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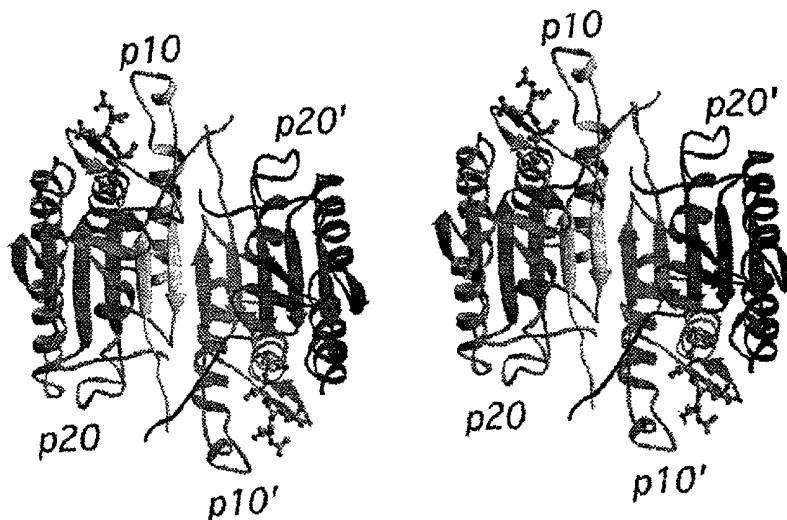
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(54) Title: CRYSTALLIZABLE COMPOSITIONS COMPRISING A CASPASE-7



(57) **Abstract:** The present invention relates to a data storage medium encoded with the structural coordinates of crystallized molecules and molecular complexes which comprise the active site binding pockets of caspase-7. Such data storage material is capable of displaying such molecules and molecular complexes, or their structural homologues, as a graphical three-dimensional representation on a computer screen. This invention also relates to methods of using the structure coordinates to solve the structure of similar or homologous proteins or protein complexes. In addition, this invention relates to methods of using the structure coordinates to screen and design compounds, including inhibitory compounds, that bind to caspase-7 or homologues thereof. This invention also relates to molecules or molecular complexes which comprise the active site binding pockets of caspase-7 or close structural homologues of the active site binding pockets. The present invention also relates to compositions and crystals of a caspase-7 in complex with a caspase inhibitor. This invention also relates to compounds and pharmaceutical compositions which are inhibitors of caspase-7.



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CRYSTALLIZABLE COMPOSITIONS COMPRISING
A CASPASE-7

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TECHNICAL FIELD OF INVENTION

The present invention relates to a data storage medium encoded with the structural coordinates of crystallized molecules and molecular complexes which
10 comprise the active site binding pockets of caspase-7. Such data storage material is capable of displaying such molecules and molecular complexes, or their structural homologues, as a graphical three-dimensional representation on a computer screen. This invention
15 also related to methods of using the structure coordinates to solve the structure of similar or homologous proteins or protein complexes. In addition, this invention relates to methods of using the structure coordinates to screen and design compounds,
20 including inhibitory compounds, that bind to caspase-7 or homologues thereof. This invention also relates to molecules or molecular complexes which comprise the active site binding pockets of caspase-7 or close structural homologues of the active site binding
25 pockets. The present invention also relates to compositions and crystals of a caspase-7 in complex with a caspase inhibitor.

BACKGROUND OF THE INVENTION

Apoptosis, or programmed cell death, is a
30 principal mechanism by which organisms eliminate unwanted cells. The deregulation of apoptosis, either excessive apoptosis or the failure to undergo it, has been implicated in a number of diseases such as cancer,

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acute inflammatory and autoimmune disorders, ischemic diseases and certain neurodegenerative disorders [see generally Science, 281, pp. 1283-1312 (1998); Ellis et al., Ann. Rev. Cell. Biol., 7, p. 663 (1991)].

5 Caspases are a family of cysteine protease enzymes that are key mediators in the signaling pathways for apoptosis and cell disassembly [N.A. Thornberry, Chem. Biol., 5, pp. R97-R103 (1998)]. These signaling pathways vary depending on cell type
10 and stimulus, but all apoptosis pathways appear to converge at a common effector pathway leading to proteolysis of key proteins. Caspases are involved in both the effector phase of the signaling pathway and further upstream at its initiation. The upstream
15 caspases involved in initiation events become activated and in turn activate other caspases that are involved in the later phases of apoptosis.

 The caspases have been classified into three groups depending on their predominant functional roles
20 and their substrate specificities [N.A. Thornberry, Chem. Biol., 5, pp. R97-R103 (1998); N.A. Thornberry & Y. Lazebnik, Science, 281, pp. 1312-1316 (1998); M. Garcia-Calvo et al., J. Biol. Chem., 273, pp. 32608-32613 (1998)].

25 The first subfamily consists of caspases-1 (ICE), 4, and 5. These caspases have been shown to be involved in pro-inflammatory cytokine processing and therefore play an important role in inflammation. Caspase-1, the most studied enzyme of this class,
30 activates the IL-1 β precursor by proteolytic cleavage. This enzyme therefore plays a key role in the inflammatory response. Caspase-1 is also involved in the processing of interferon gamma inducing factor

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(IGIF or IL-18) which stimulates the production of interferon gamma, a key immunoregulator that modulates antigen presentation, T-cell activation and cell adhesion.

5 The remaining caspases make up the second and third subfamilies. These enzymes are of central importance in the intracellular signaling pathways leading to apoptosis. One subfamily consists of the enzymes involved in initiating events in the apoptotic
10 pathway, including transduction of signals from the plasma membrane. Members of this subfamily include caspases-2, 8, 9, and 10. The other subfamily, consisting of the effector caspases 3, 6, and 7, are involved in the final downstream cleavage events that
15 result in the systematic breakdown and death of the cell by apoptosis. Caspases involved in the upstream signal transduction activate the downstream caspases, which then disable DNA repair mechanisms, fragment DNA, dismantle the cell cytoskeleton and finally fragment
20 the cell.

 The utility of caspase inhibitors to treat a variety of mammalian disease states associated with an increase in cellular apoptosis has been demonstrated using peptidic caspase inhibitors. For example, in
25 rodent models, caspase inhibitors have been shown to reduce infarct size and inhibit cardiomyocyte apoptosis after myocardial infarction, to reduce lesion volume and neurological deficit resulting from stroke, to reduce post-traumatic apoptosis and neurological
30 deficit in traumatic brain injury, to be effective in treating fulminant liver destruction, and to improve survival after endotoxic shock [H. Yaoita et al., Circulation, 97, pp. 276-281 (1998); M. Endres et al.,

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J. Cerebral Blood Flow and Metabolism, 18, pp. 238-247, (1998); Y. Cheng et al., J. Clin. Invest., 101, pp. 1992-1999 (1998); A.G. Yakovlev et al., J. Neurosci., 17, pp. 7415-7424 (1997); I. Rodriquez et al., J. Exp. Med., 184, pp. 2067-2072 (1996); Grobmyer et al., Mol. Med., 5, p. 585 (1999)].

Caspase-7 is considered a potential target for therapeutic agents. The current understanding of caspase-7 has not however led to satisfactory treatments for caspase-7 mediated disease. Thus, there is a need for more effective caspase-7 inhibitors. There is also a need for inhibitors that either inhibit caspase-7 selectively or inhibit caspase-7 as well as other caspases.

Drug discovery efforts directed towards caspase-7 have been hampered by the lack of structural information about caspase-7. Such structural information would be valuable in the discovery of selective caspase-7 inhibitors and pan-caspase inhibitors. However, efforts to determine the structure of caspase-7 have been hampered by difficulties in crystallizing caspase-7. There have been no crystals reported of a caspase-7 protein. Thus, x-ray crystallographic analysis of such proteins has not been possible.

SUMMARY OF THE INVENTION

Applicants have solved this problem by providing, for the first time, the crystallization of a caspase-7 in complex with a caspase-7 inhibitor and the structure coordinates of that complex. Solving the three-dimensional crystal structure of that complex has allowed applicants to determine key structural features

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of caspase-7, particularly the shape of its active site binding pockets.

Thus, the present invention provides molecules or molecular complexes that comprise all or parts of these binding pockets, or homologues of these binding pockets that have similar three-dimensional shapes.

The present invention relates to a data storage medium that comprises the structural coordinates of crystallized molecules and molecular complexes which comprise caspase-7, including all or any parts of the caspase-7 active site binding pockets. The data storage medium is capable of displaying the molecules and molecular complexes, or their structural homologues, as a graphical three-dimensional representation on a computer screen.

The invention also provides a method for determining at least a portion of the three-dimensional structure of molecules or molecular complexes which contain at least some structurally similar features to a caspase-7. This is achieved by using at least some of the structure coordinates obtained for caspase-7.

In addition, this invention relates to methods of using the structure coordinates to screen and design compounds, including inhibitory compounds, that bind to caspase-7 or homologues thereof.

The invention also provides crystallizable compositions and crystals of a caspase-7/inhibitor complex and methods for making such crystals.

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BRIEF DESCRIPTION OF THE FIGURES

FIGS. 1A and 1B depict a stereoview of a caspase-7 tetrameric assembly made using RIBBONS [M. Carson, J. Appl. Cryst., 24, pp. 958-961 (1991)]. The p20, p10 and their symmetry related equivalents, p20' and p10', are shown moving from left to right in each of FIG. 1A and FIG. 1B. The ball-and-stick model, near the top left of each FIG., represents the Ac-DEVD-CHO inhibitor.

FIGS. 2A, 2B, and 2C depict secondary structural elements of caspase-1, caspase-3, caspase-7, and caspase-8.

FIG. 2A depicts the conserved fold for superimposed Caspase-1, Caspase-3, Caspase-7, Caspase-8 with covalently bound tetrapeptide inhibitor, Ac-DEVD-CHO.

FIG. 2B depicts superimposed S4 loops for caspase-1 (378-386), caspase-3 (244-262), caspase-7 (270-288), and caspase-8 (451-463).

FIG. 2C depicts prime side helix-turn-helix insertion in caspase-8 ranging from residues 245-253 proximal to superimposed insertion loop of caspase-1 (residues 249-254). FIG. 2B and FIG. 2C have been rotated slightly relative to FIG. 2A.

FIG. 3 depicts the sequence alignment of caspase-1, caspase-3, caspase-7, and caspase-8. The alignment was heavily biased upon the superposition of conserved secondary structural elements and active site residues of caspase-1, caspase-3, caspase-7, and caspase-8. The alignment was performed with the MVP program and then adjusted manually [M.H. Lambert, Pract. Appl. Comput.-Aided Drug Des., pp. 243-303, P.S. Charifson, ed., Dekker, New York. (1997)]. Boxed

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residues denote direct or water-mediated interactions with Ac-DEVD-CHO as shown in FIG. 4.

FIG. 4 depicts hydrogen bonding and van der Waals interactions of covalently bound Ac-DEVD-thiohemiacetal with binding site residues of: a) caspase-1; b) caspase-3; c) caspase-7; and d) caspase-8. "Wat" indicates a water molecule.

FIG. 5A-5D depicts electrostatic potentials mapped onto molecular surface for binding site residues of caspase-1, caspase-3, caspase-7, and caspase-8. Areas of positive electrostatic potential, negative electrostatic potential, and neutral electrostatic potential are depicted. The molecular surface and electrostatic potentials calculated with GRASP [A. Nicholls et al., Proteins: Structure Function, Genetics, 11, pp. 281-296 (1991)].

FIG. 6 depicts a stereoview diagram showing the superposition of caspase-3 with caspase-7 generated by RIBBONS. The N-acetyl group of the tetrapeptide inhibitor, Ac-DEVD-CHO, bound to caspase-7 is translated approximately 2.5 Å relative to that in caspase-3 due to the substitution of proline (235) for serine at the same position of the P4-binding site.

FIG. 7 lists the atomic structure coordinates for caspase-7 in complex with a synthetic tetrapeptide inhibitor as derived by X-ray diffraction from a crystal of that complex. The preparation of the complex is described in Examples 1 and 2. The following abbreviations are used in FIG. 7:

"Atom type" refers to the element whose coordinates have been determined. Elements are defined by the first letter in the column.

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"X, Y, Z" crystallographically define the atomic position determined for each atom.

"Occ" is an occupancy factor that refers to the fraction of the molecules in which each atom occupies the position specified by the coordinates. A value of "1" indicates that each atom has the same conformation, i.e., the same position, in all molecules of the crystal.

"B" is a thermal factor that measures movement of the atom around its atomic center.

FIG. 8 shows a diagram of a system used to carry out the instructions encoded by the storage medium of FIGS. 9 and 10.

FIG. 9 shows a cross section of a magnetic storage medium.

FIG. 10 shows a cross section of an optically-readable data storage medium.

DETAILED DESCRIPTION OF THE INVENTION

The following abbreviations are used throughout the application:

A = Ala = Alanine	T = Thr = Threonine
V = Val = Valine	C = Cys = Cysteine
L = Leu = Leucine	Y = Tyr = Tyrosine
I = Ile = Isoleucine	N = Asn = Asparagine
P = Pro = Proline	Q = Gln = Glutamine
F = Phe = Phenylalanine	D = Asp = Aspartic Acid
W = Trp = Tryptophan	E = Glu = Glutamic Acid
M = Met = Methionine	K = Lys = Lysine
G = Gly = Glycine	R = Arg = Arginine
S = Ser = Serine	H = His = Histidine

Additional definitions are set forth in the specification where necessary.

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In order that the invention described herein may be more fully understood, the following detailed description is set forth.

Applicants have solved the above problems by providing, for the first time, crystallizable compositions comprising a caspase-7 in complex with a caspase-7 inhibitor.

Thus, in one embodiment of this invention is provided a crystallizable composition comprising a caspase-7 in complex with a tetrapeptide aldehyde inhibitor, acetyl-Asp-Glu-Val-Asp-CHO (Ac-DEVD-CHO). Preferably, the caspase-7 has amino acids 1-303 according to Y. Gu et al., J. Biol. Chem., 271, pp. 10816-10820 (1996).

The caspase-7 polypeptide portion of the complex is any polypeptide which has the cysteine protease activity of the naturally occurring caspase-7.

Preferably, the caspase-7 polypeptide in the compositions of this invention is the recombinantly produced caspase-7 protein that is prepared as described herein.

The caspase-7 polypeptide and Ac-DEVD-CHO may be produced by any well-known method, including synthetic methods, such as solid phase, liquid phase and combination solid phase/liquid phase syntheses; recombinant DNA methods, including cDNA cloning, optionally combined with site directed mutagenesis; and/or purification of the natural products, optionally combined with enzymatic cleavage methods to produce fragments of naturally occurring caspase-7 polypeptide. The inhibitor Ac-DEVD-CHO is commercially available (Peptides International) or may be produced by any well-known method, including synthetic methods, such as

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solid phase, liquid phase and combination solid phase/liquid phase syntheses.

In another embodiment of this invention is provided a crystal comprising a caspase-7 in complex
5 with a tetrapeptide aldehyde inhibitor, acetyl-Asp-Glu-Val-Asp-CHO (Ac-DEVD-CHO). Preferably, the caspase-7 has amino acids 1-303 according to Y. Gu et al., J. Biol. Chem., 271, pp. 10816-10820 (1996). Preferably,
the crystal has unit cell dimensions of 88.2 Å, 88.2 Å,
10 186.2 Å, $\alpha=90.0^\circ$, $\beta=90.0^\circ$, $\gamma=120.0^\circ$ and belongs to space group P₃221. More preferably, the crystallized enzyme is a tetramer.

Importantly, applicants' invention has provided, for the first time, information about the
15 shape and structure of the caspase-7 active site binding pockets.

Binding pockets are of significant utility in fields such as drug discovery. The association of natural ligands or substrates with the binding pockets
20 of their corresponding receptors or enzymes is the basis of many biological mechanisms of action. Similarly, many drugs exert their biological effects through association with the binding pockets of receptors and enzymes. Such associations may occur
25 with all or any parts of the binding pocket. An understanding of such associations will help lead to the design of drugs having more favorable associations with their target receptor or enzyme, and thus, improved biological effects. Therefore, this
30 information is valuable in designing potential inhibitors of caspase-7-like binding pockets.

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The term "binding pocket", as used herein, refers to a region of a molecule or molecular complex, that, as a result of its shape, favorably associates with another chemical entity or compound.

5 The term "caspase-7-like binding pocket" refers to a portion of a molecule or molecular complex whose shape is sufficiently similar to all or any parts of the caspase-7 active site binding pockets as to bind common ligands. This commonality of shape is defined
10 by a root mean square deviation from the structure coordinates of the backbone atoms of the amino acids that make up the binding pockets in caspase-7 (as set forth in Figure 1) of not more than 1.5 Å. How this calculation is obtained is described below.

15 The "active site binding pockets" or "active site" of caspase-7 refers to the area on the caspase-7 enzyme surface where cleavage of a substrate occurs, and where Ac-DEVD-CHO exerts its inhibitory effect.

 The terms "P binding pocket", "S pocket" "S
20 region" and the like, refer to binding subsites, or portions of the substrate binding site on the caspase molecule. The amino acid residues of the substrate are given designations according to their position relative to the scissile bond, i.e., the bond that is broken by
25 the protease. The residues are designated P1, P2, etc., for those extending toward the N-terminus of the substrate and P1', P2', etc., for those extending toward the C-terminus of the substrate. The portions of an inhibitor that correspond to the P or P' residues
30 of the substrate are also labeled P1, P1', etc., by analogy with the substrate. The binding subsites of the caspase molecule that receive the residues labeled P1, P1', etc., are designated S1, S1', etc., or may

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alternately be designated "the P1 binding pocket", "the P1' binding pocket", etc. [I. Schechter & A. Berger, Biochem. Biophys. Res. Communi., 27, pp. 157-162 (1967)].

5 In resolving the crystal structure of caspase-7, applicants have determined that caspase-7 amino acids 234, 235, 237, 276, 278, 281, and 284 are responsible for the S4-binding region of caspase-7 being more hydrophilic than the S4-binding region of
10 caspase-3. Applicants have also determined that amino acids 85, 86, 87, 88, 144, 145, 184, 186, 191, 223, 230, 231, 232, 233, 234, 235, 237, 240, 276, 278, 281, 282, and 284 are situated close enough to the Ac-DEVD-CHO inhibitor to interact with this ligand.

15 Applicants have also determined that amino acid residues 87, 184, and 233 are important in the P1 binding pocket of caspase-7; that amino acid residues 191, 230, 232, and 282 are important in the P2 binding pocket of caspase-7; that amino acid residues 86, 88,
20 233 are important in the P3 binding pocket of caspase-7; and that amino acid residues 234, 235, 237, 240, and 276 are important in the P3 binding pocket of caspase-7.

25 It will be readily apparent to those of skill in the art that the numbering of amino acids in other isoforms of caspase-7 may be different than that described herein.

30 Advantageously, the crystal provided by this invention is amenable to x-ray crystallography. Thus, this invention also provides the three-dimensional structure of a caspase-7 complex, specifically a caspase-7/Ac-DEVD-CHO complex, at 2.35 Å resolution.

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Importantly, this has provided for the first time, information about the shape and structure of caspase-7.

The three-dimensional structure of the caspase-7/inhibitor complex of this invention is defined by a set of structure coordinates as set forth in FIG. 7. The term "structure coordinates" refers to Cartesian coordinates derived from mathematical equations related to the patterns obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of a caspase-7/inhibitor complex in crystal form. The diffraction data are used to calculate an electron density map of the repeating unit of the crystal. The electron density maps are then used to establish the positions of the individual atoms of the caspase-7 or caspase-7/inhibitor complex.

Those of skill in the art will understand that a set of structure coordinates for an enzyme or an enzyme-complex or a portion thereof, is a relative set of points that define a shape in three dimensions. Thus, it is possible that an entirely different set of coordinates could define a similar or identical shape. Moreover, slight variations in the individual coordinates will have little effect on overall shape.

The variations in coordinates discussed above may be generated because of mathematical manipulations of the structure coordinates. For example, the structure coordinates set forth in FIG. 7 could be manipulated by crystallographic permutations of the structure coordinates, fractionalization of the structure coordinates, integer additions or subtractions to sets of the structure coordinates, inversion of the structure coordinates or any combination of the above.

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Alternatively, modifications in the crystal structure due to mutations, additions, substitutions, and/or deletions of amino acids, or other changes in any of the components that make up the crystal could also account for variations in structure coordinates. If such variations are within an acceptable standard error as compared to the original coordinates, the resulting three-dimensional shape is considered to be the same.

Various computational analyses are therefore necessary to determine whether a molecule or molecular complex or a portion thereof is sufficiently similar to all or parts of the caspase-7/inhibitor structure described above as to be considered the same. Such analyses may be carried out in current software applications, such as the Molecular Similarity application of QUANTA (Molecular Simulations Inc., San Diego, CA) version 4.1, and as described in the accompanying User's Guide.

The Molecular Similarity application permits comparisons between different structures, different conformations of the same structure, and different parts of the same structure. The procedure used in Molecular Similarity to compare structures is divided into four steps: 1) load the structures to be compared; 2) define the atom equivalencies in these structures; 3) perform a fitting operation; and 4) analyze the results.

Each structure is identified by a name. One structure is identified as the target (i.e., the fixed structure); all remaining structures are working structures (i.e., moving structures). Since atom equivalency within QUANTA is defined by user input, for

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the purpose of this invention we will define equivalent atoms as protein backbone atoms (N, C α , C and O) for all conserved residues between the two structures being compared. We will also consider only rigid fitting operations.

When a rigid fitting method is used, the working structure is translated and rotated to obtain an optimum fit with the target structure. The fitting operation uses an algorithm that computes the optimum translation and rotation to be applied to the moving structure, such that the root mean square difference of the fit over the specified pairs of equivalent atom is an absolute minimum. This number, given in angstroms, is reported by QUANTA.

For the purpose of this invention, any molecule or molecular complex that has a root mean square deviation of conserved residue backbone atoms (N, C α , C, O) of less than 1.5 Å when superimposed on the relevant backbone atoms described by structure coordinates listed in FIG. 7 are considered identical. More preferably, the root mean square deviation is less than 1.0 Å.

The term "root mean square deviation" means the square root of the arithmetic mean of the squares of the deviations from the mean. It is a way to express the deviation or variation from a trend or object. For purposes of this invention, the "root mean square deviation" defines the variation in the backbone of a protein or protein complex from the relevant portion of the backbone of the caspase-7 polypeptide portion of the complex as defined by the structure coordinates described herein.

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Once the structure coordinates of a protein crystal have been determined they are useful variety of purposes, such as drug discovery and x-ray crystallographic determinations of related proteins.

5 Thus, in accordance with the present invention, the structure coordinates of a caspase-7 polypeptide/inhibitor complex, and portions thereof is provided. Such data may be used for the purposes of, for example, drug design and molecular replacement.

10 Accordingly, one embodiment of this invention provides a molecule or molecular complex comprising all or any part of a binding pocket defined by structure coordinates of caspase-7 amino acids 234, 235, 237, 276, 278, 281, and 284 according to FIG. 7, or a
15 homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, and wherein said molecule or molecular complex has a S4
20 binding region that is more hydrophilic than the S4 binding region of caspase-3.

 Another embodiment of this invention provides a molecule or molecular complex comprising all or any part of a binding pocket defined by structure
25 coordinates of caspase-7 amino acids 85, 86, 87, 88, 144, 145, 184, 186, 191, 223, 230, 231, 232, 233, 234, 235, 237, 240, 276, 278, 281, 282, and 284 or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that
30 has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, and wherein said molecule or molecular complex has a S4

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binding region that is more hydrophilic than the S4 binding region of caspase-3.

Yet another embodiment of this invention provides a molecule or molecular complex defined by all or part of the structure coordinates according to FIG. 7, or a homologue thereof, wherein said homologue has a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.5 Å, and wherein said molecule or molecular complex has a S4 binding region that is more hydrophilic than the S4 binding region of caspase-3. Preferably, a molecule or molecular complex is defined by all of the structure coordinates according to FIG. 7 or a homologue thereof.

Yet another embodiment of this invention provides a molecule or molecular complex defined by all or part of the structure coordinates of caspase-7 amino acids 58-302 according to FIG. 7, or a homologue thereof, wherein said homologue has a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.5 Å, and wherein said molecule or molecular complex has a S4 binding region that is more hydrophilic than the S4 binding region of caspase-3. Preferably, the molecule or molecular complex is defined by all of the structure coordinates of caspase-7 amino acids 58-302 according to FIG. 7 or a homologue thereof.

Preferably, in any of these embodiments, the homologue has a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.0 Å.

In a more preferred embodiment, the molecule or molecular complex is defined by the structure

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coordinates of caspase-7 amino acids 58-302 according to FIG. 7.

This invention also provides a machine-readable data storage medium, comprising a data storage material encoded with machine readable data, wherein
5 said data is defined by the all or a portion of the structure coordinates of a caspase-7 complex according to FIG. 7, or a homologue of said complex, wherein said homologue comprises backbone atoms that have a root
10 mean square deviation from the backbone atoms of the complex of not more than 1.5 Å.

Preferably, the data is defined by the structure coordinates of caspase-7 amino acids 234, 235, 237, 276, 278, 281, and 284 according to FIG. 7,
15 or a homologue of said complex, wherein said homologue comprises backbone atoms that have a root mean square deviation from the backbone atoms of the complex of not more than 1.5 Å.

More preferably, the data is defined by the structure coordinates of caspase-7 amino acids 85, 86,
20 87, 88, 144, 145, 184, 186, 191, 223, 230, 231, 232, 233, 234, 235, 237, 240, 276, 278, 281, 282, and 284 according to FIG. 7, or a homologue of said complex, wherein said homologue comprises backbone atoms that
25 have a root mean square deviation from the backbone atoms of the complex of not more than 1.5 Å.

Even more preferably, the data is defined by the structure coordinates for caspase-7 amino acids 58-302 according to FIG. 7, or a homologue of said
30 molecule or molecular complex, said homologue having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

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Preferably, in any of these embodiments, the homologue has a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.0 Å.

5 More preferably, the data is defined by the structure coordinates for caspase-7 amino acids 58-302 according to FIG. 7.

 According to this invention, these caspase-7 complexes and homologues thereof have a S4 binding
10 region that is more hydrophilic than the S4 binding region of caspase-3.

 To use the structure coordinates generated for the caspase-7 complex or one of its binding pockets or homologues thereof, it is sometimes necessary to
15 convert them into a three-dimensional shape. This is achieved through the use of commercially available software that is capable of generating a three-dimensional representation of molecules or portions thereof from a set of structure coordinates. The
20 three-dimensional representations may be displayed as a graphical representation.

 Therefore, according to another embodiment of this invention is provided a machine-readable data storage medium, comprising a data storage material
25 encoded with machine readable data, when using a machine programmed with instructions for using said data, is capable of producing a three-dimensional representation of any of the molecule or molecular complexes, or homologues thereof, that are described
30 herein.

 This invention also provides a computer for producing a three-dimensional representation of:

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a. a molecule or molecular complex comprising a binding pocket defined by structure coordinates of caspase-7 amino acids 234, 235, 237, 276, 278, 281, and 284 according to FIG. 7; or

5 b. a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, wherein said computer comprises:

10 i. a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises the structure coordinates of caspase-7 amino acids 234, 235, 237, 276, 278, 281, and 284 according to FIG. 7;

15 ii. instructions for processing said machine-readable data into said three-dimensional representation.

Preferably, the computer is for producing a three-dimensional representation of a molecule or
20 molecular complex defined by the set of structure coordinates for caspase-7 amino acids 85, 86, 87, 88, 144, 145, 184, 186, 191, 223, 230, 231, 232, 233, 234, 235, 237, 240, 276, 278, 281, 282, and 284 according to FIG. 7, or a three-dimensional representation is of a
25 homologue of said molecule or molecular complex, said homologue having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

More preferably, the computer is for
30 producing a three-dimensional representation of a molecule or molecular complex defined by all or a portion of the set of structure coordinates according to FIG. 7, or a homologue of said molecule or molecular

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complex, said homologue having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

Most preferably, the computer is for
5 producing a three-dimensional defined by the set of structure coordinates of caspase-7 amino acids 58-302 according to FIG. 7, or a homologue of said molecule or molecular complex, or a homologue thereof having a root mean square deviation from the backbone atoms of said
10 amino acids of not more than 1.5 Å.

Preferably, in any of these embodiments, the homologue has a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.0 Å.

Most preferably, the computer is for
15 producing a three-dimensional defined by the set of structure coordinates of caspase-7 amino acids 58-302 according to FIG. 7.

In a preferred embodiment, a computer
20 according to this invention also comprises a working memory for storing instructions for processing the machine-readable data, a central-processing unit coupled to the working memory and to said machine-readable data storage medium for processing said
25 machine-readable data into the three-dimensional representation, or a display for displaying the three-dimensional representation. More preferably, a computer according to this invention comprises a display. Most preferably, a computer according to this
30 invention comprises the above working memory, central-processing unit, and display.

FIG. 8 demonstrates one version of these embodiments. System 10 includes a computer 11

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comprising a central processing unit ("CPU") 20, a working memory 22 which may be, e.g., RAM (random-access memory) or "core" memory, mass storage memory 24 (such as one or more disk drives or CD-ROM drives), one or more cathode-ray tube ("CRT") display terminals 26, one or more keyboards 28, one or more input lines 30, and one or more output lines 40, all of which are interconnected by a conventional bidirectional system bus 50.

10 Input hardware 36, coupled to computer 11 by input lines 30, may be implemented in a variety of ways. Machine-readable data of this invention may be inputted via the use of a modem or modems 32 connected by a telephone line or dedicated data line 34.

15 Alternatively or additionally, the input hardware 36 may comprise CD-ROM drives or disk drives 24. In conjunction with display terminal 26, keyboard 28 may also be used as an input device.

20 Output hardware 46, coupled to computer 11 by output lines 40, may similarly be implemented by conventional devices. By way of example, output hardware 46 may include CRT display terminal 26 for displaying a graphical representation of a binding pocket of this invention using a program such as QUANTA
25 as described herein. Output hardware might also include a printer 42, so that hard copy output may be produced, or a disk drive 24, to store system output for later use.

30 In operation, CPU 20 coordinates the use of the various input and output devices 36, 46, coordinates data accesses from mass storage 24 and accesses to and from working memory 22, and determines the sequence of data processing steps. A number of

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programs may be used to process the machine-readable data of this invention. Such programs are discussed in reference to the computational methods of drug discovery as described herein. Specific references to components of the hardware system 10 are included as appropriate throughout the following description of the data storage medium.

FIG. 9 shows a cross section of a magnetic data storage medium 100 which can be encoded with a machine-readable data that can be carried out by a system such as system 10 of FIG. 8. Medium 100 can be a conventional floppy diskette or hard disk, having a suitable substrate 101, which may be conventional, and a suitable coating 102, which may be conventional, on one or both sides, containing magnetic domains (not visible) whose polarity or orientation can be altered magnetically. Medium 100 may also have an opening (not shown) for receiving the spindle of a disk drive or other data storage device 24.

The magnetic domains of coating 102 of medium 100 are polarized or oriented so as to encode in manner which may be conventional, machine readable data such as that described herein, for execution by a system such as system 10 of FIG. 8.

FIG. 10 shows a cross section of an optically-readable data storage medium 110 which also can be encoded with such a machine-readable data, or set of instructions, which can be carried out by a system such as system 10 of FIG. 8. Medium 110 can be a conventional compact disk read only memory (CD-ROM) or a rewritable medium such as a magneto-optical disk which is optically readable and magneto-optically writable. Medium 100 preferably has a suitable

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substrate 111, which may be conventional, and a suitable coating 112, which may be conventional, usually of one side of substrate 111.

5 In the case of CD-ROM, as is well known, coating 112 is reflective and is impressed with a plurality of pits 113 to encode the machine-readable data. The arrangement of pits is read by reflecting laser light off the surface of coating 112. A protective coating 114, which preferably is
10 substantially transparent, is provided on top of coating 112.

In the case of a magneto-optical disk, as is well known, coating 112 has no pits 113, but has a plurality of magnetic domains whose polarity or
15 orientation can be changed magnetically when heated above a certain temperature, as by a laser (not shown). The orientation of the domains can be read by measuring the polarization of laser light reflected from coating 112. The arrangement of the domains encodes the data
20 as described above.

For the first time, the present invention permits the use of drug discovery techniques, including structure-based, rational drug design, or database screening techniques, to design, select, and/or
25 synthesize chemical entities, including inhibitory compounds that are capable of binding to caspase-7, or any portion thereof.

For example, the structure encoded by the data may be computationally evaluated for its ability
30 to associate with chemical entities. Chemical entities that associate with caspase-7 may inhibit caspase-7, and are potential drug candidates. Alternatively, the structure encoded by the data may be displayed in a

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graphical three-dimensional representation on a computer screen. This allows visual inspection of the structure, as well as visual inspection of the structure's association with chemical entities.

5 Thus, according to another embodiment, the invention relates to a method for evaluating the potential or ability of a chemical entity to associate with any of the molecules or molecular complexes set forth above. This method comprises the steps of: a)
10 employing computational means to perform a fitting operation between the chemical entity and a binding pocket of the molecule or molecular complex; and b) analyzing the results of said fitting operation to quantify the association between the chemical entity
15 and the binding pocket. The term "chemical entity", as used herein, refers to chemical compounds, complexes of at least two chemical compounds, and fragments of such compounds or complexes.

For the first time, the present invention
20 permits the use of molecular design techniques to identify, select and design chemical entities, including inhibitory compounds, capable of binding to caspase-7-like binding pockets.

Applicants' elucidation of the caspase-7
25 binding sites provides the necessary information for designing new chemical entities and compounds that may interact with the caspase-7 binding pockets, in whole or in part. This elucidation also enables the evaluation of structure-activity data for compounds
30 which bind to caspase-7 binding pockets. Applicants' elucidation of the caspase-7 binding sites also provides important structural information for comparing the requirements for interacting with caspase-7 binding

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pockets selectively or in addition to other caspase binding pockets.

Thus, according to another embodiment, the invention relates to a method for a method for
5 identifying a potential agonist or antagonist of any of the molecules or molecular complexes set forth above. This method comprises the steps of: a. generating a three-dimensional structure of the molecule or
10 molecular complex; b. employing said three-dimensional structure to design or select said potential agonist or antagonist; c. providing said potential agonist or antagonist; and d. contacting said potential agonist or antagonist to interact with said molecule.

Throughout this section, discussions about
15 the ability of an entity to bind to, associate with or inhibit a caspase-7 binding pocket refers to features of the entity alone. Assays to determine whether a compound binds to caspases are well known in the art [see for example, the assays described in WO97/22619].

20 The design of compounds that bind to or inhibit caspase-7 according to this invention generally involves consideration of two factors. First, the entity must be capable of physically and structurally associating with parts or all of the caspase-7 binding
25 pockets. Non-covalent molecular interactions important in this association include hydrogen bonding, van der Waals interactions, hydrophobic interactions and electrostatic interactions.

Second, the entity must be able to assume a
30 conformation that allows it to associate with the caspase-7 binding pocket directly. Although certain portions of the entity will not directly participate in these associations, those portions of the entity may

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still influence the overall conformation of the molecule. This, in turn, may have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity in relation to all or a portion of the binding pocket, or the spacing between functional groups of an entity comprising several chemical entities that directly interact with the caspase-7 binding pocket or homologues thereof.

The potential inhibitory or binding effect of a chemical entity on a caspase-7 binding pocket may be analyzed prior to its actual synthesis and testing by the use of computer modeling techniques. If the theoretical structure of the given entity suggests insufficient interaction and association between it and the caspase-7 binding pocket, testing of the entity is obviated. However, if computer modeling indicates a strong interaction, the molecule may then be provided or synthesized and tested for its ability to bind to a caspase-7 binding pocket. This may be achieved by testing the ability of the molecule to inhibit caspase-7 using assays that are known to those of ordinary skill in the art. In this manner, the obtaining and testing of inoperative compounds may be avoided.

A potential inhibitor of caspase-7 may be computationally evaluated by means of a series of steps in which chemical entities or fragments are screened and selected for their ability to associate with the caspase-7 binding pockets.

One skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with a caspase-7 binding pocket. This process may begin by visual inspection

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of, for example, a caspase-7 binding pocket on the computer screen based on the caspase-7 structure coordinates in FIG. 7 or other coordinates which define a similar shape generated from the machine-readable storage medium. Selected fragments or chemical entities may then be positioned in a variety of orientations, or docked, within that binding pocket as defined supra. Docking may be accomplished using software such as Quanta and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics force fields, such as CHARMM and AMBER.

Specialized computer programs may also assist in the process of selecting fragments or chemical entities. These include:

1. GRID (P. J. Goodford, "A Computational Procedure for Determining Energetically Favorable Binding Sites on Biologically Important Macromolecules", J. Med. Chem., 28, pp. 849-857 (1985)). GRID is available from Oxford University, Oxford, UK.
2. MCSS (A. Miranker et al., "Functionality Maps of Binding Sites: A Multiple Copy Simultaneous Search Method." Proteins: Structure, Function and Genetics, 11, pp. 29-34 (1991)). MCSS is available from Molecular Simulations, San Diego, CA.
3. AUTODOCK (D. S. Goodsell et al., "Automated Docking of Substrates to Proteins by Simulated Annealing", Proteins: Structure, Function, and Genetics, 8, pp. 195-202 (1990)). AUTODOCK is available from Scripps Research Institute, La Jolla, CA.
4. DOCK (I. D. Kuntz et al., "A Geometric Approach to Macromolecule-Ligand Interactions", J. Mol. Biol.,

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161, pp. 269-288 (1982)). DOCK is available from University of California, San Francisco, CA.

Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound or complex. Assembly may be preceded by
5 visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of caspase-7. This would be followed by
10 manual model building using software such as Quanta or Sybyl [Tripos Associates, St. Louis, MO].

Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include:

- 15 1. CAVEAT (P. A. Bartlett et al., "CAVEAT: A Program to Facilitate the Structure-Derived Design of Biologically Active Molecules", in Molecular Recognition in Chemical and Biological Problems", Special Pub., Royal Chem. Soc., 78, pp. 182-196 (1989);
20 G. Lauri and P. A. Bartlett, "CAVEAT: a Program to Facilitate the Design of Organic Molecules", J. Comput. Aided Mol. Des., 8, pp. 51-66 (1994)). CAVEAT is available from the University of California, Berkeley, CA.
- 25 2. 3D Database systems such as ISIS (MDL Information Systems, San Leandro, CA). This area is reviewed in Y. C. Martin, "3D Database Searching in Drug Design", J. Med. Chem., 35, pp. 2145-2154 (1992).
- 30 3. HOOK (M. B. Eisen et al., "HOOK: A Program for Finding Novel Molecular Architectures that Satisfy the Chemical and Steric Requirements of a Macromolecule Binding Site", Proteins: Struct., Funct., Genet., 19,

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pp. 199-221 (1994). HOOK is available from Molecular Simulations, San Diego, CA.

Instead of proceeding to build an inhibitor of a caspase-7 binding pocket in a step-wise fashion one fragment or chemical entity at a time as described
5 above, inhibitory or other caspase-7 binding compounds may be designed as a whole or "de novo" using either an empty binding site or optionally including some portion(s) of a known inhibitor(s). There are many de
10 novo ligand design methods including:

1. LUDI (H.-J. Bohm, "The Computer Program LUDI: A New Method for the De Novo Design of Enzyme Inhibitors", J. Comp. Aid. Molec. Design, 6, pp. 61-78 (1992)). LUDI is available from Molecular Simulations
15 Incorporated, San Diego, CA.
2. LEGEND (Y. Nishibata et al., Tetrahedron, 47, p. 8985 (1991)). LEGEND is available from Molecular Simulations Incorporated, San Diego, CA.
3. LeapFrog (available from Tripos Associates, St.
20 Louis, MO).
4. SPROUT (V. Gillet et al., "SPROUT: A Program for Structure Generation)", J. Comput. Aided Mol. Design, 7, pp. 127-153 (1993)). SPROUT is available from the University of Leeds, UK.

25 Other molecular modeling techniques may also be employed in accordance with this invention [see, e.g., N. C. Cohen et al., "Molecular Modeling Software and Methods for Medicinal Chemistry, J. Med. Chem., 33, pp. 883-894 (1990); see also, M. A. Navia and M. A.
30 Murcko, "The Use of Structural Information in Drug Design", Current Opinions in Structural Biology, 2, pp. 202-210 (1992); L. M. Balbes et al., "A Perspective of Modern Methods in Computer-Aided Drug Design", in

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Reviews in Computational Chemistry, Vol. 5, K. B. Lipkowitz and D. B. Boyd, Eds., VCH, New York, pp. 337-380 (1994); see also, W. C. Guida, "Software For Structure-Based Drug Design", Curr. Opin. Struct. Biology, 4, pp. 777-781 (1994)].

Once a compound has been designed or selected by the above methods, the efficiency with which that entity may bind to a caspase-7 binding pocket may be tested and optimized by computational evaluation. For example, an effective caspase-7 binding pocket inhibitor must preferably demonstrate a relatively small difference in energy between its bound and free states (i.e., a small deformation energy of binding). Thus, the most efficient caspase-7 binding pocket inhibitors should preferably be designed with a deformation energy of binding of not greater than about 10 kcal/mole, more preferably, not greater than 7 kcal/mole. Caspase-7 binding pocket inhibitors may interact with the binding pocket in more than one conformation that is similar in overall binding energy. In those cases, the deformation energy of binding is taken to be the difference between the energy of the free entity and the average energy of the conformations observed when the inhibitor binds to the protein.

An entity designed or selected as binding to a caspase-7 binding pocket may be further computationally optimized so that in its bound state it would preferably lack repulsive electrostatic interaction with the target enzyme and with the surrounding water molecules. Such non-complementary electrostatic interactions include repulsive charge-charge, dipole-dipole, and charge-dipole interactions.

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Specific computer software is available in the art to evaluate compound deformation energy and electrostatic interactions. Examples of programs designed for such uses include: Gaussian 94, revision C (M. J. Frisch, Gaussian, Inc., Pittsburgh, PA ©1995); AMBER, version 4.1 (P. A. Kollman, University of California at San Francisco, ©1995); QUANTA/CHARMM (Molecular Simulations, Inc., San Diego, CA ©1995); Insight II/Discover (Molecular Simulations, Inc., San Diego, CA ©1995); DelPhi (Molecular Simulations, Inc., San Diego, CA ©1995); and AMSOL (Quantum Chemistry Program Exchange, Indiana University). These programs may be implemented, for instance, using a Silicon Graphics workstation such as an Indigo² with "IMPACT" graphics. Other hardware systems and software packages will be known to those skilled in the art.

Another approach enabled by this invention, is the computational screening of small molecule databases for chemical entities or compounds that can bind in whole, or in part, to a caspase-7 binding pocket. In this screening, the quality of fit of such entities to the binding site may be judged either by shape complementarity or by estimated interaction energy [E. C. Meng et al., J. Comp. Chem., 13, pp. 505-524 (1992)].

Thus, enabled by this invention are compounds that inhibit caspase-7 by associating directly with the caspase-7 active site. Preferably, such compounds have a strain energy of 10 kcal/mol or less. More preferably, these compounds contain fewer than three secondary amide bonds. Even more preferably, these compounds have a molecular weight of less than 1000.

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Those of skill in the art will realize that association of natural ligands or substrates with the binding pockets of their corresponding receptors or enzymes is the basis of many biological mechanisms of action. Similarly, many drugs exert their biological effects through association with the binding pockets of receptors and enzymes. Such associations may occur with all or any parts of the binding pockets. An understanding of such associations will help lead to the design of drugs having more favorable associations with their target receptor or enzyme, and thus, improved biological effects. Therefore, this information is valuable in designing potential ligands or inhibitors of receptors or enzymes, such as inhibitors of caspase-7.

The term "associating with" refers to a condition of proximity between chemical entities or compounds, or portions thereof. The association may be non-covalent -- wherein the juxtaposition is energetically favored by hydrogen bonding or van der Waals or electrostatic interactions -- or it may be covalent.

Another particularly useful drug design technique enabled by this invention is iterative drug design. Iterative drug design is a method for optimizing associations between a protein and a compound by determining and evaluating the three-dimensional structures of successive sets of protein/compound complexes.

In iterative drug design, crystals of a series of protein or protein complexes are obtained and then the three-dimensional structures of each crystal is solved. Such an approach provides insight into the

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association between the proteins and compounds of each complex. This is accomplished by selecting compounds with inhibitory activity, obtaining crystals of this new protein/compound complex, solving the three-
5 dimensional structure of the complex, and comparing the associations between the new protein/compound complex and previously solved protein/compound complexes. By observing how changes in the compound affected the protein/compound associations, these associations may
10 be optimized.

In some cases, iterative drug design is carried out by forming successive protein-compound complexes and then crystallizing each new complex. Alternatively, a pre-formed protein crystal is soaked
15 in the presence of an inhibitor, thereby forming a protein/compound complex and obviating the need to crystallize each individual protein/compound complex. Advantageously, the caspase-7/inhibitor crystals provided by this invention may be soaked in the
20 presence of a compound or compounds, to provide other crystal complexes.

As used herein, the term "soaked" refers to a process in which the crystal is transferred to a solution containing the compound of interest.

25 In another embodiment of this invention is provided a method for preparing a composition comprising a caspase-7 comprising the steps described in Examples 1 and 2. Preferably, the composition comprises a caspase-7 in complex with Ac-DEVD-CHO.

30 Once the structure coordinates of a protein crystal have been determined they are useful in solving the structures of other crystals. Thus, the structure coordinates set forth in FIG. 7 can also be used to aid

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in obtaining structural information about another crystallized molecule or molecular complex. This may be achieved by any of a number of well-known techniques, including molecular replacement.

5 A machine-readable data storage medium comprising a data storage material encoded with a first set of machine readable data which, when combined with a second set of machine readable data using a machine programmed with instructions for using said first set
10 of data and said second set of data, can determine at least a portion of the structure coordinates corresponding to the second set of machine readable data, wherein: said first set of data and said second set of data comprises a Fourier transform of at least a
15 portion of the structural coordinates for caspase-7 according to FIG. 7; said second set of data comprises an X-ray diffraction pattern of a molecule or molecular complex of unknown structure.

 The structure coordinates set forth in FIG. 7
20 can also be used for determining at least a portion of the three-dimensional structure of molecules or molecular complexes which contain at least some structurally similar features to caspase-7. In particular, structural information about another
25 crystallized molecule or molecular complex may be obtained. This may be achieved by any of a number of well-known techniques, including molecular replacement.

 Therefore, in another embodiment this invention provides a method of utilizing molecular
30 replacement to obtain structural information about a crystallized molecule or molecular complex whose structure is unknown comprising the steps of:

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a) generating an X-ray diffraction pattern from said crystallized molecule or molecular complex; and

5 b) applying at least a portion of the structure coordinates set forth in FIG. 7 to the X-ray diffraction pattern to generate a three-dimensional electron density map of the molecule or molecular complex whose structure is unknown.

10 Preferably, the crystallized molecule or molecular complex comprises a caspase-7. More preferably, the crystallized molecule or molecular complex is obtained by soaking a crystal of this invention in a solution.

15 By using molecular replacement, all or part of the structure coordinates of the caspase-7 complex provided by this invention (and set forth in FIG. 7) can be used to determine the structure of a crystallized molecule or molecular complex whose structure is unknown more quickly and efficiently than
20 attempting to determine such information ab initio.

Molecular replacement provides an accurate estimation of the phases for an unknown structure. Phases are a factor in equations used to solve crystal structures that can not be determined directly.
25 Obtaining accurate values for the phases, by methods other than molecular replacement, is a time-consuming process that involves iterative cycles of approximations and refinements and greatly hinders the solution of crystal structures. However, when the
30 crystal structure of a protein containing at least a homologous portion has been solved, the phases from the known structure provide a satisfactory estimate of the phases for the unknown structure.

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Thus, this method involves generating a preliminary model of a molecule or molecular complex whose structure coordinates are unknown, by orienting and positioning the relevant portion of the caspase-7 complex according to FIG. 7 within the unit cell of the crystal of the unknown molecule or molecular complex so as best to account for the observed X-ray diffraction pattern of the crystal of the molecule or molecular complex whose structure is unknown. Phases can then be calculated from this model and combined with the observed X-ray diffraction pattern amplitudes to generate an electron density map of the structure whose coordinates are unknown. This, in turn, can be subjected to any well-known model building and structure refinement techniques to provide a final, accurate structure of the unknown crystallized molecule or molecular complex [E. Lattman, in Meth. Enzymol., 115, pp. 55-77 (1985); M. G. Rossmann, ed., Int. Sci. Rev. Ser., No. 13, Gordon & Breach, New York (1972)].

The structure of any portion of any crystallized molecule or molecular complex that is sufficiently homologous to any portion of the caspase-7 can be solved by this method.

In a preferred embodiment, the method of molecular replacement is utilized to obtain structural information about a molecule or molecular complex, wherein the complex comprises a caspase-7. Preferably the caspase-7 is the caspase-7 described herein, in complex with the inhibitor Ac-DEVD-CHO.

The structure coordinates of caspase-7 as provided by this invention are particularly useful in solving the structure of other crystal forms of caspase-7, or complexes thereof.

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The structure coordinates are also particularly useful to solve the structure of crystals of caspase-7 complexes, particularly caspase-7, co-complexed with a variety of chemical entities. This approach enables the determination of the optimal sites for interaction between chemical entities, including interaction of candidate caspase-7 inhibitors with caspase-7. For example, high resolution X-ray diffraction data collected from crystals exposed to different types of solvent allows the determination of where each type of solvent molecule resides. Small molecules that bind tightly to those sites can then be designed and synthesized and tested for their caspase-7 inhibition activity.

All of the complexes referred to above may be studied using well-known X-ray diffraction techniques and may be refined versus 1.5-3 Å resolution X-ray data to an R value of about 0.20 or less using computer software, such as X-PLOR [Yale University, ©1992, distributed by Molecular Simulations, Inc.; see, e.g., Blundell & Johnson, supra; Meth. Enzymol., vol. 114 & 115, H. W. Wyckoff et al., eds., Academic Press (1985)]. This information may thus be used to optimize known caspase inhibitors, and more importantly, to design new caspase inhibitors.

In order that this invention be more fully understood, the following examples are set forth. These examples are for the illustrative purposes only and are not to be construed as limiting the scope of this invention in any way.

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EXAMPLE 1Expression and Purification of Caspase-1, Caspase-3,
Caspase-7, and Caspase-8 for Crystallization

Recombinant human Caspase-1 was expressed in
5 *Escherichia coli* as an insoluble p32 protein spanning
residues 120-404 of the p45 precursor [N.A. Thornberry
et al., Nature, 356, pp. 768-774 (1992)]. The
insoluble p32 protein was solubilized and purified
under chaotropic conditions, then refolded and
10 autoprocessed in vitro producing the p20 and p10 active
subunits. Details, including previous X-ray
crystallographic analyses have been described elsewhere
[K.P. Wilson et al., Nature, 370, pp. 270-275 (1994);
N. Margolin et al., J. Biol. Chem., 272, pp. 7223-7228
15 (1997)]. Caspase-3 (residues 29-277) and Caspase-7
(residues 1-303) containing an N-terminal (His)₆
affinity tag and thrombin cleavable site were expressed
in *Escherichia coli* [Y. Gu et al., J. Biol. Chem., 271,
pp. 10816-10820 (1996); J.A. Lippke et al., J. Biol.
20 Chem. 271, pp. 1825-1828 (1996)]. Both caspases were
soluble and active as their p20/p10 subunits, yielding
0.05 and 1 mg/gm cells of caspase-3 and caspase-7,
respectively. For purification of either protein, cell
paste was resuspended in 10 volumes of 50 mM HEPES
25 buffer containing 10% (v/v) glycerol, 300 mM NaCl, 5 mM
 β -mercaptoethanol (β -ME), 0.05% (w/v) β -OG, 25 mM
imidazole, 0.1 mM PMSF, pH 8.0 at 4°C. Following
mechanical disruption of the cells, the soluble
fraction was harvested by centrifugation at 30,000 x g
30 for 30 min at 4°C. The supernatant was incubated
batchwise overnight with 1 ml Ni-affinity resin
(Qiagen) per 5-10 mg of expected caspase-3 or caspase-
7. The resin was washed with 50 column volumes of the

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extraction buffer, followed by 50 column volumes of the extraction buffer adjusted to pH 7.0. caspase-3 and caspase-7 were eluted with 50 and 300 mM imidazole, respectively, in 50 mM HEPES, pH 7.0 containing 10 %
5 (v/v) glycerol, 100 mM NaCl, 5 mM β -ME.

Recombinant caspase-8 (residues 233-479) was expressed as an N-terminal His-tagged fusion in High-five insect cells using a baculovirus expression vector system by conventional methods [W. Chen et al., Protein Expression and Purification, 9, pp. 69-75 (1997)].
10 Crystallization of caspase-8/Ac-DEVD-CHO was enhanced by three Lys $\rightarrow$ Arg point mutations (at residues 246, 250 and 253), and removal of Pro370 and Val371, which appeared absent from other caspases in sequence
15 alignments. Caspase-8 was processed intracellularly and secreted into the media during expression. The cell culture media was centrifuged at 1,600 x g to remove cells, and the supernatant (~ pH 6.4) adjusted to 50% (w/v) ammonium sulfate and stirred gently for 60
20 min on ice. After centrifugation at 54,000 x g for 45 min at 4°C, the supernatant was decanted, 0.2 μ m filtered and the ammonium sulfate concentration increased to 85% (w/v) and stirred for another 60 min on ice. Centrifugation at 54,000 x g for 45 min at 4°C
25 resulted in the precipitation of caspase-8. Pellets were resuspended in 2% of the starting volume of the media using 100 mM HEPES, pH 8.0, containing 100 mM NaCl, 10% glycerol (v/v) and 5 mM β -ME. The solution was incubated with 1 ml Talon affinity resin (Clontech)
30 per 5-10 mg expected caspase-8 and gently mixed overnight at 4°C. The resin washed with 150 column volumes of 20 mM HEPES, pH 7.0, containing 100 mM NaCl,

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10% glycerol (v/v) and 5 mM β -ME. A second wash of 50 column volumes was performed using the same buffer with 25 mM imidazole. Caspase-8 was eluted with wash buffer adjusted to 350 mM imidazole.

5 Characterization of Triple Mutant Caspase-8

Wild-type and mutant caspase-8 enzymes were characterized using the fluorogenic substrate Ac-DEVD-AMC (Alexis Biochemicals, San Diego, CA). The concentrations of active enzyme were determined by
10 active site titration with Ac-DEVD-CHO (Peptides International, Louisville, KY). All assays were performed in 100 mM HEPES, pH 8, containing 100 mM NaCl, 5 mM DTT and 0.1% (w/v) CHAPS at 37°C using a 96-well Fmax plate reader (Molecular Devices, Sunnyvale,
15 CA). The Ac-DEVD-AMC substrate concentration was varied between 2 and 100 μ M and the reaction was initiated by addition of 2 nM enzyme. Enzyme kinetic data were analyzed by nonlinear regression in the program EZ-Fit (Perrella Scientific, Amhurst, NH).

20

EXAMPLE 2

Crystallization of Caspase-1, Caspase-3, Caspase-7, and
Caspase-8 in Complex with Ac-DEVD-CHO

Details of protein purification and
25 crystallization of the caspase-1/Ac-DEVD-CHO complex has been reported [N. Margolin et al., J. Biol. Chem., 272, pp. 7223-7228 (1997)]. Metal affinity purified caspase-3, caspase-7 or caspase-8 were inhibited by addition of a two-fold molar excess of Ac-DEVD-CHO
30 (Peptides International). The N-terminal (His)₆ tag was then removed from caspase-3, caspase-7 or caspase-8 by thrombin cleavage (20 units of thrombin /mg caspase) at 37°C for 60 min. Thrombin was removed by a 5 min

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incubation with 100 μ l of benzamidine sepharose. The free (His)₆ tag and aggregated caspase were removed by size-exclusion chromatography using a column (60 x 1.5 cm) packed with Superdex-75 resin (Pharmacia). The column was equilibrated at 4°C in 20 mM HEPES, pH 7.0, containing 10% glycerol (v/v), 100 mM NaCl, 5 mM β -ME at a flow rate of 1 ml/min. Light-scattering (PD-2000, Precision Detectors, Franklin, MA) analyses during size-exclusion chromatography identified aggregated protein, which was excluded from the pooled fractions. Caspase-1/Ac-DEVD-CHO was purified on the same size-exclusion column except 50 mM citrate, pH 6.5, containing 2 mM DTT buffer was used. After size-exclusion, equimolar Ac-DEVD-CHO was added prior to concentration of the caspase/Ac-DEVD-CHO co-complexes for crystallization. All protein samples were stored at -70 °C.

Crystals of inhibited caspase-3 were grown by vapor diffusion and macro-seeding. Thousands of micro-crystals were initially obtained in 12 h when protein (4.6 mg/ml in 20 mM Na HEPES, 2.0 mM DTT, 0.1 M NaCl, 10% glycerol, pH 7.0) was mixed with reservoir (0.2 M ammonium acetate, 0.1 M Na citrate, 30% w/v PEG 4000) at a 3 μ l:2 μ l protein solution to reservoir ratio and allowed to stand at room temperature. A crystallization droplet setup in the same way but with 2% (v/v) methyl-pyrrolidinone (MeP) added to the reservoir produced no crystals. A micro-crystal was then transferred to this second drop and this seed crystal grew over 10 days to a size of 0.4 mm x 0.3 mm x 0.25 mm.

The autoproteolyzed active form caspase-7 was inhibited by titrating Ac-DEVD-CHO into the protein

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sample. The complex was further purified by size-exclusion chromatography. Pooled fractions were concentrated to about 5mg/ml for crystallization. Slow vapor diffusion was used to obtain X-ray quality
5 crystals of the caspase-7/Ac-DEVD-CHO complex over a few weeks at 4°C.

Caspase-8 was titrated with Ac-DEVD-CHO (12.0 mg/ml, 20 mM HEPES pH 7.0, 0.1 M NaCl, 5.0 mM β -ME) and was subsequently added to a reservoir solution (0.1 M
10 potassium phosphate, pH 6.0, 5% t-butanol, 40% (w/v) ammonium sulfate) at a 2 μ l:2 μ l ratio and suspended over 1.0 ml of reservoir at room temperature. A single crystal was harvested within two weeks and has dimensions of 0.40 X 0.20 X 0.10 mm. The same crystal
15 was flash cooled to 170°K in N₂ gas stream prior to data collection.

EXAMPLE 3

Crystal Structure Determination

20 Crystals of caspase-1-Ac-DEVD-CHO and caspase-3-Ac-DEVD-CHO were mounted in glass capillaries for X-ray data collection at -7°C and -4°C respectively. X-ray data of both caspase-1/Ac-DEVD-CHO and caspase-3 complexes were collected on a Raxis IIC
25 image plate equipped with Rigaku rotating anode generator and processed using software provided by the manufacture (Molecular Structures Corp., Woodlands, Texas). R-merge for the data was 6.1% at 2.2 Å resolution. Analysis of the unit cell dimensions
30 suggested that each asymmetric unit contained two caspase-3 heterodimers. A polyalanine model of a single caspase-1 heterodimer was used to obtain a successful rotation and translation function solution for a

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caspase-3 heterodimer using the program AMoRe [J. Navaza, Acta Crystallography, A50, pp. 157-163 (1994)]. The first solution was then held fixed while a second polyalanine model was tried in the rotation and translation function. Combining the two solutions produced a polyalanine model for the caspase-3 dimer of heterodimers with an R-factor of 45.1% for all observed reflections between 8 and 2.8 Å resolution, and an R-free of 47.5% for 10% of the reflections set aside at the start of the refinement. The resolution of the maps and model was gradually increased to 2.2 Å resolution by cycles of model building, positional refinement and thermal factor refinement, interspersed with torsional dynamics runs. All model refinement was carried out using the XPLOR suite of programs [A. Brunger, "X-PLOR, A system for X-ray crystallography and NMR" New Haven, Yale University Press (1996)].

Crystals of the caspase-7-Ac-DEVD-CHO complex were transferred to cryoprotectant and flash-cooled to 100K in N₂ gas stream prior to data collection. The diffraction images were recorded on CCD 2X2K detector at Brookhaven National Laboratories (BNL), Brookhaven, NY. The data were processed using DENZO and SCALPACK software [Z. Otwinowski & W. Minor, Methods In Enzymology (Macromolecular Crystallography, Part A), 276, pp. 307-326 (1997)]. The crystals have unit cell dimensions of 88.2 Å, 88.2 Å, 186.2 Å, $\alpha=90.0^\circ$, $\beta=90.0^\circ$, $\gamma=120.0^\circ$ and belong to space group P3221. Assuming that there is one tetramer in the asymmetric unit, the calculated Matthew's specific volume was 2.6 Å³/d. The structure was solved by molecular replacement methods using a truncated caspase-3

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tetramer molecule as the searching template. The initial R-factor and correlation coefficient factors are 44% and 65%, respectively. A polyalanine model from the solution was first refined against data
5 between 8.0 Å to 3.0 Å. The side chains of individual amino acids were modeled into the electron density map according to the protein sequence. The model was refined using XPLOR and manually corrected using QUANTA (QUANTA97, Molecular Simulations, Inc.). The final
10 model has a full tetramer assembly of 654 residues, two sulfate anions and 374 water molecules.

A single crystal of caspase-8-Ac-DEVD-CHO complex was flash cooled in N₂ cold gas stream prior to the synchrotron data collection at BNL. Data was
15 recorded on a 2X2K CCD image plate mounted on X25 beam line. The space group of the crystal was determined as C2221 with unit cell of 62.12 Å, 344.33 Å, 190.99 Å, $\alpha=90.0$, $\beta=90.0$, $\gamma=90.0$. The Matthew's specific volume calculation suggested that there are three independent
20 tetrameric molecules in the asymmetric unit giving a calculated solvent content of 54% [B.W. Matthews, Journal of Molecular Biology, 33, pp. 491-497 (1968)]. The crystal diffracts extremely anisotropically along the a*, b*, and c* axes to 2.35 Å, 2.80 Å and 2.65 Å
25 respectively. The data set was processed using DENZO and SCALPACK software to a resolution of 2.65 Å. The structure solution was obtained by using AMoRe and by using a truncated caspase-3 tetramer molecule as searching template. Rigid-body and positional
30 refinement of the polyalanine model was initially done using XPLOR. The side chains, insertions and deletions of the molecule were modeled into the electron density map manually using QUANTA programs. The final model

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contains 1454 amino acids, 316 solvent molecules and six Ac-DEVD-CHO compounds covalently attached to the active site Cysteine residue.

The coordinates of the caspase-7-Ac-DEVD-CHO structure have been deposited with the Protein Data Bank under the accession code 1F1J.

EXAMPLE 4

Crystallography

The model quality of all four structures was assessed using PROCHECK and the crystallographic statistics are given in Table 1 [R.A. Laskowski, Journal of Applied Crystallography, 26, pp. 283-291 (1993)].

Table 1. Crystallographic data and refinement statistics

	Csp1	Csp3	Csp7	Csp8
<u>X-ray experiments</u>				
Temperature (K)	298	270	100	100
<u>X-ray radiation</u>				
	rotating anode	rotating	anode	BNSL BNSL
Wavelength (Å)	1.5418	1.5418	1.10	1.09
Space group	P4 ₃ 2 ₁ 2	P2 ₁ 2 ₁ 2 ₁	P3 ₂ 2 ₁	C222 ₁
a (Å)	62.45	89.46	88.18	62.12
b (Å)	62.45	97.33	88.18	344.33
c (Å)	162.36	70.09	186.23	190.99
α(°)	90.0	90.0	90.0	90.0
β(°)	90.0	90.0	90.0	90.0
γ(°)	90.0	90.0	120.0	90.0
<u>No of p20/p10 in asym. Unit</u>				
	1	2	2	6
<u>Recording apparatus</u>				
	Raxis IIC	Raxis IIC	CCD 2X2K	CCD 2X2K
Resolution (Å)	2.5	2.2	2.35	2.65
Total observation	48936	63425	139781	189632
Unique reflection	13468	12532	34359	53183
Completeness (%)	93	92	96.6	88.2
R _{sym} * (%)	6.5	7.8	8.3	5.5

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Structure solution

Methods	ref 16.	M.R.	M.R.	M.R.
---------	---------	------	------	------

Search model

5	ref 16.	polyala of Csp1	polyala of Csp3	polyala of Csp3
---	---------	-----------------	-----------------	-----------------

Resolution range (Å)

ref 16.	8.0-2.8	16.0-4.0	16.0-4.0
---------	---------	----------	----------

Software

ref 16.	Amore	Amore	Amore
---------	-------	-------	-------

R-factor (%)

ref 16.	45.1	41.0	34.7
---------	------	------	------

Correlation coefficient Factor

10	ref 16.	54.6	61.0	72.5
----	---------	------	------	------

Refinement

Resolution range (Å)

7.5-2.4	8.0- 2.2	7.5 - 2.35	20.0- 2.6
---------	----------	------------	-----------

Sigma cut off (σ)

2.5	3.0	2.5	2.5
-----	-----	-----	-----

15	Programs	XPLOR	XPLOR	XPLOR	XPLOR
----	----------	-------	-------	-------	-------

No of reflections

14658	24890	33303	48348
-------	-------	-------	-------

R-factor# (%)

23.1	18.9	18.5	21.9
------	------	------	------

Free R-factor # (%)

28.2	24.7	26.3	28.6
------	------	------	------

20 Stereochemical parameters

R.m.s. bond distance (Å)

0.011	0.009	0.009	0.006
-------	-------	-------	-------

R.m.s. bond angle (°)

2.3	1.9	1.8	1.7
-----	-----	-----	-----

25 R.m.s. dihedral angle (°)

24.1	23.6	23.4	23.4
------	------	------	------

Non-glycine residues
in the regions of

Most favored

90.0	89.3	89.0	86.3
------	------	------	------

30 Additional allowed

9.5	9.0	10.5	13.7
-----	-----	------	------

Generously allowed

0.5	0.7	0.5	0.0
-----	-----	-----	-----

Disallowed

0	0	0	0.0
---	---	---	-----

35 $*R_{\text{sym}} = \sum |I_i - \langle I \rangle| / \sum I_i$ Where I_i and $\langle I \rangle$ are the intensities for the it observation and mean of the reflection, respectively

#R-factor = $\sum |F_{\text{obs}} - F_{\text{cal}}| / \sum |F_{\text{obs}}|$ Where F_{obs} and F_{cal} are observed and calculated model structure factors.

40 Comparison Of Caspase-7/Ac-DEVD-CHO Complex To
Caspase-3/Ac-DEVD-CHO Complex

45 The caspase-7-Ac-DEVD-CHO complex is similar to the caspase-3-Ac-DEVD-CHO complex. The refined model of caspase-7 contains a complete catalytic unit comprising two p20-p10 heterodimers. The p20 and p10

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polypeptide chains are composed of residues 57-196 and 212-302, respectively. The two interdigitating heterodimers associate to form a tetramer of globular shape. A ribbon stereo diagram of the caspase-7 complex is illustrated in FIG. 1. As expected, the overall fold of caspase-7 is very similar to that of caspase-1, caspase-3, and caspase-8. All four subunits contribute to a total of 12 strands comprising the central β sheet. This forms the core of the enzyme, which is flanked by ten α helixes approximately parallel to the β strands. In particular, the β -sheet structure of the p20 domain, which contains the catalytic His285 and Cys186 residues, has a crossing-over -1X, +2X, +1X linking topology according to Richardson's definition [J.S. Richardson, Adv. Protein Chem., 34, pp. 167-338 (1981)]. This motif has been widely observed in serine hydrolases, most notably the α/β hydrolase superfamily [D.L. Ollis et al., Protein Eng., 5, pp. 599-611 (1992)].

Among the three subfamilies of caspases, caspase-7 belongs to the second group that includes caspase-2 and caspase-3. Aside from the differences that exist in the propeptide and linker regions, caspase-7 is structurally and functionally very similar to caspase-3. In fact, caspase-7 and caspase-3 can be superimposed without any amino acid deletions or insertions along the polypeptide chains (FIG. 2a) with a root mean square (RMS) deviation of 0.37Å for backbone C α atoms. Sequence alignment and C α atom superpositioning of caspase-1, caspase-3, caspase-7 and caspase-8 spanning all three caspase subfamilies (FIGS. 2a and 3) demonstrated that the main differences between their folds are in three regions. These

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differences occur in the two loops on the prime side and a third loop proximal to the S4 binding site (FIG. 2a).

Similar to caspase-3, caspase-7 also has a
5 single-residue deletion within the strand C290-M294 (FIG. 3), which pairs with its symmetry-related equivalent forming the tetrameric assembly of the enzyme. In caspase-1 and other caspases of group 1, there is an arginine residue (R391 in caspase-1) which
10 causes a bulge in the β strand and consequently induces a rotation of one heterodimer relative to the other. In caspase-3 [P.R.E. Mittl et al., J. Biol. Chem., 272, pp. 6539-6547 (1997)] and caspase-7, the two dimeric subunits are significantly less twisted. The
15 combination of this single deletion and greater hydrophobic nature of this strand in caspase-3 and caspase-7 has not only changed the quaternary structures of these enzymes but also reshaped the central cavity formed at the interface of the two
20 heterodimers. The central cavity of the caspase-7 tetramer was occupied by 24 water molecules. As this central cavity is adjacent to the prime side of the substrate binding site, it may not effect directly substrate binding to caspase-3 and caspase-7. However,
25 the variation in the central cavity among caspases might be an important determinant of macromolecular substrate recognition in the apoptosis cascade.

Conserved Fold And Topology

Like caspase-1 and caspase-3, the mature
30 forms of caspase-7 and caspase-8 are tetramers comprised of two p20/p10 heterodimers. The heterodimers are both structurally and functionally associated to appear as a single domain. For all four

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caspases, the protein core is a six-stranded (β -sheet surrounded by five or six α -helices which lie roughly parallel to the β -strands. Weak electron density for the N-terminal helix was observed for Csp1 [K.P. Wilson
5 & D.J. Livingston, Nature, 370, pp. 270-275 (1994)], but little or no density could be observed for this helix in caspase-3, caspase-7, and caspase-8. Both p10 and p20 subunits contribute to the ligand binding site for all four caspase structures. The main differences
10 between the folds for caspases 1, 3, 7, and 8 occur in two loop regions: one on the prime side and the other proximal to the S4 binding site (FIG. 2A).

On the prime side, caspase-8 differs from the others by the presence of a helix-turn-helix insertion
15 ranging from residues 245-253 (FIG. 2C). This agrees with the recently reported caspase-8 structures expressed in *Escherichia coli* that also possess some helical content to this insertion loop [H. Blanchard et al., Structure (London), 7, pp. 1125-1133 (1999); W.
20 Watt et al., Structure (London), 7, pp. 1135-1143 (1999)]. An analysis of a sequence alignment derived from superposition of the four caspase structures (FIG. 3), suggests this insertion to be unique to caspase-8. Three of the lysines in this region
25 (Lys246, Lys250, Lys253) were mutated to arginine in order to obtain diffraction quality crystals. A comparison of wild-type and the mutant form of caspase-8 used to determine the crystal structure showed that both enzymes appear to be indistinguishable, yielding a
30 k_{cat}/K_m of $1 \times 10^5 \text{ M}^{-1}\text{s}^{-1}$ for Ac-DEVD-aminoethylcoumarin (Ac-DEVD-AMC) hydrolysis. Two of these mutated arginines are stabilized by a salt bridge with nearby glutamic residues (Arg250 with Glu249,

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Arg253 with Glu330, Arg246 with a glutamic acid from a symmetry-related neighbor. None of these mutated residues is oriented in the prime side region nor are they in close proximity to the tetrapeptide inhibitor. 5 Leu254, from this helix-turn-helix insertion, appears to point inward towards the prime side region. The spatial position of the helix-turn-helix insertion for caspase-8 most closely resembles a short insertion loop of caspase-1 (FIG. 2C: residues 249-254) which is 10 conserved among the members of the caspase-1 family.

The differences in size of the S4 loop among the four caspases in this study are striking. These loops involve the following residues: caspase-1 (378-386), caspase-3 (244-262), caspase-7 (270-288), 15 caspase-8 (451-463). FIG. 2B illustrates that this loop is largest for caspase-3 and caspase-7. Despite the fact that this loop is identical in length for these two closely related caspases, they are only 63% identical in composition. The same loop is shorter for 20 caspase-8 and shorter still for caspase-1. In each case there is an interaction between the P4 aspartic acid of the Ac-DEVD-CHO inhibitor and a residue in this loop.

25 Binding Of Ac-DEVD-CHO To Caspases From All Three families

The four caspases included in this application span three different functional and phylogenetic groups of caspases and each exhibit subtle differences in the way they bind Ac-DEVD-CHO. Although 30 there are differences in some of the protein amino acids from each caspase contributing to binding Ac-DEVD-CHO, the overall conformation of the inhibitor is highly conserved. The peptide inhibitor has adopted an

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extended conformation in all four complexes. Besides the fact that the catalytic dyad and two residues anchoring the aspartate residue in the P1 position are from the p20 domain, most of the intimate contacts are between the tetrapeptide and the groups from the p10 subunit. Although there are differences in some of the amino acid residues from each caspase that contribute to binding Ac-DEVD-CHO, the overall conformation of the inhibitor is highly conserved. A schematic comparing Ac-DEVD-CHO binding to caspase-1, caspase-3, caspase-7, and caspase-8 is shown in FIG. 4, whereas FIG. 5 shows the surface features of the respective binding sites.

Comparison Of The Binding Of Caspase-1, Caspase-2, Caspase-3 and Caspase-4 To The Tetrapeptide P1-P4 Residues

A schematic comparing Ac-DEVD-CHO binding to caspase-1, caspase-3, caspase-7, and caspase-8 is shown in FIG. 4. FIG. 5 shows the surface features of the respective binding sites.

At the P1 site, all four of the complexes show that the inhibitor is covalently bound to the nucleophilic cysteine in the active site (FIG. 4) although binding to the classic oxyanion hole was not observed. In each case, the thiohemiacetal oxygen resulting from nucleophilic thiol attack on the aldehyde carbonyl forms a hydrogen bond with the adjacent histidine that comprises the enzymes' cysteine-histidine dyad. In addition, the thiohemiacetal oxygen in all four complexes makes hydrogen bonds of varying strength to the nucleophilic cysteine backbone nitrogen and conserved glycine backbone nitrogen. Previous work has shown that some irreversible inhibitors exhibit classic oxyanion hole

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binding to caspase-1 and caspase-3 [N.P.C. Walker et al., Cell, 78, pp. 343-352 (1994); P.R.E. Mittl et al., J. Biol. Chem., 272, pp. 6539-6547 (1997)]. The other interactions at P1 are also strikingly conserved among
5 the four structures. In every case, there are charge-charge interactions between the P1 aspartate sidechain and two arginine residues, as well as a hydrogen bond with a conserved glutamine. FIG. 5 shows the conserved nature of this overwhelmingly electropositive site and
10 the buried nature of the P1 aspartate. Additionally, each complex retains a hydrogen bond between the P1 backbone nitrogen and the backbone carbonyl of a conserved serine.

For the P2 valine of Ac-DEVD-CHO the overall
15 nature of the hydrophobic interaction is conserved, but there are subtle differences in the χ_1 value for the valine sidechain depending on the residues comprising the S2 pocket. Interestingly, caspase-3 and caspase-7 possess an extra residue (phenylalanine) which
20 contributes to the S2 site and is also part of the S4 loop. Caspase-8 also possesses an aromatic residue (Tyr365) at roughly the same spatial position as Phe256 of caspase-3 and Phe282 of caspase-7, but this tyrosine residue is part of an extended strand near the C-
25 terminus of the p20 subunit. Residues corresponding to Tyr365 of caspase-8 are Pro290 (caspase-1), Leu168 (caspase-3, and Leu191 caspase-7). None of these contribute directly to the S2 site in these complexes with Ac-DEVD-CHO.

30 The P3 glutamic acid of the tetrapeptide inhibitor, makes at least one charge-charge interaction with a conserved arginine in all four caspase complexes (FIG. 4). Additionally, the P3 backbone nitrogen and

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carbonyl oxygen of the P3 glutamic acid make strong hydrogen bonds with the respective backbone carbonyl oxygen and nitrogen of the same arginine involved in the surface charge interaction. Caspase-8 also has an
5 additional charge-charge interaction from a second arginine (Arg258) which follows the helix-turn-helix insertion loop. This is in agreement with recent findings in which a similar peptide inhibitor is complexed with caspase-8 [H. Blanchard et al.,
10 Structure (London), 7, pp. 1125-1133 (1999)]. The sequence alignment presented in FIG. 3 suggests that caspase-6, caspase-9, caspase-10 and caspase-14 would also be capable of providing an extra basic amino acid at this position. Analysis of FIG. 5 shows that the P3
15 glutamic acid of the Ac-DEVD-CHO inhibitor is oriented towards this second (i.e. Arg258) arginine on the protein surface of caspase-8. A crystallographic water is observed binding to the conserved arginine for caspase-3, caspase-7, and caspase-8.

20 The major differences for the binding of Ac-DEVD-CHO to caspase-1, caspase-3, caspase-7, and caspase-8 occur at the P4 aspartic acid and the acetylated amino terminus of the tetrapeptide. All of the caspases included in this study involve either
25 direct or indirect binding by the S4 loop. FIG. 4 shows that caspase-1 interacts with the P4 aspartic acid sidechain directly through an interaction with Arg383. Caspase-3 interacts via the backbone nitrogen of Phe250 and the sidechain of Asn208. In this case,
30 there is also an interaction of the P4 aspartic acid with Trp214 through a water mediated hydrogen bond. Additionally, the P4 backbone nitrogen and carbonyl oxygen forms hydrogen bonds to two different water

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molecules both of which form hydrogen bonds to the carbonyl of Phe250. Caspase-7 binds the P4 aspartic acid through both backbone and sidechain involvement of Gln276. The P4 backbone nitrogen forms an additional
5 hydrogen bond with the backbone carbonyl of Gln276 while the P4 backbone carbonyl oxygen forms a hydrogen bond to the same crystallographic water molecule involved in another hydrogen bond with the P2 backbone nitrogen. It is interesting to note that although the
10 caspase-3 and caspase-7 sequences share 57% identity and 67% similarity (FIG. 3) there are significant differences in and around the S4 binding region. The replacement of caspase-3 residues (Asn208, Ser209, Asp211, Phe250, Phe252, Thr255, and Ala258 by their
15 respective caspase-7 residues (Ser234, Pro235, Arg237, Gln276, Asp278, His281, and Glu284) has changed the chemical content (FIG. 5) in the S4 binding region to be more hydrophilic.

Caspase-8 interacts directly with the P4
20 aspartate residue via the sidechain nitrogens of Asn414 and Trp420 that are not part of the S4 loop. However, the P4 aspartate carbonyl oxygen interacts with D455 via a water mediated hydrogen bond.

The N-acetyl P4 capping group also exhibits
25 differences in hydrogen bonding and hydrophobic interactions. Caspase-1, caspase-7, and caspase-8 all make a hydrophobic interaction between the N-acetyl terminal methyl and a proline (FIG. 4). Caspase-3 lacks this hydrophobic interaction, but makes two
30 hydrogen bonds with S209, one involving the S209 backbone nitrogen, the other with the S209 sidechain. Caspase-7 forms a water mediated hydrogen bond with both the backbone nitrogen and sidechain of Asp278.

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For caspase-8, the N-acetyl carbonyl oxygen forms a hydrogen bond to the sidechain of Asn414. No hydrogen bond is observed between caspase-1 and the N-acetyl group. One final observation regarding differences in binding the N-acetyl group occurs between caspase-3 and the other three caspases included in this study. As mentioned above, there are two strong hydrogen bonds between the N-acetyl group and S209 for caspase-3. In caspase-1, caspase-7, and caspase-8, (and caspase-9) however, the residue corresponding to Ser209 is a proline; any hydrogen bonding interactions of the N-acetyl group involve different residues. Due to the inability of the proline ring to form hydrogen bonds, the P4 N-acetyl group is translated approximately 2.5 Å. FIG. 6 illustrates this shift between caspase-3 and caspase-7. These are members of the same caspase subfamily.

The differences in hydrogen bonding of the P4 and N-acetyl groups with the associated caspase residues results in a variable width of the S4 site with caspase-8 having the widest S4 site followed by caspase-1 (FIG. 5); caspase-3 and caspase-7 have a narrower S4 site. For caspase-3 and caspase-7 the reduced width in the S4 site can be directly linked to the greater extent of the hydrogen bond network between this portion of the tetrapeptide and the S4 site which serves to "pull" the walls of the S4 pocket towards the P4 group. On this point, the electrostatic potential surfaces illustrated in FIG. 5 are informative. The surface potential of caspase-7 is unique because it is the only caspase of the four studied which has an unpaired basic residue (Arg237) near the P4 Asp. Caspase-1 and caspase-8 also have basic residues that

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contribute to the electropositive portion of the surface potential in this region, but they also have counterbalancing negative charges near by. Caspase-3 has a neutral S4 region. These observations suggest that in terms of structure and associated surface potential, there should be no absolute requirement for a negatively charged group at P4.

Structural Insights And Binding Specificity

Based on positional scanning of a combinatorial substrate library, Thornberry et al. were able to determine the optimal tetrapeptide substrate sequences for ten human caspases [N.A. Thornberry, J. Biol. Chem., 272, pp. 17907-17911 (1997)]. In this study, a cleavable Asp-AMC was held constant at P1 and the amino acids at P2 through P4 were varied. They found that group I caspases (caspase-1, caspase-4 and caspase-5) loosely preferred the sequence WEHD, while group II caspases (caspase-2, caspase-3, and caspase-7) strongly preferred the motif DEXD. Group III caspases (caspase-6, caspase-8, caspase-9, and caspase-10) preferred the motif (L/V)EXD. This information was subsequently used to design and investigate tetrapeptide aldehyde inhibitors [M. Garcia-Calvo et al., J. Biol. Chem., 273, pp. 32608-32613 (1998)]. Some traditional reversible inhibitors and irreversible inhibitors such as Z-VAD-FMK were also included in the study.

Reported Ki values (nM) from reference sequences for Ac-DEVD-CHO against caspase-1, caspase-3, caspase-7 and caspase-8, respectively, are as follows: 18nM, 0.23nM, 1.6nM, 0.92nM [M. Garcia-Calvo et al., J. Biol. Chem., 273, pp. 32608-32613 (1998)]. Although this tetrapeptide inhibitor is most potent against

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group II and group III caspases, it is the only reported tetrapeptide aldehyde that significantly inhibits representatives from all three groups of caspases. The fact that all caspases considered here
5 can accommodate a valine at P2 attests to the general tolerability for branched amino acids at this position. However, branched amino acids at P2 tend to produce less optimal substrates against caspase-1, caspase-4 and caspase-5 and are typically not present in the best
10 inhibitors for group I caspases [N.A. Thornberry, J. Biol. Chem., 272, pp. 17907-17911 (1997)]. In general, large groups are tolerated as both substrates and inhibitors for all three caspase subfamilies and even though tetrapeptide substrates containing tryptophan,
15 phenylalanine, and tyrosine at P2 are suboptimal, histidine-containing tetrapeptide substrates were generally good against group I and group III caspases [N.A. Thornberry, J. Biol. Chem., 272, pp. 17907-17911 (1997)]. Additionally, in a previous crystallographic
20 study, a non-peptidic pyridone aldehyde inhibitor containing a large 6-benzyl substituent on the pyridone ring was found to place the phenyl ring of the benzyl group over the S2 site in caspase-1 [J.M.C. Golec, Bioorg. Med. Chem. Lett., 7, pp. 2181-2186 (1997)].
25 The optimal residue identified by the combinatorial tetrapeptide substrate library at the P3 position for all three groups of caspases is glutamic acid [N.A. Thornberry et al., J. Biol. Chem., 272, pp. 17907-17911 (1997)]. All four caspases in the present
30 study make at least one charge-charge interaction with the P3 glutamic acid. The nature of this interaction involves an absolutely conserved Arg, however, this salt bridge is on the surface of the protein and is

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solvent exposed. In terms of substrate specificity, such an interaction might be optimal in terms of recognition and proper positioning of the peptide backbone, but would be expected to contribute minimally to the overall binding energetics [S. Dao-Pin, Ciba Found. Symp. (Protein Conform.) 161, pp. 52-62 (1991)]. This is illustrated by the inhibitor Ac-YVAD-CHO which shows good inhibitory potency against caspase-1 and modest inhibitory potency against group III caspases. Although the surface charge-charge interaction(s) would be lost, the P3 valine would be expected to still make the required backbone hydrogen bonds and a potential hydrophobic interaction with a either a proline (caspase-1, caspase-7, caspase-8) β -carbon of serine (caspase-3). The branched P3 valine would also serve to maintain the rigidity of the extended tetrapeptide inhibitor and could potentially improve cell potency due to one less formal charge on the molecule. A recent report of peptidomimetic caspase inhibitors shows reasonably potent inhibition of multiple caspases in a compound class that would be incapable of making a charge-charge interaction with the conserved S3 arginine [J.C. Wu & L.C. Fritz, Methods (Orlando, Fla.), 17, pp. 320-328 (1999)].

In terms of both substrate specificity and inhibitor selectivity, the P4 position offers the most variability. In general, both hydrophobic groups and the anionic aspartate are tolerated at the P4 position for both substrates and inhibitors. For group II and group III caspases, a tryptophan rests at the bottom of the S4 pocket. For group I caspases, this same residue is a smaller hydrophobic amino acid (e.g. Val or Ile, including Val348 in caspase-1). The binding of Ac-

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DEVD-CHO to Csp1 produces fewer total hydrogen bonds with S4 residues relative to the other caspases studied and this allows for a wider S4 pocket. The combination of fewer hydrogen bonds along with a neutral
5 electrostatic potential in this portion of the binding site suggests that group I caspases could accommodate larger hydrophobic groups at S4, thereby, providing an avenue to gain selectivity in the design of inhibitors. The combinatorial tetrapeptide substrate study showed
10 that WEHD was the optimal substrate for caspase-1 and was also a good substrate for the other group I caspases, caspase-4, and caspase-5 [N.A. Thornberry, J. Biol. Chem., 272, pp. 17907-17911 (1997)]. However, leucine was roughly equal to tryptophan at P4 as a
15 substrate for these two caspases. Group II caspases were shown to have a strong preference for substrates with aspartic acid at P4. As alluded to above, the replacement of hydrophobic residues in caspase-3 by charged or hydrophilic residues in caspase-7 might
20 allow these two seemingly redundant caspases to act on different substrates in different cell types or cellular compartments [J.M. Chandler et al., J. Biol. Chem., 273, 10815-10818 (1998); T. Machleidt, Federation of European Biochemical Studies, 436, pp. 51-54 (1998)] even though their *in vitro* substrate
25 preferences are identical. Group III caspases prefer either valine or leucine at the P4 position. Interestingly, in terms of inhibitors, AcWEHD-CHO showed the most potent inhibition against caspase-1
30 suggesting that the valine at the bottom of the S4 pocket leaves enough room for the P4 tryptophan to be accommodated [M. Garcia-Calvo et al., J. Biol. Chem., 273, pp. 32608-32613 (1998)]. Based on the sequence

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alignment in FIG. 3, caspase-4 and caspase-5 would be expected to possess an isoleucine instead of valine at the same position at the bottom of the S4 pocket. This one extra methyl group still allows the P4 tryptophan from AcWEHD-CHO to fit, but not quite as well (caspase-1, $K_i=0.056$ nM; Caspase-4, $K_i=97$ nM; Caspase-5, $K_i=43$ nM). AcWEHD-CHO was a poor inhibitor of all other group II and group III caspases except caspase-8 ($K_i=21$ nM). Although caspase-8 has a large tryptophan residue at the bottom of the S4 pocket, this portion of the binding site is fairly wide and can accommodate the P4 group of AcWEHD-CHO. Similar trends are observed for inhibitors containing tyrosine or benzyloxycarbonyl groups at P4. Additionally, the first selective Csp1 inhibitor to reach clinical trials, VX-740, possesses an isoquinoline group at P4. The X-ray crystallographic structure of this inhibitor clearly shows the P4 isoquinoline fitting snugly in the S4 pocket (manuscript in preparation). Thus, although it is possible to design selective Csp1 inhibitors by incorporation of large hydrophobic groups at P4, it is not clear that one can take advantage of the P4 position to design selective inhibitors of other caspases.

25

EXAMPLE 5

Use of Caspase-7 Coordinates for Inhibitor Design

The coordinates in FIG. 7 are used to design compounds, including inhibitory compounds, that associate with caspase-7 or homologues of caspase-7. This process may be aided by using a machine-readable data storage medium encoded with a set of machine-readable data storage medium encoded with a set of

30

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machine-executable instructions, wherein the recorded instructions are capable of displaying a three-dimensional representation of the caspase-7 complex or a portion thereof. The graphical representation is
5 used according to the methods described herein to design compounds, including inhibitory compounds, that bind to caspase-7. Such compounds may associate with caspase-7 at all or part of the active site.

10 While we have described a number of embodiments of this invention, it is apparent that our basic examples may be altered to provide other embodiments which utilize the products and processes of this invention. Therefore, it will be appreciated that
15 the scope of this invention is to be defined by the appended claims rather than by the specific embodiments which have been represented by way of example.

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CLAIMS

We claim:

1. A molecule or molecular complex
5 comprising all or any part of a binding pocket defined
by structure coordinates of caspase-7 amino acids 234,
235, 237, 276, 278, 281, and 284 according to FIG. 7,
or a homologue of said molecule or molecular complex,
wherein said homologue comprises a binding pocket that
10 has a root mean square deviation from the backbone
atoms of said amino acids of not more than 1.5 Å, and
wherein said molecule or molecular complex has a S4
binding region that is more hydrophilic than the S4
binding region of caspase-3.

15
2. The molecule or molecular complex
according to claim 1, wherein said homologue comprises
a binding pocket that has a root mean square deviation
from the backbone atoms of said amino acids of not more
20 than 1.0 Å.

3. The molecule or molecular complex
according to claim 1, comprising all or any part of a
binding pocket defined by structure coordinates of
25 caspase-7 amino acids 85, 86, 87, 88, 144, 145, 184,
186, 191, 223, 230, 231, 232, 233, 234, 235, 237, 240,
276, 278, 281, 282, and 284 according to FIG. 7, or a
homologue of said molecule or molecular complex,
wherein said homologue comprises a binding pocket that
30 has a root mean square deviation from the backbone
atoms of said amino acids of not more than 1.5 Å, and
wherein said molecule or molecular complex has a S4

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binding region that is more hydrophilic than the S4 binding region of caspase-3.

4. The molecule or molecular complex
5 according to claim 3, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.0 Å.

10 5. The molecule or molecular complex according to claim 3, wherein said molecule or molecular complex is defined by the structure coordinates according to FIG. 7, or a homologue thereof, wherein said homologue has a root mean square
15 deviation from the conserved backbone atoms of said amino acids of not more than 1.5 Å, and wherein said molecule or molecular complex has a S4 binding region that is more hydrophilic than the S4 binding region of caspase-3.

20 6. The molecule or molecular complex according to claim 5, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more
25 than 1.0 Å.

7. The molecule or molecular complex according to claim 1, wherein said molecule or molecular complex comprises the structure coordinates
30 of caspase-7 amino acids 58-302 according to FIG. 7.

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8. A crystallizable composition comprising a caspase-7 or homologue thereof complexed with Ac-Asp-Glu-Val-Asp-CHO.

5 9. The crystallizable composition according to claim 8, wherein the caspase-7 has amino acids 1-303.

10 10. A crystal comprising a caspase-7 or homologue thereof complexed with Ac-Asp-Glu-Val-Asp-CHO.

15 11. The crystal according to claim 10, wherein the caspase-7 has amino acids 1-303.

20 12. A machine-readable data storage medium, comprising a data storage material encoded with machine readable data, wherein said data is defined by the all or a portion of the structure coordinates of a molecule or molecular complex according to FIG. 7, or a homologue of said molecule or molecular complex, wherein said homologue comprises backbone atoms that have a root mean square deviation from the backbone atoms of the complex of not more than 1.5 Å, and
25 wherein said molecule or molecular complex has a S4 binding region that is more hydrophilic than the S4 binding region of caspase-3.

30 13. The machine-readable data storage medium according to claim 12, wherein said data is defined by all or a portion of the structure coordinates of caspase-7 amino acids 58-302 according to FIG. 7, or a homologue of said caspase-7, said homologue having a

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root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

14. A machine-readable data storage medium
5 comprising a data storage material encoded with a first set of machine readable data which, when combined with a second set of machine readable data using a machine programmed with instructions for using said first set of data and said second set of data, can determine at
10 least a portion of the structure coordinates corresponding to the second set of machine readable data, wherein: said first set of data and said second set of data comprises a Fourier transform of at least a portion of the structure coordinates of caspase-7
15 according to FIG. 7; said second set of data comprises an X-ray diffraction pattern of a molecule or molecular complex of unknown structure.

15. A computer for producing a three-
20 dimensional representation of:

a. a molecule or molecular complex comprising all or any part of a binding pocket defined by structure coordinates of caspase-7 amino acids 234, 235, 237, 276, 278, 281, and 284 according to FIG. 7;

25 or

b. a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more
30 than 1.5 Å, and wherein said molecule or molecular complex has a S4 binding region that is more hydrophilic than the S4 binding region of caspase-3, wherein said computer comprises:

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i. a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises the structure coordinates of caspase-7 amino acids 234,
5 235, 237, 276, 278, 281, and 284 according to FIG. 7; and

ii. instructions for processing said machine-readable data into said three-dimensional representation.

10

16. The computer according to claim 15, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.0 Å.

15

17. The computer according to claim 15, wherein:

a. the molecule or molecular complex comprises all or any part of a binding pocket defined
20 by structure coordinates of caspase-7 amino acids 85, 86, 87, 88, 144, 145, 184, 186, 191, 223, 230, 231, 232, 233, 234, 235, 237, 240, 276, 278, 281, 282, and 284 according to FIG. 7; or

b. a homologue of said molecule or
25 molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, and wherein said molecule or molecular complex has a S4 binding region that is more
30 hydrophilic than the S4 binding region of caspase-3 wherein said computer comprises:

i. a machine-readable data storage medium comprising a data storage material encoded with

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machine-readable data, wherein said data comprises the structure coordinates of caspase-7 amino acids 85, 86, 87, 88, 144, 145, 184, 186, 191, 223, 230, 231, 232, 233, 234, 235, 237, 240, 276, 278, 281, 282, and 284 according to FIG. 7; and

ii. instructions for processing said machine-readable data into said three-dimensional representation.

10 18. The computer according to claim 17, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.0 Å.

15 19. The computer according to claim 17, wherein:

a. said molecule or molecular complex comprises structure coordinates according to FIG. 7; or

b. a homologue of said molecule or
20 molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, and wherein said molecule or molecular complex has a S4 binding region that is more
25 hydrophilic than the S4 binding region of caspase-3 wherein said computer comprises:

i. a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises the structure coordinates according to FIG. 7;

30 ii. instructions for processing said machine-readable data into said three-dimensional representation.

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20. The computer according to claim 23,
wherein said homologue comprises a binding pocket that
has a root mean square deviation from the backbone
5 atoms of said amino acids of not more than 1.0 Å.

21. The computer according to claim 17,
wherein:

a. said molecule or molecular complex
10 comprises all or any part of a binding pocket defined
by structure coordinates of caspase-7 amino acids 58-
302 according to FIG. 7; wherein said computer
comprises:

i. a machine-readable data storage
15 medium comprising a data storage material encoded with
machine-readable data, wherein said data comprises the
structure coordinates of caspase-7 amino acids 58-302
according to FIG. 7;

ii. instructions for processing said
20 machine-readable data into said three-dimensional
representation.

22. The computer according to any one of
claims 15-21, further comprising a display for
25 displaying said three-dimensional representation.

23. A computer for determining at least a
portion of the structure coordinates corresponding to
X-ray diffraction data obtained from a molecule or
30 molecular complex, wherein said computer comprises:

a. a machine-readable data storage
medium comprising a data storage material encoded with
machine-readable data, wherein said data comprises at

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least a portion of the structure coordinates of caspase-7 according to FIG. 7;

b. a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises X-ray diffraction data obtained from said molecule or molecular complex; and

c. instructions for performing a Fourier transform of the machine readable data of (a) and for processing said machine readable data of (b) into structure coordinates.

24. The computer according to claim 23, further comprising a display for displaying said three-dimensional representation.

25. A method for evaluating the ability of a chemical entity to associate with a molecule or molecular complex according to any one of claims 1-7 comprising the steps of:

a. employing computational means to perform a fitting operation between the chemical entity and a binding pocket of the molecule or molecular complex; and

b. analyzing the results of said fitting operation to quantify the association between the chemical entity and the binding pocket.

26. A method for identifying a potential agonist or antagonist of a molecule or molecular complex according to any one of claims 1-7 comprising the steps of:

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a. generating a three-dimensional structure of the molecule or molecular complex;

b. employing said three-dimensional structure to design or select said potential agonist or antagonist;

c. providing said potential agonist or antagonist; and

d. contacting said potential agonist or antagonist to interact with said molecule.

10

27. A method of utilizing molecular replacement to obtain structural information about a molecule or a molecular complex of unknown structure by using the structure coordinates set forth in FIG. 7, comprising the steps of:

15

a. crystallizing said molecule or molecular complex;

b. generating a X-ray diffraction pattern from said crystallized molecule or molecular complex; and

20

c. applying at least a portion of the structure coordinates set forth in FIG. 7 to said X-ray diffraction pattern to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex whose structure is unknown.

25

28. The method according to claim 27, wherein the molecule or molecular complex of unknown structure comprises a polypeptide selected from a caspase-7 subunit or a capase-7 homologue.

30

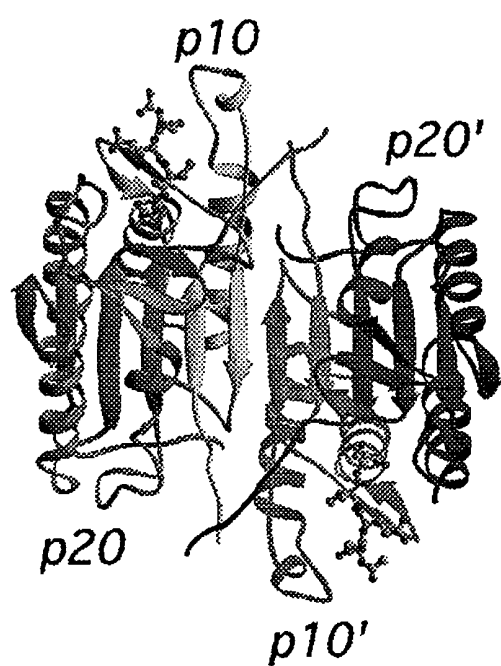


FIG. 1A

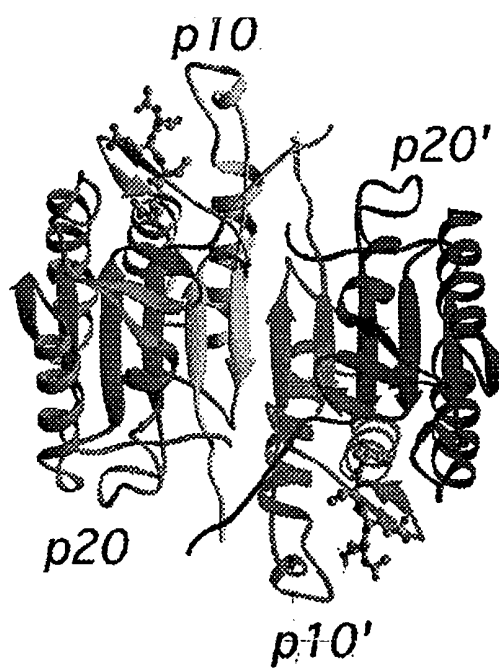
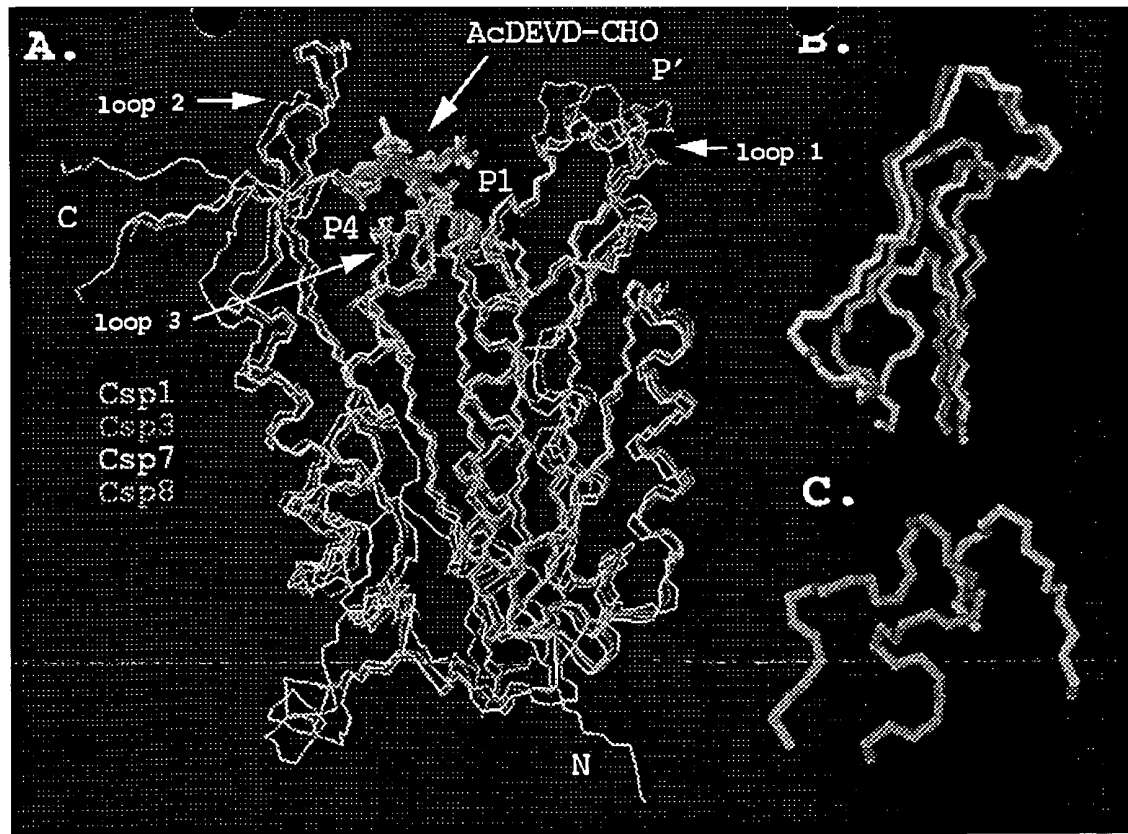


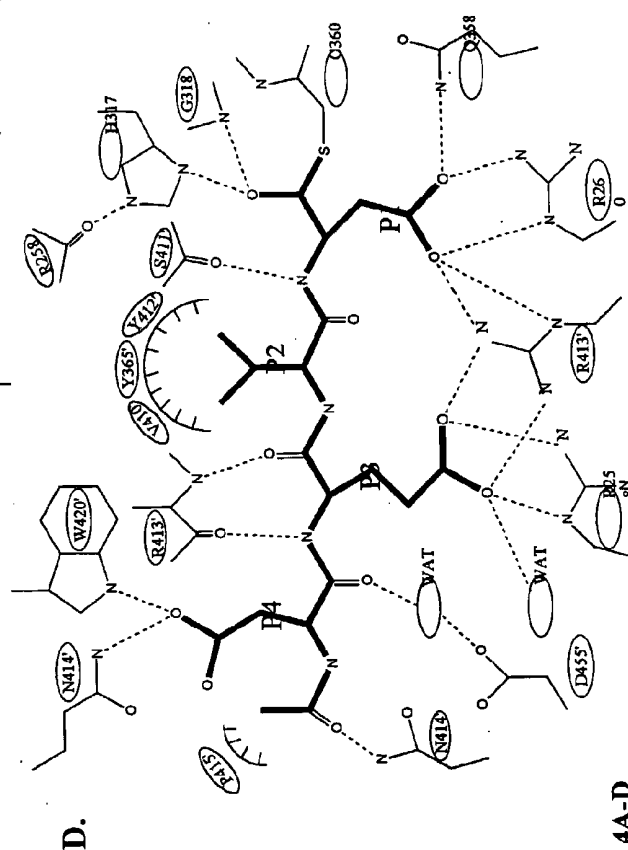
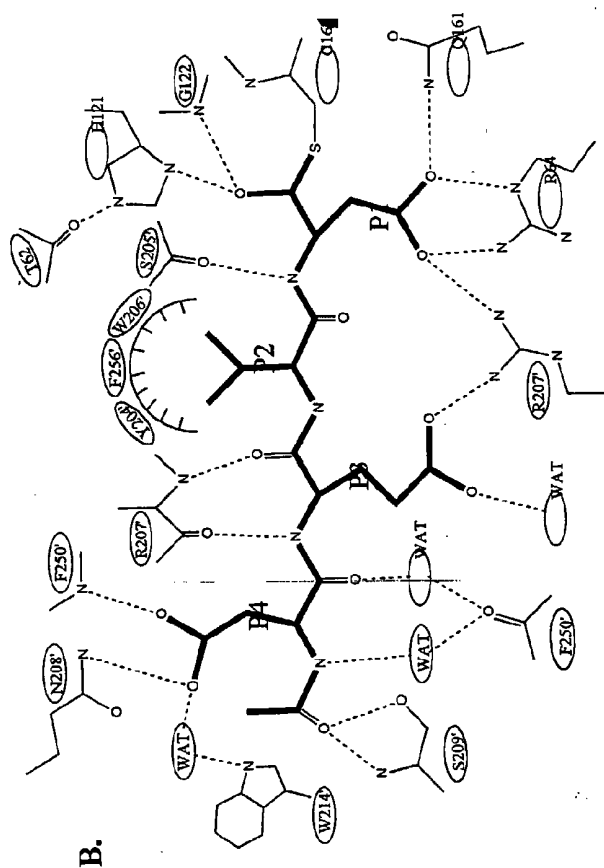
FIG. 1B



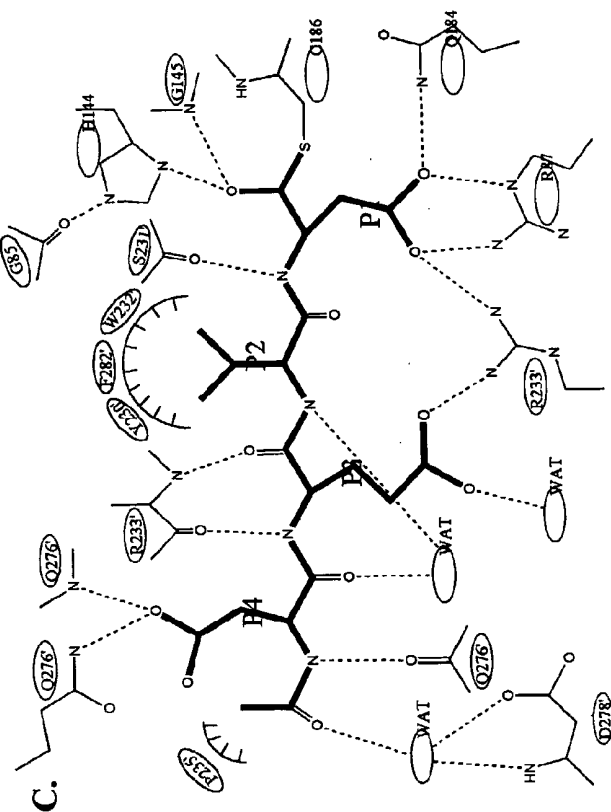
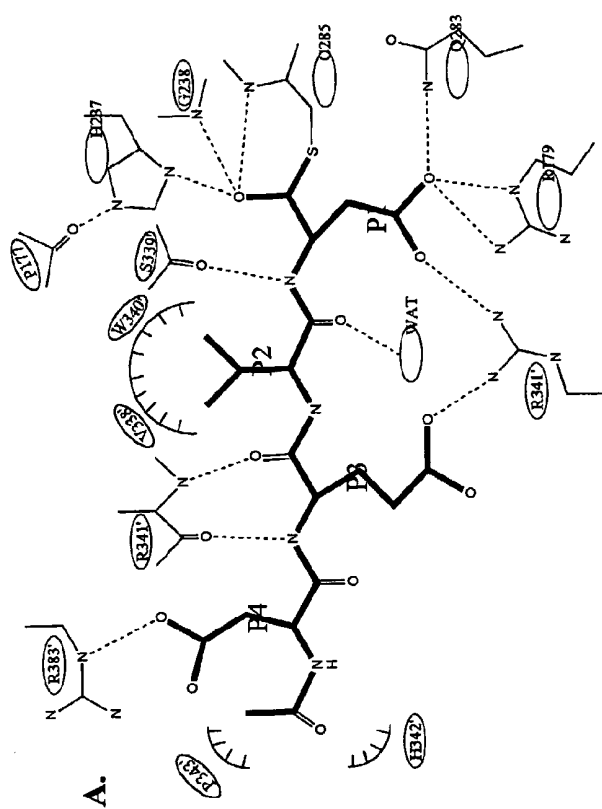
FIGS. 2A-C

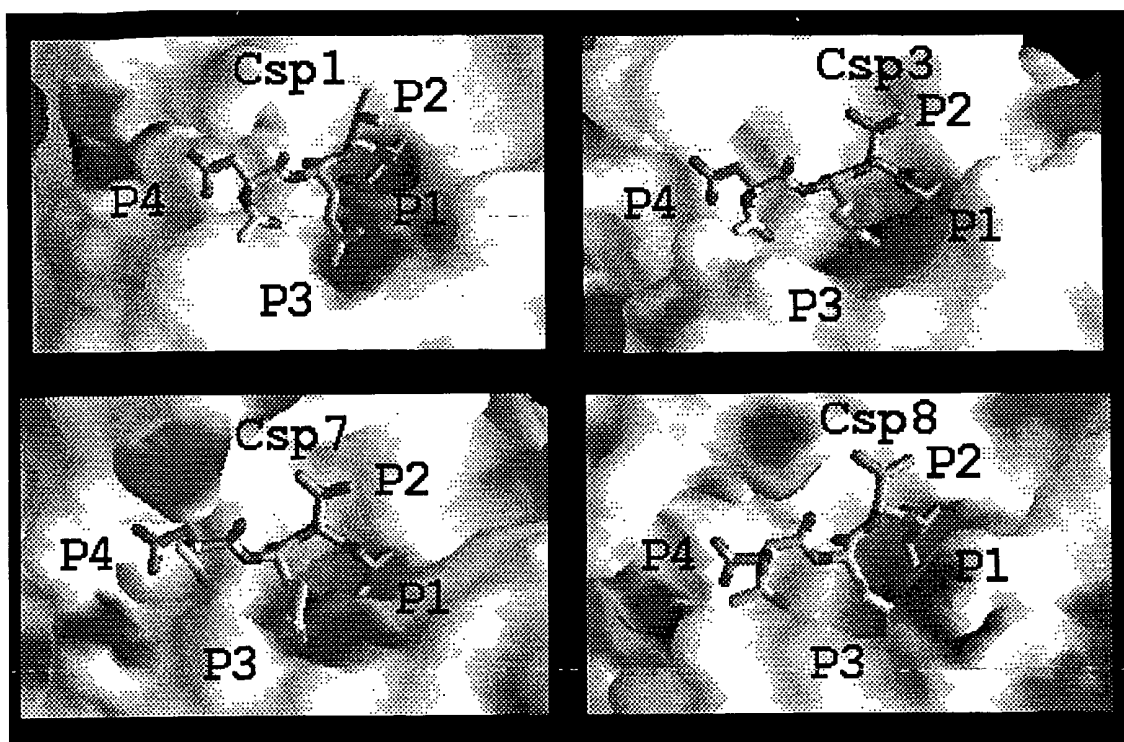
CSP01 155	████KSSRTLALIIICNEEF-----DSI████GTGAEVDITGMTMLLQ
CSP03 37	YKMDYPEMGLCIIINNKNF-----HKSTGMTSR████SGTDVDAANLRETFR
CSP07 60	YNMNFELGKCIINNKNF-----DKVTGMGVVRNGTDKDAEALFKCFR
CSP08 226	YQMSKPRGYCLIIINNHNFAKAREKVPKLHSIRDR████RNGTHLDAGALTTTFE
CSP01 195	NLGYSVDVKKNLTASDMTTELEAFAHRPEHKTS DSTFLVFMSS████HGIREGIC
CSP03 80	NLKYEVNRKNDLTREEIV-ELMRDVSKEDHSKRSSFVCVLLS████HGEEGIIF
CSP07 103	SLGFDVIVYND CSCAKMQ-DLLKKASEEDHTNAACFACILLS████HGEENVIIY
CSP08 276	ELHFEIKPHDDCTVEQIY-EILKIYQLMDHSNMDCFICCILLS████HGDKGIY
CSP01 245	GKKHSEQVPDILQLNAIFNMLNTKNCPSLKD KPKVIIIO████ACRGDSPGVVW
CSP03 129	GTNG-----PVDLKKITNFRGDRCSRSLTGKPKLFIIO████ACRGTELD CGI
CSP07 152	GKDG-----VTPIKDLTAHFRGDRCKTLLEKPKLFFIO████ACRGTELD DGI
CSP08 325	GTDGQE-----APIYELTSQFTGLKCPSLAGKPKVFFIO████ACQGDNYQKGI
CSP01 295	FKDSVGVSGNLSLPTTEEFEDDAI-----KKAHIEKDFIAFCSST
CSP03 173	ETDSGVDDDMACH-----KIPVDADFLYAYSTA
CSP07 196	QADSGPINDTDANPRY-----KIPVEADFLFAYSTV
CSP08 370	PVETDSEEQPY-----LEMDLSSPQTRYIPDEADFLLG MATV
CSP01 335	PDNV████VSWRHPTMGSVFIGRLIEHMQEYACSCDVEE IFRKVRFSFEQPDG--
CSP03 201	PGYIYSWRNSKDGSW████FIQSLCAMLKQYADKLEFMHILTRVNRKVATEFESF
CSP07 227	PGYIYSWRSP████GRGSWFVQALCSILEEHGKDLEIMQILTRVND RVARHFESQ
CSP08 407	NNC████VSYRNP████AEGTWYIQSLCQSLRERCPRGDDILTILTEVNYEVS NK---
CSP01 383	-----████RAQMPTTERVTLTRCFYLFPGH
CSP03 251	SFDATE████HAKKQIP CIV-SMLTKELYFYH
CSP07 277	S████DPHF████HEKKQIPCVV-SMLTKELYFSQ
CSP08 454	--D████KKNMGKQMPQPT-FTLRKKLVF PSD

FIG. 3



FIGS. 4A-D





FIGS. 5A-D

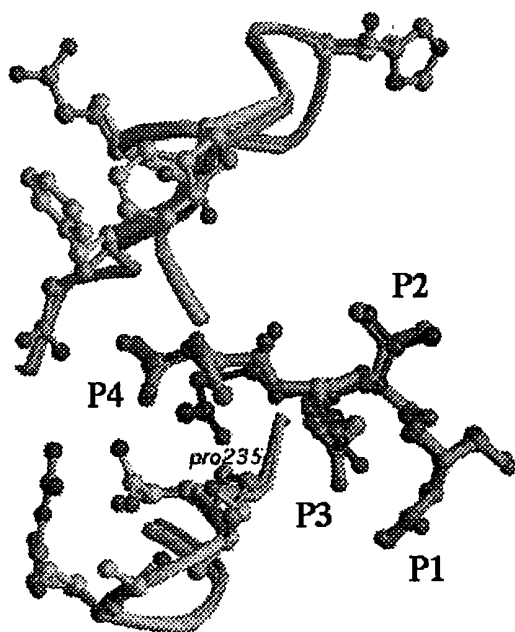


FIG. 6A

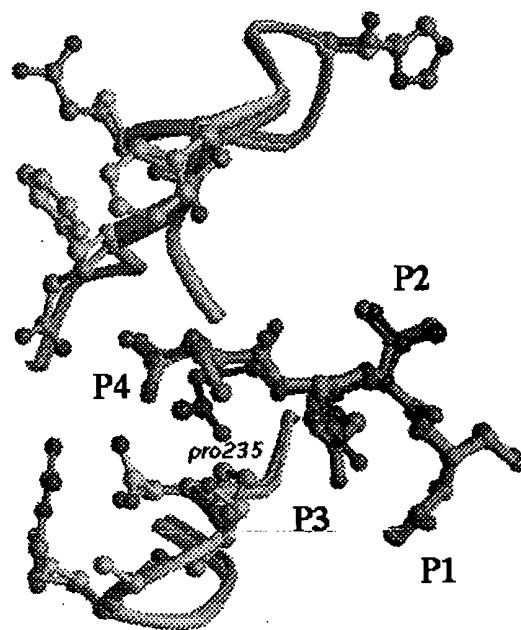


FIG. 6B

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
1	N	TYR	A	58	71.407	27.908	15.171	1	48.5
2	CA	TYR	A	58	70.067	27.257	15.182	1	49.42
3	C	TYR	A	58	69.095	27.978	14.256	1	46.64
4	O	TYR	A	58	67.912	27.652	14.226	1	46.12
5	CB	TYR	A	58	69.505	27.195	16.61	1	50.97
6	CG	TYR	A	58	70.35	26.354	17.544	1	55.34
7	CD1	TYR	A	58	70.505	24.986	17.329	1	57.69
8	CD2	TYR	A	58	71.048	26.939	18.605	1	57.76
9	CE1	TYR	A	58	71.344	24.218	18.146	1	61.9
10	CE2	TYR	A	58	71.892	26.183	19.43	1	58.39
11	CZ	TYR	A	58	72.039	24.823	19.195	1	61.08
12	OH	TYR	A	58	72.885	24.07	19.987	1	62.53
13	N	GLN	A	59	69.61	28.955	13.509	1	47.02
14	CA	GLN	A	59	68.831	29.746	12.555	1	46.86
15	C	GLN	A	59	69.432	29.608	11.171	1	43.35
16	O	GLN	A	59	70.649	29.45	11.038	1	44.53
17	CB	GLN	A	59	68.855	31.225	12.928	1	50.65
18	CG	GLN	A	59	67.582	31.724	13.566	1	59.97
19	CD	GLN	A	59	67.787	32.12	15.006	1	65.99
20	OE1	GLN	A	59	68.274	31.326	15.821	1	68.29
21	NE2	GLN	A	59	67.437	33.361	15.33	1	70.85
22	N	TYR	A	60	68.586	29.687	10.149	1	40.27
23	CA	TYR	A	60	69.058	29.585	8.772	1	35.84
24	C	TYR	A	60	69.733	30.887	8.4	1	35.18
25	O	TYR	A	60	69.156	31.955	8.596	1	34.78
26	CB	TYR	A	60	67.894	29.332	7.811	1	29.92
27	CG	TYR	A	60	67.469	27.881	7.673	1	22.93
28	CD1	TYR	A	60	68.346	26.913	7.179	1	21.17
29	CD2	TYR	A	60	66.172	27.492	7.992	1	23.95
30	CE1	TYR	A	60	67.927	25.587	7.005	1	18.01
31	CE2	TYR	A	60	65.747	26.177	7.823	1	17.97
32	CZ	TYR	A	60	66.622	25.235	7.331	1	18.02
33	OH	TYR	A	60	66.158	23.955	7.159	1	20.38
34	N	ASN	A	61	70.97	30.8	7.912	1	37.89
35	CA	ASN	A	61	71.732	31.983	7.484	1	41.04
36	C	ASN	A	61	70.945	32.713	6.414	1	42.42
37	O	ASN	A	61	70.641	32.148	5.367	1	43.98
38	CB	ASN	A	61	73.097	31.593	6.902	1	42.91
39	CG	ASN	A	61	73.856	32.793	6.313	1	43.78
40	OD1	ASN	A	61	73.565	33.95	6.628	1	41.79
41	ND2	ASN	A	61	74.831	32.512	5.461	1	42.59
42	N	MET	A	62	70.6	33.959	6.685	1	42.08
43	CA	MET	A	62	69.834	34.739	5.737	1	43.87
44	C	MET	A	62	70.707	35.763	5.019	1	45.45
45	O	MET	A	62	70.201	36.644	4.315	1	44.46
46	CB	MET	A	62	68.669	35.407	6.46	1	38.95
47	CG	MET	A	62	67.7	34.41	7.045	1	39.51
48	SD	MET	A	62	66.744	33.515	5.788	1	47.51
49	CE	MET	A	62	67.604	31.949	5.767	1	41.38
50	N	ASN	A	63	72.02	35.607	5.158	1	47.56
51	CA	ASN	A	63	72.973	36.522	4.543	1	51.28
52	C	ASN	A	63	73.281	36.191	3.083	1	49.2

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Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
53	O	ASN	A	63	74.249	35.49	2.772	1	50.08
54	CB	ASN	A	63	74.262	36.592	5.367	1	58.31
55	CG	ASN	A	63	75.293	37.544	4.767	1	65.94
56	OD1	ASN	A	63	76.437	37.153	4.504	1	73.08
57	ND2	ASN	A	63	74.895	38.8	4.549	1	65.38
58	N	PHE	A	64	72.417	36.678	2.202	1	45.79
59	CA	PHE	A	64	72.536	36.484	0.766	1	43
60	C	PHE	A	64	71.951	37.729	0.16	1	43.2
61	O	PHE	A	64	71.117	38.375	0.791	1	46.27
62	CB	PHE	A	64	71.741	35.265	0.347	1	38.99
63	CG	PHE	A	64	72.256	34.015	0.945	1	38.01
64	CD1	PHE	A	64	73.303	33.338	0.35	1	38.5
65	CD2	PHE	A	64	71.761	33.554	2.153	1	39.43
66	CE1	PHE	A	64	73.858	32.217	0.955	1	44.12
67	CE2	PHE	A	64	72.311	32.437	2.764	1	39.41
68	CZ	PHE	A	64	73.36	31.767	2.167	1	39.76
69	N	GLU	A	65	72.392	38.098	-1.037	1	42.81
70	CA	GLU	A	65	71.868	39.314	-1.649	1	41.81
71	C	GLU	A	65	70.398	39.183	-2.023	1	39.86
72	O	GLU	A	65	69.705	40.183	-2.224	1	38.62
73	CB	GLU	A	65	72.709	39.738	-2.855	1	46.32
74	CG	GLU	A	65	72.826	38.699	-3.942	1	52.04
75	CD	GLU	A	65	73.293	39.292	-5.252	1	53.57
76	OE1	GLU	A	65	74.464	39.722	-5.317	1	56.94
77	OE2	GLU	A	65	72.485	39.325	-6.21	1	57.38
78	N	LYS	A	66	69.927	37.947	-2.124	1	37.48
79	CA	LYS	A	66	68.538	37.705	-2.457	1	38.54
80	C	LYS	A	66	67.934	36.761	-1.424	1	37.76
81	O	LYS	A	66	68.609	35.841	-0.939	1	35.87
82	CB	LYS	A	66	68.416	37.034	-3.835	1	40.86
83	CG	LYS	A	66	69.016	37.794	-5.001	1	47.98
84	CD	LYS	A	66	69.283	36.873	-6.203	1	51.46
85	CE	LYS	A	66	68.037	36.593	-7.05	1	55.83
86	NZ	LYS	A	66	66.986	35.699	-6.445	1	58.66
87	N	LEU	A	67	66.678	37.016	-1.062	1	35.14
88	CA	LEU	A	67	65.964	36.123	-0.162	1	35.92
89	C	LEU	A	67	65.772	34.862	-1.004	1	38.09
90	O	LEU	A	67	66.227	33.779	-0.621	1	42.93
91	CB	LEU	A	67	64.598	36.689	0.239	1	34.01
92	CG	LEU	A	67	63.688	35.799	1.101	1	34.09
93	CD1	LEU	A	67	64.415	35.22	2.308	1	34.69
94	CD2	LEU	A	67	62.513	36.61	1.571	1	32.06
95	N	GLY	A	68	65.141	35.01	-2.17	1	35.86
96	CA	GLY	A	68	64.943	33.866	-3.032	1	33.58
97	C	GLY	A	68	63.799	34.065	-3.99	1	37.21
98	O	GLY	A	68	63.1	35.087	-3.939	1	35.73
99	N	LYS	A	69	63.63	33.105	-4.892	1	36.58
100	CA	LYS	A	69	62.556	33.172	-5.862	1	40.04
101	C	LYS	A	69	61.276	32.651	-5.237	1	36.59
102	O	LYS	A	69	61.306	31.822	-4.328	1	38.2
103	CB	LYS	A	69	62.882	32.353	-7.136	1	45.94
104	CG	LYS	A	69	61.784	32.466	-8.232	1	55.43

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
105	CD	LYS	A	69	62.031	31.622	-9.493	1	63.43
106	CE	LYS	A	69	60.987	31.967	-10.596	1	69.81
107	NZ	LYS	A	69	60.977	31.081	-11.825	1	66.84
108	N	CYS	A	70	60.153	33.147	-5.728	1	32.73
109	CA	CYS	A	70	58.867	32.701	-5.256	1	32.56
110	C	CYS	A	70	57.957	32.536	-6.475	1	30.3
111	O	CYS	A	70	57.612	33.501	-7.153	1	32.15
112	CB	CYS	A	70	58.279	33.689	-4.231	1	30.62
113	SG	CYS	A	70	56.603	33.281	-3.671	1	31.62
114	N	ILE	A	71	57.645	31.29	-6.782	1	27.79
115	CA	ILE	A	71	56.782	30.946	-7.892	1	27.99
116	C	ILE	A	71	55.359	30.768	-7.39	1	29.9
117	O	ILE	A	71	55.121	29.945	-6.511	1	36.63
118	CB	ILE	A	71	57.225	29.602	-8.51	1	24.33
119	CG1	ILE	A	71	58.574	29.759	-9.183	1	25.63
120	CG2	ILE	A	71	56.193	29.083	-9.485	1	27.32
121	CD1	ILE	A	71	59.114	28.458	-9.722	1	29.58
122	N	ILE	A	72	54.411	31.526	-7.923	1	28.72
123	CA	ILE	A	72	53.025	31.362	-7.517	1	26.62
124	C	ILE	A	72	52.26	30.814	-8.712	1	30.92
125	O	ILE	A	72	52.131	31.506	-9.726	1	32.94
126	CB	ILE	A	72	52.366	32.697	-7.115	1	25.39
127	CG1	ILE	A	72	53.003	33.246	-5.834	1	26.48
128	CG2	ILE	A	72	50.842	32.512	-6.957	1	25.06
129	CD1	ILE	A	72	52.419	34.576	-5.402	1	23.82
130	N	ILE	A	73	51.789	29.575	-8.614	1	28.7
131	CA	ILE	A	73	51.017	28.961	-9.688	1	28.94
132	C	ILE	A	73	49.549	29.177	-9.348	1	30.03
133	O	ILE	A	73	49.043	28.606	-8.403	1	30.54
134	CB	ILE	A	73	51.376	27.453	-9.847	1	28.16
135	CG1	ILE	A	73	52.774	27.322	-10.474	1	22.42
136	CG2	ILE	A	73	50.338	26.735	-10.683	1	26
137	CD1	ILE	A	73	53.292	25.917	-10.569	1	22.51
138	N	ASN	A	74	48.868	30.016	-10.115	1	31.43
139	CA	ASN	A	74	47.475	30.336	-9.843	1	28.99
140	C	ASN	A	74	46.5	29.73	-10.851	1	30.14
141	O	ASN	A	74	46.151	30.372	-11.835	1	35.04
142	CB	ASN	A	74	47.333	31.866	-9.803	1	29.68
143	CG	ASN	A	74	45.914	32.323	-9.507	1	30.21
144	OD1	ASN	A	74	45.142	31.613	-8.871	1	32.18
145	ND2	ASN	A	74	45.561	33.512	-9.984	1	24.21
146	N	ASN	A	75	46.007	28.528	-10.573	1	29.81
147	CA	ASN	A	75	45.078	27.835	-11.466	1	26.62
148	C	ASN	A	75	43.611	28.103	-11.172	1	30.34
149	O	ASN	A	75	43.039	27.522	-10.26	1	32.98
150	CB	ASN	A	75	45.339	26.327	-11.438	1	22.5
151	CG	ASN	A	75	46.705	25.959	-11.995	1	23.87
152	OD1	ASN	A	75	47.481	26.825	-12.384	1	24.05
153	ND2	ASN	A	75	47.009	24.673	-12.02	1	20.18
154	N	LYS	A	76	42.981	28.902	-12.027	1	34.35
155	CA	LYS	A	76	41.571	29.273	-11.88	1	36.59
156	C	LYS	A	76	40.565	28.631	-12.847	1	40.94

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Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
157	O	LYS	A	76	39.419	28.346	-12.473	1	41.57
158	CB	LYS	A	76	41.444	30.791	-12.002	1	32.42
159	CG	LYS	A	76	40.027	31.311	-11.89	1	28.96
160	CD	LYS	A	76	40.032	32.812	-11.737	1	26.37
161	CE	LYS	A	76	38.616	33.335	-11.633	1	29.12
162	NZ	LYS	A	76	38.604	34.817	-11.613	1	29.74
163	N	ASN	A	77	40.983	28.43	-14.092	1	43.9
164	CA	ASN	A	77	40.102	27.885	-15.124	1	44.48
165	C	ASN	A	77	40.616	26.539	-15.595	1	44.66
166	O	ASN	A	77	41.765	26.42	-16.02	1	46.73
167	CB	ASN	A	77	40.035	28.859	-16.302	1	45.58
168	CG	ASN	A	77	39.668	30.277	-15.871	1	45.93
169	OD1	ASN	A	77	38.52	30.558	-15.521	1	47.09
170	ND2	ASN	A	77	40.647	31.178	-15.903	1	46.49
171	N	PHE	A	78	39.757	25.531	-15.56	1	44.72
172	CA	PHE	A	78	40.165	24.188	-15.955	1	47.28
173	C	PHE	A	78	39.492	23.661	-17.224	1	47.72
174	O	PHE	A	78	38.438	24.156	-17.644	1	48.45
175	CB	PHE	A	78	39.95	23.221	-14.773	1	45.28
176	CG	PHE	A	78	40.743	23.591	-13.556	1	43.1
177	CD1	PHE	A	78	40.334	24.643	-12.736	1	44.57
178	CD2	PHE	A	78	41.941	22.945	-13.269	1	41.59
179	CE1	PHE	A	78	41.115	25.051	-11.646	1	43.57
180	CE2	PHE	A	78	42.723	23.345	-12.186	1	42.27
181	CZ	PHE	A	78	42.311	24.4	-11.373	1	40.21
182	N	ASP	A	79	40.141	22.687	-17.854	1	47.85
183	CA	ASP	A	79	39.616	22.061	-19.056	1	48.49
184	C	ASP	A	79	38.401	21.254	-18.636	1	52.15
185	O	ASP	A	79	38.406	20.593	-17.597	1	54.46
186	CB	ASP	A	79	40.655	21.133	-19.688	1	44.44
187	CG	ASP	A	79	41.795	21.887	-20.37	1	44.53
188	OD1	ASP	A	79	41.709	23.13	-20.533	1	41.07
189	OD2	ASP	A	79	42.779	21.217	-20.762	1	44.01
190	N	LYS	A	80	37.365	21.286	-19.458	1	56.62
191	CA	LYS	A	80	36.146	20.565	-19.151	1	60.64
192	C	LYS	A	80	36.336	19.066	-19.035	1	60.02
193	O	LYS	A	80	35.513	18.387	-18.431	1	60.12
194	CB	LYS	A	80	35.061	20.921	-20.158	1	67.39
195	CG	LYS	A	80	34.645	22.401	-20.101	1	75.39
196	CD	LYS	A	80	34.236	22.843	-18.671	1	82.45
197	CE	LYS	A	80	35.412	23.431	-17.864	1	83.7
198	NZ	LYS	A	80	35.088	23.642	-16.424	1	84.03
199	N	VAL	A	81	37.428	18.556	-19.595	1	60.7
200	CA	VAL	A	81	37.728	17.131	-19.506	1	63.7
201	C	VAL	A	81	38.061	16.757	-18.057	1	66.22
202	O	VAL	A	81	37.9	15.602	-17.656	1	69.32
203	CB	VAL	A	81	38.924	16.725	-20.409	1	63.08
204	CG1	VAL	A	81	40.202	17.451	-19.985	1	64.14
205	CG2	VAL	A	81	39.135	15.212	-20.351	1	64.32
206	N	THR	A	82	38.588	17.72	-17.299	1	67
207	CA	THR	A	82	38.932	17.496	-15.894	1	63.32
208	C	THR	A	82	37.618	17.587	-15.133	1	64.13

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
209	O	THR	A	82	37.402	16.895	-14.136	1	65
210	CB	THR	A	82	39.874	18.591	-15.353	1	58.72
211	OG1	THR	A	82	39.149	19.822	-15.224	1	53.61
212	CG2	THR	A	82	41.058	18.79	-16.286	1	56.95
213	N	GLY	A	83	36.746	18.463	-15.613	1	64.03
214	CA	GLY	A	83	35.461	18.638	-14.983	1	62.99
215	C	GLY	A	83	35.612	19.359	-13.67	1	61.81
216	O	GLY	A	83	34.852	19.099	-12.74	1	64.6
217	N	MET	A	84	36.61	20.237	-13.58	1	60.3
218	CA	MET	A	84	36.842	21.006	-12.36	1	57.68
219	C	MET	A	84	36.298	22.412	-12.556	1	56.56
220	O	MET	A	84	36.471	23.004	-13.621	1	58.86
221	CB	MET	A	84	38.329	21.061	-12.008	1	57.13
222	CG	MET	A	84	38.971	19.706	-11.704	1	59.1
223	SD	MET	A	84	38.087	18.611	-10.524	1	60.03
224	CE	MET	A	84	37.613	19.749	-9.261	1	58.1
225	N	GLY	A	85	35.649	22.947	-11.526	1	54.44
226	CA	GLY	A	85	35.067	24.275	-11.617	1	49.15
227	C	GLY	A	85	35.998	25.457	-11.441	1	49.06
228	O	GLY	A	85	37.076	25.343	-10.86	1	47.79
229	N	VAL	A	86	35.56	26.61	-11.934	1	49.11
230	CA	VAL	A	86	36.335	27.838	-11.832	1	48.55
231	C	VAL	A	86	36.502	28.172	-10.36	1	48.03
232	O	VAL	A	86	35.529	28.216	-9.599	1	48.77
233	CB	VAL	A	86	35.631	29.018	-12.556	1	48.71
234	CG1	VAL	A	86	36.409	30.31	-12.378	1	45.37
235	CG2	VAL	A	86	35.504	28.706	-14.037	1	56.13
236	N	ARG	A	87	37.746	28.38	-9.961	1	44.98
237	CA	ARG	A	87	38.048	28.709	-8.586	1	43.1
238	C	ARG	A	87	37.928	30.204	-8.345	1	42.14
239	O	ARG	A	87	38.909	30.944	-8.458	1	44.78
240	CB	ARG	A	87	39.451	28.224	-8.231	1	42.21
241	CG	ARG	A	87	39.634	26.722	-8.373	1	42.25
242	CD	ARG	A	87	41.004	26.31	-7.9	1	44.4
243	NE	ARG	A	87	41.219	26.747	-6.526	1	45.25
244	CZ	ARG	A	87	42.131	27.631	-6.145	1	45.04
245	NH1	ARG	A	87	42.943	28.187	-7.028	1	48.88
246	NH2	ARG	A	87	42.192	27.995	-4.874	1	49.32
247	N	ASN	A	88	36.724	30.652	-8.019	1	40.37
248	CA	ASN	A	88	36.503	32.06	-7.743	1	41.23
249	C	ASN	A	88	37.203	32.441	-6.464	1	40.24
250	O	ASN	A	88	37.218	31.67	-5.507	1	42.03
251	CB	ASN	A	88	35.022	32.352	-7.593	1	45.45
252	CG	ASN	A	88	34.266	32.07	-8.853	1	52.22
253	OD1	ASN	A	88	34.423	32.773	-9.854	1	50.48
254	ND2	ASN	A	88	33.479	30.999	-8.843	1	57.31
255	N	GLY	A	89	37.777	33.635	-6.458	1	38.72
256	CA	GLY	A	89	38.482	34.135	-5.3	1	33.25
257	C	GLY	A	89	39.957	33.83	-5.357	1	32.71
258	O	GLY	A	89	40.731	34.401	-4.59	1	33.54
259	N	THR	A	90	40.371	32.972	-6.284	1	33.2
260	CA	THR	A	90	41.784	32.623	-6.37	1	35.22

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
261	C	THR	A	90	42.694	33.738	-6.841	1	36.54
262	O	THR	A	90	43.868	33.765	-6.481	1	37.67
263	CB	THR	A	90	42.036	31.356	-7.188	1	37.24
264	OG1	THR	A	90	43.369	30.904	-6.932	1	34.94
265	CG2	THR	A	90	41.851	31.616	-8.674	1	34.61
266	N	ASP	A	91	42.16	34.678	-7.617	1	41.79
267	CA	ASP	A	91	42.975	35.803	-8.07	1	45.94
268	C	ASP	A	91	43.257	36.736	-6.903	1	45.71
269	O	ASP	A	91	44.347	37.323	-6.824	1	46.65
270	CB	ASP	A	91	42.315	36.561	-9.218	1	49.92
271	CG	ASP	A	91	42.399	35.814	-10.538	1	53.67
272	OD1	ASP	A	91	43.286	34.943	-10.702	1	52.51
273	OD2	ASP	A	91	41.573	36.118	-11.424	1	56.48
274	N	LYS	A	92	42.277	36.878	-6.004	1	45.75
275	CA	LYS	A	92	42.453	37.697	-4.799	1	43.9
276	C	LYS	A	92	43.576	37.079	-3.953	1	41.41
277	O	LYS	A	92	44.485	37.78	-3.486	1	40.83
278	CB	LYS	A	92	41.179	37.738	-3.961	1	48.22
279	CG	LYS	A	92	40.091	38.614	-4.496	1	53.27
280	CD	LYS	A	92	39.026	38.826	-3.436	1	59.53
281	CE	LYS	A	92	37.831	39.583	-4.005	1	65.55
282	NZ	LYS	A	92	37.142	38.809	-5.083	1	69.5
283	N	ASP	A	93	43.533	35.758	-3.79	1	36.2
284	CA	ASP	A	93	44.56	35.078	-3.02	1	35.93
285	C	ASP	A	93	45.906	35.402	-3.61	1	36.46
286	O	ASP	A	93	46.779	35.932	-2.929	1	38.24
287	CB	ASP	A	93	44.36	33.565	-3.049	1	38.02
288	CG	ASP	A	93	43.197	33.108	-2.192	1	39.44
289	OD1	ASP	A	93	42.714	33.899	-1.353	1	38.27
290	OD2	ASP	A	93	42.769	31.95	-2.359	1	38.61
291	N	ALA	A	94	46.046	35.136	-4.904	1	36.89
292	CA	ALA	A	94	47.298	35.38	-5.608	1	35.23
293	C	ALA	A	94	47.826	36.792	-5.45	1	32.19
294	O	ALA	A	94	49.002	36.984	-5.145	1	30.18
295	CB	ALA	A	94	47.155	35.038	-7.073	1	38.52
296	N	GLU	A	95	46.972	37.785	-5.648	1	31.39
297	CA	GLU	A	95	47.431	39.157	-5.52	1	32.36
298	C	GLU	A	95	47.918	39.455	-4.108	1	33.37
299	O	GLU	A	95	48.958	40.102	-3.927	1	36.46
300	CB	GLU	A	95	46.339	40.124	-5.909	1	32.06
301	CG	GLU	A	95	46.87	41.528	-6.07	1	34.41
302	CD	GLU	A	95	45.781	42.518	-6.42	1	38.44
303	OE1	GLU	A	95	44.707	42.083	-6.91	1	40.94
304	OE2	GLU	A	95	45.996	43.731	-6.195	1	39.67
305	N	ALA	A	96	47.167	38.973	-3.115	1	31.8
306	CA	ALA	A	96	47.506	39.15	-1.699	1	23.85
307	C	ALA	A	96	48.825	38.456	-1.419	1	19.43
308	O	ALA	A	96	49.763	39.058	-0.891	1	20.07
309	CB	ALA	A	96	46.42	38.554	-0.834	1	26.09
310	N	LEU	A	97	48.907	37.19	-1.807	1	17.86
311	CA	LEU	A	97	50.129	36.418	-1.62	1	23.58
312	C	LEU	A	97	51.294	37.109	-2.316	1	28.52

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
313	O	LEU	A	97	52.424	37.082	-1.825	1	35.26
314	CB	LEU	A	97	49.968	35.001	-2.171	1	25.24
315	CG	LEU	A	97	49.106	33.987	-1.409	1	26.18
316	CD1	LEU	A	97	48.793	32.805	-2.29	1	28.44
317	CD2	LEU	A	97	49.824	33.537	-0.148	1	28.31
318	N	PHE	A	98	51.014	37.735	-3.46	1	33.72
319	CA	PHE	A	98	52.032	38.436	-4.225	1	29.77
320	C	PHE	A	98	52.567	39.581	-3.381	1	29.96
321	O	PHE	A	98	53.783	39.748	-3.259	1	31.81
322	CB	PHE	A	98	51.472	38.958	-5.562	1	32.79
323	CG	PHE	A	98	52.515	39.613	-6.438	1	29.02
324	CD1	PHE	A	98	53.306	38.849	-7.287	1	31.76
325	CD2	PHE	A	98	52.764	40.977	-6.341	1	30.06
326	CE1	PHE	A	98	54.338	39.43	-8.018	1	28.75
327	CE2	PHE	A	98	53.792	41.569	-7.066	1	30.01
328	CZ	PHE	A	98	54.58	40.793	-7.903	1	30.03
329	N	LYS	A	99	51.672	40.357	-2.776	1	31.38
330	CA	LYS	A	99	52.105	41.471	-1.926	1	33.19
331	C	LYS	A	99	52.883	41.024	-0.684	1	33.09
332	O	LYS	A	99	53.939	41.583	-0.384	1	33.02
333	CB	LYS	A	99	50.926	42.353	-1.541	1	35.88
334	CG	LYS	A	99	50.361	43.08	-2.735	1	45.54
335	CD	LYS	A	99	49.182	43.975	-2.402	1	49.7
336	CE	LYS	A	99	48.713	44.732	-3.648	1	48.8
337	NZ	LYS	A	99	48.421	43.788	-4.755	1	51.85
338	N	CYS	A	100	52.423	39.962	-0.026	1	34.39
339	CA	CYS	A	100	53.102	39.455	1.169	1	35.09
340	C	CYS	A	100	54.502	38.972	0.887	1	32.42
341	O	CYS	A	100	55.467	39.519	1.422	1	38.09
342	CB	CYS	A	100	52.308	38.332	1.841	1	36.8
343	SG	CYS	A	100	50.761	38.902	2.558	1	54.06
344	N	PHE	A	101	54.632	37.972	0.021	1	31.26
345	CA	PHE	A	101	55.948	37.433	-0.289	1	25.98
346	C	PHE	A	101	56.911	38.452	-0.875	1	27.58
347	O	PHE	A	101	58.112	38.375	-0.636	1	32.95
348	CB	PHE	A	101	55.831	36.17	-1.127	1	25.98
349	CG	PHE	A	101	55.338	34.979	-0.337	1	22.23
350	CD1	PHE	A	101	54.037	34.956	0.179	1	24.66
351	CD2	PHE	A	101	56.187	33.91	-0.067	1	16.93
352	CE1	PHE	A	101	53.584	33.876	0.964	1	19.21
353	CE2	PHE	A	101	55.751	32.835	0.71	1	21.78
354	CZ	PHE	A	101	54.444	32.819	1.227	1	18.69
355	N	ARG	A	102	56.379	39.456	-1.568	1	30.63
356	CA	ARG	A	102	57.2	40.524	-2.133	1	31.8
357	C	ARG	A	102	57.732	41.323	-0.94	1	34.86
358	O	ARG	A	102	58.939	41.597	-0.842	1	32.78
359	CB	ARG	A	102	56.344	41.42	-3.027	1	32.33
360	CG	ARG	A	102	57.002	42.719	-3.475	1	36.96
361	CD	ARG	A	102	57.783	42.563	-4.77	1	35.98
362	NE	ARG	A	102	58.975	41.743	-4.609	1	35.69
363	CZ	ARG	A	102	60.162	42.21	-4.23	1	37.03
364	NH1	ARG	A	102	60.326	43.496	-3.969	1	30.68

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Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
365	NH2	ARG	A	102	61.2	41.386	-4.123	1	41.25
366	N	SER	A	103	56.826	41.661	-0.015	1	36.55
367	CA	SER	A	103	57.184	42.398	1.195	1	34.16
368	C	SER	A	103	58.279	41.635	1.91	1	32.21
369	O	SER	A	103	59.262	42.229	2.348	1	33.71
370	CB	SER	A	103	55.988	42.537	2.13	1	38.43
371	OG	SER	A	103	54.992	43.367	1.571	1	49.11
372	N	LEU	A	104	58.12	40.314	2.008	1	29.6
373	CA	LEU	A	104	59.138	39.492	2.654	1	32.83
374	C	LEU	A	104	60.463	39.626	1.903	1	36.02
375	O	LEU	A	104	61.518	39.36	2.471	1	40.1
376	CB	LEU	A	104	58.735	38.012	2.712	1	31.66
377	CG	LEU	A	104	57.562	37.575	3.583	1	31.24
378	CD1	LEU	A	104	57.436	36.068	3.522	1	26.71
379	CD2	LEU	A	104	57.788	38.035	5.013	1	30.51
380	N	GLY	A	105	60.407	39.979	0.618	1	35.72
381	CA	GLY	A	105	61.628	40.15	-0.147	1	35.63
382	C	GLY	A	105	61.937	39.061	-1.16	1	36.45
383	O	GLY	A	105	63.077	38.917	-1.6	1	38.27
384	N	PHE	A	106	60.943	38.247	-1.475	1	35.98
385	CA	PHE	A	106	61.107	37.196	-2.466	1	35.34
386	C	PHE	A	106	60.893	37.877	-3.812	1	35.87
387	O	PHE	A	106	60.208	38.905	-3.889	1	33.62
388	CB	PHE	A	106	60.001	36.147	-2.324	1	34.84
389	CG	PHE	A	106	60.266	35.098	-1.283	1	36
390	CD1	PHE	A	106	61.161	34.053	-1.541	1	34.95
391	CD2	PHE	A	106	59.587	35.125	-0.055	1	37.58
392	CE1	PHE	A	106	61.382	33.042	-0.601	1	31.19
393	CE2	PHE	A	106	59.8	34.122	0.894	1	32.18
394	CZ	PHE	A	106	60.701	33.075	0.617	1	35.75
395	N	ASP	A	107	61.487	37.319	-4.864	1	37.28
396	CA	ASP	A	107	61.297	37.837	-6.225	1	34.11
397	C	ASP	A	107	60.198	36.921	-6.751	1	30.29
398	O	ASP	A	107	60.458	35.776	-7.127	1	31.29
399	CB	ASP	A	107	62.575	37.689	-7.05	1	33.97
400	CG	ASP	A	107	63.758	38.376	-6.399	1	36.79
401	OD1	ASP	A	107	63.693	39.603	-6.134	1	38.96
402	OD2	ASP	A	107	64.752	37.671	-6.135	1	41.4
403	N	VAL	A	108	58.957	37.384	-6.647	1	28.46
404	CA	VAL	A	108	57.809	36.578	-7.054	1	29.4
405	C	VAL	A	108	57.307	36.804	-8.48	1	27.91
406	O	VAL	A	108	57.359	37.917	-9.01	1	27.03
407	CB	VAL	A	108	56.634	36.69	-5.994	1	24.46
408	CG1	VAL	A	108	56.547	38.069	-5.454	1	27.09
409	CG2	VAL	A	108	55.299	36.287	-6.585	1	25.46
410	N	ILE	A	109	56.89	35.712	-9.109	1	28.33
411	CA	ILE	A	109	56.342	35.744	-10.459	1	29.73
412	C	ILE	A	109	55.111	34.85	-10.42	1	28.18
413	O	ILE	A	109	55.199	33.709	-9.961	1	28.61
414	CB	ILE	A	109	57.376	35.225	-11.501	1	32.12
415	CG1	ILE	A	109	58.589	36.158	-11.519	1	30.55
416	CG2	ILE	A	109	56.77	35.196	-12.902	1	30.4

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Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
417	CD1	ILE	A	109	59.769	35.61	-12.253	1	33.71
418	N	VAL	A	110	53.959	35.396	-10.812	1	26.21
419	CA	VAL	A	110	52.705	34.636	-10.818	1	26.95
420	C	VAL	A	110	52.367	34.046	-12.208	1	30.53
421	O	VAL	A	110	52.259	34.782	-13.194	1	30.81
422	CB	VAL	A	110	51.524	35.515	-10.374	1	24.78
423	CG1	VAL	A	110	50.267	34.663	-10.227	1	23.23
424	CG2	VAL	A	110	51.859	36.235	-9.083	1	24.91
425	N	TYR	A	111	52.189	32.727	-12.268	1	29.25
426	CA	TYR	A	111	51.87	32.022	-13.499	1	26.71
427	C	TYR	A	111	50.427	31.533	-13.43	1	28.08
428	O	TYR	A	111	50.069	30.774	-12.535	1	30.22
429	CB	TYR	A	111	52.818	30.839	-13.688	1	25.55
430	CG	TYR	A	111	54.287	31.211	-13.668	1	32.24
431	CD1	TYR	A	111	54.908	31.788	-14.781	1	34.64
432	CD2	TYR	A	111	55.064	30.98	-12.533	1	35.84
433	CE1	TYR	A	111	56.28	32.124	-14.762	1	37.42
434	CE2	TYR	A	111	56.429	31.31	-12.5	1	39.95
435	CZ	TYR	A	111	57.034	31.879	-13.616	1	41.45
436	OH	TYR	A	111	58.387	32.168	-13.575	1	42
437	N	ASN	A	112	49.598	31.984	-14.368	1	29.6
438	CA	ASN	A	112	48.189	31.607	-14.389	1	31.94
439	C	ASN	A	112	47.828	30.391	-15.235	1	32.66
440	O	ASN	A	112	48.571	29.977	-16.123	1	36.1
441	CB	ASN	A	112	47.321	32.799	-14.77	1	36.34
442	CG	ASN	A	112	47.474	33.973	-13.8	1	42.42
443	OD1	ASN	A	112	46.765	34.062	-12.799	1	45.61
444	ND2	ASN	A	112	48.379	34.892	-14.117	1	43.6
445	N	ASP	A	113	46.689	29.808	-14.89	1	35.94
446	CA	ASP	A	113	46.134	28.615	-15.508	1	35.95
447	C	ASP	A	113	47.122	27.635	-16.126	1	36.34
448	O	ASP	A	113	46.886	27.135	-17.214	1	41.65
449	CB	ASP	A	113	45.045	28.988	-16.512	1	37.46
450	CG	ASP	A	113	43.884	29.733	-15.873	1	41.84
451	OD1	ASP	A	113	43.562	29.457	-14.706	1	45.91
452	OD2	ASP	A	113	43.29	30.602	-16.541	1	42.2
453	N	CYS	A	114	48.208	27.319	-15.427	1	35.15
454	CA	CYS	A	114	49.184	26.376	-15.97	1	33.02
455	C	CYS	A	114	48.599	24.996	-16.185	1	35.88
456	O	CYS	A	114	47.516	24.667	-15.69	1	39.06
457	CB	CYS	A	114	50.393	26.231	-15.057	1	26.33
458	SG	CYS	A	114	51.208	27.773	-14.671	1	34.09
459	N	SER	A	115	49.33	24.185	-16.935	1	37.99
460	CA	SER	A	115	48.936	22.813	-17.216	1	36.46
461	C	SER	A	115	49.992	21.987	-16.507	1	36.14
462	O	SER	A	115	51.091	22.482	-16.237	1	36.04
463	CB	SER	A	115	49.011	22.553	-18.714	1	40.9
464	OG	SER	A	115	50.321	22.824	-19.189	1	42.18
465	N	CYS	A	116	49.711	20.717	-16.271	1	36.18
466	CA	CYS	A	116	50.665	19.872	-15.558	1	40.25
467	C	CYS	A	116	52.107	19.948	-16.06	1	41.01
468	O	CYS	A	116	53.048	20.021	-15.26	1	43.93

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
469	CB	CYS	A	116	50.17	18.42	-15.527	1	38.89
470	SG	CYS	A	116	48.442	18.264	-14.982	1	44.06
471	N	ALA	A	117	52.284	19.984	-17.376	1	41.11
472	CA	ALA	A	117	53.622	20.034	-17.959	1	39.35
473	C	ALA	A	117	54.264	21.37	-17.676	1	38.99
474	O	ALA	A	117	55.457	21.455	-17.33	1	37.77
475	CB	ALA	A	117	53.554	19.798	-19.45	1	41.97
476	N	LYS	A	118	53.453	22.415	-17.822	1	38.45
477	CA	LYS	A	118	53.907	23.773	-17.591	1	36.51
478	C	LYS	A	118	54.423	23.848	-16.171	1	34.91
479	O	LYS	A	118	55.541	24.299	-15.938	1	31.57
480	CB	LYS	A	118	52.759	24.754	-17.804	1	37.42
481	CG	LYS	A	118	53.114	26.199	-17.52	1	44.32
482	CD	LYS	A	118	54.354	26.635	-18.274	1	47.22
483	CE	LYS	A	118	54.589	28.131	-18.12	1	51.63
484	NZ	LYS	A	118	55.817	28.574	-18.838	1	51.97
485	N	MET	A	119	53.633	23.307	-15.244	1	36.9
486	CA	MET	A	119	53.971	23.298	-13.821	1	35.16
487	C	MET	A	119	55.268	22.559	-13.585	1	35.31
488	O	MET	A	119	56.189	23.1	-12.966	1	35.68
489	CB	MET	A	119	52.856	22.661	-12.996	1	35.25
490	CG	MET	A	119	51.567	23.441	-12.994	1	35.85
491	SD	MET	A	119	50.396	22.877	-11.727	1	49.58
492	CE	MET	A	119	49.75	21.397	-12.449	1	39.63
493	N	GLN	A	120	55.364	21.344	-14.118	1	35.64
494	CA	GLN	A	120	56.577	20.55	-13.957	1	37.47
495	C	GLN	A	120	57.79	21.251	-14.547	1	38.4
496	O	GLN	A	120	58.898	21.162	-14.004	1	36.64
497	CB	GLN	A	120	56.411	19.176	-14.591	1	42.42
498	CG	GLN	A	120	55.508	18.238	-13.799	1	53.7
499	CD	GLN	A	120	56.039	17.923	-12.389	1	57.6
500	OE1	GLN	A	120	57.238	18.077	-12.094	1	56.38
501	NE2	GLN	A	120	55.142	17.462	-11.52	1	58.03
502	N	ASP	A	121	57.573	21.974	-15.646	1	40.69
503	CA	ASP	A	121	58.658	22.689	-16.293	1	40.5
504	C	ASP	A	121	59.089	23.869	-15.442	1	38.2
505	O	ASP	A	121	60.282	24.067	-15.211	1	37.76
506	CB	ASP	A	121	58.262	23.172	-17.689	1	43.46
507	CG	ASP	A	121	59.436	23.798	-18.434	1	45.77
508	OD1	ASP	A	121	60.482	23.115	-18.58	1	44.16
509	OD2	ASP	A	121	59.327	24.976	-18.842	1	45.64
510	N	LEU	A	122	58.104	24.656	-15.009	1	37.94
511	CA	LEU	A	122	58.304	25.832	-14.154	1	37.44
512	C	LEU	A	122	59.186	25.444	-12.967	1	37.92
513	O	LEU	A	122	60.155	26.134	-12.622	1	40.07
514	CB	LEU	A	122	56.944	26.297	-13.635	1	35.88
515	CG	LEU	A	122	56.385	27.686	-13.954	1	36.71
516	CD1	LEU	A	122	57.143	28.362	-15.064	1	33.68
517	CD2	LEU	A	122	54.906	27.567	-14.284	1	27.92
518	N	LEU	A	123	58.873	24.299	-12.371	1	37.99
519	CA	LEU	A	123	59.638	23.827	-11.236	1	35.69
520	C	LEU	A	123	60.978	23.203	-11.603	1	36.19

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Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
521	O	LEU	A	123	61.981	23.446	-10.928	1	38.3
522	CB	LEU	A	123	58.771	22.946	-10.337	1	37.57
523	CG	LEU	A	123	57.993	23.912	-9.414	1	41.64
524	CD1	LEU	A	123	56.529	24.061	-9.813	1	40.14
525	CD2	LEU	A	123	58.106	23.457	-7.982	1	45.23
526	N	LYS	A	124	61.028	22.448	-12.699	1	36.45
527	CA	LYS	A	124	62.29	21.846	-13.127	1	34.46
528	C	LYS	A	124	63.282	22.938	-13.473	1	32.35
529	O	LYS	A	124	64.437	22.91	-13.069	1	30.84
530	CB	LYS	A	124	62.072	20.974	-14.347	1	39.17
531	CG	LYS	A	124	63.337	20.33	-14.866	1	41.89
532	CD	LYS	A	124	62.992	19.262	-15.883	1	45.38
533	CE	LYS	A	124	64.151	18.303	-16.09	1	48.45
534	NZ	LYS	A	124	65.309	18.962	-16.749	1	49.12
535	N	LYS	A	125	62.805	23.913	-14.222	1	32.82
536	CA	LYS	A	125	63.631	25.024	-14.627	1	37.02
537	C	LYS	A	125	64.087	25.833	-13.426	1	38.12
538	O	LYS	A	125	65.283	26.093	-13.263	1	40.76
539	CB	LYS	A	125	62.862	25.914	-15.601	1	41.24
540	CG	LYS	A	125	62.589	25.254	-16.928	1	46.43
541	CD	LYS	A	125	63.891	24.92	-17.653	1	52.85
542	CE	LYS	A	125	63.606	24.192	-18.953	1	54.93
543	NZ	LYS	A	125	62.483	24.856	-19.68	1	59.08
544	N	ALA	A	126	63.139	26.235	-12.581	1	38.57
545	CA	ALA	A	126	63.465	27.019	-11.398	1	34.01
546	C	ALA	A	126	64.537	26.315	-10.559	1	31.22
547	O	ALA	A	126	65.52	26.931	-10.143	1	29.95
548	CB	ALA	A	126	62.216	27.289	-10.592	1	35.37
549	N	SER	A	127	64.408	25.004	-10.404	1	30.72
550	CA	SER	A	127	65.379	24.237	-9.637	1	35.02
551	C	SER	A	127	66.725	24.259	-10.311	1	38.7
552	O	SER	A	127	67.741	23.986	-9.675	1	45.94
553	CB	SER	A	127	64.947	22.777	-9.491	1	35.42
554	OG	SER	A	127	65.316	22.011	-10.623	1	37.39
555	N	GLU	A	128	66.728	24.54	-11.612	1	43.08
556	CA	GLU	A	128	67.96	24.571	-12.393	1	40.92
557	C	GLU	A	128	68.718	25.892	-12.396	1	39.21
558	O	GLU	A	128	69.846	25.954	-12.884	1	42.21
559	CB	GLU	A	128	67.693	24.071	-13.811	1	45.04
560	CG	GLU	A	128	67.323	22.586	-13.85	1	48.99
561	CD	GLU	A	128	66.741	22.126	-15.178	1	53.14
562	OE1	GLU	A	128	66.146	22.944	-15.922	1	53.83
563	OE2	GLU	A	128	66.866	20.919	-15.463	1	55.6
564	N	GLU	A	129	68.118	26.943	-11.848	1	35.1
565	CA	GLU	A	129	68.793	28.233	-11.778	1	34.43
566	C	GLU	A	129	69.928	28.2	-10.761	1	36.69
567	O	GLU	A	129	70.131	27.207	-10.064	1	40.14
568	CB	GLU	A	129	67.816	29.323	-11.38	1	34.6
569	CG	GLU	A	129	66.621	29.418	-12.283	1	40.17
570	CD	GLU	A	129	65.855	30.704	-12.089	1	44.84
571	OE1	GLU	A	129	66.486	31.73	-11.746	1	48.43
572	OE2	GLU	A	129	64.618	30.692	-12.292	1	51.71

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Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
573	N	ASP	A	130	70.662	29.297	-10.657	1	39.87
574	CA	ASP	A	130	71.753	29.366	-9.7	1	42.42
575	C	ASP	A	130	71.274	30.067	-8.439	1	43.89
576	O	ASP	A	130	71.205	31.304	-8.365	1	42.54
577	CB	ASP	A	130	72.957	30.106	-10.267	1	45.87
578	CG	ASP	A	130	74.119	30.132	-9.299	1	49.5
579	OD1	ASP	A	130	74.313	29.116	-8.609	1	51.47
580	OD2	ASP	A	130	74.831	31.156	-8.214	1	54.26
581	N	HIS	A	131	70.999	29.264	-7.421	1	45.19
582	CA	HIS	A	131	70.506	29.789	-6.16	1	42.15
583	C	HIS	A	131	71.609	30.106	-5.159	1	41.18
584	O	HIS	A	131	71.343	30.34	-3.993	1	42.94
585	CB	HIS	A	131	69.499	28.814	-5.578	1	36.74
586	CG	HIS	A	131	68.324	28.561	-6.472	1	31.38
587	ND1	HIS	A	131	67.247	29.418	-6.547	1	27.6
588	CD2	HIS	A	131	68.039	27.527	-7.3	1	31.74
589	CE1	HIS	A	131	66.345	28.921	-7.374	1	30.81
590	NE2	HIS	A	131	66.803	27.775	-7.846	1	30.66
591	N	THR	A	132	72.836	30.199	-5.648	1	40.48
592	CA	THR	A	132	73.965	30.486	-4.793	1	41.31
593	C	THR	A	132	73.839	31.792	-4.029	1	43.75
594	O	THR	A	132	74.269	31.87	-2.887	1	47.2
595	CB	THR	A	132	75.261	30.483	-5.599	1	42.49
596	OG1	THR	A	132	75.421	29.201	-6.215	1	48.71
597	CG2	THR	A	132	76.454	30.724	-4.702	1	45.27
598	N	ASN	A	133	73.243	32.812	-4.638	1	47.08
599	CA	ASN	A	133	73.089	34.117	-3.975	1	48.1
600	C	ASN	A	133	71.745	34.311	-3.265	1	46.93
601	O	ASN	A	133	71.37	35.445	-2.928	1	46.2
602	CB	ASN	A	133	73.294	35.262	-4.979	1	53.61
603	CG	ASN	A	133	74.755	35.729	-5.076	1	60.89
604	OD1	ASN	A	133	75.659	35.161	-4.451	1	62.84
605	ND2	ASN	A	133	74.985	36.774	-5.874	1	62.43
606	N	ALA	A	134	71.042	33.209	-3.011	1	45.65
607	CA	ALA	A	134	69.732	33.258	-2.364	1	44.6
608	C	ALA	A	134	69.671	32.435	-1.089	1	42.4
609	O	ALA	A	134	70.263	31.361	-1.009	1	43.61
610	CB	ALA	A	134	68.666	32.779	-3.332	1	45.16
611	N	ALA	A	135	68.939	32.933	-0.099	1	40.51
612	CA	ALA	A	135	68.804	32.225	1.171	1	38.3
613	C	ALA	A	135	67.883	31.023	1.055	1	35.64
614	O	ALA	A	135	68.138	29.973	1.633	1	36.91
615	CB	ALA	A	135	68.296	33.168	2.252	1	40.11
616	N	CYS	A	136	66.812	31.169	0.294	1	34.61
617	CA	CYS	A	136	65.873	30.078	0.145	1	35.64
618	C	CYS	A	136	65.087	30.113	-1.172	1	34.76
619	O	CYS	A	136	65.436	30.845	-2.102	1	35.17
620	CB	CYS	A	136	64.919	30.063	1.348	1	35.12
621	SG	CYS	A	136	63.807	31.483	1.511	1	36.06
622	N	PHE	A	137	64.04	29.292	-1.241	1	32.74
623	CA	PHE	A	137	63.163	29.196	-2.397	1	28.92
624	C	PHE	A	137	61.755	28.953	-1.882	1	28.4

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Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
625	O	PHE	A	137	61.562	28.15	-0.971	1	30.56
626	CB	PHE	A	137	63.577	28.012	-3.286	1	27.97
627	CG	PHE	A	137	62.595	27.707	-4.389	1	30.75
628	CD1	PHE	A	137	62.505	28.541	-5.52	1	28.82
629	CD2	PHE	A	137	61.708	26.626	-4.272	1	30.14
630	CE1	PHE	A	137	61.539	28.305	-6.509	1	24.85
631	CE2	PHE	A	137	60.739	26.381	-5.264	1	27.36
632	CZ	PHE	A	137	60.655	27.225	-6.378	1	28.45
633	N	ALA	A	138	60.778	29.632	-2.473	1	26.92
634	CA	ALA	A	138	59.385	29.451	-2.097	1	27.56
635	C	ALA	A	138	58.521	29.219	-3.333	1	29.78
636	O	ALA	A	138	58.729	29.843	-4.373	1	32.84
637	CB	ALA	A	138	58.874	30.665	-1.347	1	25.38
638	N	CYS	A	139	57.541	28.338	-3.206	1	26.42
639	CA	CYS	A	139	56.625	28.053	-4.285	1	25.86
640	C	CYS	A	139	55.235	27.894	-3.675	1	26.15
641	O	CYS	A	139	55.069	27.144	-2.727	1	27.71
642	CB	CYS	A	139	57.041	26.773	-5.013	1	26.46
643	SG	CYS	A	139	55.74	26.095	-6.081	1	27.33
644	N	ILE	A	140	54.25	28.615	-4.203	1	24.11
645	CA	ILE	A	140	52.884	28.548	-3.712	1	23.7
646	C	ILE	A	140	51.972	28.003	-4.803	1	25.48
647	O	ILE	A	140	51.934	28.548	-5.892	1	29.29
648	CB	ILE	A	140	52.389	29.95	-3.319	1	24.6
649	CG1	ILE	A	140	53.323	30.536	-2.255	1	16.02
650	CG2	ILE	A	140	50.908	29.898	-2.875	1	22.4
651	CD1	ILE	A	140	53.365	32.024	-2.251	1	16.63
652	N	LEU	A	141	51.218	26.955	-4.49	1	26.61
653	CA	LEU	A	141	50.305	26.306	-5.421	1	23.25
654	C	LEU	A	141	48.839	26.522	-5.082	1	25.03
655	O	LEU	A	141	48.364	25.993	-4.097	1	32.61
656	CB	LEU	A	141	50.563	24.806	-5.413	1	21.76
657	CG	LEU	A	141	51.931	24.366	-5.918	1	29.24
658	CD1	LEU	A	141	52.26	22.972	-5.4	1	25.14
659	CD2	LEU	A	141	51.955	24.413	-7.445	1	30.84
660	N	LEU	A	142	48.115	27.262	-5.913	1	27.94
661	CA	LEU	A	142	46.687	27.517	-5.725	1	30.59
662	C	LEU	A	142	45.936	26.733	-6.805	1	34.02
663	O	LEU	A	142	46.064	27.049	-7.985	1	37.79
664	CB	LEU	A	142	46.391	29.002	-5.931	1	30.5
665	CG	LEU	A	142	47.263	30.026	-5.212	1	32.2
666	CD1	LEU	A	142	46.717	31.415	-5.518	1	29.12
667	CD2	LEU	A	142	47.267	29.758	-3.7	1	32.3
668	N	SER	A	143	45.12	25.753	-6.434	1	35.86
669	CA	SER	A	143	44.428	24.984	-7.459	1	37.17
670	C	SER	A	143	43.484	23.954	-6.86	1	37.58
671	O	SER	A	143	43.163	24.017	-5.677	1	39.69
672	CB	SER	A	143	45.477	24.273	-8.322	1	36.91
673	OG	SER	A	143	44.895	23.693	-9.464	1	36.54
674	N	HIS	A	144	42.973	23.06	-7.705	1	35.63
675	CA	HIS	A	144	42.104	21.981	-7.252	1	34.35
676	C	HIS	A	144	43.041	20.854	-6.907	1	33.24

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Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
677	O	HIS	A	144	44.213	20.896	-7.282	1	33.11
678	CB	HIS	A	144	41.17	21.498	-8.36	1	38.58
679	CG	HIS	A	144	39.95	22.34	-8.526	1	40.57
680	ND1	HIS	A	144	38.946	22.383	-7.585	1	42.1
681	CD2	HIS	A	144	39.577	23.183	-9.516	1	42.13
682	CE1	HIS	A	144	38.005	23.221	-7.987	1	45.57
683	NE2	HIS	A	144	38.365	23.72	-9.155	1	44.82
684	N	GLY	A	145	42.547	19.839	-6.214	1	33.53
685	CA	GLY	A	145	43.429	18.75	-5.884	1	32.6
686	C	GLY	A	145	42.742	17.557	-5.297	1	36.74
687	O	GLY	A	145	41.571	17.615	-4.914	1	39.38
688	N	GLU	A	146	43.486	16.46	-5.264	1	41.15
689	CA	GLU	A	146	43.026	15.2	-4.703	1	47.98
690	C	GLU	A	146	44.178	14.753	-3.818	1	48.76
691	O	GLU	A	146	45.226	15.407	-3.766	1	50.34
692	CB	GLU	A	146	42.78	14.164	-5.798	1	54.51
693	CG	GLU	A	146	41.628	14.498	-6.728	1	65.08
694	CD	GLU	A	146	41.491	13.5	-7.86	1	71.07
695	OE1	GLU	A	146	42.358	13.499	-8.763	1	77.01
696	OE2	GLU	A	146	40.518	12.715	-7.85	1	75.81
697	N	GLU	A	147	44.011	13.635	-3.139	1	48.92
698	CA	GLU	A	147	45.068	13.179	-2.269	1	51.46
699	C	GLU	A	147	46.373	12.987	-3.018	1	49.3
700	O	GLU	A	147	46.429	12.239	-3.987	1	52.36
701	CB	GLU	A	147	44.656	11.891	-1.55	1	58.2
702	CG	GLU	A	147	45.695	11.352	-0.545	1	67.79
703	CD	GLU	A	147	46.007	12.287	0.645	1	70.79
704	OE1	GLU	A	147	45.59	13.476	0.651	1	70.08
705	OE2	GLU	A	147	46.704	11.813	1.577	1	72.85
706	N	ASN	A	148	47.394	13.729	-2.595	1	46.92
707	CA	ASN	A	148	48.748	13.657	-3.17	1	44.9
708	C	ASN	A	148	48.91	14.3	-4.54	1	42.73
709	O	ASN	A	148	50.012	14.293	-5.097	1	40.88
710	CB	ASN	A	148	49.21	12.208	-3.328	1	43.17
711	CG	ASN	A	148	49.062	11.398	-2.073	1	44.5
712	OD1	ASN	A	148	48.449	10.329	-2.088	1	49.29
713	ND2	ASN	A	148	49.646	11.872	-0.985	1	44.55
714	N	VAL	A	149	47.872	14.967	-5.025	1	41.18
715	CA	VAL	A	149	47.932	15.499	-6.363	1	40.44
716	C	VAL	A	149	47.265	16.862	-6.56	1	40.82
717	O	VAL	A	149	46.262	17.162	-5.908	1	41.37
718	CB	VAL	A	149	47.246	14.432	-7.274	1	44.49
719	CG1	VAL	A	149	45.769	14.776	-7.552	1	41.65
720	CG2	VAL	A	149	48.045	14.191	-8.522	1	50.61
721	N	ILE	A	150	47.834	17.691	-7.437	1	42.63
722	CA	ILE	A	150	47.236	18.994	-7.772	1	43.03
723	C	ILE	A	150	46.739	18.921	-9.203	1	42.53
724	O	ILE	A	150	47.227	18.126	-10.005	1	41.52
725	CB	ILE	A	150	48.212	20.198	-7.769	1	42.35
726	CG1	ILE	A	150	49.653	19.731	-7.871	1	45.24
727	CG2	ILE	A	150	47.904	21.149	-6.633	1	40.78
728	CD1	ILE	A	150	50.618	20.872	-8.044	1	53.82

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Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
729	N	TYR	A	151	45.826	19.819	-9.532	1	44.18
730	CA	TYR	A	151	45.266	19.888	-10.863	1	44.18
731	C	TYR	A	151	45.934	20.94	-11.745	1	44.2
732	O	TYR	A	151	46.138	22.079	-11.321	1	42.37
733	CB	TYR	A	151	43.771	20.212	-10.788	1	46.38
734	CG	TYR	A	151	42.866	19.004	-10.74	1	54.1
735	CD1	TYR	A	151	42.591	18.359	-9.528	1	54.9
736	CD2	TYR	A	151	42.269	18.506	-11.905	1	54.67
737	CE1	TYR	A	151	41.741	17.248	-9.474	1	55
738	CE2	TYR	A	151	41.415	17.393	-11.862	1	56.33
739	CZ	TYR	A	151	41.156	16.77	-10.641	1	55.71
740	OH	TYR	A	151	40.322	15.679	-10.579	1	54.11
741	N	GLY	A	152	46.386	20.521	-12.923	1	43.17
742	CA	GLY	A	152	46.897	21.473	-13.885	1	42.78
743	C	GLY	A	152	45.585	21.874	-14.556	1	44.25
744	O	GLY	A	152	44.518	21.408	-14.131	1	41.97
745	N	LYS	A	153	45.608	22.717	-15.585	1	45.24
746	CA	LYS	A	153	44.339	23.063	-16.229	1	44.69
747	C	LYS	A	153	43.818	21.857	-17.019	1	43.7
748	O	LYS	A	153	42.621	21.683	-17.202	1	40.52
749	CB	LYS	A	153	44.494	24.28	-17.145	1	48.27
750	CG	LYS	A	153	45.325	24.059	-18.409	1	50.35
751	CD	LYS	A	153	45.328	25.304	-19.322	1	54.64
752	CE	LYS	A	153	43.922	25.735	-19.826	1	59.84
753	NZ	LYS	A	153	43.056	26.529	-18.871	1	56.11
754	N	ASP	A	154	44.743	20.984	-17.392	1	45.97
755	CA	ASP	A	154	44.464	19.794	-18.184	1	50.29
756	C	ASP	A	154	44.332	18.458	-17.455	1	53.94
757	O	ASP	A	154	43.901	17.481	-18.058	1	59.83
758	CB	ASP	A	154	45.538	19.653	-19.267	1	52.79
759	CG	ASP	A	154	46.968	19.648	-18.698	1	58.9
760	OD1	ASP	A	154	47.184	20.18	-17.582	1	59.5
761	OD2	ASP	A	154	47.889	19.124	-19.382	1	60.66
762	N	GLY	A	155	44.722	18.395	-16.186	1	54.38
763	CA	GLY	A	155	44.636	17.14	-15.452	1	49.82
764	C	GLY	A	155	45.249	17.27	-14.074	1	48.69
765	O	GLY	A	155	45.225	18.351	-13.505	1	49.23
766	N	VAL	A	156	45.799	16.188	-13.533	1	45.38
767	CA	VAL	A	156	46.405	16.236	-12.207	1	44.24
768	C	VAL	A	156	47.844	15.746	-12.245	1	44.35
769	O	VAL	A	156	48.167	14.805	-12.969	1	44.3
770	CB	VAL	A	156	45.627	15.371	-11.152	1	44.03
771	CG1	VAL	A	156	44.178	15.736	-11.11	1	41.81
772	CG2	VAL	A	156	45.77	13.895	-11.441	1	42.14
773	N	THR	A	157	48.71	16.386	-11.469	1	43.95
774	CA	THR	A	157	50.108	15.983	-11.394	1	42.17
775	C	THR	A	157	50.471	15.83	-9.907	1	41.73
776	O	THR	A	157	49.932	16.539	-9.049	1	40.2
777	CB	THR	A	157	51.032	17	-12.127	1	40.87
778	OG1	THR	A	157	52.401	16.585	-12.032	1	41.42
779	CG2	THR	A	157	50.888	18.381	-11.539	1	41.73
780	N	PRO	A	158	51.297	14.823	-9.578	1	40.92

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Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
781	CA	PRO	A	158	51.756	14.516	-8.221	1	41.73
782	C	PRO	A	158	52.637	15.613	-7.653	1	41.96
783	O	PRO	A	158	53.679	15.942	-8.223	1	42.65
784	CB	PRO	A	158	52.573	13.235	-8.414	1	39.94
785	CG	PRO	A	158	51.96	12.611	-9.599	1	39.51
786	CD	PRO	A	158	51.768	13.79	-10.513	1	40.97
787	N	ILE	A	159	52.244	16.13	-6.496	1	41.51
788	CA	ILE	A	159	52.99	17.185	-5.827	1	40
789	C	ILE	A	159	54.427	16.72	-5.598	1	42.04
790	O	ILE	A	159	55.369	17.515	-5.68	1	42.2
791	CB	ILE	A	159	52.317	17.533	-4.486	1	40.36
792	CG1	ILE	A	159	50.861	17.926	-4.746	1	39.3
793	CG2	ILE	A	159	53.046	18.67	-3.793	1	42.07
794	CD1	ILE	A	159	49.997	17.977	-3.531	1	38.1
795	N	LYS	A	160	54.595	15.415	-5.389	1	44.22
796	CA	LYS	A	160	55.91	14.828	-5.155	1	48.23
797	C	LYS	A	160	56.837	15.083	-6.333	1	47.73
798	O	LYS	A	160	58.045	15.273	-6.165	1	46.75
799	CB	LYS	A	160	55.787	13.32	-4.919	1	56.19
800	CG	LYS	A	160	56.502	12.805	-3.658	1	66.87
801	CD	LYS	A	160	58.038	12.953	-3.711	1	73.09
802	CE	LYS	A	160	58.702	12.397	-2.436	1	75.61
803	NZ	LYS	A	160	60.198	12.396	-2.478	1	77.71
804	N	ASP	A	161	56.269	15.091	-7.529	1	48.57
805	CA	ASP	A	161	57.066	15.328	-8.72	1	48.5
806	C	ASP	A	161	57.484	16.773	-8.785	1	43.74
807	O	ASP	A	161	58.629	17.067	-9.111	1	46.62
808	CB	ASP	A	161	56.299	14.944	-9.985	1	57.55
809	CG	ASP	A	161	56.179	13.43	-10.17	1	67.33
810	OD1	ASP	A	161	56.751	12.665	-9.351	1	69.83
811	OD2	ASP	A	161	55.512	13.01	-11.149	1	72.22
812	N	LEU	A	162	56.576	17.675	-8.431	1	37.66
813	CA	LEU	A	162	56.892	19.093	-8.468	1	35.55
814	C	LEU	A	162	57.968	19.466	-7.458	1	36.67
815	O	LEU	A	162	58.829	20.301	-7.75	1	39.72
816	CB	LEU	A	162	55.651	19.951	-8.224	1	34.91
817	CG	LEU	A	162	54.532	19.95	-9.264	1	33.56
818	CD1	LEU	A	162	53.533	18.899	-8.917	1	41.12
819	CD2	LEU	A	162	53.828	21.281	-9.287	1	41.06
820	N	THR	A	163	57.964	18.811	-6.3	1	33.66
821	CA	THR	A	163	58.938	19.126	-5.252	1	31.26
822	C	THR	A	163	60.294	18.409	-5.349	1	31.23
823	O	THR	A	163	61.33	18.996	-5.022	1	29.12
824	CB	THR	A	163	58.326	18.964	-3.8	1	26.86
825	OG1	THR	A	163	58.054	17.587	-3.52	1	28.59
826	CG2	THR	A	163	57.022	19.733	-3.665	1	19.8
827	N	ALA	A	164	60.305	17.182	-5.869	1	32.34
828	CA	ALA	A	164	61.543	16.394	-5.984	1	34.54
829	C	ALA	A	164	62.711	17.062	-6.71	1	36.52
830	O	ALA	A	164	63.875	16.76	-6.434	1	38.19
831	CB	ALA	A	164	61.254	15.046	-6.598	1	35.87
832	N	HIS	A	165	62.394	17.973	-7.631	1	38.48

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
833	CA	HIS	A	165	63.39	18.723	-8.406	1	36.46
834	C	HIS	A	165	64.358	19.451	-7.477	1	38.65
835	O	HIS	A	165	65.525	19.69	-7.813	1	36.54
836	CB	HIS	A	165	62.688	19.784	-9.264	1	36.43
837	CG	HIS	A	165	61.714	19.223	-10.251	1	39.52
838	ND1	HIS	A	165	62.079	18.332	-11.242	1	40.05
839	CD2	HIS	A	165	60.384	19.427	-10.404	1	40.08
840	CE1	HIS	A	165	61.017	18.012	-11.958	1	41.14
841	NE2	HIS	A	165	59.975	18.663	-11.471	1	42.36
842	N	PHE	A	166	63.852	19.811	-6.301	1	38.57
843	CA	PHE	A	166	64.64	20.553	-5.341	1	32.81
844	C	PHE	A	166	65.4	19.717	-4.315	1	31.91
845	O	PHE	A	166	66.061	20.264	-3.429	1	33.72
846	CB	PHE	A	166	63.766	21.629	-4.696	1	29
847	CG	PHE	A	166	63.122	22.551	-5.696	1	24.05
848	CD1	PHE	A	166	61.943	22.189	-6.33	1	27.29
849	CD2	PHE	A	166	63.71	23.767	-6.019	1	23.11
850	CE1	PHE	A	166	61.356	23.024	-7.271	1	23.75
851	CE2	PHE	A	166	63.127	24.61	-6.96	1	23.97
852	CZ	PHE	A	166	61.949	24.236	-7.585	1	22.16
853	N	ARG	A	167	65.367	18.4	-4.483	1	28.58
854	CA	ARG	A	167	66.087	17.516	-3.581	1	31.59
855	C	ARG	A	167	67.551	17.913	-3.509	1	35.42
856	O	ARG	A	167	68.09	18.455	-4.474	1	41.51
857	CB	ARG	A	167	65.983	16.088	-4.056	1	25.46
858	CG	ARG	A	167	64.697	15.463	-3.677	1	28.36
859	CD	ARG	A	167	64.549	14.161	-4.381	1	32.52
860	NE	ARG	A	167	65.794	13.4	-4.397	1	34.05
861	CZ	ARG	A	167	65.839	12.085	-4.564	1	38.08
862	NH1	ARG	A	167	64.71	11.402	-4.712	1	35.29
863	NH2	ARG	A	167	67.006	11.458	-4.625	1	38.57
864	N	GLY	A	168	68.207	17.589	-2.398	1	35.31
865	CA	GLY	A	168	69.606	17.945	-2.222	1	37.41
866	C	GLY	A	168	70.512	17.472	-3.335	1	38.8
867	O	GLY	A	168	71.466	18.155	-3.724	1	40.94
868	N	ASP	A	169	70.224	16.284	-3.844	1	41.49
869	CA	ASP	A	169	71.023	15.735	-4.923	1	43.37
870	C	ASP	A	169	70.692	16.379	-6.269	1	43.84
871	O	ASP	A	169	71.487	16.287	-7.19	1	48.82
872	CB	ASP	A	169	70.899	14.198	-4.983	1	40.6
873	CG	ASP	A	169	69.458	13.702	-5.194	1	42.39
874	OD1	ASP	A	169	68.485	14.479	-5.067	1	42.17
875	OD2	ASP	A	169	69.304	12.496	-5.481	1	42.6
876	N	ARG	A	170	69.565	17.093	-6.345	1	42.95
877	CA	ARG	A	170	69.109	17.736	-7.583	1	42.69
878	C	ARG	A	170	69.179	19.259	-7.694	1	43.89
879	O	ARG	A	170	68.994	19.8	-8.796	1	47.11
880	CB	ARG	A	170	67.699	17.273	-7.923	1	39.57
881	CG	ARG	A	170	67.67	15.811	-8.169	1	39.72
882	CD	ARG	A	170	66.292	15.249	-8.273	1	38.79
883	NE	ARG	A	170	66.4	13.797	-8.281	1	41.61
884	CZ	ARG	A	170	65.371	12.969	-8.192	1	43.11

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Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
885	NH1	ARG	A	170	64.142	13.459	-8.092	1	47.82
886	NH2	ARG	A	170	65.573	11.655	-8.205	1	43.59
887	N	SER	A	171	69.381	19.949	-6.569	1	41.41
888	CA	SER	A	171	69.5	21.407	-6.562	1	34.67
889	C	SER	A	171	70.579	21.77	-5.572	1	38.64
890	O	SER	A	171	70.312	22.372	-4.539	1	42.04
891	CB	SER	A	171	68.187	22.089	-6.173	1	27.36
892	OG	SER	A	171	68.297	23.508	-6.307	1	20.67
893	N	LYS	A	172	71.815	21.432	-5.915	1	41.23
894	CA	LYS	A	172	72.965	21.708	-5.059	1	43.44
895	C	LYS	A	172	73.085	23.117	-4.504	1	39.62
896	O	LYS	A	172	73.569	23.284	-3.396	1	40.32
897	CB	LYS	A	172	74.262	21.33	-5.776	1	49.39
898	CG	LYS	A	172	74.391	19.831	-6.08	1	61.44
899	CD	LYS	A	172	74.733	19.018	-4.821	1	69.56
900	CE	LYS	A	172	76.111	19.412	-4.25	1	74.4
901	NZ	LYS	A	172	76.528	18.634	-3.039	1	73.96
902	N	THR	A	173	72.64	24.13	-5.244	1	39.25
903	CA	THR	A	173	72.757	25.507	-4.75	1	40
904	C	THR	A	173	71.724	25.887	-3.695	1	39.48
905	O	THR	A	173	71.822	26.959	-3.083	1	38.28
906	CB	THR	A	173	72.765	26.564	-5.888	1	41.08
907	OG1	THR	A	173	71.558	26.486	-6.666	1	40.51
908	CG2	THR	A	173	73.956	26.347	-6.774	1	39.56
909	N	LEU	A	174	70.71	25.031	-3.547	1	38.88
910	CA	LEU	A	174	69.647	25.202	-2.56	1	36.97
911	C	LEU	A	174	69.88	24.199	-1.432	1	38.75
912	O	LEU	A	174	69.064	24.068	-0.523	1	41.57
913	CB	LEU	A	174	68.266	24.966	-3.189	1	30.4
914	CG	LEU	A	174	67.609	26.195	-3.822	1	28.09
915	CD1	LEU	A	174	66.253	25.852	-4.373	1	23.86
916	CD2	LEU	A	174	67.491	27.295	-2.797	1	25.96
917	N	LEU	A	175	70.987	23.47	-1.508	1	38.79
918	CA	LEU	A	175	71.307	22.489	-0.487	1	39.16
919	C	LEU	A	175	71.567	23.25	0.821	1	39.98
920	O	LEU	A	175	72.111	24.365	0.805	1	39.35
921	CB	LEU	A	175	72.514	21.651	-0.923	1	38.17
922	CG	LEU	A	175	73.118	20.632	0.043	1	41.76
923	CD1	LEU	A	175	72.096	19.598	0.466	1	41.1
924	CD2	LEU	A	175	74.293	19.978	-0.629	1	43.37
925	N	GLU	A	176	71.089	22.676	1.93	1	38.23
926	CA	GLU	A	176	71.218	23.263	3.262	1	34.71
927	C	GLU	A	176	70.445	24.576	3.388	1	33.14
928	O	GLU	A	176	70.634	25.322	4.349	1	32.98
929	CB	GLU	A	176	72.689	23.468	3.646	1	35.82
930	CG	GLU	A	176	73.456	22.172	3.896	1	42.2
931	CD	GLU	A	176	74.807	22.399	4.568	1	47.32
932	OE1	GLU	A	176	74.836	22.849	5.727	1	52.48
933	OE2	GLU	A	176	75.852	22.122	3.946	1	52.39
934	N	LYS	A	177	69.576	24.848	2.414	1	30.58
935	CA	LYS	A	177	68.759	26.058	2.399	1	28.81
936	C	LYS	A	177	67.334	25.588	2.429	1	26.09

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
937	O	LYS	A	177	67.033	24.503	1.935	1	29.4
938	CB	LYS	A	177	68.993	26.883	1.124	1	32.01
939	CG	LYS	A	177	70.369	27.527	1.033	1	36.54
940	CD	LYS	A	177	70.543	28.377	-0.222	1	36.71
941	CE	LYS	A	177	71.97	28.909	-0.301	1	36.61
942	NZ	LYS	A	177	72.31	29.478	-1.634	1	41.75
943	N	PRO	A	178	66.437	26.364	3.034	1	24.46
944	CA	PRO	A	178	65.045	25.934	3.089	1	27.34
945	C	PRO	A	178	64.287	26.052	1.77	1	29.9
946	O	PRO	A	178	64.419	27.044	1.053	1	30.97
947	CB	PRO	A	178	64.444	26.828	4.18	1	24.28
948	CG	PRO	A	178	65.249	28.048	4.118	1	24.78
949	CD	PRO	A	178	66.654	27.559	3.875	1	26.31
950	N	LYS	A	179	63.485	25.034	1.477	1	30.5
951	CA	LYS	A	179	62.662	24.986	0.278	1	27.43
952	C	LYS	A	179	61.241	24.939	0.802	1	24.36
953	O	LYS	A	179	60.834	23.948	1.405	1	25.61
954	CB	LYS	A	179	62.99	23.732	-0.549	1	24.27
955	CG	LYS	A	179	64.453	23.685	-1	1	17.42
956	CD	LYS	A	179	65.08	22.346	-0.675	1	17.52
957	CE	LYS	A	179	66.501	22.557	-0.232	1	20.15
958	NZ	LYS	A	179	67.112	21.338	0.331	1	26.89
959	N	LEU	A	180	60.499	26.018	0.576	1	23.84
960	CA	LEU	A	180	59.129	26.138	1.065	1	24.64
961	C	LEU	A	180	58.03	26.031	0.008	1	23.91
962	O	LEU	A	180	58.017	26.753	-0.976	1	28.96
963	CB	LEU	A	180	58.965	27.476	1.808	1	24.7
964	CG	LEU	A	180	60.166	28.023	2.595	1	25.88
965	CD1	LEU	A	180	59.881	29.453	3.055	1	25.66
966	CD2	LEU	A	180	60.504	27.11	3.769	1	23.49
967	N	PHE	A	181	57.079	25.151	0.246	1	25.36
968	CA	PHE	A	181	55.958	24.98	-0.651	1	25.79
969	C	PHE	A	181	54.684	25.194	0.18	1	28.09
970	O	PHE	A	181	54.554	24.621	1.257	1	29.78
971	CB	PHE	A	181	55.974	23.564	-1.261	1	25.83
972	CG	PHE	A	181	57.221	23.255	-2.066	1	26.68
973	CD1	PHE	A	181	58.392	22.849	-1.439	1	25.78
974	CD2	PHE	A	181	57.23	23.406	-3.443	1	25.34
975	CE1	PHE	A	181	59.553	22.602	-2.168	1	21.55
976	CE2	PHE	A	181	58.389	23.161	-4.175	1	23.26
977	CZ	PHE	A	181	59.546	22.761	-3.537	1	24.85
978	N	PHE	A	182	53.8	26.08	-0.276	1	26.61
979	CA	PHE	A	182	52.527	26.358	0.381	1	25.97
980	C	PHE	A	182	51.441	25.849	-0.575	1	27.8
981	O	PHE	A	182	51.274	26.392	-1.654	1	32.73
982	CB	PHE	A	182	52.359	27.862	0.604	1	26.93
983	CG	PHE	A	182	53.424	28.467	1.458	1	26.43
984	CD1	PHE	A	182	54.684	28.732	0.934	1	27.63
985	CD2	PHE	A	182	53.166	28.778	2.791	1	26.2
986	CE1	PHE	A	182	55.683	29.306	1.735	1	29.27
987	CE2	PHE	A	182	54.156	29.351	3.6	1	24.09
988	CZ	PHE	A	182	55.412	29.616	3.072	1	24.31

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Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
989	N	ILE	A	183	50.655	24.862	-0.168	1	29.31
990	CA	ILE	A	183	49.662	24.313	-1.064	1	26.28
991	C	ILE	A	183	48.201	24.478	-0.688	1	28.73
992	O	ILE	A	183	47.73	23.86	0.264	1	32.84
993	CB	ILE	A	183	49.913	22.803	-1.307	1	28.73
994	CG1	ILE	A	183	51.346	22.556	-1.77	1	28.54
995	CG2	ILE	A	183	48.973	22.259	-2.369	1	27.93
996	CD1	ILE	A	183	52.288	22.205	-0.664	1	35.13
997	N	GLN	A	184	47.48	25.28	-1.47	1	30.45
998	CA	GLN	A	184	46.041	25.488	-1.295	1	29.58
999	C	GLN	A	184	45.336	24.649	-2.369	1	33
1000	O	GLN	A	184	45.327	25.007	-3.552	1	33.36
1001	CB	GLN	A	184	45.668	26.965	-1.456	1	28.75
1002	CG	GLN	A	184	44.157	27.242	-1.609	1	33.39
1003	CD	GLN	A	184	43.311	26.802	-0.41	1	35.16
1004	OE1	GLN	A	184	43.664	27.054	0.74	1	42.25
1005	NE2	GLN	A	184	42.173	26.186	-0.681	1	30.1
1006	N	ALA	A	185	44.778	23.519	-1.951	1	32.81
1007	CA	ALA	A	185	44.088	22.617	-2.854	1	34.29
1008	C	ALA	A	185	43.414	21.531	-2.027	1	35.06
1009	O	ALA	A	185	43.773	21.31	-0.873	1	39.54
1010	CB	ALA	A	185	45.085	21.994	-3.809	1	31.9
1011	N		661 A	186	42.401	20.886	-2.587	1	33.08
1012	CA		661 A	186	41.738	19.808	-1.865	1	31.53
1013	C		661 A	186	42.711	18.626	-1.739	1	30.26
1014	O		661 A	186	43.698	18.562	-2.468	1	29.59
1015	CB		661 A	186	40.454	19.382	-2.583	1	33.41
1016	SG		661 A	186	39.235	20.686	-2.354	1	35.66
1017	C2		661 A	186	33.143	26.535	-2.278	1	47.21
1018	C6		661 A	186	34.282	25.636	-1.696	1	43.81
1019	O3		661 A	186	35.096	26.072	-0.884	1	45.42
1020	N3		661 A	186	34.395	24.37	-2.053	1	39.8
1021	C3		661 A	186	35.626	23.644	-1.685	1	36.84
1022	C7		661 A	186	36.655	23.397	-2.898	1	38.95
1023	O4		661 A	186	36.232	23.433	-4.049	1	40.39
1024	N4		661 A	186	37.955	23.117	-2.671	1	35.82
1025	C4		661 A	186	38.989	22.951	-3.708	1	32.7
1026	C8		661 A	186	39.212	21.488	-3.969	1	36.53
1027	C12		661 A	186	40.356	23.612	-3.429	1	30.64
1028	C13		661 A	186	40.226	25.093	-3.712	1	30.16
1029	OD1		661 A	186	41.041	25.878	-3.194	1	24.54
1030	OD2		661 A	186	39.302	25.482	-4.458	1	35.8
1031	O5		661 A	186	40.275	21.1	-4.84	1	36.72
1032	C18		661 A	186	33.681	27.312	-3.477	1	52.51
1033	C9		661 A	186	31.665	27.578	-0.668	1	47.71
1034	N2		661 A	186	32.83	27.537	-1.274	1	47.25
1035	O6		661 A	186	30.76	26.783	-0.937	1	47.09
1036	C19		661 A	186	31.558	28.689	0.363	1	48.52
1037	C1		661 A	186	33.057	27.102	-4.849	1	58.28
1038	C5		661 A	186	32.741	28.483	-5.406	1	60.94
1039	O1		661 A	186	33.653	29.147	-5.949	1	61.97
1040	O2		661 A	186	31.575	28.917	-5.267	1	63.35

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Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
1041	C10		661 A	186	35.188	22.333	-1.018	1	36.21
1042	C11		661 A	186	34.801	21.273	-2.031	1	36.03
1043	C14		661 A	186	34.057	22.464	-0.008	1	35.13
1044	C15		661 A	186	32.062	28.342	1.756	1	48.49
1045	C16		661 A	186	32.144	29.595	2.602	1	48.63
1046	O7		661 A	186	32.305	30.705	2.053	1	52.21
1047	O8		661 A	186	32.049	29.484	3.839	1	50.69
1048	N1		661 A	186	30.252	29.308	0.427	1	51.48
1049	C17		661 A	186	29.751	29.86	-0.65	1	52.2
1050	O9		661 A	186	28.552	30.1	-0.812	1	55.72
1051	C20		661 A	186	30.801	30.183	-1.675	1	52.54
1052	N	ARG	A	187	42.476	17.74	-0.771	1	30.7
1053	CA	ARG	A	187	43.331	16.572	-0.569	1	26.97
1054	C	ARG	A	187	42.455	15.338	-0.439	1	26.1
1055	O	ARG	A	187	42.918	14.262	-0.068	1	24.95
1056	CB	ARG	A	187	44.212	16.744	0.67	1	23.39
1057	CG	ARG	A	187	45.04	18.018	0.638	1	26.9
1058	CD	ARG	A	187	45.946	18.137	1.824	1	24.82
1059	NE	ARG	A	187	46.979	17.115	1.792	1	24.78
1060	CZ	ARG	A	187	47.939	17.005	2.702	1	27.77
1061	NH1	ARG	A	187	47.984	17.855	3.723	1	28.4
1062	NH2	ARG	A	187	48.895	16.088	2.561	1	26.64
1063	N	GLY	A	188	41.189	15.503	-0.8	1	27.51
1064	CA	GLY	A	188	40.237	14.418	-0.73	1	26.99
1065	C	GLY	A	188	38.875	15.048	-0.632	1	30.54
1066	O	GLY	A	188	38.735	16.261	-0.81	1	29.14
1067	N	THR	A	189	37.877	14.252	-0.283	1	35.45
1068	CA	THR	A	189	36.527	14.776	-0.178	1	43.22
1069	C	THR	A	189	35.923	14.698	1.225	1	45.64
1070	O	THR	A	189	34.696	14.649	1.373	1	47.51
1071	CB	THR	A	189	35.588	14.079	-1.186	1	45.67
1072	OG1	THR	A	189	35.5	12.686	-0.875	1	49.86
1073	CG2	THR	A	189	36.125	14.227	-2.603	1	49.27
1074	N	GLU	A	190	36.764	14.652	2.255	1	45.71
1075	CA	GLU	A	190	36.239	14.604	3.613	1	45.3
1076	C	GLU	A	190	35.968	15.997	4.16	1	43.5
1077	O	GLU	A	190	36.704	16.951	3.877	1	42.02
1078	CB	GLU	A	190	37.166	13.842	4.554	1	48.64
1079	CG	GLU	A	190	37.148	12.34	4.362	1	55.41
1080	CD	GLU	A	190	37.682	11.607	5.573	1	59.64
1081	OE1	GLU	A	190	38.914	11.609	5.787	1	60.48
1082	OE2	GLU	A	190	36.861	11.041	6.324	1	64.46
1083	N	LEU	A	191	34.866	16.109	4.895	1	44.08
1084	CA	LEU	A	191	34.453	17.359	5.522	1	44.98
1085	C	LEU	A	191	34.641	17.204	7.026	1	46.03
1086	O	LEU	A	191	34.398	16.128	7.582	1	49.68
1087	CB	LEU	A	191	32.976	17.659	5.222	1	44.75
1088	CG	LEU	A	191	32.546	18.143	3.828	1	40.91
1089	CD1	LEU	A	191	31.036	18.185	3.736	1	38.96
1090	CD2	LEU	A	191	33.107	19.529	3.555	1	40.72
1091	N	ASP	A	192	35.128	18.259	7.665	1	46.35
1092	CA	ASP	A	192	35.339	18.259	9.102	1	45.71

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
1093	C	ASP	A	192	34.131	18.969	9.697	1	46.9
1094	O	ASP	A	192	33.969	20.178	9.542	1	44.34
1095	CB	ASP	A	192	36.637	19.003	9.444	1	46.83
1096	CG	ASP	A	192	37.049	18.842	10.896	1	46.45
1097	OD1	ASP	A	192	36.176	18.928	11.787	1	45.61
1098	OD2	ASP	A	192	38.258	18.642	11.138	1	41.01
1099	N	ASP	A	193	33.276	18.199	10.355	1	51.05
1100	CA	ASP	A	193	32.059	18.717	10.979	1	55.39
1101	C	ASP	A	193	32.353	19.709	12.098	1	54.99
1102	O	ASP	A	193	31.541	20.586	12.385	1	54.43
1103	CB	ASP	A	193	31.223	17.565	11.551	1	62.8
1104	CG	ASP	A	193	30.636	16.659	10.474	1	71.96
1105	OD1	ASP	A	193	31.4	15.999	9.732	1	77.18
1106	OD2	ASP	A	193	29.39	16.59	10.389	1	77.44
1107	N	GLY	A	194	33.507	19.557	12.737	1	54.09
1108	CA	GLY	A	194	33.867	20.44	13.83	1	54.25
1109	C	GLY	A	194	33.229	19.972	15.127	1	54.14
1110	O	GLY	A	194	32.395	19.059	15.136	1	53.26
1111	N	ILE	A	195	33.625	20.59	16.231	1	53.3
1112	CA	ILE	A	195	33.089	20.225	17.533	1	53.06
1113	C	ILE	A	195	33.092	21.473	18.401	1	54.55
1114	O	ILE	A	195	34.018	22.284	18.336	1	54.08
1115	CB	ILE	A	195	33.936	19.089	18.182	1	52.02
1116	CG1	ILE	A	195	33.272	18.565	19.457	1	51.64
1117	CG2	ILE	A	195	35.349	19.561	18.458	1	51.15
1118	CD1	ILE	A	195	32.075	17.68	19.204	1	55.06
1119	N	GLN	A	196	32.021	21.655	19.157	1	57.08
1120	CA	GLN	A	196	31.872	22.813	20.035	1	61.13
1121	C	GLN	A	196	32.543	22.553	21.381	1	60.35
1122	O	GLN	A	196	32.232	21.511	22.001	1	58.95
1123	CB	GLN	A	196	30.392	23.145	20.261	1	66.16
1124	CG	GLN	A	196	29.404	22.388	19.367	1	77.32
1125	CD	GLN	A	196	29.378	20.876	19.626	1	82.81
1126	OE1	GLN	A	196	29.22	20.084	18.692	1	84.23
1127	NE2	GLN	A	196	29.589	20.473	20.88	1	85.63
1128	OT	GLN	A	196	33.373	23.387	21.792	1	59.02
1	N	LYS	A	212	77.799	14.962	4.499	1	41.52
2	CA	LYS	A	212	76.539	14.402	3.926	1	44.49
3	C	LYS	A	212	75.244	14.936	4.561	1	45.58
4	O	LYS	A	212	75.045	14.858	5.776	1	46.9
5	CB	LYS	A	212	76.538	12.882	3.989	1	42.32
6	CG	LYS	A	212	77.041	12.176	2.761	1	38.3
7	CD	LYS	A	212	76.474	10.772	2.781	1	37.58
8	CE	LYS	A	212	77.179	9.85	1.827	1	41.77
9	NZ	LYS	A	212	76.625	8.471	1.951	1	44.72
10	N	ILE	A	213	74.367	15.45	3.704	1	46.12
11	CA	ILE	A	213	73.085	16.018	4.089	1	46.23
12	C	ILE	A	213	72.042	15.12	3.433	1	47.65
13	O	ILE	A	213	72.231	14.683	2.301	1	50.46
14	CB	ILE	A	213	72.927	17.452	3.477	1	47.89
15	CG1	ILE	A	213	74.072	18.358	3.918	1	48.74
16	CG2	ILE	A	213	71.596	18.086	3.881	1	48.72

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Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
17	CD1	ILE	A	213	74.088	18.621	5.406	1	52.08
18	N	PRO	A	214	70.956	14.782	4.147	1	46.63
19	CA	PRO	A	214	69.95	13.929	3.508	1	44.54
20	C	PRO	A	214	69.386	14.697	2.317	1	41.92
21	O	PRO	A	214	69.275	15.92	2.373	1	41.49
22	CB	PRO	A	214	68.896	13.777	4.606	1	44.27
23	CG	PRO	A	214	69.692	13.883	5.854	1	42.76
24	CD	PRO	A	214	70.612	15.031	5.556	1	44.57
25	N	VAL	A	215	69.032	13.999	1.244	1	40.74
26	CA	VAL	A	215	68.49	14.678	0.068	1	36.47
27	C	VAL	A	215	67.087	15.21	0.317	1	35.62
28	O	VAL	A	215	66.649	16.164	-0.328	1	33.76
29	CB	VAL	A	215	68.479	13.762	-1.175	1	34.07
30	CG1	VAL	A	215	69.873	13.271	-1.476	1	31.62
31	CG2	VAL	A	215	67.559	12.592	-0.964	1	38.47
32	N	GLU	A	216	66.401	14.617	1.291	1	35.87
33	CA	GLU	A	216	65.031	15.008	1.618	1	33.1
34	C	GLU	A	216	64.901	16.09	2.684	1	31.48
35	O	GLU	A	216	63.797	16.562	2.982	1	28.7
36	CB	GLU	A	216	64.238	13.772	2.006	1	31.89
37	CG	GLU	A	216	64.14	12.762	0.878	1	36.37
38	CD	GLU	A	216	63.161	13.169	-0.226	1	40.42
39	OE1	GLU	A	216	62.638	14.306	-0.213	1	42.19
40	OE2	GLU	A	216	62.895	12.329	-1.109	1	45.06
41	N	ALA	A	217	66.054	16.525	3.183	1	30.61
42	CA	ALA	A	217	66.143	17.544	4.215	1	30.01
43	C	ALA	A	217	65.833	18.945	3.719	1	32.77
44	O	ALA	A	217	65.877	19.22	2.528	1	39.89
45	CB	ALA	A	217	67.54	17.53	4.828	1	24.86
46	N	ASP	A	218	65.519	19.817	4.667	1	30.58
47	CA	ASP	A	218	65.256	21.224	4.425	1	29.43
48	C	ASP	A	218	64.032	21.652	3.616	1	29.46
49	O	ASP	A	218	63.969	22.77	3.109	1	31.27
50	CB	ASP	A	218	66.532	21.896	3.925	1	32.84
51	CG	ASP	A	218	67.696	21.767	4.921	1	35.82
52	OD1	ASP	A	218	67.683	22.457	5.961	1	36.39
53	OD2	ASP	A	218	68.634	20.984	4.663	1	36.87
54	N	PHE	A	219	63.029	20.79	3.578	1	28.66
55	CA	PHE	A	219	61.777	21.084	2.899	1	28.93
56	C	PHE	A	219	60.711	21.402	3.946	1	29.14
57	O	PHE	A	219	60.76	20.899	5.07	1	31.1
58	CB	PHE	A	219	61.267	19.848	2.152	1	31.66
59	CG	PHE	A	219	61.932	19.597	0.837	1	36.29
60	CD1	PHE	A	219	63.16	18.954	0.777	1	36.33
61	CD2	PHE	A	219	61.293	19.952	-0.351	1	36.81
62	CE1	PHE	A	219	63.745	18.662	-0.45	1	40.63
63	CE2	PHE	A	219	61.869	19.664	-1.585	1	36.62
64	CZ	PHE	A	219	63.094	19.018	-1.636	1	37.43
65	N	LEU	A	220	59.719	22.188	3.563	1	27.45
66	CA	LEU	A	220	58.611	22.47	4.443	1	26.17
67	C	LEU	A	220	57.37	22.611	3.571	1	25.82
68	O	LEU	A	220	57.368	23.399	2.629	1	28.2

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Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
69	CB	LEU	A	220	58.848	23.743	5.255	1	28.42
70	CG	LEU	A	220	57.736	24.04	6.278	1	30.26
71	CD1	LEU	A	220	58.305	24.816	7.427	1	37.22
72	CD2	LEU	A	220	56.578	24.805	5.671	1	33.22
73	N	PHE	A	221	56.339	21.819	3.853	1	23.85
74	CA	PHE	A	221	55.088	21.896	3.112	1	21.45
75	C	PHE	A	221	54.008	22.445	3.995	1	22.89
76	O	PHE	A	221	53.636	21.823	4.982	1	27.34
77	CB	PHE	A	221	54.841	20.525	2.61	1	19.93
78	CG	PHE	A	221	55.706	19.794	1.879	1	24.5
79	CD1	PHE	A	221	56.413	20.414	0.863	1	29.64
80	CD2	PHE	A	221	56.079	18.533	2.264	1	27.08
81	CE1	PHE	A	221	57.483	19.788	0.257	1	31.19
82	CE2	PHE	A	221	57.154	17.899	1.656	1	31.83
83	CZ	PHE	A	221	57.855	18.529	0.658	1	27.11
84	N	ALA	A	222	53.533	23.635	3.673	1	24.71
85	CA	ALA	A	222	52.453	24.238	4.418	1	21.89
86	C	ALA	A	222	51.152	23.95	3.659	1	24.46
87	O	ALA	A	222	50.775	24.694	2.754	1	28.55
88	CB	ALA	A	222	52.681	25.739	4.561	1	18.62
89	N	TYR	A	223	50.487	22.842	3.981	1	25.62
90	CA	TYR	A	223	49.225	22.513	3.314	1	23.31
91	C	TYR	A	223	48.081	23.279	3.943	1	26.24
92	O	TYR	A	223	48.109	23.599	5.138	1	31.12
93	CB	TYR	A	223	48.919	21.021	3.366	1	20.94
94	CG	TYR	A	223	49.817	20.165	2.506	1	23.87
95	CD1	TYR	A	223	51.029	19.694	2.994	1	24.65
96	CD2	TYR	A	223	49.426	19.782	1.22	1	26.88
97	CE1	TYR	A	223	51.833	18.861	2.241	1	29.57
98	CE2	TYR	A	223	50.223	18.938	0.451	1	28.57
99	CZ	TYR	A	223	51.43	18.475	0.97	1	28.97
100	OH	TYR	A	223	52.224	17.593	0.255	1	32.62
101	N	SER	A	224	47.049	23.531	3.155	1	23
102	CA	SER	A	224	45.91	24.289	3.633	1	26.09
103	C	SER	A	224	44.945	23.431	4.441	1	28.04
104	O	SER	A	224	44.108	23.948	5.188	1	27.28
105	CB	SER	A	224	45.166	24.899	2.439	1	26.82
106	OG	SER	A	224	44.682	23.889	1.563	1	24.02
107	N	THR	A	225	45.07	22.121	4.307	1	25.2
108	CA	THR	A	225	44.158	21.234	4.978	1	21.51
109	C	THR	A	225	44.891	19.941	5.276	1	25.62
110	O	THR	A	225	46.083	19.815	4.977	1	25.74
111	CB	THR	A	225	42.92	20.984	4.074	1	26.34
112	OG1	THR	A	225	41.832	20.496	4.863	1	27.95
113	CG2	THR	A	225	43.236	19.974	2.953	1	23.42
114	N	VAL	A	226	44.18	18.984	5.866	1	26.17
115	CA	VAL	A	226	44.777	17.707	6.225	1	25.74
116	C	VAL	A	226	44.455	16.647	5.184	1	26.68
117	O	VAL	A	226	43.42	16.721	4.511	1	28.8
118	CB	VAL	A	226	44.303	17.232	7.65	1	27.25
119	CG1	VAL	A	226	44.888	18.134	8.719	1	27.18
120	CG2	VAL	A	226	42.782	17.222	7.746	1	23.83

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
121	N	PRO	A	227	45.326	15.63	5.058	1	25.13
122	CA	PRO	A	227	45.151	14.541	4.106	1	24.49
123	C	PRO	A	227	43.735	13.98	4.148	1	30.13
124	O	PRO	A	227	43.185	13.704	5.226	1	35.19
125	CB	PRO	A	227	46.15	13.511	4.6	1	21.69
126	CG	PRO	A	227	47.256	14.331	5.112	1	20.33
127	CD	PRO	A	227	46.535	15.415	5.872	1	24.33
128	N	GLY	A	228	43.14	13.859	2.964	1	30.85
129	CA	GLY	A	228	41.803	13.319	2.826	1	23.87
130	C	GLY	A	228	40.704	14.34	2.947	1	23.86
131	O	GLY	A	228	39.537	14.009	2.731	1	26.72
132	N	TYR	A	229	41.055	15.59	3.202	1	23.75
133	CA	TYR	A	229	40.026	16.602	3.378	1	30.9
134	C	TYR	A	229	39.902	17.665	2.315	1	33.77
135	O	TYR	A	229	40.842	17.929	1.564	1	36.59
136	CB	TYR	A	229	40.192	17.291	4.738	1	32.28
137	CG	TYR	A	229	39.746	16.439	5.903	1	35.11
138	CD1	TYR	A	229	40.498	15.335	6.319	1	31.82
139	CD2	TYR	A	229	38.558	16.728	6.578	1	37.17
140	CE1	TYR	A	229	40.08	14.546	7.375	1	37.51
141	CE2	TYR	A	229	38.122	15.942	7.644	1	39.72
142	CZ	TYR	A	229	38.887	14.854	8.042	1	40.33
143	OH	TYR	A	229	38.473	14.098	9.12	1	44.64
144	N	TYR	A	230	38.722	18.276	2.274	1	33.27
145	CA	TYR	A	230	38.436	19.363	1.364	1	35.52
146	C	TYR	A	230	39.147	20.587	1.935	1	38.32
147	O	TYR	A	230	39.557	20.595	3.102	1	39.71
148	CB	TYR	A	230	36.948	19.667	1.352	1	38
149	CG	TYR	A	230	36.107	18.784	0.483	1	46.57
150	CD1	TYR	A	230	36.485	18.476	-0.822	1	50.66
151	CD2	TYR	A	230	34.869	18.34	0.931	1	51.64
152	CE1	TYR	A	230	35.63	17.755	-1.662	1	53.17
153	CE2	TYR	A	230	34.014	17.624	0.107	1	53.65
154	CZ	TYR	A	230	34.391	17.338	-1.184	1	53.99
155	OH	TYR	A	230	33.507	16.659	-1.988	1	59
156	N	SER	A	231	39.261	21.634	1.127	1	35.89
157	CA	SER	A	231	39.909	22.865	1.547	1	33
158	C	SER	A	231	38.891	23.906	1.123	1	35
159	O	SER	A	231	38.283	23.774	0.067	1	37.57
160	CB	SER	A	231	41.233	23.019	0.813	1	30.36
161	OG	SER	A	231	42.078	23.944	1.459	1	33.81
162	N	TRP	A	232	38.632	24.88	1.981	1	36.72
163	CA	TRP	A	232	37.627	25.886	1.695	1	36.91
164	C	TRP	A	232	38.115	27.193	1.117	1	38.11
165	O	TRP	A	232	39.171	27.713	1.488	1	38.32
166	CB	TRP	A	232	36.775	26.15	2.939	1	39.45
167	CG	TRP	A	232	35.928	24.973	3.32	1	42.79
168	CD1	TRP	A	232	36.291	23.916	4.109	1	43.98
169	CD2	TRP	A	232	34.581	24.717	2.899	1	43.35
170	NE1	TRP	A	232	35.259	23.019	4.205	1	42.6
171	CE2	TRP	A	232	34.195	23.482	3.474	1	42.31
172	CE3	TRP	A	232	33.669	25.405	2.088	1	41.58

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
173	CZ2	TRP	A	232	32.932	22.923	3.268	1	40.87
174	CZ3	TRP	A	232	32.414	24.852	1.88	1	41.12
175	CH2	TRP	A	232	32.059	23.618	2.471	1	43
176	N	ARG	A	233	37.266	27.761	0.268	1	38.94
177	CA	ARG	A	233	37.549	29.006	-0.41	1	38.48
178	C	ARG	A	233	36.248	29.756	-0.566	1	38.79
179	O	ARG	A	233	35.231	29.17	-0.939	1	42.35
180	CB	ARG	A	233	38.142	28.693	-1.789	1	37.71
181	CG	ARG	A	233	38.391	29.892	-2.701	1	35.14
182	CD	ARG	A	233	39.135	29.436	-3.943	1	31.83
183	NE	ARG	A	233	38.593	28.179	-4.463	1	31.63
184	CZ	ARG	A	233	37.35	28.026	-4.928	1	32.77
185	NH1	ARG	A	233	36.503	29.051	-4.955	1	34.39
186	NH2	ARG	A	233	36.94	26.833	-5.34	1	28.46
187	N	SER	A	234	36.25	31.024	-0.194	1	39.44
188	CA	SER	A	234	35.056	31.827	-0.362	1	44.1
189	C	SER	A	234	35.264	32.642	-1.637	1	45.03
190	O	SER	A	234	36.223	33.419	-1.739	1	42.63
191	CB	SER	A	234	35.169	32.709	0.892	1	44.34
192	OG	SER	A	234	34.546	33.977	0.801	1	46.7
193	N	PRO	A	235	34.379	32.467	-2.631	1	47.1
194	CA	PRO	A	235	34.414	33.158	-3.926	1	48.32
195	C	PRO	A	235	34.771	34.639	-3.833	1	48.26
196	O	PRO	A	235	35.522	35.164	-4.661	1	49.57
197	CB	PRO	A	235	32.993	32.971	-4.445	1	48.54
198	CG	PRO	A	235	32.659	31.606	-3.962	1	49.05
199	CD	PRO	A	235	33.189	31.593	-2.542	1	46.77
200	N	GLY	A	236	34.254	35.3	-2.806	1	46.38
201	CA	GLY	A	236	34.518	36.712	-2.651	1	45.93
202	C	GLY	A	236	35.693	37.141	-1.798	1	47.37
203	O	GLY	A	236	36.047	38.316	-1.842	1	49.39
204	N	ARG	A	237	36.282	36.243	-1.007	1	46.54
205	CA	ARG	A	237	37.404	36.638	-0.148	1	46.81
206	C	ARG	A	237	38.666	35.835	-0.374	1	44.18
207	O	ARG	A	237	39.751	36.233	0.05	1	43.89
208	CB	ARG	A	237	37.037	36.541	1.335	1	53.02
209	CG	ARG	A	237	36.15	37.646	1.874	1	62.35
210	CD	ARG	A	237	34.673	37.36	1.638	1	74.62
211	NE	ARG	A	237	34.169	36.237	2.43	1	84.42
212	CZ	ARG	A	237	32.964	35.69	2.273	1	90.69
213	NH1	ARG	A	237	32.136	36.162	1.343	1	94.17
214	NH2	ARG	A	237	32.577	34.685	3.053	1	92.5
215	N	GLY	A	238	38.522	34.7	-1.034	1	39.96
216	CA	GLY	A	238	39.665	33.856	-1.285	1	37.26
217	C	GLY	A	238	39.593	32.664	-0.364	1	36.2
218	O	GLY	A	238	38.631	32.505	0.396	1	34.54
219	N	SER	A	239	40.608	31.814	-0.429	1	34.92
220	CA	SER	A	239	40.65	30.631	0.408	1	34.95
221	C	SER	A	239	40.939	31.028	1.859	1	34.56
222	O	SER	A	239	41.641	32.024	2.11	1	34.26
223	CB	SER	A	239	41.713	29.665	-0.113	1	32.84
224	OG	SER	A	239	42.99	30.275	-0.135	1	39.23

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
225	N	TRP	A	240	40.427	30.235	2.804	1	33.04
226	CA	TRP	A	240	40.624	30.508	4.234	1	29.44
227	C	TRP	A	240	42.107	30.526	4.563	1	23.06
228	O	TRP	A	240	42.625	31.48	5.137	1	22.99
229	CB	TRP	A	240	39.932	29.444	5.101	1	32.47
230	CG	TRP	A	240	38.429	29.383	4.957	1	31.03
231	CD1	TRP	A	240	37.625	30.236	4.247	1	29.24
232	CD2	TRP	A	240	37.557	28.408	5.549	1	31.53
233	NE1	TRP	A	240	36.312	29.857	4.361	1	32.28
234	CE2	TRP	A	240	36.239	28.737	5.151	1	31.45
235	CE3	TRP	A	240	37.759	27.296	6.375	1	30.55
236	CZ2	TRP	A	240	35.126	27.985	5.552	1	29.57
237	CZ3	TRP	A	240	36.652	26.546	6.775	1	26.07
238	CH2	TRP	A	240	35.353	26.898	6.362	1	30.71
239	N	PHE	A	241	42.797	29.499	4.101	1	19.34
240	CA	PHE	A	241	44.212	29.355	4.349	1	19.66
241	C	PHE	A	241	45.036	30.551	3.906	1	24.1
242	O	PHE	A	241	45.991	30.938	4.583	1	29.58
243	CB	PHE	A	241	44.707	28.085	3.68	1	17.56
244	CG	PHE	A	241	46.161	27.836	3.879	1	22.84
245	CD1	PHE	A	241	46.675	27.653	5.159	1	20.77
246	CD2	PHE	A	241	47.03	27.788	2.785	1	24.47
247	CE1	PHE	A	241	48.035	27.422	5.36	1	21.32
248	CE2	PHE	A	241	48.396	27.561	2.968	1	22.25
249	CZ	PHE	A	241	48.9	27.376	4.263	1	27
250	N	VAL	A	242	44.661	31.161	2.787	1	26.69
251	CA	VAL	A	242	45.412	32.294	2.273	1	22.81
252	C	VAL	A	242	45.029	33.597	2.939	1	23.24
253	O	VAL	A	242	45.889	34.454	3.178	1	26.19
254	CB	VAL	A	242	45.319	32.367	0.739	1	24.14
255	CG1	VAL	A	242	45.966	33.654	0.211	1	18.28
256	CG2	VAL	A	242	46.02	31.143	0.152	1	17.43
257	N	GLN	A	243	43.744	33.772	3.218	1	23.41
258	CA	GLN	A	243	43.32	34.97	3.92	1	27.17
259	C	GLN	A	243	44.124	35.002	5.234	1	30.4
260	O	GLN	A	243	44.81	35.995	5.543	1	32.79
261	CB	GLN	A	243	41.84	34.885	4.259	1	28.68
262	CG	GLN	A	243	40.925	34.823	3.084	1	30.81
263	CD	GLN	A	243	39.476	34.865	3.511	1	32.26
264	OE1	GLN	A	243	39.055	35.789	4.197	1	40.86
265	NE2	GLN	A	243	38.704	33.864	3.111	1	34.67
266	N	ALA	A	244	44.085	33.872	5.953	1	31.09
267	CA	ALA	A	244	44.789	33.684	7.228	1	29.7
268	C	ALA	A	244	46.289	33.927	7.128	1	29.19
269	O	ALA	A	244	46.824	34.806	7.805	1	31.96
270	CB	ALA	A	244	44.526	32.287	7.77	1	26.82
271	N	LEU	A	245	46.953	33.15	6.272	1	30.17
272	CA	LEU	A	245	48.396	33.244	6.044	1	28.53
273	C	LEU	A	245	48.879	34.647	5.725	1	30.09
274	O	LEU	A	245	49.945	35.062	6.181	1	33.28
275	CB	LEU	A	245	48.809	32.296	4.92	1	26.79
276	CG	LEU	A	245	50.253	32.362	4.43	1	27.75

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
277	CD1	LEU	A	245	51.232	32.161	5.578	1	31.49
278	CD2	LEU	A	245	50.449	31.301	3.368	1	27.08
279	N	CYS	A	246	48.084	35.389	4.965	1	32.68
280	CA	CYS	A	246	48.454	36.742	4.596	1	33.31
281	C	CYS	A	246	48.312	37.735	5.73	1	34.36
282	O	CYS	A	246	49.181	38.597	5.895	1	34.21
283	CB	CYS	A	246	47.705	37.193	3.336	1	36.43
284	SG	CYS	A	246	48.396	36.434	1.824	1	37.11
285	N	SER	A	247	47.24	37.636	6.518	1	34.31
286	CA	SER	A	247	47.097	38.566	7.639	1	37.26
287	C	SER	A	247	48.245	38.334	8.631	1	35.07
288	O	SER	A	247	48.917	39.285	9.054	1	35.51
289	CB	SER	A	247	45.726	38.442	8.326	1	40.99
290	OG	SER	A	247	45.307	37.095	8.436	1	51.01
291	N	ILE	A	248	48.54	37.065	8.907	1	29.97
292	CA	ILE	A	248	49.615	36.745	9.824	1	28.62
293	C	ILE	A	248	50.95	37.264	9.306	1	30.39
294	O	ILE	A	248	51.646	37.983	10.022	1	32.68
295	CB	ILE	A	248	49.724	35.225	10.107	1	29.01
296	CG1	ILE	A	248	48.404	34.684	10.657	1	27.27
297	CG2	ILE	A	248	50.84	34.963	11.099	1	25.35
298	CD1	ILE	A	248	47.908	35.432	11.86	1	30.79
299	N	LEU	A	249	51.301	36.921	8.067	1	32.43
300	CA	LEU	A	249	52.575	37.355	7.483	1	32.09
301	C	LEU	A	249	52.712	38.859	7.412	1	32.87
302	O	LEU	A	249	53.797	39.403	7.63	1	30.05
303	CB	LEU	A	249	52.758	36.784	6.086	1	32.32
304	CG	LEU	A	249	53.198	35.335	5.98	1	33.35
305	CD1	LEU	A	249	53.211	34.926	4.511	1	33.21
306	CD2	LEU	A	249	54.568	35.189	6.598	1	26.29
307	N	GLU	A	250	51.619	39.531	7.08	1	38.21
308	CA	GLU	A	250	51.651	40.979	6.983	1	47.23
309	C	GLU	A	250	52.097	41.568	8.318	1	50.44
310	O	GLU	A	250	53.04	42.361	8.367	1	52.26
311	CB	GLU	A	250	50.284	41.527	6.576	1	52.32
312	CG	GLU	A	250	50.256	43.047	6.456	1	64.99
313	CD	GLU	A	250	48.923	43.601	5.956	1	73.78
314	OE1	GLU	A	250	47.914	42.851	5.944	1	77.74
315	OE2	GLU	A	250	48.889	44.801	5.578	1	77.99
316	N	GLU	A	251	51.483	41.093	9.402	1	51.5
317	CA	GLU	A	251	51.799	41.57	10.744	1	50.69
318	C	GLU	A	251	53.048	40.981	11.422	1	47.3
319	O	GLU	A	251	53.753	41.696	12.132	1	47.39
320	CB	GLU	A	251	50.587	41.383	11.657	1	59.91
321	CG	GLU	A	251	50.803	41.836	13.101	1	69.48
322	CD	GLU	A	251	49.711	41.347	14.04	1	76.13
323	OE1	GLU	A	251	49.315	40.161	13.934	1	77.63
324	OE2	GLU	A	251	49.257	42.149	14.891	1	79.7
325	N	HIS	A	252	53.338	39.7	11.202	1	43.99
326	CA	HIS	A	252	54.487	39.07	11.86	1	41.2
327	C	HIS	A	252	55.562	38.435	11.006	1	39.48
328	O	HIS	A	252	56.552	37.952	11.549	1	35.87

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
329	CB	HIS	A	252	54.002	38.023	12.853	1	42.52
330	CG	HIS	A	252	53.132	38.58	13.933	1	45.77
331	ND1	HIS	A	252	53.57	39.543	14.818	1	44.53
332	CD2	HIS	A	252	51.843	38.325	14.258	1	47.43
333	CE1	HIS	A	252	52.585	39.86	15.641	1	47.22
334	NE2	HIS	A	252	51.527	39.134	15.323	1	49.51
335	N	GLY	A	253	55.387	38.46	9.686	1	40.35
336	CA	GLY	A	253	56.335	37.846	8.767	1	34.46
337	C	GLY	A	253	57.784	38.207	8.978	1	33.55
338	O	GLY	A	253	58.679	37.386	8.773	1	33.67
339	N	LYS	A	254	58.032	39.435	9.395	1	34.68
340	CA	LYS	A	254	59.398	39.859	9.626	1	41.13
341	C	LYS	A	254	59.872	39.681	11.078	1	44.24
342	O	LYS	A	254	61.063	39.82	11.351	1	45.79
343	CB	LYS	A	254	59.609	41.303	9.151	1	44.92
344	CG	LYS	A	254	59.669	41.477	7.626	1	45.68
345	CD	LYS	A	254	58.362	42.029	7.026	1	56.44
346	CE	LYS	A	254	57.179	41.041	7.113	1	60.85
347	NZ	LYS	A	254	55.956	41.409	6.328	1	57.97
348	N	ASP	A	255	58.97	39.328	11.998	1	44.21
349	CA	ASP	A	255	59.386	39.15	13.385	1	44.96
350	C	ASP	A	255	59.218	37.778	14.054	1	42.7
351	O	ASP	A	255	59.741	37.569	15.146	1	46.32
352	CB	ASP	A	255	58.847	40.28	14.283	1	50.99
353	CG	ASP	A	255	57.337	40.244	14.456	1	60.13
354	OD1	ASP	A	255	56.812	39.232	14.971	1	65.27
355	OD2	ASP	A	255	56.676	41.252	14.11	1	65.21
356	N	LEU	A	256	58.504	36.848	13.43	1	37.48
357	CA	LEU	A	256	58.338	35.515	14.014	1	33.56
358	C	LEU	A	256	58.95	34.415	13.14	1	34.41
359	O	LEU	A	256	59.067	34.558	11.925	1	38.19
360	CB	LEU	A	256	56.86	35.192	14.242	1	28.64
361	CG	LEU	A	256	56.054	35.983	15.265	1	28.62
362	CD1	LEU	A	256	54.644	35.475	15.281	1	22.89
363	CD2	LEU	A	256	56.664	35.838	16.629	1	29.83
364	N	GLU	A	257	59.327	33.312	13.771	1	32.34
365	CA	GLU	A	257	59.889	32.165	13.075	1	28.93
366	C	GLU	A	257	58.752	31.515	12.265	1	29.95
367	O	GLU	A	257	57.577	31.591	12.652	1	30.27
368	CB	GLU	A	257	60.471	31.194	14.106	1	26.72
369	CG	GLU	A	257	61.531	30.234	13.589	1	27.17
370	CD	GLU	A	257	60.946	28.95	13.04	1	33.4
371	OE1	GLU	A	257	59.762	28.666	13.309	1	40.44
372	OE2	GLU	A	257	61.668	28.205	12.351	1	33.34
373	N	ILE	A	258	59.103	30.883	11.145	1	28.88
374	CA	ILE	A	258	58.124	30.251	10.253	1	27.66
375	C	ILE	A	258	57.095	29.356	10.951	1	24.39
376	O	ILE	A	258	55.894	29.47	10.688	1	22.36
377	CB	ILE	A	258	58.819	29.502	9.041	1	24.95
378	CG1	ILE	A	258	57.794	29.202	7.938	1	25.55
379	CG2	ILE	A	258	59.476	28.198	9.496	1	21.39
380	CD1	ILE	A	258	57.025	30.421	7.461	1	23.29

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
381	N	MET	A	259	57.555	28.466	11.827	1	26.97
382	CA	MET	A	259	56.651	27.579	12.577	1	28.71
383	C	MET	A	259	55.648	28.35	13.441	1	26.67
384	O	MET	A	259	54.503	27.923	13.581	1	25.91
385	CB	MET	A	259	57.425	26.601	13.455	1	29.68
386	CG	MET	A	259	58.149	25.502	12.703	1	32.66
387	SD	MET	A	259	57.133	24.751	11.4	1	37.72
388	CE	MET	A	259	55.573	24.391	12.232	1	37.24
389	N	GLN	A	260	56.072	29.485	14.005	1	30.03
390	CA	GLN	A	260	55.187	30.325	14.83	1	32.96
391	C	GLN	A	260	54.113	30.922	13.933	1	33.36
392	O	GLN	A	260	52.924	30.885	14.254	1	35.85
393	CB	GLN	A	260	55.946	31.468	15.498	1	33.24
394	CG	GLN	A	260	56.987	31.052	16.498	1	38.29
395	CD	GLN	A	260	57.54	32.241	17.267	1	42.31
396	OE1	GLN	A	260	58.385	32.986	16.766	1	42.11
397	NE2	GLN	A	260	57.045	32.438	18.486	1	43.55
398	N	ILE	A	261	54.546	31.478	12.808	1	31.03
399	CA	ILE	A	261	53.633	32.058	11.834	1	30.12
400	C	ILE	A	261	52.582	31.012	11.407	1	28.71
401	O	ILE	A	261	51.372	31.235	11.529	1	27.73
402	CB	ILE	A	261	54.425	32.543	10.58	1	35.02
403	CG1	ILE	A	261	55.351	33.708	10.958	1	31.51
404	CG2	ILE	A	261	53.464	32.9	9.432	1	29.99
405	CD1	ILE	A	261	56.391	34.026	9.908	1	31.07
406	N	LEU	A	262	53.052	29.859	10.938	1	29.19
407	CA	LEU	A	262	52.156	28.79	10.493	1	30.27
408	C	LEU	A	262	51.272	28.252	11.611	1	33.61
409	O	LEU	A	262	50.125	27.875	11.35	1	35.89
410	CB	LEU	A	262	52.929	27.663	9.79	1	23.35
411	CG	LEU	A	262	53.627	28.118	8.496	1	21.97
412	CD1	LEU	A	262	54.545	27.051	7.979	1	15.92
413	CD2	LEU	A	262	52.59	28.504	7.447	1	15.78
414	N	THR	A	263	51.777	28.241	12.852	1	34.28
415	CA	THR	A	263	50.955	27.78	13.973	1	30.74
416	C	THR	A	263	49.815	28.776	14.164	1	26.83
417	O	THR	A	263	48.653	28.377	14.312	1	25.94
418	CB	THR	A	263	51.763	27.597	15.265	1	34.48
419	OG1	THR	A	263	52.709	26.536	15.082	1	34.31
420	CG2	THR	A	263	50.843	27.22	16.406	1	35.89
421	N	ARG	A	264	50.126	30.066	14.044	1	23.1
422	CA	ARG	A	264	49.1	31.098	14.161	1	24.72
423	C	ARG	A	264	48.097	31.025	13.013	1	27.59
424	O	ARG	A	264	46.899	31.306	13.191	1	28.32
425	CB	ARG	A	264	49.731	32.474	14.226	1	25.55
426	CG	ARG	A	264	50.567	32.67	15.469	1	31.36
427	CD	ARG	A	264	50.978	34.112	15.645	1	35.37
428	NE	ARG	A	264	51.923	34.273	16.743	1	36.53
429	CZ	ARG	A	264	52.014	35.37	17.485	1	37.59
430	NH1	ARG	A	264	51.209	36.396	17.249	1	37.76
431	NH2	ARG	A	264	52.938	35.458	18.431	1	39.51
432	N	VAL	A	265	48.592	30.652	11.829	1	30.79

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
433	CA	VAL	A	265	47.75	30.495	10.638	1	24.83
434	C	VAL	A	265	46.823	29.313	10.923	1	21.65
435	O	VAL	A	265	45.617	29.389	10.684	1	21.47
436	CB	VAL	A	265	48.614	30.232	9.372	1	25.57
437	CG1	VAL	A	265	47.748	29.83	8.195	1	23.36
438	CG2	VAL	A	265	49.405	31.468	9.025	1	18.95
439	N	ASN	A	266	47.39	28.268	11.527	1	25.88
440	CA	ASN	A	266	46.66	27.055	11.915	1	29.21
441	C	ASN	A	266	45.516	27.422	12.851	1	29.23
442	O	ASN	A	266	44.383	26.998	12.656	1	30.93
443	CB	ASN	A	266	47.589	26.071	12.648	1	30.58
444	CG	ASN	A	266	48.136	24.977	11.743	1	31.68
445	OD1	ASN	A	266	47.656	24.781	10.635	1	34.41
446	ND2	ASN	A	266	49.139	24.246	12.225	1	27.15
447	N	ASP	A	267	45.821	28.203	13.88	1	29.37
448	CA	ASP	A	267	44.81	28.629	14.843	1	33.07
449	C	ASP	A	267	43.778	29.59	14.223	1	33.34
450	O	ASP	A	267	42.578	29.475	14.502	1	32.71
451	CB	ASP	A	267	45.502	29.249	16.067	1	38.3
452	CG	ASP	A	267	44.529	29.841	17.079	1	42.56
453	OD1	ASP	A	267	43.598	29.139	17.538	1	40.01
454	OD2	ASP	A	267	44.728	31.024	17.431	1	47.33
455	N	ARG	A	268	44.229	30.506	13.362	1	34.61
456	CA	ARG	A	268	43.334	31.465	12.708	1	33.06
457	C	ARG	A	268	42.266	30.802	11.841	1	33.33
458	O	ARG	A	268	41.095	31.174	11.893	1	35.37
459	CB	ARG	A	268	44.136	32.422	11.841	1	36.79
460	CG	ARG	A	268	43.278	33.389	11.029	1	44.09
461	CD	ARG	A	268	42.671	34.453	11.906	1	51.38
462	NE	ARG	A	268	43.692	35.092	12.74	1	61.91
463	CZ	ARG	A	268	44.386	36.18	12.403	1	64.94
464	NH1	ARG	A	268	44.178	36.785	11.236	1	67.48
465	NH2	ARG	A	268	45.312	36.655	13.233	1	64.88
466	N	VAL	A	269	42.685	29.824	11.044	1	33.13
467	CA	VAL	A	269	41.793	29.093	10.142	1	31.83
468	C	VAL	A	269	40.786	28.244	10.899	1	33.86
469	O	VAL	A	269	39.609	28.197	10.538	1	34.67
470	CB	VAL	A	269	42.608	28.173	9.163	1	30.85
471	CG1	VAL	A	269	41.693	27.212	8.424	1	21.1
472	CG2	VAL	A	269	43.363	29.027	8.153	1	30.75
473	N	ALA	A	270	41.274	27.55	11.926	1	35.33
474	CA	ALA	A	270	40.452	26.676	12.761	1	36.98
475	C	ALA	A	270	39.362	27.412	13.536	1	39.95
476	O	ALA	A	270	38.205	26.976	13.56	1	37.86
477	CB	ALA	A	270	41.34	25.905	13.734	1	35.25
478	N	ARG	A	271	39.735	28.526	14.164	1	43.08
479	CA	ARG	A	271	38.8	29.301	14.968	1	46.56
480	C	ARG	A	271	37.971	30.344	14.251	1	47.57
481	O	ARG	A	271	36.812	30.54	14.591	1	51.02
482	CB	ARG	A	271	39.522	29.95	16.148	1	50.33
483	CG	ARG	A	271	39.792	28.979	17.281	1	62.62
484	CD	ARG	A	271	40.428	29.639	18.508	1	71.12

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
485	NE	ARG	A	271	40.283	28.804	19.708	1	78.73
486	CZ	ARG	A	271	41.095	27.802	20.047	1	82.33
487	NH1	ARG	A	271	42.137	27.484	19.287	1	85.86
488	NH2	ARG	A	271	40.847	27.094	21.143	1	83.28
489	N	HIS	A	272	38.531	30.99	13.236	1	48.74
490	CA	HIS	A	272	37.807	32.051	12.542	1	48.29
491	C	HIS	A	272	37.039	31.753	11.261	1	47.63
492	O	HIS	A	272	36.485	32.666	10.654	1	50.34
493	CB	HIS	A	272	38.746	33.216	12.307	1	52.89
494	CG	HIS	A	272	39.352	33.741	13.565	1	62.11
495	ND1	HIS	A	272	38.75	34.718	14.325	1	64.64
496	CD2	HIS	A	272	40.483	33.393	14.223	1	64.98
497	CE1	HIS	A	272	39.484	34.952	15.398	1	67.25
498	NE2	HIS	A	272	40.54	34.161	15.36	1	66.34
499	N	PHE	A	273	36.945	30.49	10.871	1	44.86
500	CA	PHE	A	273	36.252	30.162	9.639	1	40.35
501	C	PHE	A	273	35.301	29.001	9.851	1	40.96
502	O	PHE	A	273	35.6	28.084	10.608	1	39.28
503	CB	PHE	A	273	37.27	29.795	8.546	1	40.1
504	CG	PHE	A	273	38.127	30.955	8.067	1	35.41
505	CD1	PHE	A	273	37.702	31.772	7.016	1	36.05
506	CD2	PHE	A	273	39.369	31.199	8.635	1	32.56
507	CE1	PHE	A	273	38.505	32.808	6.539	1	29.05
508	CE2	PHE	A	273	40.177	32.233	8.163	1	31.99
509	CZ	PHE	A	273	39.742	33.038	7.109	1	30.98
510	N	GLU	A	274	34.157	29.058	9.177	1	42.86
511	CA	GLU	A	274	33.141	28.011	9.239	1	47.61
512	C	GLU	A	274	32.301	28.138	7.966	1	46.91
513	O	GLU	A	274	31.714	29.186	7.703	1	47.59
514	CB	GLU	A	274	32.257	28.16	10.484	1	52.69
515	CG	GLU	A	274	31.337	26.96	10.718	1	59.89
516	CD	GLU	A	274	30.338	27.18	11.839	1	66.28
517	OE1	GLU	A	274	30.733	27.057	13.021	1	66.4
518	OE2	GLU	A	274	29.154	27.464	11.535	1	69.73
519	N	SER	A	275	32.226	27.063	7.195	1	47.48
520	CA	SER	A	275	31.504	27.085	5.941	1	47.08
521	C	SER	A	275	30.052	27.481	6.045	1	51.35
522	O	SER	A	275	29.353	27.113	6.987	1	51.75
523	CB	SER	A	275	31.608	25.74	5.237	1	42.69
524	OG	SER	A	275	30.545	24.889	5.612	1	41.28
525	N	GLN	A	276	29.62	28.26	5.062	1	56.66
526	CA	GLN	A	276	28.245	28.722	4.926	1	60.65
527	C	GLN	A	276	27.875	28.098	3.586	1	59.18
528	O	GLN	A	276	28.612	28.236	2.615	1	58.63
529	CB	GLN	A	276	28.184	30.252	4.808	1	67.63
530	CG	GLN	A	276	28.938	31.022	5.899	1	79.88
531	CD	GLN	A	276	29.795	32.184	5.346	1	87.1
532	OE1	GLN	A	276	29.307	33.307	5.165	1	91.49
533	NE2	GLN	A	276	31.08	31.913	5.097	1	88.07
534	N	SER	A	277	26.765	27.38	3.537	1	59.89
535	CA	SER	A	277	26.36	26.742	2.302	1	62.51
536	C	SER	A	277	24.88	26.42	2.281	1	67.28

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
537	O	SER	A	277	24.235	26.311	3.326	1	68.82
538	CB	SER	A	277	27.176	25.472	2.072	1	58.65
539	OG	SER	A	277	26.721	24.761	0.935	1	57.16
540	N	ASP	A	278	24.348	26.305	1.072	1	73.93
541	CA	ASP	A	278	22.947	25.99	0.867	1	78.76
542	C	ASP	A	278	22.785	24.488	0.899	1	78.58
543	O	ASP	A	278	21.692	23.984	1.143	1	79.84
544	CB	ASP	A	278	22.451	26.567	-0.459	1	85.91
545	CG	ASP	A	278	22.452	28.095	-0.467	1	92.81
546	OD1	ASP	A	278	21.963	28.706	0.516	1	94.66
547	OD2	ASP	A	278	22.949	28.685	-1.456	1	98.14
548	N	ASP	A	279	23.863	23.77	0.605	1	78.22
549	CA	ASP	A	279	23.807	22.322	0.668	1	78.28
550	C	ASP	A	279	24.136	22.048	2.114	1	77.24
551	O	ASP	A	279	25.265	22.266	2.55	1	79.07
552	CB	ASP	A	279	24.858	21.654	-0.224	1	80.03
553	CG	ASP	A	279	24.756	20.119	-0.213	1	82.04
554	OD1	ASP	A	279	24.081	19.547	0.675	1	81.67
555	OD2	ASP	A	279	25.353	19.475	-1.102	1	84.41
556	N	PRO	A	280	23.154	21.555	2.876	1	75.38
557	CA	PRO	A	280	23.359	21.253	4.291	1	72.89
558	C	PRO	A	280	24.539	20.306	4.48	1	69.57
559	O	PRO	A	280	25.304	20.452	5.427	1	71.02
560	CB	PRO	A	280	22.031	20.612	4.689	1	74.44
561	CG	PRO	A	280	21.551	19.99	3.41	1	75.32
562	CD	PRO	A	280	21.837	21.085	2.426	1	75.76
563	N	HIS	A	281	24.711	19.373	3.547	1	64.17
564	CA	HIS	A	281	25.813	18.422	3.598	1	61.69
565	C	HIS	A	281	27.145	19.173	3.648	1	59.46
566	O	HIS	A	281	28.148	18.647	4.137	1	60.3
567	CB	HIS	A	281	25.768	17.517	2.361	1	67.25
568	CG	HIS	A	281	26.9	16.533	2.266	1	74.72
569	ND1	HIS	A	281	28.227	16.911	2.21	1	79.02
570	CD2	HIS	A	281	26.895	15.182	2.171	1	77.86
571	CE1	HIS	A	281	28.989	15.839	2.081	1	78.89
572	NE2	HIS	A	281	28.205	14.777	2.055	1	79.31
573	N	PHE	A	282	27.162	20.39	3.118	1	55.38
574	CA	PHE	A	282	28.376	21.2	3.09	1	52
575	C	PHE	A	282	28.279	22.448	3.966	1	50.65
576	O	PHE	A	282	29.105	23.358	3.861	1	49.46
577	CB	PHE	A	282	28.692	21.603	1.643	1	49.3
578	CG	PHE	A	282	29.379	20.526	0.847	1	47.65
579	CD1	PHE	A	282	28.674	19.421	0.388	1	47.73
580	CD2	PHE	A	282	30.743	20.609	0.584	1	47.98
581	CE1	PHE	A	282	29.321	18.405	-0.322	1	50.15
582	CE2	PHE	A	282	31.4	19.606	-0.122	1	49
583	CZ	PHE	A	282	30.686	18.497	-0.576	1	50
584	N	HIS	A	283	27.321	22.461	4.882	1	49.71
585	CA	HIS	A	283	27.116	23.619	5.735	1	49.68
586	C	HIS	A	283	27.766	23.546	7.122	1	50.88
587	O	HIS	A	283	27.704	22.52	7.799	1	52.55
588	CB	HIS	A	283	25.612	23.87	5.86	1	52.08

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
589	CG	HIS	A	283	25.262	25.141	6.563	1	54.82
590	ND1	HIS	A	283	25.991	26.305	6.413	1	57.25
591	CD2	HIS	A	283	24.266	25.434	7.432	1	56.05
592	CE1	HIS	A	283	25.46	27.257	7.158	1	57.45
593	NE2	HIS	A	283	24.412	26.754	7.789	1	57.31
594	N	GLU	A	284	28.396	24.645	7.531	1	51.44
595	CA	GLU	A	284	29.03	24.758	8.847	1	50.67
596	C	GLU	A	284	30.22	23.85	9.103	1	48.76
597	O	GLU	A	284	30.485	23.474	10.242	1	47.89
598	CB	GLU	A	284	27.997	24.586	9.96	1	53.88
599	CG	GLU	A	284	27.028	25.745	10.069	1	59.11
600	CD	GLU	A	284	25.8	25.427	10.906	1	62.86
601	OE1	GLU	A	284	25.396	24.238	10.979	1	62.17
602	OE2	GLU	A	284	25.228	26.387	11.472	1	63.47
603	N	LYS	A	285	30.956	23.53	8.047	1	45.94
604	CA	LYS	A	285	32.14	22.696	8.17	1	42.36
605	C	LYS	A	285	33.325	23.536	8.664	1	39.9
606	O	LYS	A	285	33.339	24.766	8.516	1	37.53
607	CB	LYS	A	285	32.457	22.037	6.832	1	44.52
608	CG	LYS	A	285	31.315	21.196	6.316	1	45.97
609	CD	LYS	A	285	30.862	20.248	7.39	1	46.88
610	CE	LYS	A	285	29.652	19.464	6.968	1	50.67
611	NZ	LYS	A	285	29.191	18.61	8.091	1	52.52
612	N	LYS	A	286	34.311	22.869	9.255	1	37.1
613	CA	LYS	A	286	35.496	23.535	9.804	1	33.51
614	C	LYS	A	286	36.725	23.038	9.053	1	30.32
615	O	LYS	A	286	36.628	22.094	8.285	1	32.26
616	CB	LYS	A	286	35.626	23.208	11.311	1	28.06
617	CG	LYS	A	286	34.429	23.636	12.183	1	17.45
618	CD	LYS	A	286	34.337	25.146	12.324	1	12.19
619	CE	LYS	A	286	35.653	25.709	12.819	1	14.58
620	NZ	LYS	A	286	35.578	27.147	13.162	1	16.2
621	N	GLN	A	287	37.887	23.621	9.32	1	28.7
622	CA	GLN	A	287	39.103	23.202	8.639	1	24.98
623	C	GLN	A	287	40.369	23.476	9.452	1	22.94
624	O	GLN	A	287	40.478	24.511	10.103	1	25.02
625	CB	GLN	A	287	39.188	23.949	7.302	1	23.97
626	CG	GLN	A	287	40.442	23.694	6.487	1	22.06
627	CD	GLN	A	287	40.556	24.631	5.294	1	24.9
628	OE1	GLN	A	287	39.556	25.076	4.736	1	24.96
629	NE2	GLN	A	287	41.78	24.958	4.921	1	17.4
630	N	ILE	A	288	41.328	22.556	9.415	1	22.94
631	CA	ILE	A	288	42.609	22.77	10.097	1	22.93
632	C	ILE	A	288	43.761	22.506	9.102	1	23.63
633	O	ILE	A	288	43.757	21.491	8.4	1	25.05
634	CB	ILE	A	288	42.77	21.847	11.353	1	23.17
635	CG1	ILE	A	288	44.085	22.145	12.084	1	20.39
636	CG2	ILE	A	288	42.7	20.378	10.967	1	19.44
637	CD1	ILE	A	288	44.164	23.537	12.704	1	16.72
638	N	PRO	A	289	44.691	23.467	8.948	1	20.4
639	CA	PRO	A	289	45.804	23.25	8.026	1	21.33
640	C	PRO	A	289	46.736	22.123	8.497	1	25.39

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
641	O	PRO	A	289	46.454	21.43	9.469	1	28.05
642	CB	PRO	A	289	46.497	24.61	8.003	1	21.26
643	CG	PRO	A	289	45.388	25.553	8.255	1	18.41
644	CD	PRO	A	289	44.617	24.878	9.352	1	18.98
645	N	CYS	A	290	47.866	21.959	7.831	1	25.54
646	CA	CYS	A	290	48.769	20.875	8.147	1	24.96
647	C	CYS	A	290	50.153	21.293	7.692	1	27.19
648	O	CYS	A	290	50.336	21.65	6.518	1	30.73
649	CB	CYS	A	290	48.295	19.634	7.382	1	21.47
650	SG	CYS	A	290	49.379	18.193	7.304	1	32.38
651	N	VAL	A	291	51.098	21.345	8.633	1	23.78
652	CA	VAL	A	291	52.472	21.731	8.328	1	19.67
653	C	VAL	A	291	53.38	20.523	8.439	1	21.76
654	O	VAL	A	291	53.3	19.776	9.404	1	29.41
655	CB	VAL	A	291	53.016	22.798	9.307	1	19.23
656	CG1	VAL	A	291	54.362	23.289	8.834	1	15.37
657	CG2	VAL	A	291	52.032	23.953	9.473	1	16.76
658	N	VAL	A	292	54.196	20.28	7.426	1	22.6
659	CA	VAL	A	292	55.116	19.164	7.484	1	20.41
660	C	VAL	A	292	56.459	19.828	7.413	1	21.94
661	O	VAL	A	292	56.68	20.664	6.542	1	26.22
662	CB	VAL	A	292	54.934	18.204	6.313	1	20.5
663	CG1	VAL	A	292	55.929	17.041	6.426	1	18.7
664	CG2	VAL	A	292	53.499	17.687	6.297	1	19.4
665	N	SER	A	293	57.332	19.528	8.365	1	22.03
666	CA	SER	A	293	58.636	20.158	8.373	1	19.84
667	C	SER	A	293	59.763	19.186	8.437	1	23.03
668	O	SER	A	293	59.73	18.234	9.229	1	23.57
669	CB	SER	A	293	58.779	21.13	9.538	1	20.7
670	OG	SER	A	293	60.127	21.569	9.624	1	26.86
671	N	MET	A	294	60.724	19.408	7.542	1	21.49
672	CA	MET	A	294	61.942	18.617	7.463	1	20.1
673	C	MET	A	294	63.043	19.642	7.625	1	19.31
674	O	MET	A	294	64.199	19.374	7.293	1	18.94
675	CB	MET	A	294	62.1	17.881	6.119	1	20.12
676	CG	MET	A	294	61.312	16.585	5.988	1	15.4
677	SD	MET	A	294	59.593	16.982	5.841	1	28.42
678	CE	MET	A	294	58.908	15.42	5.686	1	30.02
679	N	LEU	A	295	62.678	20.832	8.112	1	20.12
680	CA	LEU	A	295	63.66	21.887	8.337	1	22.21
681	C	LEU	A	295	64.625	21.445	9.426	1	25.18
682	O	LEU	A	295	64.286	20.613	10.281	1	26.89
683	CB	LEU	A	295	62.987	23.191	8.742	1	19.14
684	CG	LEU	A	295	62.133	23.868	7.672	1	22.88
685	CD1	LEU	A	295	61.777	25.278	8.109	1	20.35
686	CD2	LEU	A	295	62.907	23.917	6.361	1	24.34
687	N	THR	A	296	65.844	21.952	9.357	1	24.83
688	CA	THR	A	296	66.853	21.599	10.333	1	26.19
689	C	THR	A	296	67.32	22.819	11.146	1	26.94
690	O	THR	A	296	68.243	22.719	11.956	1	28.19
691	CB	THR	A	296	68.038	20.945	9.632	1	26.65
692	OG1	THR	A	296	68.535	21.841	8.639	1	32.95

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Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
693	CG2	THR	A	296	67.607	19.672	8.958	1	22.69
694	N	LYS	A	297	68.653	23.955	10.948	1	27.62
695	CA	LYS	A	297	66.988	25.196	11.643	1	27.86
696	C	LYS	A	297	65.727	26.055	11.736	1	29.73
697	O	LYS	A	297	64.673	25.692	11.209	1	29.96
698	CB	LYS	A	297	68.04	25.979	10.858	1	29.72
699	CG	LYS	A	297	69.32	25.233	10.536	1	31.36
700	CD	LYS	A	297	70.221	25.107	11.752	1	38.58
701	CE	LYS	A	297	71.587	24.591	11.344	1	41.35
702	NZ	LYS	A	297	72.521	24.671	12.486	1	50.85
703	N	GLU	A	298	65.841	27.194	12.406	1	29.42
704	CA	GLU	A	298	64.734	28.121	12.556	1	32.81
705	C	GLU	A	298	64.827	29.106	11.403	1	32.32
706	O	GLU	A	298	65.918	29.579	11.071	1	32.26
707	CB	GLU	A	298	64.846	28.88	13.875	1	37.63
708	CG	GLU	A	298	64.517	28.065	15.109	1	43.35
709	CD	GLU	A	298	64.941	28.771	16.383	1	47.13
710	OE1	GLU	A	298	64.506	29.92	16.628	1	50.33
711	OE2	GLU	A	298	65.732	28.177	17.139	1	52.96
712	N	LEU	A	299	63.687	29.424	10.807	1	31.28
713	CA	LEU	A	299	63.652	30.329	9.679	1	30.42
714	C	LEU	A	299	62.985	31.653	10.021	1	31.82
715	O	LEU	A	299	61.838	31.689	10.471	1	30.26
716	CB	LEU	A	299	62.952	29.641	8.496	1	31.83
717	CG	LEU	A	299	62.741	30.399	7.173	1	30.92
718	CD1	LEU	A	299	64.072	30.781	6.536	1	30.63
719	CD2	LEU	A	299	61.941	29.522	6.222	1	32.9
720	N	TYR	A	300	63.74	32.731	9.852	1	32.3
721	CA	TYR	A	300	63.269	34.086	10.096	1	35.54
722	C	TYR	A	300	63.536	34.831	8.799	1	36.41
723	O	TYR	A	300	64.625	34.722	8.252	1	38.38
724	CB	TYR	A	300	64.083	34.746	11.211	1	38.08
725	CG	TYR	A	300	63.706	34.313	12.613	1	41.67
726	CD1	TYR	A	300	62.644	34.919	13.28	1	41.01
727	CD2	TYR	A	300	64.417	33.302	13.276	1	42.97
728	CE1	TYR	A	300	62.294	34.533	14.573	1	45.78
729	CE2	TYR	A	300	64.076	32.906	14.568	1	43.98
730	CZ	TYR	A	300	63.012	33.529	15.212	1	45.36
731	OH	TYR	A	300	62.654	33.154	16.485	1	51.23
732	N	PHE	A	301	62.541	35.53	8.272	1	37.94
733	CA	PHE	A	301	62.716	36.3	7.04	1	41.13
734	C	PHE	A	301	63.335	37.63	7.421	1	46.12
735	O	PHE	A	301	62.767	38.693	7.186	1	47.85
736	CB	PHE	A	301	61.375	36.512	6.352	1	33.45
737	CG	PHE	A	301	60.718	35.241	5.957	1	29.8
738	CD1	PHE	A	301	61.351	34.373	5.075	1	24.51
739	CD2	PHE	A	301	59.485	34.891	6.493	1	25.18
740	CE1	PHE	A	301	60.767	33.173	4.736	1	26.35
741	CE2	PHE	A	301	58.887	33.691	6.162	1	25.64
742	CZ	PHE	A	301	59.527	32.826	5.281	1	30.14
743	N	SER	A	302	64.492	37.538	8.062	1	53.63
744	CA	SER	A	302	65.242	38.69	8.54	1	61.28

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
745	C	SER	A	302	66.567	38.19	9.151	1	65.34
746	O	SER	A	302	66.592	37.047	9.683	1	65.27
747	CB	SER	A	302	64.41	39.471	9.578	1	60.95
748	OG	SER	A	302	63.845	38.612	10.568	1	64.98
749	OT	SER	A	302	67.581	38.927	9.047	1	71.46
1878	N	THR	A	357	46.338	34.018	24.506	1	64.57
1879	CA	THR	A	357	47.795	34.084	24.19	1	64.42
1880	C	THR	A	357	48.133	33.13	23.049	1	59.47
1881	O	THR	A	357	47.242	32.667	22.345	1	59.66
1882	CB	THR	A	357	48.668	33.727	25.41	1	67.32
1883	OG1	THR	A	357	47.937	32.855	26.285	1	68.95
1884	CG2	THR	A	357	49.117	34.991	26.14	1	70.89
1885	N	TYR	A	358	49.412	32.807	22.903	1	54.18
1886	CA	TYR	A	358	49.844	31.938	21.831	1	50.17
1887	C	TYR	A	358	50.387	30.594	22.285	1	48.93
1888	O	TYR	A	358	50.854	29.809	21.463	1	48.48
1889	CB	TYR	A	358	50.846	32.692	20.962	1	50.89
1890	CG	TYR	A	358	50.265	34.007	20.476	1	52
1891	CD1	TYR	A	358	49.089	34.036	19.713	1	48.89
1892	CD2	TYR	A	358	50.832	35.222	20.854	1	54.13
1893	CE1	TYR	A	358	48.494	35.235	19.353	1	49.05
1894	CE2	TYR	A	358	50.24	36.428	20.498	1	52.15
1895	CZ	TYR	A	358	49.073	36.425	19.752	1	51.42
1896	OH	TYR	A	358	48.483	37.624	19.442	1	55.21
1897	N	GLN	A	359	50.332	30.333	23.592	1	46.52
1898	CA	GLN	A	359	50.81	29.069	24.137	1	40.53
1899	C	GLN	A	359	49.659	28.221	24.595	1	37.04
1900	O	GLN	A	359	48.562	28.718	24.853	1	36.42
1901	CB	GLN	A	359	51.74	29.265	25.328	1	45.57
1902	CG	GLN	A	359	53.132	29.716	24.991	1	50.4
1903	CD	GLN	A	359	53.261	31.217	25.042	1	58.45
1904	OE1	GLN	A	359	52.421	31.95	24.502	1	63.69
1905	NE2	GLN	A	359	54.302	31.694	25.715	1	63.54
1906	N	TYR	A	360	49.917	26.925	24.675	1	35.7
1907	CA	TYR	A	360	48.924	25.983	25.142	1	35.87
1908	C	TYR	A	360	48.96	26.1	26.66	1	37.08
1909	O	TYR	A	360	50.034	26.152	27.265	1	33.82
1910	CB	TYR	A	360	49.281	24.561	24.726	1	32.23
1911	CG	TYR	A	360	48.762	24.149	23.366	1	31.28
1912	CD1	TYR	A	360	47.394	23.953	23.146	1	28.77
1913	CD2	TYR	A	360	49.65	23.867	22.324	1	29.21
1914	CE1	TYR	A	360	46.928	23.472	21.921	1	32.55
1915	CE2	TYR	A	360	49.199	23.386	21.1	1	30.52
1916	CZ	TYR	A	360	47.844	23.185	20.904	1	31.54
1917	OH	TYR	A	360	47.421	22.672	19.707	1	30.22
1918	N	ASN	A	361	47.774	26.175	27.25	1	38.56
1919	CA	ASN	A	361	47.592	26.309	28.691	1	38.93
1920	C	ASN	A	361	48.061	25.07	29.425	1	37.22
1921	O	ASN	A	361	47.435	24.013	29.343	1	37.4
1922	CB	ASN	A	361	46.114	26.59	28.999	1	42.29
1923	CG	ASN	A	361	45.79	26.514	30.482	1	44.23
1924	OD1	ASN	A	361	46.552	26.986	31.329	1	45.06

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Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
1925	ND2	ASN	A	361	44.653	25.917	30.799	1	44.31
1926	N	MET	A	362	49.186	25.206	30.113	1	37.13
1927	CA	MET	A	362	49.774	24.115	30.882	1	41.77
1928	C	MET	A	362	49.367	24.178	32.358	1	40.97
1929	O	MET	A	362	49.922	23.466	33.191	1	39.29
1930	CB	MET	A	362	51.303	24.158	30.769	1	45.27
1931	CG	MET	A	362	51.842	23.974	29.352	1	48.62
1932	SD	MET	A	362	51.488	22.346	28.65	1	52.78
1933	CE	MET	A	362	49.918	22.646	27.883	1	47.1
1934	N	ASN	A	363	48.393	25.021	32.678	1	41.1
1935	CA	ASN	A	363	47.955	25.152	34.051	1	39.37
1936	C	ASN	A	363	46.892	24.12	34.398	1	34.42
1937	O	ASN	A	363	45.707	24.43	34.517	1	29.77
1938	CB	ASN	A	363	47.442	26.561	34.304	1	50.69
1939	CG	ASN	A	363	47.364	26.886	35.78	1	61.35
1940	OD1	ASN	A	363	48.369	26.821	36.496	1	66.54
1941	ND2	ASN	A	363	46.168	27.225	36.252	1	66.52
1942	N	PHE	A	364	47.328	22.878	34.523	1	31.23
1943	CA	PHE	A	364	46.439	21.779	34.85	1	32.24
1944	C	PHE	A	364	47.083	20.985	35.995	1	37.11
1945	O	PHE	A	364	48.291	21.129	36.272	1	32.97
1946	CB	PHE	A	364	46.234	20.856	33.627	1	30.55
1947	CG	PHE	A	364	45.33	21.427	32.573	1	26.34
1948	CD1	PHE	A	364	45.807	22.36	31.655	1	25.2
1949	CD2	PHE	A	364	43.987	21.074	32.531	1	22.85
1950	CE1	PHE	A	364	44.958	22.934	30.72	1	22.54
1951	CE2	PHE	A	364	43.125	21.65	31.588	1	26.36
1952	CZ	PHE	A	364	43.614	22.582	30.686	1	20.07
1953	N	GLU	A	365	46.274	20.138	36.638	1	40.87
1954	CA	GLU	A	365	46.744	19.302	37.738	1	42.31
1955	C	GLU	A	365	47.971	18.502	37.321	1	42.39
1956	O	GLU	A	365	48.95	18.454	38.05	1	45.51
1957	CB	GLU	A	365	45.636	18.36	38.2	1	46.19
1958	CG	GLU	A	365	45.982	17.591	39.463	1	59.5
1959	CD	GLU	A	365	44.799	16.803	40.034	1	68.2
1960	OE1	GLU	A	365	43.701	17.392	40.21	1	70.64
1961	OE2	GLU	A	365	44.976	15.591	40.316	1	72.33
1962	N	LYS	A	366	47.939	17.905	36.134	1	42.15
1963	CA	LYS	A	366	49.077	17.125	35.659	1	39.42
1964	C	LYS	A	366	49.33	17.33	34.165	1	37.53
1965	O	LYS	A	366	48.417	17.692	33.416	1	36.52
1966	CB	LYS	A	366	48.83	15.651	35.955	1	37.61
1967	CG	LYS	A	366	47.623	15.12	35.258	1	39.67
1968	CD	LYS	A	366	46.947	14.051	36.054	1	43.95
1969	CE	LYS	A	366	47.829	12.862	36.263	1	51.67
1970	NZ	LYS	A	366	47.02	11.752	36.841	1	55.56
1971	N	LEU	A	367	50.562	17.066	33.737	1	36.13
1972	CA	LEU	A	367	50.945	17.213	32.327	1	34.98
1973	C	LEU	A	367	50.127	16.28	31.448	1	32.04
1974	O	LEU	A	367	49.579	16.712	30.435	1	34.39
1975	CB	LEU	A	367	52.439	16.965	32.123	1	32.37
1976	CG	LEU	A	367	52.995	17.206	30.714	1	31.26

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
1977	CD1	LEU	A	367	52.498	18.516	30.114	1	27.98
1978	CD2	LEU	A	367	54.505	17.191	30.793	1	30.38
1979	N	GLY	A	368	50.048	15.01	31.832	1	27.06
1980	CA	GLY	A	368	49.247	14.071	31.078	1	22.5
1981	C	GLY	A	368	49.841	12.696	30.945	1	22.57
1982	O	GLY	A	368	50.945	12.416	31.423	1	21.37
1983	N	LYS	A	369	49.05	11.819	30.337	1	23.66
1984	CA	LYS	A	369	49.426	10.44	30.069	1	26.4
1985	C	LYS	A	369	50.435	10.359	28.905	1	30.29
1986	O	LYS	A	369	50.445	11.207	28.004	1	32.97
1987	CB	LYS	A	369	48.161	9.648	29.733	1	30.63
1988	CG	LYS	A	369	48.381	8.172	29.523	1	40.89
1989	CD	LYS	A	369	49.084	7.525	30.721	1	51.54
1990	CE	LYS	A	369	48.211	7.478	31.987	1	56.6
1991	NZ	LYS	A	369	48.049	8.806	32.658	1	59.3
1992	N	CYS	A	370	51.302	9.356	28.949	1	28.73
1993	CA	CYS	A	370	52.302	9.156	27.922	1	24.16
1994	C	CYS	A	370	52.497	7.683	27.722	1	25.85
1995	O	CYS	A	370	53.361	7.081	28.344	1	31.03
1996	CB	CYS	A	370	53.637	9.771	28.315	1	24.06
1997	SG	CYS	A	370	54.98	9.344	27.162	1	30.03
1998	N	ILE	A	371	51.667	7.096	26.875	1	24.09
1999	CA	ILE	A	371	51.757	5.684	26.571	1	23.11
2000	C	ILE	A	371	52.916	5.396	25.598	1	27.64
2001	O	ILE	A	371	53.125	6.124	24.631	1	30.55
2002	CB	ILE	A	371	50.432	5.237	25.969	1	24.56
2003	CG1	ILE	A	371	49.339	5.447	27.008	1	21.96
2004	CG2	ILE	A	371	50.508	3.8	25.464	1	26.64
2005	CD1	ILE	A	371	47.947	5.181	26.504	1	26.72
2006	N	ILE	A	372	53.696	4.361	25.883	1	29.74
2007	CA	ILE	A	372	54.814	3.958	25.029	1	27.24
2008	C	ILE	A	372	54.614	2.488	24.618	1	29.59
2009	O	ILE	A	372	54.565	1.601	25.474	1	26.86
2010	CB	ILE	A	372	56.182	4.041	25.771	1	24.55
2011	CG1	ILE	A	372	56.498	5.475	26.197	1	21
2012	CG2	ILE	A	372	57.299	3.458	24.9	1	24.27
2013	CD1	ILE	A	372	57.87	5.594	26.867	1	14.19
2014	N	ILE	A	373	54.47	2.232	23.32	1	29.89
2015	CA	ILE	A	373	54.312	0.862	22.844	1	29.82
2016	C	ILE	A	373	55.677	0.421	22.328	1	31.48
2017	O	ILE	A	373	56.203	0.984	21.364	1	32.36
2018	CB	ILE	A	373	53.222	0.744	21.748	1	27.99
2019	CG1	ILE	A	373	51.919	1.346	22.269	1	27.04
2020	CG2	ILE	A	373	52.974	-0.715	21.407	1	27.95
2021	CD1	ILE	A	373	50.733	1.079	21.414	1	26.34
2022	N	ASN	A	374	56.276	-0.543	23.019	1	31.74
2023	CA	ASN	A	374	57.596	-1.04	22.666	1	30.28
2024	C	ASN	A	374	57.49	-2.434	22.072	1	32.22
2025	O	ASN	A	374	57.34	-3.426	22.811	1	30.73
2026	CB	ASN	A	374	58.485	-1.052	23.916	1	28.46
2027	CG	ASN	A	374	59.88	-1.55	23.637	1	28.54
2028	OD1	ASN	A	374	60.543	-1.053	22.742	1	37.53

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
2029	ND2	ASN	A	374	60.349	-2.522	24.422	1	26.1
2030	N	ASN	A	375	57.526	-2.507	20.737	1	30.03
2031	CA	ASN	A	375	57.441	-3.781	20.018	1	25.66
2032	C	ASN	A	375	58.81	-4.217	19.524	1	23.13
2033	O	ASN	A	375	59.404	-3.592	18.653	1	26.67
2034	CB	ASN	A	375	56.457	-3.68	18.866	1	27.28
2035	CG	ASN	A	375	55.039	-3.511	19.336	1	25.85
2036	OD1	ASN	A	375	54.716	-3.797	20.478	1	30.3
2037	ND2	ASN	A	375	54.176	-3.063	18.451	1	27.5
2038	N	LYS	A	376	59.283	-5.329	20.063	1	20.86
2039	CA	LYS	A	376	60.598	-5.839	19.731	1	24.75
2040	C	LYS	A	376	60.568	-7.201	19.043	1	28.73
2041	O	LYS	A	376	61.404	-7.489	18.17	1	28.72
2042	CB	LYS	A	376	61.426	-5.92	21.027	1	20.95
2043	CG	LYS	A	376	62.718	-6.69	20.933	1	16.55
2044	CD	LYS	A	376	63.611	-6.38	22.098	1	17.69
2045	CE	LYS	A	376	64.868	-7.205	22.026	1	19.94
2046	NZ	LYS	A	376	66.058	-6.503	22.595	1	29.01
2047	N	ASN	A	377	59.606	-8.027	19.444	1	29.63
2048	CA	ASN	A	377	59.459	-9.382	18.922	1	30.38
2049	C	ASN	A	377	58.169	-9.508	18.128	1	30.18
2050	O	ASN	A	377	57.09	-9.204	18.645	1	27.92
2051	CB	ASN	A	377	59.46	-10.398	20.076	1	30.16
2052	CG	ASN	A	377	60.713	-10.32	20.917	1	30.13
2053	OD1	ASN	A	377	61.806	-10.693	20.476	1	28.59
2054	ND2	ASN	A	377	60.569	-9.814	22.138	1	31.08
2055	N	PHE	A	378	58.291	-10.047	16.913	1	28.75
2056	CA	PHE	A	378	57.169	-10.198	15.977	1	30.09
2057	C	PHE	A	378	56.984	-11.648	15.545	1	27.03
2058	O	PHE	A	378	57.941	-12.421	15.558	1	30.32
2059	CB	PHE	A	378	57.418	-9.323	14.734	1	25.73
2060	CG	PHE	A	378	57.679	-7.883	15.059	1	21.48
2061	CD1	PHE	A	378	58.924	-7.482	15.513	1	22.57
2062	CD2	PHE	A	378	56.662	-6.946	14.975	1	23.07
2063	CE1	PHE	A	378	59.151	-6.166	15.89	1	22.45
2064	CE2	PHE	A	378	56.88	-5.627	15.348	1	24.1
2065	CZ	PHE	A	378	58.124	-5.238	15.808	1	25.55
2066	N	ASP	A	379	55.764	-12.013	15.163	1	27.26
2067	CA	ASP	A	379	55.497	-13.379	14.727	1	30.91
2068	C	ASP	A	379	56.289	-13.65	13.443	1	31.7
2069	O	ASP	A	379	56.52	-12.736	12.642	1	29.26
2070	CB	ASP	A	379	53.988	-13.611	14.541	1	34.72
2071	CG	ASP	A	379	53.22	-13.658	15.885	1	42.2
2072	OD1	ASP	A	379	53.851	-13.948	16.933	1	48.7
2073	OD2	ASP	A	379	51.983	-13.418	15.904	1	44.87
2074	N	LYS	A	380	56.761	-14.882	13.288	1	32.55
2075	CA	LYS	A	380	57.56	-15.264	12.127	1	36.56
2076	C	LYS	A	380	56.903	-14.857	10.807	1	36.25
2077	O	LYS	A	380	57.521	-14.186	9.968	1	34.35
2078	CB	LYS	A	380	57.781	-16.778	12.118	1	42.4
2079	CG	LYS	A	380	58.967	-17.232	11.26	1	53.8
2080	CD	LYS	A	380	58.767	-18.638	10.676	1	58.75

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Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
2081	CE	LYS	A	380	58.335	-19.653	11.729	1	61.07
2082	NZ	LYS	A	380	58.104	-21.011	11.145	1	64.54
2083	N	VAL	A	381	55.62	-15.2	10.688	1	35.04
2084	CA	VAL	A	381	54.815	-14.943	9.502	1	36.2
2085	C	VAL	A	381	54.696	-13.513	8.998	1	37.62
2086	O	VAL	A	381	54.191	-13.291	7.903	1	41.38
2087	CB	VAL	A	381	53.406	-15.525	9.66	1	34.55
2088	CG1	VAL	A	381	53.498	-17.03	9.852	1	36.82
2089	CG2	VAL	A	381	52.689	-14.871	10.817	1	35.31
2090	N	THR	A	382	55.128	-12.542	9.792	1	36.88
2091	CA	THR	A	382	55.069	-11.15	9.363	1	34.57
2092	C	THR	A	382	56.3	-10.873	8.502	1	36.19
2093	O	THR	A	382	56.366	-9.887	7.768	1	40.37
2094	CB	THR	A	382	55.083	-10.173	10.576	1	31.28
2095	OG1	THR	A	382	56.3	-10.338	11.319	1	26.85
2096	CG2	THR	A	382	53.878	-10.406	11.473	1	24.7
2097	N	GLY	A	383	57.286	-11.754	8.609	1	38.58
2098	CA	GLY	A	383	58.51	-11.567	7.871	1	40.34
2099	C	GLY	A	383	59.352	-10.545	8.603	1	44.38
2100	O	GLY	A	383	60.423	-10.169	8.126	1	48.76
2101	N	MET	A	384	58.889	-10.117	9.779	1	45.67
2102	CA	MET	A	384	59.607	-9.129	10.581	1	42.34
2103	C	MET	A	384	60.533	-9.774	11.596	1	39.55
2104	O	MET	A	384	60.214	-10.817	12.172	1	37.55
2105	CB	MET	A	384	58.625	-8.22	11.308	1	42.97
2106	CG	MET	A	384	57.845	-7.305	10.389	1	47.41
2107	SD	MET	A	384	58.899	-6.291	9.31	1	47.66
2108	CE	MET	A	384	58.502	-7.02	7.706	1	54.61
2109	N	GLY	A	385	61.68	-9.14	11.809	1	38.8
2110	CA	GLY	A	385	62.646	-9.643	12.771	1	41.35
2111	C	GLY	A	385	62.702	-8.829	14.059	1	43.68
2112	O	GLY	A	385	62.097	-7.746	14.151	1	43.44
2113	N	VAL	A	386	63.424	-9.365	15.048	1	42.99
2114	CA	VAL	A	386	63.613	-8.75	16.365	1	39.09
2115	C	VAL	A	386	64.262	-7.391	16.212	1	39.71
2116	O	VAL	A	386	65.271	-7.273	15.527	1	42.9
2117	CB	VAL	A	386	64.562	-9.589	17.24	1	36
2118	CG1	VAL	A	386	64.855	-8.865	18.538	1	36.74
2119	CG2	VAL	A	386	63.948	-10.938	17.536	1	43.43
2120	N	ARG	A	387	63.723	-6.381	16.89	1	37.43
2121	CA	ARG	A	387	64.281	-5.035	16.813	1	32.14
2122	C	ARG	A	387	65.316	-4.747	17.916	1	32.71
2123	O	ARG	A	387	65.026	-4.08	18.908	1	35.74
2124	CB	ARG	A	387	63.163	-3.994	16.844	1	27.74
2125	CG	ARG	A	387	62.176	-4.09	15.694	1	28.88
2126	CD	ARG	A	387	61.055	-3.068	15.828	1	29.98
2127	NE	ARG	A	387	61.582	-1.707	15.849	1	34.96
2128	CZ	ARG	A	387	61.452	-0.863	16.866	1	33.54
2129	NH1	ARG	A	387	60.801	-1.233	17.956	1	34
2130	NH2	ARG	A	387	62.007	0.343	16.797	1	27.28
2131	N	ASN	A	388	66.533	-5.233	17.736	1	30.21
2132	CA	ASN	A	388	67.569	-4.988	18.718	1	29.91

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
2133	C	ASN	A	388	67.81	-3.504	18.878	1	30.95
2134	O	ASN	A	388	67.874	-2.764	17.893	1	34.36
2135	CB	ASN	A	388	68.851	-5.675	18.307	1	32.07
2136	CG	ASN	A	388	68.679	-7.17	18.177	1	38.84
2137	OD1	ASN	A	388	68.042	-7.811	19.014	1	34.2
2138	ND2	ASN	A	388	69.209	-7.731	17.098	1	47.39
2139	N	GLY	A	389	67.95	-3.077	20.125	1	27.57
2140	CA	GLY	A	389	68.177	-1.679	20.438	1	22.97
2141	C	GLY	A	389	66.907	-0.996	20.907	1	21.24
2142	O	GLY	A	389	66.948	0.105	21.465	1	23.19
2143	N	THR	A	390	65.77	-1.661	20.745	1	22.02
2144	CA	THR	A	390	64.508	-1.044	21.112	1	22.09
2145	C	THR	A	390	64.299	-0.848	22.613	1	25.64
2146	O	THR	A	390	63.785	0.199	23.025	1	24.64
2147	CB	THR	A	390	63.313	-1.759	20.453	1	18.23
2148	OG1	THR	A	390	62.166	-0.905	20.493	1	21.12
2149	CG2	THR	A	390	62.995	-3.037	21.152	1	21.95
2150	N	ASP	A	391	64.723	-1.816	23.428	1	26.19
2151	CA	ASP	A	391	64.595	-1.705	24.886	1	25.51
2152	C	ASP	A	391	65.332	-0.47	25.392	1	24.4
2153	O	ASP	A	391	64.812	0.257	26.226	1	27.17
2154	CB	ASP	A	391	65.102	-2.96	25.577	1	23.36
2155	CG	ASP	A	391	64.187	-4.145	25.359	1	24.24
2156	OD1	ASP	A	391	63.035	-3.943	24.912	1	27.57
2157	OD2	ASP	A	391	64.614	-5.284	25.638	1	26.21
2158	N	LYS	A	392	66.516	-0.201	24.848	1	27.33
2159	CA	LYS	A	392	67.262	0.994	25.22	1	27.72
2160	C	LYS	A	392	66.421	2.22	24.925	1	29.42
2161	O	LYS	A	392	66.403	3.159	25.715	1	33.83
2162	CB	LYS	A	392	68.561	1.099	24.434	1	29.3
2163	CG	LYS	A	392	69.496	-0.044	24.679	1	37.31
2164	CD	LYS	A	392	70.835	0.18	24.01	1	40.85
2165	CE	LYS	A	392	71.625	-1.134	23.942	1	45.21
2166	NZ	LYS	A	392	70.976	-2.194	23.085	1	43.8
2167	N	ASP	A	393	65.723	2.208	23.789	1	33.18
2168	CA	ASP	A	393	64.859	3.323	23.388	1	32.45
2169	C	ASP	A	393	63.716	3.511	24.359	1	31.47
2170	O	ASP	A	393	63.443	4.627	24.785	1	33.96
2171	CB	ASP	A	393	64.262	3.104	21.99	1	34.53
2172	CG	ASP	A	393	65.253	3.37	20.874	1	39.45
2173	OD1	ASP	A	393	66.294	4.016	21.125	1	39.28
2174	OD2	ASP	A	393	64.983	2.937	19.734	1	40.52
2175	N	ALA	A	394	63.035	2.416	24.688	1	29.99
2176	CA	ALA	A	394	61.902	2.452	25.605	1	28.17
2177	C	ALA	A	394	62.309	2.984	26.981	1	28.94
2178	O	ALA	A	394	61.564	3.727	27.613	1	27.35
2179	CB	ALA	A	394	61.3	1.077	25.731	1	28.81
2180	N	GLU	A	395	63.507	2.618	27.422	1	31.01
2181	CA	GLU	A	395	64.032	3.062	28.706	1	34.49
2182	C	GLU	A	395	64.344	4.55	28.661	1	32.8
2183	O	GLU	A	395	63.849	5.329	29.479	1	31.43
2184	CB	GLU	A	395	65.298	2.279	29.049	1	41.02

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
2185	CG	GLU	A	395	65.87	2.596	30.416	1	52.59
2186	CD	GLU	A	395	67.323	3.031	30.352	1	60.61
2187	OE1	GLU	A	395	67.585	4.203	29.969	1	63.4
2188	OE2	GLU	A	395	68.2	2.198	30.69	1	63.34
2189	N	ALA	A	396	65.152	4.94	27.681	1	32.13
2190	CA	ALA	A	396	65.533	6.328	27.521	1	30.06
2191	C	ALA	A	396	64.302	7.209	27.426	1	31.71
2192	O	ALA	A	396	64.238	8.243	28.076	1	33.07
2193	CB	ALA	A	396	66.394	6.495	26.305	1	31.15
2194	N	LEU	A	397	63.306	6.775	26.66	1	32.69
2195	CA	LEU	A	397	62.065	7.542	26.501	1	34.4
2196	C	LEU	A	397	61.237	7.605	27.793	1	34.98
2197	O	LEU	A	397	60.731	8.665	28.161	1	32.13
2198	CB	LEU	A	397	61.208	6.971	25.351	1	31.44
2199	CG	LEU	A	397	61.632	7.195	23.884	1	30.15
2200	CD1	LEU	A	397	60.807	6.29	23.032	1	26.93
2201	CD2	LEU	A	397	61.46	8.643	23.432	1	23.81
2202	N	PHE	A	398	61.054	6.46	28.445	1	36.78
2203	CA	PHE	A	398	60.301	6.411	29.691	1	38
2204	C	PHE	A	398	60.931	7.372	30.688	1	37.62
2205	O	PHE	A	398	60.259	8.251	31.237	1	35.9
2206	CB	PHE	A	398	60.296	4.984	30.243	1	42.95
2207	CG	PHE	A	398	60.642	4.887	31.702	1	47.34
2208	CD1	PHE	A	398	59.79	5.4	32.674	1	48.95
2209	CD2	PHE	A	398	61.828	4.281	32.105	1	49.85
2210	CE1	PHE	A	398	60.118	5.306	34.016	1	50
2211	CE2	PHE	A	398	62.161	4.187	33.447	1	49.12
2212	CZ	PHE	A	398	61.307	4.697	34.4	1	50.3
2213	N	LYS	A	399	62.224	7.202	30.928	1	35.52
2214	CA	LYS	A	399	62.922	8.066	31.861	1	35.92
2215	C	LYS	A	399	62.708	9.515	31.457	1	38.13
2216	O	LYS	A	399	62.144	10.31	32.219	1	41.4
2217	CB	LYS	A	399	64.406	7.732	31.882	1	30.94
2218	CG	LYS	A	399	64.722	6.434	32.578	1	27.38
2219	CD	LYS	A	399	66.178	6.088	32.371	1	30.44
2220	CE	LYS	A	399	66.633	4.991	33.307	1	34.36
2221	NZ	LYS	A	399	66.763	5.524	34.694	1	42.3
2222	N	CYS	A	400	63.057	9.805	30.208	1	40.81
2223	CA	CYS	A	400	62.945	11.136	29.608	1	38.95
2224	C	CYS	A	400	61.563	11.803	29.708	1	35.56
2225	O	CYS	A	400	61.469	12.985	30.043	1	37.02
2226	CB	CYS	A	400	63.385	11.046	28.145	1	44.47
2227	SG	CYS	A	400	63.422	12.575	27.266	1	54.43
2228	N	PHE	A	401	60.498	11.052	29.455	1	32.25
2229	CA	PHE	A	401	59.144	11.593	29.515	1	33.91
2230	C	PHE	A	401	58.596	11.703	30.942	1	34.97
2231	O	PHE	A	401	57.689	12.512	31.21	1	36.26
2232	CB	PHE	A	401	58.203	10.801	28.595	1	34.73
2233	CG	PHE	A	401	58.239	11.267	27.155	1	35.25
2234	CD1	PHE	A	401	59.385	11.103	26.38	1	32.81
2235	CD2	PHE	A	401	57.155	11.944	26.606	1	33.22
2236	CE1	PHE	A	401	59.446	11.615	25.091	1	34.65

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
2237	CE2	PHE	A	401	57.211	12.459	25.32	1	31.46
2238	CZ	PHE	A	401	58.357	12.296	24.56	1	32.04
2239	N	ARG	A	402	59.151	10.893	31.851	1	34.95
2240	CA	ARG	A	402	58.778	10.927	33.269	1	33.53
2241	C	ARG	A	402	59.336	12.248	33.82	1	32.92
2242	O	ARG	A	402	58.618	13.019	34.46	1	31.36
2243	CB	ARG	A	402	59.386	9.744	34.025	1	28.57
2244	CG	ARG	A	402	58.908	9.629	35.462	1	24.8
2245	CD	ARG	A	402	59.535	8.443	36.172	1	22.04
2246	NE	ARG	A	402	60.992	8.465	36.064	1	24.69
2247	CZ	ARG	A	402	61.79	7.447	36.385	1	25.5
2248	NH1	ARG	A	402	61.288	6.316	36.859	1	24.78
2249	NH2	ARG	A	402	63.086	7.512	36.116	1	29.31
2250	N	SER	A	403	60.597	12.533	33.5	1	33.24
2251	CA	SER	A	403	61.243	13.769	33.92	1	36.08
2252	C	SER	A	403	60.455	14.985	33.468	1	39.09
2253	O	SER	A	403	60.506	16.031	34.116	1	42.61
2254	CB	SER	A	403	62.641	13.87	33.331	1	33.95
2255	OG	SER	A	403	63.437	12.808	33.806	1	49.49
2256	N	LEU	A	404	59.792	14.867	32.318	1	39.67
2257	CA	LEU	A	404	58.991	15.961	31.78	1	37.6
2258	C	LEU	A	404	57.733	16.184	32.599	1	36.27
2259	O	LEU	A	404	57.206	17.297	32.625	1	39.33
2260	CB	LEU	A	404	58.613	15.707	30.31	1	39.24
2261	CG	LEU	A	404	59.681	16.007	29.254	1	36.02
2262	CD1	LEU	A	404	59.182	15.585	27.884	1	35.82
2263	CD2	LEU	A	404	60.035	17.487	29.285	1	32.13
2264	N	GLY	A	405	57.235	15.122	33.232	1	32.3
2265	CA	GLY	A	405	56.041	15.243	34.047	1	26.02
2266	C	GLY	A	405	54.879	14.403	33.579	1	29.7
2267	O	GLY	A	405	53.753	14.576	34.06	1	30.76
2268	N	PHE	A	406	55.133	13.485	32.654	1	28.14
2269	CA	PHE	A	406	54.066	12.636	32.134	1	28.09
2270	C	PHE	A	406	53.932	11.385	32.999	1	26.19
2271	O	PHE	A	406	54.918	10.937	33.595	1	24.52
2272	CB	PHE	A	406	54.399	12.157	30.694	1	29.57
2273	CG	PHE	A	406	54.301	13.22	29.633	1	25.91
2274	CD1	PHE	A	406	53.067	13.548	29.066	1	27.28
2275	CD2	PHE	A	406	55.443	13.882	29.189	1	24.67
2276	CE1	PHE	A	406	52.975	14.53	28.066	1	23.79
2277	CE2	PHE	A	406	55.363	14.863	28.194	1	24.53
2278	CZ	PHE	A	406	54.126	15.186	27.632	1	25.11
2279	N	ASP	A	407	52.741	10.786	33.011	1	25.31
2280	CA	ASP	A	407	52.528	9.526	33.719	1	29.64
2281	C	ASP	A	407	52.78	8.443	32.669	1	30.51
2282	O	ASP	A	407	51.861	8.033	31.954	1	31
2283	CB	ASP	A	407	51.09	9.405	34.228	1	36.15
2284	CG	ASP	A	407	50.786	10.357	35.38	1	46.94
2285	OD1	ASP	A	407	51.697	11.076	35.852	1	51.23
2286	OD2	ASP	A	407	49.621	10.379	35.823	1	50.69
2287	N	VAL	A	408	54.018	7.981	32.562	1	29.59
2288	CA	VAL	A	408	54.332	6.986	31.554	1	30.57

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
2289	C	VAL	A	408	54.037	5.515	31.847	1	32.39
2290	O	VAL	A	408	54.358	4.986	32.917	1	35.55
2291	CB	VAL	A	408	55.768	7.194	30.959	1	30.5
2292	CG1	VAL	A	408	56.566	8.155	31.798	1	27.08
2293	CG2	VAL	A	408	56.509	5.871	30.788	1	32.72
2294	N	ILE	A	409	53.39	4.875	30.88	1	31.47
2295	CA	ILE	A	409	53.038	3.457	30.933	1	28.79
2296	C	ILE	A	409	53.753	2.835	29.727	1	30.85
2297	O	ILE	A	409	53.689	3.388	28.633	1	32.69
2298	CB	ILE	A	409	51.545	3.27	30.727	1	25.61
2299	CG1	ILE	A	409	50.774	4.177	31.681	1	24.81
2300	CG2	ILE	A	409	51.167	1.813	30.916	1	25.19
2301	CD1	ILE	A	409	49.265	4.032	31.548	1	26.5
2302	N	VAL	A	410	54.419	1.702	29.911	1	27.31
2303	CA	VAL	A	410	55.143	1.066	28.821	1	22.52
2304	C	VAL	A	410	54.599	-0.315	28.466	1	25.48
2305	O	VAL	A	410	54.668	-1.249	29.272	1	25.9
2306	CB	VAL	A	410	56.649	0.942	29.17	1	24.19
2307	CG1	VAL	A	410	57.423	0.283	28.016	1	24.21
2308	CG2	VAL	A	410	57.226	2.325	29.527	1	20.43
2309	N	TYR	A	411	54.02	-0.443	27.274	1	25.85
2310	CA	TYR	A	411	53.502	-1.737	26.838	1	22.09
2311	C	TYR	A	411	54.58	-2.435	25.983	1	22.5
2312	O	TYR	A	411	55.456	-1.777	25.428	1	22.89
2313	CB	TYR	A	411	52.169	-1.561	26.125	1	21.44
2314	CG	TYR	A	411	51.078	-0.903	26.978	1	19.34
2315	CD1	TYR	A	411	51.043	0.477	27.18	1	16.66
2316	CD2	TYR	A	411	50.045	-1.667	27.534	1	23.37
2317	CE1	TYR	A	411	50.003	1.078	27.906	1	16.34
2318	CE2	TYR	A	411	49.003	-1.068	28.263	1	20.03
2319	CZ	TYR	A	411	48.993	0.294	28.437	1	21.12
2320	OH	TYR	A	411	47.942	0.865	29.111	1	27.41
2321	N	ASN	A	412	54.557	-3.759	25.912	1	23.25
2322	CA	ASN	A	412	55.605	-4.471	25.183	1	25.72
2323	C	ASN	A	412	55.085	-5.616	24.3	1	26.77
2324	O	ASN	A	412	54.205	-6.382	24.728	1	26.56
2325	CB	ASN	A	412	56.634	-5.013	26.187	1	25.27
2326	CG	ASN	A	412	57.21	-3.927	27.077	1	29.71
2327	OD1	ASN	A	412	58.197	-3.281	26.725	1	32.28
2328	ND2	ASN	A	412	56.596	-3.719	28.241	1	33.34
2329	N	ASP	A	413	55.665	-5.752	23.095	1	26.11
2330	CA	ASP	A	413	55.275	-6.781	22.113	1	18.74
2331	C	ASP	A	413	53.764	-6.893	21.941	1	21.09
2332	O	ASP	A	413	53.184	-7.975	22.09	1	23.35
2333	CB	ASP	A	413	55.828	-8.137	22.504	1	16.68
2334	CG	ASP	A	413	57.307	-8.227	22.32	1	20.06
2335	OD1	ASP	A	413	57.904	-7.261	21.792	1	21.59
2336	OD2	ASP	A	413	57.869	-9.279	22.696	1	25.55
2337	N	CYS	A	414	53.13	-5.775	21.61	1	20.83
2338	CA	CYS	A	414	51.696	-5.754	21.463	1	23.85
2339	C	CYS	A	414	51.173	-6.322	20.164	1	28.67
2340	O	CYS	A	414	51.8	-6.214	19.117	1	32.42

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
2341	CB	CYS	A	414	51.186	-4.328	21.614	1	25.91
2342	SG	CYS	A	414	51.456	-3.597	23.251	1	32.04
2343	N	SER	A	415	50.017	-6.955	20.25	1	29.76
2344	CA	SER	A	415	49.346	-7.485	19.087	1	30.19
2345	C	SER	A	415	48.711	-6.255	18.437	1	31.91
2346	O	SER	A	415	48.784	-5.153	18.988	1	36.17
2347	CB	SER	A	415	48.239	-8.421	19.544	1	27.73
2348	OG	SER	A	415	47.272	-7.69	20.285	1	32.68
2349	N	CYS	A	416	48.052	-6.44	17.298	1	32.22
2350	CA	CYS	A	416	47.39	-5.317	16.637	1	28.73
2351	C	CYS	A	416	46.124	-4.97	17.4	1	28.64
2352	O	CYS	A	416	45.761	-3.797	17.499	1	28.85
2353	CB	CYS	A	416	47.038	-5.648	15.174	1	33.37
2354	SG	CYS	A	416	48.438	-5.66	14.031	1	29.37
2355	N	ALA	A	417	45.449	-5.994	17.929	1	29.29
2356	CA	ALA	A	417	44.214	-5.795	18.703	1	28.4
2357	C	ALA	A	417	44.521	-5.071	20.01	1	28.08
2358	O	ALA	A	417	43.724	-4.253	20.476	1	28.57
2359	CB	ALA	A	417	43.529	-7.115	18.985	1	24.39
2360	N	LYS	A	418	45.687	-5.364	20.581	1	26.4
2361	CA	LYS	A	418	46.101	-4.722	21.812	1	28.45
2362	C	LYS	A	418	46.336	-3.237	21.583	1	30.55
2363	O	LYS	A	418	45.716	-2.408	22.236	1	34.94
2364	CB	LYS	A	418	47.358	-5.37	22.366	1	28.25
2365	CG	LYS	A	418	47.768	-4.817	23.712	1	37.17
2366	CD	LYS	A	418	46.683	-5.021	24.762	1	40.63
2367	CE	LYS	A	418	47.116	-4.406	26.092	1	48.99
2368	NZ	LYS	A	418	46.07	-4.529	27.149	1	54.73
2369	N	MET	A	419	47.201	-2.895	20.633	1	33.54
2370	CA	MET	A	419	47.483	-1.491	20.338	1	31.86
2371	C	MET	A	419	46.193	-0.67	20.121	1	33.41
2372	O	MET	A	419	46.09	0.475	20.569	1	32.21
2373	CB	MET	A	419	48.397	-1.384	19.119	1	31.78
2374	CG	MET	A	419	49.722	-2.126	19.238	1	32.23
2375	SD	MET	A	419	50.87	-1.667	17.901	1	32.64
2376	CE	MET	A	419	50.065	-2.412	16.542	1	40.39
2377	N	GLN	A	420	45.2	-1.274	19.473	1	33.66
2378	CA	GLN	A	420	43.932	-0.599	19.215	1	35.96
2379	C	GLN	A	420	43.102	-0.39	20.473	1	37.43
2380	O	GLN	A	420	42.589	0.711	20.712	1	36.44
2381	CB	GLN	A	420	43.089	-1.384	18.205	1	39.14
2382	CG	GLN	A	420	43.505	-1.215	16.751	1	48.09
2383	CD	GLN	A	420	43.007	0.078	16.117	1	52.7
2384	OE1	GLN	A	420	42.216	0.824	16.703	1	53.17
2385	NE2	GLN	A	420	43.461	0.34	14.9	1	60.08
2386	N	ASP	A	421	42.94	-1.458	21.253	1	38.01
2387	CA	ASP	A	421	42.14	-1.416	22.478	1	36.23
2388	C	ASP	A	421	42.701	-0.473	23.535	1	33.56
2389	O	ASP	A	421	41.986	0.341	24.132	1	30.91
2390	CB	ASP	A	421	42.034	-2.803	23.071	1	39.68
2391	CG	ASP	A	421	40.991	-2.867	24.141	1	48.12
2392	OD1	ASP	A	421	39.859	-2.4	23.864	1	51.12

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
2393	OD2	ASP	A	421	41.304	-3.349	25.255	1	51.57
2394	N	LEU	A	422	43.992	-0.636	23.763	1	29.13
2395	CA	LEU	A	422	44.767	0.149	24.697	1	29.84
2396	C	LEU	A	422	44.62	1.629	24.359	1	32.49
2397	O	LEU	A	422	44.4	2.444	25.253	1	37.82
2398	CB	LEU	A	422	46.208	-0.343	24.597	1	26.25
2399	CG	LEU	A	422	47.525	0.326	24.925	1	26.23
2400	CD1	LEU	A	422	48.591	-0.612	24.4	1	22.3
2401	CD2	LEU	A	422	47.674	1.666	24.264	1	23.69
2402	N	LEU	A	423	44.685	1.984	23.074	1	34.22
2403	CA	LEU	A	423	44.534	3.395	22.675	1	31.9
2404	C	LEU	A	423	43.089	3.877	22.705	1	28.74
2405	O	LEU	A	423	42.832	5.046	22.996	1	31.23
2406	CB	LEU	A	423	45.148	3.661	21.298	1	34.69
2407	CG	LEU	A	423	46.675	3.691	21.278	1	36.79
2408	CD1	LEU	A	423	47.162	3.681	19.844	1	37.98
2409	CD2	LEU	A	423	47.198	4.906	22.048	1	34.46
2410	N	LYS	A	424	42.154	2.987	22.378	1	27.15
2411	CA	LYS	A	424	40.737	3.332	22.398	1	30.22
2412	C	LYS	A	424	40.36	3.677	23.84	1	32.88
2413	O	LYS	A	424	39.681	4.675	24.101	1	31.99
2414	CB	LYS	A	424	39.874	2.168	21.909	1	27.78
2415	CG	LYS	A	424	38.405	2.555	21.77	1	33.49
2416	CD	LYS	A	424	37.505	1.379	21.393	1	39.96
2417	CE	LYS	A	424	37.545	0.277	22.464	1	51.72
2418	NZ	LYS	A	424	36.481	-0.78	22.312	1	53.64
2419	N	LYS	A	425	40.855	2.87	24.774	1	33.7
2420	CA	LYS	A	425	40.587	3.072	26.19	1	34.78
2421	C	LYS	A	425	41.219	4.35	26.746	1	33.55
2422	O	LYS	A	425	40.545	5.122	27.421	1	35.52
2423	CB	LYS	A	425	40.994	1.831	26.975	1	36.97
2424	CG	LYS	A	425	39.963	0.715	26.822	1	40.59
2425	CD	LYS	A	425	40.52	-0.646	27.213	1	47.3
2426	CE	LYS	A	425	39.397	-1.684	27.363	1	48.04
2427	NZ	LYS	A	425	38.42	-1.685	26.225	1	50.35
2428	N	ALA	A	426	42.477	4.618	26.406	1	30.93
2429	CA	ALA	A	426	43.134	5.84	26.869	1	27.81
2430	C	ALA	A	426	42.333	7.075	26.467	1	30.98
2431	O	ALA	A	426	42.303	8.063	27.192	1	33.95
2432	CB	ALA	A	426	44.539	5.934	26.324	1	22.3
2433	N	SER	A	427	41.676	7.019	25.313	1	34.9
2434	CA	SER	A	427	40.884	8.15	24.838	1	35.92
2435	C	SER	A	427	39.533	8.221	25.54	1	37.28
2436	O	SER	A	427	38.881	9.265	25.534	1	38.17
2437	CB	SER	A	427	40.679	8.071	23.323	1	35.1
2438	OG	SER	A	427	39.912	6.94	22.96	1	33.26
2439	N	GLU	A	428	39.113	7.102	26.127	1	38.69
2440	CA	GLU	A	428	37.838	7.04	26.837	1	38.82
2441	C	GLU	A	428	37.998	7.44	28.3	1	40.27
2442	O	GLU	A	428	37.019	7.54	29.041	1	43.1
2443	CB	GLU	A	428	37.209	5.655	26.691	1	37.24
2444	CG	GLU	A	428	36.904	5.331	25.233	1	37.61

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
2445	CD	GLU	A	428	36.394	3.937	25.014	1	38.63
2446	OE1	GLU	A	428	36.983	2.982	25.565	1	45.47
2447	OE2	GLU	A	428	35.412	3.79	24.258	1	43.57
2448	N	GLU	A	429	39.245	7.667	28.7	1	37.97
2449	CA	GLU	A	429	39.55	8.101	30.04	1	36.05
2450	C	GLU	A	429	39.238	9.589	30.176	1	40.1
2451	O	GLU	A	429	38.853	10.244	29.204	1	40.97
2452	CB	GLU	A	429	41.008	7.838	30.349	1	31.29
2453	CG	GLU	A	429	41.314	6.374	30.48	1	35.96
2454	CD	GLU	A	429	42.784	6.118	30.73	1	45.1
2455	OE1	GLU	A	429	43.487	7.075	31.119	1	49.75
2456	OE2	GLU	A	429	43.249	4.971	30.523	1	50.37
2457	N	ASP	A	430	39.388	10.111	31.392	1	41.89
2458	CA	ASP	A	430	39.122	11.516	31.683	1	40.24
2459	C	ASP	A	430	40.449	12.273	31.712	1	38.36
2460	O	ASP	A	430	41.301	12.049	32.581	1	40.7
2461	CB	ASP	A	430	38.394	11.637	33.025	1	43.24
2462	CG	ASP	A	430	38.003	13.061	33.354	1	46.63
2463	OD1	ASP	A	430	38.91	13.907	33.517	1	50.22
2464	OD2	ASP	A	430	36.788	13.331	33.488	1	49.86
2465	N	HIS	A	431	40.623	13.176	30.761	1	32.06
2466	CA	HIS	A	431	41.853	13.936	30.686	1	28.9
2467	C	HIS	A	431	41.659	15.361	31.165	1	31.57
2468	O	HIS	A	431	42.58	16.177	31.088	1	33.37
2469	CB	HIS	A	431	42.349	13.944	29.24	1	27.13
2470	CG	HIS	A	431	42.774	12.602	28.746	1	16.87
2471	ND1	HIS	A	431	44.08	12.166	28.831	1	15.65
2472	CD2	HIS	A	431	42.055	11.562	28.261	1	16.39
2473	CE1	HIS	A	431	44.147	10.907	28.432	1	16.54
2474	NE2	HIS	A	431	42.932	10.518	28.082	1	18.27
2475	N	THR	A	432	40.461	15.648	31.664	1	31.76
2476	CA	THR	A	432	40.113	16.983	32.13	1	32.58
2477	C	THR	A	432	41.184	17.684	32.937	1	34.8
2478	O	THR	A	432	41.392	18.884	32.793	1	40.58
2479	CB	THR	A	432	38.854	16.94	32.968	1	32.87
2480	OG1	THR	A	432	37.826	16.232	32.258	1	35.7
2481	CG2	THR	A	432	38.39	18.342	33.261	1	33.69
2482	N	ASN	A	433	41.879	16.918	33.764	1	37.61
2483	CA	ASN	A	433	42.935	17.42	34.647	1	40.41
2484	C	ASN	A	433	44.337	17.412	34.036	1	40.05
2485	O	ASN	A	433	45.316	17.755	34.713	1	37.42
2486	CB	ASN	A	433	42.957	16.555	35.898	1	49.51
2487	CG	ASN	A	433	43.106	15.066	35.568	1	57.7
2488	OD1	ASN	A	433	42.403	14.525	34.695	1	59.77
2489	ND2	ASN	A	433	44.022	14.399	36.259	1	61.98
2490	N	ALA	A	434	44.428	17.02	32.767	1	38.07
2491	CA	ALA	A	434	45.695	16.923	32.06	1	34.38
2492	C	ALA	A	434	45.873	18.021	31.005	1	33.72
2493	O	ALA	A	434	44.93	18.349	30.283	1	36.16
2494	CB	ALA	A	434	45.794	15.561	31.423	1	32.41
2495	N	ALA	A	435	47.078	18.583	30.93	1	31.51
2496	CA	ALA	A	435	47.392	19.631	29.96	1	32.16

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
2497	C	ALA	A	435	47.547	19.105	28.544	1	34.66
2498	O	ALA	A	435	47.422	19.868	27.589	1	36.21
2499	CB	ALA	A	435	48.657	20.371	30.351	1	30.11
2500	N	CYS	A	436	47.861	17.822	28.399	1	36.15
2501	CA	CYS	A	436	48.035	17.237	27.077	1	35.43
2502	C	CYS	A	436	48.108	15.71	27.116	1	34.96
2503	O	CYS	A	436	47.782	15.088	28.135	1	37.82
2504	CB	CYS	A	436	49.292	17.809	26.432	1	34.9
2505	SG	CYS	A	436	50.829	17.115	26.99	1	40.7
2506	N	PHE	A	437	48.498	15.111	25.995	1	31.92
2507	CA	PHE	A	437	48.625	13.663	25.879	1	27.87
2508	C	PHE	A	437	49.752	13.324	24.921	1	27.62
2509	O	PHE	A	437	50.112	14.127	24.067	1	28.91
2510	CB	PHE	A	437	47.326	13.044	25.386	1	27.99
2511	CG	PHE	A	437	47.437	11.578	25.093	1	36.12
2512	CD1	PHE	A	437	47.303	10.637	26.111	1	33.21
2513	CD2	PHE	A	437	47.702	11.131	23.791	1	39.55
2514	CE1	PHE	A	437	47.434	9.267	25.837	1	35.78
2515	CE2	PHE	A	437	47.832	9.76	23.508	1	36.55
2516	CZ	PHE	A	437	47.699	8.833	24.528	1	36.24
2517	N	ALA	A	438	50.318	12.138	25.07	1	27.46
2518	CA	ALA	A	438	51.411	11.716	24.213	1	27.71
2519	C	ALA	A	438	51.428	10.205	24.079	1	29.32
2520	O	ALA	A	438	50.99	9.495	24.979	1	30.46
2521	CB	ALA	A	438	52.737	12.208	24.761	1	22.09
2522	N	CYS	A	439	51.86	9.738	22.91	1	30.16
2523	CA	CYS	A	439	51.971	8.31	22.591	1	29.6
2524	C	CYS	A	439	53.216	8.121	21.749	1	29.07
2525	O	CYS	A	439	53.482	8.893	20.841	1	32.96
2526	CB	CYS	A	439	50.768	7.809	21.797	1	26.87
2527	SG	CYS	A	439	50.924	6.078	21.335	1	29.05
2528	N	ILE	A	440	53.981	7.093	22.048	1	28.17
2529	CA	ILE	A	440	55.194	6.842	21.323	1	25.58
2530	C	ILE	A	440	55.16	5.41	20.831	1	31.83
2531	O	ILE	A	440	55.061	4.482	21.642	1	35.52
2532	CB	ILE	A	440	56.371	7.036	22.244	1	25.05
2533	CG1	ILE	A	440	56.319	8.451	22.823	1	25.69
2534	CG2	ILE	A	440	57.667	6.739	21.515	1	25
2535	CD1	ILE	A	440	57.304	8.692	23.92	1	27.25
2536	N	LEU	A	441	55.183	5.234	19.509	1	29.49
2537	CA	LEU	A	441	55.159	3.907	18.882	1	27.29
2538	C	LEU	A	441	56.561	3.568	18.407	1	24.53
2539	O	LEU	A	441	57.209	4.383	17.756	1	26.4
2540	CB	LEU	A	441	54.193	3.896	17.692	1	26.29
2541	CG	LEU	A	441	52.812	4.463	18.057	1	31.24
2542	CD1	LEU	A	441	51.967	4.756	16.817	1	26.83
2543	CD2	LEU	A	441	52.093	3.502	19.011	1	30.03
2544	N	LEU	A	442	57.051	2.406	18.816	1	24.45
2545	CA	LEU	A	442	58.372	1.918	18.447	1	26.59
2546	C	LEU	A	442	58.124	0.557	17.801	1	30.91
2547	O	LEU	A	442	57.805	-0.414	18.499	1	35.21
2548	CB	LEU	A	442	59.221	1.713	19.7	1	26.58

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
2549	CG	LEU	A	442	59.388	2.852	20.694	1	27.12
2550	CD1	LEU	A	442	60.083	2.324	21.946	1	26.92
2551	CD2	LEU	A	442	60.195	3.951	20.066	1	25.35
2552	N	SER	A	443	58.28	0.454	16.485	1	32.76
2553	CA	SER	A	443	58.003	-0.821	15.829	1	30.97
2554	C	SER	A	443	58.432	-0.813	14.363	1	32.32
2555	O	SER	A	443	59.064	0.136	13.89	1	32
2556	CB	SER	A	443	56.486	-1.083	15.909	1	20.56
2557	OG	SER	A	443	56.166	-2.423	15.574	1	21.75
2558	N	HIS	A	444	58.141	-1.917	13.676	1	32.18
2559	CA	HIS	A	444	58.394	-2.025	12.246	1	30.25
2560	C	HIS	A	444	57.205	-1.295	11.611	1	31.06
2561	O	HIS	A	444	56.139	-1.163	12.231	1	31.09
2562	CB	HIS	A	444	58.379	-3.489	11.781	1	25.14
2563	CG	HIS	A	444	59.655	-4.226	12.043	1	18.69
2564	ND1	HIS	A	444	60.88	-3.766	11.611	1	19.11
2565	CD2	HIS	A	444	59.893	-5.405	12.674	1	19.63
2566	CE1	HIS	A	444	61.82	-4.628	11.962	1	20.6
2567	NE2	HIS	A	444	61.246	-5.631	12.609	1	20.38
2568	N	GLY	A	445	57.375	-0.828	10.382	1	31.41
2569	CA	GLY	A	445	56.283	-0.149	9.708	1	32.28
2570	C	GLY	A	445	56.474	-0.08	8.207	1	31.17
2571	O	GLY	A	445	57.495	-0.518	7.677	1	30.99
2572	N	GLU	A	446	55.456	0.442	7.535	1	33.06
2573	CA	GLU	A	446	55.428	0.642	6.084	1	36.06
2574	C	GLU	A	446	54.537	1.874	5.943	1	37.76
2575	O	GLU	A	446	53.789	2.182	6.864	1	38.53
2576	CB	GLU	A	446	54.824	-0.567	5.376	1	35.35
2577	CG	GLU	A	446	55.688	-1.817	5.467	1	40.77
2578	CD	GLU	A	446	55.041	-3.037	4.832	1	47.48
2579	OE1	GLU	A	446	54.182	-2.872	3.948	1	52.57
2580	OE2	GLU	A	446	55.402	-4.171	5.194	1	50.79
2581	N	GLU	A	447	54.589	2.576	4.818	1	40.43
2582	CA	GLU	A	447	53.801	3.796	4.694	1	42.21
2583	C	GLU	A	447	52.382	3.705	5.23	1	39.77
2584	O	GLU	A	447	51.624	2.828	4.832	1	42.91
2585	CB	GLU	A	447	53.807	4.342	3.263	1	43.26
2586	CG	GLU	A	447	54.096	5.853	3.255	1	52.55
2587	CD	GLU	A	447	54.051	6.511	1.874	1	57.77
2588	OE1	GLU	A	447	54.728	6.023	0.936	1	57.77
2589	OE2	GLU	A	447	53.359	7.55	1.742	1	58.43
2590	N	ASN	A	448	52.076	4.559	6.208	1	36.37
2591	CA	ASN	A	448	50.745	4.64	6.836	1	35.29
2592	C	ASN	A	448	50.309	3.472	7.74	1	30.65
2593	O	ASN	A	448	49.204	3.471	8.282	1	29.69
2594	CB	ASN	A	448	49.685	4.859	5.76	1	36.7
2595	CG	ASN	A	448	50.053	5.969	4.817	1	42.47
2596	OD1	ASN	A	448	50.477	5.716	3.696	1	49.18
2597	ND2	ASN	A	448	49.942	7.208	5.278	1	44.85
2598	N	VAL	A	449	51.228	2.571	8.028	1	25.91
2599	CA	VAL	A	449	50.915	1.394	8.803	1	24.83
2600	C	VAL	A	449	52.032	1.106	9.836	1	24.66

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
2601	O	VAL	A	449	53.179	1.518	9.621	1	23.11
2602	CB	VAL	A	449	50.774	0.237	7.773	1	25.26
2603	CG1	VAL	A	449	51.577	-0.944	8.16	1	26.94
2604	CG2	VAL	A	449	49.314	-0.099	7.531	1	24.62
2605	N	ILE	A	450	51.683	0.513	10.988	1	24.57
2606	CA	ILE	A	450	52.678	0.12	12.016	1	24.2
2607	C	ILE	A	450	52.412	-1.331	12.315	1	23.18
2608	O	ILE	A	450	51.263	-1.784	12.318	1	23
2609	CB	ILE	A	450	52.605	0.87	13.398	1	25.47
2610	CG1	ILE	A	450	51.329	1.677	13.523	1	28.17
2611	CG2	ILE	A	450	53.86	1.69	13.669	1	29.41
2612	CD1	ILE	A	450	50.119	0.794	13.752	1	37.61
2613	N	TYR	A	451	53.475	-2.066	12.563	1	22.18
2614	CA	TYR	A	451	53.318	-3.462	12.86	1	25.33
2615	C	TYR	A	451	53.031	-3.764	14.314	1	29.46
2616	O	TYR	A	451	53.594	-3.135	15.214	1	29.67
2617	CB	TYR	A	451	54.594	-4.213	12.525	1	29.79
2618	CG	TYR	A	451	54.736	-4.594	11.088	1	33.23
2619	CD1	TYR	A	451	55.19	-3.668	10.149	1	33.12
2620	CD2	TYR	A	451	54.46	-5.897	10.671	1	31.84
2621	CE1	TYR	A	451	55.372	-4.028	8.831	1	40.01
2622	CE2	TYR	A	451	54.636	-6.267	9.354	1	40.05
2623	CZ	TYR	A	451	55.1	-5.328	8.437	1	40.6
2624	OH	TYR	A	451	55.328	-5.7	7.144	1	39.71
2625	N	GLY	A	452	52.107	-4.692	14.524	1	29.85
2626	CA	GLY	A	452	51.846	-5.207	15.847	1	29.69
2627	C	GLY	A	452	52.706	-6.464	15.707	1	34.3
2628	O	GLY	A	452	53.34	-6.664	14.854	1	36.71
2629	N	LYS	A	453	52.772	-7.327	16.709	1	33.54
2630	CA	LYS	A	453	53.579	-8.527	16.52	1	34.52
2631	C	LYS	A	453	52.786	-9.467	15.627	1	33.35
2632	O	LYS	A	453	53.318	-10.386	15.014	1	33.01
2633	CB	LYS	A	453	53.88	-9.211	17.855	1	39.08
2634	CG	LYS	A	453	52.673	-9.7	18.634	1	42.36
2635	CD	LYS	A	453	53.113	-10.734	19.668	1	50.7
2636	CE	LYS	A	453	51.936	-11.217	20.527	1	59.15
2637	NZ	LYS	A	453	51.549	-10.312	21.664	1	59.29
2638	N	ASP	A	454	51.497	-9.169	15.577	1	34.5
2639	CA	ASP	A	454	50.449	-9.878	14.866	1	34.86
2640	C	ASP	A	454	50.317	-9.619	13.346	1	35.68
2641	O	ASP	A	454	49.838	-10.467	12.59	1	37.69
2642	CB	ASP	A	454	49.137	-9.435	15.528	1	32.65
2643	CG	ASP	A	454	48.354	-10.573	16.073	1	43.3
2644	OD1	ASP	A	454	48.914	-11.689	16.187	1	53.9
2645	OD2	ASP	A	454	47.169	-10.356	16.383	1	43.84
2646	N	GLY	A	455	50.619	-8.403	12.922	1	34.32
2647	CA	GLY	A	455	50.455	-8.069	11.531	1	28.94
2648	C	GLY	A	455	50.61	-6.581	11.367	1	28.81
2649	O	GLY	A	455	51.545	-6.017	11.925	1	33.19
2650	N	VAL	A	456	49.627	-5.925	10.758	1	26.46
2651	CA	VAL	A	456	49.73	-4.492	10.476	1	24.43
2652	C	VAL	A	456	48.411	-3.74	10.675	1	25.33

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
2653	O	VAL	A	456	47.328	-4.293	10.459	1	28.5
2654	CB	VAL	A	456	50.257	-4.317	9.009	1	25.39
2655	CG1	VAL	A	456	49.393	-3.377	8.207	1	27.92
2656	CG2	VAL	A	456	51.69	-3.905	9.011	1	20.4
2657	N	THR	A	457	48.512	-2.467	11.048	1	25.64
2658	CA	THR	A	457	47.342	-1.624	11.298	1	27.83
2659	C	THR	A	457	47.679	-0.176	10.907	1	25.3
2660	O	THR	A	457	48.817	0.262	11.058	1	27.65
2661	CB	THR	A	457	46.851	-1.757	12.837	1	31.28
2662	OG1	THR	A	457	46.095	-0.605	13.256	1	32.32
2663	CG2	THR	A	457	48.023	-1.956	13.779	1	28.67
2664	N	PRO	A	458	46.723	0.54	10.292	1	25.33
2665	CA	PRO	A	458	46.883	1.936	9.86	1	25.08
2666	C	PRO	A	458	47.138	2.843	11.053	1	30.25
2667	O	PRO	A	458	46.381	2.806	12.042	1	30.89
2668	CB	PRO	A	458	45.511	2.278	9.269	1	24.76
2669	CG	PRO	A	458	44.987	0.965	8.817	1	25.33
2670	CD	PRO	A	458	45.407	0.01	9.892	1	25.17
2671	N	ILE	A	459	48.151	3.694	10.947	1	27.7
2672	CA	ILE	A	459	48.449	4.623	12.024	1	28.65
2673	C	ILE	A	459	47.261	5.565	12.21	1	33.41
2674	O	ILE	A	459	46.986	6.016	13.317	1	37.46
2675	CB	ILE	A	459	49.712	5.453	11.729	1	25.3
2676	CG1	ILE	A	459	50.935	4.544	11.692	1	21.31
2677	CG2	ILE	A	459	49.904	6.54	12.79	1	27.01
2678	CD1	ILE	A	459	52.212	5.258	11.37	1	24.02
2679	N	LYS	A	460	46.534	5.836	11.133	1	34.14
2680	CA	LYS	A	460	45.384	6.726	11.194	1	32.6
2681	C	LYS	A	460	44.298	6.171	12.086	1	30.96
2682	O	LYS	A	460	43.582	6.912	12.737	1	32.8
2683	CB	LYS	A	460	44.813	6.953	9.802	1	35.57
2684	CG	LYS	A	460	43.806	8.097	9.733	1	45.07
2685	CD	LYS	A	460	42.392	7.621	9.409	1	51.81
2686	CE	LYS	A	460	41.522	8.81	8.989	1	57.33
2687	NZ	LYS	A	460	40.15	8.408	8.546	1	60.53
2688	N	ASP	A	461	44.163	4.858	12.105	1	33.91
2689	CA	ASP	A	461	43.146	4.22	12.934	1	35.7
2690	C	ASP	A	461	43.433	4.287	14.435	1	31.18
2691	O	ASP	A	461	42.514	4.295	15.245	1	30.75
2692	CB	ASP	A	461	42.927	2.778	12.48	1	40.64
2693	CG	ASP	A	461	42.271	2.695	11.102	1	46.19
2694	OD1	ASP	A	461	41.921	3.761	10.526	1	43.24
2695	OD2	ASP	A	461	42.094	1.557	10.606	1	48.93
2696	N	LEU	A	462	44.709	4.362	14.784	1	28.43
2697	CA	LEU	A	462	45.142	4.444	16.17	1	30.64
2698	C	LEU	A	462	44.951	5.848	16.722	1	30.61
2699	O	LEU	A	462	44.448	6.024	17.832	1	34.8
2700	CB	LEU	A	462	46.621	4.062	16.288	1	24.93
2701	CG	LEU	A	462	47.024	2.644	15.876	1	25.85
2702	CD1	LEU	A	462	48.51	2.529	16.014	1	26.37
2703	CD2	LEU	A	462	46.32	1.583	16.733	1	26.22
2704	N	THR	A	463	45.326	6.843	15.927	1	29.25

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
2705	CA	THR	A	463	45.232	8.24	16.325	1	27.72
2706	C	THR	A	463	43.822	8.828	16.218	1	29.7
2707	O	THR	A	463	43.512	9.843	16.85	1	32.9
2708	CB	THR	A	463	46.213	9.132	15.494	1	29.31
2709	OG1	THR	A	463	45.886	9.05	14.1	1	34.19
2710	CG2	THR	A	463	47.657	8.69	15.693	1	24.05
2711	N	ALA	A	464	42.955	8.177	15.45	1	29.85
2712	CA	ALA	A	464	41.597	8.683	15.26	1	30.17
2713	C	ALA	A	464	40.832	8.789	16.568	1	31.59
2714	O	ALA	A	464	40.018	9.702	16.76	1	29.06
2715	CB	ALA	A	464	40.85	7.797	14.302	1	27.82
2716	N	HIS	A	465	41.13	7.853	17.47	1	33.36
2717	CA	HIS	A	465	40.488	7.761	18.786	1	31.4
2718	C	HIS	A	465	40.552	9.051	19.578	1	32.63
2719	O	HIS	A	465	39.634	9.359	20.342	1	34.41
2720	CB	HIS	A	465	41.144	6.669	19.616	1	24.39
2721	CG	HIS	A	465	41.036	5.31	19.013	1	19.08
2722	ND1	HIS	A	465	39.823	4.718	18.73	1	18.99
2723	CD2	HIS	A	465	41.99	4.417	18.653	1	17.35
2724	CE1	HIS	A	465	40.034	3.514	18.222	1	20.46
2725	NE2	HIS	A	465	41.34	3.309	18.166	1	22.14
2726	N	PHE	A	466	41.614	9.821	19.359	1	31.31
2727	CA	PHE	A	466	41.807	11.06	20.09	1	29.86
2728	C	PHE	A	466	41.321	12.293	19.364	1	29.11
2729	O	PHE	A	466	41.632	13.403	19.767	1	32.28
2730	CB	PHE	A	466	43.273	11.19	20.51	1	28.66
2731	CG	PHE	A	466	43.808	9.96	21.217	1	31.2
2732	CD1	PHE	A	466	44.211	8.838	20.486	1	31.59
2733	CD2	PHE	A	466	43.883	9.913	22.609	1	30.43
2734	CE1	PHE	A	466	44.677	7.694	21.122	1	28.67
2735	CE2	PHE	A	466	44.35	8.769	23.254	1	27.62
2736	CZ	PHE	A	466	44.746	7.66	22.505	1	32.92
2737	N	ARG	A	467	40.537	12.096	18.312	1	27.96
2738	CA	ARG	A	467	39.988	13.216	17.554	1	33.1
2739	C	ARG	A	467	39.08	14.019	18.46	1	33.66
2740	O	ARG	A	467	38.366	13.441	19.263	1	38.54
2741	CB	ARG	A	467	39.171	12.717	16.368	1	33.52
2742	CG	ARG	A	467	39.987	12.402	15.134	1	34.92
2743	CD	ARG	A	467	39.129	11.71	14.113	1	32.65
2744	NE	ARG	A	467	37.785	12.269	14.092	1	34.23
2745	CZ	ARG	A	467	36.886	12.009	13.153	1	38.47
2746	NH1	ARG	A	467	37.185	11.209	12.14	1	42.1
2747	NH2	ARG	A	467	35.664	12.503	13.26	1	38.77
2748	N	GLY	A	468	39.059	15.335	18.28	1	34.04
2749	CA	GLY	A	468	38.239	16.206	19.107	1	37.09
2750	C	GLY	A	468	36.84	15.723	19.441	1	40.11
2751	O	GLY	A	468	36.385	15.829	20.583	1	43.05
2752	N	ASP	A	469	36.166	15.153	18.454	1	40.89
2753	CA	ASP	A	469	34.801	14.661	18.624	1	39.82
2754	C	ASP	A	469	34.719	13.293	19.32	1	37.32
2755	O	ASP	A	469	33.638	12.793	19.631	1	36.74
2756	CB	ASP	A	469	34.104	14.605	17.243	1	39.23

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
2757	CG	ASP	A	469	34.736	13.58	16.289	1	39.56
2758	OD1	ASP	A	469	35.981	13.549	16.161	1	39.71
2759	OD2	ASP	A	469	33.977	12.802	15.664	1	40.65
2760	N	ARG	A	470	35.873	12.701	19.565	1	35.89
2761	CA	ARG	A	470	35.94	11.389	20.161	1	37.73
2762	C	ARG	A	470	36.582	11.347	21.546	1	37.13
2763	O	ARG	A	470	36.286	10.451	22.324	1	42.69
2764	CB	ARG	A	470	36.638	10.444	19.192	1	39.69
2765	CG	ARG	A	470	35.92	10.333	17.864	1	44.04
2766	CD	ARG	A	470	36.62	9.378	16.92	1	50.2
2767	NE	ARG	A	470	35.987	9.371	15.597	1	59.48
2768	CZ	ARG	A	470	36.408	8.654	14.554	1	58.34
2769	NH1	ARG	A	470	37.473	7.865	14.659	1	62.53
2770	NH2	ARG	A	470	35.755	8.722	13.403	1	57.5
2771	N	SER	A	471	37.512	12.252	21.826	1	34.4
2772	CA	SER	A	471	38.135	12.333	23.144	1	31.79
2773	C	SER	A	471	37.894	13.784	23.495	1	33.97
2774	O	SER	A	471	38.771	14.633	23.374	1	37.58
2775	CB	SER	A	471	39.639	12.029	23.106	1	30.32
2776	OG	SER	A	471	40.22	12.04	24.408	1	19.72
2777	N	LYS	A	472	36.668	14.084	23.883	1	36.28
2778	CA	LYS	A	472	36.308	15.445	24.218	1	39.36
2779	C	LYS	A	472	37.095	16.074	25.367	1	39.67
2780	O	LYS	A	472	37.32	17.288	25.364	1	40.08
2781	CB	LYS	A	472	34.79	15.54	24.388	1	43.39
2782	CG	LYS	A	472	34.067	15.318	23.041	1	52.64
2783	CD	LYS	A	472	32.626	14.816	23.149	1	59.29
2784	CE	LYS	A	472	32.537	13.389	23.727	1	65.52
2785	NZ	LYS	A	472	33.257	12.325	22.954	1	63.63
2786	N	THR	A	473	37.629	15.254	26.275	1	37.82
2787	CA	THR	A	473	38.39	15.813	27.394	1	37.51
2788	C	THR	A	473	39.786	16.274	26.995	1	36.11
2789	O	THR	A	473	40.503	16.878	27.798	1	36.76
2790	CB	THR	A	473	38.449	14.872	28.638	1	37.98
2791	OG1	THR	A	473	39.17	13.672	28.336	1	42.06
2792	CG2	THR	A	473	37.051	14.507	29.084	1	34.43
2793	N	LEU	A	474	40.2	15.944	25.774	1	35.58
2794	CA	LEU	A	474	41.498	16.4	25.291	1	31.42
2795	C	LEU	A	474	41.293	17.521	24.282	1	32.85
2796	O	LEU	A	474	42.256	18.117	23.798	1	36.28
2797	CB	LEU	A	474	42.309	15.264	24.7	1	24.5
2798	CG	LEU	A	474	43.176	14.51	25.704	1	20.93
2799	CD1	LEU	A	474	43.72	13.249	25.056	1	22.49
2800	CD2	LEU	A	474	44.304	15.394	26.213	1	15.76
2801	N	LEU	A	475	40.029	17.86	24.034	1	32.77
2802	CA	LEU	A	475	39.702	18.923	23.104	1	34.75
2803	C	LEU	A	475	40.466	20.201	23.455	1	37.09
2804	O	LEU	A	475	40.534	20.602	24.622	1	39.26
2805	CB	LEU	A	475	38.199	19.19	23.11	1	37.5
2806	CG	LEU	A	475	37.667	20.035	21.948	1	40.32
2807	CD1	LEU	A	475	37.889	19.303	20.647	1	41.82
2808	CD2	LEU	A	475	36.19	20.302	22.12	1	42.46

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
2809	N	GLU	A	476	41.059	20.811	22.428	1	37.59
2810	CA	GLU	A	476	41.848	22.046	22.522	1	32.94
2811	C	GLU	A	476	43.195	21.884	23.197	1	31.36
2812	O	GLU	A	476	43.937	22.854	23.386	1	32.44
2813	CB	GLU	A	476	41.053	23.185	23.148	1	39.49
2814	CG	GLU	A	476	39.839	23.585	22.323	1	48.51
2815	CD	GLU	A	476	39.181	24.842	22.837	1	55.54
2816	OE1	GLU	A	476	39.242	25.089	24.063	1	60.94
2817	OE2	GLU	A	476	38.608	25.589	22.012	1	62.66
2818	N	LYS	A	477	43.544	20.633	23.468	1	30.36
2819	CA	LYS	A	477	44.818	20.308	24.087	1	30.4
2820	C	LYS	A	477	45.624	19.52	23.048	1	29.21
2821	O	LYS	A	477	45.059	18.822	22.197	1	25.88
2822	CB	LYS	A	477	44.592	19.431	25.329	1	34.02
2823	CG	LYS	A	477	43.601	19.992	26.366	1	36.55
2824	CD	LYS	A	477	43.267	18.925	27.419	1	39.4
2825	CE	LYS	A	477	42.505	19.473	28.618	1	37.4
2826	NZ	LYS	A	477	42.262	18.407	29.631	1	34.16
2827	N	PRO	A	478	46.949	19.638	23.088	1	26.32
2828	CA	PRO	A	478	47.802	18.922	22.142	1	26.55
2829	C	PRO	A	478	47.848	17.409	22.38	1	29.39
2830	O	PRO	A	478	47.924	16.95	23.524	1	30.91
2831	CB	PRO	A	478	49.174	19.569	22.352	1	26.48
2832	CG	PRO	A	478	49.137	20.015	23.783	1	26
2833	CD	PRO	A	478	47.736	20.542	23.952	1	23.51
2834	N	LYS	A	479	47.811	16.648	21.284	1	30.65
2835	CA	LYS	A	479	47.869	15.186	21.291	1	26.03
2836	C	LYS	A	479	49.089	14.785	20.461	1	28.64
2837	O	LYS	A	479	49.011	14.659	19.245	1	35.07
2838	CB	LYS	A	479	46.587	14.62	20.699	1	22.45
2839	CG	LYS	A	479	45.365	15.138	21.415	1	18.52
2840	CD	LYS	A	479	44.078	14.875	20.651	1	24.25
2841	CE	LYS	A	479	43.499	16.172	20.081	1	24.44
2842	NZ	LYS	A	479	43.277	17.266	21.089	1	25.34
2843	N	LEU	A	480	50.226	14.649	21.13	1	25.52
2844	CA	LEU	A	480	51.486	14.318	20.498	1	23.83
2845	C	LEU	A	480	51.625	12.837	20.23	1	23.54
2846	O	LEU	A	480	51.162	12.02	20.998	1	26.82
2847	CB	LEU	A	480	52.649	14.78	21.387	1	26.29
2848	CG	LEU	A	480	52.496	16.115	22.14	1	26.01
2849	CD1	LEU	A	480	53.753	16.412	22.954	1	25.52
2850	CD2	LEU	A	480	52.22	17.25	21.172	1	21.63
2851	N	PHE	A	481	52.252	12.498	19.116	1	24.55
2852	CA	PHE	A	481	52.488	11.112	18.743	1	23.27
2853	C	PHE	A	481	53.886	11.098	18.165	1	24.15
2854	O	PHE	A	481	54.223	11.961	17.365	1	28.76
2855	CB	PHE	A	481	51.474	10.637	17.701	1	18.52
2856	CG	PHE	A	481	50.08	10.461	18.245	1	15.03
2857	CD1	PHE	A	481	49.206	11.544	18.324	1	17.74
2858	CD2	PHE	A	481	49.648	9.212	18.682	1	14.22
2859	CE1	PHE	A	481	47.903	11.399	18.833	1	15.46
2860	CE2	PHE	A	481	48.359	9.045	19.194	1	14.05

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
2861	CZ	PHE	A	481	47.482	10.149	19.268	1	15.59
2862	N	PHE	A	482	54.74	10.24	18.703	1	22.77
2863	CA	PHE	A	482	56.104	10.119	18.231	1	23.6
2864	C	PHE	A	482	56.14	8.71	17.683	1	27.57
2865	O	PHE	A	482	55.721	7.761	18.364	1	26.38
2866	CB	PHE	A	482	57.114	10.287	19.367	1	22.05
2867	CG	PHE	A	482	57.09	11.653	20.005	1	23.74
2868	CD1	PHE	A	482	56.12	11.983	20.953	1	22.19
2869	CD2	PHE	A	482	58.029	12.618	19.648	1	21.85
2870	CE1	PHE	A	482	56.093	13.266	21.536	1	24.22
2871	CE2	PHE	A	482	58.003	13.907	20.233	1	23
2872	CZ	PHE	A	482	57.04	14.226	21.171	1	17.32
2873	N	ILE	A	483	56.569	8.581	16.429	1	28.63
2874	CA	ILE	A	483	56.608	7.28	15.791	1	27.31
2875	C	ILE	A	483	57.968	6.932	15.222	1	28.09
2876	O	ILE	A	483	58.555	7.686	14.443	1	31.38
2877	CB	ILE	A	483	55.544	7.188	14.686	1	28.45
2878	CG1	ILE	A	483	54.179	7.575	15.257	1	25.95
2879	CG2	ILE	A	483	55.491	5.764	14.106	1	26.67
2880	CD1	ILE	A	483	53.465	8.624	14.461	1	31.52
2881	N	GLN	A	484	58.494	5.817	15.703	1	28.23
2882	CA	GLN	A	484	59.761	5.279	15.257	1	28.02
2883	C	GLN	A	484	59.385	3.969	14.564	1	28.94
2884	O	GLN	A	484	59.095	2.967	15.226	1	28.04
2885	CB	GLN	A	484	60.679	5.03	16.441	1	21.84
2886	CG	GLN	A	484	61.814	4.075	16.15	1	26.38
2887	CD	GLN	A	484	62.703	4.512	14.986	1	30.77
2888	OE1	GLN	A	484	63.077	5.683	14.862	1	28.92
2889	NE2	GLN	A	484	63.056	3.561	14.138	1	28.1
2890	N	ALA	A	485	59.306	4.03	13.232	1	29.89
2891	CA	ALA	A	485	58.947	2.894	12.376	1	28.68
2892	C	ALA	A	485	59.335	3.239	10.939	1	31.68
2893	O	ALA	A	485	59.447	4.419	10.584	1	34.07
2894	CB	ALA	A	485	57.435	2.652	12.439	1	20.86
2895	N	661 A		486	59.605	2.22	10.129	1	32.51
2896	CA	661 A		486	59.919	2.454	8.712	1	30.78
2897	C	661 A		486	58.635	2.943	8.051	1	28.02
2898	O	661 A		486	57.535	2.631	8.515	1	28.04
2899	CB	661 A		486	60.334	1.153	8.032	1	29.22
2900	SG	661 A		486	61.962	0.866	8.557	1	32.33
2901	C2	661 A		486	69.426	-1.855	10.993	1	27.94
2902	C6	661 A		486	68.305	-0.982	10.612	1	30.68
2903	O3	661 A		486	68.299	0.199	10.953	1	34.98
2904	N3	661 A		486	67.315	-1.49	9.885	1	29.27
2905	C3	661 A		486	66.212	-0.615	9.543	1	26.1
2906	C7	661 A		486	64.871	-1.121	10.04	1	24.67
2907	O4	661 A		486	64.594	-2.323	10.081	1	24.17
2908	N4	661 A		486	64.041	-0.139	10.358	1	25.58
2909	C4	661 A		486	62.718	-0.458	10.835	1	27.5
2910	C8	661 A		486	61.727	-0.586	9.678	1	29.16
2911	C12	661 A		486	62.282	0.559	11.913	1	27.4
2912	C13	661 A		486	62.828	0.097	13.248	1	27.95

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
2913	OD1		661 A	486	63.092	0.959	14.105	1	27.94
2914	OD2		661 A	486	63.014	-1.127	13.431	1	26.12
2915	O5		661 A	486	60.397	-0.974	10.048	1	32.25
2916	C18		661 A	486	68.93	-2.793	12.032	1	29.5
2917	C9		661 A	486	71.729	-1.338	11.144	1	35.5
2918	N2		661 A	486	70.504	-0.955	11.382	1	30.77
2919	O6		661 A	486	71.961	-2.354	10.495	1	38.74
2920	C19		661 A	486	72.84	-0.566	11.715	1	37.41
2921	C1		661 A	486	70.043	-3.653	12.398	1	32.38
2922	C5		661 A	486	69.578	-4.816	13.226	1	39.25
2923	O1		661 A	486	68.416	-4.908	13.664	1	40.48
2924	O2		661 A	486	70.443	-5.682	13.46	1	45.89
2925	C10		661 A	486	66.165	-0.429	8.029	1	26.65
2926	C11		661 A	486	66.018	-1.76	7.288	1	22.42
2927	C14		661 A	486	67.255	0.506	7.544	1	24.99
2928	C15		661 A	486	72.911	0.78	11.084	1	42.44
2929	C16		661 A	486	73.712	1.697	11.993	1	48.19
2930	O7		661 A	486	73.548	1.631	13.228	1	54.35
2931	O8		661 A	486	74.496	2.517	11.481	1	51.22
2932	N1		661 A	486	74.084	-1.306	11.634	1	40.55
2933	C17		661 A	486	74.43	-2.512	12.132	1	42.04
2934	O9		661 A	486	75.568	-2.967	11.98	1	46.58
2935	C20		661 A	486	73.415	-3.344	12.87	1	40.06
2936	N	ARG	A	487	58.762	3.743	7.003	1	25.93
2937	CA	ARG	A	487	57.57	4.229	6.308	1	28.03
2938	C	ARG	A	487	57.615	3.828	4.811	1	29.26
2939	O	ARG	A	487	56.933	4.425	3.962	1	25.58
2940	CB	ARG	A	487	57.412	5.743	6.492	1	25.32
2941	CG	ARG	A	487	57.4	6.197	7.953	1	28.14
2942	CD	ARG	A	487	57.307	7.697	8.073	1	17.54
2943	NE	ARG	A	487	55.982	8.173	7.701	1	15.7
2944	CZ	ARG	A	487	55.663	9.456	7.59	1	18.16
2945	NH1	ARG	A	487	56.58	10.389	7.798	1	19.97
2946	NH2	ARG	A	487	54.406	9.81	7.386	1	18.23
2947	N	GLY	A	488	58.379	2.777	4.521	1	26.65
2948	CA	GLY	A	488	58.507	2.3	3.168	1	27.62
2949	C	GLY	A	488	59.847	1.645	3.025	1	29.17
2950	O	GLY	A	488	60.447	1.272	4.029	1	32.2
2951	N	THR	A	489	60.356	1.58	1.798	1	33.28
2952	CA	THR	A	489	61.636	0.93	1.54	1	34.65
2953	C	THR	A	489	62.708	1.733	0.809	1	34.33
2954	O	THR	A	489	63.706	1.169	0.36	1	37.38
2955	CB	THR	A	489	61.429	-0.425	0.828	1	35.99
2956	OG1	THR	A	489	60.739	-0.225	-0.416	1	38.83
2957	CG2	THR	A	489	60.602	-1.36	1.714	1	35.4
2958	N	GLU	A	490	62.537	3.044	0.716	1	34.21
2959	CA	GLU	A	490	63.535	3.872	0.049	1	36.23
2960	C	GLU	A	490	64.679	4.215	1.005	1	35.72
2961	O	GLU	A	490	64.481	4.289	2.215	1	37.28
2962	CB	GLU	A	490	62.886	5.144	-0.493	1	37.65
2963	CG	GLU	A	490	61.831	4.87	-1.548	1	50.75
2964	CD	GLU	A	490	60.871	6.039	-1.765	1	61.3

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
2965	OE1	GLU	A	490	61.353	7.167	-2.039	1	66.34
2966	OE2	GLU	A	490	59.63	5.821	-1.676	1	64.42
2967	N	LEU	A	491	65.87	4.415	0.45	1	36.76
2968	CA	LEU	A	491	67.066	4.765	1.219	1	34.71
2969	C	LEU	A	491	67.553	6.137	0.775	1	35.87
2970	O	LEU	A	491	67.554	6.439	-0.411	1	40.78
2971	CB	LEU	A	491	68.181	3.737	0.985	1	33
2972	CG	LEU	A	491	68.037	2.344	1.611	1	33.44
2973	CD1	LEU	A	491	69.095	1.406	1.062	1	27.09
2974	CD2	LEU	A	491	68.157	2.455	3.134	1	35.86
2975	N	ASP	A	492	67.905	6.983	1.734	1	38.52
2976	CA	ASP	A	492	68.406	8.322	1.447	1	38.71
2977	C	ASP	A	492	69.915	8.156	1.441	1	42.71
2978	O	ASP	A	492	70.489	7.659	2.414	1	40.77
2979	CB	ASP	A	492	67.987	9.291	2.556	1	38.07
2980	CG	ASP	A	492	68.128	10.74	2.159	1	38.06
2981	OD1	ASP	A	492	69.138	11.101	1.53	1	39.16
2982	OD2	ASP	A	492	67.228	11.533	2.493	1	38.11
2983	N	ASP	A	493	70.549	8.544	0.337	1	45.51
2984	CA	ASP	A	493	71.995	8.415	0.19	1	46.6
2985	C	ASP	A	493	72.779	9.615	0.679	1	47.42
2986	O	ASP	A	493	73.979	9.515	0.939	1	49.19
2987	CB	ASP	A	493	72.351	8.116	-1.263	1	51.81
2988	CG	ASP	A	493	71.771	6.801	-1.733	1	58.84
2989	OD1	ASP	A	493	72.413	5.758	-1.488	1	63.62
2990	OD2	ASP	A	493	70.664	6.803	-2.32	1	62.21
2991	N	GLY	A	494	72.101	10.747	0.817	1	46.5
2992	CA	GLY	A	494	72.779	11.938	1.276	1	46.23
2993	C	GLY	A	494	73.521	12.603	0.137	1	47.76
2994	O	GLY	A	494	73.648	12.051	-0.948	1	51.55
2995	N	ILE	A	495	73.99	13.811	0.377	1	48.63
2996	CA	ILE	A	495	74.706	14.563	-0.625	1	50.48
2997	C	ILE	A	495	75.822	15.218	0.148	1	53.46
2998	O	ILE	A	495	75.618	15.624	1.285	1	54.12
2999	CB	ILE	A	495	73.792	15.633	-1.231	1	50.41
3000	CG1	ILE	A	495	74.526	16.401	-2.325	1	50.69
3001	CG2	ILE	A	495	73.275	16.552	-0.15	1	51.34
3002	CD1	ILE	A	495	74.874	15.54	-3.508	1	51.74
3003	N	GLN	A	496	77.004	15.285	-0.44	1	58.5
3004	CA	GLN	A	496	78.139	15.872	0.249	1	66.11
3005	C	GLN	A	496	77.925	17.36	0.579	1	69.52
3006	O	GLN	A	496	77.762	18.155	-0.377	1	71.91
3007	CB	GLN	A	496	79.414	15.665	-0.572	1	68.64
3008	CG	GLN	A	496	80.66	15.481	0.281	1	75.12
3009	CD	GLN	A	496	80.53	14.299	1.225	1	79.97
3010	OE1	GLN	A	496	80.47	14.463	2.45	1	83.35
3011	NE2	GLN	A	496	80.459	13.097	0.66	1	83.88
3012	OT	GLN	A	496	77.897	17.709	1.791	1	70.21
1	N	LYS	A	512	33.062	26.421	16.762	1	43.87
2	CA	LYS	A	512	33.483	24.999	16.78	1	41.28
3	C	LYS	A	512	34.977	24.911	16.569	1	40.21
4	O	LYS	A	512	35.629	25.924	16.322	1	39.66

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
5	CB	LYS	A	512	32.752	24.201	15.706	1	40.1
6	CG	LYS	A	512	31.301	23.971	16.038	1	42.72
7	CD	LYS	A	512	30.649	22.98	15.103	1	46.47
8	CE	LYS	A	512	30.593	23.509	13.683	1	48.27
9	NZ	LYS	A	512	29.748	22.631	12.831	1	50.18
10	N	ILE	A	513	35.508	23.705	16.721	1	40.4
11	CA	ILE	A	513	36.929	23.446	16.542	1	41.79
12	C	ILE	A	513	36.984	22.227	15.619	1	39.91
13	O	ILE	A	513	36.083	21.376	15.644	1	37.85
14	CB	ILE	A	513	37.651	23.17	17.928	1	45.34
15	CG1	ILE	A	513	38.939	23.992	18.039	1	51.99
16	CG2	ILE	A	513	38.054	21.712	18.077	1	44.31
17	CD1	ILE	A	513	38.729	25.501	17.999	1	57.62
18	N	PRO	A	514	37.977	22.184	14.716	1	37.91
19	CA	PRO	A	514	38.107	21.053	13.794	1	35.49
20	C	PRO	A	514	38.424	19.802	14.597	1	33.33
21	O	PRO	A	514	39.28	19.84	15.487	1	36.6
22	CB	PRO	A	514	39.314	21.451	12.934	1	33.51
23	CG	PRO	A	514	39.293	22.937	12.971	1	33.71
24	CD	PRO	A	514	38.98	23.221	14.416	1	37.79
25	N	VAL	A	515	37.771	18.693	14.276	1	29.98
26	CA	VAL	A	515	38.029	17.442	14.976	1	29.29
27	C	VAL	A	515	39.44	16.903	14.732	1	32.25
28	O	VAL	A	515	39.862	15.965	15.408	1	36.93
29	CB	VAL	A	515	37	16.345	14.607	1	29.6
30	CG1	VAL	A	515	35.588	16.853	14.806	1	28.42
31	CG2	VAL	A	515	37.198	15.864	13.184	1	29.47
32	N	GLU	A	516	40.168	17.485	13.775	1	30.92
33	CA	GLU	A	516	41.531	17.046	13.453	1	27.47
34	C	GLU	A	516	42.574	18.009	13.991	1	23.22
35	O	GLU	A	516	43.778	17.774	13.888	1	25.1
36	CB	GLU	A	516	41.712	16.904	11.936	1	33.36
37	CG	GLU	A	516	40.813	15.864	11.264	1	33.69
38	CD	GLU	A	516	41.207	14.415	11.56	1	40.34
39	OE1	GLU	A	516	42.16	14.18	12.341	1	44.54
40	OE2	GLU	A	516	40.561	13.498	10.997	1	41.96
41	N	ALA	A	517	42.101	19.101	14.568	1	20.8
42	CA	ALA	A	517	42.984	20.1	15.137	1	21.05
43	C	ALA	A	517	43.732	19.605	16.384	1	25.13
44	O	ALA	A	517	43.315	18.651	17.045	1	27.01
45	CB	ALA	A	517	42.183	21.343	15.471	1	19.47
46	N	ASP	A	518	44.865	20.246	16.658	1	25.98
47	CA	ASP	A	518	45.703	19.974	17.825	1	27.68
48	C	ASP	A	518	46.532	18.702	17.926	1	28.26
49	O	ASP	A	518	47.039	18.39	19.002	1	26.74
50	CB	ASP	A	518	44.912	20.22	19.11	1	26.26
51	CG	ASP	A	518	44.278	21.598	19.129	1	25.88
52	OD1	ASP	A	518	45.016	22.601	19.015	1	25.39
53	OD2	ASP	A	518	43.033	21.688	19.198	1	24.92
54	N	PHE	A	519	46.719	18.006	16.806	1	27.09
55	CA	PHE	A	519	47.559	16.81	16.773	1	18.76
56	C	PHE	A	519	48.946	17.23	16.301	1	21.09

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
57	O	PHE	A	519	49.127	18.332	15.773	1	20.61
58	CB	PHE	A	519	47.052	15.814	15.756	1	15.19
59	CG	PHE	A	519	45.902	15.003	16.216	1	15.52
60	CD1	PHE	A	519	44.622	15.549	16.258	1	17.78
61	CD2	PHE	A	519	46.085	13.663	16.559	1	17.87
62	CE1	PHE	A	519	43.527	14.763	16.633	1	15.84
63	CE2	PHE	A	519	45.003	12.866	16.938	1	15.65
64	CZ	PHE	A	519	43.724	13.414	16.972	1	17.91
65	N	LEU	A	520	49.916	16.343	16.495	1	21.47
66	CA	LEU	A	520	51.282	16.546	16.047	1	19.63
67	C	LEU	A	520	51.913	15.177	15.976	1	23.57
68	O	LEU	A	520	51.887	14.432	16.947	1	27.23
69	CB	LEU	A	520	52.088	17.438	16.978	1	20.86
70	CG	LEU	A	520	53.577	17.493	16.595	1	22.76
71	CD1	LEU	A	520	54.118	18.901	16.651	1	24
72	CD2	LEU	A	520	54.37	16.603	17.522	1	27.43
73	N	PHE	A	521	52.436	14.824	14.808	1	23.72
74	CA	PHE	A	521	53.083	13.546	14.628	1	20.75
75	C	PHE	A	521	54.501	13.859	14.315	1	24.5
76	O	PHE	A	521	54.782	14.735	13.508	1	29.3
77	CB	PHE	A	521	52.473	12.786	13.476	1	18.58
78	CG	PHE	A	521	51.009	12.626	13.592	1	21.26
79	CD1	PHE	A	521	50.159	13.589	13.091	1	24.71
80	CD2	PHE	A	521	50.474	11.551	14.264	1	24.81
81	CE1	PHE	A	521	48.791	13.489	13.253	1	26.46
82	CE2	PHE	A	521	49.108	11.444	14.432	1	26.77
83	CZ	PHE	A	521	48.267	12.422	13.928	1	25.98
84	N	ALA	A	522	55.403	13.189	15.009	1	26.47
85	CA	ALA	A	522	56.811	13.379	14.797	1	25.21
86	C	ALA	A	522	57.297	11.996	14.399	1	29.07
87	O	ALA	A	522	57.443	11.108	15.246	1	32.45
88	CB	ALA	A	522	57.467	13.844	16.08	1	20.67
89	N	TYR	A	523	57.389	11.77	13.091	1	26.52
90	CA	TYR	A	523	57.852	10.497	12.575	1	19.33
91	C	TYR	A	523	59.366	10.553	12.513	1	19.01
92	O	TYR	A	523	59.948	11.625	12.364	1	20.74
93	CB	TYR	A	523	57.301	10.247	11.174	1	21.67
94	CG	TYR	A	523	55.808	10.05	11.077	1	14.57
95	CD1	TYR	A	523	54.959	11.137	10.924	1	13.64
96	CD2	TYR	A	523	55.252	8.759	11.046	1	15.5
97	CE1	TYR	A	523	53.58	10.957	10.729	1	11.98
98	CE2	TYR	A	523	53.857	8.566	10.852	1	14.7
99	CZ	TYR	A	523	53.038	9.674	10.693	1	12.88
100	OH	TYR	A	523	51.682	9.525	10.488	1	22.38
101	N	SER	A	524	60.006	9.4	12.603	1	19.64
102	CA	SER	A	524	61.456	9.341	12.551	1	23.13
103	C	SER	A	524	62.012	9.566	11.145	1	28.32
104	O	SER	A	524	63.193	9.898	10.974	1	28.63
105	CB	SER	A	524	61.904	7.974	12.998	1	21.35
106	OG	SER	A	524	61.21	6.988	12.263	1	25.89
107	N	THR	A	525	61.172	9.348	10.14	1	27.8
108	CA	THR	A	525	61.608	9.48	8.772	1	27.77

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
109	C	THR	A	525	60.468	9.996	7.888	1	29.73
110	O	THR	A	525	59.305	10.051	8.322	1	30.33
111	CB	THR	A	525	62.107	8.113	8.277	1	25.95
112	OG1	THR	A	525	62.895	8.277	7.09	1	30.29
113	CG2	THR	A	525	60.931	7.183	8.018	1	24.18
114	N	VAL	A	526	60.825	10.438	6.681	1	26.85
115	CA	VAL	A	526	59.86	10.948	5.706	1	22.01
116	C	VAL	A	526	59.149	9.766	5.076	1	17.81
117	O	VAL	A	526	59.688	8.652	5.058	1	21.48
118	CB	VAL	A	526	60.559	11.759	4.614	1	24.13
119	CG1	VAL	A	526	61.022	13.072	5.182	1	24.57
120	CG2	VAL	A	526	61.752	11	4.076	1	22.17
121	N	PRO	A	527	57.931	9.985	4.556	1	19.11
122	CA	PRO	A	527	57.118	8.926	3.914	1	22.29
123	C	PRO	A	527	57.871	8.209	2.787	1	23.9
124	O	PRO	A	527	58.658	8.824	2.065	1	26.56
125	CB	PRO	A	527	55.92	9.691	3.353	1	19.16
126	CG	PRO	A	527	55.847	10.939	4.229	1	17.85
127	CD	PRO	A	527	57.288	11.307	4.432	1	15.26
128	N	GLY	A	528	57.665	6.904	2.677	1	24.99
129	CA	GLY	A	528	58.336	6.126	1.653	1	23.34
130	C	GLY	A	528	59.706	5.593	2.029	1	26.05
131	O	GLY	A	528	60.145	4.593	1.447	1	25.98
132	N	TYR	A	529	60.362	6.203	3.018	1	26.11
133	CA	TYR	A	529	61.7	5.767	3.434	1	26.75
134	C	TYR	A	529	61.811	4.79	4.619	1	31.13
135	O	TYR	A	529	60.857	4.589	5.382	1	34.54
136	CB	TYR	A	529	62.552	6.988	3.754	1	24.74
137	CG	TYR	A	529	62.927	7.793	2.547	1	32.82
138	CD1	TYR	A	529	61.975	8.563	1.87	1	35.95
139	CD2	TYR	A	529	64.224	7.757	2.049	1	34.27
140	CE1	TYR	A	529	62.314	9.28	0.713	1	36.11
141	CE2	TYR	A	529	64.574	8.465	0.897	1	37.85
142	CZ	TYR	A	529	63.615	9.223	0.233	1	37.93
143	OH	TYR	A	529	63.973	9.91	-0.905	1	41.43
144	N	TYR	A	530	62.983	4.169	4.749	1	30.16
145	CA	TYR	A	530	63.286	3.287	5.876	1	30.57
146	C	TYR	A	530	63.622	4.212	7.052	1	29.83
147	O	TYR	A	530	63.777	5.422	6.874	1	29.14
148	CB	TYR	A	530	64.551	2.466	5.617	1	28.97
149	CG	TYR	A	530	64.34	1.204	4.836	1	33.45
150	CD1	TYR	A	530	63.384	0.277	5.233	1	30.59
151	CD2	TYR	A	530	65.125	0.919	3.709	1	34.72
152	CE1	TYR	A	530	63.212	-0.91	4.534	1	36.41
153	CE2	TYR	A	530	64.961	-0.267	2.995	1	33.96
154	CZ	TYR	A	530	64.003	-1.178	3.414	1	36.99
155	OH	TYR	A	530	63.828	-2.36	2.733	1	39.7
156	N	SER	A	531	63.72	3.633	8.249	1	29.49
157	CA	SER	A	531	64.093	4.377	9.443	1	25.55
158	C	SER	A	531	65.21	3.53	9.993	1	25.79
159	O	SER	A	531	65.134	2.292	9.973	1	26.82
160	CB	SER	A	531	62.946	4.468	10.444	1	29.12

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
161	OG	SER	A	531	63.219	5.487	11.387	1	31.11
162	N	TRP	A	532	66.276	4.184	10.413	1	26.72
163	CA	TRP	A	532	67.438	3.482	10.916	1	31.44
164	C	TRP	A	532	67.511	3.251	12.428	1	31.68
165	O	TRP	A	532	67.052	4.072	13.229	1	28.32
166	CB	TRP	A	532	68.705	4.163	10.404	1	33.12
167	CG	TRP	A	532	68.934	3.923	8.952	1	34.28
168	CD1	TRP	A	532	68.518	4.703	7.917	1	31.72
169	CD2	TRP	A	532	69.619	2.812	8.372	1	33.78
170	NE1	TRP	A	532	68.895	4.146	6.729	1	35.32
171	CE2	TRP	A	532	69.574	2.978	6.978	1	35.16
172	CE3	TRP	A	532	70.27	1.687	8.899	1	34.98
173	CZ2	TRP	A	532	70.154	2.069	6.095	1	35.74
174	CZ3	TRP	A	532	70.849	0.782	8.032	1	32.89
175	CH2	TRP	A	532	70.787	0.976	6.641	1	37.53
176	N	ARG	A	533	68.189	2.167	12.789	1	31.44
177	CA	ARG	A	533	68.332	1.767	14.163	1	33.79
178	C	ARG	A	533	69.631	1.039	14.455	1	36.95
179	O	ARG	A	533	69.97	0.048	13.806	1	36.62
180	CB	ARG	A	533	67.143	0.892	14.548	1	33.6
181	CG	ARG	A	533	67.328	0.064	15.808	1	33.3
182	CD	ARG	A	533	66.021	-0.577	16.196	1	30.9
183	NE	ARG	A	533	65.392	-1.267	15.069	1	33.34
184	CZ	ARG	A	533	65.88	-2.355	14.471	1	31.64
185	NH1	ARG	A	533	67.02	-2.901	14.878	1	27.14
186	NH2	ARG	A	533	65.221	-2.902	13.457	1	31.62
187	N	SER	A	534	70.356	1.56	15.44	1	42.12
188	CA	SER	A	534	71.609	0.982	15.904	1	45.98
189	C	SER	A	534	71.234	0.009	17.018	1	48.53
190	O	SER	A	534	70.679	0.416	18.037	1	52.15
191	CB	SER	A	534	72.512	2.094	16.451	1	48.67
192	OG	SER	A	534	73.375	1.637	17.483	1	52.46
193	N	PRO	A	535	71.509	-1.292	16.832	1	50.47
194	CA	PRO	A	535	71.19	-2.32	17.836	1	51.21
195	C	PRO	A	535	71.818	-2.092	19.228	1	49.15
196	O	PRO	A	535	71.285	-2.54	20.246	1	48
197	CB	PRO	A	535	71.726	-3.602	17.186	1	49.52
198	CG	PRO	A	535	71.561	-3.335	15.729	1	49.97
199	CD	PRO	A	535	72.053	-1.91	15.611	1	50.64
200	N	GLY	A	536	72.941	-1.385	19.261	1	47.39
201	CA	GLY	A	536	73.62	-1.136	20.515	1	48
202	C	GLY	A	536	73.374	0.211	21.157	1	48.29
203	O	GLY	A	536	73.695	0.392	22.318	1	52.82
204	N	ARG	A	537	72.83	1.165	20.418	1	47.17
205	CA	ARG	A	537	72.583	2.48	20.983	1	44.24
206	C	ARG	A	537	71.123	2.879	20.902	1	41.77
207	O	ARG	A	537	70.668	3.761	21.632	1	40.97
208	CB	ARG	A	537	73.439	3.528	20.284	1	49.31
209	CG	ARG	A	537	74.922	3.369	20.506	1	58.85
210	CD	ARG	A	537	75.633	4.681	20.234	1	72.16
211	NE	ARG	A	537	77.09	4.563	20.324	1	84.4
212	CZ	ARG	A	537	77.907	4.421	19.277	1	90.84

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
213	NH1	ARG	A	537	77.423	4.372	18.037	1	93.69
214	NH2	ARG	A	537	79.224	4.365	19.465	1	92.89
215	N	GLY	A	538	70.394	2.221	20.008	1	41.41
216	CA	GLY	A	538	68.985	2.512	19.812	1	40.56
217	C	GLY	A	538	68.729	3.233	18.496	1	38.88
218	O	GLY	A	538	69.668	3.545	17.747	1	40.24
219	N	SER	A	539	67.462	3.494	18.197	1	33.21
220	CA	SER	A	539	67.125	4.176	16.966	1	30.88
221	C	SER	A	539	67.726	5.575	16.967	1	32.93
222	O	SER	A	539	67.924	6.169	18.029	1	37.6
223	CB	SER	A	539	65.616	4.249	16.797	1	28.56
224	OG	SER	A	539	65.039	5.073	17.782	1	33.31
225	N	TRP	A	540	67.976	6.119	15.781	1	31.87
226	CA	TRP	A	540	68.559	7.435	15.671	1	30.54
227	C	TRP	A	540	67.593	8.487	16.182	1	32.33
228	O	TRP	A	540	67.961	9.338	16.984	1	36.09
229	CB	TRP	A	540	68.925	7.739	14.227	1	33.39
230	CG	TRP	A	540	69.962	6.821	13.621	1	35.51
231	CD1	TRP	A	540	70.659	5.819	14.243	1	33.62
232	CD2	TRP	A	540	70.413	6.839	12.261	1	33.83
233	NE1	TRP	A	540	71.51	5.214	13.355	1	31.65
234	CE2	TRP	A	540	71.383	5.82	12.133	1	35.9
235	CE3	TRP	A	540	70.089	7.614	11.14	1	31.73
236	CZ2	TRP	A	540	72.033	5.558	10.924	1	35.61
237	CZ3	TRP	A	540	70.732	7.355	9.939	1	31.31
238	CH2	TRP	A	540	71.693	6.335	9.842	1	35.49
239	N	PHE	A	541	66.347	8.413	15.739	1	31.41
240	CA	PHE	A	541	65.32	9.376	16.152	1	29.6
241	C	PHE	A	541	65.228	9.448	17.677	1	30.78
242	O	PHE	A	541	65.245	10.533	18.255	1	29.89
243	CB	PHE	A	541	63.966	8.962	15.569	1	25.62
244	CG	PHE	A	541	62.858	9.954	15.806	1	17.2
245	CD1	PHE	A	541	63.031	11.294	15.513	1	15.05
246	CD2	PHE	A	541	61.62	9.526	16.282	1	15.34
247	CE1	PHE	A	541	61.983	12.199	15.685	1	18.22
248	CE2	PHE	A	541	60.576	10.415	16.455	1	14.69
249	CZ	PHE	A	541	60.754	11.757	16.155	1	14.66
250	N	VAL	A	542	65.14	8.284	18.315	1	31.68
251	CA	VAL	A	542	65.044	8.21	19.76	1	30.5
252	C	VAL	A	542	66.305	8.725	20.434	1	32.23
253	O	VAL	A	542	66.22	9.56	21.341	1	33.29
254	CB	VAL	A	542	64.705	6.811	20.227	1	30.58
255	CG1	VAL	A	542	64.736	6.759	21.747	1	30.62
256	CG2	VAL	A	542	63.309	6.429	19.704	1	24.84
257	N	GLN	A	543	67.466	8.278	19.963	1	29.5
258	CA	GLN	A	543	68.726	8.762	20.515	1	29.48
259	C	GLN	A	543	68.716	10.293	20.517	1	31.4
260	O	GLN	A	543	68.878	10.916	21.554	1	37.28
261	CB	GLN	A	543	69.929	8.291	19.679	1	30.77
262	CG	GLN	A	543	70.324	6.833	19.817	1	28.07
263	CD	GLN	A	543	71.626	6.502	19.078	1	28.74
264	OE1	GLN	A	543	72.64	7.193	19.222	1	26.15

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Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
265	NE2	GLN	A	543	71.609	5.419	18.312	1	25.79
266	N	ALA	A	544	68.472	10.896	19.362	1	33.64
267	CA	ALA	A	544	68.471	12.349	19.25	1	31.92
268	C	ALA	A	544	67.346	13.042	20.012	1	31.26
269	O	ALA	A	544	67.568	14.07	20.656	1	32.72
270	CB	ALA	A	544	68.454	12.762	17.789	1	32.48
271	N	LEU	A	545	66.14	12.493	19.934	1	31.57
272	CA	LEU	A	545	64.989	13.077	20.624	1	31.2
273	C	LEU	A	545	65.264	13.19	22.121	1	33.55
274	O	LEU	A	545	65.23	14.282	22.674	1	33.76
275	CB	LEU	A	545	63.737	12.232	20.39	1	26.73
276	CG	LEU	A	545	62.506	12.631	21.197	1	22.51
277	CD1	LEU	A	545	61.991	13.996	20.757	1	21.56
278	CD2	LEU	A	545	61.458	11.576	21.035	1	14.36
279	N	CYS	A	546	65.558	12.066	22.765	1	34.15
280	CA	CYS	A	546	65.851	12.069	24.191	1	36.46
281	C	CYS	A	546	66.974	13.044	24.522	1	36.95
282	O	CYS	A	546	66.849	13.851	25.432	1	35.9
283	CB	CYS	A	546	66.212	10.665	24.668	1	35.4
284	SG	CYS	A	546	64.772	9.59	24.808	1	39.08
285	N	SER	A	547	68.054	12.991	23.758	1	37.71
286	CA	SER	A	547	69.188	13.882	23.96	1	40.76
287	C	SER	A	547	68.78	15.366	24.004	1	41.95
288	O	SER	A	547	69.189	16.097	24.916	1	46.35
289	CB	SER	A	547	70.22	13.66	22.852	1	43.91
290	OG	SER	A	547	71.284	14.593	22.941	1	51.71
291	N	ILE	A	548	68.01	15.82	23.014	1	36.63
292	CA	ILE	A	548	67.568	17.211	22.981	1	32.36
293	C	ILE	A	548	66.606	17.471	24.136	1	34.42
294	O	ILE	A	548	66.726	18.482	24.82	1	35.88
295	CB	ILE	A	548	66.85	17.576	21.659	1	33.44
296	CG1	ILE	A	548	67.745	17.276	20.44	1	31.09
297	CG2	ILE	A	548	66.408	19.036	21.687	1	25.81
298	CD1	ILE	A	548	68.964	18.14	20.326	1	33.57
299	N	LEU	A	549	65.637	16.583	24.346	1	35.13
300	CA	LEU	A	549	64.685	16.751	25.447	1	38.89
301	C	LEU	A	549	65.418	16.842	26.787	1	44.15
302	O	LEU	A	549	65.067	17.663	27.625	1	46.43
303	CB	LEU	A	549	63.671	15.607	25.491	1	35.16
304	CG	LEU	A	549	62.484	15.662	24.52	1	32.57
305	CD1	LEU	A	549	61.616	14.423	24.718	1	26.29
306	CD2	LEU	A	549	61.658	16.929	24.737	1	27.57
307	N	GLU	A	550	66.466	16.037	26.959	1	48.95
308	CA	GLU	A	550	67.267	16.04	28.185	1	52.95
309	C	GLU	A	550	67.833	17.433	28.448	1	54.01
310	O	GLU	A	550	67.819	17.933	29.575	1	57.8
311	CB	GLU	A	550	68.455	15.079	28.073	1	54.26
312	CG	GLU	A	550	68.159	13.606	28.331	1	66.1
313	CD	GLU	A	550	69.424	12.738	28.279	1	71.53
314	OE1	GLU	A	550	70.267	12.851	29.199	1	75.39
315	OE2	GLU	A	550	69.582	11.947	27.318	1	75.63
316	N	GLU	A	551	68.335	18.055	27.393	1	52.5

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
317	CA	GLU	A	551	68.944	19.356	27.511	1	47.16
318	C	GLU	A	551	67.987	20.525	27.363	1	43.16
319	O	GLU	A	551	68.237	21.588	27.929	1	43.29
320	CB	GLU	A	551	70.071	19.465	26.488	1	54.47
321	CG	GLU	A	551	71.09	20.554	26.777	1	70.56
322	CD	GLU	A	551	71.796	20.372	28.124	1	80.1
323	OE1	GLU	A	551	72.072	19.208	28.518	1	85.38
324	OE2	GLU	A	551	72.08	21.4	28.787	1	83.64
325	N	HIS	A	552	66.872	20.335	26.655	1	38.01
326	CA	HIS	A	552	65.943	21.446	26.412	1	31.98
327	C	HIS	A	552	64.466	21.169	26.491	1	30.42
328	O	HIS	A	552	63.667	22.008	26.077	1	29.4
329	CB	HIS	A	552	66.203	22.062	25.046	1	31.13
330	CG	HIS	A	552	67.57	22.641	24.889	1	33.97
331	ND1	HIS	A	552	67.9	23.906	25.335	1	34.78
332	CD2	HIS	A	552	68.694	22.135	24.325	1	33.3
333	CE1	HIS	A	552	69.167	24.154	25.052	1	36.67
334	NE2	HIS	A	552	69.671	23.095	24.439	1	38.75
335	N	GLY	A	553	64.095	20.034	27.066	1	31.89
336	CA	GLY	A	553	62.692	19.669	27.166	1	34.23
337	C	GLY	A	553	61.81	20.639	27.922	1	38.07
338	O	GLY	A	553	60.597	20.67	27.73	1	39.4
339	N	LYS	A	554	62.41	21.433	28.794	1	42.66
340	CA	LYS	A	554	61.64	22.384	29.572	1	47.85
341	C	LYS	A	554	61.885	23.85	29.231	1	48.86
342	O	LYS	A	554	61.255	24.728	29.817	1	47.52
343	CB	LYS	A	554	61.854	22.142	31.066	1	52.14
344	CG	LYS	A	554	60.633	21.538	31.767	1	58.35
345	CD	LYS	A	554	60.844	20.084	32.163	1	60.45
346	CE	LYS	A	554	61.95	19.947	33.199	1	60.44
347	NZ	LYS	A	554	62.043	18.555	33.728	1	63.83
348	N	ASP	A	555	62.777	24.123	28.278	1	49.68
349	CA	ASP	A	555	63.051	25.504	27.904	1	46.61
350	C	ASP	A	555	62.835	25.859	26.443	1	42.46
351	O	ASP	A	555	63.036	27.005	26.062	1	45.3
352	CB	ASP	A	555	64.449	25.935	28.354	1	52.69
353	CG	ASP	A	555	65.548	25.312	27.535	1	58.61
354	OD1	ASP	A	555	65.941	25.919	26.514	1	63.18
355	OD2	ASP	A	555	66.035	24.231	27.929	1	65.46
356	N	LEU	A	556	62.483	24.887	25.61	1	40.29
357	CA	LEU	A	556	62.228	25.168	24.192	1	35.92
358	C	LEU	A	556	60.792	24.786	23.797	1	35.45
359	O	LEU	A	556	60.172	23.919	24.438	1	34.29
360	CB	LEU	A	556	63.236	24.45	23.291	1	32.29
361	CG	LEU	A	556	64.694	24.913	23.328	1	30.37
362	CD1	LEU	A	556	65.488	24.149	22.295	1	28.77
363	CD2	LEU	A	556	64.798	26.401	23.061	1	28.88
364	N	GLU	A	557	60.24	25.499	22.808	1	33.28
365	CA	GLU	A	557	58.891	25.212	22.315	1	29.54
366	C	GLU	A	557	59.055	23.906	21.525	1	28.61
367	O	GLU	A	557	60.145	23.631	20.996	1	26.72
368	CB	GLU	A	557	58.393	26.369	21.441	1	29.23

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Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
369	CG	GLU	A	557	56.883	26.35	21.152	1	29.4
370	CD	GLU	A	557	56.526	25.389	20.036	1	31.29
371	OE1	GLU	A	557	57.387	25.195	19.164	1	37.04
372	OE2	GLU	A	557	55.416	24.819	20.017	1	24.73
373	N	ILE	A	558	58	23.097	21.467	1	27.66
374	CA	ILE	A	558	58.054	21.794	20.787	1	31.95
375	C	ILE	A	558	58.664	21.772	19.367	1	31.85
376	O	ILE	A	558	59.467	20.885	19.043	1	32.8
377	CB	ILE	A	558	56.674	21.066	20.834	1	33.07
378	CG1	ILE	A	558	56.841	19.588	20.478	1	32.65
379	CG2	ILE	A	558	55.658	21.742	19.909	1	35.48
380	CD1	ILE	A	558	57.869	18.873	21.327	1	29.48
381	N	MET	A	559	58.306	22.745	18.533	1	31.38
382	CA	MET	A	559	58.864	22.826	17.182	1	31.25
383	C	MET	A	559	60.373	23.026	17.216	1	31.52
384	O	MET	A	559	61.084	22.407	16.428	1	35.59
385	CB	MET	A	559	58.202	23.929	16.347	1	29.01
386	CG	MET	A	559	56.736	23.67	16.002	1	30.75
387	SD	MET	A	559	56.451	21.992	15.348	1	43.81
388	CE	MET	A	559	57.801	21.888	14.038	1	37.68
389	N	GLN	A	560	60.865	23.846	18.151	1	31.52
390	CA	GLN	A	560	62.31	24.09	18.273	1	30.07
391	C	GLN	A	560	63.032	22.816	18.677	1	30.26
392	O	GLN	A	560	64.173	22.578	18.284	1	32.36
393	CB	GLN	A	560	62.613	25.133	19.335	1	30.53
394	CG	GLN	A	560	61.931	26.453	19.142	1	33.5
395	CD	GLN	A	560	62.271	27.43	20.251	1	31.53
396	OE1	GLN	A	560	61.524	27.566	21.218	1	35.91
397	NE2	GLN	A	560	63.408	28.088	20.132	1	30.29
398	N	ILE	A	561	62.383	22.022	19.518	1	29.95
399	CA	ILE	A	561	62.984	20.783	19.963	1	29.98
400	C	ILE	A	561	63.07	19.857	18.753	1	29.65
401	O	ILE	A	561	64.163	19.411	18.376	1	30.65
402	CB	ILE	A	561	62.166	20.157	21.147	1	30.34
403	CG1	ILE	A	561	62.349	21.015	22.407	1	29.58
404	CG2	ILE	A	561	62.598	18.707	21.429	1	27.23
405	CD1	ILE	A	561	61.33	20.729	23.5	1	30.9
406	N	LEU	A	562	61.936	19.661	18.085	1	27.96
407	CA	LEU	A	562	61.874	18.782	16.916	1	27.77
408	C	LEU	A	562	62.755	19.226	15.73	1	27.91
409	O	LEU	A	562	63.324	18.394	15.014	1	27.06
410	CB	LEU	A	562	60.416	18.584	16.504	1	25.24
411	CG	LEU	A	562	59.627	17.795	17.552	1	19.16
412	CD1	LEU	A	562	58.171	17.734	17.18	1	17.12
413	CD2	LEU	A	562	60.211	16.405	17.677	1	19.13
414	N	THR	A	563	62.905	20.529	15.542	1	25.55
415	CA	THR	A	563	63.754	21.003	14.474	1	25.2
416	C	THR	A	563	65.177	20.615	14.828	1	29.57
417	O	THR	A	563	65.92	20.125	13.968	1	33.44
418	CB	THR	A	563	63.661	22.508	14.303	1	22.79
419	OG1	THR	A	563	62.349	22.863	13.85	1	23.56
420	CG2	THR	A	563	64.666	22.977	13.301	1	21.99

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Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
421	N	ARG	A	564	65.537	20.777	16.105	1	31.88
422	CA	ARG	A	564	66.877	20.43	16.588	1	29.72
423	C	ARG	A	564	67.111	18.929	16.469	1	28.38
424	O	ARG	A	564	68.225	18.486	16.209	1	30.65
425	CB	ARG	A	564	67.101	20.92	18.026	1	34.04
426	CG	ARG	A	564	67.19	22.443	18.151	1	35.75
427	CD	ARG	A	564	67.582	22.903	19.55	1	38.52
428	NE	ARG	A	564	67.519	24.362	19.705	1	39.94
429	CZ	ARG	A	564	68.374	25.085	20.425	1	37.97
430	NH1	ARG	A	564	69.373	24.492	21.06	1	38.99
431	NH2	ARG	A	564	68.208	26.396	20.542	1	36.09
432	N	VAL	A	565	66.045	18.154	16.633	1	26.78
433	CA	VAL	A	565	66.124	16.706	16.484	1	25.41
434	C	VAL	A	565	66.336	16.402	14.988	1	27.12
435	O	VAL	A	565	67.119	15.511	14.645	1	27.79
436	CB	VAL	A	565	64.831	16.037	16.974	1	23.08
437	CG1	VAL	A	565	64.855	14.545	16.72	1	23.01
438	CG2	VAL	A	565	64.657	16.311	18.431	1	26.9
439	N	ASN	A	566	65.649	17.141	14.108	1	27.09
440	CA	ASN	A	566	65.794	16.97	12.655	1	27.15
441	C	ASN	A	566	67.25	17.177	12.257	1	29.55
442	O	ASN	A	566	67.841	16.36	11.534	1	31.03
443	CB	ASN	A	566	64.953	17.991	11.883	1	24.28
444	CG	ASN	A	566	63.522	17.572	11.728	1	21.1
445	OD1	ASN	A	566	63.15	16.46	12.086	1	22.92
446	ND2	ASN	A	566	62.701	18.463	11.194	1	20.2
447	N	ASP	A	567	67.825	18.273	12.747	1	31.43
448	CA	ASP	A	567	69.21	18.622	12.467	1	33.99
449	C	ASP	A	567	70.229	17.641	13.045	1	35.27
450	O	ASP	A	567	71.344	17.511	12.533	1	37.84
451	CB	ASP	A	567	69.509	20.027	12.983	1	37.26
452	CG	ASP	A	567	70.84	20.556	12.481	1	44.36
453	OD1	ASP	A	567	71.289	20.109	11.406	1	47.95
454	OD2	ASP	A	567	71.437	21.425	13.146	1	48.92
455	N	ARG	A	568	69.862	16.965	14.126	1	37.3
456	CA	ARG	A	568	70.755	16.011	14.765	1	34.39
457	C	ARG	A	568	70.807	14.692	14.024	1	29.6
458	O	ARG	A	568	71.877	14.147	13.788	1	27.08
459	CB	ARG	A	568	70.32	15.772	16.206	1	42.13
460	CG	ARG	A	568	71.451	15.93	17.183	1	51.05
461	CD	ARG	A	568	71.56	14.733	18.084	1	61.38
462	NE	ARG	A	568	72.682	14.891	18.998	1	73.56
463	CZ	ARG	A	568	72.726	15.781	19.987	1	78.95
464	NH1	ARG	A	568	71.7	16.6	20.206	1	78.24
465	NH2	ARG	A	568	73.811	15.864	20.753	1	83.98
466	N	VAL	A	569	69.635	14.16	13.709	1	29.38
467	CA	VAL	A	569	69.528	12.904	12.991	1	30.3
468	C	VAL	A	569	70.186	13.074	11.631	1	33.04
469	O	VAL	A	569	71.009	12.261	11.231	1	32.78
470	CB	VAL	A	569	68.049	12.513	12.795	1	33.38
471	CG1	VAL	A	569	67.923	11.162	12.083	1	33.06
472	CG2	VAL	A	569	67.359	12.47	14.131	1	33.75

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
473	N	ALA	A	570	69.866	14.174	10.957	1	36.41
474	CA	ALA	A	570	70.416	14.456	9.64	1	38.44
475	C	ALA	A	570	71.926	14.628	9.637	1	41.11
476	O	ALA	A	570	72.63	13.969	8.872	1	43.43
477	CB	ALA	A	570	69.749	15.693	9.046	1	39.71
478	N	ARG	A	571	72.421	15.494	10.514	1	43.89
479	CA	ARG	A	571	73.845	15.785	10.584	1	44.41
480	C	ARG	A	571	74.721	14.857	11.374	1	45.18
481	O	ARG	A	571	75.935	14.981	11.296	1	50.74
482	CB	ARG	A	571	74.086	17.184	11.135	1	43.37
483	CG	ARG	A	571	73.654	18.284	10.232	1	51.92
484	CD	ARG	A	571	74.184	19.613	10.715	1	58.79
485	NE	ARG	A	571	73.628	20.706	9.922	1	65.67
486	CZ	ARG	A	571	74.078	21.065	8.726	1	67.01
487	NH1	ARG	A	571	75.107	20.428	8.179	1	69.89
488	NH2	ARG	A	571	73.478	22.043	8.065	1	68.71
489	N	HIS	A	572	74.163	13.943	12.151	1	45.88
490	CA	HIS	A	572	75.049	13.116	12.957	1	45.51
491	C	HIS	A	572	75.027	11.624	12.8	1	44.25
492	O	HIS	A	572	75.817	10.933	13.434	1	45.79
493	CB	HIS	A	572	74.942	13.527	14.427	1	50.23
494	CG	HIS	A	572	75.283	14.969	14.651	1	57.47
495	ND1	HIS	A	572	76.533	15.485	14.373	1	60.13
496	CD2	HIS	A	572	74.521	16.022	15.026	1	58.59
497	CE1	HIS	A	572	76.524	16.79	14.563	1	60.7
498	NE2	HIS	A	572	75.315	17.144	14.959	1	61.82
499	N	PHE	A	573	74.18	11.123	11.914	1	40.71
500	CA	PHE	A	573	74.108	9.692	11.707	1	40.48
501	C	PHE	A	573	74.307	9.348	10.232	1	43.34
502	O	PHE	A	573	74.017	10.166	9.35	1	42.49
503	CB	PHE	A	573	72.762	9.163	12.18	1	40.14
504	CG	PHE	A	573	72.458	9.451	13.621	1	38.87
505	CD1	PHE	A	573	71.844	10.64	13.988	1	40.13
506	CD2	PHE	A	573	72.736	8.512	14.606	1	37.89
507	CE1	PHE	A	573	71.5	10.893	15.321	1	40.49
508	CE2	PHE	A	573	72.399	8.754	15.936	1	37.42
509	CZ	PHE	A	573	71.777	9.948	16.295	1	37.34
510	N	GLU	A	574	74.829	8.146	9.985	1	44.06
511	CA	GLU	A	574	75.083	7.625	8.644	1	43.09
512	C	GLU	A	574	75.323	6.139	8.83	1	42.58
513	O	GLU	A	574	76.333	5.743	9.404	1	44.71
514	CB	GLU	A	574	76.329	8.267	8.037	1	45.39
515	CG	GLU	A	574	76.552	7.897	6.579	1	51.02
516	CD	GLU	A	574	77.863	8.428	6.027	1	55.72
517	OE1	GLU	A	574	78.084	9.658	6.065	1	59.89
518	OE2	GLU	A	574	78.68	7.611	5.553	1	60.39
519	N	SER	A	575	74.415	5.32	8.316	1	42.15
520	CA	SER	A	575	74.507	3.871	8.46	1	42.15
521	C	SER	A	575	75.828	3.209	8.089	1	44.95
522	O	SER	A	575	76.521	3.625	7.164	1	45.04
523	CB	SER	A	575	73.414	3.202	7.65	1	38.5
524	OG	SER	A	575	73.617	3.497	6.287	1	39.69

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
525	N	GLN	A	576	76.161	2.163	8.834	1	48.41
526	CA	GLN	A	576	77.344	1.36	8.591	1	51.67
527	C	GLN	A	576	76.696	0.018	8.334	1	50.22
528	O	GLN	A	576	75.821	-0.392	9.087	1	49.59
529	CB	GLN	A	576	78.237	1.286	9.837	1	60.28
530	CG	GLN	A	576	79.505	0.404	9.684	1	73.42
531	CD	GLN	A	576	79.251	-1.121	9.82	1	78.71
532	OE1	GLN	A	576	79.337	-1.874	8.84	1	78.57
533	NE2	GLN	A	576	78.96	-1.568	11.038	1	80.52
534	N	SER	A	577	77.085	-0.639	7.253	1	50.16
535	CA	SER	A	577	76.517	-1.93	6.922	1	52.16
536	C	SER	A	577	77.422	-2.661	5.963	1	57.44
537	O	SER	A	577	78.126	-2.051	5.148	1	59.48
538	CB	SER	A	577	75.14	-1.77	6.282	1	49.61
539	OG	SER	A	577	74.611	-3.032	5.9	1	49.62
540	N	ASP	A	578	77.4	-3.978	6.071	1	63.65
541	CA	ASP	A	578	78.194	-4.811	5.199	1	69.6
542	C	ASP	A	578	77.608	-4.748	3.801	1	70.01
543	O	ASP	A	578	78.343	-4.561	2.823	1	73.31
544	CB	ASP	A	578	78.232	-6.246	5.72	1	75.45
545	CG	ASP	A	578	79.152	-6.4	6.918	1	80.76
546	OD1	ASP	A	578	79.829	-5.409	7.289	1	83.45
547	OD2	ASP	A	578	79.212	-7.517	7.477	1	85.16
548	N	ASP	A	579	76.286	-4.88	3.709	1	66.7
549	CA	ASP	A	579	75.619	-4.809	2.416	1	64.53
550	C	ASP	A	579	75.812	-3.375	1.939	1	63.7
551	O	ASP	A	579	75.269	-2.435	2.524	1	65.1
552	CB	ASP	A	579	74.126	-5.129	2.558	1	64.07
553	CG	ASP	A	579	73.39	-5.177	1.216	1	62.87
554	OD1	ASP	A	579	73.937	-4.726	0.187	1	65.01
555	OD2	ASP	A	579	72.243	-5.669	1.197	1	60.67
556	N	PRO	A	580	76.594	-3.187	0.867	1	61.76
557	CA	PRO	A	580	76.85	-1.851	0.325	1	58.68
558	C	PRO	A	580	75.565	-1.125	-0.058	1	55.65
559	O	PRO	A	580	75.518	0.106	-0.068	1	55.79
560	CB	PRO	A	580	77.731	-2.145	-0.884	1	60.97
561	CG	PRO	A	580	77.29	-3.522	-1.296	1	62.5
562	CD	PRO	A	580	77.206	-4.221	0.02	1	61.07
563	N	HIS	A	581	74.516	-1.891	-0.343	1	51.46
564	CA	HIS	A	581	73.23	-1.315	-0.701	1	50.02
565	C	HIS	A	581	72.647	-0.529	0.479	1	49.93
566	O	HIS	A	581	71.869	0.41	0.301	1	47.04
567	CB	HIS	A	581	72.266	-2.424	-1.127	1	51.76
568	CG	HIS	A	581	70.883	-1.935	-1.437	1	55.84
569	ND1	HIS	A	581	69.751	-2.647	-1.105	1	58.18
570	CD2	HIS	A	581	70.448	-0.793	-2.021	1	55.97
571	CE1	HIS	A	581	68.679	-1.965	-1.464	1	56.65
572	NE2	HIS	A	581	69.075	-0.835	-2.021	1	57.45
573	N	PHE	A	582	73.025	-0.921	1.687	1	48.54
574	CA	PHE	A	582	72.528	-0.264	2.879	1	47.07
575	C	PHE	A	582	73.624	0.463	3.642	1	47.83
576	O	PHE	A	582	73.409	0.908	4.771	1	50.2

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
577	CB	PHE	A	582	71.855	-1.291	3.79	1	42.9
578	CG	PHE	A	582	70.552	-1.822	3.252	1	40.43
579	CD1	PHE	A	582	69.363	-1.124	3.46	1	37.8
580	CD2	PHE	A	582	70.504	-3.03	2.577	1	37.3
581	CE1	PHE	A	582	68.143	-1.626	3.009	1	36.43
582	CE2	PHE	A	582	69.287	-3.535	2.125	1	36.63
583	CZ	PHE	A	582	68.105	-2.832	2.343	1	34.43
584	N	HIS	A	583	74.793	0.608	3.029	1	46.88
585	CA	HIS	A	583	75.904	1.27	3.702	1	48.61
586	C	HIS	A	583	75.975	2.771	3.411	1	48.68
587	O	HIS	A	583	75.684	3.204	2.304	1	51.63
588	CB	HIS	A	583	77.221	0.576	3.331	1	50.24
589	CG	HIS	A	583	78.418	1.115	4.052	1	50.56
590	ND1	HIS	A	583	78.45	1.289	5.418	1	51.68
591	CD2	HIS	A	583	79.625	1.522	3.593	1	51.68
592	CE1	HIS	A	583	79.624	1.779	5.772	1	52.93
593	NE2	HIS	A	583	80.355	1.931	4.683	1	52.53
594	N	GLU	A	584	76.319	3.555	4.432	1	47.49
595	CA	GLU	A	584	76.464	5.011	4.332	1	44.75
596	C	GLU	A	584	75.207	5.84	4.069	1	41.01
597	O	GLU	A	584	75.298	6.989	3.661	1	40.27
598	CB	GLU	A	584	77.571	5.371	3.336	1	48.79
599	CG	GLU	A	584	78.965	4.931	3.805	1	56.71
600	CD	GLU	A	584	80.074	5.156	2.777	1	61.78
601	OE1	GLU	A	584	79.775	5.528	1.62	1	65.68
602	OE2	GLU	A	584	81.257	4.943	3.13	1	62.48
603	N	LYS	A	585	74.038	5.278	4.355	1	39.91
604	CA	LYS	A	585	72.781	5.996	4.145	1	36.31
605	C	LYS	A	585	72.507	7.063	5.2	1	34.01
606	O	LYS	A	585	73.079	7.042	6.296	1	32.86
607	CB	LYS	A	585	71.605	5.017	4.055	1	37.54
608	CG	LYS	A	585	71.777	3.966	2.979	1	33.81
609	CD	LYS	A	585	72.349	4.605	1.731	1	39.59
610	CE	LYS	A	585	72.788	3.59	0.692	1	45.32
611	NZ	LYS	A	585	71.639	3.09	-0.105	1	51.74
612	N	LYS	A	586	71.58	7.954	4.874	1	31.49
613	CA	LYS	A	586	71.209	9.062	5.74	1	30.32
614	C	LYS	A	586	69.716	9.072	6.091	1	29.44
615	O	LYS	A	586	68.924	8.341	5.495	1	30.36
616	CB	LYS	A	586	71.602	10.366	5.052	1	31.59
617	CG	LYS	A	586	73.075	10.442	4.717	1	30.78
618	CD	LYS	A	586	73.923	10.762	5.928	1	31.31
619	CE	LYS	A	586	73.554	12.137	6.476	1	34.53
620	NZ	LYS	A	586	74.523	12.624	7.49	1	37.22
621	N	GLN	A	587	69.325	9.936	7.022	1	29.7
622	CA	GLN	A	587	67.931	10.006	7.459	1	29.62
623	C	GLN	A	587	67.502	11.408	7.86	1	28.3
624	O	GLN	A	587	68.316	12.206	8.309	1	31.14
625	CB	GLN	A	587	67.709	9.053	8.642	1	29.37
626	CG	GLN	A	587	66.301	9.067	9.209	1	26.27
627	CD	GLN	A	587	66.067	7.939	10.179	1	28.3
628	OE1	GLN	A	587	66.602	6.852	10.006	1	29.67

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
629	NE2	GLN	A	587	65.263	8.186	11.21	1	30.15
630	N	ILE	A	588	66.23	11.719	7.652	1	27.44
631	CA	ILE	A	588	65.695	13.019	8.026	1	31.03
632	C	ILE	A	588	64.289	12.754	8.547	1	33.38
633	O	ILE	A	588	63.537	11.988	7.929	1	35.28
634	CB	ILE	A	588	65.665	14.044	6.827	1	30.39
635	CG1	ILE	A	588	65.143	15.404	7.294	1	25.88
636	CG2	ILE	A	588	64.832	13.527	5.668	1	28.18
637	CD1	ILE	A	588	66.085	16.116	8.265	1	29.27
638	N	PRO	A	589	63.993	13.223	9.774	1	31.62
639	CA	PRO	A	589	62.687	13.061	10.417	1	29.8
640	C	PRO	A	589	61.639	13.942	9.743	1	27.26
641	O	PRO	A	589	61.971	14.876	9.018	1	27.17
642	CB	PRO	A	589	62.961	13.495	11.857	1	33.02
643	CG	PRO	A	589	64.396	13.133	12.043	1	32.2
644	CD	PRO	A	589	65.008	13.62	10.759	1	32.62
645	N	CYS	A	590	60.38	13.705	10.069	1	24.93
646	CA	CYS	A	590	59.287	14.425	9.456	1	25.25
647	C	CYS	A	590	58.264	14.821	10.51	1	25.27
648	O	CYS	A	590	57.601	13.956	11.062	1	28.81
649	CB	CYS	A	590	58.637	13.468	8.448	1	24.21
650	SG	CYS	A	590	57.154	14.04	7.639	1	30.75
651	N	VAL	A	591	58.105	16.115	10.764	1	25.17
652	CA	VAL	A	591	57.139	16.596	11.754	1	23.18
653	C	VAL	A	591	55.871	17.111	11.084	1	24.36
654	O	VAL	A	591	55.949	18.012	10.235	1	25.78
655	CB	VAL	A	591	57.707	17.812	12.565	1	24.5
656	CG1	VAL	A	591	56.71	18.249	13.647	1	18.19
657	CG2	VAL	A	591	59.069	17.481	13.153	1	24.02
658	N	VAL	A	592	54.71	16.606	11.498	1	19.99
659	CA	VAL	A	592	53.449	17.074	10.945	1	18.04
660	C	VAL	A	592	52.675	17.765	12.053	1	20.95
661	O	VAL	A	592	52.236	17.113	12.991	1	22.93
662	CB	VAL	A	592	52.599	15.935	10.434	1	14.43
663	CG1	VAL	A	592	51.466	16.497	9.623	1	15.6
664	CG2	VAL	A	592	53.429	14.988	9.61	1	18.59
665	N	SER	A	593	52.456	19.069	11.936	1	21.12
666	CA	SER	A	593	51.75	19.796	12.976	1	20.6
667	C	SER	A	593	50.383	20.347	12.655	1	23.93
668	O	SER	A	593	50.207	21.097	11.702	1	26.79
669	CB	SER	A	593	52.624	20.942	13.494	1	23.89
670	OG	SER	A	593	51.984	21.662	14.541	1	20.11
671	N	MET	A	594	49.433	20.014	13.515	1	28.21
672	CA	MET	A	594	48.057	20.498	13.43	1	28.19
673	C	MET	A	594	47.83	21.373	14.684	1	29.88
674	O	MET	A	594	46.696	21.72	15.033	1	27.37
675	CB	MET	A	594	47.057	19.329	13.437	1	30.4
676	CG	MET	A	594	46.618	18.823	12.059	1	30.86
677	SD	MET	A	594	47.966	18.118	11.106	1	34.13
678	CE	MET	A	594	48.171	16.557	11.89	1	29.1
679	N	LEU	A	595	48.916	21.712	15.373	1	28.53
680	CA	LEU	A	595	48.824	22.516	16.584	1	26.68

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Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
681	C	LEU	A	595	48.418	23.958	16.302	1	27.98
682	O	LEU	A	595	48.871	24.562	15.328	1	30.99
683	CB	LEU	A	595	50.144	22.47	17.355	1	22.12
684	CG	LEU	A	595	50.715	21.087	17.692	1	19.78
685	CD1	LEU	A	595	51.931	21.299	18.585	1	21.14
686	CD2	LEU	A	595	49.679	20.18	18.383	1	16.52
687	N	THR	A	596	47.582	24.502	17.183	1	30.77
688	CA	THR	A	596	47.075	25.862	17.072	1	25.21
689	C	THR	A	596	47.749	26.848	18.011	1	23.66
690	O	THR	A	596	47.467	28.042	17.942	1	27.4
691	CB	THR	A	596	45.553	25.903	17.315	1	28.83
692	OG1	THR	A	596	45.251	25.191	18.516	1	31.5
693	CG2	THR	A	596	44.802	25.226	16.179	1	27.15
694	N	LYS	A	597	48.612	26.363	18.904	1	23.1
695	CA	LYS	A	597	49.334	27.238	19.852	1	20.51
696	C	LYS	A	597	50.716	26.649	20.026	1	18.12
697	O	LYS	A	597	50.959	25.523	19.618	1	16.6
698	CB	LYS	A	597	48.688	27.249	21.261	1	21.25
699	CG	LYS	A	597	47.267	27.763	21.409	1	19.06
700	CD	LYS	A	597	47.173	29.251	21.09	1	23.52
701	CE	LYS	A	597	45.732	29.74	21.157	1	25.58
702	NZ	LYS	A	597	44.746	28.71	20.693	1	33.36
703	N	GLU	A	598	51.612	27.406	20.644	1	20.92
704	CA	GLU	A	598	52.954	26.93	20.942	1	24.74
705	C	GLU	A	598	52.843	26.034	22.184	1	28.37
706	O	GLU	A	598	52.083	26.319	23.108	1	27.72
707	CB	GLU	A	598	53.869	28.095	21.276	1	23.98
708	CG	GLU	A	598	53.972	29.137	20.216	1	33.96
709	CD	GLU	A	598	55.037	30.163	20.525	1	41.59
710	OE1	GLU	A	598	56.101	29.788	21.075	1	46.3
711	OE2	GLU	A	598	54.815	31.35	20.207	1	47.26
712	N	LEU	A	599	53.609	24.961	22.218	1	32.31
713	CA	LEU	A	599	53.577	24.057	23.349	1	32.74
714	C	LEU	A	599	54.904	24.124	24.062	1	34.17
715	O	LEU	A	599	55.966	24.02	23.438	1	33.96
716	CB	LEU	A	599	53.294	22.626	22.891	1	33.3
717	CG	LEU	A	599	53.481	21.47	23.873	1	34.36
718	CD1	LEU	A	599	52.615	21.647	25.119	1	30.44
719	CD2	LEU	A	599	53.108	20.19	23.165	1	32.9
720	N	TYR	A	600	54.828	24.395	25.358	1	37.24
721	CA	TYR	A	600	55.99	24.467	25.234	1	35.72
722	C	TYR	A	600	55.634	23.488	27.329	1	37.53
723	O	TYR	A	600	54.483	23.445	27.759	1	38.6
724	CB	TYR	A	600	56.131	25.864	26.816	1	30.86
725	CG	TYR	A	600	56.889	26.817	25.936	1	23.8
726	CD1	TYR	A	600	58.284	26.823	25.93	1	21.63
727	CD2	TYR	A	600	56.216	27.734	25.124	1	24.82
728	CE1	TYR	A	600	58.989	27.726	25.139	1	22.81
729	CE2	TYR	A	600	56.912	28.638	24.332	1	20.61
730	CZ	TYR	A	600	58.297	28.629	24.348	1	23.1
731	OH	TYR	A	600	58.993	29.533	23.585	1	28.55
732	N	PHE	A	601	56.578	22.645	27.717	1	41.11

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
733	CA	PHE	A	601	56.312	21.662	28.76	1	47.98
734	C	PHE	A	601	56.447	22.224	30.171	1	54.73
735	O	PHE	A	601	56.049	21.59	31.154	1	58.36
736	CB	PHE	A	601	57.201	20.444	28.56	1	44.39
737	CG	PHE	A	601	56.764	19.58	27.42	1	43.7
738	CD1	PHE	A	601	55.446	19.123	27.351	1	41.46
739	CD2	PHE	A	601	57.649	19.232	26.407	1	40.23
740	CE1	PHE	A	601	55.018	18.334	26.289	1	39.65
741	CE2	PHE	A	601	57.223	18.443	25.343	1	40.41
742	CZ	PHE	A	601	55.906	17.994	25.285	1	37.85
743	N	SER	A	602	56.967	23.443	30.237	1	60.31
744	CA	SER	A	602	57.175	24.171	31.475	1	63.67
745	C	SER	A	602	55.996	25.114	31.782	1	67.56
746	O	SER	A	602	55.575	25.153	32.96	1	71.36
747	CB	SER	A	602	58.474	24.962	31.345	1	66.05
748	OG	SER	A	602	58.714	25.29	29.976	1	66.81
749	OT	SER	A	602	55.496	25.801	30.852	1	68.24
3762	S	SO4	A	601	38.803	36.264	-8.277	1	43.08
3763	O1	SO4	A	601	39.488	36.639	-7.023	1	47.84
3764	O2	SO4	A	601	38.722	37.45	-9.135	1	51.81
3765	O3	SO4	A	601	37.439	35.765	-8.044	1	42.73
3766	O4	SO4	A	601	39.606	35.191	-8.896	1	41.45
3767	S	SO4	A	602	67.712	-4.105	23.339	1	31.88
3768	O1	SO4	A	602	68.28	-2.81	23.765	1	30.05
3769	O2	SO4	A	602	67.562	-5.026	24.482	1	37.24
3770	O3	SO4	A	602	68.577	-4.749	22.345	1	36.19
3771	O4	SO4	A	602	66.374	-3.817	22.787	1	31.43
3772	OH2	WAT	B	701	54.845	3.98	9.296	1	20.95
3773	OH2	WAT	B	702	60.222	29.77	18.646	1	32.73
3774	OH2	WAT	B	703	37.676	26.261	10.189	1	27.92
3775	OH2	WAT	B	704	46.767	22.415	27.065	1	23.22
3776	OH2	WAT	B	705	65.713	6.34	13.691	1	22.12
3777	OH2	WAT	B	706	53.271	23.904	15.338	1	24.97
3778	OH2	WAT	B	707	50.992	30.418	18.625	1	30.24
3779	OH2	WAT	B	708	47.619	16.05	-0.878	1	25.63
3780	OH2	WAT	B	709	71.499	27.873	4.721	1	34.42
3781	OH2	WAT	B	710	58.975	-5.714	38.225	1	33.97
3782	OH2	WAT	B	711	60.959	-10.683	16.233	1	28.58
3783	OH2	WAT	B	712	59.764	14.277	13.997	1	30.7
3784	OH2	WAT	B	713	43.825	-0.324	28.703	1	34.2
3785	OH2	WAT	B	714	62.014	25.685	11.819	1	29.64
3786	OH2	WAT	B	715	41.639	27.253	2.687	1	27.46
3787	OH2	WAT	B	716	51.799	7.226	8.497	1	40.96
3788	OH2	WAT	B	717	43.995	26.128	-14.35	1	36.7
3789	OH2	WAT	B	718	55.9	-6.895	18.773	1	33.38
3790	OH2	WAT	B	719	65.567	25.549	17.806	1	45.91
3791	OH2	WAT	B	720	58.741	6.927	11.397	1	24.14
3792	OH2	WAT	B	721	42.702	36.344	0.017	1	41.48
3793	OH2	WAT	B	722	65.565	31	-4.837	1	37.29
3794	OH2	WAT	B	723	40.736	16.067	21.575	1	35.63
3795	OH2	WAT	B	724	55.327	1.251	2.19	1	30.14
3796	OH2	WAT	B	725	46.657	12.739	29.192	1	23.35

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B _{eq}
3797	OH2	WAT	B	726	64.537	-11.076	21.167	1	30.68
3798	OH2	WAT	B	728	64.968	9.638	6.078	1	30.24
3799	OH2	WAT	B	729	45.956	-10.11	22.14	1	27.94
3800	OH2	WAT	B	730	68.41	18.168	1.034	1	37.18
3801	OH2	WAT	B	731	58.874	-4.961	4.735	1	63.45
3802	OH2	WAT	B	732	49.452	26.39	8.902	1	38.44
3803	OH2	WAT	B	733	69.6	29.804	4.212	1	26.44
3804	OH2	WAT	B	734	59.305	22.941	27.068	1	42.79
3805	OH2	WAT	B	735	53.991	6.146	7.586	1	32.49
3806	OH2	WAT	B	736	49.248	41.536	1.504	1	32.29
3807	OH2	WAT	B	737	50.677	39.897	18.856	1	40.12
3808	OH2	WAT	B	738	54.15	-17.129	13.063	1	60.14
3809	OH2	WAT	B	739	60.234	34.858	17.48	1	44.53
3810	OH2	WAT	B	740	42.041	24.323	19.048	1	50.63
3811	OH2	WAT	B	741	52.48	25.719	26.396	1	31.72
3812	OH2	WAT	B	742	59.688	13.52	38.138	1	41.51
3813	OH2	WAT	B	743	57.794	27.434	17.443	1	33.37
3814	OH2	WAT	B	745	68.6	21.26	-2.588	1	33.65
3815	OH2	WAT	B	746	40.208	18.376	17.62	1	25.17
3816	OH2	WAT	B	747	43.692	40.653	-3.173	1	42.45
3817	OH2	WAT	B	748	66.327	-9.177	25.893	1	40.1
3818	OH2	WAT	B	751	42.549	32.85	16.654	1	49.29
3819	OH2	WAT	B	752	62.716	1.617	19.066	1	30.35
3820	OH2	WAT	B	753	35.425	20.831	6.151	1	28.37
3821	OH2	WAT	B	754	43.688	-2.569	26.663	1	39.27
3822	OH2	WAT	B	755	44.332	32.276	-13.47	1	34.59
3823	OH2	WAT	B	756	45.325	-8.702	16.9	1	33.03
3824	OH2	WAT	B	757	36.615	-2.056	18.864	1	43.69
3825	OH2	WAT	B	758	44.677	23.641	26.29	1	30.09
3826	OH2	WAT	B	759	59.977	15.06	-10.376	1	38.15
3827	OH2	WAT	B	760	41.628	10.657	12.457	1	48.03
3828	OH2	WAT	B	761	64.662	-12.12	14.291	1	35.03
3829	OH2	WAT	B	762	45.031	22.37	-21.732	1	44.95
3830	OH2	WAT	B	763	48.068	11.633	33.303	1	63.05
3831	OH2	WAT	B	764	71.417	10.947	8.782	1	39.1
3832	OH2	WAT	B	765	49.909	9.544	-6.641	1	54.47
3833	OH2	WAT	B	766	75.719	-1.078	-3.505	1	65.13
3834	OH2	WAT	B	767	46.369	17.764	-2.452	1	48.14
3835	OH2	WAT	B	769	74.951	26.308	0.88	1	76.48
3836	OH2	WAT	B	770	43.93	11.884	13.357	1	61.37
3837	OH2	WAT	B	771	67.193	24.865	15.466	1	28.21
3838	OH2	WAT	B	772	38.216	16.912	-3.951	1	42.11
3839	OH2	WAT	B	773	67.186	2.689	-2.196	1	66.91
3840	OH2	WAT	B	774	60.658	15.906	-2.343	1	53.14
3841	OH2	WAT	B	775	68.471	2.954	35.303	1	37.03
3842	OH2	WAT	B	776	46.084	21.639	0.794	1	31.65
3843	OH2	WAT	B	778	65.026	38.012	-3.113	1	38.53
3844	OH2	WAT	B	779	53.445	41.321	4.175	1	50.72
3845	OH2	WAT	B	780	68.526	5.324	22.686	1	30.74
3846	OH2	WAT	B	781	72.9	11.958	19.98	1	48.77
3847	OH2	WAT	B	782	75.24	-1.361	17.808	1	71.19
3848	OH2	WAT	B	785	63.072	-7.223	10.057	1	43.62

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
3849	OH2	WAT	B	786	56.502	41.767	10.609	1	58.24
3850	OH2	WAT	B	787	76.011	27.004	-10.261	1	61.15
3851	OH2	WAT	B	788	43.665	30.078	-4.043	1	30.58
3852	OH2	WAT	B	789	65.657	7.045	5.685	1	37.78
3853	OH2	WAT	B	790	64.791	17.433	-11.027	1	47.63
3854	OH2	WAT	B	791	41.58	12.296	-2.464	1	55.46
3855	OH2	WAT	B	792	50.049	24.876	6.407	1	35.58
3856	OH2	WAT	B	793	65.915	35.855	16.466	1	51.78
3857	OH2	WAT	B	794	66.429	8.592	-2.331	1	39.64
3858	OH2	WAT	B	795	57.144	31.657	26.666	1	57.54
3859	OH2	WAT	B	796	57.382	28.684	29.106	1	59.34
3860	OH2	WAT	B	797	48.699	10.321	10.379	1	47.2
3861	OH2	WAT	B	798	39.242	15.257	-13.26	1	54.28
3862	OH2	WAT	B	799	59.053	11.353	1.242	1	42.97
3863	OH2	WAT	B	800	39.715	9.845	3.156	1	55.56
3864	OH2	WAT	B	801	64.908	10.538	3.319	1	39.92
3865	OH2	WAT	B	802	47.87	30.754	17.891	1	36.67
3866	OH2	WAT	B	803	70.037	-3.94	7.077	1	43.56
3867	OH2	WAT	B	804	53.869	27.65	33.113	1	68.19
3868	OH2	WAT	B	805	35.476	13.851	9.571	1	63.95
3869	OH2	WAT	B	806	43.496	11.812	9.762	1	55.48
3870	OH2	WAT	B	807	67.342	29.278	19.397	1	71.64
3871	OH2	WAT	B	808	37.175	12.004	26.982	1	45.03
3872	OH2	WAT	B	809	55.515	8.166	35.287	1	31.68
3873	OH2	WAT	B	810	40.16	18.648	9.259	1	41.48
3874	OH2	WAT	B	811	46.218	33.314	15.335	1	60.91
3875	OH2	WAT	B	812	48.764	36.706	15.572	1	54.71
3876	OH2	WAT	B	813	71.307	25.838	23.259	1	47.51
3877	OH2	WAT	B	814	73.285	18.889	14.411	1	65
3878	OH2	WAT	B	815	60.745	36.265	10.293	1	35.04
3879	OH2	WAT	B	816	31.235	31.453	-7.038	1	64.24
3880	OH2	WAT	B	817	59	-8.862	4.679	1	70.76
3881	OH2	WAT	B	818	38.024	20.12	5.89	1	40.19
3882	OH2	WAT	B	819	45.051	9.592	31.07	1	73.98
3883	OH2	WAT	B	820	54.309	44.145	-1.726	1	61.02
3884	OH2	WAT	B	821	51.737	26.105	34.15	1	63.4
3885	OH2	WAT	B	822	51.4	20.209	36.055	1	48.26
3886	OH2	WAT	B	823	70.298	31.206	-13.116	1	48.48
3887	OH2	WAT	B	824	60.241	-14.334	9.382	1	57.13
3888	OH2	WAT	B	825	36.425	2.872	28.744	1	61.75
3889	OH2	WAT	B	826	50.467	27.729	30.588	1	66.38
3890	OH2	WAT	B	827	57.944	27.791	33.656	1	73.09
3891	OH2	WAT	B	828	56.359	-8.145	4.955	1	54.1
3892	OH2	WAT	B	829	71.859	15.991	26.783	1	61.47
3893	OH2	WAT	B	830	66.781	27.434	-15.756	1	36.71
3894	OH2	WAT	B	831	63.116	16.428	30.525	1	59.82
3895	OH2	WAT	B	832	66.938	1.316	33.568	1	50.93
3896	OH2	WAT	B	833	67.869	6.024	4.656	1	36.61
3897	OH2	WAT	B	834	63.356	-10.069	23.687	1	30.72
3898	OH2	WAT	B	835	37.07	25.829	-14.694	1	56.34
3899	OH2	WAT	B	836	39.695	4.944	33.207	1	60.17
3900	OH2	WAT	B	837	52.246	5.228	34.908	1	31.32

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
3901	OH2	WAT	B	839	74.486	22.357	12.461	1	64.15
3902	OH2	WAT	B	840	29.333	19.773	14.21	1	61.72
3903	OH2	WAT	B	841	41.589	19.323	20.008	1	41.36
3904	OH2	WAT	B	842	43.944	25.847	22.178	1	62.79
3905	OH2	WAT	B	843	53.246	27.206	28.817	1	54.71
3906	OH2	WAT	B	844	39.384	19.568	29.966	1	58.08
3907	OH2	WAT	B	845	48.729	15.624	45.695	1	80.1
3908	OH2	WAT	B	846	61.392	25.589	14.851	1	30.2
3909	OH2	WAT	B	847	67.752	-10.396	19.922	1	47.29
3910	OH2	WAT	B	848	40.467	20.465	7.423	1	40.1
3911	OH2	WAT	B	850	67.031	-5.039	-0.432	1	73.49
3912	OH2	WAT	B	851	39.113	-3.167	15.191	1	73.03
3913	OH2	WAT	B	852	42.596	-5.891	25.614	1	57.48
3914	OH2	WAT	B	853	31.226	23.729	-2.001	1	92.07
3915	OH2	WAT	B	854	78.673	5.102	7.196	1	59.77
3916	OH2	WAT	B	855	42.263	24.244	27.458	1	45.49
3917	OH2	WAT	B	857	53.204	17.229	35.801	1	47.39
3918	OH2	WAT	B	858	36.479	20.198	36.174	1	59
3919	OH2	WAT	B	859	60.842	28.728	-13.94	1	48.75
3920	OH2	WAT	B	860	43.901	38.07	1.67	1	45.3
3921	OH2	WAT	B	861	67.465	37.787	3.437	1	61.96
3922	OH2	WAT	B	862	33.069	27.683	14.236	1	44.23
3923	OH2	WAT	B	863	55.186	27.396	16.917	1	30.89
3924	OH2	WAT	B	864	54.583	34.197	20.204	1	61.48
3925	OH2	WAT	B	865	57.489	35.198	19.885	1	37.8
3926	OH2	WAT	B	866	44.695	2.068	28.106	1	23.65
3927	OH2	WAT	B	868	72.117	28.318	7.208	1	45.05
3928	OH2	WAT	B	869	76.417	-4.671	8.762	1	59.94
3929	OH2	WAT	B	870	77.423	12.591	7.008	1	51.87
3930	OH2	WAT	B	871	66.651	19.624	-11.11	1	55.43
3931	OH2	WAT	B	873	45.962	1.906	32.617	1	42.25
3932	OH2	WAT	B	874	41.054	-4.424	19.549	1	52.08
3933	OH2	WAT	B	875	49.21	-8.505	23.173	1	35.05
3934	OH2	WAT	B	876	61.587	29.145	23.636	1	54.92
3935	OH2	WAT	B	877	67.329	-3.96	8.863	1	75.2
3936	OH2	WAT	B	878	70.897	-5.509	-1.401	1	80.6
3937	OH2	WAT	B	880	45.099	4.897	6.503	1	38.24
3938	OH2	WAT	B	881	38.937	11.472	-2.963	1	70.34
3939	OH2	WAT	B	883	36.555	2.469	16.796	1	60.57
3940	OH2	WAT	B	884	51.447	42.887	2.87	1	52.33
3941	OH2	WAT	B	885	62.74	-2.742	-1.671	1	72.81
3942	OH2	WAT	B	886	35.233	11.894	24.815	1	43
3943	OH2	WAT	B	887	44.442	19.798	42.122	1	57.61
3944	OH2	WAT	B	888	46.412	40.649	3.402	1	100
3945	OH2	WAT	B	889	37.822	23.102	-22.636	1	52.71
3946	OH2	WAT	B	890	42.088	36.598	8.299	1	44.32
3947	OH2	WAT	B	892	32.206	35.567	-6.693	1	54.12
3948	OH2	WAT	B	893	47.057	38.866	12.38	1	48.07
3949	OH2	WAT	B	894	53.353	25.071	18.17	1	63.96
3950	OH2	WAT	B	895	37.57	7.21	21.229	1	52.08
3951	OH2	WAT	B	896	58.672	2.49	-0.423	1	41.04
3952	OH2	WAT	B	897	53.783	21.061	33.029	1	64.02

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
3953	OH2	WAT	B	898	65.463	37.19	13.619	1	60.18
3954	OH2	WAT	B	899	62.216	10.055	-7.39	1	57.85
3955	OH2	WAT	B	900	60.775	1.879	-2.27	1	81.57
3956	OH2	WAT	B	901	43.22	-11.183	18.577	1	70.13
3957	OH2	WAT	B	902	60.392	12.348	-9.261	1	73.53
3958	OH2	WAT	B	903	39.484	-2.181	19.992	1	40.66
3959	OH2	WAT	B	904	67.433	41.209	-5.235	1	59.66
3960	OH2	WAT	B	906	45.678	12.332	32.181	1	44.03
3961	OH2	WAT	B	907	61	-3.154	6.768	1	42.63
3962	OH2	WAT	B	908	51.074	13.76	34.516	1	42.28
3963	OH2	WAT	B	909	49.491	9.238	1.16	1	61.52
3964	OH2	WAT	B	910	52.43	8.183	4.928	1	53.94
3965	OH2	WAT	B	911	61.13	15.944	1.855	1	41.3
3966	OH2	WAT	B	912	41.752	22.4	-24.925	1	60.91
3967	OH2	WAT	B	914	74.767	27.496	-2.394	1	55.11
3968	OH2	WAT	B	915	47.575	-8.276	26.122	1	44.63
3969	OH2	WAT	B	916	45.984	42.498	-2.53	1	60.09
3970	OH2	WAT	B	917	38.851	19.578	-22.562	1	48.23
3971	OH2	WAT	B	918	77.696	0.197	18.971	1	84.81
3972	OH2	WAT	B	919	52.43	13.1	-4.732	1	55.51
3973	OH2	WAT	B	920	74.064	4.288	14.082	1	50.71
3974	OH2	WAT	B	921	33.998	31.927	4.171	1	61.99
3975	OH2	WAT	B	922	50.78	15.192	4.959	1	58.89
3976	OH2	WAT	B	924	36.615	8.128	10.365	1	57.94
3977	OH2	WAT	B	925	66.529	32.641	9.569	1	45.69
3978	OH2	WAT	B	926	64.58	21.337	-17.942	1	59.95
3979	OH2	WAT	B	928	69.139	23.185	-14.854	1	43.32
3980	OH2	WAT	B	930	65.198	21.948	30.02	1	49.89
3981	OH2	WAT	B	931	36.001	34.614	4.512	1	63.32
3982	OH2	WAT	B	933	42	15.043	-14.683	1	76.89
3983	OH2	WAT	B	934	76.794	34.256	3.728	1	60.92
3984	OH2	WAT	B	935	44.075	39.635	-8.27	1	66.98
3985	OH2	WAT	B	936	48.147	14.988	9.09	1	43.97
3986	OH2	WAT	B	938	39.272	7.719	33.741	1	46.2
3987	OH2	WAT	B	941	52.251	45.457	0.661	1	78.79
3988	OH2	WAT	B	943	57.024	-17.368	15.912	1	50.97
3989	OH2	WAT	B	944	39.297	11.347	9.407	1	60.73
3990	OH2	WAT	B	945	70.909	24.263	28.837	1	89.95
3991	OH2	WAT	B	946	68.24	32.525	-7.695	1	83.64
3992	OH2	WAT	B	947	51.718	7.64	37.034	1	37.64
3993	OH2	WAT	B	948	55.723	3.389	0.273	1	44.07
3994	OH2	WAT	B	951	79.861	15.12	6.08	1	59.6
3995	OH2	WAT	B	952	54.974	15.343	2.234	1	81.2
3996	OH2	WAT	B	953	36.475	19.296	-5.615	1	60
3997	OH2	WAT	B	954	73.625	26.986	14.34	1	74.33
3998	OH2	WAT	B	955	54.246	-3.999	0.925	1	71.55
3999	OH2	WAT	B	956	53.143	31.582	17.891	1	48.17
4000	OH2	WAT	B	957	70.96	22.865	8.658	1	47.11
4001	OH2	WAT	B	959	62.709	15.108	-10	1	58.58
4002	OH2	WAT	B	960	31.736	34.279	-0.908	1	77.45
4003	OH2	WAT	B	961	39.374	9.188	11.512	1	63.57
4004	OH2	WAT	B	962	52.564	0.423	2.515	1	53.31

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
4005	OH2	WAT	B	963	68.559	3.559	27.341	1	37.62
4006	OH2	WAT	B	965	49.832	6.314	35.489	1	42.94
4007	OH2	WAT	B	966	42.916	25.9	33.268	1	52.96
4008	OH2	WAT	B	967	56.06	38.835	18.679	1	80.16
4009	OH2	WAT	B	968	49.63	12.713	8.582	1	52.64
4010	OH2	WAT	B	969	58.81	19.268	-17.628	1	79.97
4011	OH2	WAT	B	970	39.884	4.471	14.621	1	42.27
4012	OH2	WAT	B	971	41.644	11.02	6.139	1	62
4013	OH2	WAT	B	972	60.25	27.873	15.996	1	32.63
4014	OH2	WAT	B	973	50.663	-14.086	13.597	1	38.56
4015	OH2	WAT	B	974	62.352	12.118	37.1	1	30.83
4016	OH2	WAT	B	975	50.205	15.627	-0.975	1	35.31
4017	OH2	WAT	B	976	33.964	15.561	11.228	1	38.36
4018	OH2	WAT	B	977	74.048	4.871	16.847	1	40.75
4019	OH2	WAT	B	978	63.595	10.086	34.953	1	30.27
4020	OH2	WAT	B	979	51.615	29.167	-17.841	1	39.28
4021	OH2	WAT	B	980	46.076	30.908	24.693	1	86.31
4022	OH2	WAT	B	981	69.217	20.435	1.794	1	39.28
4023	OH2	WAT	B	982	45.141	10.351	-5.666	1	59.72
4024	OH2	WAT	B	983	65.318	-2.711	-0.305	1	47.28
4025	OH2	WAT	B	984	37.303	16.09	36.1	1	76.38
4026	OH2	WAT	B	985	56.447	11.729	36.534	1	52.93
4027	OH2	WAT	B	986	61.982	15.821	14.457	1	30.38
4028	OH2	WAT	B	987	68.544	-7.976	21.964	1	73.86
4029	OH2	WAT	B	988	39.044	3.56	29.34	1	34.47
4030	OH2	WAT	B	989	40.056	34.329	-15.106	1	78.18
4031	OH2	WAT	B	990	43.053	-6.508	15.194	1	58.97
4032	OH2	WAT	B	991	73.571	-3.855	8.805	1	48.59
4033	OH2	WAT	B	992	60.644	-13.25	13.533	1	53.9
4034	OH2	WAT	B	993	71.183	21.028	6.315	1	52.36
4035	OH2	WAT	B	994	28.136	28.848	8.598	1	72.65
4036	OH2	WAT	B	995	63.132	-4.607	7.686	1	60.52
4037	OH2	WAT	B	996	58.049	-0.972	-0.648	1	55.27
4038	OH2	WAT	B	997	45.376	26.309	25.763	1	48.27
4039	OH2	WAT	B	998	38.422	6.887	1.7	1	57.5
4040	OH2	WAT	B	999	45.658	13.61	10.519	1	57.84
4041	OH2	WAT	B	1001	67.523	34.555	11.439	1	76.2
4042	OH2	WAT	B	1002	69.692	3.958	-2.137	1	63.43
4043	OH2	WAT	B	1003	52.92	44.897	5.963	1	58.69
4044	OH2	WAT	B	1004	58.378	8.806	-1.432	1	58.74
4045	OH2	WAT	B	1005	72.238	30.673	14.323	1	61.15
4046	OH2	WAT	B	1006	59.133	14.144	2.125	1	57.17
4047	OH2	WAT	B	1007	81.573	-1.421	6.36	1	85.4
4048	OH2	WAT	B	1008	56.202	19.223	35.699	1	65.12
4049	OH2	WAT	B	1009	41.677	20.122	42.548	1	49.22
4050	OH2	WAT	B	1010	44.002	38.63	5.03	1	53.81
4051	OH2	WAT	B	1011	70.142	5.654	26.338	1	60.06
4052	OH2	WAT	B	1012	72.738	1.735	-2.473	1	83.93
4053	OH2	WAT	B	1014	26.147	27.561	-1.025	1	68.41
4054	OH2	WAT	B	1015	65.974	-0.026	-1.171	1	46.31
4055	OH2	WAT	B	1016	43.777	10.753	-8.919	1	82.96
4056	OH2	WAT	B	1017	28.812	30.318	-4.211	1	65.78

Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
4057	OH2	WAT	B	1018	53.036	38.244	19.461	1	64.58
4058	OH2	WAT	B	1019	60.476	23.287	11.912	1	42.87
4059	OH2	WAT	B	1020	65.919	33.753	20.847	1	72.82
4060	OH2	WAT	B	1021	64.721	-6.03	12.066	1	69.85
4061	OH2	WAT	B	1022	76.124	6.993	12.46	1	53.26
4062	OH2	WAT	B	1023	39.902	1.239	14.533	1	42.53
4063	OH2	WAT	B	1025	54.585	16.243	-0.761	1	56.58
4064	OH2	WAT	B	1026	49.688	12.674	2.75	1	64.14
4065	OH2	WAT	B	1027	48.217	15.164	-17.773	1	70.98
4066	OH2	WAT	B	1028	38.287	15.769	-7.239	1	82.57
4067	OH2	WAT	B	1029	53.837	44.096	13.723	1	79.21
4068	OH2	WAT	B	1031	56.759	-1.034	2.228	1	37.98
4069	OH2	WAT	B	1032	47.395	5.484	8.406	1	39.48
4070	OH2	WAT	B	1033	50.942	20.847	33.413	1	43.82
4071	OH2	WAT	B	1034	71.22	19.562	17.094	1	57.17
4072	OH2	WAT	B	1035	60.523	31.865	20.322	1	52.14
4073	OH2	WAT	B	1036	72.625	7.763	22.462	1	49.21
4074	OH2	WAT	B	1037	69.115	9.495	-2.156	1	52.99
4075	OH2	WAT	B	1038	29.697	33.523	-6.021	1	79.74
4076	OH2	WAT	B	1039	49.448	0.309	2.81	1	83.06
4077	OH2	WAT	B	1040	69.043	7.817	24.075	1	45.59
4078	OH2	WAT	B	1041	35.252	-2.03	15.249	1	52.42
4079	OH2	WAT	B	1042	65.285	29.973	21.338	1	61.09
4080	OH2	WAT	B	1043	71.624	25.149	7.179	1	63.79
4081	OH2	WAT	B	1044	35.758	19.27	26.31	1	62.02
4082	OH2	WAT	B	1045	60.589	43.77	0.01	1	78.89
4083	OH2	WAT	B	1046	78.475	-4.967	11.238	1	61.68
4084	OH2	WAT	B	1048	40.862	-9.718	16.833	1	81.32
4085	OH2	WAT	B	1049	35.007	25.492	21.45	1	80.65
4086	OH2	WAT	B	1051	28.029	26.842	15.413	1	75.99
4087	OH2	WAT	B	1052	59.335	-1.486	5.419	1	65.47
4088	OH2	WAT	B	1053	35.858	35.122	-10.761	1	76.15
4089	OH2	WAT	B	1054	43.843	-6.796	23.047	1	79.93
4090	OH2	WAT	B	1055	38.213	1.067	12.104	1	54.34
4091	OH2	WAT	B	1056	74.431	25.231	7.699	1	86.03
4092	OH2	WAT	B	1057	58.241	27.178	-17.818	1	56.95
4093	OH2	WAT	B	1059	39.673	0.32	17.854	1	64.18
4094	OH2	WAT	B	1060	75.701	41.487	5.047	1	72.68
4095	OH2	WAT	B	1061	69.881	-0.092	32.777	1	76.74
4096	OH2	WAT	B	1064	50.002	20.97	44.468	1	59.65
4097	OH2	WAT	B	1066	35.749	9.351	25.248	1	68.2
4098	OH2	WAT	B	1070	38.359	20.028	26.687	1	71.74
4099	OH2	WAT	B	1071	71.673	11.372	-3.519	1	78.37
4100	OH2	WAT	B	1072	83.1	2.419	3.589	1	60.94
4101	OH2	WAT	B	1073	81.543	4.615	6.257	1	71.52
4102	OH2	WAT	B	1074	76.622	4.388	12.684	1	71.94
4103	OH2	WAT	B	1075	38.741	11.835	1.075	1	78.9
4104	OH2	WAT	B	1076	46.858	13.715	45.756	1	64.13
4105	OH2	WAT	B	1077	46.805	3.316	28.934	1	54.02
4106	OH2	WAT	B	1078	39.101	6.216	11.852	1	59.83
4107	OH2	WAT	B	1079	70.615	21.91	20.555	1	81.14
4108	OH2	WAT	B	1080	40.07	22.686	27.757	1	65

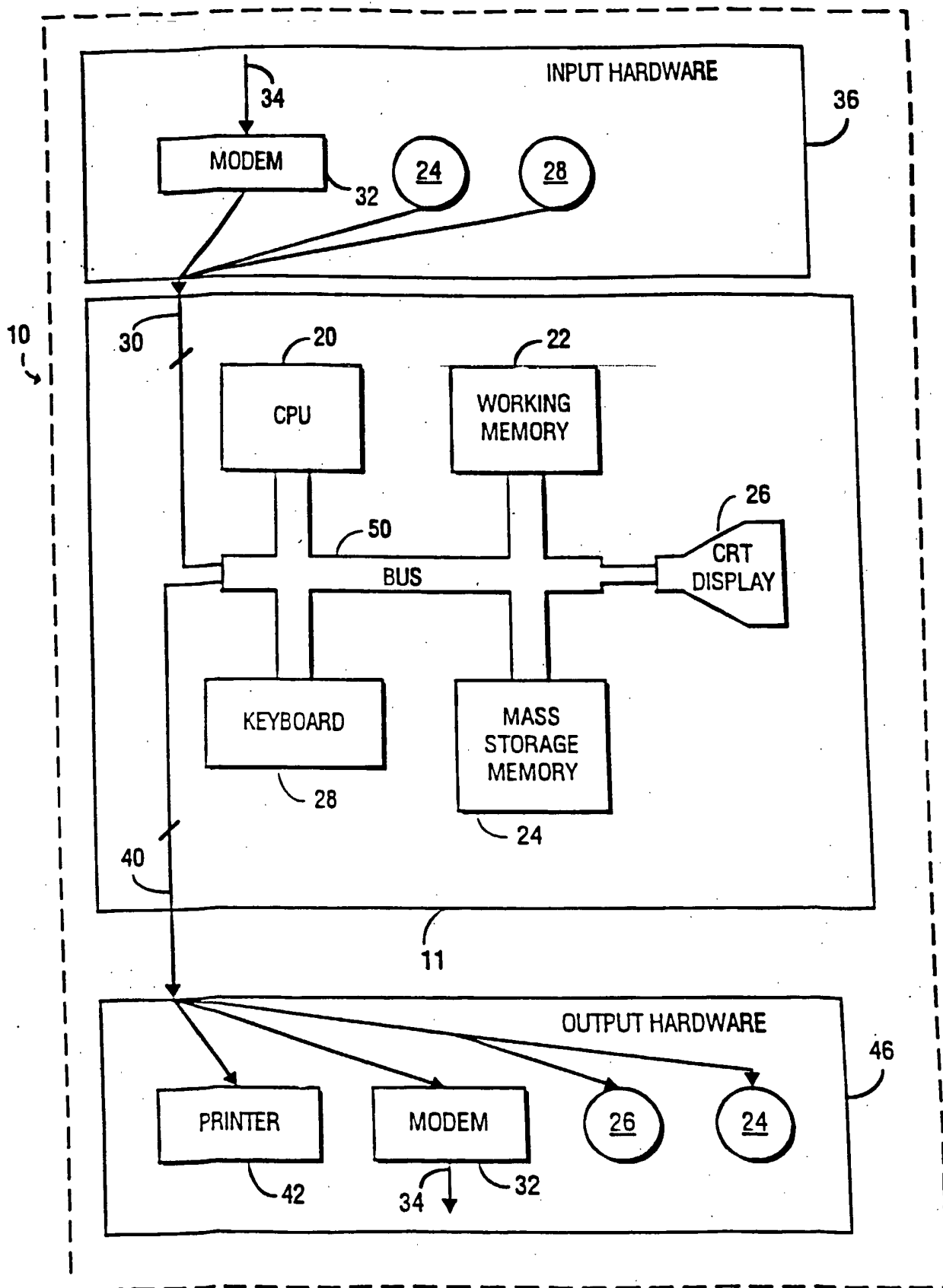
Figure 7

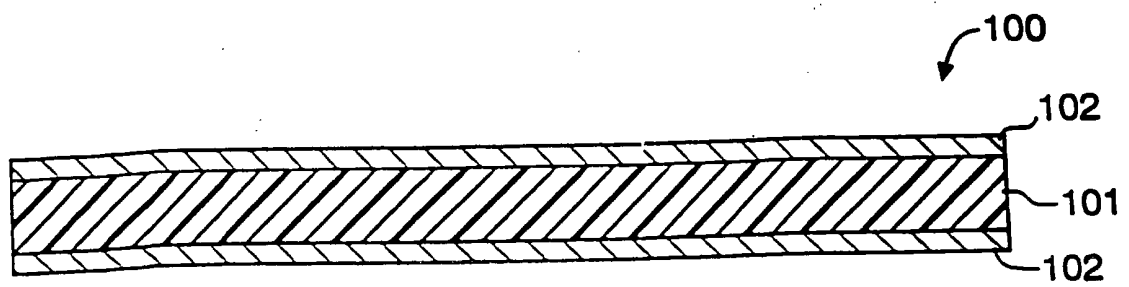
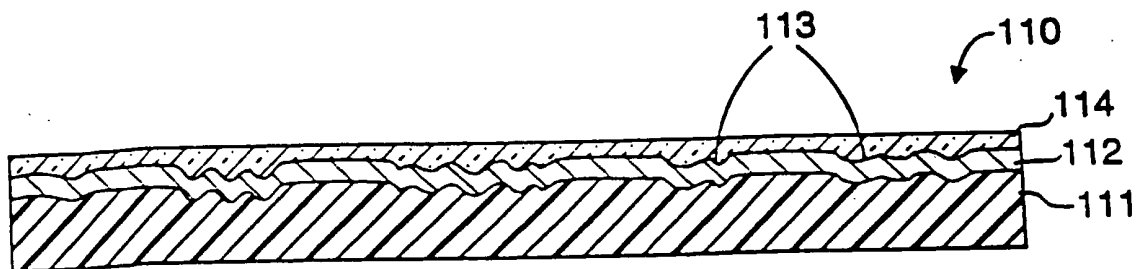
ATOM	ATOMTYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
4109	OH2	WAT	B	1082	48.55	13.994	0.721	1	65.68
4110	OH2	WAT	B	1083	57.501	31.757	22.263	1	58.14
4111	OH2	WAT	B	1104	48.667	29.925	27.693	1	68.94
4112	OH2	WAT	B	1105	34.257	19.516	38.894	1	25
4113	OH2	WAT	B	1106	34.901	25.966	-7.693	1	25
4114	OH2	WAT	B	1107	75.763	-0.064	14.754	1	25
4115	OH2	WAT	B	1108	58.034	34.344	23.444	1	25
4116	OH2	WAT	B	1109	45.838	28.705	23.98	1	25
4117	OH2	WAT	B	1110	43.931	20.666	36.5	1	25
4118	OH2	WAT	B	1111	74.902	6.326	-0.594	1	25
4119	OH2	WAT	B	1112	43.402	12.734	33.326	1	25
4120	OH2	WAT	B	1113	53.744	9.573	37.18	1	25
4121	OH2	WAT	B	1114	34.96	21.465	-9.286	1	25
4122	OH2	WAT	B	1115	37.988	5.71	16.2	1	25
4123	OH2	WAT	B	1116	57.683	14.743	-0.734	1	25
4124	OH2	WAT	B	1117	72.374	33.237	-7.446	1	25
4125	OH2	WAT	B	1118	73.632	2.428	25.085	1	25
4126	OH2	WAT	B	1119	75.101	29.931	4.817	1	25
4127	OH2	WAT	B	1120	78.014	35.55	7.109	1	25
4128	OH2	WAT	B	1121	70.136	30.475	20.537	1	25
4129	OH2	WAT	B	1122	32.547	18.773	24.158	1	25
4130	OH2	WAT	B	1123	73.804	27.842	3.686	1	25
4131	OH2	WAT	B	1124	69.99	39.213	7.787	1	25
4132	OH2	WAT	B	1125	75.599	-4.482	15.351	1	25
4133	OH2	WAT	B	1126	35.88	7.1	0.985	1	25
4134	OH2	WAT	B	1127	58.503	15.472	36.977	1	25
4135	OH2	WAT	B	1128	43.298	25.6	38.083	1	25
4136	OH2	WAT	B	1129	51.245	16.734	44.802	1	25
4137	OH2	WAT	B	1130	29.572	32.942	-1.874	1	25
4138	OH2	WAT	B	1131	70.626	24.56	-9.961	1	25
4139	OH2	WAT	B	1132	72.193	19.07	-9.087	1	25
4140	OH2	WAT	B	1133	43.776	19.286	-22.488	1	25
4141	OH2	WAT	B	1134	72.999	26.586	-13.114	1	25
4142	OH2	WAT	B	1135	34.443	-2.01	22.24	1	25
4143	OH2	WAT	B	1136	36.831	39.256	-9.779	1	25
4144	OH2	WAT	B	1137	79.109	36.668	3.045	1	25
4145	OH2	WAT	B	1138	64.441	7.77	-3.523	1	25
4146	OH2	WAT	B	1139	36.536	5.796	19.259	1	25
4147	OH2	WAT	B	1140	70.433	10.041	23.953	1	25
4148	OH2	WAT	B	1141	47.754	42.166	9.531	1	25
4149	OH2	WAT	B	1142	67.799	18.755	-13.667	1	25
4150	OH2	WAT	B	1143	80.57	-9.45	5.302	1	25
4151	OH2	WAT	B	1144	68.134	28.012	24.831	1	25
4152	OH2	WAT	B	1145	25.493	29.21	10.023	1	25
4153	OH2	WAT	B	1146	25.837	16.978	-1.423	1	25
4154	OH2	WAT	B	1147	70.554	4.283	31.333	1	25
4155	OH2	WAT	B	1148	52.065	42.638	16.562	1	25
4156	OH2	WAT	B	1149	55.603	-13.731	18.45	1	25
4157	OH2	WAT	B	1150	51.958	9.478	2.518	1	25
4158	OH2	WAT	B	1151	46.83	41.932	0.471	1	25
4159	OH2	WAT	B	1152	34.794	15.888	-12.194	1	25
4160	OH2	WAT	B	1153	50.405	47.16	7.35	1	25

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Figure 7

ATOM	ATOM TYPE	RESIDUE	SUBUNIT	#	X	Y	Z	OCC	B
4161	OH2	WAT	B	1154	66.531	33.393	-6.208	1	25
4162	OH2	WAT	B	1155	73	27.927	10.746	1	25
4163	OH2	WAT	B	1156	63.059	28.079	-19.949	1	25
4164	OH2	WAT	B	1157	55.881	8.459	-0.717	1	25
4165	OH2	WAT	B	1158	32.613	23.864	-14.809	1	25
4166	OH2	WAT	B	1159	78.466	5.638	15.735	1	25
4167	OH2	WAT	B	1160	76.849	27.181	-4.485	1	25
4168	OH2	WAT	B	1161	33.72	12.966	5.524	1	25

FIGURE 8



**FIGURE 9****FIGURE 10**