GLU  323      11.346  41.939  89.420  1.00 36.82      AAGL
ATOM   2510  O   GLU  323      10.898  42.761  90.220  1.00 35.46      AAGL
ATOM   2511  N   VAL  324      12.410  41.182  89.675  1.00 35.31      AAGL
ATOM   2512  CA  VAL  324      13.120  41.257  90.948  1.00 32.93      AAGL
ATOM   2513  CB  VAL  324      14.154  40.103  91.099  1.00 33.31      AAGL
ATOM   2514  CG1 VAL  324      13.487  38.770  90.827  1.00 32.75      AAGL
ATOM   2515  CG2 VAL  324      15.341  40.316  90.153  1.00 32.38      AAGL
ATOM   2516  C   VAL  324      13.864  42.573  91.090  1.00 33.56      AAGL
ATOM   2517  O   VAL  324      14.329  43.153  90.093  1.00 33.29      AAGL
ATOM   2518  N   TYR  325      13.974  43.045  92.328  1.00 30.85      AAGL
ATOM   2519  CA  TYR  325      14.683  44.282  92.608  1.00 31.59      AAGL
ATOM   2520  CB  TYR  325      14.228  44.910  93.929  1.00 30.31      AAGL
ATOM   2521  CG  TYR  325      12.794  45.387  93.972  1.00 31.58      AAGL
ATOM   2522  CD1 TYR  325      12.225  46.079  92.901  1.00 31.55      AAGL
ATOM   2523  CE1 TYR  325      10.908  46.548  92.970  1.00 33.68      AAGL
ATOM   2524  CD2 TYR  325      12.015  45.177  95.112  1.00 30.63      AAGL
ATOM   2525  CE2 TYR  325      10.714  45.639  95.192  1.00 30.81      AAGL
ATOM   2526  CZ  TYR  325      10.164  46.323  94.127  1.00 33.10      AAGL
ATOM   2527  OH  TYR  325       8.878  46.780  94.231  1.00 32.89      AAGL
ATOM   2528  C   TYR  325      16.169  44.003  92.714  1.00 31.02      AAGL
ATOM   2529  O   TYR  325      16.602  42.859  92.908  1.00 28.70      AAGL
ATOM   2530  N   GLU  326      16.946  45.070  92.599  1.00 31.64      AAGL
ATOM   2531  CA  GLU  326      18.398  45.010  92.684  1.00 31.11      AAGL
ATOM   2532  CB  GLU  326      18.949  46.406  92.388  1.00 34.73      AAGL
ATOM   2533  CG  GLU  326      20.432  46.588  92.571  1.00 39.05      AAGL
ATOM   2534  CD  GLU  326      20.851  47.994  92.209  1.00 41.46      AAGL
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Fig. 3 cont.

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ATOM   2535  OE1 GLU   326      20.682  48.359  91.021  1.00 42.66      AAGL
ATOM   2536  OE2 GLU   326      21.334  48.731  93.106  1.00 40.82      AAGL
ATOM   2537  C   GLU   326      18.848  44.538  94.065  1.00 29.10      AAGL
ATOM   2538  O   GLU   326      19.996  44.136  94.253  1.00 27.19      AAGL
ATOM   2539  N   SER   327      17.939  44.581  95.035  1.00 27.41      AAGL
ATOM   2540  CA  SER   327      18.265  44.147  96.387  1.00 25.31      AAGL
ATOM   2541  CB  SER   327      17.127  44.519  97.347  1.00 23.59      AAGL
ATOM   2542  OG  SER   327      15.870  44.218  96.776  1.00 25.25      AAGL
ATOM   2543  C   SER   327      18.574  42.650  96.458  1.00 24.17      AAGL
ATOM   2544  O   SER   327      19.243  42.195  97.383  1.00 25.88      AAGL
ATOM   2545  N   ILE   328      18.107  41.880  95.479  1.00 27.45      AAGL
ATOM   2546  CA  ILE   328      18.395  40.446  95.466  1.00 28.86      AAGL
ATOM   2547  CB  ILE   328      17.692  39.728  94.295  1.00 31.12      AAGL
ATOM   2548  CG2 ILE   328      18.120  38.277  94.250  1.00 35.58      AAGL
ATOM   2549  CG1 ILE   328      16.175  39.823  94.448  1.00 33.48      AAGL
ATOM   2550  CD1 ILE   328      15.647  39.194  95.727  1.00 36.80      AAGL
ATOM   2551  C   ILE   328      19.904  40.248  95.317  1.00 29.16      AAGL
ATOM   2552  O   ILE   328      20.486  39.324  95.897  1.00 27.50      AAGL
ATOM   2553  N   GLU   329      20.536  41.124  94.538  1.00 30.01      AAGL
ATOM   2554  CA  GLU   329      21.978  41.045  94.328  1.00 30.96      AAGL
ATOM   2555  CB  GLU   329      22.435  42.017  93.229  1.00 33.99      AAGL
ATOM   2556  CG  GLU   329      21.773  41.813  91.866  1.00 37.96      AAGL
ATOM   2557  CD  GLU   329      22.520  42.542  90.746  1.00 42.17      AAGL
ATOM   2558  OE1 GLU   329      22.731  43.773  90.863  1.00 42.73      AAGL
ATOM   2559  OE2 GLU   329      22.898  41.883  89.746  1.00 42.99      AAGL
ATOM   2560  C   GLU   329      22.682  41.386  95.627  1.00 29.64      AAGL
ATOM   2561  O   GLU   329      23.693  40.771  95.988  1.00 29.09      AAGL
ATOM   2562  N   THR   330      22.142  42.368  96.340  1.00 28.03      AAGL
ATOM   2563  CA  THR   330      22.720  42.776  97.611  1.00 26.58      AAGL
ATOM   2564  CB  THR   330      21.958  43.986  98.200  1.00 27.90      AAGL
ATOM   2565  OG1 THR   330      22.099  45.110  97.323  1.00 26.78      AAGL
ATOM   2566  CG2 THR   330      22.495  44.345  99.574  1.00 27.91      AAGL
ATOM   2567  C   THR   330      22.671  41.608  98.606  1.00 26.92      AAGL
ATOM   2568  O   THR   330      23.654  41.325  99.301  1.00 25.31      AAGL
ATOM   2569  N   LEU   331      21.529  40.930  98.667  1.00 25.72      AAGL
ATOM   2570  CA  LEU   331      21.368  39.791  99.571  1.00 24.97      AAGL
ATOM   2571  CB  LEU   331      19.923  39.282  99.532  1.00 24.19      AAGL
ATOM   2572  CG  LEU   331      19.567  37.968 100.247  1.00 23.31      AAGL
ATOM   2573  CD1 LEU   331      19.873  38.051 101.736  1.00 25.91      AAGL
ATOM   2574  CD2 LEU   331      18.082  37.674 100.034  1.00 23.20      AAGL
ATOM   2575  C   LEU   331      22.319  38.674  99.158  1.00 25.90      AAGL
ATOM   2576  O   LEU   331      22.971  38.054 100.001  1.00 25.54      AAGL
ATOM   2577  N   GLY   332      22.390  38.427  97.853  1.00 26.10      AAGL
ATOM   2578  CA  GLY   332      23.262  37.386  97.337  1.00 28.89      AAGL
ATOM   2579  C   GLY   332      24.738  37.631  97.594  1.00 31.12      AAGL
ATOM   2580  O   GLY   332      25.526  36.682  97.614  1.00 30.65      AAGL
ATOM   2581  N   GLU   333      25.120  38.890  97.805  1.00 31.60      AAGL
ATOM   2582  CA  GLU   333      26.524  39.229  98.044  1.00 33.74      AAGL
ATOM   2583  CB  GLU   333      26.949  40.400  97.148  1.00 34.97      AAGL
ATOM   2584  CG  GLU   333      26.639  40.205  95.673  1.00 37.79      AAGL
ATOM   2585  CD  GLU   333      26.846  41.471  94.846  1.00 41.19      AAGL
ATOM   2586  OE1 GLU   333      26.164  41.621  93.807  1.00 40.67      AAGL
ATOM   2587  OE2 GLU   333      27.694  42.309  95.225  1.00 44.05      AAGL
ATOM   2588  C   GLU   333      26.844  39.586  99.490  1.00 35.01      AAGL
ATOM   2589  O   GLU   333      27.924  40.109  99.776  1.00 33.69      AAGL
ATOM   2590  N   LEU   334      25.925  39.319 100.410  1.00 34.35      AAGL
ATOM   2591  CA  LEU   334      26.193  39.655 101.805  1.00 33.87      AAGL
ATOM   2592  CB  LEU   334      24.963  39.371 102.672  1.00 33.01      AAGL
ATOM   2593  CG  LEU   334      23.721  40.228 102.407  1.00 32.82      AAGL
ATOM   2594  CD1 LEU   334      22.611  39.797 103.347  1.00 28.38      AAGL
ATOM   2595  CD2 LEU   334      24.044  41.711 102.607  1.00 30.26      AAGL
ATOM   2596  C   LEU   334      27.396  38.881 102.344  1.00 35.69      AAGL
ATOM   2597  O   LEU   334      27.475  37.650 102.129  1.00 36.26      AAGL
ATOM   2598  OXT LEU   334      28.249  39.520 102.989  1.00 35.77      AAGL
END
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Fig. 3 cont.

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ATOM   2706  CB  ASP   359      18.203 -12.213  45.609  1.00 56.56      BLGL
ATOM   2707  CG  ASP   359      18.748 -12.887  44.366  1.00 58.60      BLGL
ATOM   2708  OD1 ASP   359      18.654 -14.130  44.268  1.00 60.63      BLGL
ATOM   2709  OD2 ASP   359      19.268 -12.166  43.485  1.00 59.51      BLGL
ATOM   2710  C   ASP   359      18.959 -11.751  47.928  1.00 51.60      BLGL
ATOM   2711  O   ASP   359      19.876 -11.837  48.742  1.00 50.90      BLGL
ATOM   2712  N   ALA   360      18.132 -10.713  47.865  1.00 51.06      BLGL
ATOM   2713  CA  ALA   360      18.226  -9.578  48.768  1.00 50.62      BLGL
ATOM   2714  CB  ALA   360      16.945  -8.767  48.697  1.00 49.16      BLGL
ATOM   2715  C   ALA   360      18.471 -10.058  50.193  1.00 50.90      BLGL
ATOM   2716  O   ALA   360      19.164  -9.403  50.973  1.00 49.67      BLGL
ATOM   2717  N   GLY   361      17.896 -11.214  50.515  1.00 52.39      BLGL
ATOM   2718  CA  GLY   361      18.042 -11.794  51.837  1.00 52.85      BLGL
ATOM   2719  C   GLY   361      19.481 -11.858  52.312  1.00 53.39      BLGL
ATOM   2720  O   GLY   361      19.809 -11.331  53.378  1.00 54.42      BLGL
ATOM   2721  N   LYS   362      20.351 -12.496  51.540  1.00 53.32      BLGL
ATOM   2722  CA  LYS   362      21.737 -12.588  51.954  1.00 54.47      BLGL
ATOM   2723  CB  LYS   362      22.081 -14.037  52.329  1.00 57.86      BLGL
ATOM   2724  CG  LYS   362      21.401 -15.120  51.495  1.00 59.76      BLGL
ATOM   2725  CD  LYS   362      22.199 -15.482  50.251  1.00 61.95      BLGL
ATOM   2726  CE  LYS   362      21.745 -16.833  49.698  1.00 63.37      BLGL
ATOM   2727  NZ  LYS   362      22.557 -17.264  48.522  1.00 62.07      BLGL
ATOM   2728  C   LYS   362      22.741 -12.034  50.953  1.00 53.61      BLGL
ATOM   2729  O   LYS   362      23.823 -12.595  50.770  1.00 54.78      BLGL
ATOM   2730  N   TRP   363      22.376 -10.921  50.323  1.00 52.09      BLGL
ATOM   2731  CA  TRP   363      23.236 -10.246  49.357  1.00 49.55      BLGL
ATOM   2732  CB  TRP   363      23.048 -10.816  47.948  1.00 53.13      BLGL
ATOM   2733  CG  TRP   363      23.559 -12.215  47.792  1.00 58.47      BLGL
ATOM   2734  CD2 TRP   363      24.840 -12.716  48.201  1.00 61.21      BLGL
ATOM   2735  CE2 TRP   363      24.867 -14.096  47.894  1.00 62.60      BLGL
ATOM   2736  CE3 TRP   363      25.966 -12.135  48.802  1.00 63.42      BLGL
ATOM   2737  CD1 TRP   363      22.885 -13.277  47.262  1.00 60.70      BLGL
ATOM   2738  NE1 TRP   363      23.663 -14.412  47.320  1.00 62.38      BLGL
ATOM   2739  CZ2 TRP   363      25.981 -14.907  48.168  1.00 63.65      BLGL
ATOM   2740  CZ3 TRP   363      27.076 -12.945  49.076  1.00 64.57      BLGL
ATOM   2741  CH2 TRP   363      27.071 -14.315  48.757  1.00 63.75      BLGL
ATOM   2742  C   TRP   363      22.900  -8.765  49.354  1.00 45.74      BLGL
ATOM   2743  O   TRP   363      23.315  -8.031  48.460  1.00 46.95      BLGL
ATOM   2744  N   PHE   364      22.143  -8.333  50.357  1.00 40.08      BLGL
ATOM   2745  CA  PHE   364      21.748  -6.939  50.478  1.00 36.02      BLGL
ATOM   2746  CB  PHE   364      20.798  -6.763  51.664  1.00 35.97      BLGL
ATOM   2747  CG  PHE   364      21.393  -7.163  52.989  1.00 35.49      BLGL
ATOM   2748  CD1 PHE   364      22.170  -6.264  53.723  1.00 34.51      BLGL
ATOM   2749  CD2 PHE   364      21.194  -8.448  53.493  1.00 34.67      BLGL
ATOM   2750  CE1 PHE   364      22.739  -6.637  54.937  1.00 33.03      BLGL
ATOM   2751  CE2 PHE   364      21.759  -8.834  54.705  1.00 33.39      BLGL
ATOM   2752  CZ  PHE   364      22.534  -7.927  55.429  1.00 33.77      BLGL
ATOM   2753  C   PHE   364      22.978  -6.061  50.655  1.00 33.99      BLGL
ATOM   2754  O   PHE   364      23.998  -6.506  51.181  1.00 34.27      BLGL
ATOM   2755  N   GLY   365      22.881  -4.816  50.208  1.00 30.67      BLGL
ATOM   2756  CA  GLY   365      24.008  -3.915  50.322  1.00 28.90      BLGL
ATOM   2757  C   GLY   365      23.806  -2.610  49.581  1.00 27.08      BLGL
ATOM   2758  O   GLY   365      22.708  -2.058  49.571  1.00 27.26      BLGL
ATOM   2759  N   GLY   366      24.863  -2.122  48.943  1.00 26.06      BLGL
ATOM   2760  CA  GLY   366      24.777  -0.860  48.230  1.00 22.87      BLGL
ATOM   2761  C   GLY   366      24.434  -0.934  46.757  1.00 22.45      BLGL
ATOM   2762  O   GLY   366      23.680  -1.800  46.312  1.00 20.99      BLGL
ATOM   2763  N   SER   367      24.996   0.004  46.002  1.00 22.77      BLGL
ATOM   2764  CA  SER   367      24.779   0.098  44.566  1.00 21.36      BLGL
ATOM   2765  CB  SER   367      25.081   1.511  44.079  1.00 19.13      BLGL
ATOM   2766  OG  SER   367      25.081   1.539  42.665  1.00 20.78      BLGL
ATOM   2767  C   SER   367      25.649  -0.877  43.802  1.00 20.92      BLGL
ATOM   2768  O   SER   367      26.828  -1.040  44.111  1.00 22.00      BLGL
ATOM   2769  N   ALA   368      25.072  -1.518  42.794  1.00 19.58      BLGL
ATOM   2770  CA  ALA   368      25.823  -2.474  41.992  1.00 19.49      BLGL
ATOM   2771  CB  ALA   368      25.069  -3.792  41.921  1.00 18.00      BLGL
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Fig. 4 cont.

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ATOM   2772  C   ALA   368      26.058  -1.928  40.595  1.00 19.35      BLGL
ATOM   2773  O   ALA   368      26.610  -2.612  39.735  1.00 19.98      BLGL
ATOM   2774  N   VAL   369      25.656  -0.679  40.387  1.00 19.26      BLGL
ATOM   2775  CA  VAL   369      25.775  -0.041  39.080  1.00 19.71      BLGL
ATOM   2776  CB  VAL   369      24.391   0.041  38.379  1.00 16.72      BLGL
ATOM   2777  CG1 VAL   369      23.863  -1.349  38.093  1.00 13.08      BLGL
ATOM   2778  CG2 VAL   369      23.411   0.804  39.265  1.00 10.69      BLGL
ATOM   2779  C   VAL   369      26.357   1.366  39.124  1.00 20.80      BLGL
ATOM   2780  O   VAL   369      26.139   2.156  38.201  1.00 21.48      BLGL
ATOM   2781  N   ASP   370      27.083   1.693  40.187  1.00 21.01      BLGL
ATOM   2782  CA  ASP   370      27.680   3.024  40.269  1.00 21.96      BLGL
ATOM   2783  CB  ASP   370      28.401   3.226  41.617  1.00 20.78      BLGL
ATOM   2784  CG  ASP   370      29.224   2.016  42.042  1.00 26.31      BLGL
ATOM   2785  OD1 ASP   370      28.640   1.027  42.529  1.00 27.68      BLGL
ATOM   2786  OD2 ASP   370      30.466   2.045  41.893  1.00 31.81      BLGL
ATOM   2787  C   ASP   370      28.649   3.264  39.098  1.00 21.03      BLGL
ATOM   2788  O   ASP   370      28.886   4.405  38.695  1.00 16.48      BLGL
ATOM   2789  N   ASN   371      29.188   2.181  38.542  1.00 20.75      BLGL
ATOM   2790  CA  ASN   371      30.126   2.291  37.431  1.00 21.39      BLGL
ATOM   2791  CB  ASN   371      31.159   1.161  37.506  1.00 19.36      BLGL
ATOM   2792  CG  ASN   371      30.554  -0.202  37.257  1.00 17.69      BLGL
ATOM   2793  OD1 ASN   371      29.412  -0.471  37.631  1.00 16.68      BLGL
ATOM   2794  ND2 ASN   371      31.329  -1.081  36.635  1.00 15.28      BLGL
ATOM   2795  C   ASN   371      29.435   2.298  36.062  1.00 22.85      BLGL
ATOM   2796  O   ASN   371      30.088   2.203  35.018  1.00 21.45      BLGL
ATOM   2797  N   GLN   372      28.109   2.405  36.074  1.00 21.57      BLGL
ATOM   2798  CA  GLN   372      27.355   2.458  34.837  1.00 21.91      BLGL
ATOM   2799  CB  GLN   372      26.432   1.248  34.702  1.00 19.34      BLGL
ATOM   2800  CG  GLN   372      27.186  -0.043  34.541  1.00 19.05      BLGL
ATOM   2801  CD  GLN   372      26.332  -1.154  33.981  1.00 18.53      BLGL
ATOM   2802  OE1 GLN   372      25.802  -1.043  32.881  1.00 16.76      BLGL
ATOM   2803  NE2 GLN   372      26.199  -2.240  34.732  1.00 19.99      BLGL
ATOM   2804  C   GLN   372      26.550   3.750  34.783  1.00 22.49      BLGL
ATOM   2805  O   GLN   372      25.693   3.927  33.920  1.00 24.48      BLGL
ATOM   2806  N   ALA   373      26.842   4.658  35.705  1.00 21.34      BLGL
ATOM   2807  CA  ALA   373      26.155   5.940  35.755  1.00 21.66      BLGL
ATOM   2808  CB  ALA   373      26.301   6.544  37.148  1.00 20.20      BLGL
ATOM   2809  C   ALA   373      26.702   6.914  34.705  1.00 22.35      BLGL
ATOM   2810  O   ALA   373      27.707   6.638  34.038  1.00 21.94      BLGL
ATOM   2811  N   LEU   374      26.025   8.048  34.555  1.00 21.60      BLGL
ATOM   2812  CA  LEU   374      26.454   9.080  33.617  1.00 21.79      BLGL
ATOM   2813  CB  LEU   374      25.273   9.548  32.763  1.00 19.88      BLGL
ATOM   2814  CG  LEU   374      24.631   8.408  31.962  1.00 19.67      BLGL
ATOM   2815  CD1 LEU   374      23.430   8.928  31.196  1.00 19.92      BLGL
ATOM   2816  CD2 LEU   374      25.650   7.809  31.011  1.00 17.34      BLGL
ATOM   2817  C   LEU   374      27.040  10.236  34.431  1.00 22.87      BLGL
ATOM   2818  O   LEU   374      27.314  11.319  33.905  1.00 21.82      BLGL
ATOM   2819  N   PHE   375      27.214   9.981  35.728  1.00 21.81      BLGL
ATOM   2820  CA  PHE   375      27.800  10.937  36.664  1.00 23.69      BLGL
ATOM   2821  CB  PHE   375      26.780  11.387  37.722  1.00 22.43      BLGL
ATOM   2822  CG  PHE   375      25.641  12.195  37.169  1.00 24.54      BLGL
ATOM   2823  CD1 PHE   375      24.652  11.592  36.389  1.00 24.54      BLGL
ATOM   2824  CD2 PHE   375      25.563  13.566  37.407  1.00 22.99      BLGL
ATOM   2825  CE1 PHE   375      23.606  12.343  35.856  1.00 21.26      BLGL
ATOM   2826  CE2 PHE   375      24.521  14.324  36.877  1.00 20.60      BLGL
ATOM   2827  CZ  PHE   375      23.543  13.712  36.101  1.00 22.10      BLGL
ATOM   2828  C   PHE   375      28.928  10.184  37.356  1.00 24.96      BLGL
ATOM   2829  O   PHE   375      28.849   8.963  37.505  1.00 26.41      BLGL
ATOM   2830  N   ASP   376      29.975  10.890  37.771  1.00 24.80      BLGL
ATOM   2831  CA  ASP   376      31.070  10.217  38.449  1.00 24.64      BLGL
ATOM   2832  CB  ASP   376      32.369  11.030  38.382  1.00 25.91      BLGL
ATOM   2833  CG  ASP   376      32.243  12.411  39.007  1.00 26.81      BLGL
ATOM   2834  OD1 ASP   376      31.528  12.566  40.022  1.00 26.23      BLGL
ATOM   2835  OD2 ASP   376      32.885  13.343  38.484  1.00 27.73      BLGL
ATOM   2836  C   ASP   376      30.698   9.969  39.899  1.00 24.00      BLGL
ATOM   2837  O   ASP   376      29.621  10.349  40.344  1.00 22.18      BLGL
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Fig. 4 cont.

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ATOM   2838  N   PHE  377      31.610   9.333  40.625  1.00 24.93      BLGL
ATOM   2839  CA  PHE  377      31.421   9.000  42.030  1.00 26.87      BLGL
ATOM   2840  CB  PHE  377      32.652   8.256  42.530  1.00 24.91      BLGL
ATOM   2841  CG  PHE  377      32.915   6.967  41.811  1.00 26.64      BLGL
ATOM   2842  CD1 PHE  377      34.185   6.394  41.837  1.00 27.20      BLGL
ATOM   2843  CD2 PHE  377      31.891   6.298  41.141  1.00 27.03      BLGL
ATOM   2844  CE1 PHE  377      34.434   5.168  41.209  1.00 27.98      BLGL
ATOM   2845  CE2 PHE  377      32.127   5.073  40.511  1.00 27.70      BLGL
ATOM   2846  CZ  PHE  377      33.402   4.505  40.546  1.00 28.28      BLGL
ATOM   2847  C   PHE  377      31.162  10.214  42.919  1.00 28.76      BLGL
ATOM   2848  O   PHE  377      30.660  10.084  44.041  1.00 29.47      BLGL
ATOM   2849  N   LYS  378      31.500  11.393  42.410  1.00 30.92      BLGL
ATOM   2850  CA  LYS  378      31.322  12.634  43.155  1.00 32.99      BLGL
ATOM   2851  CB  LYS  378      32.533  13.546  42.927  1.00 36.98      BLGL
ATOM   2852  CG  LYS  378      33.889  12.924  43.274  1.00 39.50      BLGL
ATOM   2853  CD  LYS  378      34.230  13.053  44.759  1.00 43.64      BLGL
ATOM   2854  CE  LYS  378      33.249  12.300  45.651  1.00 45.28      BLGL
ATOM   2855  NZ  LYS  378      33.467  12.607  47.092  1.00 46.72      BLGL
ATOM   2856  C   LYS  378      30.040  13.391  42.800  1.00 32.50      BLGL
ATOM   2857  O   LYS  378      29.803  14.487  43.309  1.00 31.66      BLGL
ATOM   2858  N   GLY  379      29.224  12.816  41.919  1.00 32.04      BLGL
ATOM   2859  CA  GLY  379      27.975  13.453  41.544  1.00 32.10      BLGL
ATOM   2860  C   GLY  379      28.092  14.430  40.397  1.00 33.14      BLGL
ATOM   2861  O   GLY  379      27.146  15.159  40.085  1.00 32.60      BLGL
ATOM   2862  N   ARG  380      29.261  14.451  39.771  1.00 35.05      BLGL
ATOM   2863  CA  ARG  380      29.507  15.342  38.647  1.00 35.69      BLGL
ATOM   2864  CB  ARG  380      30.958  15.817  38.660  1.00 40.31      BLGL
ATOM   2865  CG  ARG  380      31.123  17.323  38.592  1.00 48.35      BLGL
ATOM   2866  CD  ARG  380      32.569  17.728  38.876  1.00 55.04      BLGL
ATOM   2867  NE  ARG  380      33.058  17.213  40.164  1.00 61.15      BLGL
ATOM   2868  CZ  ARG  380      33.782  16.100  40.318  1.00 61.98      BLGL
ATOM   2869  NH1 ARG  380      34.117  15.362  39.267  1.00 62.74      BLGL
ATOM   2870  NH2 ARG  380      34.178  15.720  41.529  1.00 60.75      BLGL
ATOM   2871  C   ARG  380      29.216  14.587  37.354  1.00 34.09      BLGL
ATOM   2872  O   ARG  380      29.551  13.404  37.213  1.00 34.62      BLGL
ATOM   2873  N   PRO  381      28.590  15.265  36.386  1.00 30.20      BLGL
ATOM   2874  CD  PRO  381      28.201  16.683  36.407  1.00 27.18      BLGL
ATOM   2875  CA  PRO  381      28.250  14.653  35.101  1.00 28.29      BLGL
ATOM   2876  CB  PRO  381      27.395  15.723  34.438  1.00 27.26      BLGL
ATOM   2877  CG  PRO  381      28.018  16.980  34.941  1.00 26.31      BLGL
ATOM   2878  C   PRO  381      29.453  14.278  34.260  1.00 26.53      BLGL
ATOM   2879  O   PRO  381      30.436  15.014  34.221  1.00 27.34      BLGL
ATOM   2880  N   LEU  382      29.370  13.122  33.601  1.00 26.02      BLGL
ATOM   2881  CA  LEU  382      30.439  12.645  32.721  1.00 24.03      BLGL
ATOM   2882  CB  LEU  382      30.475  11.116  32.656  1.00 21.52      BLGL
ATOM   2883  CG  LEU  382      30.769  10.338  33.934  1.00 22.08      BLGL
ATOM   2884  CD1 LEU  382      30.549   8.867  33.678  1.00 21.34      BLGL
ATOM   2885  CD2 LEU  382      32.190  10.608  34.390  1.00 21.32      BLGL
ATOM   2886  C   LEU  382      30.128  13.174  31.336  1.00 23.10      BLGL
ATOM   2887  O   LEU  382      28.964  13.412  30.996  1.00 22.81      BLGL
ATOM   2888  N   PRO  383      31.160  13.364  30.511  1.00 22.83      BLGL
ATOM   2889  CD  PRO  383      32.593  13.134  30.744  1.00 21.59      BLGL
ATOM   2890  CA  PRO  383      30.919  13.873  29.159  1.00 22.58      BLGL
ATOM   2891  CB  PRO  383      32.327  13.950  28.559  1.00 22.02      BLGL
ATOM   2892  CG  PRO  383      33.101  12.953  29.345  1.00 23.42      BLGL
ATOM   2893  C   PRO  383      29.959  13.008  28.340  1.00 22.29      BLGL
ATOM   2894  O   PRO  383      29.346  13.491  27.395  1.00 23.29      BLGL
ATOM   2895  N   SER  384      29.815  11.739  28.718  1.00 23.07      BLGL
ATOM   2896  CA  SER  384      28.918  10.830  28.014  1.00 23.32      BLGL
ATOM   2897  CB  SER  384      29.189   9.387  28.438  1.00 23.43      BLGL
ATOM   2898  OG  SER  384      28.997   9.221  29.827  1.00 22.72      BLGL
ATOM   2899  C   SER  384      27.441  11.166  28.253  1.00 24.76      BLGL
ATOM   2900  O   SER  384      26.556  10.584  27.629  1.00 25.96      BLGL
ATOM   2901  N   LEU  385      27.166  12.094  29.160  1.00 23.88      BLGL
ATOM   2902  CA  LEU  385      25.792  12.474  29.419  1.00 24.72      BLGL
ATOM   2903  CB  LEU  385      25.721  13.380  30.644  1.00 22.46      BLGL
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Fig. 4 cont.

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ATOM   2904  CG  LEU   385      24.332  13.873  31.055  1.00 23.33      BLGL
ATOM   2905  CD1 LEU   385      23.424  12.687  31.367  1.00 22.86      BLGL
ATOM   2906  CD2 LEU   385      24.458  14.778  32.268  1.00 20.09      BLGL
ATOM   2907  C   LEU   385      25.250  13.207  28.193  1.00 26.26      BLGL
ATOM   2908  O   LEU   385      24.041  13.255  27.958  1.00 25.15      BLGL
ATOM   2909  N   HIS   386      26.161  13.763  27.404  1.00 28.46      BLGL
ATOM   2910  CA  HIS   386      25.789  14.512  26.213  1.00 32.60      BLGL
ATOM   2911  CB  HIS   386      26.937  15.437  25.816  1.00 37.77      BLGL
ATOM   2912  CG  HIS   386      27.172  16.539  26.799  1.00 45.65      BLGL
ATOM   2913  CD2 HIS   386      26.393  17.016  27.801  1.00 45.94      BLGL
ATOM   2914  ND1 HIS   386      28.330  17.291  26.820  1.00 48.26      BLGL
ATOM   2915  CE1 HIS   386      28.254  18.180  27.795  1.00 49.16      BLGL
ATOM   2916  NE2 HIS   386      27.089  18.033  28.405  1.00 49.07      BLGL
ATOM   2917  C   HIS   386      25.392  13.656  25.025  1.00 32.02      BLGL
ATOM   2918  O   HIS   386      25.011  14.184  23.979  1.00 34.90      BLGL
ATOM   2919  N   VAL   387      25.467  12.341  25.177  1.00 29.53      BLGL
ATOM   2920  CA  VAL   387      25.117  11.461  24.075  1.00 27.58      BLGL
ATOM   2921  CB  VAL   387      25.236   9.974  24.496  1.00 27.23      BLGL
ATOM   2922  CG1 VAL   387      24.191   9.637  25.547  1.00 25.13      BLGL
ATOM   2923  CG2 VAL   387      25.114   9.072  23.276  1.00 23.77      BLGL
ATOM   2924  C   VAL   387      23.701  11.760  23.572  1.00 26.94      BLGL
ATOM   2925  O   VAL   387      23.450  11.750  22.369  1.00 26.81      BLGL
ATOM   2926  N   PHE   388      22.788  12.060  24.491  1.00 25.61      BLGL
ATOM   2927  CA  PHE   388      21.403  12.339  24.136  1.00 26.79      BLGL
ATOM   2928  CB  PHE   388      20.586  12.619  25.390  1.00 25.81      BLGL
ATOM   2929  CG  PHE   388      20.433  11.432  26.272  1.00 26.19      BLGL
ATOM   2930  CD1 PHE   388      21.003  11.412  27.536  1.00 27.32      BLGL
ATOM   2931  CD2 PHE   388      19.728  10.317  25.834  1.00 25.78      BLGL
ATOM   2932  CE1 PHE   388      20.873  10.300  28.355  1.00 27.00      BLGL
ATOM   2933  CE2 PHE   388      19.592   9.198  26.647  1.00 26.04      BLGL
ATOM   2934  CZ  PHE   388      20.166   9.189  27.909  1.00 26.12      BLGL
ATOM   2935  C   PHE   388      21.188  13.470  23.141  1.00 29.70      BLGL
ATOM   2936  O   PHE   388      20.176  13.496  22.424  1.00 29.14      BLGL
ATOM   2937  N   GLN   389      22.125  14.412  23.102  1.00 31.10      BLGL
ATOM   2938  CA  GLN   389      22.022  15.532  22.174  1.00 32.46      BLGL
ATOM   2939  CB  GLN   389      22.603  16.797  22.793  1.00 35.41      BLGL
ATOM   2940  CG  GLN   389      22.086  17.088  24.177  1.00 44.69      BLGL
ATOM   2941  CD  GLN   389      22.807  18.261  24.818  1.00 50.70      BLGL
ATOM   2942  OE1 GLN   389      22.674  19.401  24.372  1.00 52.70      BLGL
ATOM   2943  NE2 GLN   389      23.588  17.985  25.866  1.00 53.54      BLGL
ATOM   2944  C   GLN   389      22.779  15.221  20.893  1.00 30.30      BLGL
ATOM   2945  O   GLN   389      22.270  15.416  19.790  1.00 31.42      BLGL
ATOM   2946  N   TYR   390      23.993  14.715  21.051  1.00 28.80      BLGL
ATOM   2947  CA  TYR   390      24.851  14.403  19.917  1.00 30.88      BLGL
ATOM   2948  CB  TYR   390      26.204  13.911  20.427  1.00 35.50      BLGL
ATOM   2949  CG  TYR   390      26.963  14.956  21.217  1.00 41.72      BLGL
ATOM   2950  CD1 TYR   390      28.151  14.632  21.871  1.00 45.09      BLGL
ATOM   2951  CE1 TYR   390      28.861  15.595  22.603  1.00 47.24      BLGL
ATOM   2952  CD2 TYR   390      26.496  16.273  21.313  1.00 42.36      BLGL
ATOM   2953  CE2 TYR   390      27.192  17.240  22.043  1.00 45.40      BLGL
ATOM   2954  CZ  TYR   390      28.376  16.894  22.686  1.00 47.41      BLGL
ATOM   2955  OH  TYR   390      29.078  17.841  23.406  1.00 46.59      BLGL
ATOM   2956  C   TYR   390      24.298  13.425  18.889  1.00 29.06      BLGL
ATOM   2957  O   TYR   390      24.591  13.553  17.704  1.00 29.24      BLGL
ATOM   2958  N   VAL   391      23.508  12.450  19.324  1.00 27.33      BLGL
ATOM   2959  CA  VAL   391      22.943  11.488  18.381  1.00 25.21      BLGL
ATOM   2960  CB  VAL   391      22.008  10.476  19.087  1.00 23.42      BLGL
ATOM   2961  CG1 VAL   391      22.803   9.635  20.061  1.00 19.38      BLGL
ATOM   2962  CG2 VAL   391      20.886  11.202  19.805  1.00 21.53      BLGL
ATOM   2963  C   VAL   391      22.154  12.226  17.299  1.00 26.03      BLGL
ATOM   2964  O   VAL   391      22.028  11.749  16.175  1.00 23.37      BLGL
ATOM   2965  N   ASP   392      21.635  13.400  17.647  1.00 27.71      BLGL
ATOM   2966  CA  ASP   392      20.862  14.200  16.710  1.00 30.77      BLGL
ATOM   2967  CB  ASP   392      20.134  15.323  17.448  1.00 32.83      BLGL
ATOM   2968  CG  ASP   392      18.986  14.820  18.302  1.00 34.68      BLGL
ATOM   2969  OD1 ASP   392      18.444  15.617  19.103  1.00 35.32      BLGL
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Fig. 4 cont.

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ATOM   2970  OD2 ASP   392      18.618  13.636  18.167  1.00 35.22      BLGL
ATOM   2971  C   ASP   392      21.731  14.818  15.621  1.00 33.35      BLGL
ATOM   2972  O   ASP   392      21.467  14.650  14.430  1.00 35.61      BLGL
ATOM   2973  N   THR   393      22.777  15.526  16.035  1.00 34.96      BLGL
ATOM   2974  CA  THR   393      23.664  16.215  15.105  1.00 34.87      BLGL
ATOM   2975  CB  THR   393      23.998  17.626  15.602  1.00 35.87      BLGL
ATOM   2976  OG1 THR   393      24.820  17.526  16.774  1.00 37.14      BLGL
ATOM   2977  CG2 THR   393      22.726  18.392  15.952  1.00 35.93      BLGL
ATOM   2978  C   THR   393      24.991  15.518  14.908  1.00 36.53      BLGL
ATOM   2979  O   THR   393      25.462  15.358  13.787  1.00 36.72      BLGL
ATOM   2980  N   GLY   394      25.596  15.115  16.014  1.00 38.00      BLGL
ATOM   2981  CA  GLY   394      26.896  14.481  15.961  1.00 38.77      BLGL
ATOM   2982  C   GLY   394      27.828  15.442  16.679  1.00 40.97      BLGL
ATOM   2983  O   GLY   394      27.389  16.494  17.143  1.00 40.87      BLGL
ATOM   2984  N   THR   395      29.105  15.107  16.787  1.00 43.10      BLGL
ATOM   2985  CA  THR   395      30.043  15.990  17.461  1.00 45.02      BLGL
ATOM   2986  CB  THR   395      30.967  15.197  18.393  1.00 43.84      BLGL
ATOM   2987  OG1 THR   395      31.206  13.896  17.840  1.00 43.18      BLGL
ATOM   2988  CG2 THR   395      30.340  15.054  19.753  1.00 41.53      BLGL
ATOM   2989  C   THR   395      30.883  16.752  16.443  1.00 48.88      BLGL
ATOM   2990  O   THR   395      31.470  16.155  15.536  1.00 49.70      BLGL
ATOM   2991  N   PRO   396      30.941  18.089  16.578  1.00 52.29      BLGL
ATOM   2992  CD  PRO   396      30.225  18.889  17.594  1.00 52.46      BLGL
ATOM   2993  CA  PRO   396      31.712  18.955  15.672  1.00 52.98      BLGL
ATOM   2994  CB  PRO   396      31.537  20.343  16.291  1.00 53.36      BLGL
ATOM   2995  CG  PRO   396      30.173  20.256  16.948  1.00 52.73      BLGL
ATOM   2996  C   PRO   396      33.188  18.543  15.578  1.00 53.94      BLGL
ATOM   2997  O   PRO   396      33.678  18.369  14.436  1.00 54.55      BLGL
END
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                                  9         19         29         39
---------- ---------- -ALTYRGVDW SSVVVEERAG VSYKNTNGNA QPLENILAAN   39 MT
---------- ---------- -ALQYKGVDW SSVMVEERAG VRYKNVNGQE KPLEYILAEN   39 HI
---------- ---------- -ALTYRGADI SSLLLLEDEG YSYKNLNGQT QALETILADA   39 AA
AHRDSGTAKS GLYVEKVSGL RKDFIKGVDV SSIIALEESG VAFYNESGKK QDIFNTLKEA   60 BL
        10         20         30         40         50         60

        49    54             61         71         81         91
GVNTVRQRVW VNPAD----- ---GNYNLDY NIAIAKRAKA AGLGVYIDFH YSDTWADPAH   91
GVNMVRQRVW VNPWD----- ---GNYNLDY NIQLARRAKA AGLGLYINFH YSDTWADPAH   91
GINSIRQRVW VNPSD----- ---GSYDLDY NLELAKRVKA AGMSLYLDLH LSDTWADPSD   91
GVNYVRVRIW NDPYDANGNG YGGGNNDLEK AIQIGKRANA NGMKLLADFH YSDFWADPAK  120
        70         80         90        100        110        120

       100        110        120        130        140        150
QTMPAGWP-S DIDNLSWKLY NYTLDAANKL QNAGIQPTIV SIGNEIRAGL LWPTGRTENW  150
QTTPAGWP-S DINNLAWKLY NYTLDSMNRF ADAGIQVDIV SIGNEITQGL LWPLGKTNNW  150
QTTPSGWSTT DLGTLKWQLY NYTLEVCNTF AENDIDIEII SIGNEIRAGL LWPLGETSSY  151
QKAPKAWANL NFEDKKTALY QYTKQSLKAM KAAGIDIGMV QVGNETNGGL A----GETDW  176
       130        140        150        160        170        176

       160        170        180        190        200        210
ANIARLLHSA AWGIKDSSLS PKPKIMIHLD NGWDWGTQNW WYTNVLKQGT LELSDFDMMG  210
YNIARLLHSA AWGVKDSRLN PKPKIMVHLD NGWNWDTQNW WYTNVLSQGP FEMSDFDMMG  210
SNIGALLHSG AWGVKDSNLA TTPKIMIHLD DGWSWDQQNY FYETVLATGE LLSTDFDYFG  211
AKMSQLFNAG SQAVRETD-- SNILVALHFT NPETSGRYAW IAETLHRH-- --HVDYDVFA  230
       186                204        214                230

       220        230        240        250        255        265
VSFYPFYSSS ATLSALKSSL DNMAKTWNKE IAVVETNWPI SC-----PNP RYSFPSDVKN  265
VSFYPFYSAS ATLDSLRRSL NNMVSRWGKE VAVVETNWPT SC-----PYP RYQFPADVRN  265
VSYYPFYSAS ATLASLKTSL ANLQSTYDKP VVVVETNWPV SC-----PNP AYAFPSDLSS  266
SSYYPFW--H GTLKNLTSVL TSVADTYGKK VMVAETSYTY TAEDGDGHGN TAPKNGQTLN  288
       238        248        258        268        278        288

       275        285        294
IPFSPEGQTT FITNVANIVS SVS-RGVGLF YWEPAWIH-- ---------- ----------  302
VPFSAAGQTQ YIQSVANVVS SVS-KGVGLF YWEPAWIH-- ---------- ----------  302
IPFSVAGQQE FLEKLAAVVE ATT-DGLGVY YWEPAWIG-- ---------- ----------  303
NPVTVQGQAN AVRDVIQAVS DVGEAGIGVF YWEPAWIPVG PAHRLEKNKA LWETYGSGWA  348
       298        308        318        328        338        348

                  309        318        328
---------- ---NANLGSS CADNTMFSQ- SGQALSSLSV FQRI------ --    332
---------- ---NANLGSS CADNTMFTP- SGQALSSLSV FHRI------ --    332
---------- ---NAGLGSS CADNLMVDYT TDEVYESIET LGEL------ --    334
TSYAAEYDPE DAGKWFGGSA VDNQALFDF- KGRPLPSLHV FQYVDTGTPF KN    399
       358        368        377        387        397
```

Fig. 5

```
                                  9         19         29         39
---------- ---------- -ALTYRGVDW SSVVVEERAG VSYKNTNGNA QPLENILAAN   39 MT
---------- ---------- -ALQYKGVDW SSVMVEERAG VRYKNVNGQE KPLEYILAEN   39 HI
---------- ---------- -ALTYRGADI SSLLLLEDEG YSYKNLNGQT QALETILADA   39 AA
AHRDSGTAKS GLYVEKVSGL RKDFIKGVDV SSIIALEESG VAFYNESGKK QDIFNTLKEA   60 BL
---------- ---------- -ALTYRGADI SSLLIEEDAG ISYKNLNGET QALEDILVNN   39 AT
---------- ---------M NKDFIKGADV SSVIALENSG VTFYNTNGKR QDIFTTLKQA   41 BS
---------- ----NTGVAD NTPFYVGADL SYVNEMESCG ATYRD-QGKK VDPFQLFADK   45 PF
                    6         16         26         35         45

        49    54          61         71         81         91
GVNTVRQRVW VNPAD----- ---GNYNLDY NIAIAKRAKA AGLGVYIDFH YSDTWADPAH   91
GVNMVRQRVW VNPWD----- ---GNYNLDY NIQLARRAKA AGLGLYINFH YSDTWADPAH   91
GINSIRQRVW VNPSD----- ---GSYDLDY NLELAKRVKA AGMSLYLDLH LSDTWADPSD   91
GVNYVRVRIW NDPYDANGNG YGGGNNDLEK AIQIGKRANA NGMKLLADFH YSDFWADPAK  120
GVNSIRQRVW VDPSD----- ---GSYDLDY NLKLAKRVQA AGMSIYLDLH LSDTWADPSD   91
GVNYVRVRIW NHPYDSNGNG YGGGNNDVQK AIEIGKRATA NGMKVLADFH YSDFWADPAK  101
GADLVRVRLW HNATWT---- ---KYSDLKD VSKTLKRAKN AGMKTLLDFH YSDTWTDPEK   98
        55     61          68         78         88         98

      99         109        119        129        139    145
QTMPAGWP-- SDIDNLSWKL YNYTLDAANK LQNAGIQPTI VSIGNEIRAG LLWPTG----  145
QTTPAGWP-- SDINNLAWKL YNYTLDSMNR FADAGIQVDI VSIGNEITQG LLWPLG----  145
QTTPSGWST- TDLGTLKWQL YNYTLEVCNT FAENDIDIEI ISIGNEIRAG LLWPLG----  146
QKAPKAWAN- LNFEDKKTAL YQYTKQSLKA MKAAGIDIGM VQVGNETNGG LA--------  171
QTTPTGWST- TDIDTLTWQL YNYTLEVCNT FAENDIDVEI VSIGNEISSG LLWPLG----  146
QKVPKAWAN- LSFEAKKAKL YEYTKQSLQK MIKEGVDIGM VQVGNETTGG FA--------  152
QFIPKAWAHI TDTKELAKAL YDYTTDTLAS LDQQQLLPNL VQVGNETNIE ILQAEDTLVH  158
       109        118        128        138        148        158

      155        165        175        185        195        205
RTENWANIAR LLHSAAWGIK DSSLSPKPKI MIHLDNGWDW GTQNWWYTNV LKQGTLELSD  205
KTNNWYNIAR LLHSAAWGVK DSRLNPKPKI MVHLDNGWNW DTQNWWYTNV LSQGPFEMSD  205
ETSSYSNIGA LLHSGAWGVK DSNLATTPKI MIHLDDGWSW DQQNYFYETV LATGELLSTD  206
GETDWAKMSQ LFNAGSQAVR ETD--SNILV ALHFTNPETS GRYAWIAETL HRH----HVD  225
KTSNYDNIAK LLHSGAWGVK DSDLTTTPKI MIHLDNGWDW DEQEYFYKTV LATGSLLSTD  206
GETDWTKMCQ LFNEGSRAVR ETN--SNILV ALHFTNPETA GRYSFIAETL SKN----KVD  206
GIPNWQRNAT LLNSGVNAVR DYSKKTGKPI QVVLHIAQPE NALWWFKQAK ENG----VID  214
       168        178        188        198        208        214

      215        225        235        245    252        260
FDMMGVSFYP FYSSSATLSA LKSSLDNMAK TWNKEIAVVE TNWPISC--- --PNPRYSFP  260
FDMMGVSFYP FYSASATLDS LRRSLNNMVS RWGKEVAVVE TNWPTSC--- --PYPRYQFP  260
FDYFGVSYYP FYSASATLAS LKTSLANLQS TYDKPVVVVE TNWPVSC--- --PNPAYAFP  261
YDVFASSYYP FW--HGTLKN LTSVLTSVAD TYGKKVMVAE TSYTYTAEDG DGHGNTAPKN  283
FDLMGVSYYP FYSSEATLSS LKTSLTNMQS NYDKPVVVVE TNWPVSC--- --PDPEYSFP  261
YDVFASSYYP FW--HGTLQN LTSVLKAVAN TYGKKVMVAE TSYTYTAEDG DGHGNTAPKS  264
YDVIGLSYYP QWS-EYSLPQ LPDAIAELQN TYHKPVMIVE TAYPWTLHNF DQAGNVLGEK  273
       224        233        243        253        263        273

      270        280        289        299
SDVKNIPFSP EGQTTFITNV ANIVSSVS-R GVGLFYWEPA WIH------- ----------  302
ADVRNVPFSA AGQTQYIQSV ANVVSSVS-K GVGLFYWEPA WIH------- ----------  302
SDLSSIPFSV AGQQEFLEKL AAVVEATT-D GLGVYYWEPA WIG------- ----------  303
GQTLNNPVTV QGQANAVRDV IQAVSDVGEA GIGVFYWEPA WIPVGPAHRL EKNKALWETY  333
SDLTSIPFSA AGQEEFLEKL AEVVEGVT-D GLGIYYWEPA WID------- ----------  303
GQTLPYPISV QGQATAVRDV MEAVANTGKA GLGVFYWEPA WIPVGPKTQI EKNKVLWETY  314
AVQPEFPASP RGQLTYLLTL TQLVKSAG-- GMGVIYWEPA WVSTRCR--- ----------  318
       283        293      301        311
```

Fig. 6

```
                                314        322        332
---------- --------NA NLGSSCADNT MFSQ--SGQA LSSLSVFQRI --------    332
---------- --------NA NLGSSCADNT MFTP--SGQA LSSLSVFHRI --------    332
---------- --------NA GLGSSCADNL MVDYT-TDEV YESIETLGEL --------    334
GSGWATSYAA EYDPEDAGKW FGGSAVDNQA LFDF--KGRP LPSLHVFQYV DTGTPFKN    399
---------- --------NA GLGSSCADNL MVDVN-TDEV LESVTVFEDL --------    334
GSGWASSYAA EYDPEDAGKW YGGSAVDNQA LFDF--NGHP LPSLQVFQYA --------    372
---------- --------TLW GKGSHWENAS FFDATRKNNA LPAFLFFKAD YQASAQAE    359
                  321        331        341        351
```

Fig. 6 cont.

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HEADER                                                          BLGL
ATOM      1  C   GLY    11      35.975  14.251  23.684  1.00 48.49      BLGL
ATOM      2  O   GLY    11      36.590  13.193  23.517  1.00 48.50      BLGL
ATOM      3  N   GLY    11      36.372  16.222  25.216  1.00 48.08      BLGL
ATOM      4  CA  GLY    11      36.733  15.548  23.933  1.00 47.57      BLGL
ATOM      5  N   LEU    12      34.642  14.326  23.653  1.00 48.44      BLGL
ATOM      6  CA  LEU    12      33.796  13.147  23.416  1.00 45.49      BLGL
ATOM      7  CB  LEU    12      32.592  13.139  24.371  1.00 43.64      BLGL
ATOM      8  CG  LEU    12      31.626  11.961  24.199  1.00 41.45      BLGL
ATOM      9  CD1 LEU    12      32.074  10.803  25.085  1.00 36.51      BLGL
ATOM     10  CD2 LEU    12      30.203  12.400  24.550  1.00 41.11      BLGL
ATOM     11  C   LEU    12      33.272  13.109  21.979  1.00 44.11      BLGL
ATOM     12  O   LEU    12      32.688  14.086  21.502  1.00 45.18      BLGL
ATOM     13  N   TYR    13      33.487  11.986  21.295  1.00 42.63      BLGL
ATOM     14  CA  TYR    13      33.004  11.817  19.928  1.00 41.19      BLGL
ATOM     15  CB  TYR    13      34.083  11.206  19.042  1.00 45.36      BLGL
ATOM     16  CG  TYR    13      33.594  10.996  17.624  1.00 52.03      BLGL
ATOM     17  CD1 TYR    13      33.232   9.727  17.167  1.00 53.91      BLGL
ATOM     18  CE1 TYR    13      32.703   9.545  15.872  1.00 55.69      BLGL
ATOM     19  CD2 TYR    13      33.420  12.083  16.756  1.00 53.77      BLGL
ATOM     20  CE2 TYR    13      32.890  11.914  15.466  1.00 54.66      BLGL
ATOM     21  CZ  TYR    13      32.534  10.644  15.031  1.00 56.09      BLGL
ATOM     22  OH  TYR    13      32.009  10.473  13.764  1.00 56.62      BLGL
ATOM     23  C   TYR    13      31.755  10.932  19.837  1.00 38.22      BLGL
ATOM     24  O   TYR    13      31.686   9.887  20.471  1.00 38.74      BLGL
ATOM     25  N   VAL    14      30.776  11.355  19.039  1.00 34.88      BLGL
ATOM     26  CA  VAL    14      29.537  10.604  18.845  1.00 31.50      BLGL
ATOM     27  CB  VAL    14      28.418  11.094  19.777  1.00 30.78      BLGL
ATOM     28  CG1 VAL    14      27.102  10.405  19.427  1.00 30.71      BLGL
ATOM     29  CG2 VAL    14      28.790  10.812  21.203  1.00 30.70      BLGL
ATOM     30  C   VAL    14      29.069  10.798  17.420  1.00 30.74      BLGL
ATOM     31  O   VAL    14      28.776  11.917  17.007  1.00 31.52      BLGL
ATOM     32  N   GLU    15      28.994   9.710  16.669  1.00 30.21      BLGL
ATOM     33  CA  GLU    15      28.555   9.788  15.288  1.00 30.31      BLGL
ATOM     34  CB  GLU    15      29.002   8.546  14.534  1.00 33.96      BLGL
ATOM     35  CG  GLU    15      28.509   8.486  13.113  1.00 43.05      BLGL
ATOM     36  CD  GLU    15      28.927   7.202  12.424  1.00 49.32      BLGL
ATOM     37  OE1 GLU    15      28.886   6.140  13.087  1.00 51.29      BLGL
ATOM     38  OE2 GLU    15      29.285   7.251  11.223  1.00 54.28      BLGL
ATOM     39  C   GLU    15      27.045   9.931  15.206  1.00 28.83      BLGL
ATOM     40  O   GLU    15      26.303   9.161  15.816  1.00 26.88      BLGL
ATOM     41  N   LYS    16      26.596  10.923  14.445  1.00 29.24      BLGL
ATOM     42  CA  LYS    16      25.173  11.173  14.280  1.00 30.57      BLGL
ATOM     43  CB  LYS    16      24.933  12.207  13.174  1.00 32.52      BLGL
ATOM     44  CG  LYS    16      23.454  12.496  12.948  1.00 38.94      BLGL
ATOM     45  CD  LYS    16      23.141  12.889  11.510  1.00 43.38      BLGL
ATOM     46  CE  LYS    16      23.632  14.282  11.176  1.00 46.85      BLGL
ATOM     47  NZ  LYS    16      23.276  14.648   9.776  1.00 50.40      BLGL
ATOM     48  C   LYS    16      24.399   9.902  13.938  1.00 29.87      BLGL
ATOM     49  O   LYS    16      24.836   9.090  13.121  1.00 28.75      BLGL
ATOM     50  N   VAL    17      23.249   9.733  14.575  1.00 29.36      BLGL
ATOM     51  CA  VAL    17      22.394   8.591  14.306  1.00 29.25      BLGL
ATOM     52  CB  VAL    17      21.437   8.328  15.476  1.00 28.63      BLGL
ATOM     53  CG1 VAL    17      20.469   7.201  15.127  1.00 28.74      BLGL
ATOM     54  CG2 VAL    17      22.236   7.982  16.702  1.00 30.70      BLGL
ATOM     55  C   VAL    17      21.582   8.940  13.064  1.00 30.63      BLGL
ATOM     56  O   VAL    17      20.794   9.891  13.064  1.00 30.98      BLGL
ATOM     57  N   SER    18      21.782   8.172  12.005  1.00 30.58      BLGL
ATOM     58  CA  SER    18      21.083   8.422  10.758  1.00 33.73      BLGL
ATOM     59  CB  SER    18      21.787   7.675   9.628  1.00 36.18      BLGL
ATOM     60  OG  SER    18      21.984   6.324   9.990  1.00 38.96      BLGL
ATOM     61  C   SER    18      19.611   8.032  10.800  1.00 32.04      BLGL
ATOM     62  O   SER    18      19.264   6.933  11.231  1.00 31.91      BLGL
ATOM     63  N   GLY    19      18.755   8.950  10.359  1.00 31.92      BLGL
ATOM     64  CA  GLY    19      17.328   8.697  10.327  1.00 30.75      BLGL
ATOM     65  C   GLY    19      16.601   8.894  11.638  1.00 30.09      BLGL
```

Fig. 4

ATOM	66	O	GLY	19	15.395	8.684	11.705	1.00 32.49	BLGL
ATOM	67	N	LEU	20	17.314	9.295	12.681	1.00 28.46	BLGL
ATOM	68	CA	LEU	20	16.672	9.498	13.967	1.00 28.28	BLGL
ATOM	69	CB	LEU	20	17.706	9.910	15.013	1.00 29.28	BLGL
ATOM	70	CG	LEU	20	17.141	9.983	16.436	1.00 29.10	BLGL
ATOM	71	CD1	LEU	20	16.756	8.586	16.904	1.00 27.36	BLGL
ATOM	72	CD2	LEU	20	18.165	10.598	17.359	1.00 29.58	BLGL
ATOM	73	C	LEU	20	15.565	10.548	13.890	1.00 25.87	BLGL
ATOM	74	O	LEU	20	15.821	11.686	13.535	1.00 24.28	BLGL
ATOM	75	N	ARG	21	14.342	10.147	14.226	1.00 28.07	BLGL
ATOM	76	CA	ARG	21	13.176	11.030	14.213	1.00 30.64	BLGL
ATOM	77	CB	ARG	21	11.912	10.211	14.476	1.00 31.64	BLGL
ATOM	78	CG	ARG	21	11.955	9.430	15.792	1.00 35.81	BLGL
ATOM	79	CD	ARG	21	10.892	8.339	15.840	1.00 36.79	BLGL
ATOM	80	NE	ARG	21	9.536	8.877	15.850	1.00 37.50	BLGL
ATOM	81	CZ	ARG	21	8.445	8.133	15.699	1.00 38.47	BLGL
ATOM	82	NH1	ARG	21	8.567	6.826	15.525	1.00 37.04	BLGL
ATOM	83	NH2	ARG	21	7.235	8.688	15.731	1.00 39.56	BLGL
ATOM	84	C	ARG	21	13.316	12.114	15.277	1.00 32.05	BLGL
ATOM	85	O	ARG	21	13.840	11.862	16.354	1.00 31.41	BLGL
ATOM	86	N	LYS	22	12.832	13.315	14.978	1.00 35.57	BLGL
ATOM	87	CA	LYS	22	12.927	14.428	15.916	1.00 37.84	BLGL
ATOM	88	CB	LYS	22	12.378	15.713	15.291	1.00 42.04	BLGL
ATOM	89	CG	LYS	22	13.278	16.381	14.265	1.00 47.84	BLGL
ATOM	90	CD	LYS	22	12.908	17.872	14.150	1.00 51.73	BLGL
ATOM	91	CE	LYS	22	13.460	18.518	12.882	1.00 52.80	BLGL
ATOM	92	NZ	LYS	22	12.732	18.062	11.661	1.00 52.64	BLGL
ATOM	93	C	LYS	22	12.225	14.227	17.253	1.00 36.42	BLGL
ATOM	94	O	LYS	22	12.672	14.762	18.264	1.00 37.54	BLGL
ATOM	95	N	ASP	23	11.128	13.476	17.262	1.00 34.94	BLGL
ATOM	96	CA	ASP	23	10.370	13.264	18.495	1.00 33.91	BLGL
ATOM	97	CB	ASP	23	8.869	13.257	18.181	1.00 34.54	BLGL
ATOM	98	CG	ASP	23	8.465	12.096	17.303	1.00 34.79	BLGL
ATOM	99	OD1	ASP	23	9.242	11.739	16.392	1.00 33.67	BLGL
ATOM	100	OD2	ASP	23	7.365	11.547	17.521	1.00 39.44	BLGL
ATOM	101	C	ASP	23	10.754	11.989	19.238	1.00 31.78	BLGL
ATOM	102	O	ASP	23	10.001	11.495	20.083	1.00 31.40	BLGL
ATOM	103	N	PHE	24	11.932	11.467	18.921	1.00 28.21	BLGL
ATOM	104	CA	PHE	24	12.423	10.256	19.551	1.00 25.65	BLGL
ATOM	105	CB	PHE	24	13.788	9.904	18.967	1.00 25.73	BLGL
ATOM	106	CG	PHE	24	14.281	8.538	19.337	1.00 25.81	BLGL
ATOM	107	CD1	PHE	24	15.134	8.359	20.422	1.00 25.77	BLGL
ATOM	108	CD2	PHE	24	13.930	7.431	18.573	1.00 25.98	BLGL
ATOM	109	CE1	PHE	24	15.642	7.093	20.739	1.00 25.74	BLGL
ATOM	110	CE2	PHE	24	14.431	6.161	18.881	1.00 27.08	BLGL
ATOM	111	CZ	PHE	24	15.292	5.992	19.967	1.00 24.69	BLGL
ATOM	112	C	PHE	24	12.517	10.473	21.055	1.00 22.99	BLGL
ATOM	113	O	PHE	24	12.961	11.520	21.519	1.00 23.30	BLGL
ATOM	114	N	ILE	25	12.077	9.474	21.804	1.00 19.49	BLGL
ATOM	115	CA	ILE	25	12.096	9.514	23.254	1.00 17.47	BLGL
ATOM	116	CB	ILE	25	11.137	8.465	23.820	1.00 15.37	BLGL
ATOM	117	CG2	ILE	25	11.388	8.253	25.306	1.00 13.70	BLGL
ATOM	118	CG1	ILE	25	9.706	8.883	23.524	1.00 13.77	BLGL
ATOM	119	CD1	ILE	25	8.696	7.834	23.915	1.00 18.01	BLGL
ATOM	120	C	ILE	25	13.487	9.227	23.799	1.00 17.49	BLGL
ATOM	121	O	ILE	25	14.091	8.211	23.465	1.00 16.53	BLGL
ATOM	122	N	LYS	26	13.985	10.128	24.637	1.00 16.78	BLGL
ATOM	123	CA	LYS	26	15.294	9.962	25.259	1.00 18.11	BLGL
ATOM	124	CB	LYS	26	16.213	11.096	24.825	1.00 19.07	BLGL
ATOM	125	CG	LYS	26	16.276	11.237	23.314	1.00 21.25	BLGL
ATOM	126	CD	LYS	26	16.943	12.520	22.899	1.00 23.74	BLGL
ATOM	127	CE	LYS	26	16.949	12.669	21.387	1.00 24.53	BLGL
ATOM	128	NZ	LYS	26	17.505	13.994	20.995	1.00 26.16	BLGL
ATOM	129	C	LYS	26	15.032	10.015	26.754	1.00 17.62	BLGL
ATOM	130	O	LYS	26	14.990	11.089	27.340	1.00 18.88	BLGL
ATOM	131	N	GLY	27	14.845	8.850	27.367	1.00 15.97	BLGL

Fig. 4 cont.

```
ATOM    132  CA  GLY    27      14.540   8.822  28.783  1.00 14.87      BLGL
ATOM    133  C   GLY    27      15.553   8.183  29.706  1.00 15.36      BLGL
ATOM    134  O   GLY    27      16.490   7.523  29.278  1.00 14.26      BLGL
ATOM    135  N   VAL    28      15.364   8.413  30.997  1.00 15.73      BLGL
ATOM    136  CA  VAL    28      16.233   7.847  32.002  1.00 15.81      BLGL
ATOM    137  CB  VAL    28      17.285   8.866  32.505  1.00 15.33      BLGL
ATOM    138  CG1 VAL    28      18.189   9.289  31.359  1.00 15.90      BLGL
ATOM    139  CG2 VAL    28      16.604  10.073  33.113  1.00 15.60      BLGL
ATOM    140  C   VAL    28      15.367   7.411  33.164  1.00 17.23      BLGL
ATOM    141  O   VAL    28      14.294   7.967  33.405  1.00 16.45      BLGL
ATOM    142  N   ASP    29      15.817   6.380  33.860  1.00 17.41      BLGL
ATOM    143  CA  ASP    29      15.098   5.902  35.023  1.00 18.06      BLGL
ATOM    144  CB  ASP    29      14.855   4.391  34.925  1.00 16.28      BLGL
ATOM    145  CG  ASP    29      14.123   3.832  36.138  1.00 18.27      BLGL
ATOM    146  OD1 ASP    29      13.426   2.801  35.978  1.00 15.84      BLGL
ATOM    147  OD2 ASP    29      14.258   4.409  37.246  1.00 14.09      BLGL
ATOM    148  C   ASP    29      16.006   6.248  36.201  1.00 17.72      BLGL
ATOM    149  O   ASP    29      17.075   5.670  36.362  1.00 18.18      BLGL
ATOM    150  N   VAL    30      15.592   7.228  36.994  1.00 17.06      BLGL
ATOM    151  CA  VAL    30      16.360   7.653  38.158  1.00 14.73      BLGL
ATOM    152  CB  VAL    30      16.740   9.151  38.051  1.00 13.70      BLGL
ATOM    153  CG1 VAL    30      17.688   9.354  36.880  1.00 12.16      BLGL
ATOM    154  CG2 VAL    30      15.485  10.017  37.872  1.00  9.08      BLGL
ATOM    155  C   VAL    30      15.551   7.422  39.426  1.00 14.73      BLGL
ATOM    156  O   VAL    30      15.491   8.275  40.302  1.00 16.61      BLGL
ATOM    157  N   SER    31      14.931   6.252  39.515  1.00 16.06      BLGL
ATOM    158  CA  SER    31      14.090   5.899  40.660  1.00 19.01      BLGL
ATOM    159  CB  SER    31      13.540   4.481  40.481  1.00 17.38      BLGL
ATOM    160  OG  SER    31      12.719   4.395  39.331  1.00 19.20      BLGL
ATOM    161  C   SER    31      14.769   6.007  42.030  1.00 19.31      BLGL
ATOM    162  O   SER    31      14.120   6.282  43.041  1.00 19.82      BLGL
ATOM    163  N   SER    32      16.075   5.797  42.059  1.00 18.54      BLGL
ATOM    164  CA  SER    32      16.826   5.845  43.301  1.00 19.36      BLGL
ATOM    165  CB  SER    32      18.121   5.055  43.133  1.00 18.42      BLGL
ATOM    166  OG  SER    32      18.909   5.611  42.088  1.00 16.54      BLGL
ATOM    167  C   SER    32      17.161   7.259  43.775  1.00 21.13      BLGL
ATOM    168  O   SER    32      17.612   7.442  44.902  1.00 20.54      BLGL
ATOM    169  N   ILE    33      16.931   8.256  42.925  1.00 21.96      BLGL
ATOM    170  CA  ILE    33      17.256   9.644  43.263  1.00 22.33      BLGL
ATOM    171  CB  ILE    33      16.752  10.622  42.161  1.00 21.13      BLGL
ATOM    172  CG2 ILE    33      15.234  10.621  42.095  1.00 19.56      BLGL
ATOM    173  CG1 ILE    33      17.283  12.027  42.439  1.00 20.03      BLGL
ATOM    174  CD1 ILE    33      18.794  12.117  42.425  1.00 17.45      BLGL
ATOM    175  C   ILE    33      16.796  10.152  44.636  1.00 23.71      BLGL
ATOM    176  O   ILE    33      17.549  10.858  45.309  1.00 25.43      BLGL
ATOM    177  N   ILE    34      15.581   9.797  45.059  1.00 24.35      BLGL
ATOM    178  CA  ILE    34      15.066  10.235  46.362  1.00 23.98      BLGL
ATOM    179  CB  ILE    34      13.539   9.951  46.486  1.00 23.20      BLGL
ATOM    180  CG2 ILE    34      13.170   9.637  47.922  1.00 24.75      BLGL
ATOM    181  CG1 ILE    34      12.735  11.183  46.063  1.00 20.84      BLGL
ATOM    182  CD1 ILE    34      13.078  11.696  44.729  1.00 21.81      BLGL
ATOM    183  C   ILE    34      15.815   9.598  47.550  1.00 24.38      BLGL
ATOM    184  O   ILE    34      16.186  10.290  48.502  1.00 25.31      BLGL
ATOM    185  N   ALA    35      16.041   8.290  47.500  1.00 22.66      BLGL
ATOM    186  CA  ALA    35      16.761   7.622  48.579  1.00 22.83      BLGL
ATOM    187  CB  ALA    35      16.803   6.117  48.344  1.00 20.64      BLGL
ATOM    188  C   ALA    35      18.178   8.165  48.681  1.00 23.42      BLGL
ATOM    189  O   ALA    35      18.687   8.377  49.776  1.00 25.98      BLGL
ATOM    190  N   LEU    36      18.813   8.382  47.536  1.00 23.28      BLGL
ATOM    191  CA  LEU    36      20.173   8.900  47.508  1.00 25.90      BLGL
ATOM    192  CB  LEU    36      20.726   8.908  46.073  1.00 26.42      BLGL
ATOM    193  CG  LEU    36      21.093   7.571  45.421  1.00 25.94      BLGL
ATOM    194  CD1 LEU    36      21.783   7.836  44.105  1.00 29.58      BLGL
ATOM    195  CD2 LEU    36      22.017   6.778  46.323  1.00 28.67      BLGL
ATOM    196  C   LEU    36      20.237  10.308  48.089  1.00 26.59      BLGL
ATOM    197  O   LEU    36      21.140  10.637  48.863  1.00 25.84      BLGL
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Fig. 4 cont.

ATOM	198	N	GLU	37	19.282	11.144	47.708	1.00 26.12	BLGL
ATOM	199	CA	GLU	37	19.259	12.501	48.214	1.00 28.35	BLGL
ATOM	200	CB	GLU	37	18.092	13.264	47.594	1.00 26.08	BLGL
ATOM	201	CG	GLU	37	18.409	13.814	46.220	1.00 29.12	BLGL
ATOM	202	CD	GLU	37	17.238	14.542	45.612	1.00 30.50	BLGL
ATOM	203	OE1	GLU	37	17.422	15.243	44.593	1.00 26.60	BLGL
ATOM	204	OE2	GLU	37	16.128	14.400	46.163	1.00 35.60	BLGL
ATOM	205	C	GLU	37	19.170	12.526	49.739	1.00 28.90	BLGL
ATOM	206	O	GLU	37	19.828	13.334	50.393	1.00 30.03	BLGL
ATOM	207	N	GLU	38	18.366	11.633	50.301	1.00 29.70	BLGL
ATOM	208	CA	GLU	38	18.212	11.570	51.746	1.00 31.72	BLGL
ATOM	209	CB	GLU	38	17.037	10.677	52.125	1.00 31.95	BLGL
ATOM	210	CG	GLU	38	15.752	11.052	51.450	1.00 37.83	BLGL
ATOM	211	CD	GLU	38	14.562	10.379	52.094	1.00 40.58	BLGL
ATOM	212	OE1	GLU	38	14.609	9.150	52.302	1.00 39.84	BLGL
ATOM	213	OE2	GLU	38	13.578	11.086	52.390	1.00 45.75	BLGL
ATOM	214	C	GLU	38	19.467	11.026	52.415	1.00 32.56	BLGL
ATOM	215	O	GLU	38	19.641	11.156	53.627	1.00 36.26	BLGL
ATOM	216	N	SER	39	20.335	10.402	51.632	1.00 30.07	BLGL
ATOM	217	CA	SER	39	21.553	9.842	52.176	1.00 27.49	BLGL
ATOM	218	CB	SER	39	21.939	8.602	51.379	1.00 29.09	BLGL
ATOM	219	OG	SER	39	20.872	7.667	51.376	1.00 24.83	BLGL
ATOM	220	C	SER	39	22.660	10.882	52.133	1.00 28.20	BLGL
ATOM	221	O	SER	39	23.791	10.624	52.547	1.00 29.82	BLGL
ATOM	222	N	GLY	40	22.327	12.063	51.626	1.00 28.31	BLGL
ATOM	223	CA	GLY	40	23.303	13.135	51.558	1.00 29.30	BLGL
ATOM	224	C	GLY	40	23.975	13.332	50.214	1.00 29.65	BLGL
ATOM	225	O	GLY	40	24.717	14.296	50.031	1.00 31.52	BLGL
ATOM	226	N	VAL	41	23.730	12.428	49.272	1.00 28.29	BLGL
ATOM	227	CA	VAL	41	24.333	12.540	47.948	1.00 27.33	BLGL
ATOM	228	CB	VAL	41	24.014	11.299	47.075	1.00 26.80	BLGL
ATOM	229	CG1	VAL	41	24.634	11.458	45.699	1.00 24.11	BLGL
ATOM	230	CG2	VAL	41	24.531	10.034	47.754	1.00 25.53	BLGL
ATOM	231	C	VAL	41	23.816	13.788	47.242	1.00 27.51	BLGL
ATOM	232	O	VAL	41	22.630	14.107	47.315	1.00 27.71	BLGL
ATOM	233	N	ALA	42	24.716	14.496	46.568	1.00 28.05	BLGL
ATOM	234	CA	ALA	42	24.364	15.713	45.840	1.00 27.62	BLGL
ATOM	235	CB	ALA	42	24.952	16.935	46.538	1.00 26.85	BLGL
ATOM	236	C	ALA	42	24.898	15.624	44.415	1.00 28.00	BLGL
ATOM	237	O	ALA	42	25.918	14.986	44.158	1.00 29.09	BLGL
ATOM	238	N	PHE	43	24.205	16.267	43.489	1.00 27.56	BLGL
ATOM	239	CA	PHE	43	24.625	16.244	42.101	1.00 30.30	BLGL
ATOM	240	CB	PHE	43	23.529	15.626	41.223	1.00 29.43	BLGL
ATOM	241	CG	PHE	43	23.281	14.176	41.513	1.00 29.78	BLGL
ATOM	242	CD1	PHE	43	22.538	13.791	42.630	1.00 26.98	BLGL
ATOM	243	CD2	PHE	43	23.855	13.188	40.714	1.00 28.78	BLGL
ATOM	244	CE1	PHE	43	22.373	12.442	42.957	1.00 25.96	BLGL
ATOM	245	CE2	PHE	43	23.698	11.835	41.031	1.00 28.67	BLGL
ATOM	246	CZ	PHE	43	22.954	11.461	42.160	1.00 26.33	BLGL
ATOM	247	C	PHE	43	24.954	17.651	41.632	1.00 32.38	BLGL
ATOM	248	O	PHE	43	24.351	18.622	42.096	1.00 33.12	BLGL
ATOM	249	N	TYR	44	25.915	17.759	40.719	1.00 32.89	BLGL
ATOM	250	CA	TYR	44	26.326	19.054	40.203	1.00 34.23	BLGL
ATOM	251	CB	TYR	44	27.807	19.289	40.482	1.00 33.04	BLGL
ATOM	252	CG	TYR	44	28.165	19.083	41.926	1.00 33.71	BLGL
ATOM	253	CD1	TYR	44	28.177	17.809	42.481	1.00 32.43	BLGL
ATOM	254	CE1	TYR	44	28.453	17.617	43.820	1.00 35.78	BLGL
ATOM	255	CD2	TYR	44	28.444	20.167	42.752	1.00 34.36	BLGL
ATOM	256	CE2	TYR	44	28.721	19.986	44.099	1.00 34.85	BLGL
ATOM	257	CZ	TYR	44	28.722	18.708	44.627	1.00 35.70	BLGL
ATOM	258	OH	TYR	44	28.974	18.515	45.966	1.00 37.37	BLGL
ATOM	259	C	TYR	44	26.085	19.114	38.717	1.00 35.88	BLGL
ATOM	260	O	TYR	44	25.531	18.189	38.134	1.00 36.33	BLGL
ATOM	261	N	ASN	45	26.509	20.211	38.106	1.00 39.58	BLGL
ATOM	262	CA	ASN	45	26.350	20.391	36.672	1.00 43.09	BLGL
ATOM	263	CB	ASN	45	25.429	21.581	36.391	1.00 45.50	BLGL

Fig. 4 cont.

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ATOM    264  CG  ASN    45      26.156  22.912  36.452  1.00 47.10      BLGL
ATOM    265  OD1 ASN    45      26.932  23.180  37.373  1.00 44.32      BLGL
ATOM    266  ND2 ASN    45      25.897  23.760  35.464  1.00 49.84      BLGL
ATOM    267  C   ASN    45      27.721  20.618  36.038  1.00 43.53      BLGL
ATOM    268  O   ASN    45      28.746  20.564  36.718  1.00 41.75      BLGL
ATOM    269  N   GLU    46      27.733  20.861  34.735  1.00 47.02      BLGL
ATOM    270  CA  GLU    46      28.979  21.090  34.011  1.00 51.61      BLGL
ATOM    271  CB  GLU    46      28.673  21.715  32.656  1.00 55.53      BLGL
ATOM    272  CG  GLU    46      27.635  20.976  31.820  1.00 59.75      BLGL
ATOM    273  CD  GLU    46      28.162  19.673  31.261  1.00 62.26      BLGL
ATOM    274  OE1 GLU    46      29.304  19.665  30.749  1.00 62.58      BLGL
ATOM    275  OE2 GLU    46      27.429  18.665  31.320  1.00 63.83      BLGL
ATOM    276  C   GLU    46      29.917  22.027  34.782  1.00 52.77      BLGL
ATOM    277  O   GLU    46      31.035  21.648  35.144  1.00 52.27      BLGL
ATOM    278  N   SER    47      29.440  23.248  35.029  1.00 53.78      BLGL
ATOM    279  CA  SER    47      30.197  24.288  35.723  1.00 54.29      BLGL
ATOM    280  CB  SER    47      29.312  25.518  35.940  1.00 56.24      BLGL
ATOM    281  OG  SER    47      28.822  26.029  34.707  1.00 57.54      BLGL
ATOM    282  C   SER    47      30.779  23.857  37.058  1.00 54.34      BLGL
ATOM    283  O   SER    47      31.720  24.477  37.552  1.00 56.28      BLGL
ATOM    284  N   GLY    48      30.215  22.812  37.651  1.00 53.12      BLGL
ATOM    285  CA  GLY    48      30.724  22.344  38.926  1.00 52.44      BLGL
ATOM    286  C   GLY    48      29.883  22.783  40.109  1.00 52.32      BLGL
ATOM    287  O   GLY    48      30.200  22.455  41.258  1.00 51.88      BLGL
ATOM    288  N   LYS    49      28.807  23.518  39.832  1.00 51.68      BLGL
ATOM    289  CA  LYS    49      27.919  24.009  40.882  1.00 50.92      BLGL
ATOM    290  CB  LYS    49      27.338  25.368  40.477  1.00 52.51      BLGL
ATOM    291  CG  LYS    49      26.440  25.314  39.255  1.00 54.74      BLGL
ATOM    292  CD  LYS    49      26.139  26.704  38.706  1.00 58.30      BLGL
ATOM    293  CE  LYS    49      25.326  27.551  39.672  1.00 59.50      BLGL
ATOM    294  NZ  LYS    49      25.039  28.909  39.112  1.00 61.13      BLGL
ATOM    295  C   LYS    49      26.779  23.039  41.204  1.00 49.26      BLGL
ATOM    296  O   LYS    49      26.215  22.391  40.320  1.00 50.56      BLGL
ATOM    297  N   LYS    50      26.444  22.953  42.483  1.00 46.67      BLGL
ATOM    298  CA  LYS    50      25.377  22.082  42.955  1.00 44.89      BLGL
ATOM    299  CB  LYS    50      25.229  22.272  44.465  1.00 44.47      BLGL
ATOM    300  CG  LYS    50      24.483  21.182  45.190  1.00 47.37      BLGL
ATOM    301  CD  LYS    50      24.732  21.290  46.692  1.00 50.81      BLGL
ATOM    302  CE  LYS    50      23.926  20.260  47.478  1.00 53.40      BLGL
ATOM    303  NZ  LYS    50      24.326  20.203  48.917  1.00 55.24      BLGL
ATOM    304  C   LYS    50      24.088  22.473  42.221  1.00 43.33      BLGL
ATOM    305  O   LYS    50      23.726  23.647  42.187  1.00 43.90      BLGL
ATOM    306  N   GLN    51      23.400  21.497  41.631  1.00 41.68      BLGL
ATOM    307  CA  GLN    51      22.167  21.765  40.884  1.00 38.41      BLGL
ATOM    308  CB  GLN    51      22.531  22.164  39.449  1.00 38.23      BLGL
ATOM    309  CG  GLN    51      21.352  22.358  38.507  1.00 38.66      BLGL
ATOM    310  CD  GLN    51      21.797  22.731  37.099  1.00 38.67      BLGL
ATOM    311  OE1 GLN    51      22.206  23.862  36.846  1.00 38.64      BLGL
ATOM    312  NE2 GLN    51      21.730  21.771  36.181  1.00 38.86      BLGL
ATOM    313  C   GLN    51      21.241  20.548  40.867  1.00 35.96      BLGL
ATOM    314  O   GLN    51      21.714  19.417  40.893  1.00 35.98      BLGL
ATOM    315  N   ASP    52      19.928  20.778  40.827  1.00 34.78      BLGL
ATOM    316  CA  ASP    52      18.955  19.677  40.797  1.00 34.16      BLGL
ATOM    317  CB  ASP    52      17.522  20.215  40.657  1.00 35.75      BLGL
ATOM    318  CG  ASP    52      16.475  19.100  40.603  1.00 36.25      BLGL
ATOM    319  OD1 ASP    52      15.271  19.396  40.465  1.00 35.18      BLGL
ATOM    320  OD2 ASP    52      16.857  17.919  40.703  1.00 41.59      BLGL
ATOM    321  C   ASP    52      19.269  18.760  39.610  1.00 33.33      BLGL
ATOM    322  O   ASP    52      19.475  19.231  38.483  1.00 33.59      BLGL
ATOM    323  N   ILE    53      19.294  17.454  39.856  1.00 29.47      BLGL
ATOM    324  CA  ILE    53      19.620  16.512  38.797  1.00 26.79      BLGL
ATOM    325  CB  ILE    53      19.692  15.059  39.336  1.00 25.32      BLGL
ATOM    326  CG2 ILE    53      18.304  14.567  39.715  1.00 24.80      BLGL
ATOM    327  CG1 ILE    53      20.326  14.147  38.277  1.00 25.86      BLGL
ATOM    328  CD1 ILE    53      20.638  12.753  38.777  1.00 25.81      BLGL
ATOM    329  C   ILE    53      18.644  16.588  37.631  1.00 25.41      BLGL
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Fig. 4 cont.

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ATOM    330  O   ILE   53      19.042  16.436  36.475  1.00 23.70      BLGL
ATOM    331  N   PHE   54      17.372  16.836  37.926  1.00 23.59      BLGL
ATOM    332  CA  PHE   54      16.380  16.930  36.868  1.00 25.83      BLGL
ATOM    333  CB  PHE   54      14.972  17.002  37.456  1.00 23.83      BLGL
ATOM    334  CG  PHE   54      14.526  15.723  38.072  1.00 22.74      BLGL
ATOM    335  CD1 PHE   54      14.799  15.449  39.402  1.00 25.01      BLGL
ATOM    336  CD2 PHE   54      13.885  14.760  37.306  1.00 21.32      BLGL
ATOM    337  CE1 PHE   54      14.443  14.229  39.961  1.00 27.14      BLGL
ATOM    338  CE2 PHE   54      13.525  13.537  37.856  1.00 23.72      BLGL
ATOM    339  CZ  PHE   54      13.803  13.268  39.184  1.00 24.12      BLGL
ATOM    340  C   PHE   54      16.641  18.121  35.953  1.00 27.75      BLGL
ATOM    341  O   PHE   54      16.378  18.064  34.753  1.00 27.66      BLGL
ATOM    342  N   ASN   55      17.167  19.197  36.522  1.00 30.60      BLGL
ATOM    343  CA  ASN   55      17.485  20.385  35.740  1.00 32.40      BLGL
ATOM    344  CB  ASN   55      17.927  21.528  36.665  1.00 38.72      BLGL
ATOM    345  CG  ASN   55      18.157  22.835  35.919  1.00 43.16      BLGL
ATOM    346  OD1 ASN   55      18.775  23.767  36.444  1.00 46.30      BLGL
ATOM    347  ND2 ASN   55      17.657  22.912  34.692  1.00 47.38      BLGL
ATOM    348  C   ASN   55      18.631  19.996  34.808  1.00 30.86      BLGL
ATOM    349  O   ASN   55      18.624  20.327  33.623  1.00 29.18      BLGL
ATOM    350  N   THR   56      19.608  19.281  35.363  1.00 28.42      BLGL
ATOM    351  CA  THR   56      20.765  18.824  34.606  1.00 26.82      BLGL
ATOM    352  CB  THR   56      21.769  18.101  35.514  1.00 27.58      BLGL
ATOM    353  OG1 THR   56      22.198  18.988  36.558  1.00 29.47      BLGL
ATOM    354  CG2 THR   56      22.969  17.642  34.714  1.00 22.45      BLGL
ATOM    355  C   THR   56      20.353  17.870  33.489  1.00 27.22      BLGL
ATOM    356  O   THR   56      20.851  17.952  32.366  1.00 27.23      BLGL
ATOM    357  N   LEU   57      19.441  16.961  33.805  1.00 27.52      BLGL
ATOM    358  CA  LEU   57      18.950  15.997  32.830  1.00 27.42      BLGL
ATOM    359  CB  LEU   57      17.978  15.033  33.508  1.00 26.87      BLGL
ATOM    360  CG  LEU   57      18.453  13.617  33.847  1.00 26.41      BLGL
ATOM    361  CD1 LEU   57      19.941  13.572  34.078  1.00 23.65      BLGL
ATOM    362  CD2 LEU   57      17.691  13.138  35.074  1.00 25.32      BLGL
ATOM    363  C   LEU   57      18.257  16.686  31.662  1.00 28.88      BLGL
ATOM    364  O   LEU   57      18.430  16.288  30.515  1.00 29.93      BLGL
ATOM    365  N   LYS   58      17.474  17.718  31.959  1.00 30.47      BLGL
ATOM    366  CA  LYS   58      16.757  18.455  30.926  1.00 30.56      BLGL
ATOM    367  CB  LYS   58      15.836  19.507  31.561  1.00 32.82      BLGL
ATOM    368  CG  LYS   58      15.038  20.330  30.551  1.00 33.72      BLGL
ATOM    369  CD  LYS   58      14.129  19.438  29.710  1.00 36.45      BLGL
ATOM    370  CE  LYS   58      13.279  20.253  28.732  1.00 38.35      BLGL
ATOM    371  NZ  LYS   58      12.233  19.436  28.049  1.00 36.51      BLGL
ATOM    372  C   LYS   58      17.726  19.135  29.969  1.00 30.23      BLGL
ATOM    373  O   LYS   58      17.564  19.064  28.753  1.00 31.14      BLGL
ATOM    374  N   GLU   59      18.734  19.793  30.522  1.00 30.65      BLGL
ATOM    375  CA  GLU   59      19.722  20.483  29.709  1.00 31.60      BLGL
ATOM    376  CB  GLU   59      20.668  21.275  30.610  1.00 35.74      BLGL
ATOM    377  CG  GLU   59      19.971  22.381  31.397  1.00 42.93      BLGL
ATOM    378  CD  GLU   59      20.839  22.960  32.511  1.00 48.75      BLGL
ATOM    379  OE1 GLU   59      20.327  23.818  33.264  1.00 51.01      BLGL
ATOM    380  OE2 GLU   59      22.026  22.558  32.638  1.00 51.49      BLGL
ATOM    381  C   GLU   59      20.511  19.493  28.862  1.00 30.47      BLGL
ATOM    382  O   GLU   59      21.086  19.859  27.838  1.00 30.17      BLGL
ATOM    383  N   ALA   60      20.531  18.235  29.293  1.00 29.36      BLGL
ATOM    384  CA  ALA   60      21.253  17.186  28.582  1.00 28.02      BLGL
ATOM    385  CB  ALA   60      21.611  16.065  29.543  1.00 29.83      BLGL
ATOM    386  C   ALA   60      20.461  16.623  27.406  1.00 27.47      BLGL
ATOM    387  O   ALA   60      20.975  15.807  26.643  1.00 26.82      BLGL
ATOM    388  N   GLY   61      19.208  17.048  27.269  1.00 27.12      BLGL
ATOM    389  CA  GLY   61      18.387  16.574  26.167  1.00 25.98      BLGL
ATOM    390  C   GLY   61      17.379  15.484  26.500  1.00 24.46      BLGL
ATOM    391  O   GLY   61      16.678  14.995  25.613  1.00 22.97      BLGL
ATOM    392  N   VAL   62      17.307  15.101  27.773  1.00 23.85      BLGL
ATOM    393  CA  VAL   62      16.373  14.075  28.223  1.00 22.41      BLGL
ATOM    394  CB  VAL   62      16.738  13.577  29.651  1.00 22.60      BLGL
ATOM    395  CG1 VAL   62      15.754  12.514  30.107  1.00 22.01      BLGL
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Fig. 4 cont.

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ATOM    396  CG2 VAL    62      18.146  13.018  29.664  1.00 20.65      BLGL
ATOM    397  C   VAL    62      14.958  14.658  28.230  1.00 22.28      BLGL
ATOM    398  O   VAL    62      14.743  15.783  28.686  1.00 24.37      BLGL
ATOM    399  N   ASN    63      13.997  13.896  27.721  1.00 20.64      BLGL
ATOM    400  CA  ASN    63      12.615  14.356  27.660  1.00 21.22      BLGL
ATOM    401  CB  ASN    63      12.203  14.546  26.204  1.00 20.41      BLGL
ATOM    402  CG  ASN    63      12.528  13.337  25.349  1.00 20.90      BLGL
ATOM    403  OD1 ASN    63      12.248  12.195  25.723  1.00 22.33      BLGL
ATOM    404  ND2 ASN    63      13.112  13.581  24.189  1.00 20.98      BLGL
ATOM    405  C   ASN    63      11.641  13.396  28.330  1.00 21.56      BLGL
ATOM    406  O   ASN    63      10.426  13.606  28.304  1.00 24.89      BLGL
ATOM    407  N   TYR    64      12.171  12.346  28.939  1.00 19.85      BLGL
ATOM    408  CA  TYR    64      11.323  11:360  29.578  1.00 18.37      BLGL
ATOM    409  CB  TYR    64      11.054  10.226  28.590  1.00 18.15      BLGL
ATOM    410  CG  TYR    64       9.601  10.025  28.244  1.00 18.02      BLGL
ATOM    411  CD1 TYR    64       8.724   9.446  29.155  1.00 16.59      BLGL
ATOM    412  CE1 TYR    64       7.397   9.210  28.821  1.00 17.75      BLGL
ATOM    413  CD2 TYR    64       9.109  10.375  26.985  1.00 20.14      BLGL
ATOM    414  CE2 TYR    64       7.781  10.145  26.640  1.00 17.07      BLGL
ATOM    415  CZ  TYR    64       6.935   9.560  27.562  1.00 18.10      BLGL
ATOM    416  OH  TYR    64       5.634   9.301  27.223  1.00 19.97      BLGL
ATOM    417  C   TYR    64      11.963  10.804  30.839  1.00 17.64      BLGL
ATOM    418  O   TYR    64      13.181  10.683  30.927  1.00 17.84      BLGL
ATOM    419  N   VAL    65      11.137  10.470  31.819  1.00 15.63      BLGL
ATOM    420  CA  VAL    65      11.644   9.905  33.050  1.00 16.50      BLGL
ATOM    421  CB  VAL    65      11.567  10.909  34.215  1.00 15.92      BLGL
ATOM    422  CG1 VAL    65      11.909  10.207  35.522  1.00 14.90      BLGL
ATOM    423  CG2 VAL    65      12.536  12.055  33.975  1.00 14.25      BLGL
ATOM    424  C   VAL    65      10.847   8.668  33.414  1.00 15.70      BLGL
ATOM    425  O   VAL    65       9.621   8.691  33.388  1.00 16.30      BLGL
ATOM    426  N   ARG    66      11.548   7.587  33.740  1.00 15.28      BLGL
ATOM    427  CA  ARG    66      10.898   6.343  34.126  1.00 14.69      BLGL
ATOM    428  CB  ARG    66      11.520   5.145  33.396  1.00 12.92      BLGL
ATOM    429  CG  ARG    66      10.676   3.897  33.521  1.00 16.36      BLGL
ATOM    430  CD  ARG    66      11.131   2.751  32.621  1.00 17.95      BLGL
ATOM    431  NE  ARG    66      11.997   1.835  33.347  1.00 21.82      BLGL
ATOM    432  CZ  ARG    66      11.882   0.514  33.336  1.00 20.23      BLGL
ATOM    433  NH1 ARG    66      10.933  -0.072  32.628  1.00 20.47      BLGL
ATOM    434  NH2 ARG    66      12.720  -0.218  34.050  1.00 22.65      BLGL
ATOM    435  C   ARG    66      11.049   6.155  35.627  1.00 15.52      BLGL
ATOM    436  O   ARG    66      12.097   6.461  36.194  1.00 19.23      BLGL
ATOM    437  N   VAL    67      10.003   5.663  36.277  1.00 14.45      BLGL
ATOM    438  CA  VAL    67      10.065   5.437  37.709  1.00 14.29      BLGL
ATOM    439  CB  VAL    67       9.387   6.591  38.500  1.00 14.34      BLGL
ATOM    440  CG1 VAL    67       8.010   6.866  37.946  1.00 15.07      BLGL
ATOM    441  CG2 VAL    67       9.279   6.226  39.974  1.00 14.76      BLGL
ATOM    442  C   VAL    67       9.380   4.134  38.050  1.00 13:80      BLGL
ATOM    443  O   VAL    67       8.243   3.902  37.652  1.00 16.06      BLGL
ATOM    444  N   ARG    68      10.084   3.274  38.772  1.00 12.24      BLGL
ATOM    445  CA  ARG    68       9.512   2.007  39.170  1.00 13.36      BLGL
ATOM    446  CB  ARG    68      10.613   0.987  39.505  1.00 15.94      BLGL
ATOM    447  CG  ARG    68      11.653   1.445  40.530  1.00 16.59      BLGL
ATOM    448  CD  ARG    68      12.582   0.299  40.946  1.00 17.71      BLGL
ATOM    449  NE  ARG    68      13.727   0.787  41.717  1.00 20.66      BLGL
ATOM    450  CZ  ARG    68      14.806   1.365  41.187  1.00 19.69      BLGL
ATOM    451  NH1 ARG    68      15.791   1.788  41.964  1.00 18.60      BLGL
ATOM    452  NH2 ARG    68      14.912   1.502  39.876  1.00 19.53      BLGL
ATOM    453  C   ARG    68       8.621   2.250  40.383  1.00 16.28      BLGL
ATOM    454  O   ARG    68       8.875   3.152  41.185  1.00 13.92      BLGL
ATOM    455  N   ILE    69       7.567   1.449  40.506  1.00 16.59      BLGL
ATOM    456  CA  ILE    69       6.649   1.582  41.619  1.00 17.08      BLGL
ATOM    457  CB  ILE    69       5.331   2.254  41.176  1.00 17.80      BLGL
ATOM    458  CG2 ILE    69       4.442   2.505  42.392  1.00 16.20      BLGL
ATOM    459  CG1 ILE    69       5.634   3.577  40.463  1.00 18.54      BLGL
ATOM    460  CD1 ILE    69       4.420   4.258  39.861  1.00 16.60      BLGL
ATOM    461  C   ILE-   69       6.326   0.224  42.227  1.00 19.49      BLGL
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Fig. 4 cont.

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ATOM    462  O   ILE   69       5.851  -0.684  41.537  1.00 21.07      BLGL
ATOM    463  N   TRP   70       6.613   0.088  43.518  1.00 19.80      BLGL
ATOM    464  CA  TRP   70       6.329  -1.132  44.261  1.00 20.02      BLGL
ATOM    465  CB  TRP   70       7.534  -1.548  45.108  1.00 20.03      BLGL
ATOM    466  CG  TRP   70       8.693  -2.052  44.299  1.00 20.74      BLGL
ATOM    467  CD2 TRP   70      10.078  -1.707  44.460  1.00 20.58      BLGL
ATOM    468  CE2 TRP   70      10.807  -2.445  43.496  1.00 20.35      BLGL
ATOM    469  CE3 TRP   70      10.774  -0.847  45.322  1.00 19.46      BLGL
ATOM    470  CD1 TRP   70       8.643  -2.958  43.278  1.00 20.51      BLGL
ATOM    471  NE1 TRP   70       9.906  -3.198  42.791  1.00 18.08      BLGL
ATOM    472  CZ2 TRP   70      12.200  -2.350  43.372  1.00 17.40      BLGL
ATOM    473  CZ3 TRP   70      12.162  -0.752  45.197  1.00 18.53      BLGL
ATOM    474  CH2 TRP   70      12.856  -1.501  44.227  1.00 17.88      BLGL
ATOM    475  C   TRP   70       5.145  -0.805  45.164  1.00 21.18      BLGL
ATOM    476  O   TRP   70       5.010   0.328  45.626  1.00 20.39      BLGL
ATOM    477  N   ASN   71       4.279  -1.782  45.405  1.00 21.89      BLGL
ATOM    478  CA  ASN   71       3.105  -1.553  46.238  1.00 23.11      BLGL
ATOM    479  CB  ASN   71       2.204  -2.787  46.234  1.00 21.89      BLGL
ATOM    480  CG  ASN   71       1.600  -3.059  44.875  1.00 24.42      BLGL
ATOM    481  OD1 ASN   71       2.312  -3.325  43.907  1.00 24.93      BLGL
ATOM    482  ND2 ASN   71       0.277  -2.986  44.792  1.00 24.52      BLGL
ATOM    483  C   ASN   71       3.454  -1.182  47.673  1.00 23.89      BLGL
ATOM    484  O   ASN   71       3.114  -0.093  48.150  1.00 23.65      BLGL
ATOM    485  N   ASP   72       4.139  -2.094  48.356  1.00 25.19      BLGL
ATOM    486  CA  ASP   72       4.531  -1.888  49.747  1.00 24.90      BLGL
ATOM    487  CB  ASP   72       3.576  -2.642  50.669  1.00 24.77      BLGL
ATOM    488  CG  ASP   72       3.706  -2.214  52.105  1.00 25.24      BLGL
ATOM    489  OD1 ASP   72       3.494  -3.063  52.990  1.00 26.84      BLGL
ATOM    490  OD2 ASP   72       4.006  -1.026  52.346  1.00 24.35      BLGL
ATOM    491  C   ASP   72       5.953  -2.384  49.997  1.00 24.58      BLGL
ATOM    492  O   ASP   72       6.151  -3.472  50.538  1.00 25.47      BLGL
ATOM    493  N   PRO   73       6.962  -1.586  49.619  1.00 24.27      BLGL
ATOM    494  CD  PRO   73       6.856  -0.281  48.940  1.00 23.33      BLGL
ATOM    495  CA  PRO   73       8.366  -1.962  49.805  1.00 24.32      BLGL
ATOM    496  CB  PRO   73       9.091  -1.009  48.866  1.00 24.01      BLGL
ATOM    497  CG  PRO   73       8.272   0.237  49.001  1.00 23.40      BLGL
ATOM    498  C   PRO   73       8.863  -1.840  51.248  1.00 27.14      BLGL
ATOM    499  O   PRO   73       9.987  -1.395  51.491  1.00 28.54      BLGL
ATOM    500  N   TYR   74       8.033  -2.233  52.208  1.00 27.12      BLGL
ATOM    501  CA  TYR   74       8.429  -2.147  53.609  1.00 26.57      BLGL
ATOM    502  CB  TYR   74       7.838  -0.889  54.256  1.00 25.70      BLGL
ATOM    503  CG  TYR   74       8.022   0.386  53.463  1.00 21.92      BLGL
ATOM    504  CD1 TYR   74       7.148   0.721  52.427  1.00 22.26      BLGL
ATOM    505  CE1 TYR   74       7.304   1.909  51.707  1.00 21.83      BLGL
ATOM    506  CD2 TYR   74       9.057   1.265  53.758  1.00 18.92      BLGL
ATOM    507  CE2 TYR   74       9.223   2.448  53.049  1.00 19.47      BLGL
ATOM    508  CZ  TYR   74       8.345   2.766  52.026  1.00 21.06      BLGL
ATOM    509  OH  TYR   74       8.503   3.939  51.323  1.00 21.16      BLGL
ATOM    510  C   TYR   74       7.970  -3.371  54.395  1.00 26.69      BLGL
ATOM    511  O   TYR   74       7.119  -4.131  53.928  1.00 26.70      BLGL
ATOM    512  N   ASP   75       8.547  -3.568  55.579  1.00 25.47      BLGL
ATOM    513  CA  ASP   75       8.151  -4.687  56.422  1.00 25.66      BLGL
ATOM    514  CB  ASP   75       9.348  -5.260  57.201  1.00 26.96      BLGL
ATOM    515  CG  ASP   75       9.948  -4.282  58.207  1.00 26.69      BLGL
ATOM    516  OD1 ASP   75      10.931  -4.668  58.867  1.00 25.84      BLGL
ATOM    517  OD2 ASP   75       9.455  -3.146  58.350  1.00 28.52      BLGL
ATOM    518  C   ASP   75       7.060  -4.208  57.367  1.00 26.20      BLGL
ATOM    519  O   ASP   75       6.634  -3.063  57.286  1.00 27.42      BLGL
ATOM    520  N   ALA   76       6.602  -5.078  58.255  1.00 27.05      BLGL
ATOM    521  CA  ALA   76       5.535  -4.722  59.184  1.00 28.91      BLGL
ATOM    522  CB  ALA   76       5.304  -5.869  60.153  1.00 29.44      BLGL
ATOM    523  C   ALA   76       5.793  -3.438  59.964  1.00 29.89      BLGL
ATOM    524  O   ALA   76       4.873  -2.666  60.241  1.00 31.61      BLGL
ATOM    525  N   ASN   77       7.051  -3.213  60.307  1.00 29.94      BLGL
ATOM    526  CA  ASN   77       7.445  -2.059  61.091  1.00 30.08      BLGL
ATOM    527  CB  ASN   77       8.619  -2.460  61.970  1.00 30.88      BLGL
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Fig. 4 cont.

ATOM	528	CG	ASN	77	8.337	-3.728	62.740	1.00	31.46	BLGL
ATOM	529	OD1	ASN	77	9.085	-4.700	62.659	1.00	35.40	BLGL
ATOM	530	ND2	ASN	77	7.241	-3.729	63.485	1.00	29.08	BLGL
ATOM	531	C	ASN	77	7.768	-0.802	60.294	1.00	30.14	BLGL
ATOM	532	O	ASN	77	8.048	0.249	60.874	1.00	31.47	BLGL
ATOM	533	N	GLY	78	7.742	-0.906	58.971	1.00	29.60	BLGL
ATOM	534	CA	GLY	78	7.998	0.260	58.146	1.00	30.47	BLGL
ATOM	535	C	GLY	78	9.422	0.434	57.665	1.00	30.69	BLGL
ATOM	536	O	GLY	78	9.803	1.524	57.243	1.00	31.23	BLGL
ATOM	537	N	ASN	79	10.212	-0.631	57.735	1.00	30.64	BLGL
ATOM	538	CA	ASN	79	11.599	-0.586	57.285	1.00	31.66	BLGL
ATOM	539	CB	ASN	79	12.437	-1.618	58.043	1.00	32.77	BLGL
ATOM	540	CG	ASN	79	12.478	-1.356	59.539	1.00	32.28	BLGL
ATOM	541	OD1	ASN	79	12.875	-0.277	59.981	1.00	31.97	BLGL
ATOM	542	ND2	ASN	79	12.074	-2.346	60.325	1.00	29.86	BLGL
ATOM	543	C	ASN	79	11.652	-0.888	55.788	1.00	31.40	BLGL
ATOM	544	O	ASN	79	11.253	-1.971	55.352	1.00	31.55	BLGL
ATOM	545	N	GLY	80	12.146	0.072	55.013	1.00	30.48	BLGL
ATOM	546	CA	GLY	80	12.224	-0.092	53.573	1.00	28.01	BLGL
ATOM	547	C	GLY	80	13.066	-1.265	53.132	1.00	26.92	BLGL
ATOM	548	O	GLY	80	14.104	-1.544	53.737	1.00	28.09	BLGL
ATOM	549	N	TYR	81	12.611	-1.958	52.089	1.00	25.24	BLGL
ATOM	550	CA	TYR	81	13.330	-3.110	51.539	1.00	24.70	BLGL
ATOM	551	CB	TYR	81	12.446	-3.891	50.559	1.00	26.19	BLGL
ATOM	552	CG	TYR	81	11.309	-4.704	51.155	1.00	28.51	BLGL
ATOM	553	CD1	TYR	81	10.337	-5.264	50.324	1.00	30.98	BLGL
ATOM	554	CE1	TYR	81	9.285	-6.014	50.836	1.00	33.39	BLGL
ATOM	555	CD2	TYR	81	11.202	-4.919	52.525	1.00	27.25	BLGL
ATOM	556	CE2	TYR	81	10.151	-5.673	53.053	1.00	30.71	BLGL
ATOM	557	CZ	TYR	81	9.191	-6.218	52.201	1.00	32.59	BLGL
ATOM	558	OH	TYR	81	8.134	-6.955	52.701	1.00	29.32	BLGL
ATOM	559	C	TYR	81	14.581	-2.643	50.791	1.00	23.17	BLGL
ATOM	560	O	TYR	81	15.424	-3.449	50.411	1.00	22.30	BLGL
ATOM	561	N	GLY	82	14.692	-1.337	50.575	1.00	22.25	BLGL
ATOM	562	CA	GLY	82	15.840	-0.812	49.863	1.00	22.06	BLGL
ATOM	563	C	GLY	82	15.544	-0.631	48.388	1.00	23.07	BLGL
ATOM	564	O	GLY	82	14.392	-0.466	47.994	1.00	22.83	BLGL
ATOM	565	N	GLY	83	16.582	-0.660	47.561	1.00	23.84	BLGL
ATOM	566	CA	GLY	83	16.384	-0.485	46.133	1.00	23.31	BLGL
ATOM	567	C	GLY	83	15.731	0.843	45.796	1.00	23.19	BLGL
ATOM	568	O	GLY	83	15.219	1.024	44.693	1.00	23.86	BLGL
ATOM	569	N	GLY	84	15.740	1.772	46.748	1.00	22.55	BLGL
ATOM	570	CA	GLY	84	15.142	3.075	46.514	1.00	18.60	BLGL
ATOM	571	C	GLY	84	13.832	3.262	47.243	1.00	18.25	BLGL
ATOM	572	O	GLY	84	13.282	4.354	47.254	1.00	19.59	BLGL
ATOM	573	N	ASN	85	13.339	2.199	47.867	1.00	18.82	BLGL
ATOM	574	CA	ASN	85	12.070	2.246	48.591	1.00	22.71	BLGL
ATOM	575	CB	ASN	85	12.217	3.011	49.914	1.00	22.20	BLGL
ATOM	576	CG	ASN	85	13.143	2.319	50.902	1.00	24.42	BLGL
ATOM	577	OD1	ASN	85	13.320	1.102	50.869	1.00	25.77	BLGL
ATOM	578	ND2	ASN	85	13.721	3.098	51.806	1.00	25.80	BLGL
ATOM	579	C	ASN	85	11.004	2.929	47.729	1.00	23.49	BLGL
ATOM	580	O	ASN	85	10.235	3.761	48.214	1.00	23.21	BLGL
ATOM	581	N	ASN	86	10.950	2.566	46.452	1.00	23.70	BLGL
ATOM	582	CA	ASN	86	10.001	3.196	45.546	1.00	24.44	BLGL
ATOM	583	CB	ASN	86	10.447	3.008	44.106	1.00	21.35	BLGL
ATOM	584	CG	ASN	86	11.781	3.627	43.847	1.00	21.48	BLGL
ATOM	585	OD1	ASN	86	12.811	2.972	43.976	1.00	22.65	BLGL
ATOM	586	ND2	ASN	86	11.781	4.908	43.500	1.00	20.47	BLGL
ATOM	587	C	ASN	86	8.546	2.785	45.679	1.00	25.13	BLGL
ATOM	588	O	ASN	86	8.159	1.666	45.357	1.00	23.77	BLGL
ATOM	589	N	ASP	87	7.742	3.723	46.155	1.00	25.52	BLGL
ATOM	590	CA	ASP	87	6.323	3.500	46.323	1.00	26.02	BLGL
ATOM	591	CB	ASP	87	5.954	3.547	47.803	1.00	25.67	BLGL
ATOM	592	CG	ASP	87	6.584	4.724	48.524	1.00	30.07	BLGL
ATOM	593	OD1	ASP	87	6.994	5.705	47.851	1.00	29.90	BLGL

Fig. 4 cont.

ATOM	594	OD2	ASP	87	6.656	4.668	49.771	1.00	31.21	BLGL
ATOM	595	C	ASP	87	5.625	4.613	45.566	1.00	25.13	BLGL
ATOM	596	O	ASP	87	6.276	5.396	44.877	1.00	25.07	BLGL
ATOM	597	N	LEU	88	4.307	4.693	45.694	1.00	25.05	BLGL
ATOM	598	CA	LEU	88	3.566	5.732	44.996	1.00	27.31	BLGL
ATOM	599	CB	LEU	88	2.059	5.528	45.183	1.00	25.49	BLGL
ATOM	600	CG	LEU	88	1.163	6.603	44.564	1.00	23.47	BLGL
ATOM	601	CD1	LEU	88	1.378	6.668	43.059	1.00	23.31	BLGL
ATOM	602	CD2	LEU	88	-0.283	6.294	44.880	1.00	23.48	BLGL
ATOM	603	C	LEU	88	3.956	7.146	45.440	1.00	28.05	BLGL
ATOM	604	O	LEU	88	3.942	8.072	44.633	1.00	28.88	BLGL
ATOM	605	N	GLU	89	4.310	7.312	46.713	1.00	28.47	BLGL
ATOM	606	CA	GLU	89	4.679	8.627	47.223	1.00	31.19	BLGL
ATOM	607	CB	GLU	89	4.884	8.596	48.743	1.00	38.35	BLGL
ATOM	608	CG	GLU	89	4.732	7.224	49.404	1.00	49.47	BLGL
ATOM	609	CD	GLU	89	3.309	6.673	49.355	1.00	54.88	BLGL
ATOM	610	OE1	GLU	89	3.095	5.617	48.709	1.00	55.88	BLGL
ATOM	611	OE2	GLU	89	2.413	7.297	49.968	1.00	58.86	BLGL
ATOM	612	C	GLU	89	5.931	9.157	46.547	1.00	28.83	BLGL
ATOM	613	O	GLU	89	5.958	10.293	46.083	1.00	29.30	BLGL
ATOM	614	N	LYS	90	6.970	8.337	46.486	1.00	27.00	BLGL
ATOM	615	CA	LYS	90	8.202	8.758	45.833	1.00	25.31	BLGL
ATOM	616	CB	LYS	90	9.308	7.731	46.074	1.00	24.21	BLGL
ATOM	617	CG	LYS	90	9.730	7.618	47.526	1.00	23.42	BLGL
ATOM	618	CD	LYS	90	11.003	6.815	47.664	1.00	23.39	BLGL
ATOM	619	CE	LYS	90	11.521	6.845	49.092	1.00	22.77	BLGL
ATOM	620	NZ	LYS	90	10.589	6.181	50.039	1.00	24.27	BLGL
ATOM	621	C	LYS	90	7.966	8.940	44.333	1.00	24.86	BLGL
ATOM	622	O	LYS	90	8.604	9.779	43.696	1.00	23.88	BLGL
ATOM	623	N	ALA	91	7.043	8.157	43.776	1.00	22.89	BLGL
ATOM	624	CA	ALA	91	6.727	8.252	42.362	1.00	23.29	BLGL
ATOM	625	CB	ALA	91	5.709	7.175	41.972	1.00	21.21	BLGL
ATOM	626	C	ALA	91	6.172	9.644	42.060	1.00	23.82	BLGL
ATOM	627	O	ALA	91	6.501	10.244	41.042	1.00	24.10	BLGL
ATOM	628	N	ILE	92	5.335	10.154	42.956	1.00	24.44	BLGL
ATOM	629	CA	ILE	92	4.743	11.471	42.782	1.00	25.65	BLGL
ATOM	630	CB	ILE	92	3.549	11.651	43.748	1.00	26.69	BLGL
ATOM	631	CG2	ILE	92	2.943	13.041	43.600	1.00	25.04	BLGL
ATOM	632	CG1	ILE	92	2.484	10.602	43.418	1.00	27.42	BLGL
ATOM	633	CD1	ILE	92	1.341	10.553	44.385	1.00	25.99	BLGL
ATOM	634	C	ILE	92	5.794	12.568	42.992	1.00	25.95	BLGL
ATOM	635	O	ILE	92	5.800	13.575	42.286	1.00	26.66	BLGL
ATOM	636	N	GLN	93	6.687	12.367	43.956	1.00	25.21	BLGL
ATOM	637	CA	GLN	93	7.746	13.332	44.206	1.00	25.19	BLGL
ATOM	638	CB	GLN	93	8.623	12.886	45.369	1.00	27.76	BLGL
ATOM	639	CG	GLN	93	8.285	13.505	46.705	1.00	33.90	BLGL
ATOM	640	CD	GLN	93	9.215	13.020	47.818	1.00	38.24	BLGL
ATOM	641	OE1	GLN	93	9.088	11.890	48.303	1.00	35.85	BLGL
ATOM	642	NE2	GLN	93	10.165	13.873	48.216	1.00	40.86	BLGL
ATOM	643	C	GLN	93	8.595	13.427	42.949	1.00	24.82	BLGL
ATOM	644	O	GLN	93	8.870	14.514	42.454	1.00	27.29	BLGL
ATOM	645	N	ILE	94	9.008	12.276	42.434	1.00	23.84	BLGL
ATOM	646	CA	ILE	94	9.818	12.225	41.223	1.00	21.73	BLGL
ATOM	647	CB	ILE	94	10.263	10.772	40.929	1.00	20.65	BLGL
ATOM	648	CG2	ILE	94	10.936	10.687	39.568	1.00	19.77	BLGL
ATOM	649	CG1	ILE	94	11.202	10.293	42.043	1.00	18.55	BLGL
ATOM	650	CD1	ILE	94	11.644	8.866	41.914	1.00	12.93	BLGL
ATOM	651	C	ILE	94	9.027	12.770	40.038	1.00	21.61	BLGL
ATOM	652	O	ILE	94	9.545	13.553	39.232	1.00	19.49	BLGL
ATOM	653	N	GLY	95	7.764	12.362	39.955	1.00	22.02	BLGL
ATOM	654	CA	GLY	95	6.897	12.798	38.876	1.00	23.64	BLGL
ATOM	655	C	GLY	95	6.787	14.302	38.771	1.00	24.52	BLGL
ATOM	656	O	GLY	95	6.932	14.870	37.683	1.00	24.81	BLGL
ATOM	657	N	LYS	96	6.526	14.947	39.907	1.00	26.80	BLGL
ATOM	658	CA	LYS	96	6.401	16.403	39.971	1.00	26.56	BLGL
ATOM	659	CB	LYS	96	6.095	16.844	41.401	1.00	26.83	BLGL

Fig. 4 cont.

ATOM	660	CG	LYS	96	4.653	16.630	41.818	1.00 30.58	BLGL
ATOM	661	CD	LYS	96	4.413	17.224	43.192	1.00 34.86	BLGL
ATOM	662	CE	LYS	96	2.939	17.256	43.541	1.00 38.91	BLGL
ATOM	663	NZ	LYS	96	2.712	17.810	44.909	1.00 42.19	BLGL
ATOM	664	C	LYS	96	7.663	17.106	39.474	1.00 26.13	BLGL
ATOM	665	O	LYS	96	7.592	18.041	38.676	1.00 25.77	BLGL
ATOM	666	N	ARG	97	8.818	16.649	39.946	1.00 26.45	BLGL
ATOM	667	CA	ARG	97	10.089	17.232	39.533	1.00 25.62	BLGL
ATOM	668	CB	ARG	97	11.229	16.598	40.335	1.00 26.14	BLGL
ATOM	669	CG	ARG	97	11.105	16.909	41.824	1.00 28.26	BLGL
ATOM	670	CD	ARG	97	12.157	16.228	42.687	1.00 28.70	BLGL
ATOM	671	NE	ARG	97	13.514	16.674	42.385	1.00 30.96	BLGL
ATOM	672	CZ	ARG	97	14.593	16.211	43.007	1.00 29.36	BLGL
ATOM	673	NH1	ARG	97	14.460	15.297	43.959	1.00 26.96	BLGL
ATOM	674	NH2	ARG	97	15.799	16.650	42.671	1.00 26.20	BLGL
ATOM	675	C	ARG	97	10.310	17.060	38.032	1.00 24.94	BLGL
ATOM	676	O	ARG	97	10.778	17.973	37.354	1.00 24.07	BLGL
ATOM	677	N	ALA	98	9.959	15.890	37.510	1.00 24.88	BLGL
ATOM	678	CA	ALA	98	10.104	15.626	36.084	1.00 24.73	BLGL
ATOM	679	CB	ALA	98	9.673	14.198	35.771	1.00 26.89	BLGL
ATOM	680	C	ALA	98	9.265	16.620	35.277	1.00 24.32	BLGL
ATOM	681	O	ALA	98	9.715	17.145	34.256	1.00 21.35	BLGL
ATOM	682	N	ASN	99	8.041	16.875	35.727	1.00 25.11	BLGL
ATOM	683	CA	ASN	99	7.196	17.830	35.019	1.00 27.26	BLGL
ATOM	684	CB	ASN	99	5.802	17.871	35.601	1.00 29.92	BLGL
ATOM	685	CG	ASN	99	5.039	16.631	35.330	1.00 36.77	BLGL
ATOM	686	OD1	ASN	99	3.817	16.649	35.364	1.00 43.97	BLGL
ATOM	687	ND2	ASN	99	5.743	15.529	35.063	1.00 38.67	BLGL
ATOM	688	C	ASN	99	7.766	19.229	35.096	1.00 26.84	BLGL
ATOM	689	O	ASN	99	7.850	19.919	34.090	1.00 29.38	BLGL
ATOM	690	N	ALA	100	8.143	19.652	36.298	1.00 23.90	BLGL
ATOM	691	CA	ALA	100	8.689	20.982	36.481	1.00 23.21	BLGL
ATOM	692	CB	ALA	100	9.214	21.137	37.894	1.00 20.39	BLGL
ATOM	693	C	ALA	100	9.800	21.244	35.470	1.00 25.29	BLGL
ATOM	694	O	ALA	100	10.088	22.394	35.141	1.00 26.23	BLGL
ATOM	695	N	ASN	101	10.409	20.174	34.963	1.00 25.14	BLGL
ATOM	696	CA	ASN	101	11.492	20.307	33.998	1.00 25.17	BLGL
ATOM	697	CB	ASN	101	12.696	19.515	34.483	1.00 24.95	BLGL
ATOM	698	CG	ASN	101	13.280	20.091	35.747	1.00 25.85	BLGL
ATOM	699	OD1	ASN	101	13.914	21.145	35.719	1.00 29.40	BLGL
ATOM	700	ND2	ASN	101	13.054	19.422	36.868	1.00 24.97	BLGL
ATOM	701	C	ASN	101	11.118	19.898	32.582	1.00 25.90	BLGL
ATOM	702	O	ASN	101	11.978	19.563	31.772	1.00 27.14	BLGL
ATOM	703	N	GLY	102	9.824	19.932	32.290	1.00 25.80	BLGL
ATOM	704	CA	GLY	102	9.345	19.598	30.962	1.00 24.78	BLGL
ATOM	705	C	GLY	102	9.671	18.215	30.447	1.00 25.83	BLGL
ATOM	706	O	GLY	102	10.048	18.061	29.289	1.00 27.54	BLGL
ATOM	707	N	MET	103	9.525	17.205	31.297	1.00 26.80	BLGL
ATOM	708	CA	MET	103	9.793	15.827	30.899	1.00 26.04	BLGL
ATOM	709	CB	MET	103	11.006	15.283	31.662	1.00 26.48	BLGL
ATOM	710	CG	MET	103	12.265	16.110	31.451	1.00 29.27	BLGL
ATOM	711	SD	MET	103	13.767	15.380	32.124	1.00 31.74	BLGL
ATOM	712	CE	MET	103	13.716	16.017	33.804	1.00 31.73	BLGL
ATOM	713	C	MET	103	8.559	14.978	31.191	1.00 25.31	BLGL
ATOM	714	O	MET	103	7.892	15.179	32.206	1.00 24.54	BLGL
ATOM	715	N	LYS	104	8.243	14.044	30.294	1.00 24.62	BLGL
ATOM	716	CA	LYS	104	7.082	13.174	30.484	1.00 24.42	BLGL
ATOM	717	CB	LYS	104	6.668	12.527	29.167	1.00 28.12	BLGL
ATOM	718	CG	LYS	104	6.265	13.483	28.062	1.00 32.81	BLGL
ATOM	719	CD	LYS	104	4.800	13.820	28.149	1.00 35.64	BLGL
ATOM	720	CE	LYS	104	4.294	14.402	26.843	1.00 37.37	BLGL
ATOM	721	NZ	LYS	104	2.807	14.485	26.870	1.00 40.79	BLGL
ATOM	722	C	LYS	104	7.452	12.075	31.466	1.00 22.98	BLGL
ATOM	723	O	LYS	104	8.632	11.840	31.720	1.00 23.51	BLGL
ATOM	724	N	LEU	105	6.450	11.398	32.014	1.00 21.49	BLGL
ATOM	725	CA	LEU	105	6.705	10.313	32.955	1.00 19.77	BLGL

Fig. 4 cont.

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ATOM    726  CB  LEU  105       5.975  10.559  34.279  1.00 18.76      BLGL
ATOM    727  CG  LEU  105       6.334   9.548  35.381  1.00 19.18      BLGL
ATOM    728  CD1 LEU  105       7.586  10.007  36.100  1.00 16.56      BLGL
ATOM    729  CD2 LEU  105       5.195   9.412  36.364  1.00 21.13      BLGL
ATOM    730  C   LEU  105       6.280   8.941  32.418  1.00 19.86      BLGL
ATOM    731  O   LEU  105       5.285   8.812  31.701  1.00 16.96      BLGL
ATOM    732  N   LEU  106       7.059   7.920  32.758  1.00 19.88      BLGL
ATOM    733  CA  LEU  106       6.738   6.551  32.381  1.00 19.92      BLGL
ATOM    734  CB  LEU  106       7.889   5.878  31.637  1.00 17.61      BLGL
ATOM    735  CG  LEU  106       7.550   4.607  30.838  1.00 21.29      BLGL
ATOM    736  CD1 LEU  106       8.845   3.872  30.511  1.00 18.25      BLGL
ATOM    737  CD2 LEU  106       6.627   3.689  31.604  1.00 17.96      BLGL
ATOM    738  C   LEU  106       6.567   5.877  33.730  1.00 19.81      BLGL
ATOM    739  O   LEU  106       7.546   5.660  34.437  1.00 19.58      BLGL
ATOM    740  N   ALA  107       5.327   5.581  34.102  1.00 20.44      BLGL
ATOM    741  CA  ALA  107       5.052   4.922  35.373  1.00 20.99      BLGL
ATOM    742  CB  ALA  107       3.634   5.240  35.826  1.00 21.52      BLGL
ATOM    743  C   ALA  107       5.224   3.418  35.177  1.00 21.97      BLGL
ATOM    744  O   ALA  107       4.493   2.796  34.406  1.00 23.04      BLGL
ATOM    745  N   ASP  108       6.192   2.828  35.867  1.00 21.22      BLGL
ATOM    746  CA  ASP  108       6.438   1.400  35.726  1.00 20.00      BLGL
ATOM    747  CB  ASP  108       7.932   1.175  35.463  1.00 17.66      BLGL
ATOM    748  CG  ASP  108       8.327  -0.289  35.455  1.00 17.79      BLGL
ATOM    749  OD1 ASP  108       7.448  -1.173  35.519  1.00 16.92      BLGL
ATOM    750  OD2 ASP  108       9.542  -0.562  35.385  1.00 18.27      BLGL
ATOM    751  C   ASP  108       5.966   0.625  36.953  1.00 21.24      BLGL
ATOM    752  O   ASP  108       6.635   0.614  37.984  1.00 25.51      BLGL
ATOM    753  N   PHE  109       4.801  -0.010  36.840  1.00 19.98      BLGL
ATOM    754  CA  PHE  109       4.256  -0.792  37.939  1.00 20.05      BLGL
ATOM    755  CB  PHE  109       2.739  -0.903  37.850  1.00 20.06      BLGL
ATOM    756  CG  PHE  109       2.033   0.386  38.066  1.00 21.36      BLGL
ATOM    757  CD1 PHE  109       1.751   1.225  36.995  1.00 21.28      BLGL
ATOM    758  CD2 PHE  109       1.665   0.777  39.349  1.00 21.79      BLGL
ATOM    759  CE1 PHE  109       1.110   2.442  37.194  1.00 24.40      BLGL
ATOM    760  CE2 PHE  109       1.026   1.989  39.564  1.00 23.03      BLGL
ATOM    761  CZ  PHE  109       0.745   2.828  38.482  1.00 23.74      BLGL
ATOM    762  C   PHE  109       4.822  -2.190  37.949  1.00 19.77      BLGL
ATOM    763  O   PHE  109       4.680  -2.932  36.978  1.00 18.81      BLGL
ATOM    764  N   HIS  110       5.464  -2.547  39.054  1.00 19.76      BLGL
ATOM    765  CA  HIS  110       6.023  -3.875  39.188  1.00 20.72      BLGL
ATOM    766  CB  HIS  110       7.207  -3.876  40.157  1.00 20.31      BLGL
ATOM    767  CG  HIS  110       8.497  -3.439  39.540  1.00 20.23      BLGL
ATOM    768  CD2 HIS  110       8.779  -2.456  38.653  1.00 19.83      BLGL
ATOM    769  ND1 HIS  110       9.703  -4.034  39.845  1.00 21.63      BLGL
ATOM    770  CE1 HIS  110      10.671  -3.437  39.174  1.00 20.13      BLGL
ATOM    771  NE2 HIS  110      10.137  -2.475  38.442  1.00 20.13      BLGL
ATOM    772  C   HIS  110       4.948  -4.823  39.695  1.00 20.55      BLGL
ATOM    773  O   HIS  110       5.056  -6.036  39.536  1.00 20.58      BLGL
ATOM    774  N   TYR  111       3.900  -4.267  40.291  1.00 21.08      BLGL
ATOM    775  CA  TYR  111       2.827  -5.093  40.830  1.00 23.38      BLGL
ATOM    776  CB  TYR  111       2.039  -5.759  39.695  1.00 22.62      BLGL
ATOM    777  CG  TYR  111       1.274  -4.758  38.858  1.00 23.84      BLGL
ATOM    778  CD1 TYR  111       1.551  -4.593  37.501  1.00 22.76      BLGL
ATOM    779  CE1 TYR  111       0.878  -3.641  36.742  1.00 23.56      BLGL
ATOM    780  CD2 TYR  111       0.297  -3.945  39.437  1.00 24.23      BLGL
ATOM    781  CE2 TYR  111      -0.378  -2.991  38.688  1.00 23.70      BLGL
ATOM    782  CZ  TYR  111      -0.082  -2.844  37.344  1.00 23.27      BLGL
ATOM    783  OH  TYR  111      -0.738  -1.887  36.609  1.00 24.35      BLGL
ATOM    784  C   TYR  111       3.439  -6.137  41.754  1.00 22.90      BLGL
ATOM    785  O   TYR  111       3.094  -7.317  41.718  1.00 22.52      BLGL
ATOM    786  N   SER  112       4.372  -5.668  42.574  1.00 22.56      BLGL
ATOM    787  CA  SER  112       5.071  -6.493  43.544  1.00 22.63      BLGL
ATOM    788  CB  SER  112       6.249  -7.201  42.892  1.00 22.37      BLGL
ATOM    789  OG  SER  112       7.002  -7.894  43.866  1.00 23.73      BLGL
ATOM    790  C   SER  112       5.585  -5.542  44.601  1.00 23.27      BLGL
ATOM    791  O   SER  112       5.631  -4.333  44.368  1.00 24.65      BLGL
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Fig. 4 cont.

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ATOM    792  N   ASP  113       5.968  -6.069  45.760  1.00 22.31      BLGL
ATOM    793  CA  ASP  113       6.486  -5.208  46.815  1.00 22.28      BLGL
ATOM    794  CB  ASP  113       6.202  -5.795  48.199  1.00 22.82      BLGL
ATOM    795  CG  ASP  113       4.732  -5.719  48.577  1.00 25.54      BLGL
ATOM    796  OD1 ASP  113       4.032  -4.825  48.056  1.00 23.47      BLGL
ATOM    797  OD2 ASP  113       4.281  -6.544  49.406  1.00 24.91      BLGL
ATOM    798  C   ASP  113       7.982  -4.969  46.651  1.00 21.86      BLGL
ATOM    799  O   ASP  113       8.548  -4.101  47.309  1.00 21.62      BLGL
ATOM    800  N   PHE  114       8.622  -5.738  45.775  1.00 20.23      BLGL
ATOM    801  CA  PHE  114      10.046  -5.563  45.547  1.00 20.78      BLGL
ATOM    802  CB  PHE  114      10.853  -6.387  46.549  1.00 21.28      BLGL
ATOM    803  CG  PHE  114      12.221  -5.822  46.838  1.00 24.03      BLGL
ATOM    804  CD1 PHE  114      12.420  -4.441  46.919  1.00 24.35      BLGL
ATOM    805  CD2 PHE  114      13.308  -6.666  47.064  1.00 24.49      BLGL
ATOM    806  CE1 PHE  114      13.684  -3.909  47.224  1.00 22.80      BLGL
ATOM    807  CE2 PHE  114      14.575  -6.144  47.372  1.00 20.26      BLGL
ATOM    808  CZ  PHE  114      14.761  -4.767  47.451  1.00 20.45      BLGL
ATOM    809  C   PHE  114      10.392  -5.952  44.122  1.00 21.41      BLGL
ATOM    810  O   PHE  114       9.507  -6.328  43.361  1.00 21.59      BLGL
ATOM    811  N   TRP  115      11.675  -5.856  43.768  1.00 20.29      BLGL
ATOM    812  CA  TRP  115      12.152  -6.160  42.418  1.00 19.28      BLGL
ATOM    813  CB  TRP  115      13.634  -6.577  42.445  1.00 20.57      BLGL
ATOM    814  CG  TRP  115      14.575  -5.534  42.963  1.00 21.03      BLGL
ATOM    815  CD2 TRP  115      14.942  -4.315  42.311  1.00 20.71      BLGL
ATOM    816  CE2 TRP  115      15.786  -3.607  43.198  1.00 21.97      BLGL
ATOM    817  CE3 TRP  115      14.637  -3.747  41.066  1.00 20.82      BLGL
ATOM    818  CD1 TRP  115      15.202  -5.523  44.177  1.00 19.55      BLGL
ATOM    819  NE1 TRP  115      15.929  -4.371  44.328  1.00 18.99      BLGL
ATOM    820  CZ2 TRP  115      16.329  -2.350  42.878  1.00 22.16      BLGL
ATOM    821  CZ3 TRP  115      15.177  -2.499  40.746  1.00 21.59      BLGL
ATOM    822  CH2 TRP  115      16.013  -1.815  41.653  1.00 22.47      BLGL
ATOM    823  C   TRP  115      11.361  -7.231  41.665  1.00 18.82      BLGL
ATOM    824  O   TRP  115      11.090  -8.308  42.193  1.00 17.18      BLGL
ATOM    825  N   ALA  116      10.995  -6.925  40.426  1.00 17.42      BLGL
ATOM    826  CA  ALA  116      10.277  -7.874  39.589  1.00 19.55      BLGL
ATOM    827  CB  ALA  116       8.914  -7.326  39.223  1.00 18.74      BLGL
ATOM    828  C   ALA  116      11.110  -8.105  38.331  1.00 22.25      BLGL
ATOM    829  O   ALA  116      11.457  -7.157  37.631  1.00 25.39      BLGL
ATOM    830  N   ASP  117      11.450  -9.358  38.051  1.00 21.71      BLGL
ATOM    831  CA  ASP  117      12.243  -9.672  36.872  1.00 22.29      BLGL
ATOM    832  CB  ASP  117      13.736  -9.620  37.209  1.00 22.60      BLGL
ATOM    833  CG  ASP  117      14.124 -10.578  38.309  1.00 26.69      BLGL
ATOM    834  OD1 ASP  117      13.662 -11.738  38.294  1.00 29.56      BLGL
ATOM    835  OD2 ASP  117      14.907 -10.171  39.190  1.00 30.52      BLGL
ATOM    836  C   ASP  117      11.843 -11.045  36.346  1.00 22.91      BLGL
ATOM    837  O   ASP  117      10.840 -11.601  36.784  1.00 24.06      BLGL
ATOM    838  N   PRO  118      12.617 -11.619  35.409  1.00 22.06      BLGL
ATOM    839  CD  PRO  118      13.734 -11.056  34.639  1.00 20.93      BLGL
ATOM    840  CA  PRO  118      12.252 -12.935  34.880  1.00 24.27      BLGL
ATOM    841  CB  PRO  118      13.301 -13.176  33.802  1.00 22.87      BLGL
ATOM    842  CG  PRO  118      13.629 -11.821  33.353  1.00 24.48      BLGL
ATOM    843  C   PRO  118      12.202 -14.077  35.884  1.00 26.00      BLGL
ATOM    844  O   PRO  118      11.667 -15.140  35.580  1.00 29.05      BLGL
ATOM    845  N   ALA  119      12.755 -13.868  37.071  1.00 28.00      BLGL
ATOM    846  CA  ALA  119      12.762 -14.917  38.086  1.00 28.48      BLGL
ATOM    847  CB  ALA  119      14.186 -15.188  38.543  1.00 27.97      BLGL
ATOM    848  C   ALA  119      11.899 -14.568  39.283  1.00 28.36      BLGL
ATOM    849  O   ALA  119      11.407 -15.447  39.981  1.00 30.80      BLGL
ATOM    850  N   LYS  120      11.719 -13.279  39.524  1.00 29.14      BLGL
ATOM    851  CA  LYS  120      10.920 -12.842  40.654  1.00 29.76      BLGL
ATOM    852  CB  LYS  120      11.793 -12.032  41.617  1.00 31.32      BLGL
ATOM    853  CG  LYS  120      12.940 -12.838  42.213  1.00 38.25      BLGL
ATOM    854  CD  LYS  120      13.897 -12.000  43.074  1.00 40.66      BLGL
ATOM    855  CE  LYS  120      14.801 -11.115  42.222  1.00 44.93      BLGL
ATOM    856  NZ  LYS  120      15.827 -10.373  43.027  1.00 46.70      BLGL
ATOM    857  C   LYS  120       9.708 -12.020  40.224  1.00 28.61      BLGL
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Fig. 4 cont.

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ATOM    858  O   LYS   120       9.841 -10.912  39.702  1.00 28.45      BLGL
ATOM    859  N   GLN   121       8.525 -12.589  40.425  1.00 26.27      BLGL
ATOM    860  CA  GLN   121       7.273 -11.913  40.108  1.00 25.49      BLGL
ATOM    861  CB  GLN   121       6.673 -12.457  38.805  1.00 24.33      BLGL
ATOM    862  CG  GLN   121       7.392 -12.034  37.525  1.00 20.53      BLGL
ATOM    863  CD  GLN   121       7.376 -10.528  37.291  1.00 18.36      BLGL
ATOM    864  OE1 GLN   121       6.425  -9.838  37.659  1.00 15.80      BLGL
ATOM    865  NE2 GLN   121       8.424 -10.017  36.655  1.00 17.37      BLGL
ATOM    866  C   GLN   121       6.328 -12.176  41.281  1.00 25.36      BLGL
ATOM    867  O   GLN   121       5.176 -12.571  41.099  1.00 26.22      BLGL
ATOM    868  N   LYS   122       6.843 -11.970  42.489  1.00 25.47      BLGL
ATOM    869  CA  LYS   122       6.091 -12.188  43.716  1.00 25.96      BLGL
ATOM    870  CB  LYS   122       7.031 -12.079  44.924  1.00 27.22      BLGL
ATOM    871  CG  LYS   122       6.394 -12.412  46.260  1.00 29.39      BLGL
ATOM    872  CD  LYS   122       6.870 -13.759  46.785  1.00 32.32      BLGL
ATOM    873  CE  LYS   122       7.832 -13.609  47.961  1.00 31.56      BLGL
ATOM    874  NZ  LYS   122       7.187 -12.997  49.160  1.00 32.62      BLGL
ATOM    875  C   LYS   122       4.968 -11.162  43.833  1.00 26.53      BLGL
ATOM    876  O   LYS   122       5.151  -9.988  43.504  1.00 28.15      BLGL
ATOM    877  N   ALA   123       3.804 -11.603  44.298  1.00 25.34      BLGL
ATOM    878  CA  ALA   123       2.669 -10.700  44.449  1.00 24.78      BLGL
ATOM    879  CB  ALA   123       1.377 -11.491  44.559  1.00 24.09      BLGL
ATOM    880  C   ALA   123       2.830  -9.820  45.675  1.00 23.46      BLGL
ATOM    881  O   ALA   123       3.519 -10.177  46.622  1.00 23.28      BLGL
ATOM    882  N   PRO   124       2.212  -8.636  45.660  1.00 23.79      BLGL
ATOM    883  CD  PRO   124       1.484  -7.998  44.548  1.00 21.21      BLGL
ATOM    884  CA  PRO   124       2.310  -7.738  46.811  1.00 22.77      BLGL
ATOM    885  CB  PRO   124       1.392  -6.588  46.419  1.00 21.28      BLGL
ATOM    886  CG  PRO   124       1.521  -6.547  44.927  1.00 19.51      BLGL
ATOM    887  C   PRO   124       1.791  -8.491  48.037  1.00 23.09      BLGL
ATOM    888  O   PRO   124       0.883  -9.312  47.922  1.00 22.17      BLGL
ATOM    889  N   LYS   125       2.360  -8.228  49.205  1.00 25.24      BLGL
ATOM    890  CA  LYS   125       1.910  -8.916  50.411  1.00 25.84      BLGL
ATOM    891  CB  LYS   125       2.612  -8.350  51.656  1.00 23.65      BLGL
ATOM    892  CG  LYS   125       4.109  -8.642  51.733  1.00 21.46      BLGL
ATOM    893  CD  LYS   125       4.750  -8.067  52.990  1.00 15.25      BLGL
ATOM    894  CE  LYS   125       4.683  -6.554  53.029  1.00 20.47      BLGL
ATOM    895  NZ  LYS   125       5.440  -5.911  51.912  1.00 22.44      BLGL
ATOM    896  C   LYS   125       0.391  -8.807  50.570  1.00 27.21      BLGL
ATOM    897  O   LYS   125      -0.264  -9.763  50.976  1.00 27.46      BLGL
ATOM    898  N   ALA   126      -0.170  -7.651  50.232  1.00 27.45      BLGL
ATOM    899  CA  ALA   126      -1.608  -7.438  50.360  1.00 28.44      BLGL
ATOM    900  CB  ALA   126      -1.942  -5.996  50.042  1.00 27.50      BLGL
ATOM    901  C   ALA   126      -2.445  -8.367  49.487  1.00 30.46      BLGL
ATOM    902  O   ALA   126      -3.578  -8.700  49.835  1.00 32.72      BLGL
ATOM    903  N   TRP   127      -1.893  -8.780  48.352  1.00 31.67      BLGL
ATOM    904  CA  TRP   127      -2.608  -9.663  47.436  1.00 32.34      BLGL
ATOM    905  CB  TRP   127      -2.274  -9.301  45.983  1.00 29.98      BLGL
ATOM    906  CG  TRP   127      -2.525  -7.864  45.623  1.00 26.78      BLGL
ATOM    907  CD2 TRP   127      -2.176  -7.215  44.392  1.00 25.87      BLGL
ATOM    908  CE2 TRP   127      -2.582  -5.869  44.499  1.00 24.64      BLGL
ATOM    909  CE3 TRP   127      -1.558  -7.643  43.207  1.00 25.70      BLGL
ATOM    910  CD1 TRP   127      -3.116  -6.913  46.400  1.00 25.22      BLGL
ATOM    911  NE1 TRP   127      -3.153  -5.712  45.735  1.00 25.00      BLGL
ATOM    912  CZ2 TRP   127      -2.390  -4.942  43.469  1.00 23.42      BLGL
ATOM    913  CZ3 TRP   127      -1.367  -6.723  42.183  1.00 24.22      BLGL
ATOM    914  CH2 TRP   127      -1.781  -5.387  42.323  1.00 24.78      BLGL
ATOM    915  C   TRP   127      -2.220 -11.113  47.694  1.00 34.48      BLGL
ATOM    916  O   TRP   127      -2.786 -12.039  47.101  1.00 34.45      BLGL
ATOM    917  N   ALA   128      -1.244 -11.284  48.585  1.00 37.15      BLGL
ATOM    918  CA  ALA   128      -0.704 -12.589  48.971  1.00 38.47      BLGL
ATOM    919  CB  ALA   128      -0.198 -12.528  50.396  1.00 40.00      BLGL
ATOM    920  C   ALA   128      -1.663 -13.759  48.817  1.00 39.10      BLGL
ATOM    921  O   ALA   128      -1.406 -14.671  48.032  1.00 38.72      BLGL
ATOM    922  N   ASN   129      -2.754 -13.751  49.574  1.00 40.50      BLGL
ATOM    923  CA  ASN   129      -3.716 -14.836  49.473  1.00 44.45      BLGL
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Fig. 4 cont.

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ATOM    924  CB  ASN   129      -3.794 -15.632  50.788  1.00 47.42      BLGL
ATOM    925  CG  ASN   129      -3.746 -14.751  52.018  1.00 50.55      BLGL
ATOM    926  OD1 ASN   129      -3.975 -13.545  51.941  1.00 54.24      BLGL
ATOM    927  ND2 ASN   129      -3.460 -15.356  53.168  1.00 50.85      BLGL
ATOM    928  C   ASN   129      -5.107 -14.380  49.047  1.00 44.76      BLGL
ATOM    929  O   ASN   129      -6.070 -14.460  49.813  1.00 45.16      BLGL
ATOM    930  N   LEU   130      -5.194 -13.901  47.810  1.00 44.30      BLGL
ATOM    931  CA  LEU   130      -6.452 -13.456  47.230  1.00 43.76      BLGL
ATOM    932  CB  LEU   130      -6.341 -12.018  46.731  1.00 44.19      BLGL
ATOM    933  CG  LEU   130      -6.396 -10.901  47.767  1.00 44.74      BLGL
ATOM    934  CD1 LEU   130      -6.258  -9.564  47.071  1.00 45.24      BLGL
ATOM    935  CD2 LEU   130      -7.712 -10.970  48.515  1.00 45.37      BLGL
ATOM    936  C   LEU   130      -6.727 -14.363  46.049  1.00 43.61      BLGL
ATOM    937  O   LEU   130      -5.801 -14.769  45.351  1.00 43.36      BLGL
ATOM    938  N   ASN   131      -7.991 -14.695  45.823  1.00 44.12      BLGL
ATOM    939  CA  ASN   131      -8.318 -15.549  44.690  1.00 44.97      BLGL
ATOM    940  CB  ASN   131      -9.757 -16.078  44.801  1.00 47.76      BLGL
ATOM    941  CG  ASN   131     -10.794 -14.976  44.772  1.00 51.05      BLGL
ATOM    942  OD1 ASN   131     -10.669 -13.968  45.465  1.00 55.52      BLGL
ATOM    943  ND2 ASN   131     -11.835 -15.170  43.977  1.00 52.37      BLGL
ATOM    944  C   ASN   131      -8.133 -14.706  43.436  1.00 43.17      BLGL
ATOM    945  O   ASN   131      -8.381 -13.502  43.451  1.00 42.05      BLGL
ATOM    946  N   PHE   132      -7.682 -15.338  42.360  1.00 42.47      BLGL
ATOM    947  CA  PHE   132      -7.440 -14.638  41.107  1.00 42.04      BLGL
ATOM    948  CB  PHE   132      -7.430 -15.619  39.940  1.00 42.05      BLGL
ATOM    949  CG  PHE   132      -7.126 -14.971  38.633  1.00 42.75      BLGL
ATOM    950  CD1 PHE   132      -5.870 -14.426  38.396  1.00 42.49      BLGL
ATOM    951  CD2 PHE   132      -8.103 -14.855  37.656  1.00 43.76      BLGL
ATOM    952  CE1 PHE   132      -5.594 -13.769  37.204  1.00 42.79      BLGL
ATOM    953  CE2 PHE   132      -7.834 -14.197  36.455  1.00 44.60      BLGL
ATOM    954  CZ  PHE   132      -6.579 -13.655  36.232  1.00 43.31      BLGL
ATOM    955  C   PHE   132      -8.439 -13.523  40.808  1.00 41.68      BLGL
ATOM    956  O   PHE   132      -8.050 -12.415  40.445  1.00 41.50      BLGL
ATOM    957  N   GLU   133      -9.725 -13.815  40.951  1.00 42.52      BLGL
ATOM    958  CA  GLU   133     -10.759 -12.821  40.691  1.00 42.35      BLGL
ATOM    959  CB  GLU   133     -12.138 -13.409  40.985  1.00 46.23      BLGL
ATOM    960  CG  GLU   133     -12.591 -14.433  39.967  1.00 53.21      BLGL
ATOM    961  CD  GLU   133     -12.550 -13.879  38.553  1.00 57.33      BLGL
ATOM    962  OE1 GLU   133     -13.059 -12.757  38.347  1.00 58.31      BLGL
ATOM    963  OE2 GLU   133     -12.015 -14.564  37.652  1.00 61.34      BLGL
ATOM    964  C   GLU   133     -10.573 -11.542  41.500  1.00 40.12      BLGL
ATOM    965  O   GLU   133     -10.654 -10.443  40.951  1.00 38.25      BLGL
ATOM    966  N   ASP   134     -10.326 -11.691  42.800  1.00 38.18      BLGL
ATOM    967  CA  ASP   134     -10.133 -10.547  43.684  1.00 37.03      BLGL
ATOM    968  CB  ASP   134     -10.203 -10.994  45.142  1.00 39.68      BLGL
ATOM    969  CG  ASP   134     -11.625 -11.128  45.640  1.00 40.58      BLGL
ATOM    970  OD1 ASP   134     -11.816 -11.683  46.744  1.00 40.76      BLGL
ATOM    971  OD2 ASP   134     -12.546 -10.666  44.930  1.00 42.41      BLGL
ATOM    972  C   ASP   134      -8.816  -9.822  43.434  1.00 34.44      BLGL
ATOM    973  O   ASP   134      -8.710  -8.611  43.633  1.00 33.65      BLGL
ATOM    974  N   LYS   135      -7.810 -10.570  43.003  1.00 32.43      BLGL
ATOM    975  CA  LYS   135      -6.510  -9.989  42.717  1.00 30.17      BLGL
ATOM    976  CB  LYS   135      -5.468 -11.092  42.537  1.00 28.01      BLGL
ATOM    977  CG  LYS   135      -4.058 -10.568  42.377  1.00 25.79      BLGL
ATOM    978  CD  LYS   135      -3.090 -11.647  41.928  1.00 24.80      BLGL
ATOM    979  CE  LYS   135      -2.994 -12.773  42.922  1.00 24.10      BLGL
ATOM    980  NZ  LYS   135      -1.961 -13.742  42.491  1.00 24.21      BLGL
ATOM    981  C   LYS   135      -6.615  -9.147  41.443  1.00 29.06      BLGL
ATOM    982  O   LYS   135      -6.092  -8.032  41.384  1.00 29.12      BLGL
ATOM    983  N   LYS   136      -7.303  -9.682  40.436  1.00 28.19      BLGL
ATOM    984  CA  LYS   136      -7.492  -8.986  39.166  1.00 26.63      BLGL
ATOM    985  CB  LYS   136      -8.364  -9.819  38.220  1.00 28.55      BLGL
ATOM    986  CG  LYS   136      -8.455  -9.248  36.811  1.00 33.70      BLGL
ATOM    987  CD  LYS   136      -9.739  -9.661  36.093  1.00 40.26      BLGL
ATOM    988  CE  LYS   136      -9.825 -11.171  35.873  1.00 44.05      BLGL
ATOM    989  NZ  LYS   136     -11.113 -11.590  35.228  1.00 44.46      BLGL
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Fig. 4 cont.

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ATOM    990  C   LYS  136      -8.149  -7.627  39.408  1.00 24.62      BLGL
ATOM    991  O   LYS  136      -7.714  -6.611  38.868  1.00 24.91      BLGL
ATOM    992  N   THR  137      -9.197  -7.607  40.221  1.00 23.73      BLGL
ATOM    993  CA  THR  137      -9.874  -6.356  40.519  1.00 24.53      BLGL
ATOM    994  CB  THR  137     -11.262  -6.603  41.168  1.00 26.21      BLGL
ATOM    995  OG1 THR  137     -11.679  -5.422  41.855  1.00 28.27      BLGL
ATOM    996  CG2 THR  137     -11.220  -7.759  42.134  1.00 27.71      BLGL
ATOM    997  C   THR  137      -9.017  -5.451  41.412  1.00 24.00      BLGL
ATOM    998  O   THR  137      -9.108  -4.221  41.334  1.00 23.13      BLGL
ATOM    999  N   ALA  138      -8.174  -6.054  42.248  1.00 22.08      BLGL
ATOM   1000  CA  ALA  138      -7.289  -5.277  43.115  1.00 23.30      BLGL
ATOM   1001  CB  ALA  138      -6.612  -6.182  44.128  1.00 19.73      BLGL
ATOM   1002  C   ALA  138      -6.228  -4.570  42.265  1.00 23.73      BLGL
ATOM   1003  O   ALA  138      -5.896  -3.401  42.497  1.00 23.84      BLGL
ATOM   1004  N   LEU  139      -5.700  -5.288  41.280  1.00 21.33      BLGL
ATOM   1005  CA  LEU  139      -4.690  -4.729  40.402  1.00 22.61      BLGL
ATOM   1006  CB  LEU  139      -4.144  -5.806  39.460  1.00 21.44      BLGL
ATOM   1007  CG  LEU  139      -2.895  -5.411  38.656  1.00 21.68      BLGL
ATOM   1008  CD1 LEU  139      -2.111  -6.664  38.340  1.00 22.58      BLGL
ATOM   1009  CD2 LEU  139      -3.265  -4.658  37.383  1.00 17.55      BLGL
ATOM   1010  C   LEU  139      -5.280  -3.576  39.603  1.00 23.36      BLGL
ATOM   1011  O   LEU  139      -4.629  -2.550  39.401  1.00 23.02      BLGL
ATOM   1012  N   TYR  140      -6.513  -3.747  39.141  1.00 24.62      BLGL
ATOM   1013  CA  TYR  140      -7.176  -2.697  38.381  1.00 25.60      BLGL
ATOM   1014  CB  TYR  140      -8.514  -3.206  37.833  1.00 23.98      BLGL
ATOM   1015  CG  TYR  140      -9.494  -2.109  37.498  1.00 22.17      BLGL
ATOM   1016  CD1 TYR  140     -10.389  -1.634  38.452  1.00 25.15      BLGL
ATOM   1017  CE1 TYR  140     -11.259  -0.580  38.167  1.00 25.77      BLGL
ATOM   1018  CD2 TYR  140      -9.492  -1.508  36.247  1.00 22.26      BLGL
ATOM   1019  CE2 TYR  140     -10.353  -0.457  35.950  1.00 24.44      BLGL
ATOM   1020  CZ  TYR  140     -11.235   0.003  36.911  1.00 25.75      BLGL
ATOM   1021  OH  TYR  140     -12.096   1.036  36.615  1.00 25.22      BLGL
ATOM   1022  C   TYR  140      -7.393  -1.468  39.272  1.00 27.76      BLGL
ATOM   1023  O   TYR  140      -7.167  -0.335  38.845  1.00 26.59      BLGL
ATOM   1024  N   GLN  141      -7.828  -1.698  40.508  1.00 29.36      BLGL
ATOM   1025  CA  GLN  141      -8.061  -0.605  41.446  1.00 31.47      BLGL
ATOM   1026  CB  GLN  141      -8.645  -1.134  42.758  1.00 34.45      BLGL
ATOM   1027  CG  GLN  141     -10.105  -1.525  42.664  1.00 44.36      BLGL
ATOM   1028  CD  GLN  141     -11.015  -0.331  42.408  1.00 49.85      BLGL
ATOM   1029  OE1 GLN  141     -12.161  -0.487  41.957  1.00 52.06      BLGL
ATOM   1030  NE2 GLN  141     -10.515   0.870  42.707  1.00 49.83      BLGL
ATOM   1031  C   GLN  141      -6.782   0.154  41.751  1.00 29.93      BLGL
ATOM   1032  O   GLN  141      -6.751   1.387  41.698  1.00 28.20      BLGL
ATOM   1033  N   TYR  142      -5.730  -0.593  42.079  1.00 27.46      BLGL
ATOM   1034  CA  TYR  142      -4.445  -0.002  42.413  1.00 25.44      BLGL
ATOM   1035  CB  TYR  142      -3.426  -1.105  42.694  1.00 26.98      BLGL
ATOM   1036  CG  TYR  142      -2.025  -0.585  42.928  1.00 26.89      BLGL
ATOM   1037  CD1 TYR  142      -1.752   0.281  43.979  1.00 25.19      BLGL
ATOM   1038  CE1 TYR  142      -0.473   0.768  44.189  1.00 28.95      BLGL
ATOM   1039  CD2 TYR  142      -0.979  -0.950  42.088  1.00 27.59      BLGL
ATOM   1040  CE2 TYR  142       0.305  -0.468  42.287  1.00 29.43      BLGL
ATOM   1041  CZ  TYR  142       0.553   0.390  43.341  1.00 30.68      BLGL
ATOM   1042  OH  TYR  142       1.829   0.862  43.554  1.00 32.86      BLGL
ATOM   1043  C   TYR  142      -3.922   0.912  41.311  1.00 24.17      BLGL
ATOM   1044  O   TYR  142      -3.466   2.026  41.572  1.00 22.37      BLGL
ATOM   1045  N   THR  143      -3.988   0.432  40.076  1.00 23.95      BLGL
ATOM   1046  CA  THR  143      -3.518   1.205  38.941  1.00 24.20      BLGL
ATOM   1047  CB  THR  143      -3.626   0.397  37.649  1.00 22.46      BLGL
ATOM   1048  OG1 THR  143      -3.000  -0.875  37.838  1.00 19.33      BLGL
ATOM   1049  CG2 THR  143      -2.948   1.129  36.508  1.00 20.23      BLGL
ATOM   1050  C   THR  143      -4.361   2.459  38.803  1.00 25.95      BLGL
ATOM   1051  O   THR  143      -3.836   3.568  38.689  1.00 27.54      BLGL
ATOM   1052  N   LYS  144      -5.673   2.263  38.821  1.00 27.01      BLGL
ATOM   1053  CA  LYS  144      -6.636   3.346  38.690  1.00 28.79      BLGL
ATOM   1054  CB  LYS  144      -8.053   2.779  38.818  1.00 30.43      BLGL
ATOM   1055  CG  LYS  144      -9.167   3.787  38.626  1.00 32.32      BLGL
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Fig. 4 cont.

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ATOM   1056  CD  LYS   144      -9.391   4.123  37.167  1.00 35.17      BLGL
ATOM   1057  CE  LYS   144     -10.603   5.033  37.010  1.00 36.95      BLGL
ATOM   1058  NZ  LYS   144     -11.835   4.435  37.605  1.00 37.88      BLGL
ATOM   1059  C   LYS   144      -6.401   4.421  39.748  1.00 28.67      BLGL
ATOM   1060  O   LYS   144      -6.322   5.606  39.433  1.00 29.09      BLGL
ATOM   1061  N   GLN   145      -6.287   4.010  41.004  1.00 28.65      BLGL
ATOM   1062  CA  GLN   145      -6.062   4.969  42.075  1.00 31.28      BLGL
ATOM   1063  CB  GLN   145      -6.116   4.281  43.440  1.00 35.75      BLGL
ATOM   1064  CG  GLN   145      -7.463   3.632  43.756  1.00 45.00      BLGL
ATOM   1065  CD  GLN   145      -8.638   4.586  43.565  1.00 50.27      BLGL
ATOM   1066  OE1 GLN   145      -8.697   5.651  44.189  1.00 53.13      BLGL
ATOM   1067  NE2 GLN   145      -9.580   4.206  42.699  1.00 51.05      BLGL
ATOM   1068  C   GLN   145      -4.720   5.666  41.905  1.00 30.73      BLGL
ATOM   1069  O   GLN   145      -4.653   6.895  41.883  1.00 31.69      BLGL
ATOM   1070  N   SER   146      -3.655   4.880  41.778  1.00 28.68      BLGL
ATOM   1071  CA  SER   146      -2.315   5.429  41.614  1.00 27.00      BLGL
ATOM   1072  CB  SER   146      -1.326   4.319  41.276  1.00 26.10      BLGL
ATOM   1073  OG  SER   146      -1.175   3.432  42.363  1.00 25.05      BLGL
ATOM   1074  C   SER   146      -2.258   6.485  40.529  1.00 26.20      BLGL
ATOM   1075  O   SER   146      -1.733   7.576  40.739  1.00 24.18      BLGL
ATOM   1076  N   LEU   147      -2.793   6.148  39.363  1.00 26.95      BLGL
ATOM   1077  CA  LEU   147      -2.798   7.069  38.240  1.00 28.50      BLGL
ATOM   1078  CB  LEU   147      -3.399   6.386  37.004  1.00 29.76      BLGL
ATOM   1079  CG  LEU   147      -2.403   5.891  35.949  1.00 29.50      BLGL
ATOM   1080  CD1 LEU   147      -1.214   5.237  36.616  1.00 31.84      BLGL
ATOM   1081  CD2 LEU   147      -3.098   4.918  35.010  1.00 31.26      BLGL
ATOM   1082  C   LEU   147      -3.554   8.352  38.563  1.00 28.49      BLGL
ATOM   1083  O   LEU   147      -3.059   9.448  38.291  1.00 26.93      BLGL
ATOM   1084  N   LYS   148      -4.740   8.227  39.156  1.00 29.43      BLGL
ATOM   1085  CA  LYS   148      -5.520   9.412  39.485  1.00 32.08      BLGL
ATOM   1086  CB  LYS   148      -6.897   9.041  40.039  1.00 35.85      BLGL
ATOM   1087  CG  LYS   148      -7.879  10.208  39.955  1.00 44.89      BLGL
ATOM   1088  CD  LYS   148      -9.276   9.854  40.430  1.00 48.80      BLGL
ATOM   1089  CE  LYS   148      -9.319   9.641  41.939  1.00 53.72      BLGL
ATOM   1090  NZ  LYS   148      -8.537   8.451  42.388  1.00 55.41      BLGL
ATOM   1091  C   LYS   148      -4.772  10.277  40.488  1.00 30.09      BLGL
ATOM   1092  O   LYS   148      -4.833  11.502  40.419  1.00 30.55      BLGL
ATOM   1093  N   ALA   149      -4.063   9.636  41.412  1.00 27.72      BLGL
ATOM   1094  CA  ALA   149      -3.279  10.352  42.411  1.00 27.90      BLGL
ATOM   1095  CB  ALA   149      -2.623   9.367  43.368  1.00 26.54      BLGL
ATOM   1096  C   ALA   149      -2.208  11.196  41.720  1.00 28.02      BLGL
ATOM   1097  O   ALA   149      -1.981  12.357  42.075  1.00 27.39      BLGL
ATOM   1098  N   MET   150      -1.547  10.607  40.729  1.00 27.66      BLGL
ATOM   1099  CA  MET   150      -0.511  11.319  39.996  1.00 28.87      BLGL
ATOM   1100  CB  MET   150       0.228  10.357  39.063  1.00 28.84      BLGL
ATOM   1101  CG  MET   150       1.084   9.358  39.828  1.00 31.73      BLGL
ATOM   1102  SD  MET   150       2.122   8.307  38.803  1.00 34.53      BLGL
ATOM   1103  CE  MET   150       1.218   6.808  38.827  1.00 36.46      BLGL
ATOM   1104  C   MET   150      -1.101  12.491  39.219  1.00 28.60      BLGL
ATOM   1105  O   MET   150      -0.518  13.575  39.167  1.00 25.71      BLGL
ATOM   1106  N   LYS   151      -2.269  12.274  38.626  1.00 30.33      BLGL
ATOM   1107  CA  LYS   151      -2.939  13.327  37.871  1.00 31.72      BLGL
ATOM   1108  CB  LYS   151      -4.229  12.793  37.254  1.00 32.47      BLGL
ATOM   1109  CG  LYS   151      -4.036  12.005  35.980  1.00 35.00      BLGL
ATOM   1110  CD  LYS   151      -3.833  12.927  34.789  1.00 38.64      BLGL
ATOM   1111  CE  LYS   151      -3.939  12.159  33.477  1.00 40.97      BLGL
ATOM   1112  NZ  LYS   151      -3.816  13.050  32.295  1.00 40.80      BLGL
ATOM   1113  C   LYS   151      -3.261  14.501  38.787  1.00 31.68      BLGL
ATOM   1114  O   LYS   151      -3.008  15.655  38.442  1.00 32.97      BLGL
ATOM   1115  N   ALA   152      -3.823  14.199  39.953  1.00 31.23      BLGL
ATOM   1116  CA  ALA   152      -4.176  15.228  40.921  1.00 30.30      BLGL
ATOM   1117  CB  ALA   152      -4.759  14.590  42.185  1.00 29.61      BLGL
ATOM   1118  C   ALA   152      -2.952  16.057  41.273  1.00 29.37      BLGL
ATOM   1119  O   ALA   152      -3.066  17.247  41.544  1.00 30.53      BLGL
ATOM   1120  N   ALA   153      -1.783  15.425  41.272  1.00 29.04      BLGL
ATOM   1121  CA  ALA   153      -0.543  16.124  41.596  1.00 29.10      BLGL
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Fig. 4 cont.

ATOM	1122	CB	ALA	153	0.517	15.134	42.032	1.00 30.13	BLGL
ATOM	1123	C	ALA	153	-0.056	16.910	40.391	1.00 29.10	BLGL
ATOM	1124	O	ALA	153	0.990	17.561	40.435	1.00 29.45	BLGL
ATOM	1125	N	GLY	154	-0.824	16.835	39.310	1.00 28.65	BLGL
ATOM	1126	CA	GLY	154	-0.482	17.557	38.101	1.00 26.76	BLGL
ATOM	1127	C	GLY	154	0.711	17.017	37.340	1.00 26.93	BLGL
ATOM	1128	O	GLY	154	1.406	17.770	36.661	1.00 25.28	BLGL
ATOM	1129	N	ILE	155	0.948	15.713	37.444	1.00 27.10	BLGL
ATOM	1130	CA	ILE	155	2.064	15.080	36.745	1.00 25.61	BLGL
ATOM	1131	CB	ILE	155	2.532	13.809	37.496	1.00 24.73	BLGL
ATOM	1132	CG2	ILE	155	3.661	13.118	36.724	1.00 23.73	BLGL
ATOM	1133	CG1	ILE	155	2.985	14.196	38.907	1.00 22.31	BLGL
ATOM	1134	CD1	ILE	155	3.188	13.018	39.842	1.00 21.74	BLGL
ATOM	1135	C	ILE	155	1.672	14.723	35.306	1.00 24.09	BLGL
ATOM	1136	O	ILE	155	0.568	14.240	35.056	1.00 25.01	BLGL
ATOM	1137	N	ASP	156	2.581	14.975	34.369	1.00 21.70	BLGL
ATOM	1138	CA	ASP	156	2.354	14.695	32.959	1.00 23.92	BLGL
ATOM	1139	CB	ASP	156	3.172	15.657	32.089	1.00 26.46	BLGL
ATOM	1140	CG	ASP	156	2.889	15.486	30.602	1.00 30.77	BLGL
ATOM	1141	OD1	ASP	156	3.579	16.140	29.792	1.00 33.81	BLGL
ATOM	1142	OD2	ASP	156	1.976	14.706	30.239	1.00 32.30	BLGL
ATOM	1143	C	ASP	156	2.757	13.261	32.644	1.00 23.58	BLGL
ATOM	1144	O	ASP	156	3.904	12.986	32.319	1.00 26.10	BLGL
ATOM	1145	N	ILE	157	1.805	12.348	32.750	1.00 22.55	BLGL
ATOM	1146	CA	ILE	157	2.062	10.945	32.484	1.00 21.98	BLGL
ATOM	1147	CB	ILE	157	1.070	10.058	33.254	1.00 22.84	BLGL
ATOM	1148	CG2	ILE	157	1.368	8.595	32.990	1.00 18.93	BLGL
ATOM	1149	CG1	ILE	157	1.137	10.385	34.744	1.00 23.81	BLGL
ATOM	1150	CD1	ILE	157	-0.082	9.922	35.514	1.00 26.52	BLGL
ATOM	1151	C	ILE	157	1.894	10.675	30.997	1.00 20.48	BLGL
ATOM	1152	O	ILE	157	0.819	10.885	30.443	1.00 22.51	BLGL
ATOM	1153	N	GLY	158	2.950	10.207	30.349	1.00 18.57	BLGL
ATOM	1154	CA	GLY	158	2.847	9.927	28.935	1.00 16.55	BLGL
ATOM	1155	C	GLY	158	2.758	8.445	28.632	1.00 17.26	BLGL
ATOM	1156	O	GLY	158	2.227	8.042	27.599	1.00 17.93	BLGL
ATOM	1157	N	MET	159	3.245	7.622	29.550	1.00 18.71	BLGL
ATOM	1158	CA	MET	159	3.260	6.186	29.322	1.00 19.00	BLGL
ATOM	1159	CB	MET	159	4.559	5.834	28.588	1.00 17.91	BLGL
ATOM	1160	CG	MET	159	4.563	4.506	27.872	1.00 24.08	BLGL
ATOM	1161	SD	MET	159	6.139	4.187	27.000	1.00 30.17	BLGL
ATOM	1162	CE	MET	159	6.095	5.442	25.740	1.00 26.74	BLGL
ATOM	1163	C	MET	159	3.156	5.395	30.630	1.00 19.17	BLGL
ATOM	1164	O	MET	159	3.573	5.855	31.696	1.00 16.99	BLGL
ATOM	1165	N	VAL	160	2.579	4.204	30.543	1.00 18.21	BLGL
ATOM	1166	CA	VAL	160	2.450	3.345	31.707	1.00 17.42	BLGL
ATOM	1167	CB	VAL	160	1.002	3.285	32.245	1.00 17.75	BLGL
ATOM	1168	CG1	VAL	160	0.920	2.287	33.384	1.00 16.21	BLGL
ATOM	1169	CG2	VAL	160	0.570	4.654	32.739	1.00 18.60	BLGL
ATOM	1170	C	VAL	160	2.891	1.944	31.332	1.00 17.12	BLGL
ATOM	1171	O	VAL	160	2.516	1.406	30.292	1.00 17.78	BLGL
ATOM	1172	N	GLN	161	3.704	1.360	32.192	1.00 17.31	BLGL
ATOM	1173	CA	GLN	161	4.211	0.028	31.963	1.00 17.58	BLGL
ATOM	1174	CB	GLN	161	5.709	0.018	32.272	1.00 17.55	BLGL
ATOM	1175	CG	GLN	161	6.446	-1.213	31.826	1.00 16.31	BLGL
ATOM	1176	CD	GLN	161	7.935	-1.106	32.056	1.00 16.53	BLGL
ATOM	1177	OE1	GLN	161	8.570	-0.132	31.641	1.00 17.05	BLGL
ATOM	1178	NE2	GLN	161	8.508	-2.114	32.707	1.00 12.70	BLGL
ATOM	1179	C	GLN	161	3.439	-0.903	32.893	1.00 16.74	BLGL
ATOM	1180	O	GLN	161	3.455	-0.719	34.106	1.00 17.03	BLGL
ATOM	1181	N	VAL	162	2.736	-1.882	32.330	1.00 14.93	BLGL
ATOM	1182	CA	VAL	162	1.975	-2.818	33.153	1.00 14.33	BLGL
ATOM	1183	CB	VAL	162	0.648	-3.209	32.455	1.00 14.98	BLGL
ATOM	1184	CG1	VAL	162	-0.143	-4.195	33.304	1.00 12.90	BLGL
ATOM	1185	CG2	VAL	162	-0.176	-1.964	32.213	1.00 12.73	BLGL
ATOM	1186	C	VAL	162	2.840	-4.051	33.411	1.00 15.01	BLGL
ATOM	1187	O	VAL	162	2.763	-5.046	32.691	1.00 15.57	BLGL

Fig. 4 cont.

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ATOM   1188  N   GLY  163       3.674  -3.965  34.444  1.00 13.93      BLGL
ATOM   1189  CA  GLY  163       4.568  -5.062  34.765  1.00 16.33      BLGL
ATOM   1190  C   GLY  163       6.001  -4.755  34.350  1.00 17.03      BLGL
ATOM   1191  O   GLY  163       6.239  -3.875  33.521  1.00 17.31      BLGL
ATOM   1192  N   ASN  164       6.958  -5.485  34.917  1.00 17.42      BLGL
ATOM   1193  CA  ASN  164       8.374  -5.274  34.628  1.00 16.23      BLGL
ATOM   1194  CB  ASN  164       9.035  -4.629  35.845  1.00 13.47      BLGL
ATOM   1195  CG  ASN  164      10.413  -4.117  35.556  1.00 11.45      BLGL
ATOM   1196  OD1 ASN  164      10.581  -3.019  35.026  1.00 13.59      BLGL
ATOM   1197  ND2 ASN  164      11.416  -4.912  35.889  1.00 11.01      BLGL
ATOM   1198  C   ASN  164       9.051  -6.614  34.315  1.00 17.48      BLGL
ATOM   1199  O   ASN  164       9.131  -7.490  35.175  1.00 19.59      BLGL
ATOM   1200  N   GLU  165       9.537  -6.765  33.085  1.00 17.58      BLGL
ATOM   1201  CA  GLU  165      10.197  -7.998  32.643  1.00 17.54      BLGL
ATOM   1202  CB  GLU  165      11.605  -8.093  33.244  1.00 16.33      BLGL
ATOM   1203  CG  GLU  165      12.467  -6.875  32.940  1.00 17.40      BLGL
ATOM   1204  CD  GLU  165      13.938  -7.095  33.223  1.00 17.97      BLGL
ATOM   1205  OE1 GLU  165      14.260  -7.739  34.236  1.00 20.07      BLGL
ATOM   1206  OE2 GLU  165      14.783  -6.613  32.442  1.00 15.79      BLGL
ATOM   1207  C   GLU  165       9.372  -9.248  32.982  1.00 16.57      BLGL
ATOM   1208  O   GLU  165       9.875 -10.221  33.534  1.00 14.22      BLGL
ATOM   1209  N   THR  166       8.094  -9.196  32.618  1.00 16.92      BLGL
ATOM   1210  CA  THR  166       7.146 -10.267  32.860  1.00 15.12      BLGL
ATOM   1211  CB  THR  166       5.723  -9.713  32.782  1.00 17.38      BLGL
ATOM   1212  OG1 THR  166       5.514  -9.130  31.490  1.00 16.95      BLGL
ATOM   1213  CG2 THR  166       5.511  -8.629  33.850  1.00 17.63      BLGL
ATOM   1214  C   THR  166       7.304 -11.411  31.860  1.00 15.92      BLGL
ATOM   1215  O   THR  166       6.380 -11.741  31.131  1.00 13.18      BLGL
ATOM   1216  N   ASN  167       8.488 -12.013  31.835  1.00 18.90      BLGL
ATOM   1217  CA  ASN  167       8.775 -13.122  30.933  1.00 19.84      BLGL
ATOM   1218  CB  ASN  167      10.277 -13.399  30.885  1.00 19.56      BLGL
ATOM   1219  CG  ASN  167      11.014 -12.455  29.974  1.00 19.68      BLGL
ATOM   1220  OD1 ASN  167      10.597 -11.320  29.774  1.00 21.70      BLGL
ATOM   1221  ND2 ASN  167      12.132 -12.912  29.429  1.00 19.90      BLGL
ATOM   1222  C   ASN  167       8.074 -14.397  31.343  1.00 20.80      BLGL
ATOM   1223  O   ASN  167       7.670 -15.175  30.489  1.00 22.87      BLGL
ATOM   1224  N   GLY  168       7.936 -14.615  32.647  1.00 22.03      BLGL
ATOM   1225  CA  GLY  168       7.302 -15.833  33.114  1.00 24.61      BLGL
ATOM   1226  C   GLY  168       6.216 -15.699  34.164  1.00 26.99      BLGL
ATOM   1227  O   GLY  168       5.663 -16.702  34.620  1.00 28.98      BLGL
ATOM   1228  N   GLY  169       5.898 -14.478  34.562  1.00 26.63      BLGL
ATOM   1229  CA  GLY  169       4.865 -14.319  35.558  1.00 25.86      BLGL
ATOM   1230  C   GLY  169       4.516 -12.878  35.831  1.00 27.02      BLGL
ATOM   1231  O   GLY  169       5.166 -11.959  35.334  1.00 28.44      BLGL
ATOM   1232  N   LEU  170       3.467 -12.691  36.622  1.00 26.37      BLGL
ATOM   1233  CA  LEU  170       2.996 -11.371  37.005  1.00 23.73      BLGL
ATOM   1234  CB  LEU  170       2.164 -10.751  35.875  1.00 20.57      BLGL
ATOM   1235  CG  LEU  170       1.474  -9.415  36.185  1.00 21.09      BLGL
ATOM   1236  CD1 LEU  170       2.470  -8.395  36.723  1.00 21.42      BLGL
ATOM   1237  CD2 LEU  170       0.811  -8.894  34.934  1.00 20.49      BLGL
ATOM   1238  C   LEU  170       2.158 -11.504  38.272  1.00 23.90      BLGL
ATOM   1239  O   LEU  170       1.222 -12.305  38.326  1.00 22.71      BLGL
ATOM   1240  N   ALA  171       2.522 -10.731  39.292  1.00 23.01      BLGL
ATOM   1241  CA  ALA  171       1.816 -10.724  40.567  1.00 22.14      BLGL
ATOM   1242  CB  ALA  171       0.544  -9.911  40.433  1.00 22.04      BLGL
ATOM   1243  C   ALA  171       1.488 -12.114  41.109  1.00 23.55      BLGL
ATOM   1244  O   ALA  171       0.354 -12.382  41.512  1.00 23.66      BLGL
ATOM   1245  N   GLY  172       2.479 -12.996  41.122  1.00 22.96      BLGL
ATOM   1246  CA  GLY  172       2.259 -14.337  41.632  1.00 25.97      BLGL
ATOM   1247  C   GLY  172       1.592 -15.299  40.666  1.00 27.36      BLGL
ATOM   1248  O   GLY  172       1.412 -16.474  40.980  1.00 27.94      BLGL
ATOM   1249  N   GLU  173       1.225 -14.808  39.490  1.00 28.30      BLGL
ATOM   1250  CA  GLU  173       0.584 -15.643  38.487  1.00 29.90      BLGL
ATOM   1251  CB  GLU  173      -0.540 -14.858  37.815  1.00 30.87      BLGL
ATOM   1252  CG  GLU  173      -1.888 -15.557  37.824  1.00 33.63      BLGL
ATOM   1253  CD  GLU  173      -2.308 -16.014  39.208  1.00 34.41      BLGL
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Fig. 4 cont.

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ATOM   1254  OE1 GLU   173      -2.334 -15.181  40.139  1.00 34.20      BLGL
ATOM   1255  OE2 GLU   173      -2.618 -17.214  39.359  1.00 34.57      BLGL
ATOM   1256  C   GLU   173       1.619 -16.084  37.450  1.00 30.77      BLGL
ATOM   1257  O   GLU   173       2.481 -15.302  37.053  1.00 31.69      BLGL
ATOM   1258  N   THR   174       1.539 -17.338  37.017  1.00 30.71      BLGL
ATOM   1259  CA  THR   174       2.484 -17.864  36.038  1.00 30.81      BLGL
ATOM   1260  CB  THR   174       3.366 -18.975  36.661  1.00 30.70      BLGL
ATOM   1261  OG1 THR   174       2.533 -20.027  37.167  1.00 33.92      BLGL
ATOM   1262  CG2 THR   174       4.201 -18.416  37.792  1.00 29.44      BLGL
ATOM   1263  C   THR   174       1.801 -18.426  34.792  1.00 31.23      BLGL
ATOM   1264  O   THR   174       2.470 -18.868  33.857  1.00 31.14      BLGL
ATOM   1265  N   ASP   175       0.473 -18.409  34.779  1.00 31.31      BLGL
ATOM   1266  CA  ASP   175      -0.276 -18.923  33.640  1.00 31.53      BLGL
ATOM   1267  CB  ASP   175      -1.565 -19.589  34.120  1.00 35.17      BLGL
ATOM   1268  CG  ASP   175      -2.447 -20.030  32.972  1.00 38.71      BLGL
ATOM   1269  OD1 ASP   175      -1.925 -20.654  32.023  1.00 39.79      BLGL
ATOM   1270  OD2 ASP   175      -3.665 -19.758  33.022  1.00 42.47      BLGL
ATOM   1271  C   ASP   175      -0.605 -17.796  32.674  1.00 30.63      BLGL
ATOM   1272  O   ASP   175      -1.363 -16.890  33.016  1.00 30.64      BLGL
ATOM   1273  N   TRP   176      -0.055 -17.861  31.463  1.00 27.62      BLGL
ATOM   1274  CA  TRP   176      -0.281 -16.806  30.480  1.00 27.93      BLGL
ATOM   1275  CB  TRP   176       0.403 -17.147  29.157  1.00 24.63      BLGL
ATOM   1276  CG  TRP   176       1.882 -16.910  29.193  1.00 26.55      BLGL
ATOM   1277  CD2 TRP   176       2.557 -15.666  28.966  1.00 27.36      BLGL
ATOM   1278  CE2 TRP   176       3.940 -15.900  29.148  1.00 27.27      BLGL
ATOM   1279  CE3 TRP   176       2.128 -14.375  28.625  1.00 27.01      BLGL
ATOM   1280  CD1 TRP   176       2.855 -17.820  29.498  1.00 26.56      BLGL
ATOM   1281  NE1 TRP   176       4.094 -17.222  29.473  1.00 26.37      BLGL
ATOM   1282  CZ2 TRP   176       4.899 -14.887  29.004  1.00 25.56      BLGL
ATOM   1283  CZ3 TRP   176       3.085 -13.365  28.482  1.00 25.94      BLGL
ATOM   1284  CH2 TRP   176       4.453 -13.631  28.671  1.00 25.57      BLGL
ATOM   1285  C   TRP   176      -1.739 -16.427  30.234  1.00 29.80      BLGL
ATOM   1286  O   TRP   176      -2.033 -15.289  29.857  1.00 30.42      BLGL
ATOM   1287  N   ALA   177      -2.656 -17.368  30.441  1.00 31.37      BLGL
ATOM   1288  CA  ALA   177      -4.073 -17.077  30.249  1.00 30.31      BLGL
ATOM   1289  CB  ALA   177      -4.889 -18.354  30.339  1.00 30.40      BLGL
ATOM   1290  C   ALA   177      -4.500 -16.104  31.342  1.00 31.32      BLGL
ATOM   1291  O   ALA   177      -5.199 -15.124  31.085  1.00 31.10      BLGL
ATOM   1292  N   LYS   178      -4.070 -16.379  32.569  1.00 30.35      BLGL
ATOM   1293  CA  LYS   178      -4.401 -15.507  33.680  1.00 31.58      BLGL
ATOM   1294  CB  LYS   178      -4.181 -16.235  35.008  1.00 33.69      BLGL
ATOM   1295  CG  LYS   178      -5.114 -17.410  35.234  1.00 37.35      BLGL
ATOM   1296  CD  LYS   178      -4.994 -17.911  36.664  1.00 43.39      BLGL
ATOM   1297  CE  LYS   178      -5.780 -19.196  36.897  1.00 45.38      BLGL
ATOM   1298  NZ  LYS   178      -5.125 -20.370  36.252  1.00 47.94      BLGL
ATOM   1299  C   LYS   178      -3.568 -14.217  33.637  1.00 30.97      BLGL
ATOM   1300  O   LYS   178      -4.040 -13.153  34.043  1.00 31.65      BLGL
ATOM   1301  N   MET   179      -2.333 -14.306  33.149  1.00 29.06      BLGL
ATOM   1302  CA  MET   179      -1.485 -13.126  33.062  1.00 26.50      BLGL
ATOM   1303  CB  MET   179      -0.110 -13.481  32.521  1.00 27.08      BLGL
ATOM   1304  CG  MET   179       0.789 -14.179  33.507  1.00 29.22      BLGL
ATOM   1305  SD  MET   179       2.433 -14.378  32.801  1.00 32.04      BLGL
ATOM   1306  CE  MET   179       2.432 -16.100  32.529  1.00 37.19      BLGL
ATOM   1307  C   MET   179      -2.122 -12.106  32.141  1.00 25.11      BLGL
ATOM   1308  O   MET   179      -2.206 -10.924  32.478  1.00 24.38      BLGL
ATOM   1309  N   SER   180      -2.566 -12.572  30.977  1.00 23.38      BLGL
ATOM   1310  CA  SER   180      -3.199 -11.707  29.985  1.00 23.70      BLGL
ATOM   1311  CB  SER   180      -3.725 -12.533  28.812  1.00 23.12      BLGL
ATOM   1312  OG  SER   180      -2.691 -13.297  28.223  1.00 23.86      BLGL
ATOM   1313  C   SER   180      -4.348 -10.933  30.605  1.00 24.08      BLGL
ATOM   1314  O   SER   180      -4.552  -9.756  30.313  1.00 23.86      BLGL
ATOM   1315  N   GLN   181      -5.101 -11.601  31.467  1.00 25.04      BLGL
ATOM   1316  CA  GLN   181      -6.226 -10.965  32.129  1.00 27.04      BLGL
ATOM   1317  CB  GLN   181      -7.064 -12.009  32.864  1.00 29.17      BLGL
ATOM   1318  CG  GLN   181      -7.820 -12.940  31.932  1.00 33.08      BLGL
ATOM   1319  CD  GLN   181      -8.761 -13.860  32.675  1.00 35.97      BLGL
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Fig. 4 cont.

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ATOM   1320  OE1 GLN   181      -8.558 -15.077  32.724  1.00 36.76      BLGL
ATOM   1321  NE2 GLN   181      -9.801 -13.280  33.269  1.00 37.03      BLGL
ATOM   1322  C   GLN   181      -5.774  -9.874  33.091  1.00 27.11      BLGL
ATOM   1323  O   GLN   181      -6.459  -8.864  33.252  1.00 28.46      BLGL
ATOM   1324  N   LEU   182      -4.628 -10.080  33.737  1.00 26.80      BLGL
ATOM   1325  CA  LEU   182      -4.086  -9.081  34.655  1.00 25.48      BLGL
ATOM   1326  CB  LEU   182      -2.932  -9.665  35.472  1.00 25.40      BLGL
ATOM   1327  CG  LEU   182      -3.296 -10.736  36.504  1.00 27.62      BLGL
ATOM   1328  CD1 LEU   182      -2.035 -11.268  37.156  1.00 27.60      BLGL
ATOM   1329  CD2 LEU   182      -4.229 -10.149  37.556  1.00 26.92      BLGL
ATOM   1330  C   LEU   182      -3.591  -7.899  33.823  1.00 24.10      BLGL
ATOM   1331  O   LEU   182      -3.739  -6.740  34.211  1.00 23.49      BLGL
ATOM   1332  N   PHE   183      -3.000  -8.211  32.675  1.00 21.91      BLGL
ATOM   1333  CA  PHE   183      -2.512  -7.187  31.770  1.00 22.28      BLGL
ATOM   1334  CB  PHE   183      -1.888  -7.826  30.528  1.00 21.38      BLGL
ATOM   1335  CG  PHE   183      -0.500  -8.347  30.737  1.00 20.19      BLGL
ATOM   1336  CD1 PHE   183      -0.064  -9.469  30.042  1.00 20.38      BLGL
ATOM   1337  CD2 PHE   183       0.385  -7.704  31.597  1.00 22.77      BLGL
ATOM   1338  CE1 PHE   183       1.236  -9.953  30.192  1.00 20.30      BLGL
ATOM   1339  CE2 PHE   183       1.693  -8.174  31.761  1.00 24.59      BLGL
ATOM   1340  CZ  PHE   183       2.120  -9.305  31.054  1.00 23.28      BLGL
ATOM   1341  C   PHE   183      -3.668  -6.283  31.348  1.00 22.44      BLGL
ATOM   1342  O   PHE   183      -3.548  -5.059  31.384  1.00 22.23      BLGL
ATOM   1343  N   ASN   184      -4.792  -6.881  30.954  1.00 22.00      BLGL
ATOM   1344  CA  ASN   184      -5.939  -6.087  30.533  1.00 20.53      BLGL
ATOM   1345  CB  ASN   184      -7.012  -6.964  29.895  1.00 20.92      BLGL
ATOM   1346  CG  ASN   184      -6.677  -7.345  28.474  1.00 21.95      BLGL
ATOM   1347  OD1 ASN   184      -6.162  -6.535  27.708  1.00 24.93      BLGL
ATOM   1348  ND2 ASN   184      -6.983  -8.579  28.108  1.00 26.02      BLGL
ATOM   1349  C   ASN   184      -6.538  -5.293  31.679  1.00 17.99      BLGL
ATOM   1350  O   ASN   184      -7.053  -4.199  31.474  1.00 18.30      BLGL
ATOM   1351  N   ALA   185      -6.458  -5.841  32.884  1.00 16.83      BLGL
ATOM   1352  CA  ALA   185      -6.976  -5.163  34.066  1.00 18.27      BLGL
ATOM   1353  CB  ALA   185      -6.815  -6.048  35.294  1.00 16.14      BLGL
ATOM   1354  C   ALA   185      -6.215  -3.857  34.261  1.00 18.87      BLGL
ATOM   1355  O   ALA   185      -6.812  -2.795  34.422  1.00 17.89      BLGL
ATOM   1356  N   GLY   186      -4.888  -3.945  34.244  1.00 20.07      BLGL
ATOM   1357  CA  GLY   186      -4.073  -2.756  34.409  1.00 19.75      BLGL
ATOM   1358  C   GLY   186      -4.273  -1.834  33.226  1.00 19.07      BLGL
ATOM   1359  O   GLY   186      -4.367  -0.620  33.373  1.00 20.22      BLGL
ATOM   1360  N   SER   187      -4.345  -2.424  32.042  1.00 18.72      BLGL
ATOM   1361  CA  SER   187      -4.534  -1.664  30.819  1.00 18.78      BLGL
ATOM   1362  CB  SER   187      -4.570  -2.618  29.627  1.00 19.99      BLGL
ATOM   1363  OG  SER   187      -4.606  -1.903  28.409  1.00 22.89      BLGL
ATOM   1364  C   SER   187      -5.840  -0.877  30.897  1.00 20.30      BLGL
ATOM   1365  O   SER   187      -5.879   0.311  30.582  1.00 20.23      BLGL
ATOM   1366  N   GLN   188      -6.903  -1.554  31.325  1.00 19.43      BLGL
ATOM   1367  CA  GLN   188      -8.233  -0.960  31.465  1.00 20.10      BLGL
ATOM   1368  CB  GLN   188      -9.192  -1.990  32.093  1.00 21.27      BLGL
ATOM   1369  CG  GLN   188     -10.592  -1.480  32.439  1.00 24.00      BLGL
ATOM   1370  CD  GLN   188     -11.358  -0.973  31.228  1.00 29.54      BLGL
ATOM   1371  OE1 GLN   188     -11.546  -1.695  30.242  1.00 33.67      BLGL
ATOM   1372  NE2 GLN   188     -11.808   0.274  31.295  1.00 28.21      BLGL
ATOM   1373  C   GLN   188      -8.191   0.303  32.322  1.00 20.12      BLGL
ATOM   1374  O   GLN   188      -8.779   1.322  31.984  1.00 19.92      BLGL
ATOM   1375  N   ALA   189      -7.493   0.227  33.442  1.00 20.06      BLGL
ATOM   1376  CA  ALA   189      -7.383   1.366  34.329  1.00 19.56      BLGL
ATOM   1377  CB  ALA   189      -6.587   0.982  35.563  1.00 18.86      BLGL
ATOM   1378  C   ALA   189      -6.728   2.546  33.626  1.00 19.66      BLGL
ATOM   1379  O   ALA   189      -7.150   3.681  33.805  1.00 20.48      BLGL
ATOM   1380  N   VAL   190      -5.697   2.273  32.831  1.00 19.85      BLGL
ATOM   1381  CA  VAL   190      -4.984   3.324  32.108  1.00 21.68      BLGL
ATOM   1382  CB  VAL   190      -3.717   2.755  31.378  1.00 21.13      BLGL
ATOM   1383  CG1 VAL   190      -2.955   3.875  30.675  1.00 17.97      BLGL
ATOM   1384  CG2 VAL   190      -2.809   2.069  32.376  1.00 18.02      BLGL
ATOM   1385  C   VAL   190      -5.922   3.966  31.087  1.00 22.56      BLGL
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Fig. 4 cont.

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ATOM   1386  O   VAL   190      -6.041   5.190  31.007  1.00 21.59      BLGL
ATOM   1387  N   ARG   191      -6.590   3.122  30.311  1.00 24.93      BLGL
ATOM   1388  CA  ARG   191      -7.528   3.577  29.297  1.00 24.90      BLGL
ATOM   1389  CB  ARG   191      -8.199   2.375  28.640  1.00 22.96      BLGL
ATOM   1390  CG  ARG   191      -7.687   2.059  27.236  1.00 25.30      BLGL
ATOM   1391  CD  ARG   191      -6.416   1.230  27.171  1.00 24.11      BLGL
ATOM   1392  NE  ARG   191      -5.369   1.936  26.503  1.00 24.46      BLGL
ATOM   1393  CZ  ARG   191      -4.581   1.653  25.474  1.00 21.34      BLGL
ATOM   1394  NH1 ARG   191      -3.733   2.613  25.208  1.00 22.37      BLGL
ATOM   1395  NH2 ARG   191      -4.584   0.551  24.731  1.00 21.45      BLGL
ATOM   1396  C   ARG   191      -8.590   4.492  29.892  1.00 25.14      BLGL
ATOM   1397  O   ARG   191      -8.904   5.535  29.334  1.00 27.85      BLGL
ATOM   1398  N   GLU   192      -9.145   4.098  31.026  1.00 25.90      BLGL
ATOM   1399  CA  GLU   192     -10.170   4.895  31.683  1.00 28.14      BLGL
ATOM   1400  CB  GLU   192     -10.761   4.129  32.865  1.00 28.90      BLGL
ATOM   1401  CG  GLU   192     -11.776   3.079  32.494  1.00 31.91      BLGL
ATOM   1402  CD  GLU   192     -12.200   2.266  33.697  1.00 32.43      BLGL
ATOM   1403  OE1 GLU   192     -12.359   2.874  34.772  1.00 28.80      BLGL
ATOM   1404  OE2 GLU   192     -12.378   1.033  33.569  1.00 34.08      BLGL
ATOM   1405  C   GLU   192      -9.630   6.223  32.190  1.00 28.73      BLGL
ATOM   1406  O   GLU   192     -10.352   7.219  32.278  1.00 31.92      BLGL
ATOM   1407  N   THR   193      -8.355   6.237  32.541  1.00 27.87      BLGL
ATOM   1408  CA  THR   193      -7.741   7.445  33.064  1.00 26.29      BLGL
ATOM   1409  CB  THR   193      -6.416   7.098  33.780  1.00 25.98      BLGL
ATOM   1410  OG1 THR   193      -6.697   6.231  34.884  1.00 27.07      BLGL
ATOM   1411  CG2 THR   193      -5.725   8.350  34.296  1.00 24.23      BLGL
ATOM   1412  C   THR   193      -7.488   8.500  31.990  1.00 25.40      BLGL
ATOM   1413  O   THR   193      -7.827   9.666  32.160  1.00 22.00      BLGL
ATOM   1414  N   ASP   194      -6.909   8.084  30.872  1.00 27.05      BLGL
ATOM   1415  CA  ASP   194      -6.585   9.020  29.810  1.00 27.87      BLGL
ATOM   1416  CB  ASP   194      -5.396   9.870  30.271  1.00 29.53      BLGL
ATOM   1417  CG  ASP   194      -4.956  10.881  29.243  1.00 32.75      BLGL
ATOM   1418  OD1 ASP   194      -4.131  11.746  29.606  1.00 34.57      BLGL
ATOM   1419  OD2 ASP   194      -5.418  10.816  28.081  1.00 35.03      BLGL
ATOM   1420  C   ASP   194      -6.245   8.249  28.546  1.00 27.55      BLGL
ATOM   1421  O   ASP   194      -5.389   7.368  28.565  1.00 29.57      BLGL
ATOM   1422  N   SER   195      -6.917   8.580  27.449  1.00 27.67      BLGL
ATOM   1423  CA  SER   195      -6.690   7.903  26.169  1.00 30.14      BLGL
ATOM   1424  CB  SER   195      -7.748   8.333  25.154  1.00 31.04      BLGL
ATOM   1425  OG  SER   195      -9.041   7.986  25.608  1.00 38.90      BLGL
ATOM   1426  C   SER   195      -5.314   8.137  25.553  1.00 29.28      BLGL
ATOM   1427  O   SER   195      -4.830   7.319  24.773  1.00 26.29      BLGL
ATOM   1428  N   ASN   196      -4.690   9.255  25.903  1.00 30.46      BLGL
ATOM   1429  CA  ASN   196      -3.387   9.600  25.358  1.00 32.52      BLGL
ATOM   1430  CB  ASN   196      -3.147  11.097  25.514  1.00 38.65      BLGL
ATOM   1431  CG  ASN   196      -4.246  11.919  24.892  1.00 45.74      BLGL
ATOM   1432  OD1 ASN   196      -4.436  11.902  23.672  1.00 47.81      BLGL
ATOM   1433  ND2 ASN   196      -4.996  12.637  25.729  1.00 49.19      BLGL
ATOM   1434  C   ASN   196      -2.232   8.838  25.981  1.00 30.86      BLGL
ATOM   1435  O   ASN   196      -1.141   8.779  25.411  1.00 31.65      BLGL
ATOM   1436  N   ILE   197      -2.459   8.260  27.153  1.00 28.33      BLGL
ATOM   1437  CA  ILE   197      -1.403   7.517  27.816  1.00 25.33      BLGL
ATOM   1438  CB  ILE   197      -1.771   7.224  29.282  1.00 24.62      BLGL
ATOM   1439  CG2 ILE   197      -0.720   6.335  29.919  1.00 24.24      BLGL
ATOM   1440  CG1 ILE   197      -1.873   8.542  30.053  1.00 24.08      BLGL
ATOM   1441  CD1 ILE   197      -2.239   8.380  31.513  1.00 24.86      BLGL
ATOM   1442  C   ILE   197      -1.149   6.222  27.064  1.00 23.64      BLGL
ATOM   1443  O   ILE   197      -2.081   5.487  26.748  1.00 23.83      BLGL
ATOM   1444  N   LEU   198       0.116   5.962  26.754  1.00 21.57      BLGL
ATOM   1445  CA  LEU   198       0.483   4.751  26.039  1.00 21.61      BLGL
ATOM   1446  CB  LEU   198       1.787   4.962  25.271  1.00 21.02      BLGL
ATOM   1447  CG  LEU   198       1.683   5.885  24.055  1.00 22.44      BLGL
ATOM   1448  CD1 LEU   198       3.062   6.252  23.554  1.00 22.29      BLGL
ATOM   1449  CD2 LEU   198       0.881   5.188  22.967  1.00 23.53      BLGL
ATOM   1450  C   LEU   198       0.653   3.605  27.013  1.00 21.75      BLGL
ATOM   1451  O   LEU   198       1.250   3.776  28.073  1.00 23.44      BLGL
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Fig. 4 cont.

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ATOM   1452  N   VAL  199       0.114   2.441  26.666  1.00 20.49      BLGL
ATOM   1453  CA  VAL  199       0.244   1.266  27.516  1.00 19.26      BLGL
ATOM   1454  CB  VAL  199      -1.040   0.450  27.555  1.00 19.98      BLGL
ATOM   1455  CG1 VAL  199      -0.816  -0.815  28.364  1.00 19.20      BLGL
ATOM   1456  CG2 VAL  199      -2.148   1.282  28.149  1.00 21.20      BLGL
ATOM   1457  C   VAL  199       1.352   0.376  26.979  1.00 18.65      BLGL
ATOM   1458  O   VAL  199       1.329  -0.029  25.818  1.00 16.57      BLGL
ATOM   1459  N   ALA  200       2.314   0.061  27.839  1.00 17.36      BLGL
ATOM   1460  CA  ALA  200       3.436  -0.760  27.432  1.00 17.13      BLGL
ATOM   1461  CB  ALA  200       4.701   0.087  27.427  1.00 15.68      BLGL
ATOM   1462  C   ALA  200       3.645  -1.991  28.299  1.00 16.72      BLGL
ATOM   1463  O   ALA  200       3.403  -1.960  29.501  1.00 15.94      BLGL
ATOM   1464  N   LEU  201       4.079  -3.077  27.661  1.00 17.11      BLGL
ATOM   1465  CA  LEU  201       4.390  -4.332  28.339  1.00 17.16      BLGL
ATOM   1466  CB  LEU  201       3.638  -5.502  27.706  1.00 17.16      BLGL
ATOM   1467  CG  LEU  201       2.114  -5.388  27.753  1.00 17.50      BLGL
ATOM   1468  CD1 LEU  201       1.497  -6.671  27.236  1.00 20.85      BLGL
ATOM   1469  CD2 LEU  201       1.654  -5.132  29.172  1.00 19.12      BLGL
ATOM   1470  C   LEU  201       5.907  -4.497  28.186  1.00 17.78      BLGL
ATOM   1471  O   LEU  201       6.465  -4.279  27.111  1.00 17.49      BLGL
ATOM   1472  N   HIS  202       6.568  -4.874  29.272  1.00 18.05      BLGL
ATOM   1473  CA  HIS  202       8.018  -4.981  29.294  1.00 17.54      BLGL
ATOM   1474  CB  HIS  202       8.519  -4.129  30.460  1.00 17.68      BLGL
ATOM   1475  CG  HIS  202      10.002  -4.110  30.616  1.00 19.94      BLGL
ATOM   1476  CD2 HIS  202      10.998  -4.372  29.741  1.00 20.39      BLGL
ATOM   1477  ND1 HIS  202      10.613  -3.773  31.805  1.00 21.65      BLGL
ATOM   1478  CE1 HIS  202      11.922  -3.831  31.655  1.00 22.99      BLGL
ATOM   1479  NE2 HIS  202      12.183  -4.193  30.411  1.00 23.44      BLGL
ATOM   1480  C   HIS  202       8.569  -6.400  29.402  1.00 18.30      BLGL
ATOM   1481  O   HIS  202       8.272  -7.122  30.354  1.00 18.51      BLGL
ATOM   1482  N   PHE  203       9.386  -6.790  28.429  1.00 16.01      BLGL
ATOM   1483  CA  PHE  203       9.989  -8.114  28.431  1.00 16.62      BLGL
ATOM   1484  CB  PHE  203       9.398  -8.963  27.316  1.00 13.11      BLGL
ATOM   1485  CG  PHE  203       7.912  -9.055  27.375  1.00 17.34      BLGL
ATOM   1486  CD1 PHE  203       7.116  -8.119  26.724  1.00 17.15      BLGL
ATOM   1487  CD2 PHE  203       7.299 -10.037  28.144  1.00 15.95      BLGL
ATOM   1488  CE1 PHE  203       5.738  -8.158  26.840  1.00 16.32      BLGL
ATOM   1489  CE2 PHE  203       5.925 -10.083  28.266  1.00 16.04      BLGL
ATOM   1490  CZ  PHE  203       5.141  -9.140  27.612  1.00 18.54      BLGL
ATOM   1491  C   PHE  203      11.504  -8.033  28.274  1.00 19.65      BLGL
ATOM   1492  O   PHE  203      12.051  -6.987  27.910  1.00 21.99      BLGL
ATOM   1493  N   THR  204      12.188  -9.135  28.552  1.00 17.81      BLGL
ATOM   1494  CA  THR  204      13.634  -9.133  28.426  1.00 18.21      BLGL
ATOM   1495  CB  THR  204      14.314  -8.849  29.798  1.00 17.19      BLGL
ATOM   1496  OG1 THR  204      15.726  -8.736  29.611  1.00 14.37      BLGL
ATOM   1497  CG2 THR  204      14.006  -9.951  30.809  1.00 13.65      BLGL
ATOM   1498  C   THR  204      14.161 -10.428  27.809  1.00 18.61      BLGL
ATOM   1499  O   THR  204      13.394 -11.352  27.534  1.00 16.21      BLGL
ATOM   1500  N   ASN  205      15.469 -10.473  27.580  1.00 17.26      BLGL
ATOM   1501  CA  ASN  205      16.112 -11.622  26.964  1.00 17.80      BLGL
ATOM   1502  CB  ASN  205      15.814 -12.907  27.728  1.00 18.45      BLGL
ATOM   1503  CG  ASN  205      16.601 -13.000  29.001  1.00 18.12      BLGL
ATOM   1504  OD1 ASN  205      16.070 -12.811  30.094  1.00 20.78      BLGL
ATOM   1505  ND2 ASN  205      17.890 -13.266  28.868  1.00 18.03      BLGL
ATOM   1506  C   ASN  205      15.701 -11.784  25.520  1.00 17.89      BLGL
ATOM   1507  O   ASN  205      15.129 -12.800  25.135  1.00 18.21      BLGL
ATOM   1508  N   PRO  206      15.988 -10.771  24.697  1.00 18.39      BLGL
ATOM   1509  CD  PRO  206      16.580  -9.480  25.080  1.00 15.66      BLGL
ATOM   1510  CA  PRO  206      15.657 -10.778  23.273  1.00 19.70      BLGL
ATOM   1511  CB  PRO  206      15.903  -9.334  22.867  1.00 19.33      BLGL
ATOM   1512  CG  PRO  206      17.029  -8.939  23.756  1.00 16.74      BLGL
ATOM   1513  C   PRO  206      16.500 -11.748  22.459  1.00 21.36      BLGL
ATOM   1514  O   PRO  206      16.158 -12.055  21.318  1.00 22.70      BLGL
ATOM   1515  N   GLU  207      17.601 -12.224  23.034  1.00 23.27      BLGL
ATOM   1516  CA  GLU  207      18.478 -13.154  22.324  1.00 25.47      BLGL
ATOM   1517  CB  GLU  207      19.871 -13.210  22.959  1.00 26.18      BLGL
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Fig. 4 cont.

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ATOM   1518  CG  GLU   207      20.021 -12.502  24.288  1.00 30.25      BLGL
ATOM   1519  CD  GLU   207      19.242 -13.139  25.413  1.00 29.52      BLGL
ATOM   1520  OE1 GLU   207      19.387 -14.353  25.643  1.00 33.25      BLGL
ATOM   1521  OE2 GLU   207      18.495 -12.413  26.081  1.00 29.56      BLGL
ATOM   1522  C   GLU   207      17.924 -14.561  22.258  1.00 26.20      BLGL
ATOM   1523  O   GLU   207      18.354 -15.357  21.426  1.00 29.50      BLGL
ATOM   1524  N   THR   208      16.982 -14.873  23.139  1.00 25.50      BLGL
ATOM   1525  CA  THR   208      16.384 -16.196  23.151  1.00 25.38      BLGL
ATOM   1526  CB  THR   208      15.419 -16.349  24.314  1.00 25.02      BLGL
ATOM   1527  OG1 THR   208      16.108 -16.063  25.532  1.00 24.40      BLGL
ATOM   1528  CG2 THR   208      14.871 -17.765  24.361  1.00 24.75      BLGL
ATOM   1529  C   THR   208      15.628 -16.435  21.853  1.00 24.66      BLGL
ATOM   1530  O   THR   208      14.689 -15.711  21.531  1.00 23.66      BLGL
ATOM   1531  N   SER   209      16.047 -17.455  21.114  1.00 24.67      BLGL
ATOM   1532  CA  SER   209      15.424 -17.791  19.842  1.00 25.56      BLGL
ATOM   1533  CB  SER   209      15.971 -19.120  19.334  1.00 23.59      BLGL
ATOM   1534  OG  SER   209      15.290 -19.524  18.166  1.00 26.21      BLGL
ATOM   1535  C   SER   209      13.896 -17.862  19.885  1.00 26.32      BLGL
ATOM   1536  O   SER   209      13.321 -18.668  20.632  1.00 23.52      BLGL
ATOM   1537  N   GLY   210      13.257 -17.004  19.083  1.00 26.00      BLGL
ATOM   1538  CA  GLY   210      11.803 -16.966  18.977  1.00 25.41      BLGL
ATOM   1539  C   GLY   210      10.990 -16.593  20.204  1.00 26.60      BLGL
ATOM   1540  O   GLY   210       9.768 -16.755  20.215  1.00 26.52      BLGL
ATOM   1541  N   ARG   211      11.659 -16.080  21.231  1.00 27.83      BLGL
ATOM   1542  CA  ARG   211      11.004 -15.692  22.478  1.00 25.31      BLGL
ATOM   1543  CB  ARG   211      12.046 -15.244  23.496  1.00 26.05      BLGL
ATOM   1544  CG  ARG   211      11.487 -15.024  24.881  1.00 26.98      BLGL
ATOM   1545  CD  ARG   211      12.479 -14.289  25.747  1.00 28.49      BLGL
ATOM   1546  NE  ARG   211      12.362 -14.719  27.125  1.00 32.45      BLGL
ATOM   1547  CZ  ARG   211      13.043 -15.727  27.655  1.00 34.26      BLGL
ATOM   1548  NH1 ARG   211      13.903 -16.408  26.920  1.00 33.07      BLGL
ATOM   1549  NH2 ARG   211      12.850 -16.067  28.924  1.00 40.91      BLGL
ATOM   1550  C   ARG   211       9.977 -14.580  22.294  1.00 24.24      BLGL
ATOM   1551  O   ARG   211       8.806 -14.744  22.634  1.00 24.47      BLGL
ATOM   1552  N   TYR   212      10.413 -13.440  21.768  1.00 22.57      BLGL
ATOM   1553  CA  TYR   212       9.499 -12.323  21.558  1.00 20.27      BLGL
ATOM   1554  CB  TYR   212      10.262 -11.080  21.093  1.00 18.26      BLGL
ATOM   1555  CG  TYR   212      11.063 -10.409  22.188  1.00 20.40      BLGL
ATOM   1556  CD1 TYR   212      11.669  -9.170  21.972  1.00 19.09      BLGL
ATOM   1557  CE1 TYR   212      12.387  -8.538  22.982  1.00 16.98      BLGL
ATOM   1558  CD2 TYR   212      11.204 -11.001  23.445  1.00 17.87      BLGL
ATOM   1559  CE2 TYR   212      11.919 -10.377  24.457  1.00 15.68      BLGL
ATOM   1560  CZ  TYR   212      12.505  -9.147  24.225  1.00 16.21      BLGL
ATOM   1561  OH  TYR   212      13.200  -8.514  25.235  1.00 15.74      BLGL
ATOM   1562  C   TYR   212       8.398 -12.670  20.559  1.00 20.87      BLGL
ATOM   1563  O   TYR   212       7.259 -12.237  20.712  1.00 20.22      BLGL
ATOM   1564  N   ALA   213       8.734 -13.449  19.537  1.00 19.68      BLGL
ATOM   1565  CA  ALA   213       7.742 -13.847  18.547  1.00 19.79      BLGL
ATOM   1566  CB  ALA   213       8.399 -14.687  17.454  1.00 17.89      BLGL
ATOM   1567  C   ALA   213       6.629 -14.642  19.231  1.00 19.99      BLGL
ATOM   1568  O   ALA   213       5.451 -14.479  18.911  1.00 19.71      BLGL
ATOM   1569  N   TRP   214       7.009 -15.496  20.176  1.00 20.09      BLGL
ATOM   1570  CA  TRP   214       6.039 -16.309  20.900  1.00 21.30      BLGL
ATOM   1571  CB  TRP   214       6.753 -17.375  21.732  1.00 22.71      BLGL
ATOM   1572  CG  TRP   214       5.815 -18.281  22.468  1.00 24.60      BLGL
ATOM   1573  CD2 TRP   214       5.308 -18.094  23.795  1.00 24.97      BLGL
ATOM   1574  CE2 TRP   214       4.449 -19.183  24.074  1.00 24.59      BLGL
ATOM   1575  CE3 TRP   214       5.496 -17.112  24.775  1.00 25.69      BLGL
ATOM   1576  CD1 TRP   214       5.256 -19.440  22.005  1.00 24.97      BLGL
ATOM   1577  NE1 TRP   214       4.436 -19.989  22.966  1.00 25.84      BLGL
ATOM   1578  CZ2 TRP   214       3.780 -19.319  25.294  1.00 22.78      BLGL
ATOM   1579  CZ3 TRP   214       4.829 -17.248  25.991  1.00 27.53      BLGL
ATOM   1580  CH2 TRP   214       3.981 -18.345  26.238  1.00 24.84      BLGL
ATOM   1581  C   TRP   214       5.167 -15.453  21.816  1.00 21.83      BLGL
ATOM   1582  O   TRP   214       3.948 -15.630  21.857  1.00 20.77      BLGL
ATOM   1583  N   ILE   215       5.793 -14.531  22.550  1.00 21.49      BLGL
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Fig. 4 cont.

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ATOM   1584  CA  ILE   215       5.067 -13.654  23.469  1.00 19.18      BLGL
ATOM   1585  CB  ILE   215       6.038 -12.771  24.300  1.00 19.85      BLGL
ATOM   1586  CG2 ILE   215       5.257 -11.811  25.198  1.00 15.32      BLGL
ATOM   1587  CG1 ILE   215       6.930 -13.651  25.170  1.00 18.25      BLGL
ATOM   1588  CD1 ILE   215       7.930 -12.876  25.975  1.00 15.25      BLGL
ATOM   1589  C   ILE   215       4.104 -12.740  22.725  1.00 19.79      BLGL
ATOM   1590  O   ILE   215       2.964 -12.550  23.146  1.00 18.73      BLGL
ATOM   1591  N   ALA   216       4.565 -12.163  21.621  1.00 19.35      BLGL
ATOM   1592  CA  ALA   216       3.723 -11.275  20.840  1.00 18.57      BLGL
ATOM   1593  CB  ALA   216       4.492 -10.751  19.650  1.00 18.16      BLGL
ATOM   1594  C   ALA   216       2.472 -12.020  20.378  1.00 20.55      BLGL
ATOM   1595  O   ALA   216       1.359 -11.501  20.466  1.00 16.58      BLGL
ATOM   1596  N   GLU   217       2.669 -13.242  19.890  1.00 22.90      BLGL
ATOM   1597  CA  GLU   217       1.569 -14.077  19.419  1.00 24.77      BLGL
ATOM   1598  CB  GLU   217       2.122 -15.338  18.747  1.00 28.27      BLGL
ATOM   1599  CG  GLU   217       1.063 -16.371  18.379  1.00 33.34      BLGL
ATOM   1600  CD  GLU   217      -0.002 -15.823  17.449  1.00 35.08      BLGL
ATOM   1601  OE1 GLU   217      -1.049 -16.485  17.288  1.00 39.18      BLGL
ATOM   1602  OE2 GLU   217       0.208 -14.737  16.875  1.00 35.59      BLGL
ATOM   1603  C   GLU   217       0.623 -14.468  20.560  1.00 24.16      BLGL
ATOM   1604  O   GLU   217      -0.596 -14.464  20.395  1.00 22.67      BLGL
ATOM   1605  N   THR   218       1.195 -14.805  21.713  1.00 24.08      BLGL
ATOM   1606  CA  THR   218       0.412 -15.191  22.878  1.00 23.79      BLGL
ATOM   1607  CB  THR   218       1.334 -15.684  24.027  1.00 25.12      BLGL
ATOM   1608  OG1 THR   218       1.985 -16.896  23.630  1.00 26.14      BLGL
ATOM   1609  CG2 THR   218       0.537 -15.942  25.298  1.00 23.98      BLGL
ATOM   1610  C   THR   218      -0.429 -14.014  23.362  1.00 22.94      BLGL
ATOM   1611  O   THR   218      -1.600 -14.179  23.692  1.00 24.35      BLGL
ATOM   1612  N   LEU   219       0.160 -12.825  23.401  1.00 21.92      BLGL
ATOM   1613  CA  LEU   219      -0.578 -11.644  23.846  1.00 23.28      BLGL
ATOM   1614  CB  LEU   219       0.333 -10.410  23.863  1.00 21.92      BLGL
ATOM   1615  CG  LEU   219       1.462 -10.359  24.893  1.00 18.90      BLGL
ATOM   1616  CD1 LEU   219       2.386  -9.209  24.570  1.00 14.80      BLGL
ATOM   1617  CD2 LEU   219       0.879 -10.220  26.289  1.00 16.33      BLGL
ATOM   1618  C   LEU   219      -1.753 -11.394  22.903  1.00 24.55      BLGL
ATOM   1619  O   LEU   219      -2.850 -11.031  23.322  1.00 25.23      BLGL
ATOM   1620  N   HIS   220      -1.512 -11.603  21.619  1.00 25.34      BLGL
ATOM   1621  CA  HIS   220      -2.539 -11.401  20.622  1.00 25.88      BLGL
ATOM   1622  CB  HIS   220      -1.904 -11.450  19.236  1.00 27.15      BLGL
ATOM   1623  CG  HIS   220      -2.888 -11.366  18.116  1.00 31.81      BLGL
ATOM   1624  CD2 HIS   220      -3.485 -10.300  17.529  1.00 31.02      BLGL
ATOM   1625  ND1 HIS   220      -3.388 -12.486  17.483  1.00 33.38      BLGL
ATOM   1626  CE1 HIS   220      -4.250 -12.111  16.554  1.00 33.29      BLGL
ATOM   1627  NE2 HIS   220      -4.326 -10.791  16.562  1.00 32.86      BLGL
ATOM   1628  C   HIS   220      -3.665 -12.423  20.743  1.00 26.70      BLGL
ATOM   1629  O   HIS   220      -4.839 -12.076  20.617  1.00 25.81      BLGL
ATOM   1630  N   ARG   221      -3.312 -13.679  20.993  1.00 28.18      BLGL
ATOM   1631  CA  ARG   221      -4.314 -14.730  21.133  1.00 30.04      BLGL
ATOM   1632  CB  ARG   221      -3.648 -16.090  21.361  1.00 33.95      BLGL
ATOM   1633  CG  ARG   221      -3.038 -16.680  20.095  1.00 40.22      BLGL
ATOM   1634  CD  ARG   221      -2.052 -17.802  20.368  1.00 47.28      BLGL
ATOM   1635  NE  ARG   221      -2.419 -19.012  19.696  1.00 52.72      BLGL
ATOM   1636  CZ  ARG   221      -1.881 -19.711  18.699  1.00 54.00      BLGL
ATOM   1637  NH1 ARG   221      -2.572 -20.786  18.387  1.00 56.27      BLGL
ATOM   1638  NH2 ARG   221      -0.762 -19.439  18.032  1.00 52.22      BLGL
ATOM   1639  C   ARG   221      -5.263 -14.440  22.276  1.00 29.71      BLGL
ATOM   1640  O   ARG   221      -6.441 -14.790  22.204  1.00 30.75      BLGL
ATOM   1641  N   HIS   222      -4.757 -13.803  23.331  1.00 27.89      BLGL
ATOM   1642  CA  HIS   222      -5.599 -13.482  24.477  1.00 27.09      BLGL
ATOM   1643  CB  HIS   222      -4.844 -13.728  25.782  1.00 26.93      BLGL
ATOM   1644  CG  HIS   222      -4.530 -15.168  26.023  1.00 28.56      BLGL
ATOM   1645  CD2 HIS   222      -5.196 -16.121  26.716  1.00 30.01      BLGL
ATOM   1646  ND1 HIS   222      -3.441 -15.797  25.459  1.00 31.08      BLGL
ATOM   1647  CE1 HIS   222      -3.448 -17.076  25.792  1.00 30.75      BLGL
ATOM   1648  NE2 HIS   222      -4.504 -17.298  26.554  1.00 33.11      BLGL
ATOM   1649  C   HIS   222      -6.159 -12.064  24.456  1.00 26.57      BLGL
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Fig. 4 cont.

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ATOM   1650  O   HIS   222      -6.646 -11.564  25.469  1.00 25.69      BLGL
ATOM   1651  N   HIS   223      -6.084 -11.418  23.300  1.00 25.18      BLGL
ATOM   1652  CA  HIS   223      -6.627 -10.082  23.151  1.00 26.33      BLGL
ATOM   1653  CB  HIS   223      -8.147 -10.149  23.214  1.00 30.76      BLGL
ATOM   1654  CG  HIS   223      -8.739 -11.182  22.309  1.00 38.88      BLGL
ATOM   1655  CD2 HIS   223      -9.524 -12.253  22.570  1.00 41.07      BLGL
ATOM   1656  ND1 HIS   223      -8.531 -11.182  20.945  1.00 43.14      BLGL
ATOM   1657  CE1 HIS   223      -9.161 -12.210  20.405  1.00 43.27      BLGL
ATOM   1658  NE2 HIS   223      -9.771 -12.876  21.370  1.00 45.48      BLGL
ATOM   1659  C   HIS   223      -6.149  -9.081  24.186  1.00 26.02      BLGL
ATOM   1660  O   HIS   223      -6.961  -8.345  24.750  1.00 27.73      BLGL
ATOM   1661  N   VAL   224      -4.846  -9.044  24.446  1.00 22.81      BLGL
ATOM   1662  CA  VAL   224      -4.316  -8.096  25.413  1.00 18.14      BLGL
ATOM   1663  CB  VAL   224      -2.912  -8.499  25.895  1.00 16.94      BLGL
ATOM   1664  CG1 VAL   224      -2.312  -7.399  26.758  1.00 12.94      BLGL
ATOM   1665  CG2 VAL   224      -2.998  -9.783  26.676  1.00 15.42      BLGL
ATOM   1666  C   VAL   224      -4.241  -6.742  24.734  1.00 17.57      BLGL
ATOM   1667  O   VAL   224      -3.683  -6.610  23.646  1.00 16.83      BLGL
ATOM   1668  N   ASP   225      -4.808  -5.738  25.386  1.00 16.35      BLGL
ATOM   1669  CA  ASP   225      -4.820  -4.393  24.849  1.00 17.47      BLGL
ATOM   1670  CB  ASP   225      -6.123  -3.707  25.254  1.00 17.33      BLGL
ATOM   1671  CG  ASP   225      -6.172  -2.260  24.843  1.00 19.19      BLGL
ATOM   1672  OD1 ASP   225      -5.722  -1.945  23.717  1.00 21.14      BLGL
ATOM   1673  OD2 ASP   225      -6.672  -1.444  25.643  1.00 19.74      BLGL
ATOM   1674  C   ASP   225      -3.626  -3.562  25.306  1.00 18.47      BLGL
ATOM   1675  O   ASP   225      -3.609  -3.073  26.433  1.00 19.94      BLGL
ATOM   1676  N   TYR   226      -2.626  -3.415  24.440  1.00 17.31      BLGL
ATOM   1677  CA  TYR   226      -1.441  -2.610  24.762  1.00 19.05      BLGL
ATOM   1678  CB  TYR   226      -0.315  -3.483  25.359  1.00 17.31      BLGL
ATOM   1679  CG  TYR   226       0.380  -4.417  24.386  1.00 17.91      BLGL
ATOM   1680  CD1 TYR   226      -0.315  -5.469  23.780  1.00 17.20      BLGL
ATOM   1681  CE1 TYR   226       0.317  -6.338  22.891  1.00 14.85      BLGL
ATOM   1682  CD2 TYR   226       1.737  -4.253  24.076  1.00 15.96      BLGL
ATOM   1683  CE2 TYR   226       2.380  -5.117  23.184  1.00 15.01      BLGL
ATOM   1684  CZ  TYR   226       1.661  -6.156  22.598  1.00 16.47      BLGL
ATOM   1685  OH  TYR   226       2.279  -7.019  21.725  1.00 13.64      BLGL
ATOM   1686  C   TYR   226      -0.944  -1.877  23.513  1.00 17.95      BLGL
ATOM   1687  O   TYR   226      -1.285  -2.251  22.398  1.00 17.24      BLGL
ATOM   1688  N   ASP   227      -0.141  -0.836  23.697  1.00 18.09      BLGL
ATOM   1689  CA  ASP   227       0.361  -0.075  22.557  1.00 20.63      BLGL
ATOM   1690  CB  ASP   227       0.126   1.424  22.760  1.00 23.61      BLGL
ATOM   1691  CG  ASP   227      -1.247   1.736  23.282  1.00 24.31      BLGL
ATOM   1692  OD1 ASP   227      -2.242   1.427  22.597  1.00 26.42      BLGL
ATOM   1693  OD2 ASP   227      -1.327   2.298  24.388  1.00 29.59      BLGL
ATOM   1694  C   ASP   227       1.846  -0.263  22.289  1.00 21.20      BLGL
ATOM   1695  O   ASP   227       2.283  -0.241  21.141  1.00 21.63      BLGL
ATOM   1696  N   VAL   228       2.626  -0.432  23.350  1.00 21.33      BLGL
ATOM   1697  CA  VAL   228       4.069  -0.571  23.205  1.00 18.22      BLGL
ATOM   1698  CB  VAL   228       4.822   0.572  23.961  1.00 16.56      BLGL
ATOM   1699  CG1 VAL   228       6.307   0.511  23.669  1.00 16.51      BLGL
ATOM   1700  CG2 VAL   228       4.268   1.921  23.569  1.00 16.96      BLGL
ATOM   1701  C   VAL   228       4.631  -1.892  23.700  1.00 16.80      BLGL
ATOM   1702  O   VAL   228       4.338  -2.338  24.811  1.00 16.77      BLGL
ATOM   1703  N   PHE   229       5.444  -2.510  22.858  1.00 15.66      BLGL
ATOM   1704  CA  PHE   229       6.115  -3.747  23.213  1.00 16.03      BLGL
ATOM   1705  CB  PHE   229       6.177  -4.694  22.007  1.00 15.71      BLGL
ATOM   1706  CG  PHE   229       6.773  -6.038  22.323  1.00 18.72      BLGL
ATOM   1707  CD1 PHE   229       8.148  -6.193  22.458  1.00 20.15      BLGL
ATOM   1708  CD2 PHE   229       5.957  -7.141  22.537  1.00 19.69      BLGL
ATOM   1709  CE1 PHE   229       8.698  -7.424  22.805  1.00 20.33      BLGL
ATOM   1710  CE2 PHE   229       6.502  -8.376  22.885  1.00 19.99      BLGL
ATOM   1711  CZ  PHE   229       7.873  -8.516  23.020  1.00 20.18      BLGL
ATOM   1712  C   PHE   229       7.517  -3.278  23.608  1.00 15.51      BLGL
ATOM   1713  O   PHE   229       8.336  -2.965  22.747  1.00 16.80      BLGL
ATOM   1714  N   ALA   230       7.781  -3.205  24.909  1.00 14.48      BLGL
ATOM   1715  CA  ALA   230       9.076  -2.740  25.392  1.00 16.32      BLGL
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Fig. 4 cont.

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ATOM   1716  CB  ALA   230       8.892  -1.878  26.632  1.00 15.48      BLGL
ATOM   1717  C   ALA   230      10.040  -3.878  25.691  1.00 17.75      BLGL
ATOM   1718  O   ALA   230       9.624  -4.990  26.019  1.00 19.06      BLGL
ATOM   1719  N   SER   231      11.334  -3.588  25.580  1.00 15.44      BLGL
ATOM   1720  CA  SER   231      12.363  -4.583  25.829  1.00 15.19      BLGL
ATOM   1721  CB  SER   231      12.863  -5.165  24.498  1.00 12.54      BLGL
ATOM   1722  OG  SER   231      13.966  -6.035  24.696  1.00  9.34      BLGL
ATOM   1723  C   SER   231      13.554  -4.024  26.601  1.00 16.12      BLGL
ATOM   1724  O   SER   231      13.915  -2.852  26.463  1.00 17.19      BLGL
ATOM   1725  N   SER   232      14.152  -4.865  27.434  1.00 14.04      BLGL
ATOM   1726  CA  SER   232      15.341  -4.463  28.159  1.00 15.04      BLGL
ATOM   1727  CB  SER   232      15.505  -5.272  29.447  1.00 14.50      BLGL
ATOM   1728  OG  SER   232      14.733  -4.727  30.499  1.00 17.36      BLGL
ATOM   1729  C   SER   232      16.485  -4.810  27.216  1.00 15.02      BLGL
ATOM   1730  O   SER   232      16.354  -5.696  26.374  1.00 14.13      BLGL
ATOM   1731  N   TYR   233      17.591  -4.094  27.326  1.00 14.36      BLGL
ATOM   1732  CA  TYR   233      18.738  -4.410  26.506  1.00 16.28      BLGL
ATOM   1733  CB  TYR   233      18.721  -3.697  25.152  1.00 15.72      BLGL
ATOM   1734  CG  TYR   233      19.901  -4.146  24.318  1.00 18.38      BLGL
ATOM   1735  CD1 TYR   233      19.935  -5.428  23.762  1.00 17.95      BLGL
ATOM   1736  CE1 TYR   233      21.072  -5.905  23.102  1.00 17.74      BLGL
ATOM   1737  CD2 TYR   233      21.038  -3.342  24.185  1.00 19.16      BLGL
ATOM   1738  CE2 TYR   233      22.181  -3.809  23.528  1.00 18.72      BLGL
ATOM   1739  CZ  TYR   233      22.188  -5.090  22.991  1.00 20.19      BLGL
ATOM   1740  OH  TYR   233      23.305  -5.552  22.339  1.00 21.28      BLGL
ATOM   1741  C   TYR   233      20.051  -4.096  27.204  1.00 18.26      BLGL
ATOM   1742  O   TYR   233      20.488  -2.941  27.282  1.00 19.11      BLGL
ATOM   1743  N   TYR   234      20.672  -5.148  27.715  1.00 18.61      BLGL
ATOM   1744  CA  TYR   234      21.951  -5.047  28.382  1.00 20.22      BLGL
ATOM   1745  CB  TYR   234      21.838  -5.594  29.794  1.00 18.03      BLGL
ATOM   1746  CG  TYR   234      21.020  -4.689  30.678  1.00 19.42      BLGL
ATOM   1747  CD1 TYR   234      21.536  -3.473  31.130  1.00 17.03      BLGL
ATOM   1748  CE1 TYR   234      20.778  -2.628  31.935  1.00 15.84      BLGL
ATOM   1749  CD2 TYR   234      19.718  -5.035  31.051  1.00 20.59      BLGL
ATOM   1750  CE2 TYR   234      18.950  -4.194  31.854  1.00 18.88      BLGL
ATOM   1751  CZ  TYR   234      19.489  -2.995  32.294  1.00 17.70      BLGL
ATOM   1752  OH  TYR   234      18.745  -2.180  33.108  1.00 17.67      BLGL
ATOM   1753  C   TYR   234      22.896  -5.875  27.538  1.00 20.87      BLGL
ATOM   1754  O   TYR   234      22.858  -7.104  27.570  1.00 23.14      BLGL
ATOM   1755  N   PRO   235      23.749  -5.201  26.756  1.00 21.55      BLGL
ATOM   1756  CD  PRO   235      23.983  -3.751  26.857  1.00 21.91      BLGL
ATOM   1757  CA  PRO   235      24.728  -5.825  25.864  1.00 22.81      BLGL
ATOM   1758  CB  PRO   235      25.551  -4.639  25.367  1.00 22.48      BLGL
ATOM   1759  CG  PRO   235      25.422  -3.640  26.471  1.00 21.97      BLGL
ATOM   1760  C   PRO   235      25.575  -6.912  26.508  1.00 23.83      BLGL
ATOM   1761  O   PRO   235      26.118  -7.762  25.812  1.00 26.44      BLGL
ATOM   1762  N   PHE   236      25.673  -6.894  27.834  1.00 24.38      BLGL
ATOM   1763  CA  PHE   236      26.451  -7.894  28.556  1.00 23.56      BLGL
ATOM   1764  CB  PHE   236      26.439  -7.613  30.069  1.00 22.41      BLGL
ATOM   1765  CG  PHE   236      26.751  -6.190  30.432  1.00 20.97      BLGL
ATOM   1766  CD1 PHE   236      25.769  -5.363  30.960  1.00 22.30      BLGL
ATOM   1767  CD2 PHE   236      28.018  -5.666  30.224  1.00 21.90      BLGL
ATOM   1768  CE1 PHE   236      26.043  -4.031  31.274  1.00 20.76      BLGL
ATOM   1769  CE2 PHE   236      28.304  -4.335  30.534  1.00 22.34      BLGL
ATOM   1770  CZ  PHE   236      27.310  -3.518  31.060  1.00 22.41      BLGL
ATOM   1771  C   PHE   236      25.901  -9.297  28.322  1.00 24.55      BLGL
ATOM   1772  O   PHE   236      26.664 -10.252  28.209  1.00 26.43      BLGL
ATOM   1773  N   TRP   237      24.581  -9.425  28.226  1.00 25.33      BLGL
ATOM   1774  CA  TRP   237      23.971 -10.745  28.067  1.00 26.98      BLGL
ATOM   1775  CB  TRP   237      23.270 -11.144  29.367  1.00 27.82      BLGL
ATOM   1776  CG  TRP   237      23.960 -10.698  30.606  1.00 30.90      BLGL
ATOM   1777  CD2 TRP   237      23.562  -9.632  31.466  1.00 31.06      BLGL
ATOM   1778  CE2 TRP   237      24.489  -9.585  32.535  1.00 31.99      BLGL
ATOM   1779  CE3 TRP   237      22.511  -8.711  31.443  1.00 32.34      BLGL
ATOM   1780  CD1 TRP   237      25.084 -11.238  31.162  1.00 33.44      BLGL
ATOM   1781  NE1 TRP   237      25.408 -10.577  32.324  1.00 32.26      BLGL
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Fig. 4 cont.

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ATOM   1782  CZ2 TRP   237      24.396  -8.652  33.570  1.00 32.74      BLGL
ATOM   1783  CZ3 TRP   237      22.417  -7.780  32.477  1.00 34.34      BLGL
ATOM   1784  CH2 TRP   237      23.357  -7.761  33.526  1.00 33.93      BLGL
ATOM   1785  C   TRP   237      22.938 -10.894  26.960  1.00 26.05      BLGL
ATOM   1786  O   TRP   237      22.632 -12.011  26.543  1.00 25.25      BLGL
ATOM   1787  N   HIS   238      22.401  -9.778  26.487  1.00 24.70      BLGL
ATOM   1788  CA  HIS   238      21.333  -9.824  25.504  1.00 20.96      BLGL
ATOM   1789  CB  HIS   238      20.358  -8.703  25.824  1.00 19.05      BLGL
ATOM   1790  CG  HIS   238      19.772  -8.821  27.192  1.00 17.38      BLGL
ATOM   1791  CD2 HIS   238      19.601  -9.900  27.990  1.00 16.73      BLGL
ATOM   1792  ND1 HIS   238      19.291  -7.743  27.896  1.00 20.29      BLGL
ATOM   1793  CE1 HIS   238      18.850  -8.151  29.073  1.00 20.03      BLGL
ATOM   1794  NE2 HIS   238      19.026  -9.456  29.154  1.00 19.52      BLGL
ATOM   1795  C   HIS   238      21.628  -9.863  24.019  1.00 20.65      BLGL
ATOM   1796  O   HIS   238      20.854  -9.354  23.217  1.00 22.38      BLGL
ATOM   1797  N   GLY   239      22.730 -10.489  23.643  1.00 19.61      BLGL
ATOM   1798  CA  GLY   239      23.037 -10.607  22.234  1.00 19.09      BLGL
ATOM   1799  C   GLY   239      23.345  -9.338  21.474  1.00 18.09      BLGL
ATOM   1800  O   GLY   239      23.535  -8.271  22.046  1.00 17.84      BLGL
ATOM   1801  N   THR   240      23.369  -9.476  20.158  1.00 17.37      BLGL
ATOM   1802  CA  THR   240      23.697  -8.387  19.258  1.00 18.95      BLGL
ATOM   1803  CB  THR   240      24.139  -8.949  17.896  1.00 18.49      BLGL
ATOM   1804  OG1 THR   240      23.028  -9.589  17.262  1.00 18.33      BLGL
ATOM   1805  CG2 THR   240      25.239  -9.964  18.076  1.00 14.06      BLGL
ATOM   1806  C   THR   240      22.610  -7.348  19.003  1.00 20.98      BLGL
ATOM   1807  O   THR   240      21.418  -7.604  19.169  1.00 19.90      BLGL
ATOM   1808  N   LEU   241      23.043  -6.165  18.581  1.00 21.55      BLGL
ATOM   1809  CA  LEU   241      22.115  -5.094  18.277  1.00 21.65      BLGL
ATOM   1810  CB  LEU   241      22.874  -3.780  18.086  1.00 20.04      BLGL
ATOM   1811  CG  LEU   241      23.464  -3.205  19.381  1.00 21.24      BLGL
ATOM   1812  CD1 LEU   241      24.455  -2.105  19.074  1.00 18.53      BLGL
ATOM   1813  CD2 LEU   241      22.339  -2.689  20.259  1.00 19.54      BLGL
ATOM   1814  C   LEU   241      21.350  -5.458  17.011  1.00 22.88      BLGL
ATOM   1815  O   LEU   241      20.213  -5.043  16.827  1.00 23.81      BLGL
ATOM   1816  N   LYS   242      21.971  -6.248  16.143  1.00 23.90      BLGL
ATOM   1817  CA  LYS   242      21.322  -6.659  14.902  1.00 25.71      BLGL
ATOM   1818  CB  LYS   242      22.314  -7.426  14.025  1.00 30.56      BLGL
ATOM   1819  CG  LYS   242      21.771  -7.855  12.670  1.00 36.92      BLGL
ATOM   1820  CD  LYS   242      22.735  -8.821  11.983  1.00 43.60      BLGL
ATOM   1821  CE  LYS   242      22.175  -9.333  10.664  1.00 48.93      BLGL
ATOM   1822  NZ  LYS   242      21.895  -8.217   9.709  1.00 51.96      BLGL
ATOM   1823  C   LYS   242      20.108  -7.537  15.208  1.00 24.37      BLGL
ATOM   1824  O   LYS   242      19.070  -7.444  14.551  1.00 23.45      BLGL
ATOM   1825  N   ASN   243      20.248  -8.384  16.219  1.00 23.09      BLGL
ATOM   1826  CA  ASN   243      19.178  -9.279  16.637  1.00 21.13      BLGL
ATOM   1827  CB  ASN   243      19.716 -10.285  17.653  1.00 20.66      BLGL
ATOM   1828  CG  ASN   243      18.639 -11.196  18.185  1.00 22.04      BLGL
ATOM   1829  OD1 ASN   243      18.181 -12.102  17.495  1.00 21.37      BLGL
ATOM   1830  ND2 ASN   243      18.215 -10.951  19.415  1.00 21.96      BLGL
ATOM   1831  C   ASN   243      18.041  -8.477  17.264  1.00 21.16      BLGL
ATOM   1832  O   ASN   243      16.861  -8.684  16.957  1.00 18.33      BLGL
ATOM   1833  N   LEU   244      18.408  -7.557  18.151  1.00 20.72      BLGL
ATOM   1834  CA  LEU   244      17.429  -6.712  18.821  1.00 19.78      BLGL
ATOM   1835  CB  LEU   244      18.131  -5.667  19.695  1.00 18.01      BLGL
ATOM   1836  CG  LEU   244      17.188  -4.669  20.372  1.00 16.83      BLGL
ATOM   1837  CD1 LEU   244      16.393  -5.385  21.463  1.00 13.98      BLGL
ATOM   1838  CD2 LEU   244      17.995  -3.515  20.950  1.00 16.04      BLGL
ATOM   1839  C   LEU   244      16.565  -6.000  17.792  1.00 19.53      BLGL
ATOM   1840  O   LEU   244      15.341  -6.054  17.853  1.00 20.39      BLGL
ATOM   1841  N   THR   245      17.214  -5.332  16.846  1.00 18.73      BLGL
ATOM   1842  CA  THR   245      16.505  -4.606  15.810  1.00 18.66      BLGL
ATOM   1843  CB  THR   245      17.474  -3.996  14.785  1.00 19.64      BLGL
ATOM   1844  OG1 THR   245      18.318  -3.037  15.430  1.00 21.51      BLGL
ATOM   1845  CG2 THR   245      16.697  -3.311  13.664  1.00 17.47      BLGL
ATOM   1846  C   THR   245      15.574  -5.531  15.062  1.00 19.92      BLGL
ATOM   1847  O   THR   245      14.410  -5.219  14.834  1.00 21.53      BLGL
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Fig. 4 cont.

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ATOM   1848  N   SER   246      16.109  -6.678  14.678  1.00 20.39      BLGL
ATOM   1849  CA  SER   246      15.361  -7.661  13.927  1.00 19.04      BLGL
ATOM   1850  CB  SER   246      16.303  -8.792  13.538  1.00 18.29      BLGL
ATOM   1851  OG  SER   246      15.593  -9.911  13.053  1.00 23.84      BLGL
ATOM   1852  C   SER   246      14.164  -8.205  14.695  1.00 20.89      BLGL
ATOM   1853  O   SER   246      13.034  -8.169  14.214  1.00 22.76      BLGL
ATOM   1854  N   VAL   247      14.411  -8.703  15.899  1.00 21.65      BLGL
ATOM   1855  CA  VAL   247      13.343  -9.280  16.701  1.00 21.83      BLGL
ATOM   1856  CB  VAL   247      13.923  -9.883  18.005  1.00 20.50      BLGL
ATOM   1857  CG1 VAL   247      14.342  -8.786  18.962  1.00 20.71      BLGL
ATOM   1858  CG2 VAL   247      12.912 -10.800  18.636  1.00 23.56      BLGL
ATOM   1859  C   VAL   247      12.215  -8.275  17.006  1.00 22.43      BLGL
ATOM   1860  O   VAL   247      11.031  -8.631  17.000  1.00 22.15      BLGL
ATOM   1861  N   LEU   248      12.578  -7.020  17.255  1.00 22.41      BLGL
ATOM   1862  CA  LEU   248      11.584  -5.990  17.538  1.00 22.55      BLGL
ATOM   1863  CB  LEU   248      12.251  -4.734  18.125  1.00 20.88      BLGL
ATOM   1864  CG  LEU   248      12.778  -4.816  19.563  1.00 19.44      BLGL
ATOM   1865  CD1 LEU   248      13.426  -3.498  19.954  1.00 17.12      BLGL
ATOM   1866  CD2 LEU   248      11.639  -5.143  20.505  1.00 15.29      BLGL
ATOM   1867  C   LEU   248      10.805  -5.617  16.270  1.00 23.02      BLGL
ATOM   1868  O   LEU   248       9.597  -5.381  16.318  1.00 22.01      BLGL
ATOM   1869  N   THR   249      11.496  -5.570  15.136  1.00 20.49      BLGL
ATOM   1870  CA  THR   249      10.844  -5.220  13.890  1.00 21.29      BLGL
ATOM   1871  CB  THR   249      11.836  -5.197  12.722  1.00 22.20      BLGL
ATOM   1872  OG1 THR   249      12.872  -4.246  12.994  1.00 24.83      BLGL
ATOM   1873  CG2 THR   249      11.128  -4.808  11.440  1.00 20.47      BLGL
ATOM   1874  C   THR   249       9.739  -6.214  13.573  1.00 22.84      BLGL
ATOM   1875  O   THR   249       8.706  -5.842  13.020  1.00 20.69      BLGL
ATOM   1876  N   SER   250       9.956  -7.481  13.920  1.00 23.97      BLGL
ATOM   1877  CA  SER   250       8.945  -8.509  13.667  1.00 25.77      BLGL
ATOM   1878  CB  SER   250       9.451  -9.889  14.076  1.00 27.18      BLGL
ATOM   1879  OG  SER   250      10.487 -10.310  13.213  1.00 34.71      BLGL
ATOM   1880  C   SER   250       7.686  -8.196  14.446  1.00 24.53      BLGL
ATOM   1881  O   SER   250       6.590  -8.207  13.892  1.00 24.89      BLGL
ATOM   1882  N   VAL   251       7.850  -7.919  15.736  1.00 22.02      BLGL
ATOM   1883  CA  VAL   251       6.713  -7.592  16.581  1.00 20.32      BLGL
ATOM   1884  CB  VAL   251       7.156  -7.246  18.022  1.00 19.00      BLGL
ATOM   1885  CG1 VAL   251       5.972  -6.733  18.822  1.00 19.03      BLGL
ATOM   1886  CG2 VAL   251       7.736  -8.475  18.693  1.00 17.23      BLGL
ATOM   1887  C   VAL   251       5.968  -6.401  15.984  1.00 20.70      BLGL
ATOM   1888  O   VAL   251       4.741  -6.399  15.912  1.00 20.26      BLGL
ATOM   1889  N   ALA   252       6.717  -5.396  15.546  1.00 20.84      BLGL
ATOM   1890  CA  ALA   252       6.123  -4.198  14.965  1.00 21.97      BLGL
ATOM   1891  CB  ALA   252       7.203  -3.175  14.663  1.00 21.24      BLGL
ATOM   1892  C   ALA   252       5.330  -4.497  13.701  1.00 22.61      BLGL
ATOM   1893  O   ALA   252       4.137  -4.219  13.629  1.00 23.36      BLGL
ATOM   1894  N   ASP   253       5.999  -5.069  12.711  1.00 22.58      BLGL
ATOM   1895  CA  ASP   253       5.366  -5.386  11.440  1.00 23.48      BLGL
ATOM   1896  CB  ASP   253       6.394  -5.968  10.472  1.00 23.27      BLGL
ATOM   1897  CG  ASP   253       7.403  -4.946  10.019  1.00 25.67      BLGL
ATOM   1898  OD1 ASP   253       8.372  -5.346   9.337  1.00 26.60      BLGL
ATOM   1899  OD2 ASP   253       7.224  -3.744  10.344  1.00 27.47      BLGL
ATOM   1900  C   ASP   253       4.203  -6.352  11.556  1.00 24.77      BLGL
ATOM   1901  O   ASP   253       3.174  -6.174  10.904  1.00 25.85      BLGL
ATOM   1902  N   THR   254       4.359  -7.371  12.389  1.00 24.09      BLGL
ATOM   1903  CA  THR   254       3.317  -8.374  12.537  1.00 22.38      BLGL
ATOM   1904  CB  THR   254       3.892  -9.679  13.094  1.00 21.12      BLGL
ATOM   1905  OG1 THR   254       5.000 -10.096  12.287  1.00 22.06      BLGL
ATOM   1906  CG2 THR   254       2.836 -10.765  13.073  1.00 20.31      BLGL
ATOM   1907  C   THR   254       2.123  -7.977  13.395  1.00 23.11      BLGL
ATOM   1908  O   THR   254       0.995  -8.366  13.102  1.00 26.89      BLGL
ATOM   1909  N   TYR   255       2.345  -7.201  14.444  1.00 21.45      BLGL
ATOM   1910  CA  TYR   255       1.231  -6.835  15.307  1.00 20.15      BLGL
ATOM   1911  CB  TYR   255       1.488  -7.377  16.709  1.00 20.87      BLGL
ATOM   1912  CG  TYR   255       1.670  -8.876  16.701  1.00 22.40      BLGL
ATOM   1913  CD1 TYR   255       0.568  -9.728  16.568  1.00 21.45      BLGL
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Fig. 4 cont.

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ATOM   1914  CE1 TYR   255       0.731 -11.107  16.494  1.00 21.01      BLGL
ATOM   1915  CD2 TYR   255       2.943  -9.443  16.761  1.00 19.96      BLGL
ATOM   1916  CE2 TYR   255       3.117 -10.822  16.686  1.00 20.59      BLGL
ATOM   1917  CZ  TYR   255       2.008 -11.647  16.554  1.00 21.17      BLGL
ATOM   1918  OH  TYR   255       2.179 -13.009  16.495  1.00 21.44      BLGL
ATOM   1919  C   TYR   255       0.927  -5.357  15.360  1.00 19.29      BLGL
ATOM   1920  O   TYR   255       0.056  -4.923  16.104  1.00 19.71      BLGL
ATOM   1921  N   GLY   256       1.649  -4.585  14.562  1.00 20.06      BLGL
ATOM   1922  CA  GLY   256       1.421  -3.155  14.516  1.00 21.23      BLGL
ATOM   1923  C   GLY   256       1.582  -2.454  15.847  1.00 21.40      BLGL
ATOM   1924  O   GLY   256       0.788  -1.593  16.212  1.00 22.35      BLGL
ATOM   1925  N   LYS   257       2.619  -2.815  16.581  1.00 20.19      BLGL
ATOM   1926  CA  LYS   257       2.845  -2.182  17.861  1.00 21.01      BLGL
ATOM   1927  CB  LYS   257       3.032  -3.244  18.949  1.00 20.86      BLGL
ATOM   1928  CG  LYS   257       1.863  -4.191  19.122  1.00 18.58      BLGL
ATOM   1929  CD  LYS   257       0.615  -3.458  19.566  1.00 17.81      BLGL
ATOM   1930  CE  LYS   257      -0.524  -4.428  19.765  1.00 16.84      BLGL
ATOM   1931  NZ  LYS   257      -1.801  -3.739  20.053  1.00 19.74      BLGL
ATOM   1932  C   LYS   257       4.082  -1.300  17.792  1.00 20.95      BLGL
ATOM   1933  O   LYS   257       4.934  -1.474  16.918  1.00 19.83      BLGL
ATOM   1934  N   LYS   258       4.161  -0.333  18.699  1.00 19.92      BLGL
ATOM   1935  CA  LYS   258       5.329   0.526  18.771  1.00 21.02      BLGL
ATOM   1936  CB  LYS   258       5.037   1.785  19.581  1.00 24.26      BLGL
ATOM   1937  CG  LYS   258       3.850   2.601  19.139  1.00 27.83      BLGL
ATOM   1938  CD  LYS   258       4.143   3.387  17.887  1.00 33.22      BLGL
ATOM   1939  CE  LYS   258       3.297   4.652  17.862  1.00 36.49      BLGL
ATOM   1940  NZ  LYS   258       1.845   4.362  18.036  1.00 38.07      BLGL
ATOM   1941  C   LYS   258       6.322  -0.326  19.559  1.00 21.33      BLGL
ATOM   1942  O   LYS   258       5.923  -1.248  20.276  1.00 21.62      BLGL
ATOM   1943  N   VAL   259       7.607  -0.037  19.430  1.00 18.75      BLGL
ATOM   1944  CA  VAL   259       8.604  -0.786  20.176  1.00 17.87      BLGL
ATOM   1945  CB  VAL   259       9.391  -1.762  19.271  1.00 17.66      BLGL
ATOM   1946  CG1 VAL   259       8.447  -2.789  18.686  1.00 16.47      BLGL
ATOM   1947  CG2 VAL   259      10.118  -0.997  18.171  1.00 16.36      BLGL
ATOM   1948  C   VAL   259       9.572   0.190  20.816  1.00 18.60      BLGL
ATOM   1949  O   VAL   259       9.628   1.362  20.443  1.00 19.89      BLGL
ATOM   1950  N   MET   260      10.328  -0.280  21.794  1.00 18.23      BLGL
ATOM   1951  CA  MET   260      11.295   0.583  22.452  1.00 18.93      BLGL
ATOM   1952  CB  MET   260      10.594   1.741  23.179  1.00 17.82      BLGL
ATOM   1953  CG  MET   260       9.861   1.335  24.450  1.00 18.62      BLGL
ATOM   1954  SD  MET   260       9.338   2.760  25.444  1.00 20.82      BLGL
ATOM   1955  CE  MET   260       9.092   1.989  27.061  1.00 14.70      BLGL
ATOM   1956  C   MET   260      12.109  -0.200  23.461  1.00 18.97      BLGL
ATOM   1957  O   MET   260      11.757  -1.326  23.827  1.00 18.84      BLGL
ATOM   1958  N   VAL   261      13.207   0.401  23.900  1.00 18.49      BLGL
ATOM   1959  CA  VAL   261      14.049  -0.215  24.907  1.00 19.01      BLGL
ATOM   1960  CB  VAL   261      15.545  -0.063  24.567  1.00 18.88      BLGL
ATOM   1961  CG1 VAL   261      16.399  -0.549  25.728  1.00 19.31      BLGL
ATOM   1962  CG2 VAL   261      15.867  -0.867  23.326  1.00 17.95      BLGL
ATOM   1963  C   VAL   261      13.713   0.493  26.218  1.00 17.97      BLGL
ATOM   1964  O   VAL   261      13.854   1.712  26.343  1.00 14.60      BLGL
ATOM   1965  N   ALA   262      13.228  -0.280  27.180  1.00 18.80      BLGL
ATOM   1966  CA  ALA   262      12.846   0.269  28.473  1.00 21.56      BLGL
ATOM   1967  CB  ALA   262      11.777  -0.617  29.107  1.00 20.01      BLGL
ATOM   1968  C   ALA   262      14.047   0.409  29.412  1.00 21.77      BLGL
ATOM   1969  O   ALA   262      14.079   1.297  30.262  1.00 22.42      BLGL
ATOM   1970  N   GLU   263      15.036  -0.464  29.247  1.00 20.47      BLGL
ATOM   1971  CA  GLU   263      16.214  -0.433  30.091  1.00 19.18      BLGL
ATOM   1972  CB  GLU   263      16.099  -1.464  31.211  1.00 18.99      BLGL
ATOM   1973  CG  GLU   263      15.178  -1.102  32.358  1.00 21.05      BLGL
ATOM   1974  CD  GLU   263      15.151  -2.191  33.417  1.00 19.91      BLGL
ATOM   1975  OE1 GLU   263      16.207  -2.819  33.642  1.00 20.67      BLGL
ATOM   1976  OE2 GLU   263      14.087  -2.422  34.029  1.00 22.21      BLGL
ATOM   1977  C   GLU   263      17.483  -0.729  29.319  1.00 19.96      BLGL
ATOM   1978  O   GLU   263      17.497  -1.587  28.440  1.00 20.56      BLGL
ATOM   1979  N   THR   264      18.547  -0.013  29.661  1.00 17.62      BLGL
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Fig. 4 cont.

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ATOM   1980  CA  THR   264      19.844  -0.219  29.042  1.00 15.98      BLGL
ATOM   1981  CB  THR   264      19.874   0.247  27.573  1.00 16.21      BLGL
ATOM   1982  OG1 THR   264      20.989  -0.366  26.907  1.00 15.60      BLGL
ATOM   1983  CG2 THR   264      20.036   1.771  27.494  1.00 13.52      BLGL
ATOM   1984  C   THR   264      20.872   0.578  29.820  1.00 15.21      BLGL
ATOM   1985  O   THR   264      20.532   1.477  30.579  1.00 14.74      BLGL
ATOM   1986  N   SER   265      22.136   0.240  29.621  1.00 15.34      BLGL
ATOM   1987  CA  SER   265      23.229   0.936  30.280  1.00 16.34      BLGL
ATOM   1988  CB  SER   265      23.113   0.819  31.802  1.00 16.26      BLGL
ATOM   1989  OG  SER   265      23.293  -0.517  32.249  1.00 16.64      BLGL
ATOM   1990  C   SER   265      24.531   0.312  29.826  1.00 17.34      BLGL
ATOM   1991  O   SER   265      24.543  -0.607  29.005  1.00 18.70      BLGL
ATOM   1992  N   TYR   266      25.629   0.836  30.349  1.00 18.17      BLGL
ATOM   1993  CA  TYR   266      26.939   0.307  30.039  1.00 17.93      BLGL
ATOM   1994  CB  TYR   266      27.397   0.699  28.640  1.00 15.84      BLGL
ATOM   1995  CG  TYR   266      28.485  -0.218  28.131  1.00 17.82      BLGL
ATOM   1996  CD1 TYR   266      28.192  -1.527  27.774  1.00 18.54      BLGL
ATOM   1997  CE1 TYR   266      29.186  -2.396  27.329  1.00 19.26      BLGL
ATOM   1998  CD2 TYR   266      29.816   0.210  28.035  1.00 20.22      BLGL
ATOM   1999  CE2 TYR   266      30.826  -0.656  27.591  1.00 19.11      BLGL
ATOM   2000  CZ  TYR   266      30.499  -1.962  27.238  1.00 19.47      BLGL
ATOM   2001  OH  TYR   266      31.472  -2.836  26.784  1.00 18.36      BLGL
ATOM   2002  C   TYR   266      27.911   0.846  31.064  1.00 18.90      BLGL
ATOM   2003  O   TYR   266      27.681   1.895  31.665  1.00 18.09      BLGL
ATOM   2004  N   THR   267      28.995   0.105  31.259  1.00 20.38      BLGL
ATOM   2005  CA  THR   267      30.037   0.462  32.210  1.00 21.04      BLGL
ATOM   2006  CB  THR   267      30.852  -0.773  32.580  1.00 20.00      BLGL
ATOM   2007  OG1 THR   267      31.305  -1.402  31.373  1.00 19.78      BLGL
ATOM   2008  CG2 THR   267      30.017  -1.752  33.366  1.00 19.30      BLGL
ATOM   2009  C   THR   267      31.000   1.482  31.619  1.00 21.49      BLGL
ATOM   2010  O   THR   267      31.455   1.315  30.488  1.00 24.81      BLGL
ATOM   2011  N   TYR   268      31.320   2.525  32.384  1.00 20.55      BLGL
ATOM   2012  CA  TYR   268      32.268   3.546  31.933  1.00 20.98      BLGL
ATOM   2013  CB  TYR   268      31.724   4.958  32.205  1.00 21.01      BLGL
ATOM   2014  CG  TYR   268      31.844   5.439  33.639  1.00 19.32      BLGL
ATOM   2015  CD1 TYR   268      33.019   6.027  34.105  1.00 20.87      BLGL
ATOM   2016  CE1 TYR   268      33.129   6.471  35.426  1.00 20.17      BLGL
ATOM   2017  CD2 TYR   268      30.778   5.302  34.532  1.00 21.37      BLGL
ATOM   2018  CE2 TYR   268      30.873   5.739  35.853  1.00 19.23      BLGL
ATOM   2019  CZ  TYR   268      32.049   6.322  36.295  1.00 21.74      BLGL
ATOM   2020  OH  TYR   268      32.137   6.753  37.604  1.00 22.30      BLGL
ATOM   2021  C   TYR   268      33.597   3.364  32.664  1.00 21.83      BLGL
ATOM   2022  O   TYR   268      34.590   4.013  32.344  1.00 18.94      BLGL
ATOM   2023  N   THR   269      33.600   2.479  33.657  1.00 22.82      BLGL
ATOM   2024  CA  THR   269      34.795   2.213  34.451  1.00 23.10      BLGL
ATOM   2025  CB  THR   269      34.970   3.271  35.573  1.00 20.44      BLGL
ATOM   2026  OG1 THR   269      36.161   2.989  36.311  1.00 20.91      BLGL
ATOM   2027  CG2 THR   269      33.791   3.250  36.524  1.00 18.84      BLGL
ATOM   2028  C   THR   269      34.693   0.834  35.083  1.00 23.00      BLGL
ATOM   2029  O   THR   269      33.607   0.376  35.403  1.00 25.15      BLGL
ATOM   2030  N   ALA   270      35.826   0.170  35.259  1.00 24.31      BLGL
ATOM   2031  CA  ALA   270      35.825  -1.158  35.853  1.00 24.71      BLGL
ATOM   2032  CB  ALA   270      37.058  -1.933  35.409  1.00 21.17      BLGL
ATOM   2033  C   ALA   270      35.810  -1.019  37.361  1.00 25.78      BLGL
ATOM   2034  O   ALA   270      35.538  -1.970  38.080  1.00 29.18      BLGL
ATOM   2035  N   GLU   271      36.083   0.185  37.836  1.00 27.12      BLGL
ATOM   2036  CA  GLU   271      36.133   0.448  39.263  1.00 29.78      BLGL
ATOM   2037  CB  GLU   271      36.914   1.742  39.495  1.00 32.08      BLGL
ATOM   2038  CG  GLU   271      36.864   2.261  40.920  1.00 35.54      BLGL
ATOM   2039  CD  GLU   271      37.750   3.466  41.110  1.00 36.58      BLGL
ATOM   2040  OE1 GLU   271      38.022   4.167  40.108  1.00 36.10      BLGL
ATOM   2041  OE2 GLU   271      38.160   3.714  42.262  1.00 38.61      BLGL
ATOM   2042  C   GLU   271      34.783   0.527  39.977  1.00 30.16      BLGL
ATOM   2043  O   GLU   271      33.776   0.938  39.405  1.00 31.60      BLGL
ATOM   2044  N   ASP   272      34.782   0.125  41.242  1.00 30.13      BLGL
ATOM   2045  CA  ASP   272      33.590   0.169  42.081  1.00 30.63      BLGL
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Fig. 4 cont.

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ATOM   2046  CB  ASP   272      33.333  -1.190  42.722  1.00 29.68      BLGL
ATOM   2047  CG  ASP   272      32.488  -1.081  43.968  1.00 29.93      BLGL
ATOM   2048  OD1 ASP   272      31.427  -0.428  43.896  1.00 29.02      BLGL
ATOM   2049  OD2 ASP   272      32.884  -1.640  45.014  1.00 30.80      BLGL
ATOM   2050  C   ASP   272      33.865   1.188  43.178  1.00 31.65      BLGL
ATOM   2051  O   ASP   272      34.705   0.946  44.045  1.00 33.92      BLGL
ATOM   2052  N   GLY   273      33.163   2.318  43.157  1.00 31.58      BLGL
ATOM   2053  CA  GLY   273      33.420   3.340  44.158  1.00 32.18      BLGL
ATOM   2054  C   GLY   273      32.476   3.304  45.333  1.00 31.14      BLGL
ATOM   2055  O   GLY   273      32.407   4.250  46.116  1.00 32.09      BLGL
ATOM   2056  N   ASP   274      31.786   2.184  45.472  1.00 30.99      BLGL
ATOM   2057  CA  ASP   274      30.790   2.002  46.511  1.00 30.40      BLGL
ATOM   2058  CB  ASP   274      29.550   1.377  45.871  1.00 31.29      BLGL
ATOM   2059  CG  ASP   274      28.304   1.620  46.659  1.00 32.35      BLGL
ATOM   2060  OD1 ASP   274      27.319   0.902  46.433  1.00 34.84      BLGL
ATOM   2061  OD2 ASP   274      28.299   2.539  47.495  1.00 38.43      BLGL
ATOM   2062  C   ASP   274      31.264   1.104  47.649  1.00 30.15      BLGL
ATOM   2063  O   ASP   274      31.075   1.408  48.827  1.00 28.39      BLGL
ATOM   2064  N   GLY   275      31.867  -0.017  47.283  1.00 28.33      BLGL
ATOM   2065  CA  GLY   275      32.311  -0.956  48.283  1.00 29.05      BLGL
ATOM   2066  C   GLY   275      31.486  -2.210  48.099  1.00 28.72      BLGL
ATOM   2067  O   GLY   275      31.881  -3.298  48.519  1.00 31.31      BLGL
ATOM   2068  N   HIS   276      30.325  -2.046  47.472  1.00 26.86      BLGL
ATOM   2069  CA  HIS   276      29.431  -3.164  47.191  1.00 24.43      BLGL
ATOM   2070  CB  HIS   276      27.974  -2.726  47.336  1.00 23.89      BLGL
ATOM   2071  CG  HIS   276      26.986  -3.842  47.172  1.00 26.16      BLGL
ATOM   2072  CD2 HIS   276      26.329  -4.297  46.078  1.00 24.85      BLGL
ATOM   2073  ND1 HIS   276      26.595  -4.652  48.217  1.00 26.36      BLGL
ATOM   2074  CE1 HIS   276      25.741  -5.557  47.776  1.00 24.78      BLGL
ATOM   2075  NE2 HIS   276      25.562  -5.363  46.481  1.00 25.01      BLGL
ATOM   2076  C   HIS   276      29.691  -3.597  45.748  1.00 24.24      BLGL
ATOM   2077  O   HIS   276      29.512  -2.808  44.822  1.00 23.66      BLGL
ATOM   2078  N   GLY   277      30.108  -4.844  45.562  1.00 23.41      BLGL
ATOM   2079  CA  GLY   277      30.397  -5.343  44.225  1.00 23.85      BLGL
ATOM   2080  C   GLY   277      29.405  -4.987  43.130  1.00 24.88      BLGL
ATOM   2081  O   GLY   277      28.185  -5.064  43.320  1.00 25.03      BLGL
ATOM   2082  N   ASN   278      29.935  -4.616  41.966  1.00 24.25      BLGL
ATOM   2083  CA  ASN   278      29.114  -4.238  40.822  1.00 22.79      BLGL
ATOM   2084  CB  ASN   278      29.827  -3.150  40.027  1.00 21.96      BLGL
ATOM   2085  CG  ASN   278      29.928  -1.844  40.797  1.00 23.90      BLGL
ATOM   2086  ND2 ASN   278      30.661  -0.934  40.410  1.00 26.25      BLGL
ATOM   2087  OD1 ASN   278      29.177  -1.742  41.889  1.00 21.34      BLGL
ATOM   2088  C   ASN   278      28.748  -5.407  39.910  1.00 23.33      BLGL
ATOM   2089  O   ASN   278      29.408  -6.443  39.898  1.00 22.97      BLGL
ATOM   2090  N   THR   279      27.675  -5.226  39.152  1.00 23.75      BLGL
ATOM   2091  CA  THR   279      27.188  -6.247  38.241  1.00 24.46      BLGL
ATOM   2092  CB  THR   279      25.821  -5.857  37.666  1.00 25.31      BLGL
ATOM   2093  OG1 THR   279      24.874  -5.729  38.728  1.00 27.04      BLGL
ATOM   2094  CG2 THR   279      25.331  -6.910  36.701  1.00 28.22      BLGL
ATOM   2095  C   THR   279      28.137  -6.482  37.078  1.00 24.01      BLGL
ATOM   2096  O   THR   279      28.356  -7.613  36.659  1.00 24.35      BLGL
ATOM   2097  N   ALA   280      28.687  -5.401  36.547  1.00 24.16      BLGL
ATOM   2098  CA  ALA   280      29.599  -5.495  35.422  1.00 24.11      BLGL
ATOM   2099  CB  ALA   280      28.857  -5.182  34.137  1.00 21.63      BLGL
ATOM   2100  C   ALA   280      30.749  -4.522  35.616  1.00 25.17      BLGL
ATOM   2101  O   ALA   280      30.638  -3.565  36.379  1.00 26.21      BLGL
ATOM   2102  N   PRO   281      31.881  -4.766  34.942  1.00 25.93      BLGL
ATOM   2103  CD  PRO   281      32.977  -3.790  34.829  1.00 26.64      BLGL
ATOM   2104  CA  PRO   281      32.106  -5.896  34.037  1.00 27.75      BLGL
ATOM   2105  CB  PRO   281      33.155  -5.353  33.084  1.00 27.25      BLGL
ATOM   2106  CG  PRO   281      34.001  -4.545  33.998  1.00 28.42      BLGL
ATOM   2107  C   PRO   281      32.590  -7.142  34.773  1.00 29.21      BLGL
ATOM   2108  O   PRO   281      33.055  -7.071  35.902  1.00 31.08      BLGL
ATOM   2109  N   LYS   282      32.468  -8.287  34.123  1.00 31.67      BLGL
ATOM   2110  CA  LYS   282      32.902  -9.546  34.705  1.00 35.33      BLGL
ATOM   2111  CB  LYS   282      31.788 -10.169  35.537  1.00 34.90      BLGL
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Fig. 4 cont.

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ATOM   2112  CG  LYS   282      31.527  -9.495  36.861  1.00 37.13      BLGL
ATOM   2113  CD  LYS   282      30.496 -10.301  37.636  1.00 38.88      BLGL
ATOM   2114  CE  LYS   282      30.386  -9.846  39.077  1.00 40.27      BLGL
ATOM   2115  NZ  LYS   282      29.540 -10.796  39.851  1.00 42.22      BLGL
ATOM   2116  C   LYS   282      33.270 -10.495  33.583  1.00 38.11      BLGL
ATOM   2117  O   LYS   282      32.931 -10.251  32.429  1.00 39.52      BLGL
ATOM   2118  N   ASN   283      33.967 -11.575  33.920  1.00 42.82      BLGL
ATOM   2119  CA  ASN   283      34.355 -12.558  32.914  1.00 46.20      BLGL
ATOM   2120  CB  ASN   283      35.290 -13.614  33.512  1.00 50.82      BLGL
ATOM   2121  CG  ASN   283      36.534 -13.010  34.122  1.00 56.85      BLGL
ATOM   2122  OD1 ASN   283      36.474 -12.369  35.175  1.00 61.22      BLGL
ATOM   2123  ND2 ASN   283      37.672 -13.200  33.461  1.00 58.97      BLGL
ATOM   2124  C   ASN   283      33.100 -13.246  32.382  1.00 45.60      BLGL
ATOM   2125  O   ASN   283      32.163 -13.532  33.138  1.00 44.14      BLGL
ATOM   2126  N   GLY   284      33.081 -13.507  31.080  1.00 44.05      BLGL
ATOM   2127  CA  GLY   284      31.927 -14.166  30.499  1.00 42.01      BLGL
ATOM   2128  C   GLY   284      30.920 -13.195  29.918  1.00 40.47      BLGL
ATOM   2129  O   GLY   284      30.072 -13.590  29.114  1.00 41.73      BLGL
ATOM   2130  N   GLN   285      30.997 -11.929  30.321  1.00 36.97      BLGL
ATOM   2131  CA  GLN   285      30.081 -10.934  29.794  1.00 32.62      BLGL
ATOM   2132  CB  GLN   285      29.904  -9.781  30.771  1.00 31.11      BLGL
ATOM   2133  CG  GLN   285      29.440 -10.187  32.149  1.00 29.26      BLGL
ATOM   2134  CD  GLN   285      29.234  -8.985  33.046  1.00 27.08      BLGL
ATOM   2135  OE1 GLN   285      29.922  -7.973  32.910  1.00 26.10      BLGL
ATOM   2136  NE2 GLN   285      28.296  -9.091  33.974  1.00 25.79      BLGL
ATOM   2137  C   GLN   285      30.634 -10.397  28.487  1.00 30.85      BLGL
ATOM   2138  O   GLN   285      31.844 -10.301  28.302  1.00 31.43      BLGL
ATOM   2139  N   THR   286      29.735 -10.047  27.581  1.00 29.00      BLGL
ATOM   2140  CA  THR   286      30.119  -9.516  26.292  1.00 26.23      BLGL
ATOM   2141  CB  THR   286      29.000  -9.741  25.280  1.00 26.60      BLGL
ATOM   2142  OG1 THR   286      28.755 -11.147  25.159  1.00 26.51      BLGL
ATOM   2143  CG2 THR   286      29.370  -9.150  23.928  1.00 26.18      BLGL
ATOM   2144  C   THR   286      30.401  -8.030  26.413  1.00 25.38      BLGL
ATOM   2145  O   THR   286      29.553  -7.266  26.859  1.00 25.73      BLGL
ATOM   2146  N   LEU   287      31.596  -7.619  26.016  1.00 25.58      BLGL
ATOM   2147  CA  LEU   287      31.957  -6.219  26.098  1.00 25.95      BLGL
ATOM   2148  CB  LEU   287      33.036  -6.034  27.159  1.00 23.53      BLGL
ATOM   2149  CG  LEU   287      32.593  -6.516  28.539  1.00 22.29      BLGL
ATOM   2150  CD1 LEU   287      33.742  -6.413  29.523  1.00 21.57      BLGL
ATOM   2151  CD2 LEU   287      31.409  -5.692  28.998  1.00 20.26      BLGL
ATOM   2152  C   LEU   287      32.446  -5.739  24.748  1.00 28.08      BLGL
ATOM   2153  O   LEU   287      33.648  -5.666  24.503  1.00 29.85      BLGL
ATOM   2154  N   ASN   288      31.508  -5.406  23.870  1.00 29.45      BLGL
ATOM   2155  CA  ASN   288      31.869  -4.949  22.537  1.00 31.56      BLGL
ATOM   2156  CB  ASN   288      30.641  -4.928  21.632  1.00 35.67      BLGL
ATOM   2157  CG  ASN   288      30.039  -6.306  21.456  1.00 41.56      BLGL
ATOM   2158  OD1 ASN   288      30.766  -7.298  21.320  1.00 42.80      BLGL
ATOM   2159  ND2 ASN   288      28.707  -6.380  21.449  1.00 43.66      BLGL
ATOM   2160  C   ASN   288      32.533  -3.590  22.523  1.00 30.88      BLGL
ATOM   2161  O   ASN   288      33.295  -3.281  21.615  1.00 32.37      BLGL
ATOM   2162  N   ASN   289      32.242  -2.767  23.520  1.00 30.69      BLGL
ATOM   2163  CA  ASN   289      32.849  -1.447  23.583  1.00 29.17      BLGL
ATOM   2164  CB  ASN   289      31.778  -0.364  23.737  1.00 29.80      BLGL
ATOM   2165  CG  ASN   289      31.108  -0.018  22.420  1.00 34.65      BLGL
ATOM   2166  OD1 ASN   289      31.733   0.562  21.529  1.00 36.80      BLGL
ATOM   2167  ND2 ASN   289      29.834  -0.382  22.285  1.00 34.27      BLGL
ATOM   2168  C   ASN   289      33.818  -1.386  24.746  1.00 28.28      BLGL
ATOM   2169  O   ASN   289      33.698  -2.144  25.718  1.00 26.00      BLGL
ATOM   2170  N   PRO   290      34.815  -0.497  24.654  1.00 26.69      BLGL
ATOM   2171  CD  PRO   290      35.116   0.459  23.576  1.00 25.39      BLGL
ATOM   2172  CA  PRO   290      35.783  -0.375  25.740  1.00 24.60      BLGL
ATOM   2173  CB  PRO   290      36.796   0.616  25.184  1.00 23.11      BLGL
ATOM   2174  CG  PRO   290      35.977   1.470  24.294  1.00 24.06      BLGL
ATOM   2175  C   PRO   290      35.098   0.132  27.006  1.00 25.03      BLGL
ATOM   2176  O   PRO   290      34.140   0.916  26.951  1.00 24.16      BLGL
ATOM   2177  N   VAL   291      35.582  -0.334  28.149  1.00 23.84      BLGL
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Fig. 4 cont.

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ATOM   2178  CA  VAL   291      35.019   0.083  29.420  1.00 21.28      BLGL
ATOM   2179  CB  VAL   291      35.340  -0.945  30.520  1.00 21.94      BLGL
ATOM   2180  CG1 VAL   291      34.752  -0.488  31.852  1.00 20.42      BLGL
ATOM   2181  CG2 VAL   291      34.775  -2.309  30.114  1.00 17.11      BLGL
ATOM   2182  C   VAL   291      35.607   1.448  29.760  1.00 20.16      BLGL
ATOM   2183  O   VAL   291      36.504   1.574  30.588  1.00 19.20      BLGL
ATOM   2184  N   THR   292      35.100   2.464  29.070  1.00 19.49      BLGL
ATOM   2185  CA  THR   292      35.532   3.842  29.250  1.00 18.74      BLGL
ATOM   2186  CB  THR   292      36.660   4.228  28.251  1.00 18.53      BLGL
ATOM   2187  OG1 THR   292      36.111   4.400  26.939  1.00 17.67      BLGL
ATOM   2188  CG2 THR   292      37.716   3.148  28.196  1.00 17.15      BLGL
ATOM   2189  C   THR   292      34.335   4.759  28.994  1.00 19.39      BLGL
ATOM   2190  O   THR   292      33.275   4.308  28.568  1.00 19.27      BLGL
ATOM   2191  N   VAL   293      34.514   6.048  29.252  1.00 20.06      BLGL
ATOM   2192  CA  VAL   293      33.446   7.005  29.039  1.00 20.55      BLGL
ATOM   2193  CB  VAL   293      33.865   8.406  29.544  1.00 20.16      BLGL
ATOM   2194  CG1 VAL   293      32.857   9.451  29.100  1.00 20.66      BLGL
ATOM   2195  CG2 VAL   293      33.936   8.390  31.074  1.00 16.78      BLGL
ATOM   2196  C   VAL   293      33.051   7.044  27.562  1.00 20.97      BLGL
ATOM   2197  O   VAL   293      31.864   7.124  27.234  1.00 21.53      BLGL
ATOM   2198  N   GLN   294      34.039   6.962  26.674  1.00 20.45      BLGL
ATOM   2199  CA  GLN   294      33.770   6.956  25.238  1.00 21.64      BLGL
ATOM   2200  CB  GLN   294      35.066   7.058  24.431  1.00 25.60      BLGL
ATOM   2201  CG  GLN   294      35.192   8.341  23.619  1.00 29.52      BLGL
ATOM   2202  CD  GLN   294      34.031   8.562  22.666  1.00 29.94      BLGL
ATOM   2203  OE1 GLN   294      33.739   9.696  22.296  1.00 34.05      BLGL
ATOM   2204  NE2 GLN   294      33.371   7.485  22.260  1.00 28.56      BLGL
ATOM   2205  C   GLN   294      33.058   5.672  24.834  1.00 22.39      BLGL
ATOM   2206  O   GLN   294      32.199   5.677  23.950  1.00 19.94      BLGL
ATOM   2207  N   GLY   295      33.444   4.566  25.468  1.00 22.59      BLGL
ATOM   2208  CA  GLY   295      32.814   3.295  25.173  1.00 20.59      BLGL
ATOM   2209  C   GLY   295      31.349   3.362  25.564  1.00 22.43      BLGL
ATOM   2210  O   GLY   295      30.464   3.047  24.767  1.00 23.22      BLGL
ATOM   2211  N   GLN   296      31.099   3.787  26.798  1.00 19.02      BLGL
ATOM   2212  CA  GLN   296      29.750   3.905  27.313  1.00 19.21      BLGL
ATOM   2213  CB  GLN   296      29.789   4.581  28.683  1.00 19.90      BLGL
ATOM   2214  CG  GLN   296      28.467   4.668  29.419  1.00 18.48      BLGL
ATOM   2215  CD  GLN   296      28.572   5.536  30.669  1.00 17.80      BLGL
ATOM   2216  OE1 GLN   296      29.027   6.679  30.595  1.00 16.03      BLGL
ATOM   2217  NE2 GLN   296      28.152   4.999  31.818  1.00 15.03      BLGL
ATOM   2218  C   GLN   296      28.906   4.719  26.336  1.00 19.79      BLGL
ATOM   2219  O   GLN   296      27.777   4.347  26.016  1.00 20.36      BLGL
ATOM   2220  N   ALA   297      29.458   5.825  25.851  1.00 18.99      BLGL
ATOM   2221  CA  ALA   297      28.733   6.669  24.905  1.00 18.45      BLGL
ATOM   2222  CB  ALA   297      29.546   7.916  24.578  1.00 14.36      BLGL
ATOM   2223  C   ALA   297      28.416   5.895  23.630  1.00 19.50      BLGL
ATOM   2224  O   ALA   297      27.301   5.978  23.104  1.00 20.34      BLGL
ATOM   2225  N   ASN   298      29.395   5.142  23.135  1.00 19.83      BLGL
ATOM   2226  CA  ASN   298      29.196   4.352  21.926  1.00 21.45      BLGL
ATOM   2227  CB  ASN   298      30.442   3.524  21.592  1.00 24.97      BLGL
ATOM   2228  CG  ASN   298      31.563   4.358  20.999  1.00 26.63      BLGL
ATOM   2229  OD1 ASN   298      31.329   5.440  20.459  1.00 25.65      BLGL
ATOM   2230  ND2 ASN   298      32.791   3.843  21.078  1.00 27.74      BLGL
ATOM   2231  C   ASN   298      28.027   3.405  22.133  1.00 21.39      BLGL
ATOM   2232  O   ASN   298      27.130   3.306  21.297  1.00 21.38      BLGL
ATOM   2233  N   ALA   299      28.061   2.713  23.266  1.00 19.25      BLGL
ATOM   2234  CA  ALA   299      27.038   1.754  23.633  1.00 17.97      BLGL
ATOM   2235  CB  ALA   299      27.294   1.264  25.030  1.00 16.35      BLGL
ATOM   2236  C   ALA   299      25.638   2.339  23.537  1.00 19.35      BLGL
ATOM   2237  O   ALA   299      24.763   1.771  22.881  1.00 17.73      BLGL
ATOM   2238  N   VAL   300      25.432   3.474  24.201  1.00 20.77      BLGL
ATOM   2239  CA  VAL   300      24.134   4.146  24.202  1.00 20.54      BLGL
ATOM   2240  CB  VAL   300      24.141   5.382  25.141  1.00 19.20      BLGL
ATOM   2241  CG1 VAL   300      22.786   6.081  25.108  1.00 16.54      BLGL
ATOM   2242  CG2 VAL   300      24.467   4.948  26.556  1.00 16.81      BLGL
ATOM   2243  C   VAL   300      23.761   4.597  22.795  1.00 20.62      BLGL
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Fig. 4 cont.

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ATOM   2244  O   VAL   300      22.643   4.383  22.332  1.00 22.02      BLGL
ATOM   2245  N   ARG   301      24.711   5.220  22.117  1.00 19.80      BLGL
ATOM   2246  CA  ARG   301      24.485   5.699  20.770  1.00 20.87      BLGL
ATOM   2247  CB  ARG   301      25.764   6.370  20.273  1.00 20.72      BLGL
ATOM   2248  CG  ARG   301      25.697   6.960  18.884  1.00 19.75      BLGL
ATOM   2249  CD  ARG   301      25.963   5.909  17.841  1.00 20.20      BLGL
ATOM   2250  NE  ARG   301      25.950   6.479  16.502  1.00 21.66      BLGL
ATOM   2251  CZ  ARG   301      25.770   5.763  15.400  1.00 21.05      BLGL
ATOM   2252  NH1 ARG   301      25.593   4.453  15.484  1.00 23.39      BLGL
ATOM   2253  NH2 ARG   301      25.741   6.359  14.223  1.00 19.98      BLGL
ATOM   2254  C   ARG   301      24.050   4.575  19.824  1.00 21.51      BLGL
ATOM   2255  O   ARG   301      23.190   4.774  18.967  1.00 23.05      BLGL
ATOM   2256  N   ASP   302      24.633   3.394  19.989  1.00 20.34      BLGL
ATOM   2257  CA  ASP   302      24.306   2.262  19.138  1.00 19.74      BLGL
ATOM   2258  CB  ASP   302      25.378   1.190  19.260  1.00 22.07      BLGL
ATOM   2259  CG  ASP   302      26.659   1.571  18.548  1.00 26.74      BLGL
ATOM   2260  OD1 ASP   302      27.647   0.818  18.676  1.00 31.70      BLGL
ATOM   2261  OD2 ASP   302      26.686   2.618  17.857  1.00 28.72      BLGL
ATOM   2262  C   ASP   302      22.947   1.648  19.408  1.00 20.74      BLGL
ATOM   2263  O   ASP   302      22.329   1.083  18.509  1.00 23.13      BLGL
ATOM   2264  N   VAL   303      22.482   1.740  20.644  1.00 18.00      BLGL
ATOM   2265  CA  VAL   303      21.182   1.189  20.971  1.00 18.00      BLGL
ATOM   2266  CB  VAL   303      20.971   1.110  22.503  1.00 17.67      BLGL
ATOM   2267  CG1 VAL   303      19.626   0.483  22.813  1.00 17.30      BLGL
ATOM   2268  CG2 VAL   303      22.075   0.299  23.132  1.00 20.13      BLGL
ATOM   2269  C   VAL   303      20.126   2.099  20.346  1.00 18.76      BLGL
ATOM   2270  O   VAL   303      19.099   1.638  19.854  1.00 16.54      BLGL
ATOM   2271  N   ILE   304      20.392   3.401  20.367  1.00 19.37      BLGL
ATOM   2272  CA  ILE   304      19.471   4.371  19.793  1.00 20.60      BLGL
ATOM   2273  CB  ILE   304      19.955   5.820  20.067  1.00 21.68      BLGL
ATOM   2274  CG2 ILE   304      19.113   6.835  19.293  1.00 19.25      BLGL
ATOM   2275  CG1 ILE   304      19.853   6.108  21.567  1.00 21.33      BLGL
ATOM   2276  CD1 ILE   304      20.334   7.482  21.961  1.00 21.10      BLGL
ATOM   2277  C   ILE   304      19.387   4.102  18.294  1.00 21.62      BLGL
ATOM   2278  O   ILE   304      18.316   4.130  17.695  1.00 22.05      BLGL
ATOM   2279  N   GLN   305      20.531   3.820  17.694  1.00 21.95      BLGL
ATOM   2280  CA  GLN   305      20.579   3.523  16.279  1.00 22.70      BLGL
ATOM   2281  CB  GLN   305      22.031   3.274  15.855  1.00 25.34      BLGL
ATOM   2282  CG  GLN   305      22.203   2.958  14.381  1.00 28.30      BLGL
ATOM   2283  CD  GLN   305      22.031   4.178  13.505  1.00 30.27      BLGL
ATOM   2284  OE1 GLN   305      22.915   5.030  13.430  1.00 30.12      BLGL
ATOM   2285  NE2 GLN   305      20.884   4.273  12.841  1.00 32.34      BLGL
ATOM   2286  C   GLN   305      19.736   2.278  16.006  1.00 22.92      BLGL
ATOM   2287  O   GLN   305      18.925   2.258  15.080  1.00 23.46      BLGL
ATOM   2288  N   ALA   306      19.931   1.247  16.831  1.00 22.84      BLGL
ATOM   2289  CA  ALA   306      19.221  -0.031  16.693  1.00 21.78      BLGL
ATOM   2290  CB  ALA   306      19.708  -1.019  17.743  1.00 18.27      BLGL
ATOM   2291  C   ALA   306      17.704   0.090  16.773  1.00 22.33      BLGL
ATOM   2292  O   ALA   306      16.987  -0.569  16.018  1.00 23.37      BLGL
ATOM   2293  N   VAL   307      17.219   0.919  17.691  1.00 20.00      BLGL
ATOM   2294  CA  VAL   307      15.788   1.112  17.844  1.00 20.55      BLGL
ATOM   2295  CB  VAL   307      15.450   1.823  19.169  1.00 20.50      BLGL
ATOM   2296  CG1 VAL   307      13.959   2.106  19.248  1.00 17.36      BLGL
ATOM   2297  CG2 VAL   307      15.878   0.960  20.337  1.00 19.55      BLGL
ATOM   2298  C   VAL   307      15.274   1.959  16.696  1.00 21.97      BLGL
ATOM   2299  O   VAL   307      14.164   1.750  16.195  1.00 22.69      BLGL
ATOM   2300  N   SER   308      16.097   2.916  16.283  1.00 21.64      BLGL
ATOM   2301  CA  SER   308      15.750   3.818  15.197  1.00 21.48      BLGL
ATOM   2302  CB  SER   308      16.809   4.916  15.073  1.00 22.23      BLGL
ATOM   2303  OG  SER   308      16.510   5.812  14.018  1.00 26.06      BLGL
ATOM   2304  C   SER   308      15.633   3.059  13.885  1.00 20.97      BLGL
ATOM   2305  O   SER   308      14.781   3.372  13.054  1.00 17.14      BLGL
ATOM   2306  N   ASP   309      16.490   2.057  13.709  1.00 21.61      BLGL
ATOM   2307  CA  ASP   309      16.480   1.252  12.494  1.00 23.50      BLGL
ATOM   2308  CB  ASP   309      17.698   0.332  12.434  1.00 25.27      BLGL
ATOM   2309  CG  ASP   309      18.971   1.069  12.064  1.00 29.05      BLGL
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Fig. 4 cont.

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ATOM   2310  OD1 ASP   309      18.874   2.130  11.401  1.00 26.38      BLGL
ATOM   2311  OD2 ASP   309      20.066   0.576  12.423  1.00 30.01      BLGL
ATOM   2312  C   ASP   309      15.225   0.412  12.339  1.00 24.33      BLGL
ATOM   2313  O   ASP   309      14.972  -0.124  11.265  1.00 26.71      BLGL
ATOM   2314  N   VAL   310      14.450   0.280  13.409  1.00 24.29      BLGL
ATOM   2315  CA  VAL   310      13.219  -0.490  13.344  1.00 23.62      BLGL
ATOM   2316  CB  VAL   310      12.582  -0.647  14.730  1.00 23.06      BLGL
ATOM   2317  CG1 VAL   310      11.232  -1.336  14.606  1.00 21.23      BLGL
ATOM   2318  CG2 VAL   310      13.509  -1.443  15.632  1.00 21.91      BLGL
ATOM   2319  C   VAL   310      12.248   0.247  12.440  1.00 23.63      BLGL
ATOM   2320  O   VAL   310      11.360  -0.352  11.834  1.00 25.38      BLGL
ATOM   2321  N   GLY   311      12.438   1.555  12.343  1.00 23.71      BLGL
ATOM   2322  CA  GLY   311      11.573   2.373  11.519  1.00 23.98      BLGL
ATOM   2323  C   GLY   311      10.628   3.201  12.366  1.00 27.47      BLGL
ATOM   2324  O   GLY   311      10.919   3.565  13.514  1.00 28.40      BLGL
ATOM   2325  N   GLU   312       9.469   3.474  11.783  1.00 27.49      BLGL
ATOM   2326  CA  GLU   312       8.438   4.262  12.419  1.00 27.36      BLGL
ATOM   2327  CB  GLU   312       7.210   4.291  11.514  1.00 32.86      BLGL
ATOM   2328  CG  GLU   312       6.318   5.503  11.705  1.00 43.92      BLGL
ATOM   2329  CD  GLU   312       4.950   5.314  11.071  1.00 50.44      BLGL
ATOM   2330  OE1 GLU   312       4.889   4.793   9.930  1.00 51.60      BLGL
ATOM   2331  OE2 GLU   312       3.939   5.694  11.713  1.00 53.86      BLGL
ATOM   2332  C   GLU   312       8.039   3.746  13.805  1.00 25.87      BLGL
ATOM   2333  O   GLU   312       7.717   4.537  14.683  1.00 27.15      BLGL
ATOM   2334  N   ALA   313       8.067   2.431  14.003  1.00 22.50      BLGL
ATOM   2335  CA  ALA   313       7.671   1.814  15.273  1.00 19.75      BLGL
ATOM   2336  CB  ALA   313       7.480   0.315  15.077  1.00 19.28      BLGL
ATOM   2337  C   ALA   313       8.608   2.054  16.454  1.00 18.86      BLGL
ATOM   2338  O   ALA   313       8.167   2.049  17.602  1.00 15.56      BLGL
ATOM   2339  N   GLY   314       9.897   2.238  16.173  1.00 19.40      BLGL
ATOM   2340  CA  GLY   314      10.868   2.476  17.232  1.00 21.12      BLGL
ATOM   2341  C   GLY   314      10.667   3.878  17.787  1.00 22.30      BLGL
ATOM   2342  O   GLY   314      11.016   4.865  17.135  1.00 23.19      BLGL
ATOM   2343  N   ILE   315      10.122   3.973  18.997  1.00 19.98      BLGL
ATOM   2344  CA  ILE   315       9.841   5.267  19.580  1.00 18.06      BLGL
ATOM   2345  CB  ILE   315       8.457   5.265  20.248  1.00 17.92      BLGL
ATOM   2346  CG2 ILE   315       7.402   4.928  19.221  1.00 16.03      BLGL
ATOM   2347  CG1 ILE   315       8.417   4.242  21.378  1.00 17.81      BLGL
ATOM   2348  CD1 ILE   315       7.113   4.236  22.116  1.00 16.57      BLGL
ATOM   2349  C   ILE   315      10.852   5.818  20.563  1.00 18.49      BLGL
ATOM   2350  O   ILE   315      10.851   7.012  20.836  1.00 19.85      BLGL
ATOM   2351  N   GLY   316      11.719   4.974  21.101  1.00 18.64      BLGL
ATOM   2352  CA  GLY   316      12.692   5.492  22.042  1.00 17.78      BLGL
ATOM   2353  C   GLY   316      13.562   4.510  22.803  1.00 18.38      BLGL
ATOM   2354  O   GLY   316      13.500   3.290  22.618  1.00 17.99      BLGL
ATOM   2355  N   VAL   317      14.381   5.081  23.680  1.00 17.69      BLGL
ATOM   2356  CA  VAL   317      15.312   4.328  24.512  1.00 17.45      BLGL
ATOM   2357  CB  VAL   317      16.727   4.367  23.916  1.00 17.12      BLGL
ATOM   2358  CG1 VAL   317      17.710   3.738  24.882  1.00 16.69      BLGL
ATOM   2359  CG2 VAL   317      16.753   3.642  22.586  1.00 16.13      BLGL
ATOM   2360  C   VAL   317      15.385   4.902  25.921  1.00 17.08      BLGL
ATOM   2361  O   VAL   317      15.386   6.116  26.101  1.00 19.09      BLGL
ATOM   2362  N   PHE   318      15.441   4.032  26.920  1.00 17.11      BLGL
ATOM   2363  CA  PHE   318      15.547   4.488  28.298  1.00 16.85      BLGL
ATOM   2364  CB  PHE   318      14.389   3.976  29.146  1.00 17.66      BLGL
ATOM   2365  CG  PHE   318      13.154   4.821  29.068  1.00 19.59      BLGL
ATOM   2366  CD1 PHE   318      12.208   4.615  28.063  1.00 17.88      BLGL
ATOM   2367  CD2 PHE   318      12.922   5.811  30.017  1.00 18.14      BLGL
ATOM   2368  CE1 PHE   318      11.041   5.383  28.007  1.00 15.40      BLGL
ATOM   2369  CE2 PHE   318      11.760   6.585  29.968  1.00 20.01      BLGL
ATOM   2370  CZ  PHE   318      10.815   6.367  28.960  1.00 16.53      BLGL
ATOM   2371  C   PHE   318      16.839   3.996  28.914  1.00 17.63      BLGL
ATOM   2372  O   PHE   318      17.132   2.802  28.878  1.00 19.56      BLGL
ATOM   2373  N   TYR   319      17.619   4.914  29.471  1.00 17.12      BLGL
ATOM   2374  CA  TYR   319      18.859   4.531  30.127  1.00 17.31      BLGL
ATOM   2375  CB  TYR   319      19.876   5.676  30.103  1.00 15.56      BLGL
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Fig. 4 cont.

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ATOM   2376  CG  TYR  319      21.255   5.211  30.495  1.00 17.60      BLGL
ATOM   2377  CD1 TYR  319      22.257   5.060  29.541  1.00 16.51      BLGL
ATOM   2378  CE1 TYR  319      23.503   4.568  29.886  1.00 17.94      BLGL
ATOM   2379  CD2 TYR  319      21.541   4.860  31.815  1.00 17.35      BLGL
ATOM   2380  CE2 TYR  319      22.781   4.366  32.174  1.00 18.20      BLGL
ATOM   2381  CZ  TYR  319      23.761   4.220  31.207  1.00 18.82      BLGL
ATOM   2382  OH  TYR  319      24.993   3.717  31.560  1.00 17.43      BLGL
ATOM   2383  C   TYR  319      18.465   4.214  31.568  1.00 15.84      BLGL
ATOM   2384  O   TYR  319      17.852   5.040  32.231  1.00 17.43      BLGL
ATOM   2385  N   TRP  320      18.811   3.024  32.050  1.00 15.86      BLGL
ATOM   2386  CA  TRP  320      18.448   2.622  33.408  1.00 14.37      BLGL
ATOM   2387  CB  TRP  320      18.286   1.099  33.489  1.00 13.03      BLGL
ATOM   2388  CG  TRP  320      17.673   0.644  34.786  1.00 13.67      BLGL
ATOM   2389  CD2 TRP  320      18.348  -0.001  35.873  1.00 13.63      BLGL
ATOM   2390  CE2 TRP  320      17.408  -0.123  36.930  1.00 16.14      BLGL
ATOM   2391  CE3 TRP  320      19.654  -0.480  36.063  1.00 12.95      BLGL
ATOM   2392  CD1 TRP  320      16.388   0.865  35.210  1.00 10.20      BLGL
ATOM   2393  NE1 TRP  320      16.225   0.413  36.491  1.00 11.94      BLGL
ATOM   2394  CZ2 TRP  320      17.736  -0.706  38.171  1.00 14.00      BLGL
ATOM   2395  CZ3 TRP  320      19.984  -1.057  37.292  1.00 14.81      BLGL
ATOM   2396  CH2 TRP  320      19.023  -1.163  38.332  1.00 15.77      BLGL
ATOM   2397  C   TRP  320      19.428   3.071  34.484  1.00 14.79      BLGL
ATOM   2398  O   TRP  320      20.624   2.786  34.403  1.00 13.40      BLGL
ATOM   2399  N   GLU  321      18.898   3.770  35.487  1.00 14.52      BLGL
ATOM   2400  CA  GLU  321      19.671   4.261  36.630  1.00 16.07      BLGL
ATOM   2401  CB  GLU  321      19.878   3.117  37.634  1.00 16.50      BLGL
ATOM   2402  CG  GLU  321      18.605   2.675  38.362  1.00 15.22      BLGL
ATOM   2403  CD  GLU  321      18.179   3.653  39.439  1.00 15.33      BLGL
ATOM   2404  OE1 GLU  321      17.190   3.375  40.156  1.00 13.74      BLGL
ATOM   2405  OE2 GLU  321      18.840   4.703  39.573  1.00 17.28      BLGL
ATOM   2406  C   GLU  321      21.015   4.890  36.267  1.00 16.30      BLGL
ATOM   2407  O   GLU  321      22.078   4.321  36.533  1.00 19.88      BLGL
ATOM   2408  N   PRO  322      20.985   6.085  35.664  1.00 13.95      BLGL
ATOM   2409  CD  PRO  322      19.800   6.807  35.166  1.00 13.71      BLGL
ATOM   2410  CA  PRO  322      22.207   6.776  35.269  1.00 13.32      BLGL
ATOM   2411  CB  PRO  322      21.727   7.665  34.136  1.00 13.68      BLGL
ATOM   2412  CG  PRO  322      20.397   8.108  34.648  1.00 11.78      BLGL
ATOM   2413  C   PRO  322      22.826   7.588  36.391  1.00 14.16      BLGL
ATOM   2414  O   PRO  322      23.849   8.235  36.191  1.00 17.47      BLGL
ATOM   2415  N   ALA  323      22.215   7.564  37.568  1.00 12.38      BLGL
ATOM   2416  CA  ALA  323      22.742   8.345  38.676  1.00 11.98      BLGL
ATOM   2417  CB  ALA  323      21.979   9.660  38.786  1.00  8.04      BLGL
ATOM   2418  C   ALA  323      22.736   7.619  40.012  1.00 12.24      BLGL
ATOM   2419  O   ALA  323      22.580   8.245  41.060  1.00 10.55      BLGL
ATOM   2420  N   TRP  324      22.910   6.300  39.980  1.00 14.35      BLGL
ATOM   2421  CA  TRP  324      22.933   5.515  41.215  1.00 15.62      BLGL
ATOM   2422  CB  TRP  324      22.422   4.094  40.973  1.00 15.22      BLGL
ATOM   2423  CG  TRP  324      21.843   3.473  42.201  1.00 16.28      BLGL
ATOM   2424  CD2 TRP  324      20.827   2.465  42.257  1.00 18.02      BLGL
ATOM   2425  CE2 TRP  324      20.595   2.181  43.622  1.00 18.70      BLGL
ATOM   2426  CE3 TRP  324      20.086   1.776  41.287  1.00 16.37      BLGL
ATOM   2427  CD1 TRP  324      22.178   3.748  43.494  1.00 17.37      BLGL
ATOM   2428  NE1 TRP  324      21.434   2.978  44.354  1.00 19.41      BLGL
ATOM   2429  CZ2 TRP  324      19.655   1.231  44.044  1.00 19.78      BLGL
ATOM   2430  CZ3 TRP  324      19.154   0.834  41.703  1.00 16.22      BLGL
ATOM   2431  CH2 TRP  324      18.944   0.570  43.071  1.00 18.68      BLGL
ATOM   2432  C   TRP  324      24.378   5.467  41.707  1.00 16.46      BLGL
ATOM   2433  O   TRP  324      24.986   4.405  41.823  1.00 13.25      BLGL
ATOM   2434  N   ILE  325      24.916   6.645  41.994  1.00 18.45      BLGL
ATOM   2435  CA  ILE  325      26.284   6.781  42.453  1.00 20.02      BLGL
ATOM   2436  CB  ILE  325      26.796   8.203  42.189  1.00 19.48      BLGL
ATOM   2437  CG2 ILE  325      26.652   8.518  40.706  1.00 18.33      BLGL
ATOM   2438  CG1 ILE  325      26.021   9.212  43.032  1.00 17.13      BLGL
ATOM   2439  CD1 ILE  325      26.493  10.630  42.843  1.00 14.92      BLGL
ATOM   2440  C   ILE  325      26.448   6.429  43.926  1.00 21.37      BLGL
ATOM   2441  O   ILE  325      25.473   6.373  44.675  1.00 20.25      BLGL
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Fig. 4 cont.

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ATOM   2442  N   PRO  326      27.697   6.188  44.358  1.00 22.85      BLGL
ATOM   2443  CD  PRO  326      28.935   6.258  43.557  1.00 21.92      BLGL
ATOM   2444  CA  PRO  326      27.988   5.827  45.750  1.00 23.11      BLGL
ATOM   2445  CB  PRO  326      29.488   5.535  45.724  1.00 21.79      BLGL
ATOM   2446  CG  PRO  326      29.992   6.401  44.613  1.00 23.00      BLGL
ATOM   2447  C   PRO  326      27.604   6.851  46.806  1.00 22.87      BLGL
ATOM   2448  O   PRO  326      27.666   8.055  46.564  1.00 22.51      BLGL
ATOM   2449  N   VAL  327      27.189   6.360  47.975  1.00 22.78      BLGL
ATOM   2450  CA  VAL  327      26.812   7.236  49.083  1.00 24.67      BLGL
ATOM   2451  CB  VAL  327      25.918   6.519  50.133  1.00 26.26      BLGL
ATOM   2452  CG1 VAL  327      24.651   5.996  49.478  1.00 27.07      BLGL
ATOM   2453  CG2 VAL  327      26.691   5.393  50.805  1.00 23.81      BLGL
ATOM   2454  C   VAL  327      28.072   7.697  49.798  1.00 25.35      BLGL
ATOM   2455  O   VAL  327      28.036   8.643  50.582  1.00 25.02      BLGL
ATOM   2456  N   GLY  328      29.176   7.007  49.516  1.00 26.68      BLGL
ATOM   2457  CA  GLY  328      30.459   7.315  50.120  1.00 27.54      BLGL
ATOM   2458  C   GLY  328      31.540   6.412  49.551  1.00 29.31      BLGL
ATOM   2459  O   GLY  328      31.219   5.392  48.938  1.00 29.16      BLGL
ATOM   2460  N   PRO  329      32.830   6.751  49.743  1.00 30.18      BLGL
ATOM   2461  CD  PRO  329      33.277   7.948  50.477  1.00 30.73      BLGL
ATOM   2462  CA  PRO  329      33.989   5.994  49.255  1.00 30.09      BLGL
ATOM   2463  CB  PRO  329      35.166   6.722  49.891  1.00 30.88      BLGL
ATOM   2464  CG  PRO  329      34.685   8.128  49.959  1.00 31.43      BLGL
ATOM   2465  C   PRO  329      33.966   4.520  49.614  1.00 29.93      BLGL
ATOM   2466  O   PRO  329      33.416   4.132  50.639  1.00 30.03      BLGL
ATOM   2467  N   ALA  330      34.582   3.706  48.768  1.00 29.86      BLGL
ATOM   2468  CA  ALA  330      34.614   2.272  48.987  1.00 32.93      BLGL
ATOM   2469  CB  ALA  330      35.343   1.585  47.833  1.00 31.50      BLGL
ATOM   2470  C   ALA  330      35.265   1.911  50.313  1.00 35.35      BLGL
ATOM   2471  O   ALA  330      34.894   0.916  50.940  1.00 35.56      BLGL
ATOM   2472  N   HIS  331      36.228   2.721  50.749  1.00 37.94      BLGL
ATOM   2473  CA  HIS  331      36.922   2.440  52.001  1.00 40.82      BLGL
ATOM   2474  CB  HIS  331      38.282   3.143  52.049  1.00 41.19      BLGL
ATOM   2475  CG  HIS  331      38.195   4.632  52.171  1.00 42.83      BLGL
ATOM   2476  CD2 HIS  331      38.170   5.436  53.261  1.00 42.69      BLGL
ATOM   2477  ND1 HIS  331      38.130   5.469  51.077  1.00 43.41      BLGL
ATOM   2478  CE1 HIS  331      38.073   6.725  51.488  1.00 42.26      BLGL
ATOM   2479  NE2 HIS  331      38.096   6.732  52.809  1.00 42.43      BLGL
ATOM   2480  C   HIS  331      36.130   2.805  53.254  1.00 42.32      BLGL
ATOM   2481  O   HIS  331      36.674   2.788  54.354  1.00 43.73      BLGL
ATOM   2482  N   ARG  332      34.857   3.149  53.105  1.00 43.54      BLGL
ATOM   2483  CA  ARG  332      34.041   3.478  54.264  1.00 43.67      BLGL
ATOM   2484  CB  ARG  332      33.446   4.878  54.152  1.00 46.16      BLGL
ATOM   2485  CG  ARG  332      34.428   6.031  54.232  1.00 51.93      BLGL
ATOM   2486  CD  ARG  332      33.693   7.258  54.754  1.00 55.92      BLGL
ATOM   2487  NE  ARG  332      32.323   7.299  54.240  1.00 62.04      BLGL
ATOM   2488  CZ  ARG  332      31.376   8.138  54.664  1.00 64.85      BLGL
ATOM   2489  NH1 ARG  332      30.154   8.095  54.132  1.00 64.81      BLGL
ATOM   2490  NH2 ARG  332      31.640   9.023  55.622  1.00 65.83      BLGL
ATOM   2491  C   ARG  332      32.899   2.482  54.368  1.00 43.46      BLGL
ATOM   2492  O   ARG  332      31.882   2.766  54.999  1.00 42.10      BLGL
ATOM   2493  N   LEU  333      33.077   1.318  53.748  1.00 43.54      BLGL
ATOM   2494  CA  LEU  333      32.058   0.277  53.739  1.00 44.90      BLGL
ATOM   2495  CB  LEU  333      32.700  -1.104  53.605  1.00 44.71      BLGL
ATOM   2496  CG  LEU  333      32.076  -1.981  52.511  1.00 47.14      BLGL
ATOM   2497  CD1 LEU  333      32.702  -3.370  52.561  1.00 47.53      BLGL
ATOM   2498  CD2 LEU  333      30.561  -2.068  52.691  1.00 46.62      BLGL
ATOM   2499  C   LEU  333      31.154   0.282  54.959  1.00 46.15      BLGL
ATOM   2500  O   LEU  333      29.931   0.378  54.833  1.00 47.20      BLGL
ATOM   2501  N   GLU  334      31.755   0.183  56.139  1.00 47.86      BLGL
ATOM   2502  CA  GLU  334      30.989   0.159  57.384  1.00 48.83      BLGL
ATOM   2503  CB  GLU  334      31.934   0.012  58.584  1.00 51.92      BLGL
ATOM   2504  CG  GLU  334      32.639  -1.345  58.641  1.00 58.71      BLGL
ATOM   2505  CD  GLU  334      31.663  -2.521  58.588  1.00 61.85      BLGL
ATOM   2506  OE1 GLU  334      30.824  -2.642  59.510  1.00 62.23      BLGL
ATOM   2507  OE2 GLU  334      31.734  -3.319  57.622  1.00 63.86      BLGL
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Fig. 4 cont.

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ATOM   2508  C   GLU   334      30.083   1.374  57.584  1.00 46.21      BLGL
ATOM   2509  O   GLU   334      28.939   1.246  58.030  1.00 45.37      BLGL
ATOM   2510  N   LYS   335      30.583   2.552  57.251  1.00 44.31      BLGL
ATOM   2511  CA  LYS   335      29.783   3.752  57.415  1.00 43.94      BLGL
ATOM   2512  CB  LYS   335      30.687   4.980  57.370  1.00 48.35      BLGL
ATOM   2513  CG  LYS   335      30.158   6.168  58.168  1.00 51.85      BLGL
ATOM   2514  CD  LYS   335      29.958   5.809  59.653  1.00 56.01      BLGL
ATOM   2515  CE  LYS   335      31.207   5.161  60.270  1.00 57.13      BLGL
ATOM   2516  NZ  LYS   335      32.440   5.982  60.078  1.00 58.45      BLGL
ATOM   2517  C   LYS   335      28.717   3.843  56.318  1.00 42.75      BLGL
ATOM   2518  O   LYS   335      27.664   4.458  56.508  1.00 40.92      BLGL
ATOM   2519  N   ASN   336      28.999   3.229  55.169  1.00 40.89      BLGL
ATOM   2520  CA  ASN   336      28.068   3.233  54.050  1.00 36.25      BLGL
ATOM   2521  CB  ASN   336      28.758   2.764  52.774  1.00 34.22      BLGL
ATOM   2522  CG  ASN   336      29.754   3.770  52.252  1.00 33.73      BLGL
ATOM   2523  OD1 ASN   336      29.698   4.949  52.593  1.00 33.95      BLGL
ATOM   2524  ND2 ASN   336      30.661   3.316  51.401  1.00 34.13      BLGL
ATOM   2525  C   ASN   336      26.883   2.332  54.333  1.00 35.83      BLGL
ATOM   2526  O   ASN   336      25.742   2.702  54.050  1.00 35.07      BLGL
ATOM   2527  N   LYS   337      27.161   1.147  54.882  1.00 34.86      BLGL
ATOM   2528  CA  LYS   337      26.116   0.171  55.209  1.00 33.18      BLGL
ATOM   2529  CB  LYS   337      26.712  -1.023  55.953  1.00 31.58      BLGL
ATOM   2530  CG  LYS   337      27.594  -1.901  55.095  1.00 32.46      BLGL
ATOM   2531  CD  LYS   337      28.112  -3.095  55.881  1.00 33.49      BLGL
ATOM   2532  CE  LYS   337      28.869  -4.046  54.967  1.00 38.20      BLGL
ATOM   2533  NZ  LYS   337      29.366  -5.262  55.679  1.00 41.08      BLGL
ATOM   2534  C   LYS   337      25.042   0.812  56.069  1.00 32.37      BLGL
ATOM   2535  O   LYS   337      23.866   0.477  55.971  1.00 30.10      BLGL
ATOM   2536  N   ALA   338      25.466   1.738  56.917  1.00 32.27      BLGL
ATOM   2537  CA  ALA   338      24.543   2.434  57.793  1.00 32.10      BLGL
ATOM   2538  CB  ALA   338      25.313   3.383  58.712  1.00 30.46      BLGL
ATOM   2539  C   ALA   338      23.533   3.211  56.951  1.00 31.53      BLGL
ATOM   2540  O   ALA   338      22.332   3.174  57.217  1.00 32.87      BLGL
ATOM   2541  N   LEU   339      24.025   3.915  55.937  1.00 29.75      BLGL
ATOM   2542  CA  LEU   339      23.165   4.703  55.064  1.00 28.75      BLGL
ATOM   2543  CB  LEU   339      24.019   5.580  54.149  1.00 29.58      BLGL
ATOM   2544  CG  LEU   339      24.839   6.671  54.842  1.00 29.29      BLGL
ATOM   2545  CD1 LEU   339      25.763   7.358  53.858  1.00 30.28      BLGL
ATOM   2546  CD2 LEU   339      23.889   7.674  55.457  1.00 30.12      BLGL
ATOM   2547  C   LEU   339      22.246   3.824  54.217  1.00 28.58      BLGL
ATOM   2548  O   LEU   339      21.035   4.049  54.154  1.00 28.13      BLGL
ATOM   2549  N   TRP   340      22.828   2.828  53.557  1.00 27.39      BLGL
ATOM   2550  CA  TRP   340      22.052   1.925  52.719  1.00 26.49      BLGL
ATOM   2551  CB  TRP   340      22.900   0.746  52.236  1.00 23.72      BLGL
ATOM   2552  CG  TRP   340      24.091  -1.114  51.444  1.00 22.86      BLGL
ATOM   2553  CD2 TRP   340      25.305   0.366  51.336  1.00 23.48      BLGL
ATOM   2554  CE2 TRP   340      26.154   1.077  50.458  1.00 23.45      BLGL
ATOM   2555  CE3 TRP   340      25.760  -0.839  51.895  1.00 23.20      BLGL
ATOM   2556  CD1 TRP   340      24.243   2.214  50.651  1.00 22.87      BLGL
ATOM   2557  NE1 TRP   340      25.480   2.200  50.056  1.00 22.68      BLGL
ATOM   2558  CZ2 TRP   340      27.437   0.626  50.123  1.00 23.93      BLGL
ATOM   2559  CZ3 TRP   340      27.036  -1.288  51.561  1.00 24.91      BLGL
ATOM   2560  CH2 TRP   340      27.859  -0.553  50.682  1.00 23.29      BLGL
ATOM   2561  C   TRP   340      20.891   1.359  53.505  1.00 26.35      BLGL
ATOM   2562  O   TRP   340      19.777   1.252  53.005  1.00 26.95      BLGL
ATOM   2563  N   GLU   341      21.179   0.990  54.743  1.00 27.03      BLGL
ATOM   2564  CA  GLU   341      20.206   0.383  55.629  1.00 27.61      BLGL
ATOM   2565  CB  GLU   341      20.939  -0.239  56.818  1.00 29.81      BLGL
ATOM   2566  CG  GLU   341      20.338  -1.534  57.345  1.00 32.17      BLGL
ATOM   2567  CD  GLU   341      20.490  -2.693  56.384  1.00 34.50      BLGL
ATOM   2568  OE1 GLU   341      20.087  -3.811  56.756  1.00 38.21      BLGL
ATOM   2569  OE2 GLU   341      21.003  -2.503  55.261  1.00 35.23      BLGL
ATOM   2570  C   GLU   341      19.150   1.366  56.112  1.00 27.16      BLGL
ATOM   2571  O   GLU   341      17.967   1.044  56.169  1.00 27.02      BLGL
ATOM   2572  N   THR   342      19.569   2.572  56.452  1.00 27.11      BLGL
ATOM   2573  CA  THR   342      18.624   3.562  56.940  1.00 27.99      BLGL
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Fig. 4 cont.

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ATOM   2574  CB  THR   342      19.356   4.706  57.658  1.00 27.99      BLGL
ATOM   2575  OG1 THR   342      20.097   4.174  58.759  1.00 29.52      BLGL
ATOM   2576  CG2 THR   342      18.365   5.731  58.173  1.00 28.27      BLGL
ATOM   2577  C   THR   342      17.732   4.169  55.860  1.00 27.72      BLGL
ATOM   2578  O   THR   342      16.527   4.283  56.047  1.00 27.61      BLGL
ATOM   2579  N   TYR   343      18.319   4.554  54.732  1.00 28.64      BLGL
ATOM   2580  CA  TYR   343      17.544   5.185  53.675  1.00 29.90      BLGL
ATOM   2581  CB  TYR   343      18.260   6.448  53.209  1.00 31.83      BLGL
ATOM   2582  CG  TYR   343      18.573   7.381  54.350  1.00 35.78      BLGL
ATOM   2583  CD1 TYR   343      19.798   7.313  55.013  1.00 36.95      BLGL
ATOM   2584  CE1 TYR   343      20.078   8.151  56.085  1.00 38.42      BLGL
ATOM   2585  CD2 TYR   343      17.631   8.313  54.792  1.00 35.14      BLGL
ATOM   2586  CE2 TYR   343      17.901   9.153  55.864  1.00 36.75      BLGL
ATOM   2587  CZ  TYR   343      19.128   9.067  56.503  1.00 38.36      BLGL
ATOM   2588  OH  TYR   343      19.417   9.904  57.554  1.00 40.88      BLGL
ATOM   2589  C   TYR   343      17.202   4.327  52.469  1.00 28.69      BLGL
ATOM   2590  O   TYR   343      16.524   4.788  51.554  1.00 28.30      BLGL
ATOM   2591  N   GLY   344      17.652   3.081  52.470  1.00 28.37      BLGL
ATOM   2592  CA  GLY   344      17.375   2.204  51.347  1.00 29.03      BLGL
ATOM   2593  C   GLY   344      18.001   2.730  50.068  1.00 28.56      BLGL
ATOM   2594  O   GLY   344      17.425   2.603  48.987  1.00 27.04      BLGL
ATOM   2595  N   SER   345      19.187   3.320  50.199  1.00 27.20      BLGL
ATOM   2596  CA  SER   345      19.903   3.888  49.067  1.00 25.65      BLGL
ATOM   2597  CB  SER   345      20.754   5.061  49.530  1.00 25.43      BLGL
ATOM   2598  OG  SER   345      21.600   4.654  50.582  1.00 31.71      BLGL
ATOM   2599  C   SER   345      20.780   2.853  48.380  1.00 25.28      BLGL
ATOM   2600  O   SER   345      21.554   3.183  47.479  1.00 24.47      BLGL
ATOM   2601  N   GLY   346      20.662   1.604  48.823  1.00 24.37      BLGL
ATOM   2602  CA  GLY   346      21.414   0.518  48.220  1.00 21.46      BLGL
ATOM   2603  C   GLY   346      20.430  -0.252  47.360  1.00 20.92      BLGL
ATOM   2604  O   GLY   346      19.286   0.183  47.216  1.00 21.35      BLGL
ATOM   2605  N   TRP   347      20.834  -1.385  46.795  1.00 18.57      BLGL
ATOM   2606  CA  TRP   347      19.915  -2.145  45.959  1.00 18.47      BLGL
ATOM   2607  CB  TRP   347      20.677  -3.115  45.057  1.00 19.55      BLGL
ATOM   2608  CG  TRP   347      20.976  -4.426  45.700  1.00 24.39      BLGL
ATOM   2609  CD2 TRP   347      20.205  -5.626  45.576  1.00 26.03      BLGL
ATOM   2610  CE2 TRP   347      20.843  -6.616  46.361  1.00 27.34      BLGL
ATOM   2611  CE3 TRP   347      19.035  -5.963  44.878  1.00 25.88      BLGL
ATOM   2612  CD1 TRP   347      22.023  -4.725  46.533  1.00 24.43      BLGL
ATOM   2613  NE1 TRP   347      21.950  -6.039  46.931  1.00 24.87      BLGL
ATOM   2614  CZ2 TRP   347      20.344  -7.926  46.467  1.00 27.61      BLGL
ATOM   2615  CZ3 TRP   347      18.541  -7.268  44.982  1.00 26.42      BLGL
ATOM   2616  CH2 TRP   347      19.195  -8.229  45.770  1.00 25.85      BLGL
ATOM   2617  C   TRP   347      18.910  -2.916  46.807  1.00 17.94      BLGL
ATOM   2618  O   TRP   347      17.820  -3.255  46.347  1.00 16.07      BLGL
ATOM   2619  N   ALA   348      19.296  -3.197  48.047  1.00 19.28      BLGL
ATOM   2620  CA  ALA   348      18.444  -3.918  48.984  1.00 21.94      BLGL
ATOM   2621  CB  ALA   348      18.387  -5.394  48.607  1.00 20.51      BLGL
ATOM   2622  C   ALA   348      18.948  -3.767  50.422  1.00 24.22      BLGL
ATOM   2623  O   ALA   348      20.138  -3.549  50.659  1.00 25.24      BLGL
ATOM   2624  N   THR   349      18.030  -3.870  51.379  1.00 25.44      BLGL
ATOM   2625  CA  THR   349      18.378  -3.774  52.789  1.00 25.50      BLGL
ATOM   2626  CB  THR   349      17.509  -2.738  53.553  1.00 26.44      BLGL
ATOM   2627  OG1 THR   349      16.167  -3.228  53.679  1.00 25.28      BLGL
ATOM   2628  CG2 THR   349      17.500  -1.400  52.823  1.00 24.16      BLGL
ATOM   2629  C   THR   349      18.102  -5.139  53.383  1.00 26.30      BLGL
ATOM   2630  O   THR   349      17.382  -5.942  52.791  1.00 26.26      BLGL
ATOM   2631  N   SER   350      18.671  -5.403  54.551  1.00 27.06      BLGL
ATOM   2632  CA  SER   350      18.463  -6.685  55.208  1.00 26.38      BLGL
ATOM   2633  CB  SER   350      19.252  -6.738  56.514  1.00 23.71      BLGL
ATOM   2634  OG  SER   350      18.812  -5.726  57.400  1.00 21.01      BLGL
ATOM   2635  C   SER   350      16.975  -6.911  55.490  1.00 26.83      BLGL
ATOM   2636  O   SER   350      16.509  -8.046  55.520  1.00 26.17      BLGL
ATOM   2637  N   TYR   351      16.225  -5.830  55.683  1.00 28.04      BLGL
ATOM   2638  CA  TYR   351      14.796  -5.946  55.965  1.00 30.41      BLGL
ATOM   2639  CB  TYR   351      14.208  -4.566  56.244  1.00 32.17      BLGL
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Fig. 4 cont.

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ATOM   2640  CG  TYR   351      14.911  -3.829  57.352  1.00 33.63      BLGL
ATOM   2641  CD1 TYR   351      15.961  -2.951  57.083  1.00 35.43      BLGL
ATOM   2642  CE1 TYR   351      16.623  -2.279  58.114  1.00 35.75      BLGL
ATOM   2643  CD2 TYR   351      14.539  -4.020  58.677  1.00 35.69      BLGL
ATOM   2644  CE2 TYR   351      15.193  -3.355  59.717  1.00 36.21      BLGL
ATOM   2645  CZ  TYR   351      16.231  -2.488  59.427  1.00 35.60      BLGL
ATOM   2646  OH  TYR   351      16.865  -1.828  60.451  1.00 36.59      BLGL
ATOM   2647  C   TYR   351      14.012  -6.626  54.836  1.00 30.90      BLGL
ATOM   2648  O   TYR   351      12.921  -7.159  55.055  1.00 30.86      BLGL
ATOM   2649  N   ALA   352      14.572  -6.604  53.633  1.00 30.77      BLGL
ATOM   2650  CA  ALA   352      13.936  -7.220  52.476  1.00 31.75      BLGL
ATOM   2651  CB  ALA   352      14.611  -6.744  51.202  1.00 30.75      BLGL
ATOM   2652  C   ALA   352      13.989  -8.745  52.545  1.00 33.29      BLGL
ATOM   2653  O   ALA   352      13.411  -9.434  51.700  1.00 33.71      BLGL
ATOM   2654  N   ALA   353      14.680  -9.273  53.549  1.00 33.30      BLGL
ATOM   2655  CA  ALA   353      14.804 -10.718  53.706  1.00 33.02      BLGL
ATOM   2656  CB  ALA   353      15.687 -11.033  54.908  1.00 34.24      BLGL
ATOM   2657  C   ALA   353      13.449 -11.409  53.856  1.00 32.34      BLGL
ATOM   2658  O   ALA   353      13.270 -12.545  53.422  1.00 30.15      BLGL
ATOM   2659  N   GLU   354      12.496 -10.716  54.466  1.00 33.65      BLGL
ATOM   2660  CA  GLU   354      11.176 -11.284  54.668  1.00 35.34      BLGL
ATOM   2661  CB  GLU   354      10.345 -10.375  55.578  1.00 35.98      BLGL
ATOM   2662  CG  GLU   354       9.744  -9.163  54.894  1.00 37.66      BLGL
ATOM   2663  CD  GLU   354       8.831  -8.378  55.818  1.00 40.92      BLGL
ATOM   2664  OE1 GLU   354       8.010  -7.584  55.310  1.00 42.14      BLGL
ATOM   2665  OE2 GLU   354       8.935  -8.548  57.055  1.00 41.70      BLGL
ATOM   2666  C   GLU   354      10.437 -11.503  53.343  1.00 36.54      BLGL
ATOM   2667  O   GLU   354       9.614 -12.416  53.228  1.00 36.40      BLGL
ATOM   2668  N   TYR   355      10.735 -10.673  52.345  1.00 36.32      BLGL
ATOM   2669  CA  TYR   355      10.072 -10.778  51.046  1.00 35.27      BLGL
ATOM   2670  CB  TYR   355       9.800  -9.381  50.496  1.00 32.38      BLGL
ATOM   2671  CG  TYR   355       8.715  -9.339  49.445  1.00 32.93      BLGL
ATOM   2672  CD1 TYR   355       9.022  -9.211  48.087  1.00 31.94      BLGL
ATOM   2673  CE1 TYR   355       8.014  -9.141  47.126  1.00 30.60      BLGL
ATOM   2674  CD2 TYR   355       7.372  -9.403  49.812  1.00 31.34      BLGL
ATOM   2675  CE2 TYR   355       6.364  -9.333  48.864  1.00 31.48      BLGL
ATOM   2676  CZ  TYR   355       6.688  -9.198  47.524  1.00 32.10      BLGL
ATOM   2677  OH  TYR   355       5.679  -9.084  46.593  1.00 32.53      BLGL
ATOM   2678  C   TYR   355      10.873 -11.590  50.034  1.00 36.46      BLGL
ATOM   2679  O   TYR   355      10.306 -12.262  49.177  1.00 33.16      BLGL
ATOM   2680  N   ASP   356      12.196 -11.513  50.133  1.00 39.53      BLGL
ATOM   2681  CA  ASP   356      13.079 -12.251  49.241  1.00 42.86      BLGL
ATOM   2682  CB  ASP   356      13.568 -11.355  48.096  1.00 43.64      BLGL
ATOM   2683  CG  ASP   356      14.568 -12.064  47.182  1.00 44.35      BLGL
ATOM   2684  OD1 ASP   356      15.202 -11.382  46.349  1.00 42.98      BLGL
ATOM   2685  OD2 ASP   356      14.715 -13.303  47.293  1.00 45.31      BLGL
ATOM   2686  C   ASP   356      14.278 -12.741  50.045  1.00 45.45      BLGL
ATOM   2687  O   ASP   356      15.302 -12.058  50.133  1.00 47.13      BLGL
ATOM   2688  N   PRO   357      14.165 -13.931  50.650  1.00 46.19      BLGL
ATOM   2689  CD  PRO   357      12.983 -14.810  50.688  1.00 45.78      BLGL
ATOM   2690  CA  PRO   357      15.260 -14.493  51.447  1.00 46.80      BLGL
ATOM   2691  CB  PRO   357      14.578 -15.627  52.196  1.00 46.98      BLGL
ATOM   2692  CG  PRO   357      13.567 -16.109  51.196  1.00 46.25      BLGL
ATOM   2693  C   PRO   357      16.412 -14.990  50.581  1.00 48.11      BLGL
ATOM   2694  O   PRO   357      17.562 -15.006  51.007  1.00 48.32      BLGL
ATOM   2695  N   GLU   358      16.075 -15.381  49.358  1.00 49.36      BLGL
ATOM   2696  CA  GLU   358      17.019 -15.911  48.385  1.00 51.27      BLGL
ATOM   2697  CB  GLU   358      16.257 -16.304  47.125  1.00 53.72      BLGL
ATOM   2698  CG  GLU   358      15.040 -17.170  47.389  1.00 58.04      BLGL
ATOM   2699  CD  GLU   358      15.414 -18.587  47.774  1.00 62.05      BLGL
ATOM   2700  OE1 GLU   358      15.886 -19.331  46.886  1.00 63.62      BLGL
ATOM   2701  OE2 GLU   358      15.244 -18.955  48.961  1.00 64.62      BLGL
ATOM   2702  C   GLU   358      18.142 -14.958  47.995  1.00 52.75      BLGL
ATOM   2703  O   GLU   358      19.319 -15.232  48.240  1.00 53.92      BLGL
ATOM   2704  N   ASP   359      17.768 -13.850  47.366  1.00 53.56      BLGL
ATOM   2705  CA  ASP   359      18.717 -12.847  46.902  1.00 53.46      BLGL
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Fig. 4 cont.