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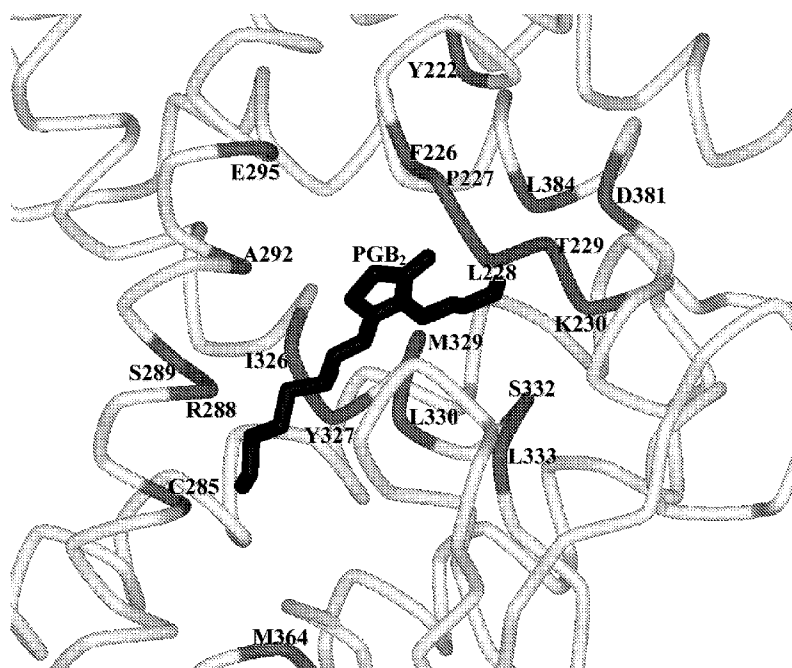
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(54) Title: PROSTAGLANDIN-BINDING POCKET OF PPAR PROTEIN AND USE THEREOF



(57) **Abstract:** Described are methods for evaluating the ability of a chemical entity to associate with a prostaglandin-binding pocket or part of a prostaglandin-binding pocket of a PPAR, PPAR γ or PPAR γ -like protein using structure coordinates of the prostaglandin-binding pocket as described herein, as well as methods for identifying, selecting, designing and/or optimizing chemical entities binding PPAR, PPAR γ or PPAR γ -like protein using such coordinates, as well as computer systems comprising data storage media comprising data defining such coordinates.

WO 2008/015276 A1

PROSTAGLANDIN-BINDING POCKET OF PPAR PROTEIN AND USE THEREOF

FIELD OF THE INVENTION

The present invention relates to methods of using the structure coordinates of a prostaglandin-binding pocket in PPAR γ . The invention provides a three-dimensional model of the prostaglandin-binding pocket and means for identifying, designing, screening, evaluating, selecting and/or optimising of chemical entities by rational drug design.

BACKGROUND OF THE INVENTION

The peroxisome proliferator-activated receptors, PPAR α , PPAR γ , and PPAR δ , are examples of orphan nuclear receptors (ONR) involved in transcriptional regulation of metabolic pathways.

The nuclear receptor PPAR γ is a central regulator of adipose tissue development and an important modulator of gene expression in a number of specialized cell types including adipocytes, epithelial cells, and macrophages. PPAR γ signaling pathways impact both cellular and systemic lipid metabolism and have links to obesity, diabetes, and cardiovascular disease (Walczak et al., 2002; Willson et al., 2000). In addition, a dependence between PPAR γ activation by 15-Deoxy $\Delta^{12,14}$ -prostaglandin J₂, a natural ligand to PPAR γ , and a reduction in cancer development (Nosjean and Boutin, 2002; Sawai et al., 2006; Coyle et al., 2005) have been shown. Thiazolidinediones (TZDs) like Rosiglitazone, originally discovered to possess the ability to lower blood glucose and used in treatment of type 2 diabetes, also may inhibit growth and invasiveness of cancer cell lines (Ferruzzi et al., 2005; Han and Roman, 2006).

The crystals structure of the ligand binding domain (LBD) of PPAR γ in complex with Rosiglitazone has been reported (Nolte et al., 1998) and coordinates, accession number 2PRG, have been deposited in the Protein Data Bank (PDB, www.rcsb.org/pdb; Berman et al., 2000). In the same paper (Nolte et al., 1998) the apo structure of the LBD PPAR γ is described and the coordinates deposited in the PDB with the accession number 1PRG.

SUMMARY OF THE INVENTION

The present invention provides methods for evaluating the ability of a chemical entity to associate with a prostaglandin-binding pocket or part of a prostaglandin-binding pocket of a PPAR γ or PPAR γ -like protein using structure coordinates of the prostaglandin-binding pocket as described herein, as well as methods for identifying, selecting, designing and/or optimizing

chemical entities binding PPAR γ or PPAR γ -like protein using such coordinates, as well as computer systems comprising data storage media comprising data defining such coordinates.

BRIEF DESCRIPTION OF THE DRAWINGS

Figure 1 lists the atomic structure coordinates of one of the crystallographic independent molecules of the prostaglandin B₂-complex with LBD PPAR γ (chains P and A, respectively) as derived by X-ray diffraction. A residue type of "E2P" indicates the prostaglandin B₂ molecule while that of "D" indicates a dimethyl sulfoxide (DMSO) molecule. The following abbreviations are used in Figure 1: "Atom type" refers to the element whose coordinates are measured. The first letter in the column defines the element. The "#" sign is an abbreviation for "number" in a numbering of atoms and residues. Residues further have a chain name indicated by a letter in front of the digits as part of the residue numbering. "Resid" refers to the amino acid residue identity in the molecular model. "X, Y, Z" define the atomic position of the element measured. "B" is a thermal factor that measures movement of the atom around its atomic center. "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 the atom has the same position in all symmetry related molecules of the crystal.

Figure 2 lists the atomic structure coordinates of the second crystallographic independent molecule of the prostaglandin B₂ and LBD PPAR γ -complex as (chains P and B, respectively) derived by X-ray diffraction. A residue type of "E2P" indicates the prostaglandin B₂ molecule. The abbreviations are the same as those in Figure 1.

Figure 3 shows a detailed representation of the prostaglandin B₂-binding part of the PPAR γ prostaglandin-binding pocket, in complex with prostaglandin B₂. In black; the prostaglandin B₂ molecule, labelled PGB₂, binding to the PPAR γ A molecule (Figure 1). In light and dark gray; the C α -trace of the PPAR γ A molecule. Dark gray colored residues were, by the CONTACT software program, calculated to be within 5 Å distance from the bound Prostaglandin B₂ molecule, and are labelled with their residue type and number according to Figure 1. Light gray coloured residues are more than 5 Å away from the bound prostaglandin B₂ molecule and are not labelled.

DETAILED DESCRIPTION OF THE INVENTION

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

The present invention is based, in part, on the discovery of a prostaglandin-binding pocket in the PPAR γ structure. Briefly, as described in Example 1, from re-refinement of the so called apo-LBD-PPAR γ structure (Nolte *et al.*, 1998; deposited under accession number 1PRG in the Protein Data Bank), it was discovered that the PPAR γ protein molecule was not in an apo state, but actually bound a ligand. The ligand was recognized to be a prostaglandin molecule; prostaglandin B₂, which is closely related to the natural PPAR γ ligand, 15-Deoxy $\Delta^{12,14}$ -prostaglandin J₂. Further, based on the close contact between atom O12 of the prostaglandin B₂ molecule and the main-chain oxygen of the LEU 228 residue of the PPAR γ molecule (Figure 3), it was discovered that the enol form of the prostaglandin B₂ molecule could make a hydrogen bond to the main chain oxygen of LEU 228. It was also found that the keto form could form a hydrogen-bond to the main-chain amide hydrogen of LEU 228. As shown in Figure 3, adjacent residues also involved in the interaction with the central ring part of the Prostaglandin B₂ molecule included PHE 226, PRO 227, and MET 329. Without being limited to theory, Leu-228-based interactions could be mechanisms by which other prostaglandin such as, e.g., 15-deoxy- $\Delta^{12,14}$ -Prostaglandin J₂, or novel prostaglandin-like chemical entities could bind to the PPAR ligand-binding domain (LBD) described herein.

The binding site of the prostaglandin molecule was found to differ from the Rosiglitazone binding site (Nolte *et al.*, 1998), and only a few atoms of one of the hydrocarbon tails of the prostaglandin molecule were found to reach the Rosiglitazone binding site. Simplified, the complete binding pocket could be described as T-shaped (Nolte *et al.*, 1998), with Rosiglitazone situated in the vertical part of the T-shaped pocket and prostaglandin B₂ situated in the one of side bars of the horizontal part of the T-shape.

The prostaglandin-binding pocket of PPAR γ was also discovered to comprise parts not immediately occupied by prostaglandin B₂, comprising residues ILE 296, ILE 325, THR 328, ALA 331, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380 and LEU 435. The residues defining these parts could be useful in designing novel chemical entities targeting the prostaglandin-binding pocket described herein, or the LBD of PPAR γ or a PPAR γ -like protein.

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; and H = His = Histidine.

As used herein, the following definitions shall apply unless otherwise indicated.

Throughout the specification, the word "comprise", or variations such as "comprises" or "comprising" will be understood to imply the inclusion of a stated integer or groups of integers but not exclusion of any other integer or groups of integers.

- 5 All residue numbers of the PPAR γ structure described in the present patent specification use the numbering scheme as in Figure 1 and SEQ ID NO:1). SEQ ID NO:1 is the full-length sequence of mature PPAR γ , corresponding to SwissProt entry UNIPROT:P37231, identifier PPARG_HUMAN, Version 87 without the 28-amino acid signal sequence. SEQ ID NO:2 is the LBD PPAR γ sequence of Chain A, also shown by structure coordinates in Figure 1. SEQ ID
- 10 NO:3 is the LBD PPAR γ sequence of Chain B, as also shown by structure coordinates in Figure 2. SEQ ID NO:2 (Chain A) and 3 (Chain B) have the same amino acid sequence. The first amino acid residue of SEQ ID NOS:2 and 3, a Glu residue, corresponds to residue number 207 in SEQ ID NO:1, which also is seen in Figure 1. The last amino acid of SEQ ID NOS:2 and 3 corresponds to residue 476 of SEQ ID NO:1. The term "about" when used in the context of
- 15 RMSD values takes into consideration the standard error of the RMSD value, which is ± 0.1 Å.

The term "associating with" refers to a condition of proximity between a chemical entity or compound, or portions thereof, and a prostaglandin-binding pocket or binding site on a protein. The association may be non-covalent wherein the juxtaposition is energetically favoured by hydrogen bonding or by van der Waals or electrostatic interactions or it may be covalent.

- 20 The term "to quantify" refers in the present context to compile calculated values from the computational calculations of said fitting operation between the chemical entity and the prostaglandin-binding pocket.

- As examples of quantification of association mention can be made of the two computer programmes FlexX (A fast flexible docking method using an incremental construction algorithm. M. Rarey, B. Kramer, T. Lengauer, and G. Klebe. Journal of Molecular Biology, 261(3):470–489, 1996) and GOLD (Development and Validation of a Genetic Algorithm for Flexible Docking. G. Jones, P. Willett, R. C. Glen, A. R. Leach and R. Taylor, Journal of Molecular Biology, 267, 727-748, 1997). FlexX calculates a binding energy (expressed in kJ/mol with smaller, more negative energies being more favourable, -10 kJ/mol or less being a typical value for an association between a chemical entity and a binding pocket), whereas GOLD calculates only a
- 25
- 30 binding score (expressed in unitless numbers, with higher numbers being more favourable).

The term "PPAR protein" refers to orphan nuclear receptors (ONR) from the orphan nuclear receptor family. Examples of this family of orphan nuclear receptors include but are not limited to PPAR α , PPAR γ , and PPAR δ .

"Prostaglandin-binding pocket" refers to a binding pocket of a molecule or molecular complex defined by the structure coordinates of a certain set of amino acid residues present in the PPAR γ or PPAR γ -like protein structure, as described below. In general, the ligand for the prostaglandin-binding pocket is a lipid such as prostaglandin. In one aspect of the invention, the prostaglandin-binding pocket is located in the ligand binding domain (LBD) of the PPAR γ molecule. In the protein molecule, PPAR γ , the prostaglandin-binding pocket is buried between the following structure elements (numbering as in Nolte *et al*, 1998 incorporated herein by reference): The loop between helix 1 and 2, the loop between strand 3 and 4, and between helices 3, 5, 8 and 10. The LBD of the PPAR γ protein comprises amino acid residues 207-476 of SEQ ID NO:1, corresponding to SEQ ID NO:2 and 3.

The term "prostaglandin" designates a member of a group of lipid compounds, prostaglandins, that are derived from fatty acids. Prostaglandins contain 20 carbon atoms of which 5 forms a ring structure which may also contain double bonds, a ketone, or alcohol groups. They are also unsaturated carboxylic acids. Prostaglandins are mediators with strong physiological effects.

The term "PPAR γ -like" refers to all or a portion of a molecule or molecular complex that has a commonality of shape and/or sequence identity to all or a portion of the PPAR γ protein. Typically, a PPAR γ -like protein comprises a sequence segment which is at least 65% identical to the LBD of PPAR γ , i.e., residues 207-476 of SEQ ID NO:1. In specific and separate embodiments, the sequence identity between a sequence segment of a PPAR γ -like protein and the LBD of PPAR γ is at least 70%, at least 80%, at least 90%, at least 95%, or at least 99%. In the segment or portion of the PPAR γ -like protein aligned with the LBD of PPAR γ , at least 3, alternatively all four, of PHE 226, PRO 227, LEU 228, and MET 329 may also be conserved. Additionally, in a PPAR γ -like prostaglandin-binding pocket, the commonality of shape may be defined by a root mean square deviation of the structure coordinates of the backbone atoms between the amino acids in a PPAR γ -like prostaglandin-binding pocket and the amino acids in the PPAR γ prostaglandin-binding pocket (as set forth in Figures 1 or 2). Compared to an amino acid in the PPAR γ prostaglandin-binding pocket, the corresponding amino acids in the PPAR γ -like prostaglandin-binding pocket may or may not be identical. Depending on the PPAR γ amino acid residues that define the PPAR γ prostaglandin binding pocket, one skilled in the art would be able to locate the corresponding amino acid residues that define a PPAR γ -like-

prostaglandin binding pocket in a protein based upon sequence and structural homology. In one aspect of the invention, the PPAR γ -like protein is a PPAR γ homologue.

The term "PPAR γ protein complex" or "PPAR γ homologue complex" refers to a molecular complex formed by associating the PPAR γ protein or PPAR γ homologue with a chemical entity.

- 5 The term "binding pocket" refers to a region of a molecule or molecular complex that, as a result of its shape, electrostatic complementarity and hydrophobicity, favourably associates with another chemical entity or compound. The term "pocket" includes, but is not limited to, cleft, channel or site. PPAR, PPAR γ or PPAR γ -like molecules may have binding pockets which include, but are not limited to, peptide or substrate binding, lipid-binding, like the pro-
- 10 taglandin-binding pocket and antibody binding sites.

- The term "ligand" refers to a chemical entity that, as a result of its shape, electrostatic complementarity and hydrophobicity, favourably associates with another chemical entity or compound. The term "ligand" includes, but is not limited to, a lipid, a substrate, an agonist, an antagonist, an inhibitor, an antibody, a drug, a peptide, a protein, DNA, RNA, PNA or a com-
- 15 pound.

- The term "chemical entity" refers to a chemical compound, a complex of at least two chemical compounds, and a fragment of such a compound or complex. The chemical entity may be, for example, a ligand, a lipid, a substrate, an agonist, an antagonist, an inhibitor, an antibody, a drug, a peptide, a protein, DNA, RNA, PNA or a compound. In one aspect, the chemical entity
- 20 is selected from the group consisting of prostaglandins, a prostaglandin analogue and a ligand to the prostaglandin-binding pocket.

- "Conservative substitutions" refers to residues that are physically or functionally similar to the corresponding reference residues. That is, a conservative substitution and its reference residue have similar size, shape, electric charge, chemical properties including the ability to form covalent or hydrogen bonds, or the like. Preferred conservative substitutions are those fulfilling the criteria defined for an accepted point mutation in Dayhoff et al., Atlas of Protein Sequence and Structure, 5, pp. 345-352 (1978 & Supp.), which is incorporated herein by reference. Examples of conservative substitutions are substitutions including but not limited to the following groups: (a) valine, glycine; (b) glycine, alanine; (c) valine, isoleucine, leucine; (d)
- 25 aspartic acid, glutamic acid; (e) asparagine, glutamine; (f) serine, threonine; (g) lysine, arginine, methionine; and (h) phenylalanine, tyrosine, tryptophan.
- 30

The term "corresponding amino acid" or "residue which corresponds to" refers to a particular amino acid or analogue thereof in a PPAR γ protein or PPAR γ -like protein molecule such as a PPAR γ homologue that is identical or functionally equivalent to an amino acid in PPAR γ according to SEQ ID NOS: 1 or 2/3.

- 5 Methods for identifying a corresponding amino acid are known in the art and are based upon sequence, structural alignment, its functional position or a combination thereof as compared to the PPAR γ protein molecule.

For example, corresponding amino acids may be identified by superimposing the backbone atoms of the amino acids in PPAR γ and the PPAR γ homologue using well known software applications, such as QUANTA (Accelrys Inc., San Diego, ©2001, 2002). The corresponding amino
10 acids may also be identified using sequence alignment programs such as the "bestfit" program available from the Genetics Computer Group which uses the local homology algorithm described by Smith and Waterman in Advances in Applied Mathematics 2,482 (1981), which is incorporated herein by reference.

- 15 The term "domain" refers to a portion of the PPAR γ protein or PPAR γ -like protein that can be separated based on its biological function, for example, ligand binding, DNA binding or Zinc fingers. The domain may comprise a binding pocket, a sequence or a structural motif.

The term "fitting operation" refers to an operation that utilizes the structure coordinates of a chemical entity, binding pocket, molecule or molecular complex, or portion thereof, to associate the chemical entity with the binding pocket, molecule or molecular complex, or portion
20 thereof. This may be achieved by positioning, rotating or translating the chemical entity in the binding pocket to match the shape and electrostatic complementarity of the binding pocket. Covalent interactions, non-covalent interactions such as hydrogen bond, electrostatic, hydrophobic, van der Waals interactions, and non-complementary electrostatic interactions such as
25 repulsive charge-charge, dipole-dipole and charge-dipole interactions may be optimized. Alternatively, one may minimize the deformation energy of binding of the chemical entity to the binding pocket.

The term "generating a three-dimensional structure" or "generating a three-dimensional representation" refers to converting the lists of structure coordinates into structural models or
30 graphical representation in three-dimensional space. This can be achieved through commercially or publicly available software. The three-dimensional structure may be displayed or used

to perform computer modelling or fitting operations. In addition, the structure coordinates themselves may be used to perform computer and fitting operations.

The term "homology model" refers to a structural model derived from known three-dimensional structure (s). Generation of the homology model, termed "homology modelling", can include sequence alignment, residue replacement, residue conformation adjustment through energy minimization, or a combination thereof.

The term "homologue of PPAR γ " or "PPAR γ homologue" refers to a molecule that is homologous to PPAR γ by structure or sequence. Examples of homologues include but are not limited to human PPAR γ and PPAR γ from another species with conservative substitutions, additions, deletions or a combination thereof; or another member of the PPAR family including, but not limited to, PPAR α and PPAR δ , with conservative substitutions, additions, deletions or a combination thereof.

The term "homologue of PPAR γ ligand binding domain (LBD)" or "PPAR γ LBD homologues" refer to a molecule having amino acids which correspond to the amino acids in the PPAR γ LBD. Examples of homologues include but are not limited to the LB domain of human PPAR γ and PPAR γ from another species with conservative substitutions; or the LBD of another member of the PPAR family including, but not limited to, PPAR α and PPAR δ , or with conservative substitutions.

The term "molecular complex" or "complex" refers to a molecule associated with at least one chemical entity.

The term "part of a binding pocket" refers to less than all of the amino acid residues that define the binding pocket. For example, the structure coordinates of residues that constitute part of a binding pocket may be specific for defining the chemical environment of the binding pocket, or useful in designing fragments of an inhibitor that may interact with those residues. For example, the portion of residues may be key residues that play a role in ligand binding, or may be residues that are spatially related and define a three-dimensional compartment of the binding pocket. The residues may be contiguous or non-contiguous in primary sequence.

The term "part of a PPAR γ ligand binding domain (LBD)" or "part of a PPAR γ -like ligand binding domain (LBD)" refers to less than all of the PPAR γ or PPAR γ -like LBD, respectively. The structure coordinates of residues that constitute part of a PPAR γ or PPAR γ -LBD may be specific for defining the chemical environment of the domain, or useful in designing fragments of an in-

hibitor that interact with those residues. For example, the portion of residues may be residues that play a role in ligand binding, or may be residues that are spatially related and define a three-dimensional compartment of the domain. The residues may be contiguous or non-contiguous in primary sequence. For example, part of a PPAR γ -LBD can be the ligand binding site, the co-activator site, the lipid binding pocket, the prostaglandin-binding pocket, the AF-2 helix.

The term "part of a PPAR γ protein" or "part of a PPAR γ homologue" refers to less than all of the amino acid residues of a PPAR γ protein or homologue. In one aspect, part of a PPAR γ protein or homologue defines the binding pockets, domains, and motifs of the protein or homologue. The structure coordinates of residues that constitute part of a PPAR γ protein or homologue may be specific for defining the chemical environment of the protein, or useful in designing fragments of an inhibitor that may interact with those residues. The portion of residues may also be residues that are spatially related and define a three-dimensional compartment of a binding pocket, motif or domain. The residues may be contiguous or non-contiguous in primary sequence. For example, the portion of residues may be key residues that play a role in ligand or substrate binding, peptide binding, co-activator binding, DNA binding, metal ion binding, antibody binding, catalysis, structural stabilization or degradation.

The term "root mean square deviation" or "RMSD" 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 from the backbone of the PPAR γ protein molecule, a binding pocket, a motif, a domain, or portion thereof, as defined by the structure coordinates of PPAR γ protein molecule described herein. It would be apparent to the skilled worker that the calculation of RMSD involves a standard error.

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 protein or protein 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 molecule or molecular complex.

Once a chemical entity has been designed or selected according to the invention, the efficiency with which that chemical entity may bind to the PPAR γ or PPAR γ -like prostaglandin-binding pocket as defined herein may be tested and optimized by computational evaluation.

For example, an effective PPAR γ prostaglandin-binding pocket ligand 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 PPAR γ prostaglandin-binding pocket ligands 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. PPAR γ prostaglandin-binding pocket inhibitors may interact with the prostaglandin-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 chemical entity and the average energy of the conformations observed when the inhibitor binds to the protein.

- 10 The term "sufficiently homologous to PPAR γ " refers to a protein that has a sequence homology of at least 20% compared to PPAR γ protein. In one aspect, the sequence homology is at least 40%, 50%, 60%, 70%, 80%, 90%, 95%, 96%, 97%, 98%, or 99%.

The term "three-dimensional structural information" refers to information obtained from the structure coordinates. Structural information generated can include the three-dimensional structure or graphical representation of the structure. Structural information can also be generated when subtracting distances between atoms in the structure coordinates, calculating chemical energies for a PPAR γ molecule or molecular complex or homologues thereof, calculating or minimizing energies for an association of a PPAR γ molecule or molecular complex or homologues thereof to a chemical entity.

- 20 The PPAR γ protein or its homologue 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 cloning, optionally combined with site directed mutagenesis; and/or purification of the natural products. In a preferred aspect, the protein is overexpressed in a baculovirus system, an E. coli system, or a Pichia pastoris system,
- 25

Prostaglandin-binding Pocket of PPAR γ Protein, Protein Complexes or Homologues thereof

- As disclosed above, applicants have provided the three-dimensional X-ray crystal structures of a PPAR γ prostaglandin complex. The invention may in one aspect be useful for inhibitor or activator design for novel drugs to be used in the treatment of cancer or other prostaglandin- and/or PPAR γ -related diseases or conditions, and to study the role of PPAR γ in cell signalling. The atomic coordinate data is presented in Figures 1-2.
- 30

In order to use the structure coordinates generated for the binding pocket it is often necessary to convert the structure coordinates into a three-dimensional shape. This is achieved through the use of commercially available software that is capable of generating three-dimensional graphical representations of molecules or portions thereof from a set of structure coordinates.

Binding pockets, also referred to as binding sites in the present invention, are of significant utility in fields such as drug discovery. The 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 part 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 information is valuable in designing potential inhibitors of the binding pockets of biologically important targets. The prostaglandin-binding pocket of this invention may be important for drug design.

In one aspect, the prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids that comprises amino acid residues corresponding to four or more selected from the group consisting of TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, CYS 285, ARG 288, SER 289, ALA 292, GLU 295, ILE 296, ILE 325, ILE 326, TYR 327, THR 328, MET 329, LEU 330, ALA 331, SER 332, LEU 333, MET 364, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380, ASP 381, LEU 384, and LEU 435 of SEQ ID NO:1

In another aspect, the PPAR γ or PPAR γ -like protein molecule comprises an amino acid sequence at least 65% identical to residues 207-476 of SEQ ID NO:1, and the prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids that comprises (i) an amino acid residue corresponding to LEU 228, and (ii) three or more amino acids corresponding to amino acid residues selected from the group consisting of TYR 222, PHE 226, PRO 227, THR 229, LYS 230, CYS 285, ARG 288, SER 289, ALA 292, GLU 295, ILE 296, ILE 325, ILE 326, TYR 327, THR 328, MET 329, LEU 330, ALA 331, SER 332, LEU 333, MET 364, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380, ASP 381, LEU 384, and LEU 435 of SEQ ID NO:1.

In one embodiment of any of the preceding aspects, the PPAR γ or PPAR γ -like protein molecule comprises an amino acid sequence at least 65% identical to residues 207-476 of SEQ ID

NO:1, and the prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids comprising an amino acid residue corresponding to LEU 228 and six or more corresponding to amino acid residues selected from the group consisting of TYR 222, PHE 226, PRO 227, THR 229, LYS 230, CYS 285, ARG 288, SER 289, ALA 292, GLU 295, ILE 326, TYR 327, MET 329, LEU 330, SER 332, LEU 333, MET 364, ASP 381, and LEU 384.

In an additional or alternative embodiment, the prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids comprising an amino acid residue corresponding to LEU 228 and ten or more corresponding to amino acid residues selected from the group consisting of TYR 222, PHE 226, PRO 227, THR 229, LYS 230, CYS 285, ARG 288, SER 289, ALA 292, GLU 295, ILE 326, TYR 327, MET 329, LEU 330, SER 332, LEU 333, MET 364, ASP 381, and LEU 384.

In another additional or alternative embodiment, the prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids comprises amino acid residues corresponding to PHE 226, PRO 227, LEU 228 and MET 329.

In another additional or alternative embodiment, the prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids comprising amino acid residues corresponding to TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, ALA 292, GLU 295, MET 329, SER 332, LEU 333, ASP 381, and LEU 384.

In another additional or alternative embodiment, the prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids comprising amino acid residues corresponding to one or more selected from the group consisting of CYS 285, ARG 288, SER 289, ILE 326, TYR 327, LEU 330 and MET 364.

In another additional or alternative embodiment, the prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids comprising amino acid residues corresponding to TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, CYS 285, ARG 288, SER 289, ALA 292, GLU 295, ILE 326, TYR 327, MET 329, LEU 330, SER 332, LEU 333, MET 364, ASP 381, and LEU 384.

In another additional or alternative embodiment, the prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids comprising amino acid residues corresponding to one or more selected from the group consisting of ILE 296, ILE

325, THR 328, ALA 331, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380 and LEU 435.

In another additional or alternative embodiment, the prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids comprising amino acid residues corresponding to ILE 296, ILE 325, THR 328, ALA 331, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380 and LEU 435.

In another additional or alternative embodiment, the prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids comprising amino acid residues corresponding to TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, CYS 285, ARG 288, SER 289, ALA 292, GLU 295, ILE 296, ILE 325, ILE 326, TYR 327, THR 328, MET 329, LEU 330, ALA 331, SER 332, LEU 333, MET 364, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380, ASP 381, LEU 384, and LEU 435.

In another aspect, the prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids that correspond to four or more PPAR γ amino acid residues selected from the group consisting of TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, ALA 292, GLU 295, ILE 296, ILE 325, THR 328, MET 329, ALA 331, SER 332, LEU 333, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380, ASP 381, LEU 384, and LEU 435 and optionally one or more selected from the group consisting of CYS 285, ARG 288, SER 289, ILE 326, TYR 327, LEU 330 and MET 364 according to figure 1, wherein the root mean square deviation of the backbone atoms between said amino acid residues and said PPAR γ residues is not greater than about 3 Å. In one aspect, the RMSD is not greater than about 2.0. In one aspect, the RMSD is not greater than about 1.5. In one aspect, the RMSD is not greater than about 1.0. In one aspect, the RMSD is not greater than about 0.8. In one aspect, the RMSD is not greater than about 0.5. In one aspect, the RMSD is not greater than about 0.3. In one aspect, the RMSD is not greater than about 0.2.

In another aspect, the prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids that correspond to PPAR γ amino acid residues selected from the group consisting of PHE 226, PRO 227, LEU 228 and MET 329 according to figure 1, wherein the root mean square deviation of the backbone atoms between said amino acid residues and said PPAR γ residues is not greater than about 3 Å. In one aspect, the RMSD is not greater than about 2.0. In one aspect, the RMSD is not greater than about 1.5. In one aspect, the RMSD is not greater than about 1.0. In one aspect, the RMSD is not greater than about

0.8. In one aspect, the RMSD is not greater than about 0.5. In one aspect, the RMSD is not greater than about 0.3. In one aspect, the RMSD is not greater than about 0.2.

In another aspect, the prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids that correspond to four or more PPAR γ amino acid residues selected from the group consisting of TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, ALA 292, GLU 295, MET 329, SER 332, LEU 333, ASP 381, and LEU 384 and optionally one or more selected from the group consisting of CYS 285, ARG 288, SER 289, ILE 326, TYR 327, LEU 330 and MET 364 according to figure 1, wherein the root mean square deviation of the backbone atoms between said amino acid residues and said PPAR γ residues is not greater than about 3 Å. In one aspect, the RMSD is not greater than about 2.0. In one aspect, the RMSD is not greater than about 1.5. In one aspect, the RMSD is not greater than about 1.0. In one aspect, the RMSD is not greater than about 0.8. In one aspect, the RMSD is not greater than about 0.5. In one aspect, the RMSD is not greater than about 0.3. In one aspect, the RMSD is not greater than about 0.2.

In another aspect, the prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids that correspond to PPAR γ amino acid residues PHE 226, PRO 227, LEU 228 and MET 329 and optionally one or more selected from the group consisting of TYR 222, THR 229, LYS 230, ALA 292, GLU 295, ILE 296, ILE 325, THR 328, ALA 331, SER 332, LEU 333, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380, ASP 381, LEU 384, and LEU 435 and optionally one or more selected from the group consisting of CYS 285, ARG 288, SER 289, ILE 326, TYR 327, LEU 330 and MET 364 according to figure 1, wherein the root mean square deviation of the backbone atoms between said amino acid residues and said PPAR γ residues is not greater than about 3 Å. In one aspect, the RMSD is not greater than about 2.0. In one aspect, the RMSD is not greater than about 1.5. In one aspect, the RMSD is not greater than about 1.0. In one aspect, the RMSD is not greater than about 0.8. In one aspect, the RMSD is not greater than about 0.5. In one aspect, the RMSD is not greater than about 0.3. In one aspect, the RMSD is not greater than about 0.2.

In another aspect, the prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids that correspond to PPAR γ amino acid residues PHE 226, PRO 227, LEU 228 and MET 329 and optionally one or more selected from the group consisting of TYR 222, THR 229, LYS 230, ALA 292, GLU 295, SER 332, LEU 333, ASP 381, and LEU 384 and optionally one or more selected from the group consisting of CYS 285, ARG 288, SER 289, ILE 326, TYR 327, LEU 330 and MET 364 according to figure 1, wherein the root mean square deviation of the backbone atoms between said amino acid residues and said PPAR γ

residues is not greater than about 3 Å. In one aspect, the RMSD is not greater than about 2.0. In one aspect, the RMSD is not greater than about 1.5. In one aspect, the RMSD is not greater than about 1.0. In one aspect, the RMSD is not greater than about 0.8. In one aspect, the RMSD is not greater than about 0.5. In one aspect, the RMSD is not greater than about 0.3. In one aspect, the RMSD is not greater than about 0.2.

In another aspect, the prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids that correspond to PPAR γ amino acid residues TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, ALA 292, GLU 295, MET 329, SER 332, LEU 333, ASP 381, and LEU 384 and optionally one or more selected from the group consisting of CYS 285, ARG 288, SER 289, ILE 326, TYR 327, LEU 330 and MET 364 according to figure 1, wherein the root mean square deviation of the backbone atoms between said amino acid residues and said PPAR γ residues is not greater than about 3 Å. In one aspect, the RMSD is not greater than about 2.0. In one aspect, the RMSD is not greater than about 1.5. In one aspect, the RMSD is not greater than about 1.0. In one aspect, the RMSD is not greater than about 0.8. In one aspect, the RMSD is not greater than about 0.5. In one aspect, the RMSD is not greater than about 0.3. In one aspect, the RMSD is not greater than about 0.2.

In another aspect, the prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids that correspond to PPAR γ amino acid residues TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, ALA 292, GLU 295, ILE 296, ILE 325, THR 328, MET 329, ALA 331, SER 332, LEU 333, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380, ASP 381, LEU 384, and LEU 435 and optionally one or more selected from the group consisting of CYS 285, ARG 288, SER 289, ILE 326, TYR 327, LEU 330 and MET 364 according to figure 1, wherein the root mean square deviation of the backbone atoms between said amino acid residues and said PPAR γ residues is not greater than about 3 Å. In one aspect, the RMSD is not greater than about 2.0. In one aspect, the RMSD is not greater than about 1.5. In one aspect, the RMSD is not greater than about 1.0. In one aspect, the RMSD is not greater than about 0.8. In one aspect, the RMSD is not greater than about 0.5. In one aspect, the RMSD is not greater than about 0.3. In one aspect, the RMSD is not greater than about 0.2.

In another aspect, the prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids that correspond to PPAR γ amino acid residues TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, CYS 285, ARG 288, SER 289, ALA 292, GLU 295, ILE 326, TYR 327, MET 329, LEU 330, SER 332, LEU 333, MET 364, ASP 381, and LEU 384 according to figure 1, wherein the root mean square deviation of the backbone atoms be-

tween said amino acid residues and said PPAR γ residues is not greater than about 3 Å. In one aspect, the RMSD is not greater than about 2.0. In one aspect, the RMSD is not greater than about 1.5. In one aspect, the RMSD is not greater than about 1.0. In one aspect, the RMSD is not greater than about 0.8. In one aspect, the RMSD is not greater than about 0.5. In one aspect, the RMSD is not greater than about 0.3. In one aspect, the RMSD is not greater than about 0.2.

In another aspect, the prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids that correspond to PPAR γ amino acid residues TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, CYS 285, ARG 288, SER 289, ALA 292, GLU 295, ILE 296, ILE 325, ILE 326, TYR 327, THR 328, MET 329, LEU 330, ALA 331, SER 332, LEU 333, MET 364, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380, ASP 381, LEU 384, and LEU 435 according to figure 1, wherein the root mean square deviation of the backbone atoms between said amino acid residues and said PPAR γ residues is not greater than about 3 Å. In one aspect, the RMSD is not greater than about 2.0. In one aspect, the RMSD is not greater than about 1.5. In one aspect, the RMSD is not greater than about 1.0. In one aspect, the RMSD is not greater than about 0.8. In one aspect, the RMSD is not greater than about 0.5. In one aspect, the RMSD is not greater than about 0.3. In one aspect, the RMSD is not greater than about 0.2.

In another aspect, the prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids that correspond to PPAR γ amino acid residues TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, CYS 285, ARG 288, SER 289, ALA 292, GLU 295, ILE 326, TYR 327, MET 329, LEU 330, SER 332, LEU 333, MET 364, ASP 381, and LEU 384 according to the structure of PPAR γ -complex in Figure 1. These above-identified amino acid residues was found to be within 5 Å distance of the ligand bound in the prostaglandin-binding pocket of PPAR γ identified using the program QUANTA (Accelrys Inc., San Diego, ©2001, 2002) and the CONTACT software program of the CCP4 program package (Bailey, 1994), Table 1 and Table 2, which allow the display and output of all residues within 5 Å from the inhibitor.

Further, the LBD of the PPAR γ molecule, with or without any bound ligands, can be run through the VOIDOO software program (Kleywegt and Jones, 1994). From the output of the program voids, pockets within the PPAR γ molecule not filled with atoms, around the position for the prostaglandin B₂ site can predict residues which could be reached and utilized in a drug design process. The amino acid residues which were found using this method was ILE 296, ILE 325, THR 328, ALA 331, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379,

ASP 380 and LEU 435. These residues were situated more than 5 Å from the prostaglandin B2 molecule, but were found to form part of the prostaglandin-binding pocket.

It will be readily apparent to those of skill in the art that the numbering of amino acids in other homologues of PPAR γ may be different than that set forth for PPAR γ . Corresponding
5 amino acids in homologues of PPAR γ are easily identified by visual inspection of the amino acid sequences or by using commercially available sequence homology, structural homology or structure superimposition software programs.

In one aspect of the invention, the PPAR γ or PPAR γ -like protein comprises the amino acid sequence of SEQ ID NO:2 or a homologous sequence.

- 10 In another aspect of the invention, the PPAR γ protein comprises the amino acid sequence of SEQ ID NO:1.

Those of skill in the art understand that a set of structure coordinates for a molecule or a molecular-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
15 similar or identical shape. Moreover, slight variations in the individual coordinates will have little effect on overall shape. In terms of binding pockets, these variations would not be expected to significantly alter the nature of ligands that could associate with those pockets.

The variations in coordinates discussed above may be generated as a result of mathematical manipulations of the PPAR γ structure coordinates. For example, the structure coordinates set
20 forth in Figure 1 or 2 could be manipulated by crystallographic permutations of the structure coordinates, integer additions or subtractions to sets of the structure coordinates, translation or rotation of the structure coordinates or any combination of the above.

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
25 crystal could also account for variations in structure coordinates. If such variations are within a certain root mean square deviation as compared to the original coordinates, the resulting three-dimensional shape is considered encompassed by this invention. Thus, for example, a ligand that binds to the prostaglandin-binding pocket of PPAR γ would also be expected to bind to another binding pocket whose structure coordinates define a shape that falls within the acceptable root mean square deviation.
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Various computational analyses may be necessary to determine whether a prostaglandin-binding pocket of a molecule or molecular complex is sufficiently similar to the prostaglandin-binding pocket of PPAR γ . Such analyses may be carried out using well known software applications, such as ProFit (A. C. R. Martin, SciTech Software, ProFit version 2.5, University College London, <http://www.bioinf.org.uk/software>), Swiss-Pdb Viewer (Guex et al., pp. 2714-2723 (1997)), the Molecular Similarity application of QUANTA (Accelrys Inc., San Diego, ©2001, 2002) and as described in the accompanying User's Guide, which are incorporated herein by reference.

The above programs permit comparisons between different structures, different conformations of the same structure, and different parts of the same structure.

The procedure used in QUANTA (Accelrys Inc., San Diego, ©2001, 2002) and Swiss-Pdb Viewer to compare structures is divided into four steps: 1) load the structures to be compared; 2) define the atom equivalences in these structures; 3) perform a fitting operation on the structures; and 4) analyze the results.

The procedure used in ProFit to compare structures includes the following steps load the structures to be compared; 2) specify selected residues of interest; 3) define the atom equivalences in the selected residues; 4) perform a fitting operation on the selected residues; and 5) analyze the results.

Each structure in the comparison 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 the above programs is defined by user input, for the purpose of this invention we will define equivalent atoms as protein backbone atoms (N, C and for PPAR γ amino acids and corresponding amino acids in the structures being compared).

The corresponding amino acids may be identified by sequence alignment programs such as the "bestfit" program available from the Genetics Computer Group which uses the local homology algorithm described by Smith and Waterman in *Advances in Applied Mathematics* 2,482 (1981), which is incorporated herein by reference. A suitable amino acid sequence alignment will require that the proteins being aligned share minimum percentage of identical amino acids. Generally, a first protein being aligned with a second protein should share in excess of about 35% identical amino acids [Hanks et al., *Science*, 241,42 (1988); Hanks and Quinn, *Methods in Enzymology*, 200,38 (1991)]. The identification of equivalent residues can

also be assisted by secondary structure alignment, for example, aligning the α -helices, β -sheets in the structure. The program Swiss-Pdb Viewer has its own best fit algorithm that is based on secondary sequence alignment.

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 the above programs. The Swiss-Pdb Viewer program sets an RMSD cutoff for eliminating pairs of equivalent atoms that have high RMSD values. An RMSD cutoff value can be used to exclude pairs of equivalent atoms with extreme individual RMSD values. In the program ProFit, the RMSD cutoff value can be specified by the user.

The RMSD values are averages of individual RMSD values calculated for the backbone atoms (C, N and Ca) of all residues in the LBD or prostaglandin-binding pocket between the reference structure and the other PPAR γ -inhibitor complex structures.

Computer Systems

According to another aspect, this invention provides a machine-readable data storage medium, comprising a data storage material encoded with machine-readable data, wherein said data defines the above-mentioned prostaglandin-binding pockets by comprising the structure coordinates of said amino acid residues according to any one of Figures 1-2.

In one aspect of the invention, a computer comprising: (a) a machine-readable data storage medium, comprising a data storage material encoded with machine-readable data, wherein said data defines a prostaglandin-binding pocket of a PPAR protein molecule, which prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids that comprises amino acid residues corresponding to four or more selected from the group consisting of TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, CYS 285, ARG 288, SER 289, ALA 292, GLU 295, ILE 296, ILE 325, ILE 326, TYR 327, THR 328, MET 329, LEU 330, ALA 331, SER 332, LEU 333, MET 364, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380, ASP 381, LEU 384, and LEU 435 of SEQ ID NO:1; (b) a working memory for storing instructions for processing said machine-readable data; (c) a central processing unit coupled to said working memory and to said machine-readable data storage medium for processing said machine-readable data and means for generating three-

dimensional structural information of said binding pocket; and (d) output hardware coupled to said central processing unit for outputting three-dimensional structural information of said binding pocket, or information produced using said three-dimensional structural information of said binding pocket, is provided.

- 5 In another aspect of the invention, a computer comprising: (a) a machine-readable data storage medium, comprising a data storage material encoded with machine-readable data, wherein said data defines a prostaglandin-binding pocket of a PPAR γ or PPAR γ -like protein molecule comprising an amino acid sequence at least 65% identical to residues 207-476 of SEQ ID NO:1, which prostaglandin-binding pocket is defined by three-dimensional structure
- 10 coordinates of a set of amino acids that comprises (i) an amino acid residue corresponding to LEU 228, and (ii) three or more amino acids corresponding to amino acid residues selected from the group consisting of TYR 222, PHE 226, PRO 227, THR 229, LYS 230, CYS 285, ARG 288, SER 289, ALA 292, GLU 295, ILE 296, ILE 325, ILE 326, TYR 327, THR 328, MET 329, LEU 330, ALA 331, SER 332, LEU 333, MET 364, PHE 374, ASN 375, ALA 376, LEU 377, GLU
- 15 378, LEU 379, ASP 380, ASP 381, LEU 384, and LEU 435 of SEQ ID NO:1; (b) a working memory for storing instructions for processing said machine-readable data; (c) a central processing unit coupled to said working memory and to said machine-readable data storage medium for processing said machine-readable data and means for generating three-dimensional structural information of said binding pocket; and (d) output hardware coupled to
- 20 said central processing unit for outputting three-dimensional structural information of said binding pocket, or information produced using said three-dimensional structural information of said binding pocket, is provided. In another aspect of the invention, a computer comprising: (a) a machine-readable data storage medium, comprising a data storage material encoded with machine-readable data, wherein said data defines a prostaglandin-binding pocket of a
- 25 PPAR γ or PPAR γ -like protein molecule, which prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids that correspond to four or more PPAR γ amino acid residues selected from the group consisting of TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, ALA 292, GLU 295, ILE 296, ILE 325, THR 328, MET 329, ALA 331, SER 332, LEU 333, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380, ASP 381, LEU 384, and LEU 435 and optionally one or more selected from the group consisting of CYS 285, ARG 288, SER 289, ILE 326, TYR 327, LEU 330 and MET 364 according to figure 1, wherein the root mean square deviation of the backbone atoms between amino acid
- 30 residues of said molecule and said PPAR γ residues is not greater than about 3 Å; (b) a working memory for storing instructions for processing said machine-readable data; (c) a central processing unit coupled to said working memory and to said machine-readable data storage medium for processing said machine-readable data and means for generating three-
- 35

dimensional structural information of said binding pocket; and (d) output hardware coupled to said central processing unit for outputting three-dimensional structural information of said binding pocket, or information produced using said three-dimensional structural information of said binding pocket, is provided.

5 To use the structure coordinates generated for PPAR γ , homologues thereof, or its prostaglandin-binding pocket, it is at times necessary to convert them into a three-dimensional shape. This is achieved through the use of commercially or publicly available software that is capable of generating a three-dimensional structure of molecules or portions thereof from a set of structure coordinates. The three-dimensional structure may be displayed as a graphical
10 representation.

Therefore, according to another aspect, this invention provides a machine-readable data storage medium comprising a data storage material encoded with machine readable data. In one aspect, a machine programmed with instructions for using said data, is capable of generating a three-dimensional structure of any of the prostaglandin-binding pockets that are defined
15 herein.

This invention also provides a computer comprising: (a) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data defines any one of the above defined prostaglandin-binding pockets; (b) a working memory for storing instructions for processing said machine-readable data; (c) a central
20 processing unit (CPU) coupled to said working memory and to said machine-readable data storage medium for processing said machine readable data and means for generating three-dimensional structural information of said binding pockets; and (d) output hardware coupled to said central processing unit for outputting three-dimensional structural information of said prostaglandin-binding pockets, or information produced using said three-dimensional structural information of said prostaglandin-binding pockets.
25

Three-dimensional data generation may be provided by an instruction or set of instructions such as a computer program or commands for generating a three-dimensional structure or graphical representation from structure coordinates, or by calculating distances between atoms, calculating chemical energies for a PPAR γ molecule or molecular complex or homologues thereof, or calculating or minimizing energies for an association of a PPAR γ molecule or molecular complex or homologues thereof to a chemical entity. The graphical representation can be generated or displayed by commercially available software programs. Examples of software programs include but are not limited to QUANTA (Accelrys Inc., San Diego, © 2001,
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2002), O (Jones et al. Acta A47, pp. 110-119 (1991)) and RIBBONS (Carson, Appl. Crystallogr., 24, pp. 9589-961 (1991)), which are incorporated herein by reference. Certain software programs may imbue this representation with physico-chemical attributes which are known from the chemical composition of the molecule, such as residue charge, hydrophobicity, torsional and rotational degrees of freedom for the residue or segment, etc. Examples of software programs for calculating chemical energies are described in the Rational Drug Design section.

In one aspect, the computer is executing instruction(s) such as a computer program for three-dimensional data generation.

- 10 Information of said binding pocket or information produced by using said binding pocket can be outputted through display terminals, touchscreens, facsimile machines, modems, CD-ROMs, printers or disk drives. The information can be in graphical or alphanumeric form.

The "Computer system" includes in one aspect of the invention a computer comprising a central processing unit ("CPU"), a working memory which may be, e. g., RAM (random-access memory) or "core" memory, mass storage memory (such as one or more disk drives, DVD or CD-ROM drives), one or more cathode-ray tube ("CRT") displays or liquid-crystal-display (LCDs) terminals, one or more keyboards, one or more input lines using e.g. Ethernet cable, USB or Firewire cables, RSR232, parallel cables or so called wire-less connection, and one or more output lines using e.g. Ethernet cable, USB or Firewire cables, RSR232, parallel cables or so called wire-less connection, all of which are interconnected by a conventional bi-directional system bus.

Input hardware, coupled to computer by input lines, 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 connected by a telephone line dedicated data line or so called wire-less connection.

- 25 Alternatively or additionally, the input hardware may comprise CD-ROM drives, DVD drives, disk drives or various sorts of flash memory drives. In conjunction with display terminal, keyboard mouse or pen tablets may also be used as an input device.

Output hardware, coupled to computer by output lines, may similarly be implemented by conventional devices. By way of example, output hardware may include CRT display or LCD terminal for displaying a graphical representation of a prostaglandin-binding pocket of this invention using a program such as QUANTA as described herein. Output hardware may also include

a printer, so that hard copy output may be produced, or a disk drive, to store system output for later use. Output hardware may also include a CD or DVD recorder, ZIP, USB drives, various sorts of flash memory or other machine-readable data storage device.

In operation, CPU coordinates the use of the various input and output devices, coordinates data accesses from mass storage and accesses to and from working memory, and determines the sequence of data processing steps. A number of 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 are included as appropriate throughout the following description of the data storage medium.

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

The magnetic domains of coating of medium 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.

A cross section of an optically-readable data storage medium 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 a system described above. Medium 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 writeable. Medium preferably has a suitable substrate, which may be conventional, and a suitable coating, which may be conventional, usually of one side of substrate.

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

In the case of a magneto-optical disk, as is well known, coating has no pits, but has a plurality of magnetic domains whose polarity or orientation can be changed magnetically when heated above a certain temperature, as by a laser. The orientation of the domains can be read by measuring the polarization of laser light reflected from coating. The arrangement of the domains encodes the data as described above.

In one aspect, the structure coordinates of PPAR γ - or PPAR γ -like molecules are produced by homology modelling (Sali, A. "Modeling mutations and homologous proteins," *Curr. Opin. Biotech.*, 6, 437-451 (1995)) of at least a portion of the structure coordinates of Figure 1 or 2. Homology modelling can be used to generate structural models of PPAR γ homologues or other homologous proteins based on the known structure of PPAR γ . This can be achieved by performing one or more of the following steps: performing sequence alignment between the amino acid sequence of an unknown molecule against the amino acid sequence of PPAR γ ; identifying conserved and variable regions by sequence or structure; generating structure coordinates for structurally conserved residues of the unknown structure from those of PPAR γ ; generating conformations for the structurally variable residues in the unknown structure; replacing the non-conserved residues of PPAR γ with residues in the unknown structure; building side chain conformations; and refining and/or evaluating the unknown structure.

For example, since the protein sequence of the ligand binding domain of PPAR γ and PPAR α or PPAR δ can be aligned relative to each other, it is possible to construct models of the structures of PPAR α or PPAR δ , particularly in the regions of the binding pockets, using the PPAR γ structure, or the opposite way, making PPAR γ models using PPAR α or PPAR δ molecular structures. Software programs that are useful in homology modelling include XALIGN (Wishart, D. S. et al., *Comput. Appl. Biosci.*, 10, pp. 687-88 (1994)) and CLUSTAL W Alignment Tool (Higgins D. G. et al., *Methods Enzymol.*, 266, pp. 383-402 (1996)). See also, U. S. Patent No. 5,884, 230. These references are incorporated herein by reference.

To perform the sequence alignment, programs such as available from the Genetics Computer Group (Waterman in *Advances in Applied Mathematics* 2, 482 (1981), which is incorporated herein by reference) and CLUSTAL W Alignment Tool (Higgins D. G. et al., *Methods Enzymol.*, 266, pp. 383-402 (1996), which is incorporated by reference) can be used. To model the amino acid side chains of PPAR α or PPAR δ , the amino acid residues in PPAR γ can be replaced, using a computer graphics program such as "O" (Jones et al, (1991) *Acta Cryst. Sect. A*, 47: 110-119), by those of the homologous protein, where they differ. The same orientation or a different orientation of the amino acid can be used. Insertions and deletions of amino acid residues may be necessary where gaps occur in the sequence alignment.

Homology modelling can be performed using, for example, the computer programs SWISS-MODEL available through Glaxo Wellcome Experimental Research in Geneva, Switzerland; WHATIF available on EMBL servers ; Schnare et al., J. Mol. Biol, 256: 701-719 (1996); Blundell et al., Nature 326: 347-352 (1987); Fetrow and Bryant, Bio/Technology 11: 479-484 (1993); Greer, Methods in Enzymology 202: 239-252 (1991); and Johnson et Crit. Rev. Biochem. Mol Biol. 29: 1-68 (1994). An example of homology modelling can be found, for example, in Szklarz G. D., Life Sci. 61: 2507-2520 (1997). These references are incorporated herein by reference.

Thus, in accordance with the present invention, data capable of generating the three-dimensional structure of the above prostaglandin-binding pockets, can be stored in a machine-readable storage medium, which is capable of displaying a graphical three-dimensional representation of the structure.

Rational Drug Design

The PPAR γ structure coordinates as described above or the three-dimensional graphical representation generated from these coordinates may be used in conjunction with a computer for a variety of purposes, including drug discovery.

For example, the structure encoded by the data may be computationally evaluated for its ability to associate with chemical entities. Chemical entities that associate with PPAR γ may inhibit or activate PPAR γ or its homologues, and are potential drug candidates. Alternatively, the structure encoded by the data may be displayed in a 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.

In a further aspect of the invention, a method for screening for chemical entities useful for the treatment of prostaglandin and/or PPAR related diseases such as cancer (especially in lung, skin, breast, colon, pancreas, prostate, liposarcoma), inflammation, skin and hair disorders, diabetes, obesity, hypertension, and impaired glucose tolerance, is provided. In one embodiment, the invention provides a method for screening for chemical entities useful for the treatment of cancer (especially in lung, skin, breast, colon, pancreas, prostate, and/or liposarcoma).

In one aspect, the invention thus provides a method for evaluating the ability of a chemical entity to associate with a prostaglandin-binding pocket of a PPAR protein molecule, which

prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids that comprises amino acid residues corresponding to four or more selected from the group consisting of TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, CYS 285, ARG 288, SER 289, ALA 292, GLU 295, ILE 296, ILE 325, ILE 326, TYR 327, THR 328, MET 329, LEU 330, ALA 331, SER 332, LEU 333, MET 364, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380, ASP 381, LEU 384, and LEU 435 of SEQ ID NO:1, comprising the steps of: (a) providing the structure coordinates of said prostaglandin-binding pocket on a computer comprising the means for generating three-dimensional structural information from said structure coordinates; (b) employing computational means to perform a fitting operation between the chemical entity and the prostaglandin-binding pocket; and (c) analyzing the results of said fitting operation to evaluate the association between the chemical entity and the prostaglandin-binding pocket. In a further aspect of the invention, step (c) further comprises that the association is quantified. In another aspect, the invention provides a method for evaluating the ability of a chemical entity to associate with prostaglandin-binding pocket of a PPAR γ or PPAR γ -like protein molecule comprising an amino acid sequence at least 65% identical to residues 207-476 of SEQ ID NO:1, which prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids that comprises (i) an amino acid residue corresponding to LEU 228, and (ii) three or more amino acids corresponding to amino acid residues selected from the group consisting of TYR 222, PHE 226, PRO 227, THR 229, LYS 230, CYS 285, ARG 288, SER 289, ALA 292, GLU 295, ILE 296, ILE 325, ILE 326, TYR 327, THR 328, MET 329, LEU 330, ALA 331, SER 332, LEU 333, MET 364, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380, ASP 381, LEU 384, and LEU 435 of SEQ ID NO:1, comprising the steps of: (a) providing the structure coordinates of said prostaglandin-binding pocket on a computer comprising the means for generating three-dimensional structural information from said structure coordinates; (b) employing computational means to perform a fitting operation between the chemical entity and the prostaglandin-binding pocket; and (c) analyzing the results of said fitting operation to evaluate the association between the chemical entity and the prostaglandin-binding pocket. In a further aspect of the invention, step (c) further comprises that the association is quantified.

In another aspect, the invention provides a method for evaluating the ability of a chemical entity to associate with a prostaglandin-binding pocket of a PPAR γ or PPAR γ -like protein molecule, which prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids that correspond to four or more PPAR γ amino acid residues selected from the group consisting of TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, ALA 292, GLU 295, ILE 296, ILE 325, THR 328, MET 329, ALA 331, SER 332, LEU 333, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380, ASP 381, LEU 384, and LEU

435 and optionally one or more selected from the group consisting of CYS 285, ARG 288, SER 289, ILE 326, TYR 327, LEU 330 and MET 364 according to figure 1, wherein the root mean square deviation of the backbone atoms between amino acid residues of said molecule and said PPAR γ residues is not greater than about 3 Å, comprising the steps of: (a) providing the structure coordinates of said prostaglandin-binding pocket on a computer comprising the means for generating three-dimensional structural information from said structure coordinates; (b) employing computational means to perform a fitting operation between the chemical entity and the prostaglandin-binding pocket; and (c) analyzing the results of said fitting operation to evaluate the association between the chemical entity and the prostaglandin-binding pocket. In a further aspect of the invention, step (c) further comprises that the association is quantified.

In a further aspect, the above method further comprises generating a three-dimensional graphical representation of the prostaglandin-binding pocket prior to step (b).

In above aspect of the invention and in the following aspects the prostaglandin-binding pocket can be further defined as follows:

In one aspect of the invention, the prostaglandin-binding pocket is defined by structure coordinates of a set of amino acids that correspond to four or more PPAR γ amino acid residues selected from the group consisting of TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, ALA 292, GLU 295, MET 329, SER 332, LEU 333, ASP 381, and LEU 384.

In a further aspect of the invention, the prostaglandin-binding pocket is defined by structure coordinates of a set of amino acids that correspond to PPAR γ amino acid residues PHE 226, PRO 227, LEU 228 and MET 329 and optionally one or more selected from the group consisting of TYR 222, THR 229, LYS 230, ALA 292, GLU 295, ILE 296, ILE 325, THR 328, ALA 331, SER 332, LEU 333, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380, ASP 381, LEU 384, and LEU 435.

In a further aspect of the invention, the prostaglandin-binding pocket is defined by structure coordinates of a set of amino acids that correspond to PPAR γ amino acid residues PHE 226, PRO 227, LEU 228 and MET 329 and optionally one or more selected from the group consisting of TYR 222, THR 229, LYS 230, ALA 292, GLU 295, SER 332, LEU 333, ASP 381, and LEU 384.

In a further aspect of the invention, the prostaglandin-binding pocket is defined by structure coordinates of a set of amino acids that correspond to PPAR γ amino acid residues TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, ALA 292, GLU 295, MET 329, SER 332, LEU 333, ASP 381, and LEU 384.

- 5 In a further aspect of the invention, the prostaglandin-binding pocket is defined by structure coordinates of a set of amino acids that correspond to PPAR γ amino acid residues TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, ALA 292, GLU 295, ILE 296, ILE 325, THR 328, MET 329, ALA 331, SER 332, LEU 333, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380, ASP 381, LEU 384, and LEU 435.
- 10 In a further aspect of the invention, the prostaglandin-binding pocket is defined by structure coordinates of a set of above amino acids and further comprises one or more amino acids that correspond to PPAR γ amino acid residues selected from the group consisting of CYS 285, ARG 288, SER 289, ILE 326, TYR 327, LEU 330 and MET 364.

- 15 In a further aspect of the invention, the prostaglandin-binding pocket is defined by structure coordinates of a set of amino acids that correspond to PPAR γ amino acid residues TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, CYS 285, ARG 288, SER 289, ALA 292, GLU 295, ILE 326, TYR 327, MET 329, LEU 330, SER 332, LEU 333, MET 364, ASP 381, and LEU 384.

- 20 In a further aspect of the invention, the prostaglandin-binding pocket is defined by structure coordinates of a set of amino acids that correspond to PPAR γ amino acid residues TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, CYS 285, ARG 288, SER 289, ALA 292, GLU 295, ILE 296, ILE 325, ILE 326, TYR 327, THR 328, MET 329, LEU 330, ALA 331, SER 332, LEU 333, MET 364, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380, ASP 381, LEU 384, and LEU 435.

- 25 In another aspect, the invention provides a method of designing a compound or complex that associates with a prostaglandin-binding pocket of a PPAR protein molecule, which prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids that comprises amino acid residues corresponding to four or more selected from the group consisting of TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, CYS 285,
- 30 ARG 288, SER 289, ALA 292, GLU 295, ILE 296, ILE 325, ILE 326, TYR 327, THR 328, MET 329, LEU 330, ALA 331, SER 332, LEU 333, MET 364, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380, ASP 381, LEU 384, and LEU 435 of SEQ ID NO:1, comprising the

steps of: (a) providing the structure coordinates of said prostaglandin-binding pocket on a computer comprising the means for generating three- dimensional structural information from said structure coordinates; and (b) using the computer to perform a fitting operation to associate a first chemical entity with the prostaglandin-binding pocket; (c) performing a fitting operation to associate at least a second chemical entity with the prostaglandin-binding pocket; (d) quantifying the association between the first and second chemical entity and the prostaglandin-binding pocket; (e) optionally repeating steps b) to d) with another first and second chemical entity, selecting a first and a second chemical entity based on said quantified association of all of said first and second chemical entity; (f) optionally, visually inspecting the relationship of the first and second chemical entity to each other in relation to the prostaglandin-binding pocket on a computer screen using the three-dimensional graphical representation of the prostaglandin-binding pocket and said first and second chemical entity; and (g) assembling the first and second chemical entity into a compound or complex that associates with said prostaglandin-binding pocket by model building.

In another aspect, the invention provides a method of designing a compound or complex that associates with a prostaglandin-binding pocket of a PPAR γ or PPAR γ -like protein molecule comprising an amino acid sequence at least 65% identical to residues 207-476 of SEQ ID NO:1, which prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids that comprises (i) an amino acid residue corresponding to LEU 228, and (ii) three or more amino acids corresponding to amino acid residues selected from the group consisting of TYR 222, PHE 226, PRO 227, THR 229, LYS 230, CYS 285, ARG 288, SER 289, ALA 292, GLU 295, ILE 296, ILE 325, ILE 326, TYR 327, THR 328, MET 329, LEU 330, ALA 331, SER 332, LEU 333, MET 364, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380, ASP 381, LEU 384, and LEU 435 of SEQ ID NO:1, comprising the steps of: (a) providing the structure coordinates of said prostaglandin-binding pocket on a computer comprising the means for generating three- dimensional structural information from said structure coordinates; and (b) using the computer to perform a fitting operation to associate a first chemical entity with the prostaglandin-binding pocket; (c) performing a fitting operation to associate at least a second chemical entity with the prostaglandin-binding pocket; (d) quantifying the association between the first and second chemical entity and the prostaglandin-binding pocket; (e) optionally repeating steps b) to d) with another first and second chemical entity, selecting a first and a second chemical entity based on said quantified association of all of said first and second chemical entity; (f) optionally, visually inspecting the relationship of the first and second chemical entity to each other in relation to the prostaglandin-binding pocket on a computer screen using the three-dimensional graphical representation of the prostaglandin-binding pocket and said first and second chemical entity; and

(g) assembling the first and second chemical entity into a compound or complex that associates with said prostaglandin-binding pocket by model building.

In another aspect, the invention provides a method of designing a compound or complex that associates with a prostaglandin-binding pocket of a PPAR γ or PPAR γ -like protein molecule, which prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids that correspond to four or more PPAR γ amino acid residues selected from the group consisting of TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, ALA 292, GLU 295, ILE 296, ILE 325, THR 328, MET 329, ALA 331, SER 332, LEU 333, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380, ASP 381, LEU 384, and LEU 435 and optionally one or more selected from the group consisting of CYS 285, ARG 288, SER 289, ILE 326, TYR 327, LEU 330 and MET 364 according to figure 1, wherein the root mean square deviation of the backbone atoms between amino acid residues of said molecule and said PPAR γ residues is not greater than about 3 Å, comprising the steps of: (a) providing the structure coordinates of said prostaglandin-binding pocket on a computer comprising the means for generating three-dimensional structural information from said structure coordinates; and (b) using the computer to perform a fitting operation to associate a first chemical entity with the prostaglandin-binding pocket; (c) performing a fitting operation to associate at least a second chemical entity with the prostaglandin-binding pocket; (d) quantifying the association between the first and second chemical entity and the prostaglandin-binding pocket; (e) optionally repeating steps b) to d) with another first and second chemical entity, selecting a first and a second chemical entity based on said quantified association of all of said first and second chemical entity; (f) optionally, visually inspecting the relationship of the first and second chemical entity to each other in relation to the prostaglandin-binding pocket on a computer screen using the three-dimensional graphical representation of the prostaglandin-binding pocket and said first and second chemical entity; and (g) assembling the first and second chemical entity into a compound or complex that associates with said prostaglandin-binding pocket by model building.

According to another aspect, the invention provides a method for designing, selecting and/or optimizing a chemical entity that binds a prostaglandin-binding pocket of a PPAR protein molecule, which prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids that comprises amino acid residues corresponding to four or more selected from the group consisting of TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, CYS 285, ARG 288, SER 289, ALA 292, GLU 295, ILE 296, ILE 325, ILE 326, TYR 327, THR 328, MET 329, LEU 330, ALA 331, SER 332, LEU 333, MET 364, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380, ASP 381, LEU 384, and LEU 435 of SEQ ID

NO:1, comprising the steps of: (a) providing the structure coordinates of said prostaglandin-binding pocket on a computer comprising the means for generating three-dimensional structural information from said structure coordinates; and (b) designing, selecting and/or optimizing said chemical entity by performing a fitting operation between said chemical entity and said three-dimensional structural information of said prostaglandin-binding pocket.

According to another aspect, the invention provides a method for designing, selecting and/or optimizing a chemical entity that binds a prostaglandin-binding pocket of a PPAR γ or PPAR γ -like protein molecule comprising an amino acid sequence at least 65% identical to residues 207-476 of SEQ ID NO:1, which prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids that comprises (i) an amino acid residue corresponding to LEU 228, and (ii) three or more amino acids corresponding to amino acid residues selected from the group consisting of TYR 222, PHE 226, PRO 227, THR 229, LYS 230, CYS 285, ARG 288, SER 289, ALA 292, GLU 295, ILE 296, ILE 325, ILE 326, TYR 327, THR 328, MET 329, LEU 330, ALA 331, SER 332, LEU 333, MET 364, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380, ASP 381, LEU 384, and LEU 435 of SEQ ID NO:1, comprising the steps of: (a) providing the structure coordinates of said prostaglandin-binding pocket on a computer comprising the means for generating three-dimensional structural information from said structure coordinates; and (b) designing, selecting and/or optimizing said chemical entity by performing a fitting operation between said chemical entity and said three-dimensional structural information of said prostaglandin-binding pocket.

According to another aspect, the invention provides a method for designing, selecting and/or optimizing a chemical entity that binds the prostaglandin-binding pocket of a PPAR γ or PPAR γ -like protein molecule, which prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids that correspond to four or more PPAR γ amino acid residues selected from the group consisting of TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, ALA 292, GLU 295, ILE 296, ILE 325, THR 328, MET 329, ALA 331, SER 332, LEU 333, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380, ASP 381, LEU 384, and LEU 435 and optionally one or more selected from the group consisting of CYS 285, ARG 288, SER 289, ILE 326, TYR 327, LEU 330 and MET 364 according to figure 1, wherein the root mean square deviation of the backbone atoms between amino acid residues of said molecule and said PPAR γ residues is not greater than about 3 Å comprising the steps of: (a) providing the structure coordinates of said prostaglandin-binding pocket on a computer comprising the means for generating three-dimensional structural information from said structure coordinates; and (b) designing, selecting and/or optimizing said chemical entity by

performing a fitting operation between said chemical entity and said three-dimensional structural information of said prostaglandin-binding pocket.

In one aspect, the above methods for designing, selecting, and/or optimizing a chemical entity further comprises the following steps before step (a): (c) producing a crystal of a molecule or molecular complex comprising PPAR γ or homologue thereof; (d) determining the three-dimensional structure coordinates of the molecule or molecular complex by X-ray diffraction of the crystal; and (e) identifying the prostaglandin-binding pocket.

Three-dimensional structural information in step (a) may be generated by instructions such as a computer program or commands that can generate a three-dimensional structure or graphical representation; subtract distances between atoms; calculate chemical energies for a PPAR γ molecule, molecular complex or homologues thereof; or calculate or minimize energies of an association of PPAR γ molecule, molecular complex or homologues thereof to a chemical entity. These types of computer programs are known in the art. The graphical representation can be generated or displayed by commercially available software programs. Examples of software programs include but are not limited to QUANTA (Accelrys Inc., San Diego, ©2001, 2002), O (Jones et al., Acta A47, pp. 110-119 (1991)) and RIBBONS (Carson, J. Appl. 24, pp. 9589-961 (1991)), which are incorporated herein by reference. Certain software programs may imbue this representation with physico-chemical attributes which are known from the chemical composition of the molecule, such as residue charge, hydrophobicity, torsional and rotational degrees of freedom for the residue or segment, etc. Examples of software programs for calculating chemical energies are described below.

In one aspect, the method is for evaluating the ability of a chemical entity to associate with a prostaglandin-binding pocket as defined above.

This method comprises the steps of: (a) employing computational means to perform a fitting operation between the chemical entity and the prostaglandin-binding pocket as described before; (b) analyzing the results of said fitting operation to quantify the association between the chemical entity and the prostaglandin-binding pocket; and optionally (c) outputting said quantified association to a suitable output hardware, such as a CRT display terminal or LCD monitor, a CD or DVD recorder, a disk drive, or other machine-readable data storage device, as described previously. The method may further comprise generating a three-dimensional structure, graphical representation thereof, or both of all or part of the molecule or molecular complex prior to step (a).

In another aspect, the invention provides a method for screening a plurality of chemical entities to associate more strongly than a given threshold value, such as a deformation energy of binding of less than 7 kcal/mol, with said prostaglandin-binding pocket:

(a) employing computational means, which utilize said structure coordinates to perform a fitting operation between one of said chemical entities from the plurality of chemical entities and said prostaglandin-binding pocket;

(b) quantifying the binding between the chemical entity and the prostaglandin-binding pocket; (c) repeating steps (a) and (b) for each remaining chemical entity; and (d) outputting to a suitable output hardware a set of chemical entities that associate with the prostaglandin-binding pocket more strongly than a chosen threshold value, optionally defined as an upper quantile yielding the desired fraction of chemical entities.

In another aspect, the method comprises the steps of: (a) constructing a computer model of a prostaglandin-binding pocket; b) selecting a chemical entity to be evaluated by a method selected from the group consisting of assembling said chemical entity; selecting a chemical entity from a small molecule database; *de novo* ligand design of said chemical entity; and modifying a known agonist or inhibitor, or a portion thereof, of an PPAR γ protein or homologue thereof; (c) employing computational means to perform a fitting operation between computer models of said chemical entity to be evaluated and said prostaglandin-binding pocket in order to provide an energy-minimized configuration of said chemical entity in the prostaglandin-binding pocket; and (d) evaluating the results of said fitting operation to quantify the association between said chemical entity and the prostaglandin-binding pocket model, whereby evaluating the ability of said chemical entity to associate with said prostaglandin-binding pocket.

In another aspect, the invention provides a method of using a computer for evaluating the ability of a chemical entity to associate with a prostaglandin-binding pocket of a PPAR γ or PPAR γ -like protein molecule comprising an amino acid sequence at least 65% identical to residues 207-476 of SEQ ID NO:1, which prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids that comprises (i) an amino acid residue corresponding to LEU 228, and (ii) three or more amino acids corresponding to amino acid residues selected from the group consisting of TYR 222, PHE 226, PRO 227, THR 229, LYS 230, CYS 285, ARG 288, SER 289, ALA 292, GLU 295, ILE 296, ILE 325, ILE 326, TYR 327, THR 328, MET 329, LEU 330, ALA 331, SER 332, LEU 333, MET 364, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380, ASP 381, LEU 384, and LEU 435 of SEQ ID

NO:1, wherein said computer comprises a machine-readable data storage medium comprising a data storage material encoded with said structure coordinates defining said prostaglandin-binding pocket and means for generating a three-dimensional graphical representation of the prostaglandin-binding pocket, and wherein said method comprises the steps of: (a) position-
5 ing a first chemical entity within said prostaglandin-binding pocket using a graphical three-dimensional representation of the structure of the chemical entity and the prostaglandin-binding pocket; (b) performing a fitting operation between said chemical entity and said prostaglandin-binding pocket by employing computational means; and (c) analyzing the results of said fitting operation to quantify the association between said chemical entity and the prostaglandin-binding pocket and optionally (d) outputting said quantified association to a suitable
10 output hardware.

In another aspect, the invention provides a method of using a computer for evaluating the ability of a chemical entity to associate with a prostaglandin-binding pocket of a PPAR γ or PPAR γ -like protein molecule, which prostaglandin-binding pocket is defined by three-
15 dimensional structure coordinates of a set of amino acids that correspond to four or more PPAR γ amino acid residues selected from the group consisting of TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, ALA 292, GLU 295, ILE 296, ILE 325, THR 328, MET 329, ALA 331, SER 332, LEU 333, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380, ASP 381, LEU 384, and LEU 435 and optionally one or more selected from the group consist-
20 ing of CYS 285, ARG 288, SER 289, ILE 326, TYR 327, LEU 330 and MET 364 according to figure 1, wherein the root mean square deviation of the backbone atoms between amino acid residues of said molecule and said PPAR γ residues is not greater than about 3 Å, wherein said computer comprises a machine-readable data storage medium comprising a data storage material encoded with said structure coordinates defining said prostaglandin-binding pocket and
25 means for generating a three-dimensional graphical representation of the prostaglandin-binding pocket, and wherein said method comprises the steps of: (a) positioning a first chemical entity within said prostaglandin-binding pocket using a graphical three-dimensional representation of the structure of the chemical entity and the prostaglandin-binding pocket; (b) performing a fitting operation between said chemical entity and said prostaglandin-binding
30 pocket by employing computational means; and (c) analyzing the results of said fitting operation to quantify the association between said chemical entity and the prostaglandin-binding pocket and optionally (d) outputting said quantified association to a suitable output hardware.

The above methods may further comprise the steps of: (e) repeating steps (a) through (d) with a second chemical entity; and (f) selecting at least one of said first or second chemical

entity that associates with said prostaglandin-binding pocket based on said quantified association of said first or second chemical entity.

In yet another aspect of the invention, a method for identifying a ligand of a prostaglandin-binding pocket of a PPAR protein molecule, which prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids that comprises amino acid residues corresponding to four or more selected from the group consisting of TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, CYS 285, ARG 288, SER 289, ALA 292, GLU 295, ILE 296, ILE 325, ILE 326, TYR 327, THR 328, MET 329, LEU 330, ALA 331, SER 332, LEU 333, MET 364, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380, ASP 381, LEU 384, and LEU 435 of SEQ ID NO:1, comprising the steps of: (a) using a three-dimensional structure of the prostaglandin-binding pocket to design, select and/or optimize a chemical entity; (b) contacting the chemical entity with the molecule; and (c) identifying any chemical entity capable of binding the molecule as a ligand, is provided.

In another aspect of the invention, a method for identifying a ligand of a prostaglandin-binding pocket of a PPAR γ or PPAR γ -like protein molecule comprising an amino acid sequence at least 65% identical to residues 207-476 of SEQ ID NO:1, which prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids that comprises (i) an amino acid residue corresponding to LEU 228, and (ii) three or more amino acids corresponding to amino acid residues selected from the group consisting of TYR 222, PHE 226, PRO 227, THR 229, LYS 230, CYS 285, ARG 288, SER 289, ALA 292, GLU 295, ILE 296, ILE 325, ILE 326, TYR 327, THR 328, MET 329, LEU 330, ALA 331, SER 332, LEU 333, MET 364, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380, ASP 381, LEU 384, and LEU 435 of SEQ ID NO:1, comprising the steps of: (a) using a three-dimensional structure of the prostaglandin-binding pocket to design, select and/or optimize a chemical entity; (b) contacting the chemical entity with the molecule; and (c) identifying any chemical entity capable of binding the molecule as a ligand, is provided.

In another aspect of the invention, a method for identifying a ligand of a prostaglandin-binding pocket of a PPAR γ or PPAR γ -like protein molecule, which prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids that correspond to four or more PPAR γ amino acid residues selected from the group consisting of TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, ALA 292, GLU 295, ILE 296, ILE 325, THR 328, MET 329, ALA 331, SER 332, LEU 333, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380, ASP 381, LEU 384, and LEU 435 and optionally one or more selected from the group consisting of CYS 285, ARG 288, SER 289, ILE 326, TYR 327, LEU 330 and MET 364

according to figure 1, wherein the root mean square deviation of the backbone atoms between amino acid residues of said molecule and said PPAR γ residues is not greater than about 3 Å, comprising the steps of: (a) using a three-dimensional structure of the prostaglandin-binding pocket to design, select and/or optimize a chemical entity; (b) contacting the chemical entity with the molecule; and (c) identifying any chemical entity capable of binding the molecule as a ligand, is provided.

Alternatively, the structure coordinates of the prostaglandin-binding pocket as defined above may be utilized in a method for identifying an agonist or antagonist of a molecule comprising a prostaglandin-binding pocket of PPAR γ . This method comprises the steps of: (a) using a three-dimensional structure of the prostaglandin-binding pocket to design, select and/or optimize a chemical entity; (b) contacting the chemical entity with the molecule or molecular complex; (c) monitoring the activity of the molecule or molecular complex; and (d) classifying the chemical entity as an agonist or antagonist based on the effect of the chemical entity on the activity of the molecule or molecular complex.

In one aspect, step (a) is using a three-dimensional structure of the prostaglandin-binding pocket of the molecule or molecular complex. In another aspect, the three-dimensional structure is displayed as a graphical representation.

In another aspect, the method comprises the steps of: (a) constructing a computer model of a prostaglandin-binding pocket of the molecule or molecular complex; (b) selecting a chemical entity to be evaluated by a method selected from the group consisting of assembling said chemical entity; selecting a chemical entity from a small molecule database; *de novo* ligand design of said chemical entity; and modifying a known agonist or inhibitor, or a portion thereof, of an PPAR γ protein or homologue thereof; (c) employing computational means to perform a fitting operation between computer models of said chemical entity to be evaluated and said prostaglandin-binding pocket in order to provide an energy-minimized configuration of said chemical entity in the prostaglandin-binding pocket; and (d) evaluating the results of said fitting operation to quantify the association between said chemical entity and the prostaglandin-binding pocket model, whereby evaluating the ability of said chemical entity to associate with said prostaglandin-binding pocket; (e) synthesizing said chemical entity; and (f) contacting said chemical entity with said molecule or molecular complex to determine the ability of said compound to activate or inhibit said molecule.

In one aspect, the invention provides a method of designing a compound or complex that associates with the prostaglandin-binding pocket comprising the steps of: (a) providing the

structure coordinates of said prostaglandin-binding pocket or protein on a computer comprising the means for generating three-dimensional structural information from said structure coordinates; and (b) using the computer to perform a fitting operation to associate a first chemical entity with the prostaglandin-binding pocket; (c) performing a fitting operation to associate at least a second chemical entity with all or, part of the prostaglandin-binding pocket; (d) quantifying the association between the first and second chemical entity and the prostaglandin-binding pocket; (e) optionally repeating steps (b) to (d) with another first and second chemical entity, selecting a first and a second chemical entity based on said quantified association of all of said first and second chemical entity; (f) optionally, visually inspecting the relationship of the first and second chemical entity to each other in relation to the prostaglandin-binding pocket on a computer screen using the three-dimensional graphical representation of the prostaglandin-binding pocket and said first and second chemical entity; and (g) assembling the first and second chemical entity into a compound or complex that associates with said prostaglandin-binding pocket by model building.

In one aspect, the present invention permits the use of molecular design techniques to identify, select and design chemical entities, including inhibitory compounds, capable of binding to PPAR, PPAR γ or PPAR γ -like prostaglandin-binding pockets.

The present elucidation of the prostaglandin-binding pocket on PPAR γ can provide the necessary information for designing new chemical entities and compounds that may interact with PPAR γ substrate or prostaglandin-binding pockets or PPAR γ -like substrate or prostaglandin-binding pockets, in whole or in part. Due to the homology in the binding pocket core between PPAR γ , PPAR α and PPAR δ , compounds that inhibit or activate PPAR γ are also expected to inhibit PPAR α and PPAR δ , especially those compounds that bind to the prostaglandin-binding pocket.

Throughout this section, discussions about the ability of a chemical entity to bind to, associate with or inhibit PPAR γ prostaglandin-binding pockets refer to features of the entity alone.

Assays to determine if a compound binds to a PPAR protein, PPAR γ , or a PPAR γ -like protein are well known in the art and are for example as described below as assay method 1 and assay method 2.

Assay method 1: PPAR γ receptor binding assay:

This assay can be used to, with use of a suitable ligand toward the prostaglandin-binding pocket, hereafter called the "Start-ligand", identify chemical entities such as, e.g., low molecular weight compounds, which displace the Start-ligand from the Ligand-binding-domain (LBD) of the Perox-
isome proliferator-activated receptor γ (PPAR γ). Exemplary "Start-ligands" include Prostaglandin
5 J₂, Prostaglandin B₂, 15-Deoxy $\Delta^{12,14}$ -prostaglandin J₂, as well as other suitable ligands known in
the art. When new ligands are designed, these may serve as new Start-ligands for further drug
testing and development.

The method is a ligand binding assay based upon IPA (imaging proximity assay) particles and is
based on the assay by Nichols *et al.* (Nichols *et al.*, 1998a; Nichols *et al.*, 1998b).

- 10 The method can be described as follows: The Start-ligand is marked with ^3H , while GST-PPAR γ -LBD is
marked with biotin and the scintillation proximity assay SPA particles are coated with Streptavidin
(SA). The receptor is coupled to Glutathiontransferase (GST); GST is a tag that is used to purify the
receptor from homogenized cells. When the SPA particles are added they bind to the biotin residues on
the GST-PPAR γ -LBD. ^3H -Start-ligand binds to GST-PPAR γ -LBD, and the proximity between the
15 radioactive tritium and the SPA particle results in emission of light from the SPA particles. The amount
of light emitted is proportional to the amount of ^3H -Start-ligand bound to the binding protein. When a
compound that displaces the Start-ligand is present it results in a decrease in the amount of light
emitted. Following the binding constant (K_d) can be determined. Compounds with a K_d value < 1 mM is
regarded as a "Hit" and can be used further in the drug design process. The Hit is preferably tested
20 also by assay method 2.

Assay method 2: A cell based transfection assay:

- With this PPAR response element (PPRE) reporter assay, the selective transactivation of PPAR γ
in chosen cancer cell line after treatment by small molecule compounds, like ligand Hits from
assay 1, can be evaluated. Differences in transactivation between different ligands for a cho-
25 sen cell lines is screened. The assay is based on the Allred and Kilgore published assay (Allred
and Kilgore, 2005) as described in the following.

- The PPRE reporter plasmid: A reporter construct, 3XPPRE-TK-pGL3, contains three copies of a
PPRE sequence (AGGACAAAGGTCA) upstream of the mTK promoter between the *Xho*I and
*Hind*III restriction enzyme sites of the pGL3 basic vector (Promega, Madison, WI). *Bam*HI and
30 *Bgl*/II is used to release a 2.2 kb fragment containing the 3XPPRE-mTK-Luciferase. This frag-
ment is ligated into the BamH I receptor site of pRL-TK plasmid (Promega) completing the

new reporter which contains both Luciferase and Renilla in a single expression plasmid. Renilla expression is used as a transfection efficiency control.

The transfection assay: Cells are transiently transfected with 5 μ g of PPRE reporter plasmid per 12-well plate. Chosen cancer cells are transfected with ESCORT transfection reagent (Sigma-Aldrich) for 4 h. Cells are subsequently treated with the substance to be tested in about micro-molar concentration for 18 h. PPAR γ ligand concentrations for each compound used are those shown to be maximally effective following dose response studies. Proper vehicle controls including ethanol, DMSO, and methyl acetate are run for each treatment group. Following treatment, cells are lysed in 50 μ l passive lysis buffer and treated according to manufacturer's instructions (Promega dual luciferase assay kit). Luminometry are performed and data are calculated as raw Luciferase Units (RLUs) divided by raw Renilla units. Mean fold induction is obtained by dividing the RLU data from each treatment well by the mean values of the vehicle control appropriate for each treatment. Each set of treatments are performed in replicates of six in three separate experiments. Showing more than 1.05 fold induction change such a compound is regarded as a "hit" and can be used further in the drug design process.

Other methods are readily known by and available to the skilled person in the field.

The design of compounds that bind to or inhibit a PPAR, PPAR γ or PPAR γ -like prostaglandin-binding pocket according to this invention generally involves consideration of two factors. First, the chemical entity must be capable of physically and structurally associating with parts or all of the prostaglandin-binding pocket. Non-covalent molecular interactions important in this association include hydrogen bonding, van der Waals' interactions, hydrophobic interactions and electrostatic interactions.

Second, the chemical entity must be able to assume a conformation that allows it to associate with the PPAR, PPAR γ or PPAR γ -like prostaglandin-binding pocket directly. Although certain portions of the chemical entity will not directly participate in these associations, those portions of the chemical entity may 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 prostaglandin-binding pocket, or the spacing between functional groups of a chemical entity comprising several chemical entities that directly interact with the PPAR, PPAR γ or PPAR γ -like prostaglandin-binding pockets.

The potential inhibitory or binding effect of a chemical entity on a prostaglandin-binding pocket may be analyzed prior to its actual synthesis and testing by the use of computer modelling techniques. If the theoretical structure of the given entity suggests insufficient interaction and association between it and the prostaglandin-binding pocket, testing of the entity is obviated.

However, if computer modelling indicates a strong interaction, the molecule may then be synthesized and tested for its ability to bind to a prostaglandin-binding pocket. This may be achieved by testing the ability of the molecule to bind and/or inhibit/activate a PPAR protein such as PPAR γ or a PPAR γ -like protein using the assays described above. In this manner, synthesis of inoperative compounds may be avoided.

A potential inhibitor of a prostaglandin-binding pocket of, e.g., PPAR γ , 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 PPAR γ prostaglandin-binding pocket.

One skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with a prostaglandin-binding pocket of, e.g., PPAR γ . This process may begin by visual inspection of, for example, a PPAR γ prostaglandin-binding pocket on the computer screen based on the PPAR γ structure coordinates in any of Figures 1-2 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 prostaglandin-binding pocket as defined supra. Docking may be accomplished using software such as QUANTA (Accelrys Inc., San Diego, ©2001, 2002) and Sybyl (Tripos Associates, St. Louis, MO), 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", *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: 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.*

5 Mol. 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 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 PPAR γ . This would be followed by manual model building using software such as QUANTA (Accelrys Inc., San Diego, ©2001, 2002) 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); G. Lauri and P. A. Bartlett, "CAVEAT: a Program to Facilitate the Design of Organic Molecules", *Comput. Aided Mol. Des.*, 8, pp. 51-66 (1994)). CAVEAT is available from the University of California, Berkeley, CA.

20 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).

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

Instead of proceeding to build an inhibitor of a PPAR γ prostaglandin-binding pocket in a step-wise fashion one fragment or chemical entity at a time as described above, inhibitory or other PPAR γ binding compounds may be designed as a whole or "*de novo*" using either an empty

30

binding pocket or optionally including some portion (s) of a known inhibitor (s). There are many *de novo* ligand design methods including:

1. LUDI (H.-J. 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 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. Louis, MO).

4. SPROUT (V. Gillet et al., "SPROUT : A Program for Structure Generation)", Comput. Aided Mol. Design, pp. 127-153 (1993)). SPROUT is available from the University of Leeds, UK.

Other molecular modelling techniques may also be employed in accordance with this invention (see, e. g., N. C. Cohen et al., "Molecular Modelling Software and Methods for Medicinal Chemistry, J. Med. Chem., 33, pp. 883-894 (1990); see also, M. A. Navia and M. A. 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", 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 chemical entity has been designed or selected by the above methods, the efficiency with which that chemical entity may bind to the prostaglandin-binding pocket of, e.g., PPAR γ , may be tested and optimized by computational evaluation. For example, an effective prostaglandin-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 prostaglandin-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. PPAR γ prostaglandin-binding pocket inhibitors may interact with the prostaglandin-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 chemical entity and the average energy of the conformations observed when the inhibitor binds to the protein.

A chemical entity designed or selected as binding to a prostaglandin-binding pocket of, e.g., PPAR γ , 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.

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 ; QUANTA/CHARMM (Accelrys Inc., San Diego, ©2001, 2002); Insight II/Discover (Molecular Simulations, Inc., San Diego, CA ©1998; DelPhi (Molecular Simulations, Inc., San Diego, CA©1998 ; 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 to the prostaglandin-binding pocket of, e.g., PPAR γ . In this screening, the quality of fit of such entities to the prostaglandin-binding pocket 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)).

According to another aspect, the invention provides compounds which associate with the prostaglandin-binding pocket of, e.g., PPAR γ , produced or identified by the method set forth above.

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 structure of each crystal is solved.

Such an approach provides insight into the 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-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 be optimized.

In some cases, iterative drug design is carried out by forming successive protein-compound complexes and then crystallizing each new complex. High throughput crystallization assays may be used to find a new crystallization condition or to optimize the original protein or complex crystallization condition for the new complex. Alternatively, a pre-formed protein crystal may be soaked in the presence of an inhibitor, thereby forming a protein/compound complex and obviating the need to crystallize each individual protein/compound complex.

10 Structure Determination of Other Molecules

The structure coordinates set forth in Figures 1-2 can also be used to aid in obtaining structural information about other crystallized molecules or molecular complexes. This may be achieved by any of a number of well-known techniques, including molecular replacement.

According to an alternate aspect, the machine-readable data storage medium comprises a data storage material encoded with a first set of machine readable data which comprises the Fourier transform of at least a portion of the structure coordinates set forth in Figures 1-2 or homology model thereof, and which, when using a machine programmed with instructions for using said data, can be combined with a second set of machine readable data comprising the X-ray diffraction pattern of a molecule or molecular complex to determine at least a portion of the structure coordinates corresponding to the second set of machine readable data.

In another aspect, the invention provides a computer for determining at least a portion of the structure coordinates corresponding to X-ray diffraction data obtained from a molecule or 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 least a portion of the structure coordinates of PPAR γ according to any one of Figures 1-2 or homology model thereof; (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.

For example, the Fourier transform of at least a portion of the structure coordinates set forth in any one of Figures 1-2 or homology model thereof may be used to determine at least a portion of the structure coordinates of PPAR γ homologues. In one aspect, the molecule is a PPAR γ homologue. In another aspect, the molecular complex is selected from the group consisting of PPAR γ complex and PPAR γ homologue complex.

Therefore, in another aspect this invention provides a method of utilizing molecular replacement to obtain structural information about a molecule or a molecular complex of unknown structure wherein the molecule or molecular complex is sufficiently homologous to PPAR γ , comprising the steps of: (a) crystallizing said molecule or molecular complex of unknown structure; (b) generating an X-ray diffraction pattern from said crystallized molecule or molecular complex; (c) applying at least a portion of the PPAR γ structure coordinates set forth in one of Figures 1-2 or a homology model thereof to the 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; and (d) generating a structural model of the molecule or molecular complex from the three-dimensional electron density map.

In one aspect, the method is performed using a computer. In another aspect, the molecule is selected from the group consisting of PPAR γ and PPAR γ homologues. In another aspect, the molecule is a PPAR molecular complex or homologue thereof.

By using molecular replacement, all or part of the structure coordinates of the PPAR γ as provided by this invention or homology model thereof (and set forth in any one of Figures 1-2) can be used to determine the structure of a crystallized molecule or molecular complex whose structure is unknown more quickly and efficiently than 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. 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 crystal structure of a protein containing at least a homologous portion has been solved, the phases from the known structure may provide a satisfactory estimate of the phases for the unknown structure.

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 PPAR γ according to any one of Figures 1-2 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, "Use of the Rotation and Translation Functions", in Meth. 115, pp. 55-77 (1985); M. G. Rossmann, ed., "The Molecular Replacement Method", 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 PPAR γ can be resolved by this method.

In one aspect, the method of molecular replacement is utilized to obtain structural information about a PPAR γ homologue. The structure coordinates of PPAR γ as provided by this invention are particularly useful in solving the structure of PPAR γ complexes that are bound by ligands, substrates and inhibitors.

Furthermore, the structure coordinates of PPAR γ as provided by this invention are useful in solving the structure of PPAR γ proteins that have amino acid substitutions, additions and/or deletions (referred to collectively as "PPAR γ mutants", as compared to naturally occurring PPAR γ). These PPAR γ mutants may optionally be crystallized in co-complex with a chemical entity, such as a non-hydrolyzable prostaglandin analogue or a suicide substrate. The crystal structures of a series of such complexes may then be solved by molecular replacement and compared with that of wild-type PPAR γ . Potential sites for modification within the various binding pockets of the enzyme may thus be identified. This information provides an additional tool for determining the most efficient binding interactions, for example, increased hydrophobic interactions, between PPAR γ and a chemical entity or compound.

The structure coordinates are also particularly useful in solving the structure of crystals of PPAR γ or PPAR γ homologues co-complexed with a variety of chemical entities. This approach enables the determination of the optimal sites for interaction between chemical entities, including candidate PPAR γ inhibitors. 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 PPAR γ inhibition activity.

All of the complexes referred to above may be studied using well-known X-ray diffraction techniques and may be refined using 1.5-3.4 resolution X-ray data to an R value of about 0.30 or less using computer software, such as X-PLOR (Yale distributed by Molecular Simulations, Inc.; see, e.g., Blundell & Johnson, *supra*; Meth. Enzymol., vol. 114 & 115, H. W. Wyckoff et al., Academic Press (1985)) or CNS (Brunger et al., Acta Cryst., D54, pp. 905-921, (1998)).

The features disclosed in the foregoing description may, both separately and in any combination thereof, be material for realising the invention in diverse forms thereof.

The following formulation examples are illustrative only and are not intended to limit the scope of the invention in any way.

EXAMPLES

EXAMPLE 1 – Re-Refinement of PPAR γ Structure

Crystallographic coordinates of the in the Protein Data Bank (Berman et al., 2000) accession code 1PRG deposited Peroxisome Proliferator-Activated Receptor- γ (PPAR γ), ligand binding domain, (Nolte et al., 1998) were downloaded along with deposited structure factors, accession code r1prgsf. The structure was reported as an Apo structure of PPAR γ , a structure without any bound ligand. To check this, REFMAC5 of the CCP4 crystallographic program package (Bailey, 1994) was used to re-refine the structure. CCP4 was run using the CCP4i interface (Liz Potterton (*CCP4 Newsletter 34, September 1997*) <http://www.ccp4.ac.uk/newsletters.php>). The 1PRG coordinates were stripped of any water molecules and 50 cycles of maximum likelihood restrained refinement was performed using the deposited structure factors with data between 45.3 and 2.0 Å resolution. Bulk solvent correction was used. The crystallographic space group number 5 was used for refinement. The refinement ended in with an R-value of 0.264 and with a root-mean-square deviation (RMSD) from ideal bond lengths of 0.020 Å. SigmaA weighted electron density maps, 2Fo-Fc and Fo-Fc, were generated after the last cycle. The crystallographic refinement was followed by computer graphics inspection of the electron density maps using the Coot program (Emsley and Cowtan, 2004). The Coot command "Validate/Unmodelled blobs", using 3 sigma cut-off on the Fo-Fc map, gave a list of

three "blobs", unmodelled electron densities larger than water molecules in size. The first and second "blob" in the list pointed to the same location of the crystallographically independent molecules A and B, respectively, the first "blob" showing a highest sigma value of 5 in the Fo-Fc map and 2.5 in the 2Fo-Fc map. The second "blob" was showing a 5.6 sigma high peak in the Fo-Fc map and 2.7 sigma in the 2Fo-Fc map.

The shape of the blobs, a central disk-shape with arms protruding on opposite sides of the disk and pointing away from each other, reminded very much of the shape of a prostaglandin molecule, a natural ligand of PPAR γ . Different types of prostaglandin molecules were therefore modeled into the difference electron density, among those the natural PPAR γ ligand 15-Deoxy $\Delta^{12,14}$ -prostaglandin J₂, using the Coot program followed by REFMAC5 refinement, an then model and map inspection by the Coot program. It was concluded that Prostaglandin B₂ fitted the electron density best. Prostaglandin B₂ is a non-native prostaglandin commonly used as an internal standard for HPLC-traced extractions and chromatograms which makes it probable to have been used during the purification of the PPAR γ molecule. Despite its non-native nature, the prostaglandin B₂ molecule is similar enough to most likely occupy the same binding site, with slight deviations, as would 15-Deoxy $\Delta^{12,14}$ -prostaglandin J₂. The prostaglandin B₂ molecule fits very well with the electron density with the exception of the two last carbons of the hydrocarbon arm containing the carboxyl group. For those two moieties there is no electron density seen.

The third "blob" found by the Coot program was situated in a mostly hydrophobic pocket on the surface of the PPAR γ A molecule formed by residues like Leu237, Val248, Pro246 and Phe347. It was interpreted as DMSO (dimethyl sulfoxide) molecule and inserted by the Coot program and refined in REFMAC5. Moreover, a disordered part of the main-chain, amino acid 239 to 244, of the A molecule, was modelled in two discrete conformations. Thereafter water molecules were added by the ARP_WARP program software (Perrakis et al., 1999) implemented by the CCP4i procedure of REFMAC5. For statistics from the final refinement, see Table 1.

The amino acid residues within a 5 Å radius of the prostaglandin B₂ molecule was calculated with the help of the CONTACT software program of the CCP4 program package, Table 2 and 3, and in QUANTA. From the close contact between P O12 and Leu 228 O, Table 2 and Table 3, it is clear that it has to be the enol form of the prostaglandin B₂ molecule making a hydrogen bond to the main chain oxygen of PPAR γ . The LBD PPAR γ amino acid residues within 5 Å distance from the bound prostaglandin B₂ molecule were TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, CYS 285, ARG 288, SER 289, ALA 292, GLU 295, ILE 326, TYR 327, MET

329, LEU 330, SER 332, LEU 333, MET 364, ASP 381, and LEU 384.

Further, the PPAR γ molecule, without any bound ligands, was run through the VOIDOO software program (Kleywegt and Jones, 1994). From the output of the program voids, pockets within the PPAR γ molecule not filled with atoms, around the position for the prostaglandin B₂ site was used to predict residues which could be reached and utilized in a drug design process. The amino acid residues which were added, thus extending the pocket filled by the prostaglandin B₂ molecule, were ILE 296, ILE 325, THR 328, ALA 331, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380 and LEU 435.

Table 1:

10 DATA USED IN REFINEMENT.

RESOLUTION RANGE HIGH (ANGSTROMS) : 2.00
 RESOLUTION RANGE LOW (ANGSTROMS) : 115.47
 DATA CUTOFF (SIGMA(F)) : NONE
 COMPLETENESS FOR RANGE (%) : 76.06
 15 NUMBER OF REFLECTIONS : 31793

FIT TO DATA USED IN REFINEMENT.

CROSS-VALIDATION METHOD : THROUGHOUT
 FREE R VALUE TEST SET SELECTION : RANDOM
 20 R VALUE (WORKING + TEST SET) : 0.24317
 R VALUE (WORKING SET) : 0.24007
 FREE R VALUE : 0.30111
 FREE R VALUE TEST SET SIZE (%) : 5.1
 FREE R VALUE TEST SET COUNT : 1693

25

FIT IN THE HIGHEST RESOLUTION BIN.

TOTAL NUMBER OF BINS USED : 20
 BIN RESOLUTION RANGE HIGH : 2.001
 BIN RESOLUTION RANGE LOW : 2.053
 30 REFLECTION IN BIN (WORKING SET) : 1219
 BIN COMPLETENESS (WORKING+TEST) (%) : 39.27
 BIN R VALUE (WORKING SET) : 0.330
 BIN FREE R VALUE SET COUNT : 62
 BIN FREE R VALUE : 0.365

35

RMS DEVIATIONS FROM IDEAL VALUES COUNT RMS WEIGHT
 BOND LENGTHS REFINED ATOMS (A): 4312 ; 0.017 ; 0.022
 BOND ANGLES REFINED ATOMS (DEGREES): 5801 ; 1.775 ; 1.999
 TORSION ANGLES, PERIOD 1 (DEGREES): 522 ; 6.838 ; 5.000

5

Table 2:

PPAR γ – prostaglandin B₂ interactions of the A and P residue chain, respectively. A cut-off of 5.0 Å was used. The contacts were identified by the CONTACT computer program of the CCP4 suite. In the last column "****" indicates a strong possibility for a hydrogen bond at this contact (distance < 3.3 Å) as calculated by CONTACT, " *" indicates a weak possibility (distance > 3.3 Å). Blank indicates that the program considered there to be no possibility of a hydrogen bond.

10

PPAR γ			Prostaglandin			
Res. Type	Res. # and Chain	Atom name	Res. # and Chain	Atom name	Distance [Å]	Possibly H-bond
Tyr	222A	CE1	2P	C18	4.49	
Tyr	222A	CZ	2P	C17	4.59	
			2P	C18	4.08	
Tyr	222A	OH	2P	C16	4.45	
			2P	C17	3.40	
			2P	C18	2.91	
Phe	226A	CA	2P	C11	4.79	
			2P	C12	4.63	
			2P	O12	3.91	
Phe	226A	CB	2P	C11	4.74	
			2P	C12	4.16	
			2P	O12	3.42	
Phe	226A	CG	2P	C12	4.78	
			2P	O12	4.34	
Phe	226A	CD1	2P	C11	4.77	
			2P	C12	4.55	
			2P	O12	4.48	
Phe	226A	C	2P	C11	4.87	
			2P	C12	4.68	
			2P	O12	3.76	
Phe	226A	O	2P	O12	4.21	*
Pro	227A	N	2P	C11	4.44	
			2P	C12	4.60	
			2P	O12	3.85	*
Pro	227A	CA	2P	O12	4.62	
Pro	227A	CG	2P	C11	4.23	
			2P	O12	4.74	
Pro	227A	CD	2P	C11	3.72	

PPAR γ			Prostaglandin			
Res. Type	Res. # and Chain	Atom name	Res. # and Chain	Atom name	Distance [Å]	Possibly H-bond
			2P	C12	4.37	
			2P	O12	3.99	
Pro	227A	C	2P	O12	4.21	
Leu	228A	N	2P	C11	4.32	
			2P	C12	3.97	
			2P	O12	3.06	***
Leu	228A	CA	2P	C11	4.94	
			2P	C12	4.30	
			2P	O12	3.43	
Leu	228A	CB	2P	C13	4.91	
			2P	C11	4.66	
			2P	C12	4.18	
			2P	O12	3.72	
Leu	228A	CG	2P	O12	4.74	
Leu	228A	C	2P	C13	4.93	
			2P	C15	4.42	
			2P	C12	4.23	
			2P	O12	3.24	
Leu	228A	O	2P	C13	3.92	
			2P	C14	4.00	
			2P	C15	3.23	
			2P	C16	4.23	
			2P	C17	4.23	
			2P	C11	4.69	
			2P	C12	3.42	
			2P	O12	2.53	***
Thr	229A	N	2P	O12	4.41	*
Thr	229A	CA	2P	C17	4.70	
			2P	O12	5.00	
Thr	229A	C	2P	C15	4.94	
			2P	C17	4.31	
Lys	230A	N	2P	C15	4.91	
			2P	C16	4.77	
			2P	C17	3.66	
			2P	C18	4.45	
Lys	230A	CA	2P	C17	4.14	
			2P	C18	4.80	
Lys	230A	CB	2P	C17	4.11	
			2P	C18	4.28	
Cys	285A	CA	2P	C2	4.94	
Cys	285A	CB	2P	C2	4.39	
Cys	285A	SG	2P	C2	4.45	
Cys	285A	C	2P	C2	4.96	
Cys	285A	O	2P	C3	4.28	
			2P	C4	4.97	
			2P	C2	4.31	
Arg	288A	CA	2P	C4	4.99	
Arg	288A	CB	2P	C3	4.73	
			2P	C4	4.19	
			2P	C5	4.60	

PPAR γ			Prostaglandin			
Res. Type	Res. # and Chain	Atom name	Res. # and Chain	Atom name	Distance [Å]	Possibly H-bond
Arg	288A	C	2P	C3	4.63	
			2P	C4	4.48	
			2P	C5	4.29	
Arg	288A	O	2P	C4	4.71	
			2P	C5	4.11	
Ser	289A	N	2P	C3	4.10	
			2P	C4	4.41	
			2P	C5	4.41	
Ser	289A	CA	2P	C3	4.12	
			2P	C4	4.65	
			2P	C5	4.39	
Ser	289A	CB	2P	C3	4.11	
Ser	289A	OG	2P	C3	3.07	
			2P	C4	4.31	
			2P	C5	4.69	
			2P	C2	3.74	
			2P	C1	4.07	
Ala	292A	CB	2P	C8	4.84	
			2P	C10	4.75	
			2P	C5	4.08	
			2P	C6	4.54	
			2P	O6	4.48	
			2P	C7	4.12	
Glu	295A	CD	2P	C10	4.15	
			2P	C11	3.77	
			2P	C12	4.90	
Glu	295A	OE1	2P	C13	4.73	
			2P	C9	4.34	
			2P	C10	3.32	
			2P	C11	3.16	
			2P	C12	4.14	
			2P	O12	4.73	*
Glu	295A	OE2	2P	C10	4.11	
			2P	C11	3.61	
			2P	C12	4.93	
Ile	326A	CA	2P	O6	4.05	
Ile	326A	CB	2P	O6	4.43	
Ile	326A	CG1	2P	C5	4.90	
			2P	O6	4.62	
Ile	326A	CG2	2P	C3	3.76	
			2P	C4	4.47	
			2P	C5	4.16	
			2P	C6	4.65	
			2P	O6	3.97	
			2P	C2	4.63	
			2P	C1	4.30	
Ile	326A	C	2P	O6	3.93	
Ile	326A	O	2P	C5	4.89	
			2P	C6	4.30	
			2P	O6	3.06	***

PPAR γ			Prostaglandin			
Res. Type	Res. # and Chain	Atom name	Res. # and Chain	Atom name	Distance [Å]	Possibly H-bond
Tyr	327A	CD1	2P	C1	4.48	
Tyr	327A	CE1	2P	C1	3.86	
Tyr	327A	CZ	2P	C1	4.89	
Tyr	327A	OH	2P	C1	4.92	
Met	329A	CA	2P	C14	4.43	
			2P	C15	4.54	
			2P	C16	3.59	
			2P	C17	4.42	
			2P	C18	4.13	
			2P	O6	4.79	
Met	329A	CB	2P	C13	4.93	
			2P	C14	3.97	
			2P	C15	4.25	
			2P	C16	3.55	
			2P	C17	4.53	
			2P	C18	4.34	
			2P	C8	4.67	
			2P	O6	4.37	
Met	329A	CG	2P	C14	4.88	
			2P	C15	4.88	
			2P	C16	4.04	
			2P	C17	4.67	
			2P	C18	4.10	
Met	329A	SD	2P	C14	4.89	
			2P	C15	4.94	
			2P	C16	4.49	
			2P	C18	4.78	
Met	329A	CE	2P	C13	4.67	
			2P	C14	4.22	
			2P	C15	3.86	
			2P	C16	3.46	
			2P	C17	3.81	
			2P	C18	3.64	
			2P	O12	4.94	
Met	329A	C	2P	C14	3.93	
			2P	C15	4.26	
			2P	C16	3.57	
			2P	C17	4.59	
			2P	C18	4.74	
			2P	C8	4.57	
			2P	O6	4.09	
Met	329A	O	2P	C13	4.51	
			2P	C14	3.09	
			2P	C15	3.33	
			2P	C16	2.82	
			2P	C17	3.90	
			2P	C18	4.41	
			2P	C8	4.14	
			2P	C9	4.86	
			2P	O6	4.36	*

PPAR γ			Prostaglandin			
Res. Type	Res. # and Chain	Atom name	Res. # and Chain	Atom name	Distance [Å]	Possibly H-bond
Leu	330A	N	2P	C14	4.91	
			2P	C16	4.85	
			2P	C8	4.94	
			2P	C6	4.77	
			2P	O6	3.79	*
Leu	330A	CA	2P	C8	4.87	
			2P	C6	4.35	
			2P	O6	3.73	
Leu	330A	CB	2P	C6	4.23	
			2P	O6	3.68	
Leu	330A	CG	2P	C6	4.80	
			2P	O6	4.64	
Leu	330A	CD1	2P	C3	4.82	
			2P	C4	4.11	
			2P	C5	4.72	
			2P	C6	4.09	
			2P	O6	4.37	
			2P	C2	4.64	
Leu	330A	CD2	2P	C2	4.73	
			2P	C1	4.32	
Ser	332A	CA	2P	C16	4.77	
			2P	C17	4.66	
Ser	332A	CB	2P	C14	4.94	
			2P	C15	4.19	
			2P	C16	3.40	
			2P	C17	3.19	
			2P	C18	3.71	
Ser	332A	OG	2P	C15	4.39	
			2P	C16	3.26	
			2P	C17	2.80	
			2P	C18	2.74	
Leu	333A	CG	2P	C13	4.95	
			2P	C14	4.17	
			2P	C15	4.60	
			2P	C8	4.58	
Leu	333A	CD1	2P	C13	4.68	
			2P	C14	4.28	
			2P	C8	3.77	
			2P	C9	4.41	
			2P	C6	4.24	
			2P	O6	4.88	
			2P	C7	4.14	
Leu	333A	CD2	2P	C13	4.60	
			2P	C14	3.96	
			2P	C15	4.11	
			2P	C16	4.80	
			2P	C8	4.92	
Met	364A	SD	2P	C2	4.89	
			2P	C1	4.45	
Met	364A	CE	2P	C1	4.98	

PPAR γ			Prostaglandin			
Res. Type	Res. # and Chain	Atom name	Res. # and Chain	Atom name	Distance [Å]	Possibly H-bond
Asp	381A	OD1	2P	C17	4.05	
			2P	C18	3.94	
Leu	384A	CB	2P	C18	4.67	
Leu	384A	CG	2P	C18	4.46	
Leu	384A	CD1	2P	C17	4.52	
			2P	C18	3.21	

Table 3:

PPAR γ – prostaglandin B₂ interactions of the B and P residue chain, respectively. A cut-off of 5.0 Å was used. The contacts were identified by the CONTACT computer program of the CCP4 suite. In the last column "****" indicates a strong possibility for a hydrogen bond at this contact (distance < 3.3 Å) as calculated by CONTACT, " *" indicates a weak possibility (distance > 3.3 Å). Blank indicates that the program considered there to be no possibility of a hydrogen bond.

PPAR γ			Prostaglandin			
Res. Type	Res. # and Chain	Atom name	Res. # and Chain	Atom name	Distance [Å]	Possibly H-bond
Tyr	222B	CE1	3P	C17	4.99	
			3P	C18	4.95	
Tyr	222B	CZ	3P	C17	4.20	
			3P	C18	3.89	
Tyr	222B	OH	3P	C16	4.31	
			3P	C17	3.13	
			3P	C18	2.66	
Tyr	222B	CE2	3P	C17	4.89	
			3P	C18	4.41	
Phe	226B	CA	3P	C11	4.64	
			3P	C12	4.64	
			3P	O12	4.11	
Phe	226B	CB	3P	C11	4.71	
			3P	C12	4.28	
			3P	O12	3.70	
Phe	226B	CG	3P	O12	4.70	
Phe	226B	CD1	3P	C11	4.91	
			3P	C12	4.78	
			3P	O12	4.81	
Phe	226B	C	3P	C11	4.74	
			3P	C12	4.69	
			3P	O12	3.94	

PPAR γ			Prostaglandin			
Res. Type	Res. # and Chain	Atom name	Res. # and Chain	Atom name	Distance [Å]	Possibly H-bond
Phe	226B	O	3P	O12	4.25	*
Pro	227B	N	3P	C11	4.41	
			3P	C12	4.72	
			3P	O12	4.14	*
Pro	227B	CA	3P	O12	4.79	
Pro	227B	CG	3P	C11	3.87	
			3P	C12	4.80	
			3P	O12	4.71	
Pro	227B	CD	3P	C11	3.93	
			3P	C12	4.69	
			3P	O12	4.49	
Pro	227B	C	3P	O12	4.33	
Leu	228B	N	3P	C11	4.26	
			3P	C12	4.02	
			3P	O12	3.20	***
Leu	228B	CA	3P	C11	4.93	
			3P	C12	4.36	
			3P	O12	3.48	
Leu	228B	CB	3P	C15	4.93	
			3P	C11	4.43	
			3P	C12	3.89	
			3P	O12	3.37	
			3P	C13	4.68	
Leu	228B	CG	3P	O12	4.76	
Leu	228B	C	3P	C15	4.57	
			3P	C12	4.41	
			3P	O12	3.32	
Leu	228B	O	3P	C14	4.33	
			3P	C15	3.37	
			3P	C16	4.20	
			3P	C17	3.97	
			3P	C11	4.89	
			3P	C12	3.69	
			3P	O12	2.61	***
			3P	C13	4.34	
Thr	229B	N	3P	O12	4.51	*
Thr	229B	CA	3P	C17	4.85	
Thr	229B	C	3P	C17	4.44	
Lys	230B	N	3P	C16	4.83	
			3P	C17	3.75	
			3P	C18	4.46	
Lys	230B	CA	3P	C17	4.26	
			3P	C18	4.71	
Lys	230B	CB	3P	C17	4.11	
			3P	C18	4.03	
Cys	285B	CA	3P	C2	4.68	
			3P	C3	4.88	
Cys	285B	CB	3P	C2	4.14	
			3P	C3	4.83	
			3P	C1	4.86	

PPAR γ			Prostaglandin			
Res. Type	Res. # and Chain	Atom name	Res. # and Chain	Atom name	Distance [Å]	Possibly H-bond
Cys	285B	SG	3P	C2	4.53	
Cys	285B	C	3P	C2	4.72	
			3P	C3	4.69	
Cys	285B	O	3P	C2	4.01	
			3P	C3	3.73	
			3P	C4	4.93	
			3P	C1	4.61	
Arg	288B	CB	3P	C3	4.70	
			3P	C4	4.60	
			3P	C5	4.91	
Arg	288B	C	3P	C3	4.32	
			3P	C4	4.58	
			3P	C5	4.37	
Arg	288B	O	3P	C7	4.73	
			3P	C3	4.63	
			3P	C4	4.60	
			3P	C5	3.98	
Ser	289B	N	3P	C3	3.89	
			3P	C4	4.57	
			3P	C5	4.54	
Ser	289B	CA	3P	C3	3.78	
			3P	C4	4.55	
			3P	C5	4.25	
Ser	289B	CB	3P	C2	4.25	
			3P	C3	3.39	
			3P	C4	4.55	
			3P	C5	4.55	
			3P	C1	4.17	
Ser	289B	OG	3P	C3	4.43	
			3P	C1	4.81	
Ala	292B	CB	3P	C7	3.91	
			3P	C8	4.74	
			3P	C10	4.91	
			3P	C5	3.96	
			3P	C6	4.35	
			3P	O6	4.37	
Glu	295B	CD	3P	C10	3.83	
			3P	C11	3.72	
			3P	C12	4.94	
Glu	295B	OE1	3P	C8	4.92	
			3P	C9	4.09	
			3P	C10	3.08	
			3P	C11	3.24	
			3P	C12	4.26	
			3P	C13	4.66	
Glu	295B	OE2	3P	C10	3.73	
			3P	C11	3.41	
			3P	C12	4.81	
Ile	326B	CA	3P	O6	4.26	
Ile	326B	CB	3P	C5	4.99	

PPAR γ			Prostaglandin			
Res. Type	Res. # and Chain	Atom name	Res. # and Chain	Atom name	Distance [Å]	Possibly H-bond
			3P	O6	4.60	
Ile	326B	CG1	3P	C5	4.90	
			3P	O6	4.79	
Ile	326B	CG2	3P	C2	4.50	
			3P	C3	4.19	
			3P	C4	4.46	
			3P	C5	4.09	
			3P	C6	4.71	
			3P	O6	4.11	
			3P	C1	3.83	
Ile	326B	C	3P	O6	4.19	
Ile	326B	O	3P	C6	4.58	
			3P	O6	3.38	*
Tyr	327B	CD1	3P	C1	4.56	
Tyr	327B	CE1	3P	C1	3.82	
Tyr	327B	CZ	3P	C1	4.66	
Tyr	327B	OH	3P	C1	4.65	
Met	329B	CA	3P	C14	4.48	
			3P	C15	4.68	
			3P	C16	3.79	
			3P	C17	4.64	
			3P	C18	4.20	
			3P	O6	4.74	
Met	329B	CB	3P	C14	3.87	
			3P	C15	4.12	
			3P	C16	3.42	
			3P	C17	4.37	
			3P	C18	4.18	
			3P	C8	4.70	
			3P	C13	4.78	
			3P	O6	4.30	
Met	329B	CG	3P	C14	4.99	
			3P	C16	4.17	
			3P	C17	4.78	
			3P	C18	4.31	
Met	329B	SD	3P	C16	4.54	
			3P	C18	4.90	
Met	329B	CE	3P	C14	4.36	
			3P	C15	3.89	
			3P	C16	3.35	
			3P	C17	3.56	
			3P	C18	3.62	
			3P	O12	4.91	
			3P	C13	4.75	
Met	329B	C	3P	C14	4.07	
			3P	C15	4.51	
			3P	C16	3.88	
			3P	C17	4.93	
			3P	C18	4.81	
			3P	C8	4.86	

PPAR γ			Prostaglandin			
Res. Type	Res. # and Chain	Atom name	Res. # and Chain	Atom name	Distance [Å]	Possibly H-bond
			3P	O6	4.17	
Met	329B	O	3P	C14	3.41	
			3P	C15	3.74	
			3P	C16	3.21	
			3P	C17	4.26	
			3P	C18	4.38	
			3P	C8	4.69	
			3P	C13	4.82	
			3P	O6	4.61	*
Leu	330B	N	3P	C14	4.94	
			3P	C6	4.73	
			3P	O6	3.76	*
Leu	330B	CA	3P	C6	4.67	
			3P	O6	4.06	
Leu	330B	CB	3P	C6	4.90	
			3P	O6	4.37	
Leu	330B	CG	3P	C2	4.55	
			3P	C4	4.38	
			3P	C5	4.98	
			3P	C6	4.67	
			3P	O6	4.54	
			3P	C1	4.85	
Leu	330B	CD1	3P	C2	4.61	
			3P	C1	4.60	
Leu	330B	CD2	3P	C2	4.81	
			3P	C4	4.33	
			3P	C6	4.66	
			3P	O6	4.88	
Ser	332B	CA	3P	C16	4.85	
			3P	C17	4.92	
			3P	C18	4.76	
Ser	332B	CB	3P	C15	4.36	
			3P	C16	3.52	
			3P	C17	3.43	
			3P	C18	3.34	
Ser	332B	OG	3P	C15	4.85	
			3P	C16	3.70	
			3P	C17	3.38	
			3P	C18	2.67	
Leu	333B	CG	3P	C14	3.99	
			3P	C15	4.55	
			3P	C8	4.79	
			3P	C13	4.82	
Leu	333B	CD1	3P	C14	4.12	
			3P	C7	4.48	
			3P	C8	3.95	
			3P	C9	4.51	
			3P	C13	4.59	
			3P	C6	4.46	
			3P	O6	4.96	

PPAR γ			Prostaglandin			
Res. Type	Res. # and Chain	Atom name	Res. # and Chain	Atom name	Distance [Å]	Possibly H-bond
Leu	333B	CD2	3P	C14	3.78	
			3P	C15	4.04	
			3P	C16	4.78	
			3P	C13	4.46	
Asp	381B	OD2	3P	C17	4.35	
			3P	C18	4.27	
Leu	384B	CB	3P	C18	4.77	
Leu	384B	CG	3P	C18	4.87	
Leu	384B	CD1	3P	C18	3.97	

Table 4:

PPAR γ -LBD residues within 5 Å radius of prostaglandin B2 molecule 1. See also Figure 3.

Tyr	222
Phe	226
Pro	227
Leu	228
Thr	229
Lys	230
Cys	285
Arg	288
Ser	289
Ala	292
Glu	295
Ile	326
Tyr	327
Met	329
Leu	330
Ser	332
Leu	333
Met	364
Asp	381
Leu	384

5 References

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EXEMPLARY EMBODIMENTS

- 15 The following are exemplary embodiments of the invention.

1. A prostaglandin-binding pocket of a PPAR protein molecule, which prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids that comprises amino acids corresponding to four or more selected from the group consisting of TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, CYS 285, ARG 288, SER 289,
20 ALA 292, GLU 295, ILE 296, ILE 325, ILE 326, TYR 327, THR 328, MET 329, LEU 330, ALA 331, SER 332, LEU 333, MET 364, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380, ASP 381, LEU 384, and LEU 435 of SEQ ID NO:1.
2. A prostaglandin-binding pocket of a PPAR γ or PPAR γ -like protein molecule comprising an amino acid sequence at least 65% identical to residues 207-476 of SEQ ID NO:1, which
25 prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids that comprises (i) an amino acid corresponding to LEU 228, and (ii) amino acids corresponding to three or more selected from the group consisting of TYR

222, PHE 226, PRO 227, THR 229, LYS 230, CYS 285, ARG 288, SER 289, ALA 292, GLU 295, ILE 296, ILE 325, ILE 326, TYR 327, THR 328, MET 329, LEU 330, ALA 331, SER 332, LEU 333, MET 364, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380, ASP 381, LEU 384, and LEU 435 of SEQ ID NO:1.

- 5 3. A prostaglandin-binding pocket according to any one of embodiments 1-2, wherein the set of amino acids comprises an amino acid corresponding to LEU 228 and amino acids corresponding to six or more selected from the group consisting of TYR 222, PHE 226, PRO 227, THR 229, LYS 230, CYS 285, ARG 288, SER 289, ALA 292, GLU 295, ILE 326, TYR 327, MET 329, LEU 330, SER 332, LEU 333, MET 364, ASP 381, and LEU 384.
- 10 4. A prostaglandin-binding pocket according to any one of embodiments 1-3, wherein the set of amino acids comprises an amino acid corresponding to LEU 228 and amino acids corresponding to ten or more selected from the group consisting of TYR 222, PHE 226, PRO 227, THR 229, LYS 230, CYS 285, ARG 288, SER 289, ALA 292, GLU 295, ILE 326, TYR 327, MET 329, LEU 330, SER 332, LEU 333, MET 364, ASP 381, and LEU 384.
- 15 5. A prostaglandin-binding pocket according to any one of embodiments 1-4, wherein the set of amino acids comprises amino acids corresponding to PHE 226, PRO 227, LEU 228 and MET 329.
- 20 6. A prostaglandin-binding pocket according to any one of embodiments 1-5, wherein the set of amino acids comprises amino acids corresponding to TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, ALA 292, GLU 295, MET 329, SER 332, LEU 333, ASP 381, and LEU 384.
- 25 7. A prostaglandin-binding pocket according to any one of embodiments 1-6, wherein the set of amino acids comprises amino acids corresponding to one or more selected from the group consisting of CYS 285, ARG 288, SER 289, ILE 326, TYR 327, LEU 330 and MET 364.
8. A prostaglandin-binding pocket according to any one of embodiments 1-7, wherein the set of amino acids comprises amino acids corresponding to TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, CYS 285, ARG 288, SER 289, ALA 292, GLU 295, ILE 326, TYR 327, MET 329, LEU 330, SER 332, LEU 333, MET 364, ASP 381, and LEU 384.

9. A prostaglandin-binding pocket according to any one of embodiments 1-8, wherein the set of amino acids comprises amino acids corresponding to one or more selected from the group consisting of ILE 296, ILE 325, THR 328, ALA 331, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380 and LEU 435.
- 5 10. A prostaglandin-binding pocket according to any one of embodiments 1-9, wherein the set of amino acids comprises amino acids corresponding to ILE 296, ILE 325, THR 328, ALA 331, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380 and LEU 435.
- 10 11. A prostaglandin-binding pocket according to any one of embodiments 1-10, wherein the set of amino acids comprises amino acids corresponding to TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, CYS 285, ARG 288, SER 289, ALA 292, GLU 295, ILE 296, ILE 325, ILE 326, TYR 327, THR 328, MET 329, LEU 330, ALA 331, SER 332, LEU 333, MET 364, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380, ASP 381, LEU 384, and LEU 435.
- 15 12. A method for evaluating the ability of a chemical entity to associate with the prostaglandin-binding pocket of any of embodiments 1-11, comprising the steps of: (a) providing the structure coordinates of said prostaglandin-binding pocket on a computer comprising the means for generating three-dimensional structural information from said structure coordinates; (b) employing computational means to perform a fitting operation between the chemical entity and the prostaglandin-binding pocket; and (c) analyzing the results of said fitting operation to evaluate the association between the chemical entity and the prostaglandin-binding pocket.
- 20 13. The method according to embodiment 12, further comprising in step (c) to quantify the association between the chemical entity and the prostaglandin-binding pocket.
- 25 14. A method of using a computer for evaluating the ability of a chemical entity to associate with a prostaglandin-binding pocket according to any of embodiments 1-11, wherein said computer comprises a machine-readable data storage medium comprising a data storage material encoded with said structure coordinates defining said prostaglandin-binding pocket and means for generating a three-dimensional graphical representation of the prostaglandin-binding pocket, and wherein said method comprises the steps of: (a) positioning a first chemical entity within said prostaglandin-binding pocket using a graphical three-dimensional representation of the structure of the chemical entity and the prostaglandin-binding pocket ; (b) performing a fitting operation between said chemical entity
- 30

and said prostaglandin-binding pocket by employing computational means; and (c) analyzing the results of said fitting operation to quantify the association between said chemical entity and the prostaglandin-binding pocket.

15. The method according to embodiment 14, further comprising the steps of: (d) repeating
5 steps (a) through (c) with a second chemical entity; and (e) selecting at least one of said first or second chemical entity that associates with said prostaglandin-binding pocket based on said quantified association of said first or second chemical entity.

16. A method for identifying a ligand of the prostaglandin-binding pocket of any of embodi-
10 ments 1-11, comprising the steps of: (a) using a three-dimensional structure of the prostaglandin-binding pocket to design, select and/or optimize a chemical entity; (b) contacting the chemical entity with the molecule; and (c) identifying any chemical entity capable of binding the molecule as a ligand.

17. A method for designing, selecting and/or optimizing a chemical entity that binds to the
15 prostaglandin-binding pocket of any of embodiments 1-11, comprising the steps of: (a) providing the structure coordinates of said prostaglandin-binding pocket on a computer comprising the means for generating three-dimensional structural information from said structure coordinates; and (b) designing, selecting and/or optimizing said chemical entity by performing a fitting operation between said chemical entity and said three-dimensional structural information of said prostaglandin-binding pocket.

20 18. A method of designing a compound or complex that associates with the prostaglandin-binding pocket of any of embodiments 1-11, comprising the steps of: (a) providing the structure coordinates of said prostaglandin-binding pocket on a computer comprising the means for generating three-dimensional structural information from said structure coordinates; and (b) using the computer to perform a fitting operation to associate a first
25 chemical entity with the prostaglandin-binding pocket; (c) performing a fitting operation to associate at least a second chemical entity with the prostaglandin-binding pocket; (d) quantifying the association between the first and second chemical entity and the prostaglandin-binding pocket; (e) optionally repeating steps b) to d) with another first and second chemical entity, selecting a first and a second chemical entity based on said quantified association of all of said first and second chemical entity; (f) optionally, visually inspecting the relationship of the first and second chemical entity to each other in relation to
30 the prostaglandin-binding pocket on a computer screen using the three-dimensional graphical representation of the prostaglandin-binding pocket and said first and second

chemical entity; and (g) assembling the first and second chemical entity into a compound or complex that associates with said prostaglandin-binding pocket by model building.

19. The method according to any one of embodiments 1-18 for screening for chemical entities useful for the treatment of prostaglandin- and/or PPAR-related diseases.

5 20. The method according to embodiment 19, wherein the prostaglandin- and/or PPAR-related diseases is cancer, inflammation, skin and hair disorders, diabetes, obesity, hypertension, and impaired glucose tolerance.

21. The method according to embodiment 20, wherein the prostaglandin- and/or PPAR-related diseases is cancer.

10 22. A computer comprising: (a) a machine-readable data storage medium, comprising a data storage material encoded with machine-readable data, wherein said data defines the prostaglandin-binding pocket of any of embodiments 1-11; (b) a working memory for storing instructions for processing said machine-readable data; (c) a central processing unit coupled to said working memory and to said machine-readable data storage medium for
15 processing said machine-readable data and means for generating three-dimensional structural information of said prostaglandin-binding pocket; and (d) output hardware coupled to said central processing unit for outputting three-dimensional structural information of said prostaglandin-binding pocket, or information produced using said three-dimensional structural information of said prostaglandin-binding pocket.

20 23. The computer according to embodiment 22, wherein said means for generating three-dimensional structural information is provided by means for generating a three-dimensional graphical representation of said prostaglandin-binding pocket.

24. The computer according to any one of embodiments 22-23, wherein said output hardware is a display terminal, a printer, CD or DID recorder, ZIP or JAZ drive, USB drive, a disk
25 drive, memory stick or other machine-readable data storage device.

25. The prostaglandin-binding pocket, method, or computer according to any one of embodiments 1-24, wherein the root mean square deviation of the backbone atoms between amino acids of said molecule and said PPAR γ residues is not greater than about 3 Å.

26. The prostaglandin-binding pocket, method, or computer according to any one of embodiments 1-24, wherein the root mean square deviation of the backbone atoms between amino acids of said molecule and said PPAR γ residues is not greater than about 1.5 Å.

27. The prostaglandin-binding pocket, method, or computer according to any one of embodiments 1-24, wherein the PPAR γ -like protein molecule comprises an amino acid sequence at least 80% identical to SEQ ID NO:2.

28. The prostaglandin-binding pocket, method, or computer according to any one of embodiments 1-24, wherein the PPAR γ -like protein molecule comprises an amino acid sequence at least 90% identical to SEQ ID NO:2.

29. The prostaglandin-binding pocket, method, or computer according to any one of embodiments 1-24, wherein the PPAR γ -like protein molecule comprises an amino acid sequence at least 95% identical to SEQ ID NO:2.

30. The prostaglandin-binding pocket, method, or computer according to any one of embodiments 1-24, wherein the PPAR γ protein molecule comprises the amino acid sequence of SEQ ID NO:2.

31. The prostaglandin-binding pocket, method, or computer according to any one of embodiments 1-24, wherein the PPAR γ protein molecule comprises the amino acid sequence of SEQ ID NO:1.

All references, including publications, patent applications and patents, cited herein are hereby incorporated by reference to the same extent as if each reference was individually and specifically indicated to be incorporated by reference and was set forth in its entirety herein.

All headings and sub-headings are used herein for convenience only and should not be construed as limiting the invention in any way,

Any combination of the above-described elements in all possible variations thereof is encompassed by the invention unless otherwise indicated herein or otherwise clearly contradicted by context.

The terms "a" and "an" and "the" and similar referents as used in the context of de-scribing the invention are to be construed to cover both the singular and the plural, unless otherwise indicated herein or clearly contradicted by context.

Recitation of ranges of values herein are merely intended to serve as a shorthand method of referring individually to each separate value falling within the range, unless other-wise indicated herein, and each separate value is incorporated into the specification as if it were individually recited herein. Unless otherwise stated, all exact values provided herein are representative of corresponding approximate values (e.g., all exact exemplary values provided with respect to a particular factor or measurement can be considered to also provide a corresponding approximate measurement, modified by "about," where appropriate).

All methods described herein can be performed in any suitable order unless other-wise indicated herein or otherwise clearly contradicted by context.

The use of any and all examples, or exemplary language (e.g., "such as") provided herein, is intended merely to better illuminate the invention and does not pose a limitation on the scope of the invention unless otherwise indicated. No language in the specification should be construed as indicating any element is essential to the practice of the invention unless as much is explicitly stated.

The citation and incorporation of patent documents herein is done for convenience only and does not reflect any view of the validity, patentability and/or enforceability of such patent documents,

The description herein of any aspect or embodiment of the invention using terms such as "comprising", "having", "including" or "containing" with reference to an element or elements is intended to provide support for a similar aspect or embodiment of the invention that "consists of", "consists essentially of", or "substantially comprises" that particular element or elements, unless otherwise stated or clearly contradicted by context (e.g., a composition described herein as comprising a particular element should be understood as also describing a composition consisting of that element, unless otherwise stated or clearly contradicted by context).

This invention includes all modifications and equivalents of the subject matter recited in the aspects or claims presented herein to the maximum extent permitted by applicable law.

CLAIMS

1. A method for evaluating the ability of a chemical entity to associate with a prostaglandin-binding pocket of a PPAR γ or PPAR γ -like protein molecule comprising an amino acid sequence at least 65% identical to residues 207-476 of SEQ ID NO:1, which prostaglandin-binding pocket is defined by three-dimensional structure coordinates of a set of amino acids that comprises (i) an amino acid corresponding to LEU 228, and (ii) amino acids corresponding to three or more selected from the group consisting of TYR 222, PHE 226, PRO 227, THR 229, LYS 230, CYS 285, ARG 288, SER 289, ALA 292, GLU 295, ILE 296, ILE 325, ILE 326, TYR 327, THR 328, MET 329, LEU 330, ALA 331, SER 332, LEU 333, MET 364, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380, ASP 381, LEU 384, and LEU 435 of SEQ ID NO:1, the method comprising the steps of: (a) providing the structure coordinates of said prostaglandin-binding pocket on a computer comprising the means for generating three-dimensional structural information from said structure coordinates; (b) employing computational means to perform a fitting operation between the chemical entity and the prostaglandin-binding pocket; and (c) analyzing the results of said fitting operation to evaluate the association between the chemical entity and the prostaglandin-binding pocket.
2. The method according to claim 1, wherein the set of amino acids comprises an amino acid corresponding to LEU 228 and amino acids corresponding to six or more selected from the group consisting of TYR 222, PHE 226, PRO 227, THR 229, LYS 230, CYS 285, ARG 288, SER 289, ALA 292, GLU 295, ILE 326, TYR 327, MET 329, LEU 330, SER 332, LEU 333, MET 364, ASP 381, and LEU 384.
3. The method according to any one of claims 1-2, wherein the set of amino acids comprises an amino acid corresponding to LEU 228 and amino acids corresponding to ten or more selected from the group consisting of TYR 222, PHE 226, PRO 227, THR 229, LYS 230, CYS 285, ARG 288, SER 289, ALA 292, GLU 295, ILE 326, TYR 327, MET 329, LEU 330, SER 332, LEU 333, MET 364, ASP 381, and LEU 384.
4. The method according to any one of claims 1-3, wherein the set of amino acids comprises amino acids corresponding to PHE 226, PRO 227, LEU 228 and MET 329.
5. The method according to any one of claims 1-4, wherein the set of amino acids comprises amino acids corresponding to TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, ALA 292, GLU 295, MET 329, SER 332, LEU 333, ASP 381, and LEU 384.

6. The method according to any one of claims 1-5, wherein the set of amino acids comprises amino acids corresponding to one or more selected from the group consisting of CYS 285, ARG 288, SER 289, ILE 326, TYR 327, LEU 330 and MET 364.
- 5 7. The method according to any one of claims 1-6, wherein the set of amino acids comprises amino acids corresponding to TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, CYS 285, ARG 288, SER 289, ALA 292, GLU 295, ILE 326, TYR 327, MET 329, LEU 330, SER 332, LEU 333, MET 364, ASP 381, and LEU 384.
- 10 8. The method according to any one of claims 1-7, wherein the set of amino acids comprises amino acids corresponding to one or more selected from the group consisting of ILE 296, ILE 325, THR 328, ALA 331, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380 and LEU 435.
9. The method according to any one of claims 1-8, wherein the set of amino acids comprises amino acids corresponding to ILE 296, ILE 325, THR 328, ALA 331, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380 and LEU 435.
- 15 10. The method according to any one of claims 1-9, wherein the set of amino acids comprises amino acids corresponding to TYR 222, PHE 226, PRO 227, LEU 228, THR 229, LYS 230, CYS 285, ARG 288, SER 289, ALA 292, GLU 295, ILE 296, ILE 325, ILE 326, TYR 327, THR 328, MET 329, LEU 330, ALA 331, SER 332, LEU 333, MET 364, PHE 374, ASN 375, ALA 376, LEU 377, GLU 378, LEU 379, ASP 380, ASP 381, LEU 384, and LEU 435.
- 20 11. The method according to any one of claims 1-10, further comprising in step (c) to quantify the association between the chemical entity and the prostaglandin-binding pocket.
12. The method according to any one of claims 1-11, wherein the PPAR γ protein molecule comprises the amino acid sequence of SEQ ID NO:2.
- 25 13. The method according to any one of claims 1-12, wherein the PPAR γ protein molecule comprises the amino acid sequence of SEQ ID NO:1.
14. The method according to any one of claims 1-13 for use in the designing of, or screening for, chemical entities useful for the treatment of a prostaglandin- and/or PPAR-related disease.

15. The method according to claim 14, wherein the disease is cancer.

1/75

	Atom				Coordinates			Occ	B
	#	Type	Resid Type	#	X	Y	Z		
ATOM	1	N	GLU A 207		-6.164	34.314	28.458	1.00	50.42
ATOM	2	CA	GLU A 207		-6.818	34.409	27.106	1.00	49.62
ATOM	3	CB	GLU A 207		-8.248	34.992	27.222	1.00	49.95
ATOM	4	CG	GLU A 207		-9.113	34.883	25.961	1.00	50.58
ATOM	5	CD	GLU A 207		-9.417	33.437	25.508	1.00	53.11
ATOM	6	OE1	GLU A 207		-9.126	33.099	24.325	1.00	53.55
ATOM	7	OE2	GLU A 207		-9.954	32.651	26.322	1.00	51.93
ATOM	8	C	GLU A 207		-6.005	35.159	26.033	1.00	48.88
ATOM	9	O	GLU A 207		-5.691	36.356	26.174	1.00	49.09
ATOM	10	N	SER A 208		-5.711	34.447	24.949	1.00	47.26
ATOM	11	CA	SER A 208		-5.186	35.047	23.740	1.00	46.26
ATOM	12	CB	SER A 208		-4.891	33.963	22.690	1.00	46.73
ATOM	13	OG	SER A 208		-6.005	33.113	22.453	1.00	47.65
ATOM	14	C	SER A 208		-6.117	36.130	23.176	1.00	45.44
ATOM	15	O	SER A 208		-5.660	37.078	22.534	1.00	45.19
ATOM	16	N	ALA A 209		-7.415	36.015	23.449	1.00	44.29
ATOM	17	CA	ALA A 209		-8.387	37.009	22.992	1.00	43.43
ATOM	18	CB	ALA A 209		-9.822	36.561	23.286	1.00	43.16
ATOM	19	C	ALA A 209		-8.107	38.375	23.618	1.00	42.91
ATOM	20	O	ALA A 209		-8.158	39.362	22.932	1.00	42.71
ATOM	21	N	ASP A 210		-7.799	38.414	24.916	1.00	42.65
ATOM	22	CA	ASP A 210		-7.472	39.673	25.610	1.00	42.72
ATOM	23	CB	ASP A 210		-7.465	39.472	27.129	1.00	43.46
ATOM	24	CG	ASP A 210		-8.840	39.611	27.732	1.00	45.87
ATOM	25	OD1	ASP A 210		-9.630	40.476	27.241	1.00	48.94
ATOM	26	OD2	ASP A 210		-9.123	38.852	28.695	1.00	47.10
ATOM	27	C	ASP A 210		-6.140	40.284	25.198	1.00	41.61
ATOM	28	O	ASP A 210		-5.961	41.497	25.266	1.00	41.42
ATOM	29	N	LEU A 211		-5.194	39.437	24.818	1.00	41.46
ATOM	30	CA	LEU A 211		-3.924	39.880	24.205	1.00	40.84
ATOM	31	CB	LEU A 211		-2.864	38.778	24.249	1.00	40.24
ATOM	32	CG	LEU A 211		-2.560	38.130	25.608	1.00	41.74
ATOM	33	CD1	LEU A 211		-1.623	36.964	25.409	1.00	39.20
ATOM	34	CD2	LEU A 211		-1.971	39.166	26.579	1.00	39.24
ATOM	35	C	LEU A 211		-4.092	40.343	22.760	1.00	41.45
ATOM	36	O	LEU A 211		-3.231	41.033	22.237	1.00	41.43
ATOM	37	N	ARG A 212		-5.171	39.919	22.105	1.00	41.32
ATOM	38	CA	ARG A 212		-5.427	40.330	20.745	1.00	42.13
ATOM	39	CB	ARG A 212		-6.418	39.387	20.034	1.00	41.39
ATOM	40	CG	ARG A 212		-5.760	38.165	19.497	1.00	42.86
ATOM	41	CD	ARG A 212		-4.284	38.456	19.234	1.00	47.31
ATOM	42	NE	ARG A 212		-4.076	38.967	17.881	1.00	49.59
ATOM	43	CZ	ARG A 212		-2.992	39.605	17.446	1.00	49.82
ATOM	44	NH1	ARG A 212		-1.958	39.850	18.247	1.00	46.02
ATOM	45	NH2	ARG A 212		-2.956	39.999	16.176	1.00	49.34
ATOM	46	C	ARG A 212		-5.952	41.746	20.800	1.00	41.66
ATOM	47	O	ARG A 212		-5.478	42.592	20.065	1.00	42.56
ATOM	48	N	ALA A 213		-6.927	41.968	21.682	1.00	42.22
ATOM	49	CA	ALA A 213		-7.530	43.283	21.987	1.00	42.70
ATOM	50	CB	ALA A 213		-8.578	43.114	23.056	1.00	42.43
ATOM	51	C	ALA A 213		-6.498	44.324	22.451	1.00	43.15
ATOM	52	O	ALA A 213		-6.614	45.510	22.157	1.00	43.54
ATOM	53	N	LEU A 214		-5.508	43.875	23.206	1.00	43.52

2/75

ATOM	54	CA	LEU	A	214	-4.402	44.741	23.583	1.00	42.59
ATOM	55	CB	LEU	A	214	-3.534	44.100	24.665	1.00	42.91
ATOM	56	CG	LEU	A	214	-2.391	44.997	25.179	1.00	40.78
ATOM	57	CD1	LEU	A	214	-2.871	46.263	25.878	1.00	38.59
ATOM	58	CD2	LEU	A	214	-1.490	44.228	26.156	1.00	41.16
ATOM	59	C	LEU	A	214	-3.568	45.124	22.366	1.00	43.56
ATOM	60	O	LEU	A	214	-3.263	46.295	22.210	1.00	42.88
ATOM	61	N	ALA	A	215	-3.203	44.136	21.528	1.00	43.53
ATOM	62	CA	ALA	A	215	-2.474	44.365	20.281	1.00	44.07
ATOM	63	CB	ALA	A	215	-2.282	43.036	19.500	1.00	43.48
ATOM	64	C	ALA	A	215	-3.176	45.386	19.397	1.00	43.54
ATOM	65	O	ALA	A	215	-2.538	46.246	18.789	1.00	43.53
ATOM	66	N	LYS	A	216	-4.496	45.267	19.322	1.00	44.72
ATOM	67	CA	LYS	A	216	-5.320	46.048	18.421	1.00	43.30
ATOM	68	CB	LYS	A	216	-6.772	45.501	18.375	1.00	44.72
ATOM	69	CG	LYS	A	216	-7.179	44.569	17.174	1.00	46.49
ATOM	70	CD	LYS	A	216	-6.353	43.224	17.140	1.00	51.58
ATOM	71	CE	LYS	A	216	-6.973	42.160	16.204	1.00	51.18
ATOM	72	NZ	LYS	A	216	-8.176	41.492	16.822	1.00	54.84
ATOM	73	C	LYS	A	216	-5.340	47.458	18.984	1.00	42.75
ATOM	74	O	LYS	A	216	-5.235	48.415	18.243	1.00	42.50
ATOM	75	N	HIS	A	217	-5.529	47.568	20.302	1.00	41.79
ATOM	76	CA	HIS	A	217	-5.615	48.836	20.983	1.00	40.79
ATOM	77	CB	HIS	A	217	-5.721	48.604	22.496	1.00	42.37
ATOM	78	CG	HIS	A	217	-5.512	49.856	23.297	1.00	45.84
ATOM	79	ND1	HIS	A	217	-6.391	50.924	23.235	1.00	50.65
ATOM	80	CE1	HIS	A	217	-5.955	51.901	24.013	1.00	49.66
ATOM	81	NE2	HIS	A	217	-4.812	51.520	24.547	1.00	45.02
ATOM	82	CD2	HIS	A	217	-4.508	50.246	24.112	1.00	45.87
ATOM	83	C	HIS	A	217	-4.342	49.620	20.741	1.00	39.74
ATOM	84	O	HIS	A	217	-4.343	50.816	20.492	1.00	38.90
ATOM	85	N	LEU	A	218	-3.230	48.948	20.891	1.00	37.23
ATOM	86	CA	LEU	A	218	-1.958	49.611	20.759	1.00	37.64
ATOM	87	CB	LEU	A	218	-0.851	48.700	21.335	1.00	37.76
ATOM	88	CG	LEU	A	218	-0.826	48.486	22.848	1.00	37.03
ATOM	89	CD1	LEU	A	218	0.255	47.466	23.119	1.00	34.75
ATOM	90	CD2	LEU	A	218	-0.566	49.801	23.699	1.00	32.25
ATOM	91	C	LEU	A	218	-1.664	49.970	19.305	1.00	38.87
ATOM	92	O	LEU	A	218	-1.086	51.064	19.006	1.00	38.75
ATOM	93	N	TYR	A	219	-2.093	49.104	18.372	1.00	39.05
ATOM	94	CA	TYR	A	219	-1.847	49.423	16.947	1.00	39.85
ATOM	95	CB	TYR	A	219	-2.245	48.279	16.016	1.00	40.46
ATOM	96	CG	TYR	A	219	-1.984	48.521	14.538	1.00	40.89
ATOM	97	CD1	TYR	A	219	-0.908	49.271	14.113	1.00	42.48
ATOM	98	CE1	TYR	A	219	-0.665	49.512	12.759	1.00	44.03
ATOM	99	CZ	TYR	A	219	-1.481	48.977	11.810	1.00	45.61
ATOM	100	OH	TYR	A	219	-1.193	49.228	10.489	1.00	47.23
ATOM	101	CE2	TYR	A	219	-2.570	48.200	12.192	1.00	47.16
ATOM	102	CD2	TYR	A	219	-2.805	47.979	13.581	1.00	44.43
ATOM	103	C	TYR	A	219	-2.606	50.715	16.616	1.00	41.97
ATOM	104	O	TYR	A	219	-2.057	51.646	16.003	1.00	43.06
ATOM	105	N	ASP	A	220	-3.867	50.751	17.051	1.00	41.97
ATOM	106	CA	ASP	A	220	-4.762	51.913	16.912	1.00	42.05
ATOM	107	CB	ASP	A	220	-6.011	51.623	17.737	1.00	42.33
ATOM	108	CG	ASP	A	220	-7.117	52.599	17.501	1.00	41.41
ATOM	109	OD1	ASP	A	220	-7.610	52.658	16.366	1.00	44.78
ATOM	110	OD2	ASP	A	220	-7.500	53.301	18.474	1.00	43.08
ATOM	111	C	ASP	A	220	-4.125	53.222	17.354	1.00	41.93

3/75

ATOM	112	O	ASP	A	220	-4.345	54.255	16.703	1.00	42.52
ATOM	113	N	SER	A	221	-3.404	53.193	18.482	1.00	41.10
ATOM	114	CA	SER	A	221	-2.918	54.379	19.157	1.00	40.91
ATOM	115	CB	SER	A	221	-2.617	54.119	20.636	1.00	42.58
ATOM	116	OG	SER	A	221	-3.721	53.565	21.341	1.00	47.99
ATOM	117	C	SER	A	221	-1.636	54.794	18.521	1.00	40.85
ATOM	118	O	SER	A	221	-1.328	55.964	18.470	1.00	40.16
ATOM	119	N	TYR	A	222	-0.816	53.806	18.161	1.00	40.52
ATOM	120	CA	TYR	A	222	0.330	54.003	17.331	1.00	41.27
ATOM	121	CB	TYR	A	222	0.851	52.600	17.002	1.00	40.55
ATOM	122	CG	TYR	A	222	2.007	52.557	16.076	1.00	39.93
ATOM	123	CD1	TYR	A	222	3.322	52.497	16.557	1.00	40.22
ATOM	124	CE1	TYR	A	222	4.365	52.458	15.681	1.00	39.72
ATOM	125	CZ	TYR	A	222	4.093	52.451	14.331	1.00	37.48
ATOM	126	OH	TYR	A	222	5.071	52.346	13.420	1.00	41.09
ATOM	127	CE2	TYR	A	222	2.830	52.475	13.848	1.00	31.91
ATOM	128	CD2	TYR	A	222	1.802	52.513	14.719	1.00	37.53
ATOM	129	C	TYR	A	222	0.022	54.813	16.038	1.00	41.96
ATOM	130	O	TYR	A	222	0.665	55.815	15.736	1.00	42.89
ATOM	131	N	ILE	A	223	-0.973	54.371	15.273	1.00	43.27
ATOM	132	CA	ILE	A	223	-1.388	55.050	14.061	1.00	42.14
ATOM	133	CB	ILE	A	223	-2.551	54.260	13.339	1.00	43.48
ATOM	134	CG1	ILE	A	223	-2.112	52.859	12.869	1.00	39.52
ATOM	135	CD1	ILE	A	223	-0.937	52.834	11.960	1.00	42.43
ATOM	136	CG2	ILE	A	223	-3.093	55.002	12.166	1.00	42.66
ATOM	137	C	ILE	A	223	-1.826	56.472	14.372	1.00	43.06
ATOM	138	O	ILE	A	223	-1.585	57.397	13.577	1.00	43.25
ATOM	139	N	LYS	A	224	-2.487	56.655	15.514	1.00	42.22
ATOM	140	CA	LYS	A	224	-3.047	57.969	15.844	1.00	40.87
ATOM	141	CB	LYS	A	224	-4.131	57.810	16.932	1.00	40.57
ATOM	142	CG	LYS	A	224	-5.434	57.165	16.430	1.00	40.62
ATOM	143	CD	LYS	A	224	-6.379	56.802	17.561	1.00	40.23
ATOM	144	CE	LYS	A	224	-7.773	56.468	16.997	1.00	40.07
ATOM	145	NZ	LYS	A	224	-8.668	55.896	18.043	1.00	41.48
ATOM	146	C	LYS	A	224	-1.905	58.896	16.304	1.00	40.15
ATOM	147	O	LYS	A	224	-1.969	60.121	16.199	1.00	37.96
ATOM	148	N	SER	A	225	-0.833	58.296	16.794	1.00	39.09
ATOM	149	CA	SER	A	225	0.301	59.060	17.380	1.00	39.05
ATOM	150	CB	SER	A	225	0.872	58.305	18.608	1.00	38.63
ATOM	151	OG	SER	A	225	-0.087	58.166	19.604	1.00	38.04
ATOM	152	C	SER	A	225	1.496	59.394	16.462	1.00	38.44
ATOM	153	O	SER	A	225	2.237	60.339	16.738	1.00	38.61
ATOM	154	N	PHE	A	226	1.764	58.555	15.469	1.00	38.33
ATOM	155	CA	PHE	A	226	2.933	58.713	14.593	1.00	38.87
ATOM	156	CB	PHE	A	226	3.830	57.459	14.641	1.00	38.32
ATOM	157	CG	PHE	A	226	4.337	57.161	16.027	1.00	39.20
ATOM	158	CD1	PHE	A	226	5.270	58.012	16.645	1.00	38.82
ATOM	159	CE1	PHE	A	226	5.734	57.757	17.975	1.00	36.43
ATOM	160	CZ	PHE	A	226	5.216	56.694	18.660	1.00	36.34
ATOM	161	CE2	PHE	A	226	4.263	55.834	18.049	1.00	35.55
ATOM	162	CD2	PHE	A	226	3.819	56.097	16.755	1.00	37.98
ATOM	163	C	PHE	A	226	2.458	58.985	13.198	1.00	38.94
ATOM	164	O	PHE	A	226	1.882	58.084	12.545	1.00	40.77
ATOM	165	N	PRO	A	227	2.665	60.222	12.715	1.00	40.18
ATOM	166	CA	PRO	A	227	2.011	60.546	11.454	1.00	40.57
ATOM	167	CB	PRO	A	227	2.170	62.085	11.341	1.00	41.60
ATOM	168	CG	PRO	A	227	3.396	62.385	12.158	1.00	41.41
ATOM	169	CD	PRO	A	227	3.468	61.345	13.241	1.00	39.70

4/75

ATOM	170	C	PRO	A	227	2.612	59.803	10.245	1.00	41.66
ATOM	171	O	PRO	A	227	1.901	59.581	9.269	1.00	42.31
ATOM	172	N	LEU	A	228	3.875	59.384	10.318	1.00	42.23
ATOM	173	CA	LEU	A	228	4.491	58.637	9.210	1.00	42.75
ATOM	174	CB	LEU	A	228	5.755	59.359	8.663	1.00	42.81
ATOM	175	CG	LEU	A	228	6.535	58.644	7.547	1.00	42.60
ATOM	176	CD1	LEU	A	228	5.716	58.476	6.312	1.00	43.54
ATOM	177	CD2	LEU	A	228	7.811	59.382	7.209	1.00	43.84
ATOM	178	C	LEU	A	228	4.791	57.176	9.580	1.00	41.99
ATOM	179	O	LEU	A	228	5.703	56.909	10.298	1.00	42.02
ATOM	180	N	THR	A	229	4.004	56.237	9.055	1.00	41.61
ATOM	181	CA	THR	A	229	4.085	54.835	9.461	1.00	40.14
ATOM	182	CB	THR	A	229	2.752	54.126	9.149	1.00	40.57
ATOM	183	OG1	THR	A	229	2.445	54.322	7.776	1.00	38.52
ATOM	184	CG2	THR	A	229	1.616	54.731	9.965	1.00	38.42
ATOM	185	C	THR	A	229	5.195	54.156	8.677	1.00	39.85
ATOM	186	O	THR	A	229	5.598	54.640	7.629	1.00	40.44
ATOM	187	N	LYS	A	230	5.693	53.035	9.157	1.00	37.80
ATOM	188	CA	LYS	A	230	6.619	52.267	8.360	1.00	36.61
ATOM	189	CB	LYS	A	230	7.016	50.962	9.098	1.00	36.34
ATOM	190	CG	LYS	A	230	7.915	50.068	8.289	1.00	32.86
ATOM	191	CD	LYS	A	230	8.486	48.915	9.094	1.00	35.06
ATOM	192	CE	LYS	A	230	9.588	48.359	8.298	1.00	40.59
ATOM	193	NZ	LYS	A	230	10.198	47.141	8.890	1.00	45.56
ATOM	194	C	LYS	A	230	6.001	51.949	6.995	1.00	37.01
ATOM	195	O	LYS	A	230	6.672	52.043	5.967	1.00	38.60
ATOM	196	N	ALA	A	231	4.722	51.572	6.968	1.00	37.48
ATOM	197	CA	ALA	A	231	4.036	51.241	5.714	1.00	36.80
ATOM	198	CB	ALA	A	231	2.632	50.726	5.987	1.00	37.24
ATOM	199	C	ALA	A	231	4.014	52.426	4.694	1.00	36.49
ATOM	200	O	ALA	A	231	4.186	52.199	3.515	1.00	36.13
ATOM	201	N	LYS	A	232	3.841	53.668	5.155	1.00	36.83
ATOM	202	CA	LYS	A	232	3.997	54.847	4.267	1.00	37.01
ATOM	203	CB	LYS	A	232	3.423	56.083	4.926	1.00	36.83
ATOM	204	CG	LYS	A	232	3.343	57.337	4.077	1.00	39.31
ATOM	205	CD	LYS	A	232	2.473	58.354	4.852	1.00	41.47
ATOM	206	CE	LYS	A	232	2.704	59.788	4.401	1.00	43.78
ATOM	207	NZ	LYS	A	232	2.652	59.805	2.927	1.00	47.38
ATOM	208	C	LYS	A	232	5.467	55.067	3.921	1.00	36.77
ATOM	209	O	LYS	A	232	5.801	55.384	2.784	1.00	36.68
ATOM	210	N	ALA	A	233	6.353	54.847	4.893	1.00	36.21
ATOM	211	CA	ALA	A	233	7.784	54.966	4.630	1.00	35.80
ATOM	212	CB	ALA	A	233	8.549	54.786	5.922	1.00	36.68
ATOM	213	C	ALA	A	233	8.305	54.018	3.519	1.00	36.51
ATOM	214	O	ALA	A	233	9.032	54.443	2.614	1.00	37.15
ATOM	215	N	ARG	A	234	7.973	52.730	3.588	1.00	36.54
ATOM	216	CA	ARG	A	234	8.416	51.788	2.557	1.00	36.73
ATOM	217	CB	ARG	A	234	8.201	50.312	2.953	1.00	38.10
ATOM	218	CG	ARG	A	234	8.423	49.891	4.425	1.00	39.71
ATOM	219	CD	ARG	A	234	9.699	50.322	5.046	1.00	45.68
ATOM	220	NE	ARG	A	234	10.863	50.073	4.217	1.00	50.63
ATOM	221	CZ	ARG	A	234	12.081	50.521	4.517	1.00	53.33
ATOM	222	NH1	ARG	A	234	12.287	51.229	5.617	1.00	49.98
ATOM	223	NH2	ARG	A	234	13.101	50.252	3.716	1.00	56.09
ATOM	224	C	ARG	A	234	7.729	52.020	1.241	1.00	35.66
ATOM	225	O	ARG	A	234	8.309	51.760	0.218	1.00	36.25
ATOM	226	N	ALA	A	235	6.494	52.515	1.235	1.00	36.55
ATOM	227	CA	ALA	A	235	5.815	52.831	-0.043	1.00	36.40

5/75

ATOM	228	CB	ALA	A	235	4.367	53.172	0.181	1.00	36.52
ATOM	229	C	ALA	A	235	6.527	53.978	-0.732	1.00	36.70
ATOM	230	O	ALA	A	235	6.675	53.959	-1.942	1.00	38.29
ATOM	231	N	ILE	A	236	6.992	54.962	0.045	1.00	36.22
ATOM	232	CA	ILE	A	236	7.795	56.066	-0.498	1.00	35.57
ATOM	233	CB	ILE	A	236	8.006	57.181	0.537	1.00	35.77
ATOM	234	CG1	ILE	A	236	6.678	57.820	0.887	1.00	33.16
ATOM	235	CD1	ILE	A	236	6.693	58.569	2.241	1.00	27.84
ATOM	236	CG2	ILE	A	236	9.007	58.259	0.028	1.00	35.99
ATOM	237	C	ILE	A	236	9.141	55.610	-0.987	1.00	35.14
ATOM	238	O	ILE	A	236	9.557	56.005	-2.057	1.00	34.70
ATOM	239	N	LEU	A	237	9.807	54.756	-0.211	1.00	35.24
ATOM	240	CA	LEU	A	237	11.143	54.257	-0.560	1.00	36.99
ATOM	241	CB	LEU	A	237	11.828	53.658	0.685	1.00	37.27
ATOM	242	CG	LEU	A	237	12.177	54.458	1.935	1.00	39.44
ATOM	243	CD1	LEU	A	237	12.458	53.532	3.146	1.00	39.92
ATOM	244	CD2	LEU	A	237	13.377	55.316	1.630	1.00	43.77
ATOM	245	C	LEU	A	237	11.215	53.192	-1.690	1.00	37.66
ATOM	246	O	LEU	A	237	12.239	53.038	-2.345	1.00	36.80
ATOM	247	N	THR	A	238	10.147	52.425	-1.874	1.00	39.11
ATOM	248	CA	THR	A	238	10.149	51.354	-2.857	1.00	40.48
ATOM	249	CB	THR	A	238	9.426	50.093	-2.332	1.00	40.63
ATOM	250	OG1	THR	A	238	8.111	50.438	-1.878	1.00	42.59
ATOM	251	CG2	THR	A	238	10.178	49.513	-1.162	1.00	42.35
ATOM	252	C	THR	A	238	9.610	51.808	-4.223	1.00	41.16
ATOM	253	O	THR	A	238	9.791	51.114	-5.252	1.00	41.62
ATOM	254	N	AGLY	A	239	8.864	52.911	-4.231	0.67	41.71
ATOM	255	N	BGLY	A	239	9.064	53.025	-4.243	0.33	40.35
ATOM	256	CA	AGLY	A	239	8.233	53.386	-5.462	0.67	41.35
ATOM	257	CA	BGLY	A	239	8.807	53.763	-5.479	0.33	39.03
ATOM	258	C	AGLY	A	239	6.775	52.980	-5.697	0.67	41.18
ATOM	259	C	BGLY	A	239	7.664	53.236	-6.319	0.33	38.32
ATOM	260	O	AGLY	A	239	6.345	52.874	-6.860	0.67	40.94
ATOM	261	O	BGLY	A	239	6.491	53.557	-6.086	0.33	38.20
ATOM	262	N	ALYS	A	240	6.013	52.750	-4.620	0.67	40.52
ATOM	263	N	BLYS	A	240	8.012	52.428	-7.307	0.33	37.26
ATOM	264	CA	ALYS	A	240	4.554	52.514	-4.753	0.67	40.16
ATOM	265	CA	BLYS	A	240	7.023	51.836	-8.191	0.33	36.31
ATOM	266	CB	ALYS	A	240	3.959	51.835	-3.511	0.67	39.69
ATOM	267	CB	BLYS	A	240	6.388	50.605	-7.536	0.33	36.48
ATOM	268	CG	ALYS	A	240	4.716	50.586	-3.037	0.67	41.89
ATOM	269	CG	BLYS	A	240	7.238	49.339	-7.612	0.33	36.95
ATOM	270	CD	ALYS	A	240	4.838	49.524	-4.149	0.67	44.90
ATOM	271	CD	BLYS	A	240	6.389	48.106	-7.353	0.33	37.22
ATOM	272	CE	ALYS	A	240	6.173	48.769	-4.099	0.67	45.44
ATOM	273	CE	BLYS	A	240	7.097	46.830	-7.794	0.33	37.38
ATOM	274	NZ	ALYS	A	240	6.620	48.346	-5.480	0.67	45.86
ATOM	275	NZ	BLYS	A	240	7.020	46.567	-9.257	0.33	36.19
ATOM	276	C	ALYS	A	240	3.769	53.796	-5.106	0.67	39.58
ATOM	277	C	BLYS	A	240	5.952	52.849	-8.576	0.33	35.27
ATOM	278	O	ALYS	A	240	4.138	54.894	-4.692	0.67	39.29
ATOM	279	O	BLYS	A	240	5.104	52.570	-9.424	0.33	34.97
ATOM	280	N	ATHR	A	241	2.679	53.636	-5.864	0.67	38.77
ATOM	281	N	BTHR	A	241	6.016	54.029	-7.965	0.33	34.13
ATOM	282	CA	ATHR	A	241	1.930	54.757	-6.437	0.67	37.95
ATOM	283	CA	BTHR	A	241	4.943	55.017	-8.074	0.33	33.03
ATOM	284	CB	ATHR	A	241	1.326	54.390	-7.806	0.67	37.93
ATOM	285	CB	BTHR	A	241	4.039	55.023	-6.823	0.33	33.26

6/75

ATOM	286	OG1ATHR	A	241	0.248	53.469	-7.613	0.67	37.32	
ATOM	287	OG1BTHR	A	241	4.630	55.833	-5.796	0.33	33.47	
ATOM	288	CG2ATHR	A	241	2.394	53.769	-8.721	0.67	38.10	
ATOM	289	CG2BTHR	A	241	3.824	53.605	-6.303	0.33	33.47	
ATOM	290	C	ATHR	A	241	0.807	55.257	-5.537	0.67	37.56
ATOM	291	C	BTHR	A	241	5.437	56.440	-8.280	0.33	32.15
ATOM	292	O	ATHR	A	241	0.012	56.096	-5.932	0.67	37.88
ATOM	293	O	BTHR	A	241	6.567	56.781	-7.938	0.33	31.78
ATOM	294	N	ATHR	A	242	0.764	54.716	-4.334	0.67	37.58
ATOM	295	N	BTHR	A	242	4.554	57.280	-8.804	0.33	30.94
ATOM	296	CA	ATHR	A	242	0.017	55.274	-3.215	0.67	37.03
ATOM	297	CA	BTHR	A	242	4.893	58.661	-9.083	0.33	30.33
ATOM	298	CB	ATHR	A	242	-0.186	54.217	-2.139	0.67	36.35
ATOM	299	CB	BTHR	A	242	4.296	59.139	-10.416	0.33	30.34
ATOM	300	OG1ATHR	A	242	1.102	53.815	-1.614	0.67	34.49	
ATOM	301	OG1BTHR	A	242	2.889	58.857	-10.451	0.33	29.24	
ATOM	302	CG2ATHR	A	242	-0.910	52.995	-2.722	0.67	33.13	
ATOM	303	CG2BTHR	A	242	4.991	58.459	-11.579	0.33	30.17	
ATOM	304	C	ATHR	A	242	0.790	56.471	-2.629	0.67	37.95
ATOM	305	C	BTHR	A	242	4.452	59.624	-7.998	0.33	30.46
ATOM	306	O	ATHR	A	242	0.195	57.393	-2.089	0.67	37.42
ATOM	307	O	BTHR	A	242	5.035	60.693	-7.834	0.33	29.77
ATOM	308	N	AASP	A	243	2.118	56.452	-2.747	0.67	38.90
ATOM	309	N	BASP	A	243	3.418	59.257	-7.253	0.33	31.16
ATOM	310	CA	AASP	A	243	2.932	57.558	-2.256	0.67	39.43
ATOM	311	CA	BASP	A	243	2.826	60.228	-6.363	0.33	32.36
ATOM	312	CB	AASP	A	243	3.581	57.205	-0.945	0.67	39.68
ATOM	313	CB	BASP	A	243	1.871	59.565	-5.366	0.33	32.10
ATOM	314	CG	AASP	A	243	2.567	56.903	0.123	0.67	40.75
ATOM	315	CG	BASP	A	243	0.800	58.748	-6.044	0.33	33.01
ATOM	316	OD1AASP	A	243	2.063	57.856	0.755	0.67	43.76	
ATOM	317	OD1BASP	A	243	0.712	57.543	-5.758	0.33	34.00	
ATOM	318	OD2AASP	A	243	2.289	55.710	0.339	0.67	41.86	
ATOM	319	OD2BASP	A	243	0.048	59.300	-6.883	0.33	35.60	
ATOM	320	C	AASP	A	243	3.945	58.116	-3.255	0.67	40.10
ATOM	321	C	BASP	A	243	3.968	60.948	-5.659	0.33	33.38
ATOM	322	O	AASP	A	243	4.181	57.549	-4.342	0.67	40.55
ATOM	323	O	BASP	A	243	4.699	61.751	-6.269	0.33	33.63
ATOM	324	N	ALYS	A	244	4.523	59.252	-2.878	0.67	39.55
ATOM	325	N	BLYS	A	244	4.142	60.629	-4.386	0.33	34.35
ATOM	326	CA	ALYS	A	244	5.074	60.197	-3.848	0.67	38.91
ATOM	327	CA	BLYS	A	244	5.172	61.253	-3.590	0.33	35.62
ATOM	328	CB	ALYS	A	244	4.378	61.566	-3.714	0.67	38.68
ATOM	329	CB	BLYS	A	244	4.672	61.484	-2.155	0.33	36.03
ATOM	330	CG	ALYS	A	244	3.237	61.812	-4.696	0.67	39.01
ATOM	331	CG	BLYS	A	244	3.782	62.725	-1.983	0.33	35.46
ATOM	332	CD	ALYS	A	244	2.068	60.815	-4.565	0.67	40.35
ATOM	333	CD	BLYS	A	244	2.374	62.498	-2.508	0.33	35.52
ATOM	334	CE	ALYS	A	244	1.269	60.684	-5.829	0.67	39.85
ATOM	335	CE	BLYS	A	244	1.817	63.772	-3.148	0.33	33.52
ATOM	336	NZ	ALYS	A	244	2.126	60.433	-7.022	0.67	39.78
ATOM	337	NZ	BLYS	A	244	1.256	63.487	-4.507	0.33	31.97
ATOM	338	C	ALYS	A	244	6.572	60.289	-3.632	0.67	38.59
ATOM	339	C	BLYS	A	244	6.471	60.442	-3.639	0.33	36.42
ATOM	340	O	ALYS	A	244	7.064	59.915	-2.579	0.67	38.21
ATOM	341	O	BLYS	A	244	6.659	59.494	-2.879	0.33	36.14
ATOM	342	N	SER	A	245	7.298	60.794	-4.626	1.00	37.77
ATOM	343	CA	SER	A	245	8.731	60.504	-4.721	1.00	37.49

7/75

ATOM	344	CB	SER	A	245	9.173	60.700	-6.177	1.00	37.75
ATOM	345	OG	SER	A	245	8.520	59.814	-7.061	1.00	38.99
ATOM	346	C	SER	A	245	9.510	61.515	-3.907	1.00	36.96
ATOM	347	O	SER	A	245	9.220	62.723	-4.004	1.00	35.50
ATOM	348	N	PRO	A	246	10.537	61.056	-3.162	1.00	35.90
ATOM	349	CA	PRO	A	246	11.295	62.055	-2.402	1.00	35.47
ATOM	350	CB	PRO	A	246	11.989	61.230	-1.305	1.00	35.56
ATOM	351	CG	PRO	A	246	11.921	59.798	-1.730	1.00	36.44
ATOM	352	CD	PRO	A	246	11.073	59.696	-2.993	1.00	36.19
ATOM	353	C	PRO	A	246	12.295	62.839	-3.268	1.00	35.33
ATOM	354	O	PRO	A	246	12.770	62.325	-4.291	1.00	34.72
ATOM	355	N	PHE	A	247	12.552	64.101	-2.901	1.00	35.69
ATOM	356	CA	PHE	A	247	13.669	64.862	-3.466	1.00	35.69
ATOM	357	CB	PHE	A	247	13.485	66.368	-3.321	1.00	35.28
ATOM	358	CG	PHE	A	247	14.617	67.170	-3.933	1.00	37.24
ATOM	359	CD1	PHE	A	247	14.526	67.672	-5.246	1.00	36.38
ATOM	360	CE1	PHE	A	247	15.567	68.396	-5.807	1.00	37.06
ATOM	361	CZ	PHE	A	247	16.723	68.617	-5.081	1.00	37.34
ATOM	362	CE2	PHE	A	247	16.833	68.120	-3.786	1.00	37.05
ATOM	363	CD2	PHE	A	247	15.788	67.402	-3.220	1.00	37.82
ATOM	364	C	PHE	A	247	14.915	64.438	-2.709	1.00	35.45
ATOM	365	O	PHE	A	247	14.894	64.373	-1.487	1.00	36.35
ATOM	366	N	VAL	A	248	16.011	64.199	-3.419	1.00	35.15
ATOM	367	CA	VAL	A	248	17.134	63.441	-2.849	1.00	34.77
ATOM	368	CB	VAL	A	248	17.471	62.220	-3.757	1.00	34.83
ATOM	369	CG1	VAL	A	248	18.835	61.633	-3.411	1.00	34.85
ATOM	370	CG2	VAL	A	248	16.351	61.159	-3.684	1.00	34.51
ATOM	371	C	VAL	A	248	18.373	64.327	-2.638	1.00	34.37
ATOM	372	O	VAL	A	248	18.873	64.931	-3.585	1.00	34.07
ATOM	373	N	ILE	A	249	18.825	64.427	-1.385	1.00	34.81
ATOM	374	CA	ILE	A	249	20.037	65.194	-1.042	1.00	34.48
ATOM	375	CB	ILE	A	249	19.991	65.896	0.387	1.00	34.88
ATOM	376	CG1	ILE	A	249	18.674	66.640	0.726	1.00	35.76
ATOM	377	CD1	ILE	A	249	17.902	67.225	-0.428	1.00	40.28
ATOM	378	CG2	ILE	A	249	21.235	66.745	0.595	1.00	32.99
ATOM	379	C	ILE	A	249	21.227	64.260	-0.970	1.00	34.23
ATOM	380	O	ILE	A	249	21.302	63.440	-0.068	1.00	35.08
ATOM	381	N	TYR	A	250	22.181	64.416	-1.869	1.00	34.32
ATOM	382	CA	TYR	A	250	23.325	63.507	-1.927	1.00	34.86
ATOM	383	CB	TYR	A	250	23.264	62.614	-3.185	1.00	34.15
ATOM	384	CG	TYR	A	250	23.318	63.406	-4.490	1.00	33.61
ATOM	385	CD1	TYR	A	250	24.499	63.497	-5.222	1.00	32.31
ATOM	386	CE1	TYR	A	250	24.552	64.243	-6.407	1.00	32.94
ATOM	387	CZ	TYR	A	250	23.418	64.896	-6.856	1.00	31.52
ATOM	388	OH	TYR	A	250	23.486	65.647	-8.013	1.00	32.44
ATOM	389	CE2	TYR	A	250	22.244	64.820	-6.146	1.00	28.65
ATOM	390	CD2	TYR	A	250	22.191	64.080	-4.976	1.00	30.14
ATOM	391	C	TYR	A	250	24.636	64.281	-1.877	1.00	35.64
ATOM	392	O	TYR	A	250	25.698	63.692	-1.786	1.00	36.29
ATOM	393	N	ASP	A	251	24.560	65.602	-1.959	1.00	36.54
ATOM	394	CA	ASP	A	251	25.745	66.436	-1.880	1.00	38.01
ATOM	395	CB	ASP	A	251	26.624	66.352	-3.153	1.00	37.58
ATOM	396	CG	ASP	A	251	25.949	66.908	-4.405	1.00	38.62
ATOM	397	OD1	ASP	A	251	24.784	67.375	-4.348	1.00	38.72
ATOM	398	OD2	ASP	A	251	26.611	66.874	-5.466	1.00	37.90
ATOM	399	C	ASP	A	251	25.374	67.859	-1.506	1.00	38.64
ATOM	400	O	ASP	A	251	24.241	68.136	-1.120	1.00	39.05
ATOM	401	N	MET	A	252	26.346	68.743	-1.603	1.00	39.92

8/75

ATOM	402	CA	MET	A	252	26.187	70.119	-1.182	1.00	41.51
ATOM	403	CB	MET	A	252	27.555	70.813	-1.109	1.00	41.75
ATOM	404	CG	MET	A	252	28.465	70.299	0.012	1.00	42.84
ATOM	405	SD	MET	A	252	27.722	70.473	1.640	1.00	46.61
ATOM	406	CE	MET	A	252	27.279	72.219	1.605	1.00	46.55
ATOM	407	C	MET	A	252	25.238	70.887	-2.082	1.00	41.84
ATOM	408	O	MET	A	252	24.374	71.606	-1.589	1.00	41.80
ATOM	409	N	ASN	A	253	25.409	70.735	-3.394	1.00	42.75
ATOM	410	CA	ASN	A	253	24.543	71.380	-4.370	1.00	43.74
ATOM	411	CB	ASN	A	253	25.131	71.205	-5.774	1.00	44.40
ATOM	412	CG	ASN	A	253	24.359	71.966	-6.853	1.00	46.40
ATOM	413	OD1	ASN	A	253	24.764	73.055	-7.299	1.00	46.92
ATOM	414	ND2	ASN	A	253	23.252	71.375	-7.304	1.00	48.95
ATOM	415	C	ASN	A	253	23.087	70.879	-4.275	1.00	44.13
ATOM	416	O	ASN	A	253	22.144	71.666	-4.374	1.00	44.31
ATOM	417	N	SER	A	254	22.883	69.582	-4.060	1.00	44.27
ATOM	418	CA	SER	A	254	21.511	69.107	-3.918	1.00	44.88
ATOM	419	CB	SER	A	254	21.405	67.600	-4.129	1.00	44.24
ATOM	420	OG	SER	A	254	22.487	66.935	-3.536	1.00	44.37
ATOM	421	C	SER	A	254	20.873	69.556	-2.592	1.00	45.53
ATOM	422	O	SER	A	254	19.666	69.797	-2.542	1.00	45.22
ATOM	423	N	LEU	A	255	21.675	69.698	-1.535	1.00	46.60
ATOM	424	CA	LEU	A	255	21.169	70.250	-0.275	1.00	48.12
ATOM	425	CB	LEU	A	255	22.252	70.290	0.804	1.00	47.91
ATOM	426	CG	LEU	A	255	21.998	71.206	2.013	1.00	47.62
ATOM	427	CD1	LEU	A	255	20.765	70.788	2.819	1.00	46.96
ATOM	428	CD2	LEU	A	255	23.203	71.221	2.886	1.00	46.50
ATOM	429	C	LEU	A	255	20.619	71.643	-0.476	1.00	49.45
ATOM	430	O	LEU	A	255	19.534	71.952	0.012	1.00	49.35
ATOM	431	N	MET	A	256	21.398	72.463	-1.185	1.00	51.41
ATOM	432	CA	MET	A	256	21.063	73.837	-1.563	1.00	54.02
ATOM	433	CB	MET	A	256	22.171	74.370	-2.480	1.00	53.71
ATOM	434	CG	MET	A	256	22.566	75.819	-2.281	1.00	54.63
ATOM	435	SD	MET	A	256	23.974	76.310	-3.326	1.00	55.55
ATOM	436	CE	MET	A	256	25.390	75.697	-2.402	1.00	56.80
ATOM	437	C	MET	A	256	19.702	73.937	-2.279	1.00	55.23
ATOM	438	O	MET	A	256	18.890	74.823	-1.978	1.00	55.27
ATOM	439	N	MET	A	257	19.468	73.017	-3.220	1.00	56.89
ATOM	440	CA	MET	A	257	18.227	72.970	-3.985	1.00	58.24
ATOM	441	CB	MET	A	257	18.472	72.308	-5.342	1.00	58.62
ATOM	442	CG	MET	A	257	19.339	73.119	-6.320	1.00	60.12
ATOM	443	SD	MET	A	257	18.571	74.611	-7.032	1.00	64.60
ATOM	444	CE	MET	A	257	17.187	73.916	-7.954	1.00	63.21
ATOM	445	C	MET	A	257	17.106	72.245	-3.237	1.00	59.15
ATOM	446	O	MET	A	257	15.954	72.250	-3.677	1.00	59.37
ATOM	447	N	GLY	A	258	17.450	71.616	-2.113	1.00	60.20
ATOM	448	CA	GLY	A	258	16.475	70.932	-1.254	1.00	61.31
ATOM	449	C	GLY	A	258	15.532	71.913	-0.583	1.00	62.25
ATOM	450	O	GLY	A	258	14.321	71.696	-0.521	1.00	62.10
ATOM	451	N	GLU	A	259	16.107	73.001	-0.083	1.00	63.25
ATOM	452	CA	GLU	A	259	15.351	74.115	0.471	1.00	64.47
ATOM	453	CB	GLU	A	259	16.327	75.147	1.044	1.00	64.51
ATOM	454	CG	GLU	A	259	17.449	74.524	1.904	1.00	65.03
ATOM	455	CD	GLU	A	259	18.694	75.408	2.038	1.00	65.31
ATOM	456	OE1	GLU	A	259	19.349	75.340	3.105	1.00	66.30
ATOM	457	OE2	GLU	A	259	19.026	76.157	1.086	1.00	65.98
ATOM	458	C	GLU	A	259	14.450	74.733	-0.614	1.00	64.82
ATOM	459	O	GLU	A	259	13.312	75.136	-0.344	1.00	64.97

9/75

ATOM	460	N	ASP	A	260	14.960	74.773	-1.845	1.00	65.19
ATOM	461	CA	ASP	A	260	14.215	75.289	-2.992	1.00	65.57
ATOM	462	CB	ASP	A	260	15.103	76.217	-3.823	1.00	65.73
ATOM	463	CG	ASP	A	260	14.306	77.126	-4.729	1.00	65.96
ATOM	464	OD1	ASP	A	260	13.529	77.952	-4.201	1.00	65.79
ATOM	465	OD2	ASP	A	260	14.469	77.021	-5.967	1.00	66.25
ATOM	466	C	ASP	A	260	13.688	74.161	-3.878	1.00	65.60
ATOM	467	O	ASP	A	260	12.668	73.542	-3.578	1.00	65.51
ATOM	468	N	LYS	A	275	26.633	79.543	9.911	1.00	48.69
ATOM	469	CA	LYS	A	275	25.857	78.406	10.367	1.00	48.27
ATOM	470	CB	LYS	A	275	24.378	78.810	10.460	1.00	48.30
ATOM	471	CG	LYS	A	275	23.493	77.845	11.258	1.00	49.21
ATOM	472	CD	LYS	A	275	22.082	78.404	11.462	1.00	48.66
ATOM	473	CE	LYS	A	275	21.283	77.553	12.439	1.00	48.23
ATOM	474	NZ	LYS	A	275	20.244	78.342	13.155	1.00	46.85
ATOM	475	C	LYS	A	275	26.076	77.248	9.374	1.00	48.33
ATOM	476	O	LYS	A	275	25.192	76.934	8.578	1.00	48.28
ATOM	477	N	GLU	A	276	27.262	76.629	9.415	1.00	47.80
ATOM	478	CA	GLU	A	276	27.699	75.684	8.364	1.00	46.63
ATOM	479	CB	GLU	A	276	29.132	75.203	8.598	1.00	46.84
ATOM	480	CG	GLU	A	276	29.255	74.247	9.782	1.00	48.26
ATOM	481	CD	GLU	A	276	30.483	73.359	9.715	1.00	50.38
ATOM	482	OE1	GLU	A	276	30.571	72.554	8.752	1.00	52.12
ATOM	483	OE2	GLU	A	276	31.344	73.455	10.630	1.00	49.07
ATOM	484	C	GLU	A	276	26.780	74.474	8.230	1.00	45.53
ATOM	485	O	GLU	A	276	26.103	74.084	9.181	1.00	45.47
ATOM	486	N	VAL	A	277	26.777	73.887	7.034	1.00	44.26
ATOM	487	CA	VAL	A	277	25.938	72.735	6.721	1.00	42.65
ATOM	488	CB	VAL	A	277	26.248	72.131	5.298	1.00	42.57
ATOM	489	CG1	VAL	A	277	27.728	71.851	5.108	1.00	42.92
ATOM	490	CG2	VAL	A	277	25.446	70.874	5.050	1.00	41.18
ATOM	491	C	VAL	A	277	25.927	71.686	7.835	1.00	41.81
ATOM	492	O	VAL	A	277	24.854	71.351	8.319	1.00	42.46
ATOM	493	N	ALA	A	278	27.094	71.192	8.259	1.00	41.05
ATOM	494	CA	ALA	A	278	27.165	70.061	9.213	1.00	40.38
ATOM	495	CB	ALA	A	278	28.605	69.746	9.600	1.00	40.30
ATOM	496	C	ALA	A	278	26.335	70.320	10.452	1.00	39.95
ATOM	497	O	ALA	A	278	25.564	69.461	10.867	1.00	40.47
ATOM	498	N	ILE	A	279	26.483	71.512	11.024	1.00	39.82
ATOM	499	CA	ILE	A	279	25.767	71.937	12.233	1.00	39.60
ATOM	500	CB	ILE	A	279	26.270	73.330	12.745	1.00	39.83
ATOM	501	CG1	ILE	A	279	27.794	73.362	12.895	1.00	39.85
ATOM	502	CD1	ILE	A	279	28.322	73.346	14.313	1.00	39.32
ATOM	503	CG2	ILE	A	279	25.580	73.731	14.046	1.00	39.14
ATOM	504	C	ILE	A	279	24.274	72.033	11.988	1.00	39.41
ATOM	505	O	ILE	A	279	23.502	71.621	12.831	1.00	40.05
ATOM	506	N	ARG	A	280	23.889	72.591	10.835	1.00	40.11
ATOM	507	CA	ARG	A	280	22.484	72.799	10.428	1.00	39.99
ATOM	508	CB	ARG	A	280	22.395	73.619	9.121	1.00	39.95
ATOM	509	CG	ARG	A	280	22.845	75.072	9.273	1.00	40.61
ATOM	510	CD	ARG	A	280	22.333	76.006	8.134	1.00	41.61
ATOM	511	NE	ARG	A	280	22.603	75.454	6.800	1.00	45.59
ATOM	512	CZ	ARG	A	280	23.462	75.952	5.914	1.00	46.51
ATOM	513	NH1	ARG	A	280	24.147	77.069	6.168	1.00	47.88
ATOM	514	NH2	ARG	A	280	23.613	75.335	4.747	1.00	46.69
ATOM	515	C	ARG	A	280	21.718	71.505	10.278	1.00	39.66
ATOM	516	O	ARG	A	280	20.571	71.409	10.727	1.00	40.77
ATOM	517	N	ILE	A	281	22.345	70.509	9.659	1.00	38.85

10/75

ATOM	518	CA	ILE	A	281	21.771	69.154	9.580	1.00	38.26
ATOM	519	CB	ILE	A	281	22.616	68.250	8.704	1.00	38.07
ATOM	520	CG1	ILE	A	281	22.661	68.795	7.288	1.00	36.86
ATOM	521	CD1	ILE	A	281	23.787	68.219	6.509	1.00	37.60
ATOM	522	CG2	ILE	A	281	22.058	66.821	8.676	1.00	37.83
ATOM	523	C	ILE	A	281	21.650	68.546	10.969	1.00	38.30
ATOM	524	O	ILE	A	281	20.631	67.937	11.290	1.00	38.43
ATOM	525	N	PHE	A	282	22.679	68.740	11.798	1.00	39.20
ATOM	526	CA	PHE	A	282	22.665	68.231	13.168	1.00	39.98
ATOM	527	CB	PHE	A	282	24.018	68.405	13.871	1.00	40.11
ATOM	528	CG	PHE	A	282	24.041	67.773	15.239	1.00	40.49
ATOM	529	CD1	PHE	A	282	24.252	66.407	15.377	1.00	40.65
ATOM	530	CE1	PHE	A	282	24.217	65.809	16.630	1.00	40.64
ATOM	531	CZ	PHE	A	282	23.962	66.576	17.759	1.00	40.65
ATOM	532	CE2	PHE	A	282	23.731	67.931	17.634	1.00	40.96
ATOM	533	CD2	PHE	A	282	23.757	68.520	16.372	1.00	40.23
ATOM	534	C	PHE	A	282	21.518	68.831	14.009	1.00	40.46
ATOM	535	O	PHE	A	282	20.709	68.111	14.610	1.00	40.40
ATOM	536	N	GLN	A	283	21.459	70.154	14.039	1.00	41.03
ATOM	537	CA	GLN	A	283	20.338	70.871	14.637	1.00	42.32
ATOM	538	CB	GLN	A	283	20.642	72.372	14.651	1.00	42.15
ATOM	539	CG	GLN	A	283	21.326	72.783	15.968	1.00	44.00
ATOM	540	CD	GLN	A	283	21.778	74.236	16.004	1.00	43.75
ATOM	541	OE1	GLN	A	283	21.913	74.827	17.081	1.00	46.17
ATOM	542	NE2	GLN	A	283	22.015	74.822	14.828	1.00	46.64
ATOM	543	C	GLN	A	283	18.964	70.535	14.009	1.00	42.48
ATOM	544	O	GLN	A	283	17.970	70.380	14.714	1.00	41.96
ATOM	545	N	GLY	A	284	18.919	70.407	12.689	1.00	43.45
ATOM	546	CA	GLY	A	284	17.760	69.829	12.017	1.00	44.58
ATOM	547	C	GLY	A	284	17.355	68.496	12.626	1.00	45.87
ATOM	548	O	GLY	A	284	16.176	68.262	12.867	1.00	45.46
ATOM	549	N	CYS	A	285	18.327	67.622	12.889	1.00	47.02
ATOM	550	CA	CYS	A	285	18.048	66.342	13.546	1.00	48.67
ATOM	551	CB	CYS	A	285	19.213	65.372	13.407	1.00	48.98
ATOM	552	SG	CYS	A	285	19.203	64.568	11.818	1.00	58.53
ATOM	553	C	CYS	A	285	17.676	66.473	15.017	1.00	47.78
ATOM	554	O	CYS	A	285	16.852	65.704	15.511	1.00	46.78
ATOM	555	N	GLN	A	286	18.300	67.431	15.715	1.00	48.22
ATOM	556	CA	GLN	A	286	17.903	67.771	17.093	1.00	48.34
ATOM	557	CB	GLN	A	286	18.596	69.057	17.578	1.00	48.78
ATOM	558	CG	GLN	A	286	19.837	68.880	18.440	1.00	49.55
ATOM	559	CD	GLN	A	286	20.334	70.227	18.987	1.00	49.36
ATOM	560	OE1	GLN	A	286	19.621	70.921	19.723	1.00	48.02
ATOM	561	NE2	GLN	A	286	21.552	70.604	18.602	1.00	51.50
ATOM	562	C	GLN	A	286	16.403	67.983	17.173	1.00	47.71
ATOM	563	O	GLN	A	286	15.735	67.401	18.001	1.00	47.75
ATOM	564	N	PHE	A	287	15.902	68.838	16.291	1.00	48.25
ATOM	565	CA	PHE	A	287	14.499	69.242	16.243	1.00	48.66
ATOM	566	CB	PHE	A	287	14.349	70.482	15.326	1.00	50.59
ATOM	567	CG	PHE	A	287	13.074	70.516	14.519	1.00	53.03
ATOM	568	CD1	PHE	A	287	13.051	70.016	13.207	1.00	55.29
ATOM	569	CE1	PHE	A	287	11.879	70.032	12.454	1.00	56.15
ATOM	570	CZ	PHE	A	287	10.705	70.558	13.015	1.00	55.80
ATOM	571	CE2	PHE	A	287	10.715	71.073	14.324	1.00	57.82
ATOM	572	CD2	PHE	A	287	11.902	71.058	15.063	1.00	56.52
ATOM	573	C	PHE	A	287	13.584	68.088	15.850	1.00	47.87
ATOM	574	O	PHE	A	287	12.501	67.963	16.394	1.00	48.39
ATOM	575	N	ARG	A	288	14.037	67.226	14.950	1.00	46.40

11/75

ATOM	576	CA	ARG	A	288	13.266	66.056	14.546	1.00	45.82
ATOM	577	CB	ARG	A	288	13.889	65.355	13.305	1.00	45.87
ATOM	578	CG	ARG	A	288	13.946	66.207	11.970	1.00	47.01
ATOM	579	CD	ARG	A	288	15.003	65.646	10.877	1.00	48.68
ATOM	580	NE	ARG	A	288	15.365	66.614	9.789	1.00	49.20
ATOM	581	CZ	ARG	A	288	16.477	66.582	9.031	1.00	46.81
ATOM	582	NH1	ARG	A	288	17.401	65.637	9.194	1.00	47.81
ATOM	583	NH2	ARG	A	288	16.672	67.505	8.102	1.00	43.91
ATOM	584	C	ARG	A	288	13.084	65.101	15.753	1.00	44.63
ATOM	585	O	ARG	A	288	11.993	64.571	15.935	1.00	43.77
ATOM	586	N	SER	A	289	14.124	64.909	16.585	1.00	42.90
ATOM	587	CA	SER	A	289	14.018	64.042	17.778	1.00	42.46
ATOM	588	CB	SER	A	289	15.364	63.890	18.479	1.00	41.88
ATOM	589	OG	SER	A	289	16.323	63.269	17.675	1.00	45.22
ATOM	590	C	SER	A	289	13.083	64.608	18.832	1.00	41.51
ATOM	591	O	SER	A	289	12.545	63.869	19.626	1.00	42.10
ATOM	592	N	VAL	A	290	12.982	65.923	18.909	1.00	40.62
ATOM	593	CA	VAL	A	290	12.133	66.547	19.918	1.00	40.46
ATOM	594	CB	VAL	A	290	12.398	68.080	20.042	1.00	40.86
ATOM	595	CG1	VAL	A	290	11.154	68.831	20.520	1.00	42.83
ATOM	596	CG2	VAL	A	290	13.572	68.364	20.991	1.00	38.76
ATOM	597	C	VAL	A	290	10.685	66.220	19.535	1.00	40.72
ATOM	598	O	VAL	A	290	9.897	65.754	20.378	1.00	39.96
ATOM	599	N	GLU	A	291	10.353	66.424	18.254	1.00	39.66
ATOM	600	CA	GLU	A	291	9.028	66.031	17.756	1.00	40.25
ATOM	601	CB	GLU	A	291	8.887	66.314	16.263	1.00	40.93
ATOM	602	CG	GLU	A	291	9.259	67.730	15.989	1.00	43.74
ATOM	603	CD	GLU	A	291	8.893	68.195	14.611	1.00	51.08
ATOM	604	OE1	GLU	A	291	8.060	69.114	14.522	1.00	51.45
ATOM	605	OE2	GLU	A	291	9.441	67.654	13.618	1.00	54.24
ATOM	606	C	GLU	A	291	8.732	64.564	18.076	1.00	38.94
ATOM	607	O	GLU	A	291	7.667	64.258	18.567	1.00	38.30
ATOM	608	N	ALA	A	292	9.702	63.685	17.838	1.00	37.33
ATOM	609	CA	ALA	A	292	9.522	62.252	18.092	1.00	36.49
ATOM	610	CB	ALA	A	292	10.702	61.430	17.560	1.00	34.72
ATOM	611	C	ALA	A	292	9.328	62.050	19.565	1.00	35.92
ATOM	612	O	ALA	A	292	8.524	61.221	19.975	1.00	36.21
ATOM	613	N	VAL	A	293	10.050	62.811	20.391	1.00	35.83
ATOM	614	CA	VAL	A	293	9.868	62.676	21.846	1.00	35.00
ATOM	615	CB	VAL	A	293	10.941	63.461	22.637	1.00	35.61
ATOM	616	CG1	VAL	A	293	10.466	63.767	24.066	1.00	35.59
ATOM	617	CG2	VAL	A	293	12.272	62.706	22.660	1.00	33.06
ATOM	618	C	VAL	A	293	8.440	63.052	22.244	1.00	35.84
ATOM	619	O	VAL	A	293	7.858	62.485	23.170	1.00	35.99
ATOM	620	N	GLN	A	294	7.864	64.023	21.567	1.00	36.51
ATOM	621	CA	GLN	A	294	6.522	64.430	21.914	1.00	38.83
ATOM	622	CB	GLN	A	294	6.171	65.810	21.360	1.00	39.31
ATOM	623	CG	GLN	A	294	4.640	66.194	21.597	1.00	45.61
ATOM	624	CD	GLN	A	294	4.182	66.278	23.119	1.00	49.55
ATOM	625	OE1	GLN	A	294	4.482	67.275	23.824	1.00	49.34
ATOM	626	NE2	GLN	A	294	3.436	65.245	23.594	1.00	44.64
ATOM	627	C	GLN	A	294	5.493	63.412	21.461	1.00	39.22
ATOM	628	O	GLN	A	294	4.473	63.245	22.139	1.00	40.94
ATOM	629	N	GLU	A	295	5.776	62.699	20.355	1.00	38.90
ATOM	630	CA	GLU	A	295	4.854	61.700	19.816	1.00	37.66
ATOM	631	CB	GLU	A	295	5.212	61.343	18.379	1.00	36.85
ATOM	632	CG	GLU	A	295	4.869	62.425	17.301	1.00	38.50
ATOM	633	CD	GLU	A	295	5.711	62.232	16.032	1.00	38.83

12/75

ATOM	634	OE1	GLU	A	295	6.582	61.328	15.991	1.00	42.06
ATOM	635	OE2	GLU	A	295	5.513	62.975	15.076	1.00	40.44
ATOM	636	C	GLU	A	295	4.937	60.467	20.688	1.00	36.16
ATOM	637	O	GLU	A	295	3.937	59.916	21.081	1.00	36.40
ATOM	638	N	ILE	A	296	6.149	60.042	20.987	1.00	35.50
ATOM	639	CA	ILE	A	296	6.365	58.888	21.862	1.00	34.78
ATOM	640	CB	ILE	A	296	7.889	58.597	22.053	1.00	34.21
ATOM	641	CG1	ILE	A	296	8.565	58.250	20.715	1.00	32.85
ATOM	642	CD1	ILE	A	296	10.121	58.379	20.715	1.00	34.11
ATOM	643	CG2	ILE	A	296	8.110	57.562	23.173	1.00	35.72
ATOM	644	C	ILE	A	296	5.732	59.160	23.212	1.00	36.04
ATOM	645	O	ILE	A	296	5.152	58.253	23.789	1.00	37.69
ATOM	646	N	THR	A	297	5.830	60.392	23.742	1.00	36.57
ATOM	647	CA	THR	A	297	5.182	60.683	25.003	1.00	38.19
ATOM	648	CB	THR	A	297	5.516	62.072	25.509	1.00	38.34
ATOM	649	OG1	THR	A	297	6.940	62.170	25.687	1.00	40.79
ATOM	650	CG2	THR	A	297	4.852	62.291	26.851	1.00	38.46
ATOM	651	C	THR	A	297	3.651	60.532	24.927	1.00	38.69
ATOM	652	O	THR	A	297	3.019	59.980	25.826	1.00	37.79
ATOM	653	N	GLU	A	298	3.079	61.003	23.837	1.00	39.73
ATOM	654	CA	GLU	A	298	1.637	60.888	23.621	1.00	41.46
ATOM	655	CB	GLU	A	298	1.261	61.686	22.381	1.00	41.35
ATOM	656	CG	GLU	A	298	-0.249	61.694	22.069	1.00	45.57
ATOM	657	CD	GLU	A	298	-0.617	62.429	20.772	1.00	44.43
ATOM	658	OE1	GLU	A	298	-1.317	63.466	20.844	1.00	53.35
ATOM	659	OE2	GLU	A	298	-0.237	61.977	19.681	1.00	46.31
ATOM	660	C	GLU	A	298	1.239	59.396	23.490	1.00	41.22
ATOM	661	O	GLU	A	298	0.230	58.957	24.038	1.00	42.19
ATOM	662	N	TYR	A	299	2.038	58.627	22.764	1.00	40.51
ATOM	663	CA	TYR	A	299	1.789	57.195	22.625	1.00	40.62
ATOM	664	CB	TYR	A	299	2.865	56.561	21.752	1.00	40.13
ATOM	665	CG	TYR	A	299	2.711	55.078	21.588	1.00	37.02
ATOM	666	CD1	TYR	A	299	1.574	54.564	21.000	1.00	34.80
ATOM	667	CE1	TYR	A	299	1.407	53.233	20.816	1.00	35.52
ATOM	668	CZ	TYR	A	299	2.391	52.340	21.289	1.00	41.02
ATOM	669	OH	TYR	A	299	2.204	51.002	21.071	1.00	39.65
ATOM	670	CE2	TYR	A	299	3.543	52.811	21.883	1.00	35.59
ATOM	671	CD2	TYR	A	299	3.700	54.188	22.047	1.00	40.54
ATOM	672	C	TYR	A	299	1.811	56.493	23.971	1.00	41.36
ATOM	673	O	TYR	A	299	0.912	55.759	24.299	1.00	43.38
ATOM	674	N	ALA	A	300	2.862	56.719	24.740	1.00	41.16
ATOM	675	CA	ALA	A	300	3.028	56.090	26.056	1.00	40.32
ATOM	676	CB	ALA	A	300	4.241	56.682	26.750	1.00	39.52
ATOM	677	C	ALA	A	300	1.758	56.197	26.950	1.00	40.26
ATOM	678	O	ALA	A	300	1.337	55.209	27.583	1.00	39.76
ATOM	679	N	LYS	A	301	1.159	57.384	26.998	1.00	38.32
ATOM	680	CA	LYS	A	301	-0.106	57.613	27.698	1.00	39.23
ATOM	681	CB	LYS	A	301	-0.622	59.073	27.502	1.00	38.72
ATOM	682	CG	LYS	A	301	0.202	60.078	28.256	1.00	40.68
ATOM	683	CD	LYS	A	301	0.054	61.568	27.849	1.00	41.41
ATOM	684	CE	LYS	A	301	-1.375	62.130	27.956	1.00	43.21
ATOM	685	NZ	LYS	A	301	-1.509	63.660	28.136	1.00	44.43
ATOM	686	C	LYS	A	301	-1.206	56.613	27.347	1.00	39.40
ATOM	687	O	LYS	A	301	-2.077	56.383	28.182	1.00	40.20
ATOM	688	N	SER	A	302	-1.190	56.042	26.134	1.00	39.33
ATOM	689	CA	SER	A	302	-2.221	55.087	25.717	1.00	40.38
ATOM	690	CB	SER	A	302	-2.338	55.072	24.207	1.00	40.26
ATOM	691	OG	SER	A	302	-1.320	54.263	23.626	1.00	42.02

13/75

ATOM	692	C	SER	A	302	-1.913	53.662	26.176	1.00	40.89
ATOM	693	O	SER	A	302	-2.765	52.792	26.076	1.00	42.93
ATOM	694	N	ILE	A	303	-0.698	53.402	26.641	1.00	40.31
ATOM	695	CA	ILE	A	303	-0.342	52.061	27.152	1.00	38.83
ATOM	696	CB	ILE	A	303	1.167	51.944	27.362	1.00	39.67
ATOM	697	CG1	ILE	A	303	1.902	52.347	26.060	1.00	37.58
ATOM	698	CD1	ILE	A	303	3.441	52.289	26.095	1.00	37.54
ATOM	699	CG2	ILE	A	303	1.528	50.501	27.950	1.00	36.80
ATOM	700	C	ILE	A	303	-1.107	51.741	28.460	1.00	40.19
ATOM	701	O	ILE	A	303	-0.932	52.422	29.478	1.00	40.20
ATOM	702	N	PRO	A	304	-2.031	50.760	28.425	1.00	39.90
ATOM	703	CA	PRO	A	304	-2.844	50.630	29.619	1.00	39.84
ATOM	704	CB	PRO	A	304	-3.681	49.389	29.313	1.00	40.91
ATOM	705	CG	PRO	A	304	-3.823	49.439	27.819	1.00	39.69
ATOM	706	CD	PRO	A	304	-2.431	49.782	27.400	1.00	39.63
ATOM	707	C	PRO	A	304	-1.992	50.452	30.867	1.00	40.99
ATOM	708	O	PRO	A	304	-1.018	49.695	30.859	1.00	41.99
ATOM	709	N	GLY	A	305	-2.350	51.164	31.935	1.00	40.73
ATOM	710	CA	GLY	A	305	-1.578	51.161	33.122	1.00	40.19
ATOM	711	C	GLY	A	305	-0.541	52.257	33.253	1.00	40.04
ATOM	712	O	GLY	A	305	-0.234	52.631	34.366	1.00	40.67
ATOM	713	N	PHE	A	306	-0.023	52.777	32.143	1.00	39.11
ATOM	714	CA	PHE	A	306	1.040	53.786	32.191	1.00	38.66
ATOM	715	CB	PHE	A	306	1.611	54.104	30.792	1.00	37.45
ATOM	716	CG	PHE	A	306	2.809	55.016	30.837	1.00	36.31
ATOM	717	CD1	PHE	A	306	4.082	54.500	31.020	1.00	36.57
ATOM	718	CE1	PHE	A	306	5.202	55.345	31.112	1.00	36.15
ATOM	719	CZ	PHE	A	306	5.030	56.732	31.013	1.00	36.82
ATOM	720	CE2	PHE	A	306	3.746	57.252	30.847	1.00	36.71
ATOM	721	CD2	PHE	A	306	2.651	56.392	30.796	1.00	35.37
ATOM	722	C	PHE	A	306	0.718	55.059	32.989	1.00	38.88
ATOM	723	O	PHE	A	306	1.440	55.383	33.925	1.00	39.50
ATOM	724	N	VAL	A	307	-0.334	55.794	32.637	1.00	38.51
ATOM	725	CA	VAL	A	307	-0.676	56.980	33.399	1.00	38.09
ATOM	726	CB	VAL	A	307	-1.755	57.828	32.676	1.00	39.01
ATOM	727	CG1	VAL	A	307	-1.295	58.157	31.257	1.00	37.11
ATOM	728	CG2	VAL	A	307	-3.132	57.104	32.649	1.00	36.69
ATOM	729	C	VAL	A	307	-1.058	56.763	34.891	1.00	39.23
ATOM	730	O	VAL	A	307	-1.259	57.725	35.631	1.00	38.75
ATOM	731	N	ASN	A	308	-1.141	55.513	35.347	1.00	39.18
ATOM	732	CA	ASN	A	308	-1.586	55.262	36.698	1.00	39.38
ATOM	733	CB	ASN	A	308	-2.526	54.059	36.794	1.00	39.86
ATOM	734	CG	ASN	A	308	-3.692	54.152	35.854	1.00	41.48
ATOM	735	OD1	ASN	A	308	-4.579	55.009	36.015	1.00	44.33
ATOM	736	ND2	ASN	A	308	-3.710	53.273	34.851	1.00	39.57
ATOM	737	C	ASN	A	308	-0.375	54.981	37.530	1.00	39.82
ATOM	738	O	ASN	A	308	-0.494	54.748	38.712	1.00	40.12
ATOM	739	N	LEU	A	309	0.794	54.987	36.903	1.00	39.88
ATOM	740	CA	LEU	A	309	2.042	54.758	37.620	1.00	40.17
ATOM	741	CB	LEU	A	309	3.163	54.390	36.643	1.00	39.38
ATOM	742	CG	LEU	A	309	3.032	52.982	36.047	1.00	39.45
ATOM	743	CD1	LEU	A	309	4.034	52.830	34.967	1.00	37.78
ATOM	744	CD2	LEU	A	309	3.259	51.946	37.126	1.00	41.63
ATOM	745	C	LEU	A	309	2.398	56.023	38.368	1.00	39.47
ATOM	746	O	LEU	A	309	1.997	57.107	37.987	1.00	39.22
ATOM	747	N	ASP	A	310	3.133	55.878	39.451	1.00	40.22
ATOM	748	CA	ASP	A	310	3.733	57.030	40.086	1.00	39.55
ATOM	749	CB	ASP	A	310	4.781	56.608	41.101	1.00	39.90

14/75

ATOM	750	CG	ASP	A	310	5.431	57.796	41.787	1.00	41.08
ATOM	751	OD1	ASP	A	310	5.184	58.017	42.998	1.00	44.49
ATOM	752	OD2	ASP	A	310	6.168	58.538	41.105	1.00	42.98
ATOM	753	C	ASP	A	310	4.344	57.911	39.001	1.00	39.75
ATOM	754	O	ASP	A	310	5.034	57.432	38.098	1.00	38.92
ATOM	755	N	LEU	A	311	4.066	59.204	39.129	1.00	40.80
ATOM	756	CA	LEU	A	311	4.435	60.235	38.183	1.00	42.34
ATOM	757	CB	LEU	A	311	3.971	61.571	38.734	1.00	43.05
ATOM	758	CG	LEU	A	311	4.363	62.897	38.082	1.00	46.77
ATOM	759	CD1	LEU	A	311	3.224	63.881	38.309	1.00	47.77
ATOM	760	CD2	LEU	A	311	5.671	63.478	38.706	1.00	48.22
ATOM	761	C	LEU	A	311	5.930	60.271	37.926	1.00	42.36
ATOM	762	O	LEU	A	311	6.368	60.407	36.780	1.00	42.62
ATOM	763	N	ASN	A	312	6.698	60.177	39.008	1.00	41.85
ATOM	764	CA	ASN	A	312	8.152	60.166	38.938	1.00	41.56
ATOM	765	CB	ASN	A	312	8.740	60.142	40.332	1.00	41.74
ATOM	766	CG	ASN	A	312	8.611	61.476	41.025	1.00	42.55
ATOM	767	OD1	ASN	A	312	9.178	62.466	40.576	1.00	46.46
ATOM	768	ND2	ASN	A	312	7.862	61.513	42.109	1.00	41.51
ATOM	769	C	ASN	A	312	8.658	59.007	38.118	1.00	41.10
ATOM	770	O	ASN	A	312	9.574	59.159	37.326	1.00	42.28
ATOM	771	N	ASP	A	313	8.015	57.860	38.257	1.00	40.67
ATOM	772	CA	ASP	A	313	8.370	56.717	37.461	1.00	38.90
ATOM	773	CB	ASP	A	313	7.753	55.457	38.047	1.00	38.61
ATOM	774	CG	ASP	A	313	8.450	54.973	39.291	1.00	38.74
ATOM	775	OD1	ASP	A	313	9.571	55.447	39.636	1.00	40.49
ATOM	776	OD2	ASP	A	313	7.871	54.072	39.930	1.00	35.23
ATOM	777	C	ASP	A	313	7.952	56.912	36.005	1.00	38.87
ATOM	778	O	ASP	A	313	8.655	56.485	35.095	1.00	38.77
ATOM	779	N	GLN	A	314	6.817	57.570	35.768	1.00	39.01
ATOM	780	CA	GLN	A	314	6.399	57.843	34.403	1.00	38.02
ATOM	781	CB	GLN	A	314	5.079	58.617	34.343	1.00	38.23
ATOM	782	CG	GLN	A	314	3.828	57.749	34.550	1.00	37.98
ATOM	783	CD	GLN	A	314	2.588	58.578	34.636	1.00	40.59
ATOM	784	OE1	GLN	A	314	1.841	58.500	35.606	1.00	41.67
ATOM	785	NE2	GLN	A	314	2.362	59.392	33.630	1.00	37.91
ATOM	786	C	GLN	A	314	7.490	58.624	33.714	1.00	37.87
ATOM	787	O	GLN	A	314	7.798	58.385	32.557	1.00	37.92
ATOM	788	N	VAL	A	315	8.072	59.574	34.435	1.00	38.18
ATOM	789	CA	VAL	A	315	9.128	60.416	33.898	1.00	37.09
ATOM	790	CB	VAL	A	315	9.298	61.692	34.769	1.00	37.42
ATOM	791	CG1	VAL	A	315	10.463	62.562	34.279	1.00	36.31
ATOM	792	CG2	VAL	A	315	7.988	62.489	34.746	1.00	35.62
ATOM	793	C	VAL	A	315	10.425	59.630	33.695	1.00	37.55
ATOM	794	O	VAL	A	315	11.146	59.862	32.718	1.00	38.37
ATOM	795	N	THR	A	316	10.701	58.670	34.578	1.00	37.72
ATOM	796	CA	THR	A	316	11.918	57.834	34.462	1.00	37.24
ATOM	797	CB	THR	A	316	12.203	57.046	35.787	1.00	38.02
ATOM	798	OG1	THR	A	316	12.579	57.969	36.821	1.00	36.12
ATOM	799	CG2	THR	A	316	13.344	55.983	35.589	1.00	37.89
ATOM	800	C	THR	A	316	11.858	56.879	33.265	1.00	37.55
ATOM	801	O	THR	A	316	12.838	56.698	32.536	1.00	36.70
ATOM	802	N	LEU	A	317	10.685	56.301	33.048	1.00	37.57
ATOM	803	CA	LEU	A	317	10.463	55.411	31.926	1.00	38.83
ATOM	804	CB	LEU	A	317	9.109	54.719	32.064	1.00	38.75
ATOM	805	CG	LEU	A	317	8.976	53.765	33.259	1.00	38.97
ATOM	806	CD1	LEU	A	317	7.511	53.359	33.402	1.00	40.47
ATOM	807	CD2	LEU	A	317	9.896	52.551	33.103	1.00	38.84

15/75

ATOM	808	C	LEU	A	317	10.561	56.116	30.578	1.00	39.00
ATOM	809	O	LEU	A	317	11.097	55.551	29.621	1.00	39.29
ATOM	810	N	LEU	A	318	10.050	57.345	30.507	1.00	39.65
ATOM	811	CA	LEU	A	318	10.176	58.154	29.317	1.00	39.93
ATOM	812	CB	LEU	A	318	9.257	59.390	29.380	1.00	40.05
ATOM	813	CG	LEU	A	318	7.779	59.154	29.075	1.00	42.11
ATOM	814	CD1	LEU	A	318	6.945	60.423	29.340	1.00	42.75
ATOM	815	CD2	LEU	A	318	7.583	58.650	27.681	1.00	41.53
ATOM	816	C	LEU	A	318	11.621	58.579	29.133	1.00	40.04
ATOM	817	O	LEU	A	318	12.155	58.495	28.024	1.00	40.53
ATOM	818	N	LYS	A	319	12.244	59.042	30.212	1.00	40.66
ATOM	819	CA	LYS	A	319	13.631	59.540	30.180	1.00	41.46
ATOM	820	CB	LYS	A	319	14.176	59.879	31.588	1.00	41.09
ATOM	821	CG	LYS	A	319	15.640	60.383	31.565	1.00	42.18
ATOM	822	CD	LYS	A	319	16.203	60.730	32.973	1.00	42.27
ATOM	823	CE	LYS	A	319	17.393	61.726	32.919	1.00	42.03
ATOM	824	NZ	LYS	A	319	17.398	62.633	34.144	1.00	44.65
ATOM	825	C	LYS	A	319	14.556	58.569	29.474	1.00	41.57
ATOM	826	O	LYS	A	319	15.305	58.968	28.573	1.00	41.69
ATOM	827	N	TYR	A	320	14.463	57.296	29.861	1.00	42.11
ATOM	828	CA	TYR	A	320	15.347	56.259	29.346	1.00	41.90
ATOM	829	CB	TYR	A	320	15.694	55.234	30.429	1.00	41.11
ATOM	830	CG	TYR	A	320	16.599	55.803	31.502	1.00	40.51
ATOM	831	CD1	TYR	A	320	16.072	56.321	32.673	1.00	37.82
ATOM	832	CE1	TYR	A	320	16.903	56.858	33.672	1.00	39.87
ATOM	833	CZ	TYR	A	320	18.271	56.870	33.497	1.00	39.79
ATOM	834	OH	TYR	A	320	19.087	57.398	34.509	1.00	40.89
ATOM	835	CE2	TYR	A	320	18.818	56.351	32.334	1.00	39.21
ATOM	836	CD2	TYR	A	320	17.987	55.817	31.341	1.00	39.48
ATOM	837	C	TYR	A	320	14.794	55.566	28.131	1.00	42.48
ATOM	838	O	TYR	A	320	15.551	55.159	27.278	1.00	43.88
ATOM	839	N	GLY	A	321	13.479	55.459	28.015	1.00	42.82
ATOM	840	CA	GLY	A	321	12.885	54.789	26.866	1.00	41.99
ATOM	841	C	GLY	A	321	12.884	55.571	25.566	1.00	41.86
ATOM	842	O	GLY	A	321	13.024	55.013	24.472	1.00	41.03
ATOM	843	N	VAL	A	322	12.689	56.869	25.666	1.00	42.38
ATOM	844	CA	VAL	A	322	12.519	57.697	24.485	1.00	42.44
ATOM	845	CB	VAL	A	322	12.245	59.163	24.926	1.00	43.80
ATOM	846	CG1	VAL	A	322	13.092	60.152	24.184	1.00	45.35
ATOM	847	CG2	VAL	A	322	10.729	59.441	24.822	1.00	42.87
ATOM	848	C	VAL	A	322	13.592	57.496	23.397	1.00	42.45
ATOM	849	O	VAL	A	322	13.251	57.263	22.245	1.00	41.28
ATOM	850	N	HIS	A	323	14.878	57.464	23.748	1.00	42.75
ATOM	851	CA	HIS	A	323	15.888	57.335	22.692	1.00	43.30
ATOM	852	CB	HIS	A	323	17.243	57.916	23.103	1.00	44.62
ATOM	853	CG	HIS	A	323	17.302	59.400	22.942	1.00	47.67
ATOM	854	ND1	HIS	A	323	17.457	60.005	21.711	1.00	51.96
ATOM	855	CE1	HIS	A	323	17.431	61.318	21.859	1.00	49.48
ATOM	856	NE2	HIS	A	323	17.236	61.586	23.136	1.00	48.79
ATOM	857	CD2	HIS	A	323	17.130	60.403	23.833	1.00	49.59
ATOM	858	C	HIS	A	323	15.994	55.968	22.031	1.00	43.22
ATOM	859	O	HIS	A	323	16.087	55.864	20.813	1.00	43.17
ATOM	860	N	GLU	A	324	15.940	54.908	22.826	1.00	42.75
ATOM	861	CA	GLU	A	324	15.775	53.556	22.291	1.00	41.62
ATOM	862	CB	GLU	A	324	15.570	52.628	23.469	1.00	41.35
ATOM	863	CG	GLU	A	324	16.838	52.397	24.237	1.00	41.38
ATOM	864	CD	GLU	A	324	16.619	51.639	25.515	1.00	41.62
ATOM	865	OE1	GLU	A	324	15.484	51.226	25.806	1.00	45.82

16/75

ATOM	866	OE2	GLU	A	324	17.588	51.475	26.251	1.00	42.56
ATOM	867	C	GLU	A	324	14.617	53.406	21.300	1.00	41.21
ATOM	868	O	GLU	A	324	14.670	52.604	20.374	1.00	40.50
ATOM	869	N	ILE	A	325	13.552	54.176	21.529	1.00	41.18
ATOM	870	CA	ILE	A	325	12.399	54.246	20.617	1.00	40.35
ATOM	871	CB	ILE	A	325	11.158	54.715	21.388	1.00	40.18
ATOM	872	CG1	ILE	A	325	10.830	53.704	22.468	1.00	39.01
ATOM	873	CD1	ILE	A	325	9.627	54.030	23.296	1.00	37.88
ATOM	874	CG2	ILE	A	325	9.957	54.903	20.454	1.00	39.29
ATOM	875	C	ILE	A	325	12.649	55.118	19.356	1.00	40.94
ATOM	876	O	ILE	A	325	12.258	54.773	18.261	1.00	42.02
ATOM	877	N	ILE	A	326	13.331	56.238	19.511	1.00	40.75
ATOM	878	CA	ILE	A	326	13.734	57.042	18.358	1.00	40.72
ATOM	879	CB	ILE	A	326	14.469	58.306	18.837	1.00	40.75
ATOM	880	CG1	ILE	A	326	13.405	59.304	19.273	1.00	40.57
ATOM	881	CD1	ILE	A	326	13.833	60.155	20.271	1.00	37.97
ATOM	882	CG2	ILE	A	326	15.391	58.860	17.741	1.00	38.07
ATOM	883	C	ILE	A	326	14.556	56.265	17.341	1.00	40.70
ATOM	884	O	ILE	A	326	14.320	56.386	16.160	1.00	41.32
ATOM	885	N	TYR	A	327	15.521	55.467	17.797	1.00	40.86
ATOM	886	CA	TYR	A	327	16.364	54.684	16.878	1.00	41.01
ATOM	887	CB	TYR	A	327	17.695	54.291	17.540	1.00	40.94
ATOM	888	CG	TYR	A	327	18.427	55.512	18.087	1.00	42.41
ATOM	889	CD1	TYR	A	327	18.483	56.702	17.344	1.00	42.56
ATOM	890	CE1	TYR	A	327	19.117	57.841	17.834	1.00	40.48
ATOM	891	CZ	TYR	A	327	19.722	57.805	19.055	1.00	39.90
ATOM	892	OH	TYR	A	327	20.352	58.956	19.508	1.00	44.08
ATOM	893	CE2	TYR	A	327	19.690	56.654	19.844	1.00	39.45
ATOM	894	CD2	TYR	A	327	19.031	55.501	19.360	1.00	40.62
ATOM	895	C	TYR	A	327	15.643	53.467	16.269	1.00	40.84
ATOM	896	O	TYR	A	327	15.883	53.152	15.115	1.00	41.12
ATOM	897	N	THR	A	328	14.795	52.775	17.043	1.00	40.28
ATOM	898	CA	THR	A	328	13.857	51.777	16.479	1.00	39.49
ATOM	899	CB	THR	A	328	12.934	51.177	17.573	1.00	39.04
ATOM	900	OG1	THR	A	328	13.763	50.556	18.589	1.00	37.25
ATOM	901	CG2	THR	A	328	12.019	50.103	16.981	1.00	36.37
ATOM	902	C	THR	A	328	12.977	52.337	15.339	1.00	40.73
ATOM	903	O	THR	A	328	12.829	51.727	14.290	1.00	41.27
ATOM	904	N	MET	A	329	12.364	53.483	15.568	1.00	42.49
ATOM	905	CA	MET	A	329	11.398	54.041	14.667	1.00	43.82
ATOM	906	CB	MET	A	329	10.521	54.962	15.481	1.00	43.47
ATOM	907	CG	MET	A	329	9.597	54.169	16.343	1.00	46.68
ATOM	908	SD	MET	A	329	8.293	55.207	16.913	1.00	52.80
ATOM	909	CE	MET	A	329	7.147	54.959	15.561	1.00	50.89
ATOM	910	C	MET	A	329	12.069	54.791	13.523	1.00	42.16
ATOM	911	O	MET	A	329	11.459	55.145	12.485	1.00	41.79
ATOM	912	N	LEU	A	330	13.348	55.030	13.692	1.00	39.63
ATOM	913	CA	LEU	A	330	14.079	55.777	12.712	1.00	38.08
ATOM	914	CB	LEU	A	330	15.335	56.370	13.354	1.00	37.38
ATOM	915	CG	LEU	A	330	16.402	56.877	12.420	1.00	36.54
ATOM	916	CD1	LEU	A	330	15.925	58.145	11.741	1.00	36.12
ATOM	917	CD2	LEU	A	330	17.741	57.035	13.157	1.00	35.46
ATOM	918	C	LEU	A	330	14.457	54.830	11.601	1.00	37.94
ATOM	919	O	LEU	A	330	14.579	55.230	10.448	1.00	37.28
ATOM	920	N	ALA	A	331	14.649	53.567	11.977	1.00	37.75
ATOM	921	CA	ALA	A	331	14.959	52.497	11.063	1.00	37.61
ATOM	922	CB	ALA	A	331	15.120	51.196	11.862	1.00	37.62
ATOM	923	C	ALA	A	331	13.912	52.296	10.010	1.00	37.50

17/75

ATOM	924	O	ALA	A	331	14.220	51.860	8.917	1.00	37.39
ATOM	925	N	SER	A	332	12.645	52.514	10.380	1.00	37.94
ATOM	926	CA	SER	A	332	11.527	52.428	9.453	1.00	36.32
ATOM	927	CB	SER	A	332	10.299	52.915	10.132	1.00	35.59
ATOM	928	OG	SER	A	332	9.979	52.086	11.196	1.00	34.71
ATOM	929	C	SER	A	332	11.707	53.340	8.237	1.00	37.00
ATOM	930	O	SER	A	332	11.229	53.016	7.153	1.00	35.27
ATOM	931	N	LEU	A	333	12.382	54.471	8.467	1.00	36.45
ATOM	932	CA	LEU	A	333	12.636	55.501	7.467	1.00	37.04
ATOM	933	CB	LEU	A	333	12.753	56.843	8.203	1.00	37.55
ATOM	934	CG	LEU	A	333	11.790	57.237	9.318	1.00	40.36
ATOM	935	CD1	LEU	A	333	12.139	58.635	9.916	1.00	42.00
ATOM	936	CD2	LEU	A	333	10.407	57.281	8.744	1.00	44.58
ATOM	937	C	LEU	A	333	13.944	55.266	6.712	1.00	37.49
ATOM	938	O	LEU	A	333	14.298	56.051	5.841	1.00	38.39
ATOM	939	N	MET	A	334	14.669	54.194	7.046	1.00	37.10
ATOM	940	CA	MET	A	334	15.978	53.959	6.476	1.00	37.47
ATOM	941	CB	MET	A	334	16.987	53.732	7.588	1.00	36.94
ATOM	942	CG	MET	A	334	17.298	54.981	8.414	1.00	35.41
ATOM	943	SD	MET	A	334	18.548	54.617	9.645	1.00	36.61
ATOM	944	CE	MET	A	334	19.276	56.241	9.904	1.00	35.42
ATOM	945	C	MET	A	334	16.039	52.780	5.533	1.00	38.53
ATOM	946	O	MET	A	334	15.242	51.868	5.605	1.00	38.83
ATOM	947	N	ASN	A	335	16.992	52.835	4.625	1.00	39.84
ATOM	948	CA	ASN	A	335	17.497	51.646	3.939	1.00	40.64
ATOM	949	CB	ASN	A	335	16.904	51.454	2.529	1.00	39.38
ATOM	950	CG	ASN	A	335	17.191	52.602	1.605	1.00	39.71
ATOM	951	OD1	ASN	A	335	18.257	53.216	1.675	1.00	41.82
ATOM	952	ND2	ASN	A	335	16.241	52.913	0.724	1.00	36.21
ATOM	953	C	ASN	A	335	19.003	51.780	3.917	1.00	41.05
ATOM	954	O	ASN	A	335	19.543	52.685	4.532	1.00	41.59
ATOM	955	N	LYS	A	336	19.682	50.881	3.211	1.00	42.68
ATOM	956	CA	LYS	A	336	21.137	50.883	3.143	1.00	42.77
ATOM	957	CB	LYS	A	336	21.606	49.895	2.058	1.00	43.96
ATOM	958	CG	LYS	A	336	22.205	48.637	2.570	1.00	46.54
ATOM	959	CD	LYS	A	336	23.147	48.915	3.749	1.00	52.33
ATOM	960	CE	LYS	A	336	24.388	47.997	3.785	1.00	53.76
ATOM	961	NZ	LYS	A	336	25.140	48.191	5.057	1.00	55.63
ATOM	962	C	LYS	A	336	21.665	52.244	2.761	1.00	41.82
ATOM	963	O	LYS	A	336	22.755	52.626	3.173	1.00	41.82
ATOM	964	N	ASP	A	337	20.895	52.963	1.950	1.00	40.84
ATOM	965	CA	ASP	A	337	21.466	54.062	1.181	1.00	40.67
ATOM	966	CB	ASP	A	337	21.001	53.978	-0.263	1.00	40.33
ATOM	967	CG	ASP	A	337	21.584	52.772	-0.992	1.00	43.04
ATOM	968	OD1	ASP	A	337	22.775	52.435	-0.776	1.00	45.79
ATOM	969	OD2	ASP	A	337	20.843	52.144	-1.761	1.00	44.84
ATOM	970	C	ASP	A	337	21.174	55.441	1.756	1.00	39.61
ATOM	971	O	ASP	A	337	21.753	56.432	1.329	1.00	40.20
ATOM	972	N	GLY	A	338	20.274	55.504	2.715	1.00	38.98
ATOM	973	CA	GLY	A	338	19.857	56.796	3.251	1.00	37.26
ATOM	974	C	GLY	A	338	18.583	56.730	4.051	1.00	35.96
ATOM	975	O	GLY	A	338	18.078	55.637	4.349	1.00	35.95
ATOM	976	N	VAL	A	339	18.080	57.918	4.398	1.00	33.92
ATOM	977	CA	VAL	A	339	16.977	58.068	5.325	1.00	32.83
ATOM	978	CB	VAL	A	339	17.495	58.502	6.727	1.00	32.80
ATOM	979	CG1	VAL	A	339	18.342	59.826	6.643	1.00	31.59
ATOM	980	CG2	VAL	A	339	16.412	58.571	7.763	1.00	30.32
ATOM	981	C	VAL	A	339	16.004	59.111	4.803	1.00	32.98

18/75

ATOM	982	O	VAL	A	339	16.412	60.122	4.256	1.00	32.16
ATOM	983	N	LEU	A	340	14.719	58.832	4.985	1.00	32.34
ATOM	984	CA	LEU	A	340	13.676	59.793	4.671	1.00	33.15
ATOM	985	CB	LEU	A	340	12.303	59.139	4.688	1.00	32.41
ATOM	986	CG	LEU	A	340	11.979	58.189	3.499	1.00	30.57
ATOM	987	CD1	LEU	A	340	10.652	57.539	3.855	1.00	29.93
ATOM	988	CD2	LEU	A	340	11.838	58.925	2.197	1.00	32.36
ATOM	989	C	LEU	A	340	13.709	60.916	5.687	1.00	33.86
ATOM	990	O	LEU	A	340	13.927	60.669	6.893	1.00	33.69
ATOM	991	N	ILE	A	341	13.522	62.127	5.172	1.00	34.72
ATOM	992	CA	ILE	A	341	13.494	63.370	5.957	1.00	35.89
ATOM	993	CB	ILE	A	341	14.775	64.194	5.779	1.00	35.69
ATOM	994	CG1	ILE	A	341	14.934	64.664	4.344	1.00	35.92
ATOM	995	CD1	ILE	A	341	15.949	65.826	4.188	1.00	37.05
ATOM	996	CG2	ILE	A	341	15.993	63.352	6.222	1.00	35.46
ATOM	997	C	ILE	A	341	12.267	64.181	5.572	1.00	36.69
ATOM	998	O	ILE	A	341	11.495	63.734	4.726	1.00	35.30
ATOM	999	N	SER	A	342	12.140	65.390	6.141	1.00	38.16
ATOM	1000	CA	SER	A	342	10.873	66.171	6.227	1.00	39.95
ATOM	1001	CB	SER	A	342	10.971	67.612	5.689	1.00	40.46
ATOM	1002	OG	SER	A	342	10.943	67.756	4.270	1.00	44.28
ATOM	1003	C	SER	A	342	9.536	65.477	5.902	1.00	40.48
ATOM	1004	O	SER	A	342	8.971	65.644	4.807	1.00	40.54
ATOM	1005	N	GLU	A	343	9.058	64.692	6.875	1.00	39.89
ATOM	1006	CA	GLU	A	343	7.840	63.894	6.715	1.00	41.06
ATOM	1007	CB	GLU	A	343	6.587	64.812	6.646	1.00	41.19
ATOM	1008	CG	GLU	A	343	6.155	65.574	7.946	1.00	42.93
ATOM	1009	CD	GLU	A	343	5.264	66.816	7.653	1.00	45.11
ATOM	1010	OE1	GLU	A	343	5.760	67.727	6.955	1.00	50.34
ATOM	1011	OE2	GLU	A	343	4.087	66.891	8.114	1.00	49.15
ATOM	1012	C	GLU	A	343	7.866	63.014	5.441	1.00	40.00
ATOM	1013	O	GLU	A	343	6.804	62.736	4.883	1.00	40.62
ATOM	1014	N	GLY	A	344	9.034	62.576	4.968	1.00	38.35
ATOM	1015	CA	GLY	A	344	9.106	61.703	3.793	1.00	36.13
ATOM	1016	C	GLY	A	344	9.261	62.377	2.445	1.00	35.88
ATOM	1017	O	GLY	A	344	9.420	61.679	1.412	1.00	36.05
ATOM	1018	N	GLN	A	345	9.217	63.720	2.438	1.00	34.98
ATOM	1019	CA	GLN	A	345	9.342	64.552	1.232	1.00	34.27
ATOM	1020	CB	GLN	A	345	8.852	65.975	1.511	1.00	35.17
ATOM	1021	CG	GLN	A	345	7.347	66.079	1.754	1.00	38.39
ATOM	1022	CD	GLN	A	345	6.981	67.045	2.877	1.00	43.82
ATOM	1023	OE1	GLN	A	345	6.288	66.670	3.833	1.00	49.11
ATOM	1024	NE2	GLN	A	345	7.449	68.278	2.783	1.00	44.81
ATOM	1025	C	GLN	A	345	10.761	64.621	0.672	1.00	33.37
ATOM	1026	O	GLN	A	345	10.972	65.019	-0.476	1.00	32.25
ATOM	1027	N	GLY	A	346	11.742	64.249	1.479	1.00	31.04
ATOM	1028	CA	GLY	A	346	13.107	64.279	1.036	1.00	31.46
ATOM	1029	C	GLY	A	346	13.789	63.001	1.446	1.00	31.58
ATOM	1030	O	GLY	A	346	13.247	62.254	2.230	1.00	32.83
ATOM	1031	N	PHE	A	347	14.965	62.746	0.915	1.00	32.35
ATOM	1032	CA	PHE	A	347	15.709	61.555	1.302	1.00	33.86
ATOM	1033	CB	PHE	A	347	15.394	60.422	0.302	1.00	33.67
ATOM	1034	CG	PHE	A	347	16.207	59.161	0.483	1.00	32.71
ATOM	1035	CD1	PHE	A	347	15.780	58.161	1.347	1.00	32.19
ATOM	1036	CE1	PHE	A	347	16.503	56.963	1.469	1.00	33.75
ATOM	1037	CZ	PHE	A	347	17.691	56.760	0.717	1.00	31.80
ATOM	1038	CE2	PHE	A	347	18.126	57.736	-0.149	1.00	33.45
ATOM	1039	CD2	PHE	A	347	17.364	58.947	-0.279	1.00	32.01

19/75

ATOM	1040	C	PHE	A	347	17.165	61.960	1.281	1.00	33.85
ATOM	1041	O	PHE	A	347	17.647	62.440	0.271	1.00	34.63
ATOM	1042	N	MET	A	348	17.859	61.818	2.407	1.00	35.29
ATOM	1043	CA	MET	A	348	19.282	62.183	2.492	1.00	35.61
ATOM	1044	CB	MET	A	348	19.524	63.018	3.766	1.00	35.92
ATOM	1045	CG	MET	A	348	20.909	63.694	3.943	1.00	38.16
ATOM	1046	SD	MET	A	348	20.895	64.973	5.278	1.00	39.36
ATOM	1047	CE	MET	A	348	20.215	66.357	4.311	1.00	37.51
ATOM	1048	C	MET	A	348	20.114	60.900	2.501	1.00	35.06
ATOM	1049	O	MET	A	348	19.832	59.970	3.258	1.00	34.36
ATOM	1050	N	THR	A	349	21.147	60.874	1.669	1.00	35.40
ATOM	1051	CA	THR	A	349	22.003	59.720	1.467	1.00	36.22
ATOM	1052	CB	THR	A	349	22.863	59.968	0.210	1.00	36.74
ATOM	1053	OG1	THR	A	349	21.989	60.253	-0.896	1.00	41.55
ATOM	1054	CG2	THR	A	349	23.708	58.752	-0.146	1.00	39.16
ATOM	1055	C	THR	A	349	22.906	59.440	2.683	1.00	35.38
ATOM	1056	O	THR	A	349	23.372	60.388	3.327	1.00	35.28
ATOM	1057	N	ARG	A	350	23.151	58.161	2.970	1.00	34.63
ATOM	1058	CA	ARG	A	350	24.077	57.717	4.008	1.00	36.11
ATOM	1059	CB	ARG	A	350	24.078	56.182	4.118	1.00	36.02
ATOM	1060	CG	ARG	A	350	25.024	55.531	5.146	1.00	35.58
ATOM	1061	CD	ARG	A	350	24.886	54.004	5.059	1.00	37.33
ATOM	1062	NE	ARG	A	350	25.561	53.241	6.122	1.00	41.52
ATOM	1063	CZ	ARG	A	350	25.366	51.937	6.322	1.00	41.82
ATOM	1064	NH1	ARG	A	350	24.528	51.286	5.528	1.00	44.29
ATOM	1065	NH2	ARG	A	350	26.004	51.272	7.291	1.00	41.46
ATOM	1066	C	ARG	A	350	25.473	58.261	3.716	1.00	36.99
ATOM	1067	O	ARG	A	350	26.156	58.729	4.627	1.00	37.17
ATOM	1068	N	GLU	A	351	25.857	58.240	2.432	1.00	37.65
ATOM	1069	CA	GLU	A	351	27.101	58.818	1.940	1.00	39.14
ATOM	1070	CB	GLU	A	351	27.239	58.522	0.447	1.00	39.97
ATOM	1071	CG	GLU	A	351	28.593	58.028	0.020	1.00	45.37
ATOM	1072	CD	GLU	A	351	28.808	56.567	0.385	1.00	52.22
ATOM	1073	OE1	GLU	A	351	28.359	55.678	-0.393	1.00	53.83
ATOM	1074	OE2	GLU	A	351	29.440	56.312	1.444	1.00	54.32
ATOM	1075	C	GLU	A	351	27.293	60.334	2.189	1.00	38.97
ATOM	1076	O	GLU	A	351	28.386	60.751	2.581	1.00	38.47
ATOM	1077	N	PHE	A	352	26.278	61.157	1.909	1.00	38.92
ATOM	1078	CA	PHE	A	352	26.357	62.598	2.174	1.00	39.91
ATOM	1079	CB	PHE	A	352	25.117	63.340	1.676	1.00	38.90
ATOM	1080	CG	PHE	A	352	25.093	64.809	2.052	1.00	38.93
ATOM	1081	CD1	PHE	A	352	26.127	65.664	1.674	1.00	37.77
ATOM	1082	CE1	PHE	A	352	26.103	67.028	2.028	1.00	37.17
ATOM	1083	CZ	PHE	A	352	25.035	67.533	2.758	1.00	35.82
ATOM	1084	CE2	PHE	A	352	24.009	66.706	3.132	1.00	34.93
ATOM	1085	CD2	PHE	A	352	24.039	65.338	2.789	1.00	37.76
ATOM	1086	C	PHE	A	352	26.572	62.889	3.675	1.00	40.56
ATOM	1087	O	PHE	A	352	27.389	63.723	4.056	1.00	41.58
ATOM	1088	N	LEU	A	353	25.823	62.173	4.496	1.00	41.67
ATOM	1089	CA	LEU	A	353	25.895	62.236	5.940	1.00	42.70
ATOM	1090	CB	LEU	A	353	24.792	61.371	6.559	1.00	42.31
ATOM	1091	CG	LEU	A	353	23.418	62.039	6.499	1.00	42.78
ATOM	1092	CD1	LEU	A	353	22.314	61.070	6.848	1.00	40.28
ATOM	1093	CD2	LEU	A	353	23.417	63.292	7.435	1.00	45.29
ATOM	1094	C	LEU	A	353	27.270	61.792	6.429	1.00	43.21
ATOM	1095	O	LEU	A	353	27.789	62.361	7.379	1.00	43.23
ATOM	1096	N	LYS	A	354	27.854	60.792	5.769	1.00	43.14
ATOM	1097	CA	LYS	A	354	29.187	60.338	6.134	1.00	43.99

20/75

ATOM	1098	CB	LYS	A	354	29.479	58.952	5.553	1.00	44.14
ATOM	1099	CG	LYS	A	354	30.658	58.253	6.197	1.00	46.77
ATOM	1100	CD	LYS	A	354	30.466	56.737	6.284	1.00	51.21
ATOM	1101	CE	LYS	A	354	30.608	56.036	4.915	1.00	53.78
ATOM	1102	NZ	LYS	A	354	31.344	54.710	4.993	1.00	55.83
ATOM	1103	C	LYS	A	354	30.265	61.354	5.733	1.00	43.72
ATOM	1104	O	LYS	A	354	31.327	61.393	6.335	1.00	44.02
ATOM	1105	N	SER	A	355	29.979	62.197	4.744	1.00	43.45
ATOM	1106	CA	SER	A	355	30.950	63.180	4.263	1.00	42.96
ATOM	1107	CB	SER	A	355	30.610	63.576	2.825	1.00	42.56
ATOM	1108	OG	SER	A	355	29.704	64.655	2.803	1.00	40.91
ATOM	1109	C	SER	A	355	31.088	64.442	5.146	1.00	43.41
ATOM	1110	O	SER	A	355	31.905	65.321	4.856	1.00	43.55
ATOM	1111	N	LEU	A	356	30.293	64.543	6.205	1.00	43.57
ATOM	1112	CA	LEU	A	356	30.199	65.793	6.949	1.00	44.45
ATOM	1113	CB	LEU	A	356	28.916	65.856	7.792	1.00	44.17
ATOM	1114	CG	LEU	A	356	27.604	65.988	6.990	1.00	43.50
ATOM	1115	CD1	LEU	A	356	26.367	65.657	7.834	1.00	43.85
ATOM	1116	CD2	LEU	A	356	27.442	67.359	6.338	1.00	42.02
ATOM	1117	C	LEU	A	356	31.459	66.051	7.770	1.00	45.31
ATOM	1118	O	LEU	A	356	32.276	65.150	7.965	1.00	45.67
ATOM	1119	N	ARG	A	357	31.633	67.294	8.211	1.00	46.28
ATOM	1120	CA	ARG	A	357	32.833	67.690	8.934	1.00	46.81
ATOM	1121	CB	ARG	A	357	32.821	69.199	9.196	1.00	46.96
ATOM	1122	CG	ARG	A	357	33.967	69.712	10.026	1.00	47.59
ATOM	1123	CD	ARG	A	357	33.562	69.878	11.496	1.00	48.68
ATOM	1124	NE	ARG	A	357	32.832	71.126	11.720	1.00	47.83
ATOM	1125	CZ	ARG	A	357	32.497	71.595	12.917	1.00	47.75
ATOM	1126	NH1	ARG	A	357	32.828	70.920	14.012	1.00	48.39
ATOM	1127	NH2	ARG	A	357	31.833	72.740	13.015	1.00	47.09
ATOM	1128	C	ARG	A	357	33.002	66.870	10.212	1.00	46.86
ATOM	1129	O	ARG	A	357	32.028	66.544	10.881	1.00	46.95
ATOM	1130	N	LYS	A	358	34.262	66.576	10.521	1.00	47.65
ATOM	1131	CA	LYS	A	358	34.716	65.523	11.441	1.00	47.93
ATOM	1132	CB	LYS	A	358	35.940	65.989	12.247	1.00	48.31
ATOM	1133	CG	LYS	A	358	36.933	66.884	11.466	1.00	49.08
ATOM	1134	CD	LYS	A	358	37.403	66.238	10.151	1.00	49.88
ATOM	1135	CE	LYS	A	358	37.876	67.279	9.156	1.00	51.00
ATOM	1136	NZ	LYS	A	358	39.246	67.797	9.503	1.00	52.93
ATOM	1137	C	LYS	A	358	33.652	64.887	12.341	1.00	48.38
ATOM	1138	O	LYS	A	358	33.034	63.871	11.951	1.00	48.58
ATOM	1139	N	PRO	A	359	33.387	65.497	13.521	1.00	47.89
ATOM	1140	CA	PRO	A	359	32.509	64.793	14.461	1.00	47.19
ATOM	1141	CB	PRO	A	359	32.408	65.755	15.660	1.00	47.33
ATOM	1142	CG	PRO	A	359	32.871	67.106	15.135	1.00	46.96
ATOM	1143	CD	PRO	A	359	33.809	66.831	14.006	1.00	47.29
ATOM	1144	C	PRO	A	359	31.127	64.501	13.867	1.00	47.05
ATOM	1145	O	PRO	A	359	30.570	63.410	14.091	1.00	47.60
ATOM	1146	N	PHE	A	360	30.577	65.440	13.096	1.00	45.82
ATOM	1147	CA	PHE	A	360	29.187	65.308	12.654	1.00	44.74
ATOM	1148	CB	PHE	A	360	28.651	66.634	12.142	1.00	43.63
ATOM	1149	CG	PHE	A	360	28.654	67.714	13.173	1.00	42.58
ATOM	1150	CD1	PHE	A	360	29.705	68.613	13.249	1.00	41.20
ATOM	1151	CE1	PHE	A	360	29.720	69.610	14.197	1.00	38.75
ATOM	1152	CZ	PHE	A	360	28.686	69.727	15.093	1.00	39.62
ATOM	1153	CE2	PHE	A	360	27.625	68.844	15.052	1.00	40.60
ATOM	1154	CD2	PHE	A	360	27.612	67.826	14.088	1.00	41.93
ATOM	1155	C	PHE	A	360	29.032	64.230	11.596	1.00	45.08

21/75

ATOM	1156	O	PHE	A	360	27.929	63.787	11.318	1.00	44.80
ATOM	1157	N	GLY	A	361	30.155	63.795	11.041	1.00	45.47
ATOM	1158	CA	GLY	A	361	30.153	62.869	9.933	1.00	46.25
ATOM	1159	C	GLY	A	361	29.985	61.449	10.384	1.00	46.78
ATOM	1160	O	GLY	A	361	29.889	60.546	9.564	1.00	46.77
ATOM	1161	N	ASP	A	362	29.968	61.230	11.692	1.00	47.77
ATOM	1162	CA	ASP	A	362	29.748	59.873	12.184	1.00	48.68
ATOM	1163	CB	ASP	A	362	31.015	59.259	12.828	1.00	49.36
ATOM	1164	CG	ASP	A	362	31.866	60.275	13.532	1.00	51.03
ATOM	1165	OD1	ASP	A	362	31.355	60.925	14.478	1.00	54.27
ATOM	1166	OD2	ASP	A	362	33.049	60.410	13.149	1.00	51.08
ATOM	1167	C	ASP	A	362	28.510	59.710	13.053	1.00	48.08
ATOM	1168	O	ASP	A	362	28.226	58.624	13.548	1.00	48.57
ATOM	1169	N	PHE	A	363	27.754	60.783	13.212	1.00	47.42
ATOM	1170	CA	PHE	A	363	26.537	60.705	13.976	1.00	46.95
ATOM	1171	CB	PHE	A	363	25.904	62.090	14.159	1.00	47.43
ATOM	1172	CG	PHE	A	363	26.229	62.701	15.491	1.00	49.92
ATOM	1173	CD1	PHE	A	363	25.457	62.406	16.605	1.00	51.39
ATOM	1174	CE1	PHE	A	363	25.770	62.933	17.852	1.00	51.96
ATOM	1175	CZ	PHE	A	363	26.880	63.766	17.995	1.00	51.33
ATOM	1176	CE2	PHE	A	363	27.676	64.044	16.893	1.00	52.86
ATOM	1177	CD2	PHE	A	363	27.348	63.514	15.649	1.00	51.71
ATOM	1178	C	PHE	A	363	25.543	59.674	13.453	1.00	46.01
ATOM	1179	O	PHE	A	363	24.973	58.922	14.240	1.00	46.15
ATOM	1180	N	MET	A	364	25.364	59.588	12.140	1.00	45.35
ATOM	1181	CA	MET	A	364	24.284	58.755	11.629	1.00	44.66
ATOM	1182	CB	MET	A	364	23.606	59.388	10.424	1.00	44.69
ATOM	1183	CG	MET	A	364	22.598	60.479	10.802	1.00	45.45
ATOM	1184	SD	MET	A	364	21.276	60.055	11.959	1.00	47.54
ATOM	1185	CE	MET	A	364	20.142	59.200	10.891	1.00	44.80
ATOM	1186	C	MET	A	364	24.642	57.292	11.390	1.00	44.28
ATOM	1187	O	MET	A	364	23.789	56.413	11.489	1.00	43.35
ATOM	1188	N	GLU	A	365	25.919	57.033	11.165	1.00	44.35
ATOM	1189	CA	GLU	A	365	26.386	55.707	10.769	1.00	44.71
ATOM	1190	CB	GLU	A	365	27.908	55.755	10.531	1.00	45.22
ATOM	1191	CG	GLU	A	365	28.475	54.586	9.749	1.00	46.29
ATOM	1192	CD	GLU	A	365	27.794	54.360	8.411	1.00	46.74
ATOM	1193	OE1	GLU	A	365	27.237	55.319	7.835	1.00	44.88
ATOM	1194	OE2	GLU	A	365	27.829	53.204	7.929	1.00	49.79
ATOM	1195	C	GLU	A	365	25.963	54.536	11.700	1.00	44.66
ATOM	1196	O	GLU	A	365	25.445	53.528	11.220	1.00	44.78
ATOM	1197	N	PRO	A	366	26.133	54.674	13.029	1.00	44.36
ATOM	1198	CA	PRO	A	366	25.680	53.539	13.845	1.00	44.41
ATOM	1199	CB	PRO	A	366	26.096	53.907	15.278	1.00	44.71
ATOM	1200	CG	PRO	A	366	26.774	55.227	15.223	1.00	44.84
ATOM	1201	CD	PRO	A	366	26.684	55.781	13.835	1.00	44.98
ATOM	1202	C	PRO	A	366	24.169	53.281	13.802	1.00	44.17
ATOM	1203	O	PRO	A	366	23.748	52.172	14.162	1.00	43.70
ATOM	1204	N	LYS	A	367	23.383	54.305	13.408	1.00	43.19
ATOM	1205	CA	LYS	A	367	21.916	54.207	13.298	1.00	42.82
ATOM	1206	CB	LYS	A	367	21.233	55.581	13.263	1.00	41.89
ATOM	1207	CG	LYS	A	367	21.955	56.699	14.030	1.00	43.74
ATOM	1208	CD	LYS	A	367	21.711	56.686	15.492	1.00	42.53
ATOM	1209	CE	LYS	A	367	22.944	57.189	16.303	1.00	44.54
ATOM	1210	NZ	LYS	A	367	23.152	58.680	16.400	1.00	44.72
ATOM	1211	C	LYS	A	367	21.564	53.404	12.045	1.00	42.72
ATOM	1212	O	LYS	A	367	20.705	52.525	12.100	1.00	43.96
ATOM	1213	N	PHE	A	368	22.249	53.696	10.942	1.00	41.03

22/75

ATOM	1214	CA	PHE	A	368	22.137	52.935	9.702	1.00	40.39
ATOM	1215	CB	PHE	A	368	23.014	53.559	8.638	1.00	39.83
ATOM	1216	CG	PHE	A	368	22.398	54.724	7.946	1.00	38.47
ATOM	1217	CD1	PHE	A	368	21.332	54.555	7.114	1.00	35.63
ATOM	1218	CE1	PHE	A	368	20.768	55.644	6.453	1.00	36.36
ATOM	1219	CZ	PHE	A	368	21.309	56.900	6.596	1.00	38.57
ATOM	1220	CE2	PHE	A	368	22.399	57.075	7.406	1.00	36.69
ATOM	1221	CD2	PHE	A	368	22.944	55.987	8.071	1.00	39.00
ATOM	1222	C	PHE	A	368	22.562	51.487	9.849	1.00	41.53
ATOM	1223	O	PHE	A	368	21.898	50.584	9.329	1.00	42.07
ATOM	1224	N	GLU	A	369	23.695	51.265	10.528	1.00	41.56
ATOM	1225	CA	GLU	A	369	24.155	49.910	10.793	1.00	41.99
ATOM	1226	CB	GLU	A	369	25.470	49.904	11.537	1.00	42.00
ATOM	1227	CG	GLU	A	369	26.696	50.218	10.699	1.00	43.41
ATOM	1228	CD	GLU	A	369	27.923	50.370	11.583	1.00	47.90
ATOM	1229	OE1	GLU	A	369	27.820	49.992	12.778	1.00	47.72
ATOM	1230	OE2	GLU	A	369	28.973	50.882	11.100	1.00	48.95
ATOM	1231	C	GLU	A	369	23.137	49.115	11.566	1.00	41.46
ATOM	1232	O	GLU	A	369	22.886	47.978	11.248	1.00	41.14
ATOM	1233	N	PHE	A	370	22.569	49.714	12.596	1.00	42.58
ATOM	1234	CA	PHE	A	370	21.426	49.131	13.295	1.00	43.06
ATOM	1235	CB	PHE	A	370	21.045	49.961	14.530	1.00	42.90
ATOM	1236	CG	PHE	A	370	19.700	49.576	15.129	1.00	43.07
ATOM	1237	CD1	PHE	A	370	19.566	48.434	15.925	1.00	43.19
ATOM	1238	CE1	PHE	A	370	18.348	48.097	16.477	1.00	41.82
ATOM	1239	CZ	PHE	A	370	17.238	48.872	16.212	1.00	41.52
ATOM	1240	CE2	PHE	A	370	17.361	50.002	15.437	1.00	40.37
ATOM	1241	CD2	PHE	A	370	18.581	50.352	14.901	1.00	41.15
ATOM	1242	C	PHE	A	370	20.194	48.956	12.403	1.00	43.56
ATOM	1243	O	PHE	A	370	19.540	47.886	12.405	1.00	42.92
ATOM	1244	N	ALA	A	371	19.843	50.009	11.665	1.00	44.38
ATOM	1245	CA	ALA	A	371	18.607	49.944	10.907	1.00	44.60
ATOM	1246	CB	ALA	A	371	18.356	51.208	10.147	1.00	44.36
ATOM	1247	C	ALA	A	371	18.689	48.744	9.984	1.00	45.77
ATOM	1248	O	ALA	A	371	17.761	47.946	9.935	1.00	45.90
ATOM	1249	N	VAL	A	372	19.827	48.598	9.300	1.00	46.84
ATOM	1250	CA	VAL	A	372	20.040	47.538	8.326	1.00	47.11
ATOM	1251	CB	VAL	A	372	21.429	47.693	7.636	1.00	47.27
ATOM	1252	CG1	VAL	A	372	22.001	46.371	7.210	1.00	48.76
ATOM	1253	CG2	VAL	A	372	21.289	48.586	6.451	1.00	47.00
ATOM	1254	C	VAL	A	372	19.741	46.125	8.852	1.00	47.06
ATOM	1255	O	VAL	A	372	18.991	45.402	8.212	1.00	47.13
ATOM	1256	N	LYS	A	373	20.288	45.756	10.013	1.00	47.17
ATOM	1257	CA	LYS	A	373	19.935	44.478	10.660	1.00	47.49
ATOM	1258	CB	LYS	A	373	20.963	43.964	11.685	1.00	48.25
ATOM	1259	CG	LYS	A	373	22.144	44.849	12.047	1.00	51.64
ATOM	1260	CD	LYS	A	373	23.383	44.015	12.376	1.00	53.45
ATOM	1261	CE	LYS	A	373	24.642	44.891	12.640	1.00	54.90
ATOM	1262	NZ	LYS	A	373	24.711	45.526	14.027	1.00	56.42
ATOM	1263	C	LYS	A	373	18.563	44.436	11.298	1.00	46.61
ATOM	1264	O	LYS	A	373	17.924	43.385	11.281	1.00	47.21
ATOM	1265	N	PHE	A	374	18.110	45.558	11.865	1.00	44.83
ATOM	1266	CA	PHE	A	374	16.769	45.585	12.452	1.00	43.23
ATOM	1267	CB	PHE	A	374	16.455	46.917	13.145	1.00	42.22
ATOM	1268	CG	PHE	A	374	15.203	46.882	14.009	1.00	42.04
ATOM	1269	CD1	PHE	A	374	15.185	46.175	15.220	1.00	41.97
ATOM	1270	CE1	PHE	A	374	14.060	46.157	16.034	1.00	39.28
ATOM	1271	CZ	PHE	A	374	12.930	46.842	15.658	1.00	42.25

23/75

ATOM	1272	CE2	PHE	A	374	12.918	47.558	14.436	1.00	40.79
ATOM	1273	CD2	PHE	A	374	14.060	47.583	13.631	1.00	40.96
ATOM	1274	C	PHE	A	374	15.745	45.333	11.381	1.00	42.50
ATOM	1275	O	PHE	A	374	14.780	44.589	11.601	1.00	42.39
ATOM	1276	N	ASN	A	375	15.938	45.996	10.244	1.00	41.75
ATOM	1277	CA	ASN	A	375	14.966	45.998	9.172	1.00	41.42
ATOM	1278	CB	ASN	A	375	15.296	47.060	8.146	1.00	41.79
ATOM	1279	CG	ASN	A	375	14.789	48.454	8.553	1.00	40.58
ATOM	1280	OD1	ASN	A	375	14.052	48.627	9.526	1.00	41.43
ATOM	1281	ND2	ASN	A	375	15.178	49.435	7.787	1.00	37.46
ATOM	1282	C	ASN	A	375	14.846	44.656	8.507	1.00	42.27
ATOM	1283	O	ASN	A	375	13.807	44.346	7.913	1.00	42.35
ATOM	1284	N	ALA	A	376	15.898	43.852	8.646	1.00	41.94
ATOM	1285	CA	ALA	A	376	15.913	42.505	8.123	1.00	43.20
ATOM	1286	CB	ALA	A	376	17.302	41.922	8.206	1.00	42.00
ATOM	1287	C	ALA	A	376	14.902	41.609	8.851	1.00	43.38
ATOM	1288	O	ALA	A	376	14.573	40.537	8.349	1.00	43.74
ATOM	1289	N	LEU	A	377	14.432	42.050	10.018	1.00	42.77
ATOM	1290	CA	LEU	A	377	13.384	41.344	10.755	1.00	43.75
ATOM	1291	CB	LEU	A	377	13.338	41.778	12.231	1.00	42.07
ATOM	1292	CG	LEU	A	377	14.549	41.444	13.124	1.00	45.00
ATOM	1293	CD1	LEU	A	377	14.241	41.746	14.578	1.00	47.22
ATOM	1294	CD2	LEU	A	377	15.048	39.975	12.999	1.00	47.39
ATOM	1295	C	LEU	A	377	12.014	41.470	10.080	1.00	44.07
ATOM	1296	O	LEU	A	377	11.126	40.653	10.333	1.00	44.88
ATOM	1297	N	GLU	A	378	11.845	42.496	9.236	1.00	44.33
ATOM	1298	CA	GLU	A	378	10.602	42.726	8.462	1.00	44.86
ATOM	1299	CB	GLU	A	378	10.349	41.582	7.473	1.00	45.45
ATOM	1300	CG	GLU	A	378	11.376	41.454	6.326	1.00	47.20
ATOM	1301	CD	GLU	A	378	11.127	40.227	5.451	1.00	48.01
ATOM	1302	OE1	GLU	A	378	10.144	39.479	5.705	1.00	54.43
ATOM	1303	OE2	GLU	A	378	11.924	39.978	4.524	1.00	52.34
ATOM	1304	C	GLU	A	378	9.375	42.948	9.359	1.00	43.82
ATOM	1305	O	GLU	A	378	8.306	42.384	9.113	1.00	44.24
ATOM	1306	N	LEU	A	379	9.545	43.769	10.401	1.00	41.90
ATOM	1307	CA	LEU	A	379	8.491	44.014	11.339	1.00	41.39
ATOM	1308	CB	LEU	A	379	9.026	44.581	12.660	1.00	40.19
ATOM	1309	CG	LEU	A	379	9.821	43.534	13.493	1.00	41.62
ATOM	1310	CD1	LEU	A	379	10.034	44.070	14.871	1.00	38.57
ATOM	1311	CD2	LEU	A	379	9.121	42.143	13.597	1.00	35.36
ATOM	1312	C	LEU	A	379	7.584	44.997	10.645	1.00	41.19
ATOM	1313	O	LEU	A	379	8.026	45.735	9.760	1.00	39.80
ATOM	1314	N	ASP	A	380	6.309	44.933	10.950	1.00	41.30
ATOM	1315	CA	ASP	A	380	5.444	45.937	10.389	1.00	43.10
ATOM	1316	CB	ASP	A	380	4.343	45.338	9.520	1.00	43.18
ATOM	1317	CG	ASP	A	380	3.430	44.413	10.272	1.00	47.20
ATOM	1318	OD1	ASP	A	380	3.417	44.470	11.506	1.00	50.02
ATOM	1319	OD2	ASP	A	380	2.695	43.633	9.612	1.00	48.53
ATOM	1320	C	ASP	A	380	4.957	46.841	11.510	1.00	42.21
ATOM	1321	O	ASP	A	380	5.381	46.671	12.653	1.00	43.31
ATOM	1322	N	ASP	A	381	4.095	47.803	11.222	1.00	41.87
ATOM	1323	CA	ASP	A	381	3.733	48.721	12.268	1.00	41.06
ATOM	1324	CB	ASP	A	381	2.860	49.874	11.749	1.00	42.00
ATOM	1325	CG	ASP	A	381	3.588	50.801	10.799	1.00	40.56
ATOM	1326	OD1	ASP	A	381	4.577	51.500	11.196	1.00	38.25
ATOM	1327	OD2	ASP	A	381	3.133	50.842	9.642	1.00	38.91
ATOM	1328	C	ASP	A	381	2.960	48.022	13.366	1.00	41.61
ATOM	1329	O	ASP	A	381	3.016	48.458	14.495	1.00	41.62

24/75

ATOM	1330	N	SER	A	382	2.141	47.015	13.040	1.00	42.13
ATOM	1331	CA	SER	A	382	1.313	46.356	14.079	1.00	41.51
ATOM	1332	CB	SER	A	382	0.312	45.382	13.478	1.00	42.08
ATOM	1333	OG	SER	A	382	0.979	44.290	12.898	1.00	40.52
ATOM	1334	C	SER	A	382	2.195	45.661	15.112	1.00	41.03
ATOM	1335	O	SER	A	382	1.876	45.663	16.313	1.00	41.24
ATOM	1336	N	ASP	A	383	3.312	45.098	14.645	1.00	41.16
ATOM	1337	CA	ASP	A	383	4.378	44.519	15.533	1.00	40.78
ATOM	1338	CB	ASP	A	383	5.445	43.859	14.688	1.00	40.16
ATOM	1339	CG	ASP	A	383	4.903	42.767	13.840	1.00	40.37
ATOM	1340	OD1	ASP	A	383	3.993	42.067	14.333	1.00	42.11
ATOM	1341	OD2	ASP	A	383	5.395	42.603	12.700	1.00	38.96
ATOM	1342	C	ASP	A	383	5.135	45.526	16.408	1.00	41.31
ATOM	1343	O	ASP	A	383	5.420	45.277	17.589	1.00	40.05
ATOM	1344	N	LEU	A	384	5.555	46.621	15.776	1.00	41.16
ATOM	1345	CA	LEU	A	384	6.408	47.647	16.421	1.00	40.56
ATOM	1346	CB	LEU	A	384	6.953	48.639	15.358	1.00	40.28
ATOM	1347	CG	LEU	A	384	7.986	48.263	14.275	1.00	40.56
ATOM	1348	CD1	LEU	A	384	8.149	49.335	13.145	1.00	36.60
ATOM	1349	CD2	LEU	A	384	9.348	48.070	14.904	1.00	39.60
ATOM	1350	C	LEU	A	384	5.627	48.388	17.469	1.00	41.02
ATOM	1351	O	LEU	A	384	6.180	48.802	18.477	1.00	41.15
ATOM	1352	N	ALA	A	385	4.329	48.596	17.251	1.00	39.58
ATOM	1353	CA	ALA	A	385	3.545	49.269	18.272	1.00	39.88
ATOM	1354	CB	ALA	A	385	2.062	49.390	17.834	1.00	39.43
ATOM	1355	C	ALA	A	385	3.641	48.533	19.617	1.00	39.68
ATOM	1356	O	ALA	A	385	3.681	49.152	20.695	1.00	39.12
ATOM	1357	N	ILE	A	386	3.654	47.204	19.559	1.00	38.47
ATOM	1358	CA	ILE	A	386	3.728	46.434	20.783	1.00	36.93
ATOM	1359	CB	ILE	A	386	3.242	44.971	20.662	1.00	37.02
ATOM	1360	CG1	ILE	A	386	1.794	44.885	20.180	1.00	36.80
ATOM	1361	CD1	ILE	A	386	1.357	43.469	19.701	1.00	35.19
ATOM	1362	CG2	ILE	A	386	3.216	44.435	22.085	1.00	34.47
ATOM	1363	C	ILE	A	386	5.174	46.411	21.307	1.00	38.21
ATOM	1364	O	ILE	A	386	5.395	46.445	22.529	1.00	39.38
ATOM	1365	N	PHE	A	387	6.153	46.398	20.399	1.00	37.60
ATOM	1366	CA	PHE	A	387	7.553	46.351	20.808	1.00	37.97
ATOM	1367	CB	PHE	A	387	8.418	46.210	19.567	1.00	38.35
ATOM	1368	CG	PHE	A	387	9.903	46.310	19.824	1.00	38.43
ATOM	1369	CD1	PHE	A	387	10.564	45.359	20.632	1.00	38.05
ATOM	1370	CE1	PHE	A	387	11.934	45.415	20.859	1.00	36.98
ATOM	1371	CZ	PHE	A	387	12.700	46.391	20.242	1.00	38.90
ATOM	1372	CE2	PHE	A	387	12.077	47.356	19.404	1.00	38.34
ATOM	1373	CD2	PHE	A	387	10.663	47.284	19.180	1.00	38.58
ATOM	1374	C	PHE	A	387	7.958	47.601	21.550	1.00	39.43
ATOM	1375	O	PHE	A	387	8.744	47.546	22.493	1.00	39.77
ATOM	1376	N	ILE	A	388	7.506	48.735	21.017	1.00	39.17
ATOM	1377	CA	ILE	A	388	7.711	50.085	21.546	1.00	39.79
ATOM	1378	CB	ILE	A	388	7.150	51.084	20.466	1.00	41.04
ATOM	1379	CG1	ILE	A	388	8.095	51.159	19.245	1.00	41.47
ATOM	1380	CD1	ILE	A	388	9.527	51.450	19.634	1.00	44.56
ATOM	1381	CG2	ILE	A	388	6.844	52.464	20.978	1.00	42.95
ATOM	1382	C	ILE	A	388	7.061	50.257	22.932	1.00	40.20
ATOM	1383	O	ILE	A	388	7.524	51.058	23.760	1.00	41.05
ATOM	1384	N	ALA	A	389	5.966	49.540	23.186	1.00	38.81
ATOM	1385	CA	ALA	A	389	5.298	49.553	24.478	1.00	38.32
ATOM	1386	CB	ALA	A	389	3.895	48.877	24.343	1.00	39.23
ATOM	1387	C	ALA	A	389	6.151	48.783	25.451	1.00	38.28

25/75

ATOM	1388	O	ALA	A	389	6.334	49.176	26.595	1.00	39.58
ATOM	1389	N	VAL	A	390	6.679	47.672	24.980	1.00	38.38
ATOM	1390	CA	VAL	A	390	7.573	46.859	25.813	1.00	37.72
ATOM	1391	CB	VAL	A	390	8.036	45.611	25.063	1.00	37.32
ATOM	1392	CG1	VAL	A	390	9.139	44.912	25.858	1.00	37.06
ATOM	1393	CG2	VAL	A	390	6.833	44.669	24.786	1.00	35.13
ATOM	1394	C	VAL	A	390	8.823	47.637	26.268	1.00	38.29
ATOM	1395	O	VAL	A	390	9.284	47.481	27.426	1.00	39.89
ATOM	1396	N	ILE	A	391	9.463	48.340	25.335	1.00	38.30
ATOM	1397	CA	ILE	A	391	10.626	49.182	25.662	1.00	37.70
ATOM	1398	CB	ILE	A	391	11.177	49.965	24.481	1.00	38.13
ATOM	1399	CG1	ILE	A	391	11.643	49.039	23.351	1.00	35.26
ATOM	1400	CD1	ILE	A	391	12.405	49.776	22.248	1.00	32.09
ATOM	1401	CG2	ILE	A	391	12.259	50.888	24.958	1.00	36.74
ATOM	1402	C	ILE	A	391	10.324	50.212	26.718	1.00	39.11
ATOM	1403	O	ILE	A	391	11.112	50.386	27.655	1.00	40.26
ATOM	1404	N	ILE	A	392	9.229	50.960	26.565	1.00	39.52
ATOM	1405	CA	ILE	A	392	8.885	51.978	27.565	1.00	40.30
ATOM	1406	CB	ILE	A	392	7.587	52.702	27.199	1.00	39.43
ATOM	1407	CG1	ILE	A	392	7.762	53.394	25.840	1.00	39.25
ATOM	1408	CD1	ILE	A	392	6.453	53.969	25.273	1.00	39.15
ATOM	1409	CG2	ILE	A	392	7.273	53.738	28.279	1.00	39.90
ATOM	1410	C	ILE	A	392	8.730	51.419	28.987	1.00	41.08
ATOM	1411	O	ILE	A	392	9.292	51.956	29.948	1.00	42.54
ATOM	1412	N	LEU	A	393	7.973	50.340	29.123	1.00	41.29
ATOM	1413	CA	LEU	A	393	7.689	49.773	30.444	1.00	41.24
ATOM	1414	CB	LEU	A	393	6.363	49.009	30.431	1.00	40.75
ATOM	1415	CG	LEU	A	393	5.030	49.772	30.468	1.00	34.98
ATOM	1416	CD1	LEU	A	393	4.737	50.245	31.893	1.00	35.69
ATOM	1417	CD2	LEU	A	393	5.030	50.957	29.579	1.00	32.00
ATOM	1418	C	LEU	A	393	8.827	48.860	30.898	1.00	43.53
ATOM	1419	O	LEU	A	393	8.604	47.716	31.270	1.00	42.79
ATOM	1420	N	SER	A	394	10.055	49.356	30.941	1.00	45.12
ATOM	1421	CA	SER	A	394	11.124	48.452	31.435	1.00	47.28
ATOM	1422	CB	SER	A	394	12.493	48.896	30.977	1.00	47.10
ATOM	1423	OG	SER	A	394	12.509	48.744	29.581	1.00	48.78
ATOM	1424	C	SER	A	394	11.094	48.106	32.935	1.00	48.71
ATOM	1425	O	SER	A	394	10.588	47.043	33.328	1.00	50.76
ATOM	1426	N	GLY	A	395	11.593	48.954	33.805	1.00	49.34
ATOM	1427	CA	GLY	A	395	11.648	48.486	35.204	1.00	50.16
ATOM	1428	C	GLY	A	395	12.999	47.984	35.647	1.00	50.55
ATOM	1429	O	GLY	A	395	13.218	47.712	36.831	1.00	50.77
ATOM	1430	N	ASP	A	396	13.918	47.844	34.703	1.00	50.98
ATOM	1431	CA	ASP	A	396	15.320	47.741	35.057	1.00	50.93
ATOM	1432	CB	ASP	A	396	16.016	46.582	34.294	1.00	52.35
ATOM	1433	CG	ASP	A	396	16.000	45.200	35.099	1.00	56.79
ATOM	1434	OD1	ASP	A	396	15.621	45.143	36.313	1.00	59.53
ATOM	1435	OD2	ASP	A	396	16.407	44.149	34.516	1.00	61.46
ATOM	1436	C	ASP	A	396	15.972	49.122	34.848	1.00	49.41
ATOM	1437	O	ASP	A	396	17.184	49.244	34.884	1.00	49.75
ATOM	1438	N	ARG	A	397	15.157	50.169	34.648	1.00	47.70
ATOM	1439	CA	ARG	A	397	15.681	51.563	34.544	1.00	45.92
ATOM	1440	CB	ARG	A	397	14.577	52.561	34.094	1.00	45.23
ATOM	1441	CG	ARG	A	397	13.826	52.231	32.759	1.00	43.06
ATOM	1442	CD	ARG	A	397	14.788	52.012	31.619	1.00	40.96
ATOM	1443	NE	ARG	A	397	14.137	52.076	30.306	1.00	39.75
ATOM	1444	CZ	ARG	A	397	14.712	51.797	29.136	1.00	38.47
ATOM	1445	NH1	ARG	A	397	15.977	51.396	29.095	1.00	36.71

26/75

ATOM	1446	NH2	ARG	A	397	14.007	51.894	28.004	1.00	34.06
ATOM	1447	C	ARG	A	397	16.279	52.043	35.885	1.00	45.10
ATOM	1448	O	ARG	A	397	15.728	51.736	36.934	1.00	45.86
ATOM	1449	N	PRO	A	398	17.410	52.776	35.864	1.00	44.30
ATOM	1450	CA	PRO	A	398	17.867	53.360	37.121	1.00	43.51
ATOM	1451	CB	PRO	A	398	19.111	54.167	36.717	1.00	43.59
ATOM	1452	CG	PRO	A	398	19.593	53.515	35.486	1.00	45.17
ATOM	1453	CD	PRO	A	398	18.349	53.054	34.763	1.00	43.97
ATOM	1454	C	PRO	A	398	16.870	54.289	37.802	1.00	42.64
ATOM	1455	O	PRO	A	398	16.263	55.146	37.156	1.00	42.27
ATOM	1456	N	GLY	A	399	16.737	54.108	39.114	1.00	41.75
ATOM	1457	CA	GLY	A	399	16.045	55.049	39.990	1.00	40.50
ATOM	1458	C	GLY	A	399	14.531	54.954	40.048	1.00	39.59
ATOM	1459	O	GLY	A	399	13.901	55.825	40.629	1.00	38.90
ATOM	1460	N	LEU	A	400	13.948	53.910	39.454	1.00	38.91
ATOM	1461	CA	LEU	A	400	12.498	53.668	39.548	1.00	38.61
ATOM	1462	CB	LEU	A	400	12.088	52.461	38.684	1.00	38.87
ATOM	1463	CG	LEU	A	400	12.078	52.712	37.169	1.00	37.87
ATOM	1464	CD1	LEU	A	400	11.816	51.450	36.369	1.00	40.54
ATOM	1465	CD2	LEU	A	400	11.048	53.747	36.836	1.00	36.51
ATOM	1466	C	LEU	A	400	12.097	53.445	40.989	1.00	38.75
ATOM	1467	O	LEU	A	400	12.843	52.854	41.740	1.00	38.17
ATOM	1468	N	LEU	A	401	10.934	53.944	41.379	1.00	39.51
ATOM	1469	CA	LEU	A	401	10.486	53.850	42.770	1.00	39.83
ATOM	1470	CB	LEU	A	401	9.650	55.092	43.155	1.00	39.91
ATOM	1471	CG	LEU	A	401	10.254	56.523	43.028	1.00	40.45
ATOM	1472	CD1	LEU	A	401	9.248	57.604	43.450	1.00	40.38
ATOM	1473	CD2	LEU	A	401	11.498	56.704	43.835	1.00	37.79
ATOM	1474	C	LEU	A	401	9.720	52.522	43.020	1.00	40.64
ATOM	1475	O	LEU	A	401	10.054	51.776	43.952	1.00	40.22
ATOM	1476	N	ASN	A	402	8.720	52.211	42.182	1.00	41.32
ATOM	1477	CA	ASN	A	402	7.968	50.937	42.283	1.00	42.02
ATOM	1478	CB	ASN	A	402	6.458	51.153	42.511	1.00	42.94
ATOM	1479	CG	ASN	A	402	6.135	52.351	43.402	1.00	45.44
ATOM	1480	OD1	ASN	A	402	5.290	53.198	43.048	1.00	44.96
ATOM	1481	ND2	ASN	A	402	6.795	52.427	44.561	1.00	47.36
ATOM	1482	C	ASN	A	402	8.115	50.086	41.030	1.00	41.74
ATOM	1483	O	ASN	A	402	7.280	50.184	40.110	1.00	41.31
ATOM	1484	N	VAL	A	403	9.143	49.246	41.011	1.00	40.78
ATOM	1485	CA	VAL	A	403	9.535	48.421	39.857	1.00	41.66
ATOM	1486	CB	VAL	A	403	10.885	47.685	40.117	1.00	41.82
ATOM	1487	CG1	VAL	A	403	11.150	46.665	39.062	1.00	40.50
ATOM	1488	CG2	VAL	A	403	12.043	48.674	40.170	1.00	40.88
ATOM	1489	C	VAL	A	403	8.482	47.392	39.455	1.00	42.92
ATOM	1490	O	VAL	A	403	8.312	47.108	38.253	1.00	44.51
ATOM	1491	N	LYS	A	404	7.749	46.885	40.448	1.00	43.59
ATOM	1492	CA	LYS	A	404	6.759	45.805	40.276	1.00	43.65
ATOM	1493	CB	LYS	A	404	6.324	45.256	41.637	1.00	44.35
ATOM	1494	CG	LYS	A	404	5.860	43.823	41.623	1.00	45.28
ATOM	1495	CD	LYS	A	404	4.374	43.719	41.476	1.00	47.89
ATOM	1496	CE	LYS	A	404	3.828	42.557	42.317	1.00	47.39
ATOM	1497	NZ	LYS	A	404	3.543	42.970	43.743	1.00	47.90
ATOM	1498	C	LYS	A	404	5.525	46.059	39.418	1.00	43.16
ATOM	1499	O	LYS	A	404	5.222	45.222	38.569	1.00	43.44
ATOM	1500	N	PRO	A	405	4.750	47.143	39.681	1.00	42.44
ATOM	1501	CA	PRO	A	405	3.632	47.420	38.781	1.00	41.55
ATOM	1502	CB	PRO	A	405	3.038	48.735	39.335	1.00	41.40
ATOM	1503	CG	PRO	A	405	4.062	49.285	40.228	1.00	41.97

27/75

ATOM	1504	CD	PRO	A	405	4.759	48.095	40.806	1.00	42.57
ATOM	1505	C	PRO	A	405	4.019	47.604	37.321	1.00	40.35
ATOM	1506	O	PRO	A	405	3.180	47.424	36.451	1.00	39.92
ATOM	1507	N	ILE	A	406	5.263	48.011	37.094	1.00	39.99
ATOM	1508	CA	ILE	A	406	5.842	48.183	35.762	1.00	39.36
ATOM	1509	CB	ILE	A	406	7.172	49.026	35.795	1.00	38.83
ATOM	1510	CG1	ILE	A	406	6.866	50.462	36.252	1.00	39.01
ATOM	1511	CD1	ILE	A	406	8.091	51.331	36.660	1.00	38.30
ATOM	1512	CG2	ILE	A	406	7.810	49.072	34.409	1.00	37.98
ATOM	1513	C	ILE	A	406	6.087	46.839	35.094	1.00	39.49
ATOM	1514	O	ILE	A	406	5.731	46.638	33.938	1.00	39.76
ATOM	1515	N	GLU	A	407	6.708	45.927	35.833	1.00	39.87
ATOM	1516	CA	GLU	A	407	6.989	44.598	35.345	1.00	40.81
ATOM	1517	CB	GLU	A	407	7.882	43.864	36.354	1.00	40.17
ATOM	1518	CG	GLU	A	407	9.272	44.502	36.411	1.00	41.50
ATOM	1519	CD	GLU	A	407	10.326	43.692	37.155	1.00	42.77
ATOM	1520	OE1	GLU	A	407	9.989	42.969	38.135	1.00	43.12
ATOM	1521	OE2	GLU	A	407	11.515	43.831	36.762	1.00	46.98
ATOM	1522	C	GLU	A	407	5.721	43.828	35.054	1.00	40.81
ATOM	1523	O	GLU	A	407	5.645	43.136	34.056	1.00	41.76
ATOM	1524	N	ASP	A	408	4.716	43.948	35.912	1.00	41.73
ATOM	1525	CA	ASP	A	408	3.403	43.367	35.632	1.00	41.99
ATOM	1526	CB	ASP	A	408	2.426	43.667	36.750	1.00	42.07
ATOM	1527	CG	ASP	A	408	2.743	42.908	38.014	1.00	43.91
ATOM	1528	OD1	ASP	A	408	3.771	42.152	38.065	1.00	45.34
ATOM	1529	OD2	ASP	A	408	1.936	43.081	38.963	1.00	45.22
ATOM	1530	C	ASP	A	408	2.822	43.818	34.293	1.00	41.47
ATOM	1531	O	ASP	A	408	2.430	42.978	33.505	1.00	42.78
ATOM	1532	N	ILE	A	409	2.767	45.130	34.018	1.00	41.68
ATOM	1533	CA	ILE	A	409	2.353	45.627	32.698	1.00	39.76
ATOM	1534	CB	ILE	A	409	2.435	47.164	32.561	1.00	41.09
ATOM	1535	CG1	ILE	A	409	1.581	47.899	33.606	1.00	41.23
ATOM	1536	CD1	ILE	A	409	2.108	49.322	33.895	1.00	40.86
ATOM	1537	CG2	ILE	A	409	1.938	47.624	31.160	1.00	40.97
ATOM	1538	C	ILE	A	409	3.225	45.058	31.587	1.00	39.50
ATOM	1539	O	ILE	A	409	2.712	44.620	30.546	1.00	38.11
ATOM	1540	N	GLN	A	410	4.550	45.076	31.788	1.00	38.45
ATOM	1541	CA	GLN	A	410	5.430	44.708	30.723	1.00	38.16
ATOM	1542	CB	GLN	A	410	6.897	44.945	31.045	1.00	37.92
ATOM	1543	CG	GLN	A	410	7.769	44.896	29.768	1.00	37.19
ATOM	1544	CD	GLN	A	410	9.271	44.765	30.112	1.00	36.46
ATOM	1545	OE1	GLN	A	410	10.124	45.491	29.561	1.00	39.71
ATOM	1546	NE2	GLN	A	410	9.592	43.837	31.000	1.00	38.78
ATOM	1547	C	GLN	A	410	5.261	43.263	30.417	1.00	38.31
ATOM	1548	O	GLN	A	410	5.407	42.880	29.268	1.00	38.77
ATOM	1549	N	ASP	A	411	5.028	42.456	31.449	1.00	40.24
ATOM	1550	CA	ASP	A	411	4.818	41.031	31.278	1.00	41.12
ATOM	1551	CB	ASP	A	411	4.612	40.365	32.640	1.00	42.21
ATOM	1552	CG	ASP	A	411	5.931	40.154	33.435	1.00	45.68
ATOM	1553	OD1	ASP	A	411	7.018	40.692	33.050	1.00	45.82
ATOM	1554	OD2	ASP	A	411	5.853	39.438	34.478	1.00	48.81
ATOM	1555	C	ASP	A	411	3.572	40.864	30.410	1.00	40.86
ATOM	1556	O	ASP	A	411	3.532	40.058	29.499	1.00	40.75
ATOM	1557	N	ASN	A	412	2.551	41.659	30.673	1.00	41.49
ATOM	1558	CA	ASN	A	412	1.365	41.652	29.769	1.00	41.78
ATOM	1559	CB	ASN	A	412	0.253	42.545	30.307	1.00	42.01
ATOM	1560	CG	ASN	A	412	-1.089	42.133	29.765	1.00	45.54
ATOM	1561	OD1	ASN	A	412	-1.212	41.018	29.285	1.00	52.88

28/75

ATOM	1562	ND2	ASN	A	412	-2.098	43.007	29.824	1.00	45.51
ATOM	1563	C	ASN	A	412	1.680	41.976	28.271	1.00	41.44
ATOM	1564	O	ASN	A	412	1.304	41.245	27.323	1.00	42.02
ATOM	1565	N	LEU	A	413	2.412	43.064	28.086	1.00	39.96
ATOM	1566	CA	LEU	A	413	2.941	43.473	26.812	1.00	37.24
ATOM	1567	CB	LEU	A	413	3.756	44.755	27.014	1.00	37.03
ATOM	1568	CG	LEU	A	413	2.907	45.972	27.419	1.00	31.94
ATOM	1569	CD1	LEU	A	413	3.906	47.071	27.799	1.00	31.22
ATOM	1570	CD2	LEU	A	413	1.948	46.429	26.300	1.00	35.96
ATOM	1571	C	LEU	A	413	3.792	42.469	26.135	1.00	37.15
ATOM	1572	O	LEU	A	413	3.716	42.332	24.950	1.00	38.76
ATOM	1573	N	LEU	A	414	4.672	41.803	26.879	1.00	37.47
ATOM	1574	CA	LEU	A	414	5.510	40.797	26.314	1.00	37.22
ATOM	1575	CB	LEU	A	414	6.451	40.311	27.392	1.00	36.65
ATOM	1576	CG	LEU	A	414	7.658	41.190	27.708	1.00	34.37
ATOM	1577	CD1	LEU	A	414	8.410	40.597	28.918	1.00	39.52
ATOM	1578	CD2	LEU	A	414	8.596	41.232	26.483	1.00	36.08
ATOM	1579	C	LEU	A	414	4.661	39.651	25.790	1.00	37.84
ATOM	1580	O	LEU	A	414	4.964	39.061	24.736	1.00	38.84
ATOM	1581	N	GLN	A	415	3.590	39.349	26.527	1.00	37.97
ATOM	1582	CA	GLN	A	415	2.676	38.257	26.186	1.00	38.44
ATOM	1583	CB	GLN	A	415	1.603	38.093	27.277	1.00	38.84
ATOM	1584	CG	GLN	A	415	1.755	36.898	28.204	1.00	40.03
ATOM	1585	CD	GLN	A	415	0.553	36.741	29.129	1.00	40.63
ATOM	1586	OE1	GLN	A	415	0.379	37.488	30.119	1.00	43.23
ATOM	1587	NE2	GLN	A	415	-0.275	35.742	28.833	1.00	41.43
ATOM	1588	C	GLN	A	415	2.021	38.518	24.858	1.00	38.78
ATOM	1589	O	GLN	A	415	2.093	37.678	23.977	1.00	38.92
ATOM	1590	N	ALA	A	416	1.375	39.694	24.745	1.00	38.16
ATOM	1591	CA	ALA	A	416	0.820	40.256	23.503	1.00	38.94
ATOM	1592	CB	ALA	A	416	0.292	41.667	23.787	1.00	37.84
ATOM	1593	C	ALA	A	416	1.760	40.290	22.290	1.00	38.97
ATOM	1594	O	ALA	A	416	1.369	39.943	21.176	1.00	39.12
ATOM	1595	N	LEU	A	417	2.995	40.750	22.504	1.00	39.31
ATOM	1596	CA	LEU	A	417	4.010	40.740	21.440	1.00	39.25
ATOM	1597	CB	LEU	A	417	5.252	41.451	21.919	1.00	38.71
ATOM	1598	CG	LEU	A	417	6.470	41.585	21.019	1.00	38.63
ATOM	1599	CD1	LEU	A	417	6.113	42.147	19.659	1.00	37.50
ATOM	1600	CD2	LEU	A	417	7.447	42.501	21.785	1.00	36.81
ATOM	1601	C	LEU	A	417	4.381	39.337	20.965	1.00	38.90
ATOM	1602	O	LEU	A	417	4.551	39.099	19.776	1.00	39.89
ATOM	1603	N	GLU	A	418	4.521	38.402	21.891	1.00	38.58
ATOM	1604	CA	GLU	A	418	4.754	37.009	21.520	1.00	37.51
ATOM	1605	CB	GLU	A	418	4.856	36.140	22.794	1.00	37.02
ATOM	1606	CG	GLU	A	418	5.118	34.662	22.478	1.00	38.45
ATOM	1607	CD	GLU	A	418	5.464	33.841	23.699	1.00	38.25
ATOM	1608	OE1	GLU	A	418	4.832	34.085	24.757	1.00	43.96
ATOM	1609	OE2	GLU	A	418	6.348	32.969	23.588	1.00	40.27
ATOM	1610	C	GLU	A	418	3.650	36.468	20.593	1.00	37.36
ATOM	1611	O	GLU	A	418	3.943	35.956	19.510	1.00	38.24
ATOM	1612	N	LEU	A	419	2.395	36.573	21.020	1.00	36.84
ATOM	1613	CA	LEU	A	419	1.240	36.112	20.227	1.00	36.43
ATOM	1614	CB	LEU	A	419	-0.038	36.307	21.060	1.00	36.05
ATOM	1615	CG	LEU	A	419	-1.395	35.796	20.538	1.00	36.79
ATOM	1616	CD1	LEU	A	419	-1.389	34.304	20.354	1.00	34.69
ATOM	1617	CD2	LEU	A	419	-2.465	36.181	21.502	1.00	35.78
ATOM	1618	C	LEU	A	419	1.193	36.913	18.888	1.00	37.33
ATOM	1619	O	LEU	A	419	1.079	36.346	17.807	1.00	35.58

29/75

ATOM	1620	N	GLN	A	420	1.358	38.231	18.957	1.00	38.10
ATOM	1621	CA	GLN	A	420	1.388	39.065	17.744	1.00	39.67
ATOM	1622	CB	GLN	A	420	1.769	40.526	18.091	1.00	39.12
ATOM	1623	CG	GLN	A	420	2.117	41.371	16.850	1.00	38.99
ATOM	1624	CD	GLN	A	420	0.943	41.601	15.876	1.00	41.63
ATOM	1625	OE1	GLN	A	420	-0.230	41.396	16.214	1.00	43.62
ATOM	1626	NE2	GLN	A	420	1.270	42.047	14.664	1.00	37.85
ATOM	1627	C	GLN	A	420	2.354	38.504	16.726	1.00	40.72
ATOM	1628	O	GLN	A	420	1.986	38.238	15.569	1.00	42.40
ATOM	1629	N	LEU	A	421	3.588	38.265	17.150	1.00	41.77
ATOM	1630	CA	LEU	A	421	4.612	37.772	16.222	1.00	41.79
ATOM	1631	CB	LEU	A	421	6.004	37.892	16.854	1.00	42.05
ATOM	1632	CG	LEU	A	421	6.526	39.304	17.177	1.00	41.77
ATOM	1633	CD1	LEU	A	421	7.830	39.228	18.004	1.00	42.13
ATOM	1634	CD2	LEU	A	421	6.727	40.146	15.879	1.00	40.98
ATOM	1635	C	LEU	A	421	4.359	36.344	15.705	1.00	42.62
ATOM	1636	O	LEU	A	421	4.711	35.972	14.570	1.00	41.91
ATOM	1637	N	LYS	A	422	3.779	35.526	16.565	1.00	43.27
ATOM	1638	CA	LYS	A	422	3.486	34.138	16.230	1.00	43.48
ATOM	1639	CB	LYS	A	422	3.083	33.401	17.527	1.00	43.63
ATOM	1640	CG	LYS	A	422	2.522	31.999	17.387	1.00	45.34
ATOM	1641	CD	LYS	A	422	1.845	31.525	18.704	1.00	45.58
ATOM	1642	CE	LYS	A	422	2.774	30.657	19.597	1.00	49.25
ATOM	1643	NZ	LYS	A	422	2.580	29.151	19.453	1.00	47.40
ATOM	1644	C	LYS	A	422	2.383	34.129	15.157	1.00	42.70
ATOM	1645	O	LYS	A	422	2.402	33.318	14.223	1.00	42.68
ATOM	1646	N	LEU	A	423	1.435	35.054	15.312	1.00	42.50
ATOM	1647	CA	LEU	A	423	0.270	35.225	14.426	1.00	41.89
ATOM	1648	CB	LEU	A	423	-0.876	35.943	15.160	1.00	40.87
ATOM	1649	CG	LEU	A	423	-1.537	35.150	16.291	1.00	40.35
ATOM	1650	CD1	LEU	A	423	-2.707	35.892	16.892	1.00	40.39
ATOM	1651	CD2	LEU	A	423	-1.962	33.711	15.818	1.00	39.01
ATOM	1652	C	LEU	A	423	0.615	35.943	13.115	1.00	42.35
ATOM	1653	O	LEU	A	423	0.270	35.479	12.027	1.00	42.62
ATOM	1654	N	ASN	A	424	1.341	37.043	13.229	1.00	42.18
ATOM	1655	CA	ASN	A	424	1.668	37.859	12.080	1.00	42.73
ATOM	1656	CB	ASN	A	424	1.945	39.294	12.557	1.00	42.30
ATOM	1657	CG	ASN	A	424	1.896	40.305	11.424	1.00	41.38
ATOM	1658	OD1	ASN	A	424	1.294	40.055	10.385	1.00	34.54
ATOM	1659	ND2	ASN	A	424	2.573	41.432	11.612	1.00	38.04
ATOM	1660	C	ASN	A	424	2.827	37.306	11.244	1.00	42.98
ATOM	1661	O	ASN	A	424	2.885	37.549	10.034	1.00	42.87
ATOM	1662	N	HIS	A	425	3.753	36.565	11.872	1.00	42.95
ATOM	1663	CA	HIS	A	425	4.879	35.962	11.145	1.00	43.40
ATOM	1664	CB	HIS	A	425	6.213	36.610	11.481	1.00	43.25
ATOM	1665	CG	HIS	A	425	6.278	38.059	11.153	1.00	45.48
ATOM	1666	ND1	HIS	A	425	5.690	39.019	11.942	1.00	46.04
ATOM	1667	CE1	HIS	A	425	5.881	40.209	11.404	1.00	46.84
ATOM	1668	NE2	HIS	A	425	6.585	40.055	10.297	1.00	48.87
ATOM	1669	CD2	HIS	A	425	6.858	38.719	10.124	1.00	47.33
ATOM	1670	C	HIS	A	425	5.014	34.483	11.444	1.00	44.35
ATOM	1671	O	HIS	A	425	6.044	34.059	11.968	1.00	45.30
ATOM	1672	N	PRO	A	426	4.012	33.674	11.075	1.00	44.85
ATOM	1673	CA	PRO	A	426	4.080	32.248	11.356	1.00	45.32
ATOM	1674	CB	PRO	A	426	2.849	31.688	10.628	1.00	45.88
ATOM	1675	CG	PRO	A	426	1.886	32.851	10.593	1.00	46.05
ATOM	1676	CD	PRO	A	426	2.780	34.038	10.358	1.00	45.73
ATOM	1677	C	PRO	A	426	5.344	31.566	10.850	1.00	45.46

30/75

ATOM	1678	O	PRO	A	426	5.839	30.657	11.497	1.00	46.19
ATOM	1679	N	GLU	A	427	5.870	31.991	9.709	1.00	45.74
ATOM	1680	CA	GLU	A	427	6.991	31.304	9.094	1.00	46.29
ATOM	1681	CB	GLU	A	427	7.167	31.748	7.638	1.00	46.66
ATOM	1682	CG	GLU	A	427	7.850	33.132	7.464	1.00	47.95
ATOM	1683	CD	GLU	A	427	6.936	34.347	7.673	1.00	48.05
ATOM	1684	OE1	GLU	A	427	5.726	34.215	7.961	1.00	49.96
ATOM	1685	OE2	GLU	A	427	7.447	35.470	7.552	1.00	48.65
ATOM	1686	C	GLU	A	427	8.266	31.549	9.861	1.00	46.55
ATOM	1687	O	GLU	A	427	9.205	30.766	9.767	1.00	46.16
ATOM	1688	N	SER	A	428	8.294	32.644	10.616	1.00	46.78
ATOM	1689	CA	SER	A	428	9.525	33.137	11.214	1.00	47.71
ATOM	1690	CB	SER	A	428	9.512	34.651	11.266	1.00	47.77
ATOM	1691	OG	SER	A	428	10.841	35.110	11.327	1.00	51.66
ATOM	1692	C	SER	A	428	9.778	32.576	12.596	1.00	47.25
ATOM	1693	O	SER	A	428	9.369	33.142	13.615	1.00	47.07
ATOM	1694	N	SER	A	429	10.458	31.441	12.604	1.00	47.57
ATOM	1695	CA	SER	A	429	10.871	30.760	13.833	1.00	47.07
ATOM	1696	CB	SER	A	429	11.716	29.517	13.493	1.00	47.43
ATOM	1697	OG	SER	A	429	11.570	28.470	14.458	1.00	49.17
ATOM	1698	C	SER	A	429	11.657	31.750	14.711	1.00	45.76
ATOM	1699	O	SER	A	429	12.625	32.384	14.252	1.00	45.10
ATOM	1700	N	GLN	A	430	11.179	31.902	15.949	1.00	44.17
ATOM	1701	CA	GLN	A	430	11.901	32.597	17.001	1.00	42.99
ATOM	1702	CB	GLN	A	430	13.250	31.919	17.229	1.00	42.58
ATOM	1703	CG	GLN	A	430	13.559	31.684	18.686	1.00	42.42
ATOM	1704	CD	GLN	A	430	12.551	30.796	19.357	1.00	36.76
ATOM	1705	OE1	GLN	A	430	12.031	29.883	18.738	1.00	39.11
ATOM	1706	NE2	GLN	A	430	12.257	31.069	20.625	1.00	32.08
ATOM	1707	C	GLN	A	430	12.125	34.078	16.751	1.00	42.39
ATOM	1708	O	GLN	A	430	13.128	34.633	17.190	1.00	41.95
ATOM	1709	N	LEU	A	431	11.188	34.725	16.064	1.00	42.20
ATOM	1710	CA	LEU	A	431	11.298	36.148	15.809	1.00	41.08
ATOM	1711	CB	LEU	A	431	10.240	36.610	14.797	1.00	41.55
ATOM	1712	CG	LEU	A	431	10.242	38.084	14.412	1.00	39.56
ATOM	1713	CD1	LEU	A	431	11.564	38.474	13.793	1.00	36.81
ATOM	1714	CD2	LEU	A	431	9.098	38.338	13.428	1.00	40.36
ATOM	1715	C	LEU	A	431	11.181	36.922	17.119	1.00	41.11
ATOM	1716	O	LEU	A	431	11.823	37.957	17.302	1.00	42.06
ATOM	1717	N	PHE	A	432	10.339	36.432	18.019	1.00	40.55
ATOM	1718	CA	PHE	A	432	10.174	37.053	19.340	1.00	39.91
ATOM	1719	CB	PHE	A	432	9.099	36.298	20.131	1.00	40.18
ATOM	1720	CG	PHE	A	432	8.895	36.779	21.529	1.00	41.13
ATOM	1721	CD1	PHE	A	432	8.435	38.057	21.788	1.00	38.23
ATOM	1722	CE1	PHE	A	432	8.217	38.490	23.114	1.00	40.04
ATOM	1723	CZ	PHE	A	432	8.449	37.617	24.178	1.00	37.70
ATOM	1724	CE2	PHE	A	432	8.902	36.356	23.931	1.00	38.21
ATOM	1725	CD2	PHE	A	432	9.112	35.916	22.613	1.00	40.00
ATOM	1726	C	PHE	A	432	11.529	37.078	20.039	1.00	39.32
ATOM	1727	O	PHE	A	432	12.007	38.130	20.407	1.00	38.57
ATOM	1728	N	ALA	A	433	12.194	35.929	20.148	1.00	39.51
ATOM	1729	CA	ALA	A	433	13.544	35.924	20.715	1.00	40.34
ATOM	1730	CB	ALA	A	433	14.092	34.482	20.826	1.00	39.55
ATOM	1731	C	ALA	A	433	14.534	36.867	19.970	1.00	41.12
ATOM	1732	O	ALA	A	433	15.216	37.676	20.605	1.00	41.16
ATOM	1733	N	LYS	A	434	14.576	36.803	18.634	1.00	41.83
ATOM	1734	CA	LYS	A	434	15.524	37.611	17.841	1.00	41.70
ATOM	1735	CB	LYS	A	434	15.480	37.255	16.348	1.00	41.64

31/75

ATOM	1736	CG	LYS	A	434	15.520	35.748	16.026	1.00	43.75
ATOM	1737	CD	LYS	A	434	16.905	35.194	15.679	1.00	41.62
ATOM	1738	CE	LYS	A	434	17.119	33.812	16.332	1.00	43.50
ATOM	1739	NZ	LYS	A	434	18.328	33.068	15.820	1.00	39.11
ATOM	1740	C	LYS	A	434	15.283	39.100	18.051	1.00	42.59
ATOM	1741	O	LYS	A	434	16.219	39.865	18.222	1.00	43.07
ATOM	1742	N	LEU	A	435	14.021	39.503	18.052	1.00	42.36
ATOM	1743	CA	LEU	A	435	13.647	40.875	18.365	1.00	42.71
ATOM	1744	CB	LEU	A	435	12.124	41.046	18.190	1.00	42.56
ATOM	1745	CG	LEU	A	435	11.589	42.437	18.552	1.00	42.86
ATOM	1746	CD1	LEU	A	435	12.390	43.536	17.790	1.00	45.51
ATOM	1747	CD2	LEU	A	435	10.074	42.592	18.341	1.00	41.33
ATOM	1748	C	LEU	A	435	14.116	41.404	19.757	1.00	43.74
ATOM	1749	O	LEU	A	435	14.603	42.550	19.871	1.00	42.80
ATOM	1750	N	LEU	A	436	13.976	40.582	20.811	1.00	44.23
ATOM	1751	CA	LEU	A	436	14.350	41.013	22.168	1.00	44.36
ATOM	1752	CB	LEU	A	436	13.845	40.046	23.241	1.00	43.17
ATOM	1753	CG	LEU	A	436	12.328	39.898	23.350	1.00	43.59
ATOM	1754	CD1	LEU	A	436	11.975	39.064	24.536	1.00	44.11
ATOM	1755	CD2	LEU	A	436	11.576	41.267	23.414	1.00	41.24
ATOM	1756	C	LEU	A	436	15.856	41.225	22.279	1.00	44.99
ATOM	1757	O	LEU	A	436	16.321	42.093	23.016	1.00	45.07
ATOM	1758	N	GLN	A	437	16.639	40.456	21.538	1.00	46.03
ATOM	1759	CA	GLN	A	437	18.070	40.693	21.561	1.00	46.52
ATOM	1760	CB	GLN	A	437	18.791	39.508	20.933	1.00	47.27
ATOM	1761	CG	GLN	A	437	18.466	38.178	21.630	1.00	48.09
ATOM	1762	CD	GLN	A	437	19.287	37.055	21.110	1.00	51.38
ATOM	1763	OE1	GLN	A	437	20.502	37.014	21.323	1.00	52.83
ATOM	1764	NE2	GLN	A	437	18.639	36.105	20.430	1.00	53.61
ATOM	1765	C	GLN	A	437	18.474	42.038	20.904	1.00	46.94
ATOM	1766	O	GLN	A	437	19.597	42.468	21.043	1.00	46.98
ATOM	1767	N	LYS	A	438	17.561	42.701	20.198	1.00	47.28
ATOM	1768	CA	LYS	A	438	17.889	43.993	19.540	1.00	48.14
ATOM	1769	CB	LYS	A	438	16.894	44.349	18.411	1.00	47.76
ATOM	1770	CG	LYS	A	438	16.964	43.381	17.198	1.00	47.00
ATOM	1771	CD	LYS	A	438	18.136	43.689	16.279	1.00	44.33
ATOM	1772	CE	LYS	A	438	18.280	42.663	15.133	1.00	46.05
ATOM	1773	NZ	LYS	A	438	19.003	41.392	15.507	1.00	47.93
ATOM	1774	C	LYS	A	438	18.110	45.173	20.494	1.00	48.42
ATOM	1775	O	LYS	A	438	18.765	46.140	20.135	1.00	48.35
ATOM	1776	N	MET	A	439	17.599	45.066	21.718	1.00	50.00
ATOM	1777	CA	MET	A	439	17.914	46.024	22.786	1.00	51.20
ATOM	1778	CB	MET	A	439	17.308	45.618	24.108	1.00	51.51
ATOM	1779	CG	MET	A	439	16.240	46.571	24.528	1.00	55.93
ATOM	1780	SD	MET	A	439	14.855	46.179	23.490	1.00	59.07
ATOM	1781	CE	MET	A	439	14.404	44.520	24.088	1.00	58.95
ATOM	1782	C	MET	A	439	19.375	46.317	23.041	1.00	51.21
ATOM	1783	O	MET	A	439	19.716	47.470	23.316	1.00	52.16
ATOM	1784	N	THR	A	440	20.240	45.310	22.988	1.00	50.96
ATOM	1785	CA	THR	A	440	21.636	45.609	23.255	1.00	51.30
ATOM	1786	CB	THR	A	440	22.533	44.362	23.572	1.00	51.55
ATOM	1787	OG1	THR	A	440	23.876	44.807	23.806	1.00	53.23
ATOM	1788	CG2	THR	A	440	22.530	43.296	22.450	1.00	51.72
ATOM	1789	C	THR	A	440	22.202	46.502	22.146	1.00	51.26
ATOM	1790	O	THR	A	440	23.034	47.376	22.409	1.00	51.18
ATOM	1791	N	ASP	A	441	21.688	46.319	20.927	1.00	50.50
ATOM	1792	CA	ASP	A	441	22.123	47.097	19.784	1.00	50.08
ATOM	1793	CB	ASP	A	441	21.563	46.513	18.471	1.00	50.63

32/75

ATOM	1794	CG	ASP	A	441	22.028	45.084	18.208	1.00	51.46
ATOM	1795	OD1	ASP	A	441	23.107	44.920	17.619	1.00	52.12
ATOM	1796	OD2	ASP	A	441	21.316	44.128	18.587	1.00	54.44
ATOM	1797	C	ASP	A	441	21.683	48.546	19.984	1.00	49.26
ATOM	1798	O	ASP	A	441	22.445	49.468	19.684	1.00	49.06
ATOM	1799	N	LEU	A	442	20.473	48.712	20.527	1.00	48.89
ATOM	1800	CA	LEU	A	442	19.857	50.027	20.831	1.00	48.80
ATOM	1801	CB	LEU	A	442	18.354	49.876	21.069	1.00	47.71
ATOM	1802	CG	LEU	A	442	17.521	49.591	19.826	1.00	47.70
ATOM	1803	CD1	LEU	A	442	16.113	49.251	20.218	1.00	43.13
ATOM	1804	CD2	LEU	A	442	17.525	50.826	18.888	1.00	50.78
ATOM	1805	C	LEU	A	442	20.501	50.795	22.009	1.00	49.12
ATOM	1806	O	LEU	A	442	20.802	51.974	21.858	1.00	49.02
ATOM	1807	N	ARG	A	443	20.724	50.135	23.158	1.00	49.27
ATOM	1808	CA	ARG	A	443	21.468	50.761	24.269	1.00	49.83
ATOM	1809	CB	ARG	A	443	21.561	49.839	25.509	1.00	50.65
ATOM	1810	CG	ARG	A	443	20.423	50.010	26.583	1.00	51.31
ATOM	1811	CD	ARG	A	443	20.911	50.632	27.948	1.00	53.75
ATOM	1812	NE	ARG	A	443	19.803	50.857	28.900	1.00	52.57
ATOM	1813	CZ	ARG	A	443	19.892	51.434	30.103	1.00	53.54
ATOM	1814	NH1	ARG	A	443	21.070	51.853	30.575	1.00	55.29
ATOM	1815	NH2	ARG	A	443	18.794	51.576	30.863	1.00	51.43
ATOM	1816	C	ARG	A	443	22.862	51.289	23.854	1.00	49.39
ATOM	1817	O	ARG	A	443	23.286	52.348	24.304	1.00	49.53
ATOM	1818	N	GLN	A	444	23.554	50.573	22.975	1.00	49.69
ATOM	1819	CA	GLN	A	444	24.902	50.956	22.555	1.00	49.19
ATOM	1820	CB	GLN	A	444	25.636	49.763	21.944	1.00	50.00
ATOM	1821	CG	GLN	A	444	25.852	48.571	22.922	1.00	53.66
ATOM	1822	CD	GLN	A	444	27.096	48.707	23.829	1.00	58.04
ATOM	1823	OE1	GLN	A	444	27.915	49.632	23.671	1.00	60.17
ATOM	1824	NE2	GLN	A	444	27.243	47.766	24.778	1.00	57.23
ATOM	1825	C	GLN	A	444	24.921	52.159	21.607	1.00	48.06
ATOM	1826	O	GLN	A	444	25.884	52.923	21.584	1.00	48.09
ATOM	1827	N	ILE	A	445	23.868	52.309	20.808	1.00	47.30
ATOM	1828	CA	ILE	A	445	23.692	53.482	19.968	1.00	46.26
ATOM	1829	CB	ILE	A	445	22.499	53.302	19.012	1.00	47.23
ATOM	1830	CG1	ILE	A	445	22.804	52.216	17.989	1.00	47.46
ATOM	1831	CD1	ILE	A	445	21.571	51.570	17.525	1.00	51.63
ATOM	1832	CG2	ILE	A	445	22.186	54.585	18.287	1.00	45.76
ATOM	1833	C	ILE	A	445	23.484	54.718	20.857	1.00	45.78
ATOM	1834	O	ILE	A	445	24.135	55.763	20.665	1.00	45.30
ATOM	1835	N	VAL	A	446	22.600	54.575	21.843	1.00	44.47
ATOM	1836	CA	VAL	A	446	22.354	55.628	22.840	1.00	44.43
ATOM	1837	CB	VAL	A	446	21.328	55.177	23.910	1.00	43.76
ATOM	1838	CG1	VAL	A	446	21.173	56.231	24.993	1.00	43.90
ATOM	1839	CG2	VAL	A	446	19.982	54.892	23.242	1.00	43.06
ATOM	1840	C	VAL	A	446	23.652	56.123	23.487	1.00	44.17
ATOM	1841	O	VAL	A	446	23.970	57.314	23.457	1.00	44.40
ATOM	1842	N	THR	A	447	24.414	55.187	24.022	1.00	44.08
ATOM	1843	CA	THR	A	447	25.759	55.461	24.548	1.00	43.97
ATOM	1844	CB	THR	A	447	26.397	54.138	24.971	1.00	44.12
ATOM	1845	OG1	THR	A	447	25.584	53.545	25.997	1.00	43.90
ATOM	1846	CG2	THR	A	447	27.824	54.350	25.495	1.00	44.48
ATOM	1847	C	THR	A	447	26.714	56.234	23.628	1.00	43.95
ATOM	1848	O	THR	A	447	27.376	57.184	24.062	1.00	44.17
ATOM	1849	N	GLU	A	448	26.828	55.818	22.377	1.00	43.92
ATOM	1850	CA	GLU	A	448	27.771	56.456	21.471	1.00	44.16
ATOM	1851	CB	GLU	A	448	27.987	55.604	20.217	1.00	45.03

33/75

ATOM	1852	CG	GLU	A	448	28.957	54.426	20.442	1.00	49.15
ATOM	1853	CD	GLU	A	448	28.691	53.219	19.537	1.00	53.73
ATOM	1854	OE1	GLU	A	448	28.378	53.401	18.332	1.00	53.79
ATOM	1855	OE2	GLU	A	448	28.821	52.081	20.046	1.00	55.80
ATOM	1856	C	GLU	A	448	27.290	57.856	21.132	1.00	43.40
ATOM	1857	O	GLU	A	448	28.090	58.791	21.033	1.00	43.09
ATOM	1858	N	HIS	A	449	25.974	57.995	20.993	1.00	42.13
ATOM	1859	CA	HIS	A	449	25.334	59.278	20.777	1.00	41.64
ATOM	1860	CB	HIS	A	449	23.815	59.089	20.630	1.00	42.56
ATOM	1861	CG	HIS	A	449	23.103	60.291	20.086	1.00	44.28
ATOM	1862	ND1	HIS	A	449	22.344	61.132	20.875	1.00	47.56
ATOM	1863	CE1	HIS	A	449	21.872	62.122	20.138	1.00	45.72
ATOM	1864	NE2	HIS	A	449	22.287	61.946	18.898	1.00	47.75
ATOM	1865	CD2	HIS	A	449	23.062	60.812	18.838	1.00	45.16
ATOM	1866	C	HIS	A	449	25.650	60.266	21.906	1.00	41.30
ATOM	1867	O	HIS	A	449	26.119	61.372	21.636	1.00	41.48
ATOM	1868	N	VAL	A	450	25.421	59.858	23.155	1.00	40.19
ATOM	1869	CA	VAL	A	450	25.528	60.742	24.300	1.00	40.28
ATOM	1870	CB	VAL	A	450	25.037	60.081	25.614	1.00	40.42
ATOM	1871	CG1	VAL	A	450	25.244	61.027	26.783	1.00	42.61
ATOM	1872	CG2	VAL	A	450	23.558	59.706	25.525	1.00	41.68
ATOM	1873	C	VAL	A	450	26.966	61.216	24.452	1.00	40.24
ATOM	1874	O	VAL	A	450	27.212	62.403	24.692	1.00	39.83
ATOM	1875	N	GLN	A	451	27.915	60.298	24.274	1.00	39.87
ATOM	1876	CA	GLN	A	451	29.315	60.687	24.295	1.00	40.45
ATOM	1877	CB	GLN	A	451	30.282	59.505	24.513	1.00	40.60
ATOM	1878	CG	GLN	A	451	29.984	58.216	23.743	1.00	42.28
ATOM	1879	CD	GLN	A	451	31.144	57.230	23.785	1.00	43.08
ATOM	1880	OE1	GLN	A	451	31.674	56.831	22.733	1.00	45.44
ATOM	1881	NE2	GLN	A	451	31.577	56.862	25.006	1.00	43.42
ATOM	1882	C	GLN	A	451	29.682	61.548	23.096	1.00	39.37
ATOM	1883	O	GLN	A	451	30.456	62.457	23.250	1.00	38.91
ATOM	1884	N	LEU	A	452	29.087	61.328	21.922	1.00	38.80
ATOM	1885	CA	LEU	A	452	29.295	62.283	20.833	1.00	38.44
ATOM	1886	CB	LEU	A	452	28.720	61.798	19.503	1.00	39.11
ATOM	1887	CG	LEU	A	452	29.800	61.327	18.522	1.00	40.23
ATOM	1888	CD1	LEU	A	452	29.150	60.753	17.278	1.00	41.22
ATOM	1889	CD2	LEU	A	452	30.813	62.442	18.146	1.00	39.38
ATOM	1890	C	LEU	A	452	28.808	63.700	21.185	1.00	38.35
ATOM	1891	O	LEU	A	452	29.528	64.686	20.937	1.00	38.32
ATOM	1892	N	LEU	A	453	27.631	63.802	21.806	1.00	37.48
ATOM	1893	CA	LEU	A	453	27.143	65.085	22.334	1.00	37.28
ATOM	1894	CB	LEU	A	453	25.804	64.937	23.022	1.00	37.91
ATOM	1895	CG	LEU	A	453	24.546	64.846	22.166	1.00	36.68
ATOM	1896	CD1	LEU	A	453	24.814	64.357	20.808	1.00	37.17
ATOM	1897	CD2	LEU	A	453	23.601	63.941	22.881	1.00	38.38
ATOM	1898	C	LEU	A	453	28.084	65.758	23.308	1.00	37.38
ATOM	1899	O	LEU	A	453	28.296	66.967	23.205	1.00	38.16
ATOM	1900	N	GLN	A	454	28.618	65.005	24.272	1.00	36.98
ATOM	1901	CA	GLN	A	454	29.653	65.549	25.175	1.00	36.82
ATOM	1902	CB	GLN	A	454	30.207	64.485	26.139	1.00	36.61
ATOM	1903	CG	GLN	A	454	29.325	64.152	27.368	1.00	38.54
ATOM	1904	CD	GLN	A	454	29.209	65.305	28.416	1.00	43.55
ATOM	1905	OE1	GLN	A	454	28.112	65.846	28.630	1.00	44.90
ATOM	1906	NE2	GLN	A	454	30.339	65.671	29.071	1.00	41.31
ATOM	1907	C	GLN	A	454	30.784	66.166	24.381	1.00	36.47
ATOM	1908	O	GLN	A	454	31.318	67.190	24.791	1.00	37.24
ATOM	1909	N	VAL	A	455	31.163	65.551	23.255	1.00	36.37

34/75

ATOM	1910	CA	VAL	A	455	32.257	66.088	22.420	1.00	36.92
ATOM	1911	CB	VAL	A	455	32.753	65.083	21.318	1.00	37.17
ATOM	1912	CG1	VAL	A	455	33.687	65.769	20.318	1.00	36.10
ATOM	1913	CG2	VAL	A	455	33.489	63.906	21.948	1.00	37.02
ATOM	1914	C	VAL	A	455	31.883	67.438	21.808	1.00	36.99
ATOM	1915	O	VAL	A	455	32.674	68.386	21.854	1.00	36.30
ATOM	1916	N	ILE	A	456	30.671	67.505	21.256	1.00	37.11
ATOM	1917	CA	ILE	A	456	30.132	68.716	20.626	1.00	37.51
ATOM	1918	CB	ILE	A	456	28.851	68.386	19.863	1.00	37.69
ATOM	1919	CG1	ILE	A	456	29.094	67.268	18.872	1.00	38.74
ATOM	1920	CD1	ILE	A	456	27.821	66.755	18.385	1.00	38.17
ATOM	1921	CG2	ILE	A	456	28.367	69.580	19.066	1.00	38.57
ATOM	1922	C	ILE	A	456	29.775	69.824	21.615	1.00	37.05
ATOM	1923	O	ILE	A	456	29.832	70.998	21.283	1.00	36.94
ATOM	1924	N	LYS	A	457	29.348	69.440	22.809	1.00	36.82
ATOM	1925	CA	LYS	A	457	29.163	70.367	23.902	1.00	36.98
ATOM	1926	CB	LYS	A	457	29.007	69.560	25.206	1.00	37.44
ATOM	1927	CG	LYS	A	457	28.551	70.314	26.453	1.00	38.18
ATOM	1928	CD	LYS	A	457	27.047	70.091	26.725	1.00	41.58
ATOM	1929	CE	LYS	A	457	26.607	70.601	28.110	1.00	40.79
ATOM	1930	NZ	LYS	A	457	27.017	72.029	28.373	1.00	41.54
ATOM	1931	C	LYS	A	457	30.400	71.286	23.961	1.00	36.72
ATOM	1932	O	LYS	A	457	30.271	72.507	24.027	1.00	36.19
ATOM	1933	N	LYS	A	458	31.581	70.674	23.849	1.00	36.49
ATOM	1934	CA	LYS	A	458	32.860	71.310	24.172	1.00	36.74
ATOM	1935	CB	LYS	A	458	33.812	70.273	24.773	1.00	36.22
ATOM	1936	CG	LYS	A	458	33.265	69.603	26.030	1.00	36.80
ATOM	1937	CD	LYS	A	458	34.357	68.925	26.815	1.00	37.24
ATOM	1938	CE	LYS	A	458	33.843	68.363	28.147	1.00	38.23
ATOM	1939	NZ	LYS	A	458	33.109	69.456	29.033	1.00	38.23
ATOM	1940	C	LYS	A	458	33.519	72.050	23.010	1.00	36.78
ATOM	1941	O	LYS	A	458	34.035	73.156	23.191	1.00	37.62
ATOM	1942	N	THR	A	459	33.516	71.449	21.829	1.00	37.60
ATOM	1943	CA	THR	A	459	34.127	72.079	20.649	1.00	38.15
ATOM	1944	CB	THR	A	459	34.639	71.029	19.612	1.00	38.42
ATOM	1945	OG1	THR	A	459	33.541	70.278	19.071	1.00	38.87
ATOM	1946	CG2	THR	A	459	35.633	70.076	20.240	1.00	38.58
ATOM	1947	C	THR	A	459	33.166	73.037	19.943	1.00	38.64
ATOM	1948	O	THR	A	459	33.602	73.908	19.185	1.00	38.51
ATOM	1949	N	GLU	A	460	31.856	72.834	20.158	1.00	39.38
ATOM	1950	CA	GLU	A	460	30.836	73.725	19.603	1.00	40.20
ATOM	1951	CB	GLU	A	460	29.862	72.958	18.675	1.00	40.78
ATOM	1952	CG	GLU	A	460	30.506	72.177	17.489	1.00	40.02
ATOM	1953	CD	GLU	A	460	31.532	73.014	16.704	1.00	40.79
ATOM	1954	OE1	GLU	A	460	32.651	72.481	16.358	1.00	39.36
ATOM	1955	OE2	GLU	A	460	31.241	74.218	16.463	1.00	41.64
ATOM	1956	C	GLU	A	460	30.093	74.521	20.710	1.00	41.04
ATOM	1957	O	GLU	A	460	28.906	74.321	20.950	1.00	40.92
ATOM	1958	N	THR	A	461	30.813	75.441	21.350	1.00	41.93
ATOM	1959	CA	THR	A	461	30.285	76.269	22.455	1.00	43.09
ATOM	1960	CB	THR	A	461	31.379	77.212	23.038	1.00	42.93
ATOM	1961	OG1	THR	A	461	32.112	77.828	21.971	1.00	44.06
ATOM	1962	CG2	THR	A	461	32.353	76.442	23.938	1.00	43.46
ATOM	1963	C	THR	A	461	29.013	77.101	22.146	1.00	43.21
ATOM	1964	O	THR	A	461	28.100	77.236	23.040	1.00	43.11
ATOM	1965	N	ASP	A	462	28.953	77.653	20.904	1.00	43.59
ATOM	1966	CA	ASP	A	462	27.772	78.406	20.493	1.00	44.26
ATOM	1967	CB	ASP	A	462	28.115	79.405	19.393	1.00	44.25

ATOM	1968	CG	ASP	A	462	28.680	78.742	18.145	1.00	44.51
ATOM	1969	OD1	ASP	A	462	29.445	77.710	18.277	1.00	44.62
ATOM	1970	OD2	ASP	A	462	28.376	79.282	17.028	1.00	45.22
ATOM	1971	C	ASP	A	462	26.616	77.529	20.031	1.00	45.30
ATOM	1972	O	ASP	A	462	25.579	78.038	19.610	1.00	45.65
ATOM	1973	N	MET	A	463	26.783	76.218	20.099	1.00	46.01
ATOM	1974	CA	MET	A	463	25.717	75.342	19.673	1.00	47.77
ATOM	1975	CB	MET	A	463	26.272	74.089	19.038	1.00	47.30
ATOM	1976	CG	MET	A	463	25.462	73.649	17.871	1.00	48.60
ATOM	1977	SD	MET	A	463	25.971	72.023	17.354	1.00	50.22
ATOM	1978	CE	MET	A	463	25.086	71.019	18.546	1.00	49.51
ATOM	1979	C	MET	A	463	24.873	74.992	20.860	1.00	47.68
ATOM	1980	O	MET	A	463	25.401	74.764	21.955	1.00	47.50
ATOM	1981	N	SER	A	464	23.563	74.958	20.647	1.00	48.64
ATOM	1982	CA	SER	A	464	22.635	74.699	21.741	1.00	50.13
ATOM	1983	CB	SER	A	464	21.606	75.833	21.884	1.00	50.16
ATOM	1984	OG	SER	A	464	21.377	76.494	20.653	1.00	50.95
ATOM	1985	C	SER	A	464	21.956	73.347	21.634	1.00	50.52
ATOM	1986	O	SER	A	464	21.711	72.855	20.532	1.00	51.96
ATOM	1987	N	LEU	A	465	21.695	72.722	22.778	1.00	50.66
ATOM	1988	CA	LEU	A	465	20.896	71.504	22.806	1.00	51.06
ATOM	1989	CB	LEU	A	465	21.598	70.405	23.599	1.00	51.25
ATOM	1990	CG	LEU	A	465	21.036	68.975	23.509	1.00	51.49
ATOM	1991	CD1	LEU	A	465	21.274	68.296	22.141	1.00	53.84
ATOM	1992	CD2	LEU	A	465	21.644	68.131	24.610	1.00	52.71
ATOM	1993	C	LEU	A	465	19.527	71.815	23.402	1.00	51.21
ATOM	1994	O	LEU	A	465	19.436	72.475	24.446	1.00	51.56
ATOM	1995	N	HIS	A	466	18.470	71.362	22.725	1.00	51.19
ATOM	1996	CA	HIS	A	466	17.091	71.583	23.175	1.00	50.80
ATOM	1997	CB	HIS	A	466	16.097	70.849	22.276	1.00	50.44
ATOM	1998	CG	HIS	A	466	14.689	71.334	22.422	1.00	50.96
ATOM	1999	ND1	HIS	A	466	13.917	71.055	23.529	1.00	51.91
ATOM	2000	CE1	HIS	A	466	12.729	71.617	23.391	1.00	52.42
ATOM	2001	NE2	HIS	A	466	12.705	72.260	22.236	1.00	52.16
ATOM	2002	CD2	HIS	A	466	13.917	72.096	21.610	1.00	51.87
ATOM	2003	C	HIS	A	466	16.943	71.115	24.620	1.00	50.53
ATOM	2004	O	HIS	A	466	17.340	70.000	24.934	1.00	50.62
ATOM	2005	N	PRO	A	467	16.396	71.972	25.508	1.00	50.40
ATOM	2006	CA	PRO	A	467	16.381	71.608	26.943	1.00	50.48
ATOM	2007	CB	PRO	A	467	15.634	72.778	27.602	1.00	50.40
ATOM	2008	CG	PRO	A	467	15.767	73.916	26.642	1.00	50.26
ATOM	2009	CD	PRO	A	467	15.782	73.292	25.272	1.00	50.31
ATOM	2010	C	PRO	A	467	15.679	70.265	27.233	1.00	50.06
ATOM	2011	O	PRO	A	467	16.078	69.529	28.150	1.00	49.57
ATOM	2012	N	LEU	A	468	14.639	69.979	26.452	1.00	50.12
ATOM	2013	CA	LEU	A	468	13.927	68.712	26.517	1.00	50.16
ATOM	2014	CB	LEU	A	468	12.789	68.694	25.496	1.00	49.93
ATOM	2015	CG	LEU	A	468	11.704	67.620	25.496	1.00	49.65
ATOM	2016	CD1	LEU	A	468	12.160	66.437	24.687	1.00	52.07
ATOM	2017	CD2	LEU	A	468	11.298	67.175	26.908	1.00	49.90
ATOM	2018	C	LEU	A	468	14.953	67.604	26.284	1.00	50.43
ATOM	2019	O	LEU	A	468	15.067	66.689	27.101	1.00	50.76
ATOM	2020	N	LEU	A	469	15.741	67.734	25.216	1.00	50.74
ATOM	2021	CA	LEU	A	469	16.843	66.815	24.923	1.00	51.78
ATOM	2022	CB	LEU	A	469	17.469	67.149	23.564	1.00	51.14
ATOM	2023	CG	LEU	A	469	17.074	66.288	22.339	1.00	50.79
ATOM	2024	CD1	LEU	A	469	15.881	65.393	22.548	1.00	46.75
ATOM	2025	CD2	LEU	A	469	16.871	67.164	21.117	1.00	50.65

36/75

ATOM	2026	C	LEU	A	469	17.904	66.797	26.023	1.00	52.96
ATOM	2027	O	LEU	A	469	18.392	65.733	26.402	1.00	52.92
ATOM	2028	N	GLN	A	470	18.238	67.974	26.540	1.00	54.54
ATOM	2029	CA	GLN	A	470	19.190	68.102	27.649	1.00	56.80
ATOM	2030	CB	GLN	A	470	19.478	69.564	27.927	1.00	56.61
ATOM	2031	CG	GLN	A	470	20.851	69.992	27.480	1.00	56.79
ATOM	2032	CD	GLN	A	470	21.112	71.441	27.780	1.00	56.24
ATOM	2033	OE1	GLN	A	470	20.808	71.929	28.879	1.00	53.48
ATOM	2034	NE2	GLN	A	470	21.676	72.148	26.801	1.00	55.27
ATOM	2035	C	GLN	A	470	18.771	67.413	28.957	1.00	58.35
ATOM	2036	O	GLN	A	470	19.608	66.796	29.632	1.00	58.29
ATOM	2037	N	GLU	A	471	17.485	67.527	29.302	1.00	60.46
ATOM	2038	CA	GLU	A	471	16.932	66.885	30.489	1.00	62.17
ATOM	2039	CB	GLU	A	471	15.481	67.302	30.723	1.00	62.45
ATOM	2040	CG	GLU	A	471	14.975	66.960	32.123	1.00	65.24
ATOM	2041	CD	GLU	A	471	13.562	66.384	32.128	1.00	69.46
ATOM	2042	OE1	GLU	A	471	12.646	67.087	32.617	1.00	71.17
ATOM	2043	OE2	GLU	A	471	13.364	65.231	31.654	1.00	70.56
ATOM	2044	C	GLU	A	471	17.032	65.369	30.419	1.00	62.98
ATOM	2045	O	GLU	A	471	17.331	64.738	31.431	1.00	63.14
ATOM	2046	N	ILE	A	472	16.789	64.787	29.245	1.00	64.23
ATOM	2047	CA	ILE	A	472	16.813	63.327	29.118	1.00	66.00
ATOM	2048	CB	ILE	A	472	15.976	62.757	27.901	1.00	65.83
ATOM	2049	CG1	ILE	A	472	16.657	62.980	26.561	1.00	66.06
ATOM	2050	CD1	ILE	A	472	15.667	62.991	25.429	1.00	67.96
ATOM	2051	CG2	ILE	A	472	14.549	63.283	27.881	1.00	64.82
ATOM	2052	C	ILE	A	472	18.229	62.726	29.146	1.00	67.70
ATOM	2053	O	ILE	A	472	18.442	61.642	29.701	1.00	67.87
ATOM	2054	N	TYR	A	473	19.194	63.423	28.560	1.00	69.66
ATOM	2055	CA	TYR	A	473	20.558	62.922	28.556	1.00	71.79
ATOM	2056	CB	TYR	A	473	21.420	63.713	27.572	1.00	72.31
ATOM	2057	CG	TYR	A	473	21.020	63.576	26.111	1.00	73.30
ATOM	2058	CD1	TYR	A	473	20.688	62.336	25.562	1.00	73.01
ATOM	2059	CE1	TYR	A	473	20.341	62.217	24.223	1.00	73.63
ATOM	2060	CZ	TYR	A	473	20.335	63.348	23.412	1.00	73.98
ATOM	2061	OH	TYR	A	473	19.998	63.261	22.070	1.00	74.39
ATOM	2062	CE2	TYR	A	473	20.666	64.583	23.938	1.00	74.04
ATOM	2063	CD2	TYR	A	473	21.014	64.687	25.276	1.00	73.88
ATOM	2064	C	TYR	A	473	21.160	62.974	29.965	1.00	73.04
ATOM	2065	O	TYR	A	473	21.139	64.032	30.614	1.00	73.18
ATOM	2066	N	LYS	A	474	21.668	61.821	30.427	1.00	74.39
ATOM	2067	CA	LYS	A	474	22.366	61.669	31.728	1.00	75.35
ATOM	2068	CB	LYS	A	474	21.357	61.608	32.885	1.00	75.05
ATOM	2069	CG	LYS	A	474	21.839	62.175	34.218	1.00	75.10
ATOM	2070	CD	LYS	A	474	22.472	63.586	34.134	1.00	74.41
ATOM	2071	CE	LYS	A	474	21.762	64.589	33.192	1.00	72.71
ATOM	2072	NZ	LYS	A	474	20.279	64.669	33.296	1.00	70.19
ATOM	2073	C	LYS	A	474	23.267	60.417	31.701	1.00	76.15
ATOM	2074	O	LYS	A	474	22.975	59.397	32.361	1.00	76.33
ATOM	2075	N	ASP	A	475	24.355	60.532	30.924	1.00	76.77
ATOM	2076	CA	ASP	A	475	25.277	59.435	30.571	1.00	77.31
ATOM	2077	CB	ASP	A	475	26.311	59.892	29.513	1.00	77.50
ATOM	2078	CG	ASP	A	475	27.092	61.168	29.918	1.00	78.07
ATOM	2079	OD1	ASP	A	475	28.338	61.085	30.074	1.00	76.95
ATOM	2080	OD2	ASP	A	475	26.469	62.254	30.054	1.00	78.17
ATOM	2081	C	ASP	A	475	25.997	58.746	31.736	1.00	77.67
ATOM	2082	O	ASP	A	475	27.019	59.236	32.247	1.00	77.72
ATOM	2083	N	LEU	A	476	25.454	57.600	32.143	1.00	77.86

37/75

ATOM	2084	CA	LEU	A	476	26.099	56.737	33.131	1.00	77.94
ATOM	2085	CB	LEU	A	476	25.411	56.838	34.512	1.00	77.90
ATOM	2086	CG	LEU	A	476	25.985	57.755	35.625	1.00	78.23
ATOM	2087	CD1	LEU	A	476	25.955	59.269	35.304	1.00	77.58
ATOM	2088	CD2	LEU	A	476	25.287	57.487	36.966	1.00	77.88
ATOM	2089	C	LEU	A	476	26.124	55.306	32.585	1.00	77.86
ATOM	2090	O	LEU	A	476	27.199	54.739	32.364	1.00	77.70
ATOM	2091	OXT	LEU	A	476	25.076	54.706	32.317	1.00	77.71
ATOM	4201	O	DMS	D	1	13.333	56.468	-4.310	1.00	74.31
ATOM	4202	S	DMS	D	1	14.657	56.911	-3.171	1.00	74.75
ATOM	4203	C2	DMS	D	1	15.789	55.516	-2.907	1.00	73.86
ATOM	4204	C1	DMS	D	1	13.851	57.049	-1.562	1.00	73.98
ATOM	4205	C1	E2P	P	2	18.438	60.701	15.328	1.00	41.81
ATOM	4206	C2	E2P	P	2	17.393	61.545	14.537	1.00	43.73
ATOM	4207	C3	E2P	P	2	15.974	61.533	15.164	1.00	42.97
ATOM	4208	C4	E2P	P	2	14.901	61.367	14.075	1.00	42.84
ATOM	4209	C5	E2P	P	2	13.542	60.977	14.669	1.00	41.19
ATOM	4210	C6	E2P	P	2	12.882	59.772	13.934	1.00	39.46
ATOM	4211	O6	E2P	P	2	12.786	58.627	14.748	1.00	43.16
ATOM	4212	C7	E2P	P	2	11.440	60.083	13.736	1.00	39.48
ATOM	4213	C8	E2P	P	2	10.577	59.102	13.316	1.00	38.62
ATOM	4214	C9	E2P	P	2	9.242	59.419	13.145	1.00	39.09
ATOM	4215	C10	E2P	P	2	8.545	60.781	13.374	1.00	38.48
ATOM	4216	C11	E2P	P	2	7.084	60.488	12.988	1.00	36.12
ATOM	4217	C12	E2P	P	2	7.104	59.014	12.603	1.00	39.00
ATOM	4218	O12	E2P	P	2	6.060	58.471	12.260	1.00	40.37
ATOM	4219	C13	E2P	P	2	8.387	58.437	12.710	1.00	38.93
ATOM	4220	C14	E2P	P	2	9.061	57.091	12.466	1.00	39.12
ATOM	4221	C15	E2P	P	2	8.283	56.051	12.041	1.00	38.15
ATOM	4222	C16	E2P	P	2	8.666	54.789	12.456	1.00	37.93
ATOM	4223	C17	E2P	P	2	7.860	53.710	12.034	1.00	42.11
ATOM	4224	C18	E2P	P	2	7.943	52.532	12.969	1.00	38.60

Fig. 1/3

38/75

	Atom				Coordinates			Occ	B
	#	Type	Type	#	X	Y	Z		
ATOM	2092	N	GLU B	207	8.673	19.407	17.391	1.00	56.02
ATOM	2093	CA	GLU B	207	8.392	18.065	17.990	1.00	56.38
ATOM	2094	CB	GLU B	207	9.038	16.975	17.150	1.00	56.62
ATOM	2095	CG	GLU B	207	8.203	16.564	15.957	1.00	58.14
ATOM	2096	CD	GLU B	207	7.096	15.605	16.329	1.00	59.42
ATOM	2097	OE1	GLU B	207	7.156	15.031	17.451	1.00	59.05
ATOM	2098	OE2	GLU B	207	6.175	15.423	15.491	1.00	60.74
ATOM	2099	C	GLU B	207	8.917	17.989	19.415	1.00	56.17
ATOM	2100	O	GLU B	207	10.132	17.955	19.632	1.00	56.32
ATOM	2101	N	SER B	208	7.998	17.941	20.377	1.00	55.60
ATOM	2102	CA	SER B	208	8.318	18.209	21.792	1.00	54.89
ATOM	2103	CB	SER B	208	7.046	18.197	22.649	1.00	54.79
ATOM	2104	OG	SER B	208	6.216	17.107	22.286	1.00	56.29
ATOM	2105	C	SER B	208	9.405	17.319	22.391	1.00	54.09
ATOM	2106	O	SER B	208	10.317	17.816	23.071	1.00	53.82
ATOM	2107	N	ALA B	209	9.308	16.019	22.124	1.00	53.40
ATOM	2108	CA	ALA B	209	10.290	15.023	22.585	1.00	52.95
ATOM	2109	CB	ALA B	209	9.799	13.598	22.288	1.00	52.83
ATOM	2110	C	ALA B	209	11.726	15.220	22.064	1.00	52.21
ATOM	2111	O	ALA B	209	12.682	14.876	22.760	1.00	52.19
ATOM	2112	N	ASP B	210	11.865	15.748	20.847	1.00	51.26
ATOM	2113	CA	ASP B	210	13.162	16.089	20.283	1.00	50.53
ATOM	2114	CB	ASP B	210	13.030	16.534	18.822	1.00	51.57
ATOM	2115	CG	ASP B	210	12.719	15.388	17.857	1.00	52.84
ATOM	2116	OD1	ASP B	210	11.986	14.444	18.216	1.00	55.05
ATOM	2117	OD2	ASP B	210	13.194	15.458	16.700	1.00	55.73
ATOM	2118	C	ASP B	210	13.801	17.232	21.078	1.00	49.67
ATOM	2119	O	ASP B	210	15.009	17.247	21.293	1.00	50.04
ATOM	2120	N	LEU B	211	12.986	18.194	21.493	1.00	48.05
ATOM	2121	CA	LEU B	211	13.464	19.318	22.303	1.00	46.55
ATOM	2122	CB	LEU B	211	12.469	20.482	22.306	1.00	45.22
ATOM	2123	CG	LEU B	211	12.088	21.009	20.918	1.00	43.85
ATOM	2124	CD1	LEU B	211	10.862	21.869	20.944	1.00	40.05
ATOM	2125	CD2	LEU B	211	13.243	21.695	20.220	1.00	42.07
ATOM	2126	C	LEU B	211	13.761	18.851	23.725	1.00	46.41
ATOM	2127	O	LEU B	211	14.718	19.312	24.340	1.00	45.12
ATOM	2128	N	ARG B	212	12.951	17.927	24.244	1.00	46.23
ATOM	2129	CA	ARG B	212	13.241	17.373	25.567	1.00	46.51
ATOM	2130	CB	ARG B	212	12.094	16.550	26.116	1.00	46.63
ATOM	2131	CG	ARG B	212	10.964	17.360	26.730	1.00	49.64
ATOM	2132	CD	ARG B	212	11.233	17.846	28.165	1.00	53.06
ATOM	2133	NE	ARG B	212	11.480	16.755	29.113	1.00	57.61
ATOM	2134	CZ	ARG B	212	12.685	16.436	29.603	1.00	60.17
ATOM	2135	NH1	ARG B	212	13.758	17.140	29.234	1.00	59.31
ATOM	2136	NH2	ARG B	212	12.819	15.418	30.468	1.00	58.88
ATOM	2137	C	ARG B	212	14.517	16.556	25.520	1.00	46.41
ATOM	2138	O	ARG B	212	15.265	16.545	26.482	1.00	46.76
ATOM	2139	N	ALA B	213	14.769	15.882	24.397	1.00	46.11
ATOM	2140	CA	ALA B	213	16.002	15.129	24.222	1.00	44.98
ATOM	2141	CB	ALA B	213	15.946	14.289	22.945	1.00	45.27
ATOM	2142	C	ALA B	213	17.200	16.087	24.212	1.00	45.05
ATOM	2143	O	ALA B	213	18.239	15.826	24.826	1.00	43.95
ATOM	2144	N	LEU B	214	17.040	17.213	23.525	1.00	44.26

39/75

ATOM	2145	CA	LEU	B	214	18.088	18.207	23.483	1.00	43.80
ATOM	2146	CB	LEU	B	214	17.734	19.330	22.523	1.00	43.82
ATOM	2147	CG	LEU	B	214	18.752	20.418	22.217	1.00	42.82
ATOM	2148	CD1	LEU	B	214	20.174	19.904	21.917	1.00	41.04
ATOM	2149	CD2	LEU	B	214	18.173	21.187	21.051	1.00	42.82
ATOM	2150	C	LEU	B	214	18.419	18.754	24.868	1.00	43.29
ATOM	2151	O	LEU	B	214	19.588	18.843	25.187	1.00	43.67
ATOM	2152	N	ALA	B	215	17.401	19.096	25.670	1.00	42.39
ATOM	2153	CA	ALA	B	215	17.598	19.696	26.997	1.00	42.80
ATOM	2154	CB	ALA	B	215	16.274	20.101	27.620	1.00	42.26
ATOM	2155	C	ALA	B	215	18.356	18.762	27.927	1.00	43.43
ATOM	2156	O	ALA	B	215	19.275	19.177	28.632	1.00	44.43
ATOM	2157	N	LYS	B	216	17.990	17.489	27.895	1.00	43.37
ATOM	2158	CA	LYS	B	216	18.646	16.454	28.684	1.00	43.64
ATOM	2159	CB	LYS	B	216	17.868	15.130	28.550	1.00	44.18
ATOM	2160	CG	LYS	B	216	17.743	14.334	29.842	1.00	46.65
ATOM	2161	CD	LYS	B	216	19.059	13.664	30.265	1.00	48.87
ATOM	2162	CE	LYS	B	216	19.010	13.039	31.667	1.00	48.82
ATOM	2163	NZ	LYS	B	216	19.314	14.022	32.766	1.00	51.38
ATOM	2164	C	LYS	B	216	20.102	16.244	28.282	1.00	42.81
ATOM	2165	O	LYS	B	216	20.963	16.049	29.139	1.00	43.03
ATOM	2166	N	HIS	B	217	20.376	16.226	26.981	1.00	42.27
ATOM	2167	CA	HIS	B	217	21.748	16.098	26.505	1.00	42.08
ATOM	2168	CB	HIS	B	217	21.798	16.104	24.967	1.00	43.06
ATOM	2169	CG	HIS	B	217	23.186	16.049	24.413	1.00	41.86
ATOM	2170	ND1	HIS	B	217	23.841	17.164	23.952	1.00	43.21
ATOM	2171	CE1	HIS	B	217	25.049	16.824	23.541	1.00	42.06
ATOM	2172	NE2	HIS	B	217	25.196	15.525	23.706	1.00	44.13
ATOM	2173	CD2	HIS	B	217	24.046	15.018	24.256	1.00	45.26
ATOM	2174	C	HIS	B	217	22.627	17.222	27.059	1.00	41.88
ATOM	2175	O	HIS	B	217	23.729	16.982	27.568	1.00	42.11
ATOM	2176	N	LEU	B	218	22.129	18.451	26.956	1.00	40.18
ATOM	2177	CA	LEU	B	218	22.870	19.625	27.373	1.00	39.21
ATOM	2178	CB	LEU	B	218	22.180	20.906	26.853	1.00	37.78
ATOM	2179	CG	LEU	B	218	22.068	21.110	25.347	1.00	37.22
ATOM	2180	CD1	LEU	B	218	21.154	22.348	25.041	1.00	31.58
ATOM	2181	CD2	LEU	B	218	23.483	21.296	24.802	1.00	30.50
ATOM	2182	C	LEU	B	218	23.027	19.708	28.874	1.00	39.83
ATOM	2183	O	LEU	B	218	24.070	20.127	29.340	1.00	38.39
ATOM	2184	N	TYR	B	219	21.974	19.358	29.624	1.00	41.74
ATOM	2185	CA	TYR	B	219	22.079	19.195	31.079	1.00	43.31
ATOM	2186	CB	TYR	B	219	20.752	18.779	31.729	1.00	44.15
ATOM	2187	CG	TYR	B	219	20.925	18.431	33.203	1.00	45.07
ATOM	2188	CD1	TYR	B	219	21.011	19.439	34.163	1.00	45.57
ATOM	2189	CE1	TYR	B	219	21.191	19.145	35.528	1.00	44.75
ATOM	2190	CZ	TYR	B	219	21.290	17.825	35.938	1.00	45.89
ATOM	2191	OH	TYR	B	219	21.470	17.587	37.292	1.00	47.36
ATOM	2192	CE2	TYR	B	219	21.222	16.776	35.004	1.00	44.11
ATOM	2193	CD2	TYR	B	219	21.048	17.080	33.644	1.00	46.65
ATOM	2194	C	TYR	B	219	23.150	18.151	31.428	1.00	43.89
ATOM	2195	O	TYR	B	219	23.972	18.368	32.325	1.00	44.89
ATOM	2196	N	ASP	B	220	23.131	17.008	30.758	1.00	43.48
ATOM	2197	CA	ASP	B	220	24.188	16.037	30.981	1.00	43.79
ATOM	2198	CB	ASP	B	220	23.885	14.727	30.288	1.00	43.93
ATOM	2199	CG	ASP	B	220	22.775	13.962	30.964	1.00	45.64
ATOM	2200	OD1	ASP	B	220	22.450	14.230	32.143	1.00	45.54
ATOM	2201	OD2	ASP	B	220	22.220	13.069	30.307	1.00	49.06
ATOM	2202	C	ASP	B	220	25.632	16.502	30.716	1.00	43.87

40/75

ATOM	2203	O	ASP	B	220	26.508	16.171	31.476	1.00	44.82
ATOM	2204	N	SER	B	221	25.932	17.244	29.660	1.00	44.05
ATOM	2205	CA	SER	B	221	27.339	17.660	29.537	1.00	43.31
ATOM	2206	CB	SER	B	221	27.788	17.854	28.101	1.00	43.19
ATOM	2207	OG	SER	B	221	26.947	18.753	27.456	1.00	44.60
ATOM	2208	C	SER	B	221	27.721	18.882	30.378	1.00	42.47
ATOM	2209	O	SER	B	221	28.881	19.040	30.702	1.00	41.90
ATOM	2210	N	TYR	B	222	26.753	19.739	30.690	1.00	42.73
ATOM	2211	CA	TYR	B	222	26.939	20.860	31.631	1.00	42.08
ATOM	2212	CB	TYR	B	222	25.601	21.554	31.831	1.00	40.41
ATOM	2213	CG	TYR	B	222	25.481	22.624	32.907	1.00	38.64
ATOM	2214	CD1	TYR	B	222	25.152	22.278	34.225	1.00	40.35
ATOM	2215	CE1	TYR	B	222	25.002	23.247	35.207	1.00	37.99
ATOM	2216	CZ	TYR	B	222	25.090	24.606	34.827	1.00	39.08
ATOM	2217	OH	TYR	B	222	24.895	25.555	35.782	1.00	38.59
ATOM	2218	CE2	TYR	B	222	25.408	24.984	33.540	1.00	34.79
ATOM	2219	CD2	TYR	B	222	25.575	23.992	32.577	1.00	38.40
ATOM	2220	C	TYR	B	222	27.429	20.246	32.938	1.00	42.70
ATOM	2221	O	TYR	B	222	28.454	20.650	33.454	1.00	44.05
ATOM	2222	N	ILE	B	223	26.724	19.240	33.435	1.00	43.08
ATOM	2223	CA	ILE	B	223	27.143	18.510	34.634	1.00	44.04
ATOM	2224	CB	ILE	B	223	26.087	17.423	34.979	1.00	44.22
ATOM	2225	CG1	ILE	B	223	24.798	18.090	35.471	1.00	43.67
ATOM	2226	CD1	ILE	B	223	24.930	18.964	36.700	1.00	43.47
ATOM	2227	CG2	ILE	B	223	26.618	16.370	35.958	1.00	43.42
ATOM	2228	C	ILE	B	223	28.562	17.923	34.593	1.00	44.78
ATOM	2229	O	ILE	B	223	29.236	17.820	35.637	1.00	46.05
ATOM	2230	N	LYS	B	224	29.019	17.510	33.413	1.00	45.54
ATOM	2231	CA	LYS	B	224	30.355	16.907	33.301	1.00	45.63
ATOM	2232	CB	LYS	B	224	30.412	15.913	32.140	1.00	46.41
ATOM	2233	CG	LYS	B	224	29.339	14.821	32.234	1.00	49.06
ATOM	2234	CD	LYS	B	224	29.361	14.039	33.628	1.00	51.92
ATOM	2235	CE	LYS	B	224	28.015	13.302	33.970	1.00	50.56
ATOM	2236	NZ	LYS	B	224	26.746	14.029	33.482	1.00	48.89
ATOM	2237	C	LYS	B	224	31.423	17.976	33.154	1.00	45.41
ATOM	2238	O	LYS	B	224	32.577	17.755	33.512	1.00	45.83
ATOM	2239	N	SER	B	225	31.017	19.139	32.643	1.00	44.28
ATOM	2240	CA	SER	B	225	31.895	20.259	32.350	1.00	43.74
ATOM	2241	CB	SER	B	225	31.329	21.027	31.159	1.00	43.87
ATOM	2242	OG	SER	B	225	31.817	20.425	29.999	1.00	44.91
ATOM	2243	C	SER	B	225	32.102	21.248	33.503	1.00	44.09
ATOM	2244	O	SER	B	225	33.224	21.732	33.708	1.00	43.82
ATOM	2245	N	PHE	B	226	31.012	21.569	34.215	1.00	43.54
ATOM	2246	CA	PHE	B	226	31.042	22.503	35.330	1.00	43.14
ATOM	2247	CB	PHE	B	226	29.955	23.541	35.150	1.00	42.39
ATOM	2248	CG	PHE	B	226	29.970	24.162	33.795	1.00	41.33
ATOM	2249	CD1	PHE	B	226	30.917	25.125	33.474	1.00	41.44
ATOM	2250	CE1	PHE	B	226	30.953	25.702	32.214	1.00	38.85
ATOM	2251	CZ	PHE	B	226	30.060	25.300	31.249	1.00	42.61
ATOM	2252	CE2	PHE	B	226	29.102	24.317	31.538	1.00	39.64
ATOM	2253	CD2	PHE	B	226	29.074	23.751	32.821	1.00	39.92
ATOM	2254	C	PHE	B	226	30.943	21.771	36.661	1.00	44.12
ATOM	2255	O	PHE	B	226	29.837	21.378	37.090	1.00	44.53
ATOM	2256	N	PRO	B	227	32.109	21.565	37.320	1.00	44.48
ATOM	2257	CA	PRO	B	227	32.223	20.815	38.579	1.00	44.61
ATOM	2258	CB	PRO	B	227	33.721	20.953	38.941	1.00	44.41
ATOM	2259	CG	PRO	B	227	34.189	22.151	38.137	1.00	45.35
ATOM	2260	CD	PRO	B	227	33.429	22.048	36.869	1.00	44.69

41/75

ATOM	2261	C	PRO	B	227	31.311	21.320	39.736	1.00	43.88
ATOM	2262	O	PRO	B	227	30.724	20.508	40.453	1.00	43.41
ATOM	2263	N	LEU	B	228	31.192	22.633	39.902	1.00	43.00
ATOM	2264	CA	LEU	B	228	30.386	23.181	40.977	1.00	41.88
ATOM	2265	CB	LEU	B	228	31.045	24.460	41.515	1.00	41.82
ATOM	2266	CG	LEU	B	228	31.149	24.817	42.990	1.00	41.27
ATOM	2267	CD1	LEU	B	228	31.733	26.213	43.122	1.00	40.42
ATOM	2268	CD2	LEU	B	228	29.852	24.719	43.708	1.00	35.77
ATOM	2269	C	LEU	B	228	29.002	23.518	40.423	1.00	42.17
ATOM	2270	O	LEU	B	228	28.796	24.564	39.819	1.00	41.19
ATOM	2271	N	THR	B	229	28.011	22.678	40.658	1.00	42.59
ATOM	2272	CA	THR	B	229	26.697	23.035	40.126	1.00	41.59
ATOM	2273	CB	THR	B	229	25.708	21.870	40.164	1.00	41.45
ATOM	2274	OG1	THR	B	229	25.476	21.460	41.519	1.00	41.06
ATOM	2275	CG2	THR	B	229	26.225	20.716	39.357	1.00	43.89
ATOM	2276	C	THR	B	229	26.091	24.215	40.871	1.00	41.60
ATOM	2277	O	THR	B	229	26.394	24.443	42.027	1.00	39.84
ATOM	2278	N	LYS	B	230	25.188	24.945	40.209	1.00	40.37
ATOM	2279	CA	LYS	B	230	24.346	25.876	40.925	1.00	40.77
ATOM	2280	CB	LYS	B	230	23.399	26.562	39.942	1.00	40.71
ATOM	2281	CG	LYS	B	230	22.183	27.127	40.614	1.00	40.01
ATOM	2282	CD	LYS	B	230	21.625	28.312	39.927	1.00	37.69
ATOM	2283	CE	LYS	B	230	20.780	29.044	40.919	1.00	38.86
ATOM	2284	NZ	LYS	B	230	20.001	30.137	40.291	1.00	37.67
ATOM	2285	C	LYS	B	230	23.573	25.220	42.108	1.00	41.30
ATOM	2286	O	LYS	B	230	23.451	25.818	43.173	1.00	41.39
ATOM	2287	N	ALA	B	231	23.068	23.996	41.941	1.00	41.92
ATOM	2288	CA	ALA	B	231	22.396	23.304	43.054	1.00	43.25
ATOM	2289	CB	ALA	B	231	21.877	21.942	42.639	1.00	42.89
ATOM	2290	C	ALA	B	231	23.343	23.167	44.244	1.00	44.29
ATOM	2291	O	ALA	B	231	22.954	23.413	45.379	1.00	45.10
ATOM	2292	N	LYS	B	232	24.592	22.802	43.953	1.00	45.79
ATOM	2293	CA	LYS	B	232	25.664	22.660	44.931	1.00	46.55
ATOM	2294	CB	LYS	B	232	26.924	22.130	44.236	1.00	46.77
ATOM	2295	CG	LYS	B	232	27.682	21.027	44.977	1.00	50.75
ATOM	2296	CD	LYS	B	232	28.253	21.491	46.344	1.00	53.87
ATOM	2297	CE	LYS	B	232	29.686	21.029	46.496	1.00	53.72
ATOM	2298	NZ	LYS	B	232	29.704	19.596	46.919	1.00	57.28
ATOM	2299	C	LYS	B	232	26.003	23.975	45.616	1.00	46.19
ATOM	2300	O	LYS	B	232	26.080	24.022	46.840	1.00	45.62
ATOM	2301	N	ALA	B	233	26.229	25.018	44.813	1.00	45.48
ATOM	2302	CA	ALA	B	233	26.548	26.356	45.309	1.00	46.07
ATOM	2303	CB	ALA	B	233	26.877	27.293	44.159	1.00	45.35
ATOM	2304	C	ALA	B	233	25.450	26.954	46.175	1.00	47.02
ATOM	2305	O	ALA	B	233	25.752	27.543	47.212	1.00	47.71
ATOM	2306	N	ARG	B	234	24.183	26.821	45.744	1.00	47.87
ATOM	2307	CA	ARG	B	234	23.033	27.264	46.546	1.00	47.90
ATOM	2308	CB	ARG	B	234	21.723	27.089	45.793	1.00	48.32
ATOM	2309	CG	ARG	B	234	21.594	27.968	44.495	1.00	49.17
ATOM	2310	CD	ARG	B	234	21.496	29.461	44.845	1.00	51.95
ATOM	2311	NE	ARG	B	234	22.609	30.224	44.298	1.00	52.30
ATOM	2312	CZ	ARG	B	234	22.774	31.538	44.427	1.00	51.23
ATOM	2313	NH1	ARG	B	234	21.913	32.285	45.130	1.00	48.76
ATOM	2314	NH2	ARG	B	234	23.833	32.096	43.854	1.00	48.07
ATOM	2315	C	ARG	B	234	22.982	26.539	47.880	1.00	48.47
ATOM	2316	O	ARG	B	234	22.887	27.180	48.924	1.00	48.17
ATOM	2317	N	ALA	B	235	23.090	25.211	47.851	1.00	48.56
ATOM	2318	CA	ALA	B	235	23.122	24.426	49.067	1.00	48.69

42/75

ATOM	2319	CB	ALA	B	235	23.382	22.967	48.751	1.00	48.55
ATOM	2320	C	ALA	B	235	24.160	24.974	50.048	1.00	49.15
ATOM	2321	O	ALA	B	235	23.951	24.943	51.247	1.00	49.28
ATOM	2322	N	ILE	B	236	25.261	25.512	49.529	1.00	49.99
ATOM	2323	CA	ILE	B	236	26.304	26.136	50.358	1.00	50.32
ATOM	2324	CB	ILE	B	236	27.665	26.152	49.630	1.00	49.77
ATOM	2325	CG1	ILE	B	236	28.115	24.721	49.329	1.00	49.61
ATOM	2326	CD1	ILE	B	236	29.188	24.588	48.241	1.00	48.20
ATOM	2327	CG2	ILE	B	236	28.685	26.867	50.462	1.00	49.25
ATOM	2328	C	ILE	B	236	25.951	27.551	50.862	1.00	51.32
ATOM	2329	O	ILE	B	236	26.150	27.852	52.035	1.00	50.98
ATOM	2330	N	LEU	B	237	25.413	28.401	49.989	1.00	52.28
ATOM	2331	CA	LEU	B	237	25.227	29.835	50.284	1.00	53.84
ATOM	2332	CB	LEU	B	237	24.836	30.586	49.012	1.00	52.79
ATOM	2333	CG	LEU	B	237	25.950	30.704	47.976	1.00	51.59
ATOM	2334	CD1	LEU	B	237	25.349	30.848	46.622	1.00	49.71
ATOM	2335	CD2	LEU	B	237	26.896	31.847	48.283	1.00	51.53
ATOM	2336	C	LEU	B	237	24.219	30.144	51.407	1.00	55.71
ATOM	2337	O	LEU	B	237	24.116	29.389	52.359	1.00	55.54
ATOM	2338	N	THR	B	238	23.530	31.290	51.288	1.00	58.02
ATOM	2339	CA	THR	B	238	22.252	31.598	51.981	1.00	59.81
ATOM	2340	CB	THR	B	238	21.384	32.647	51.158	1.00	60.27
ATOM	2341	OG1	THR	B	238	21.808	32.686	49.777	1.00	59.87
ATOM	2342	CG2	THR	B	238	21.509	34.055	51.741	1.00	60.56
ATOM	2343	C	THR	B	238	21.432	30.324	52.306	1.00	60.80
ATOM	2344	O	THR	B	238	21.129	30.053	53.484	1.00	61.40
ATOM	2345	N	GLY	B	239	21.090	29.553	51.265	1.00	61.84
ATOM	2346	CA	GLY	B	239	20.712	28.148	51.407	1.00	63.09
ATOM	2347	C	GLY	B	239	21.711	27.461	52.322	1.00	64.44
ATOM	2348	O	GLY	B	239	22.782	27.055	51.880	1.00	64.90
ATOM	2349	N	LYS	B	240	21.348	27.385	53.605	1.00	65.37
ATOM	2350	CA	LYS	B	240	22.151	26.854	54.714	1.00	66.38
ATOM	2351	CB	LYS	B	240	21.207	26.453	55.856	1.00	66.58
ATOM	2352	CG	LYS	B	240	21.851	25.666	57.003	1.00	67.33
ATOM	2353	CD	LYS	B	240	20.824	24.812	57.749	1.00	68.26
ATOM	2354	CE	LYS	B	240	19.652	25.641	58.246	1.00	68.34
ATOM	2355	NZ	LYS	B	240	19.127	25.087	59.515	1.00	69.03
ATOM	2356	C	LYS	B	240	23.061	25.671	54.424	1.00	66.77
ATOM	2357	O	LYS	B	240	24.280	25.811	54.440	1.00	67.13
ATOM	2358	N	THR	B	241	22.444	24.515	54.179	1.00	67.17
ATOM	2359	CA	THR	B	241	23.112	23.205	54.188	1.00	67.46
ATOM	2360	CB	THR	B	241	22.903	22.452	52.846	1.00	67.51
ATOM	2361	OG1	THR	B	241	21.603	22.767	52.328	1.00	67.49
ATOM	2362	CG2	THR	B	241	23.006	20.942	53.040	1.00	67.66
ATOM	2363	C	THR	B	241	24.589	23.259	54.649	1.00	67.42
ATOM	2364	O	THR	B	241	25.521	23.403	53.829	1.00	67.39
ATOM	2365	N	THR	B	242	24.752	23.188	55.978	1.00	67.30
ATOM	2366	CA	THR	B	242	26.055	23.139	56.666	1.00	67.12
ATOM	2367	CB	THR	B	242	26.052	23.872	58.066	1.00	67.48
ATOM	2368	OG1	THR	B	242	25.006	24.855	58.142	1.00	67.67
ATOM	2369	CG2	THR	B	242	27.413	24.524	58.342	1.00	67.43
ATOM	2370	C	THR	B	242	26.535	21.680	56.863	1.00	66.77
ATOM	2371	O	THR	B	242	26.449	21.096	57.970	1.00	66.29
ATOM	2372	N	ASP	B	243	27.014	21.097	55.766	1.00	65.97
ATOM	2373	CA	ASP	B	243	27.741	19.833	55.801	1.00	65.31
ATOM	2374	CB	ASP	B	243	27.525	19.040	54.495	1.00	65.69
ATOM	2375	CG	ASP	B	243	26.111	19.236	53.897	1.00	66.58
ATOM	2376	OD1	ASP	B	243	25.105	19.031	54.623	1.00	66.60

43/75

ATOM	2377	OD2	ASP	B	243	26.016	19.600	52.695	1.00	67.23
ATOM	2378	C	ASP	B	243	29.230	20.171	56.027	1.00	64.40
ATOM	2379	O	ASP	B	243	29.940	19.432	56.723	1.00	64.28
ATOM	2380	N	LYS	B	244	29.675	21.293	55.434	1.00	62.85
ATOM	2381	CA	LYS	B	244	31.001	21.909	55.679	1.00	61.09
ATOM	2382	CB	LYS	B	244	32.138	21.107	55.004	1.00	61.81
ATOM	2383	CG	LYS	B	244	32.252	21.207	53.445	1.00	63.65
ATOM	2384	CD	LYS	B	244	31.481	20.103	52.691	1.00	65.83
ATOM	2385	CE	LYS	B	244	30.122	20.586	52.184	1.00	66.95
ATOM	2386	NZ	LYS	B	244	29.326	19.501	51.530	1.00	67.13
ATOM	2387	C	LYS	B	244	31.033	23.393	55.244	1.00	58.97
ATOM	2388	O	LYS	B	244	31.152	23.694	54.054	1.00	58.83
ATOM	2389	N	SER	B	245	30.918	24.318	56.200	1.00	56.35
ATOM	2390	CA	SER	B	245	30.883	25.761	55.861	1.00	53.64
ATOM	2391	CB	SER	B	245	30.297	26.593	56.992	1.00	53.60
ATOM	2392	OG	SER	B	245	30.525	25.961	58.231	1.00	55.53
ATOM	2393	C	SER	B	245	32.239	26.322	55.397	1.00	50.89
ATOM	2394	O	SER	B	245	33.283	25.910	55.910	1.00	50.86
ATOM	2395	N	PRO	B	246	32.222	27.257	54.412	1.00	47.81
ATOM	2396	CA	PRO	B	246	33.468	27.714	53.830	1.00	45.20
ATOM	2397	CB	PRO	B	246	33.030	28.322	52.502	1.00	44.79
ATOM	2398	CG	PRO	B	246	31.673	28.766	52.701	1.00	45.72
ATOM	2399	CD	PRO	B	246	31.063	27.952	53.811	1.00	47.62
ATOM	2400	C	PRO	B	246	34.175	28.763	54.683	1.00	42.98
ATOM	2401	O	PRO	B	246	33.581	29.328	55.600	1.00	42.02
ATOM	2402	N	PHE	B	247	35.441	29.012	54.361	1.00	41.05
ATOM	2403	CA	PHE	B	247	36.228	30.031	55.033	1.00	39.10
ATOM	2404	CB	PHE	B	247	37.704	29.887	54.654	1.00	39.27
ATOM	2405	CG	PHE	B	247	38.621	30.736	55.474	1.00	39.50
ATOM	2406	CD1	PHE	B	247	39.030	30.321	56.750	1.00	40.57
ATOM	2407	CE1	PHE	B	247	39.878	31.115	57.541	1.00	39.54
ATOM	2408	CZ	PHE	B	247	40.332	32.337	57.051	1.00	39.94
ATOM	2409	CE2	PHE	B	247	39.921	32.764	55.778	1.00	40.31
ATOM	2410	CD2	PHE	B	247	39.077	31.959	54.991	1.00	39.47
ATOM	2411	C	PHE	B	247	35.666	31.350	54.550	1.00	37.55
ATOM	2412	O	PHE	B	247	35.462	31.515	53.365	1.00	37.22
ATOM	2413	N	VAL	B	248	35.377	32.270	55.462	1.00	35.77
ATOM	2414	CA	VAL	B	248	34.800	33.560	55.070	1.00	33.96
ATOM	2415	CB	VAL	B	248	33.577	33.950	55.938	1.00	33.47
ATOM	2416	CG1	VAL	B	248	33.064	35.308	55.557	1.00	32.36
ATOM	2417	CG2	VAL	B	248	32.466	32.914	55.779	1.00	32.47
ATOM	2418	C	VAL	B	248	35.854	34.660	55.063	1.00	33.14
ATOM	2419	O	VAL	B	248	36.601	34.826	56.030	1.00	32.92
ATOM	2420	N	ILE	B	249	35.918	35.385	53.951	1.00	31.85
ATOM	2421	CA	ILE	B	249	36.892	36.450	53.785	1.00	30.85
ATOM	2422	CB	ILE	B	249	37.768	36.229	52.505	1.00	30.79
ATOM	2423	CG1	ILE	B	249	38.762	35.085	52.743	1.00	31.93
ATOM	2424	CD1	ILE	B	249	38.945	34.173	51.559	1.00	32.27
ATOM	2425	CG2	ILE	B	249	38.561	37.489	52.162	1.00	29.65
ATOM	2426	C	ILE	B	249	36.157	37.784	53.781	1.00	29.81
ATOM	2427	O	ILE	B	249	35.433	38.102	52.842	1.00	29.33
ATOM	2428	N	TYR	B	250	36.358	38.556	54.842	1.00	29.03
ATOM	2429	CA	TYR	B	250	35.563	39.747	55.126	1.00	29.20
ATOM	2430	CB	TYR	B	250	34.577	39.452	56.292	1.00	28.09
ATOM	2431	CG	TYR	B	250	35.273	38.977	57.536	1.00	29.29
ATOM	2432	CD1	TYR	B	250	35.764	39.889	58.455	1.00	27.03
ATOM	2433	CE1	TYR	B	250	36.435	39.484	59.574	1.00	28.94
ATOM	2434	CZ	TYR	B	250	36.642	38.155	59.797	1.00	27.64

44/75

ATOM	2435	OH	TYR	B	250	37.318	37.816	60.946	1.00	28.87
ATOM	2436	CE2	TYR	B	250	36.164	37.215	58.927	1.00	26.08
ATOM	2437	CD2	TYR	B	250	35.489	37.625	57.784	1.00	28.78
ATOM	2438	C	TYR	B	250	36.502	40.926	55.464	1.00	29.46
ATOM	2439	O	TYR	B	250	36.052	42.073	55.671	1.00	28.97
ATOM	2440	N	ASP	B	251	37.806	40.611	55.462	1.00	29.62
ATOM	2441	CA	ASP	B	251	38.867	41.399	56.076	1.00	30.71
ATOM	2442	CB	ASP	B	251	39.141	40.905	57.517	1.00	29.79
ATOM	2443	CG	ASP	B	251	38.754	41.887	58.501	1.00	30.58
ATOM	2444	OD1	ASP	B	251	38.117	42.848	58.056	1.00	33.16
ATOM	2445	OD2	ASP	B	251	39.079	41.745	59.697	1.00	32.29
ATOM	2446	C	ASP	B	251	40.181	41.277	55.374	1.00	31.14
ATOM	2447	O	ASP	B	251	40.459	40.250	54.765	1.00	31.44
ATOM	2448	N	MET	B	252	41.024	42.294	55.542	1.00	32.37
ATOM	2449	CA	MET	B	252	42.442	42.157	55.244	1.00	34.15
ATOM	2450	CB	MET	B	252	43.164	43.479	55.494	1.00	35.03
ATOM	2451	CG	MET	B	252	42.740	44.576	54.507	1.00	36.89
ATOM	2452	SD	MET	B	252	43.262	44.220	52.806	1.00	42.53
ATOM	2453	CE	MET	B	252	42.399	45.496	51.863	1.00	39.54
ATOM	2454	C	MET	B	252	43.082	40.979	56.012	1.00	34.60
ATOM	2455	O	MET	B	252	43.878	40.191	55.399	1.00	34.85
ATOM	2456	N	ASN	B	253	42.679	40.807	57.334	1.00	35.80
ATOM	2457	CA	ASN	B	253	43.232	39.652	58.064	1.00	37.47
ATOM	2458	CB	ASN	B	253	43.063	39.801	59.602	1.00	37.23
ATOM	2459	CG	ASN	B	253	44.155	40.804	60.123	1.00	39.50
ATOM	2460	OD1	ASN	B	253	44.463	41.814	59.468	1.00	42.23
ATOM	2461	ND2	ASN	B	253	44.782	40.501	61.397	1.00	40.61
ATOM	2462	C	ASN	B	253	42.687	38.309	57.573	1.00	37.47
ATOM	2463	O	ASN	B	253	43.529	37.371	57.386	1.00	37.91
ATOM	2464	N	SER	B	254	41.258	38.210	57.689	1.00	38.27
ATOM	2465	CA	SER	B	254	40.726	36.910	57.124	1.00	38.53
ATOM	2466	CB	SER	B	254	39.150	36.816	57.085	1.00	38.39
ATOM	2467	OG	SER	B	254	38.606	37.966	56.426	1.00	34.88
ATOM	2468	C	SER	B	254	41.306	36.589	55.724	1.00	39.71
ATOM	2469	O	SER	B	254	41.421	35.415	55.355	1.00	39.54
ATOM	2470	N	LEU	B	255	41.690	37.601	54.946	1.00	41.51
ATOM	2471	CA	LEU	B	255	42.225	37.328	53.599	1.00	43.99
ATOM	2472	CB	LEU	B	255	42.288	38.591	52.736	1.00	43.58
ATOM	2473	CG	LEU	B	255	43.083	38.456	51.436	1.00	43.03
ATOM	2474	CD1	LEU	B	255	42.240	37.832	50.344	1.00	41.59
ATOM	2475	CD2	LEU	B	255	43.608	39.794	51.014	1.00	43.09
ATOM	2476	C	LEU	B	255	43.597	36.661	53.691	1.00	45.76
ATOM	2477	O	LEU	B	255	43.793	35.549	53.180	1.00	45.73
ATOM	2478	N	MET	B	256	44.521	37.352	54.357	1.00	47.81
ATOM	2479	CA	MET	B	256	45.863	36.844	54.607	1.00	50.82
ATOM	2480	CB	MET	B	256	46.693	37.836	55.440	1.00	51.00
ATOM	2481	CG	MET	B	256	46.407	39.341	55.233	1.00	52.70
ATOM	2482	SD	MET	B	256	47.314	40.266	53.950	1.00	55.33
ATOM	2483	CE	MET	B	256	47.967	41.617	54.954	1.00	52.95
ATOM	2484	C	MET	B	256	45.838	35.484	55.317	1.00	52.19
ATOM	2485	O	MET	B	256	46.601	34.591	54.954	1.00	52.72
ATOM	2486	N	MET	B	257	44.977	35.333	56.327	1.00	53.85
ATOM	2487	CA	MET	B	257	44.741	34.021	56.948	1.00	55.47
ATOM	2488	CB	MET	B	257	43.884	34.146	58.213	1.00	55.68
ATOM	2489	CG	MET	B	257	44.546	34.917	59.363	1.00	56.85
ATOM	2490	SD	MET	B	257	45.690	33.955	60.403	1.00	59.25
ATOM	2491	CE	MET	B	257	46.602	35.264	61.235	1.00	57.38
ATOM	2492	C	MET	B	257	44.111	33.017	55.966	1.00	56.45

45/75

ATOM	2493	O	MET	B	257	44.363	31.818	56.050	1.00	56.48
ATOM	2494	N	GLY	B	258	43.322	33.516	55.019	1.00	57.48
ATOM	2495	CA	GLY	B	258	42.604	32.658	54.081	1.00	59.27
ATOM	2496	C	GLY	B	258	43.429	32.130	52.935	1.00	60.46
ATOM	2497	O	GLY	B	258	43.222	31.003	52.483	1.00	60.09
ATOM	2498	N	GLU	B	259	44.349	32.962	52.456	1.00	62.16
ATOM	2499	CA	GLU	B	259	45.350	32.552	51.463	1.00	63.91
ATOM	2500	CB	GLU	B	259	46.321	33.706	51.173	1.00	63.96
ATOM	2501	CG	GLU	B	259	45.803	34.757	50.188	1.00	64.02
ATOM	2502	CD	GLU	B	259	46.850	35.810	49.839	1.00	63.93
ATOM	2503	OE1	GLU	B	259	47.404	36.452	50.765	1.00	62.92
ATOM	2504	OE2	GLU	B	259	47.104	35.998	48.628	1.00	64.46
ATOM	2505	C	GLU	B	259	46.152	31.363	51.984	1.00	64.89
ATOM	2506	O	GLU	B	259	46.466	30.428	51.244	1.00	65.27
ATOM	2507	N	ASP	B	260	46.454	31.424	53.276	1.00	66.06
ATOM	2508	CA	ASP	B	260	47.332	30.492	53.958	1.00	67.13
ATOM	2509	CB	ASP	B	260	47.812	31.131	55.255	1.00	67.04
ATOM	2510	CG	ASP	B	260	49.260	30.856	55.527	1.00	67.31
ATOM	2511	OD1	ASP	B	260	49.776	29.840	55.014	1.00	67.54
ATOM	2512	OD2	ASP	B	260	49.883	31.664	56.246	1.00	67.41
ATOM	2513	C	ASP	B	260	46.654	29.170	54.275	1.00	67.89
ATOM	2514	O	ASP	B	260	47.313	28.139	54.394	1.00	68.03
ATOM	2515	N	LYS	B	261	45.335	29.214	54.423	1.00	68.99
ATOM	2516	CA	LYS	B	261	44.552	28.033	54.772	1.00	70.11
ATOM	2517	CB	LYS	B	261	43.503	28.377	55.842	1.00	70.15
ATOM	2518	CG	LYS	B	261	44.114	29.010	57.108	1.00	70.46
ATOM	2519	CD	LYS	B	261	43.067	29.348	58.177	1.00	70.44
ATOM	2520	CE	LYS	B	261	43.491	30.526	59.087	1.00	70.65
ATOM	2521	NZ	LYS	B	261	44.928	30.525	59.510	1.00	69.27
ATOM	2522	C	LYS	B	261	43.923	27.397	53.531	1.00	70.75
ATOM	2523	O	LYS	B	261	44.048	26.185	53.325	1.00	70.74
ATOM	2524	N	ILE	B	262	43.273	28.219	52.704	1.00	71.45
ATOM	2525	CA	ILE	B	262	42.682	27.758	51.450	1.00	72.32
ATOM	2526	CB	ILE	B	262	41.593	28.757	50.934	1.00	72.16
ATOM	2527	CG1	ILE	B	262	40.300	28.019	50.581	1.00	71.73
ATOM	2528	CD1	ILE	B	262	39.052	28.845	50.826	1.00	69.68
ATOM	2529	CG2	ILE	B	262	42.103	29.650	49.777	1.00	72.44
ATOM	2530	C	ILE	B	262	43.765	27.464	50.391	1.00	73.16
ATOM	2531	O	ILE	B	262	44.905	27.940	50.495	1.00	72.96
ATOM	2532	N	LYS	B	263	43.404	26.664	49.389	1.00	74.33
ATOM	2533	CA	LYS	B	263	44.315	26.325	48.293	1.00	75.11
ATOM	2534	CB	LYS	B	263	43.882	24.999	47.613	1.00	75.24
ATOM	2535	CG	LYS	B	263	44.765	24.503	46.432	1.00	74.68
ATOM	2536	CD	LYS	B	263	46.054	23.780	46.867	1.00	73.83
ATOM	2537	CE	LYS	B	263	47.195	24.751	47.170	1.00	73.49
ATOM	2538	NZ	LYS	B	263	48.526	24.104	47.061	1.00	72.46
ATOM	2539	C	LYS	B	263	44.429	27.470	47.271	1.00	75.56
ATOM	2540	O	LYS	B	263	43.781	27.441	46.213	1.00	75.84
ATOM	2541	N	PHE	B	264	45.236	28.484	47.583	1.00	75.89
ATOM	2542	CA	PHE	B	264	45.557	29.471	46.552	1.00	76.35
ATOM	2543	CB	PHE	B	264	45.306	30.930	46.980	1.00	76.53
ATOM	2544	CG	PHE	B	264	45.336	31.906	45.818	1.00	77.14
ATOM	2545	CD1	PHE	B	264	44.538	31.685	44.676	1.00	77.46
ATOM	2546	CE1	PHE	B	264	44.564	32.567	43.576	1.00	76.24
ATOM	2547	CZ	PHE	B	264	45.396	33.686	43.613	1.00	77.09
ATOM	2548	CE2	PHE	B	264	46.208	33.921	44.748	1.00	77.80
ATOM	2549	CD2	PHE	B	264	46.174	33.028	45.842	1.00	77.65
ATOM	2550	C	PHE	B	264	46.949	29.244	45.932	1.00	76.42

46/75

ATOM	2551	O	PHE	B	264	47.985	29.666	46.470	1.00	76.58
ATOM	2552	N	LYS	B	265	46.934	28.557	44.791	1.00	76.38
ATOM	2553	CA	LYS	B	265	48.115	28.311	43.961	1.00	75.87
ATOM	2554	CB	LYS	B	265	47.767	27.327	42.837	1.00	75.98
ATOM	2555	CG	LYS	B	265	46.282	27.296	42.466	1.00	75.05
ATOM	2556	CD	LYS	B	265	45.935	26.194	41.468	1.00	75.16
ATOM	2557	CE	LYS	B	265	46.659	24.873	41.722	1.00	73.96
ATOM	2558	NZ	LYS	B	265	46.486	24.333	43.093	1.00	74.62
ATOM	2559	C	LYS	B	265	48.706	29.603	43.384	1.00	75.99
ATOM	2560	O	LYS	B	265	48.344	30.034	42.266	1.00	75.62
ATOM	2561	N	HIS	B	266	49.574	30.225	44.192	1.00	75.87
ATOM	2562	CA	HIS	B	266	50.477	31.305	43.769	1.00	75.89
ATOM	2563	CB	HIS	B	266	49.756	32.656	43.639	1.00	75.86
ATOM	2564	CG	HIS	B	266	50.393	33.586	42.645	1.00	75.94
ATOM	2565	ND1	HIS	B	266	51.764	33.730	42.526	1.00	75.58
ATOM	2566	CE1	HIS	B	266	52.032	34.607	41.574	1.00	75.39
ATOM	2567	NE2	HIS	B	266	50.885	35.048	41.077	1.00	75.36
ATOM	2568	CD2	HIS	B	266	49.844	34.425	41.729	1.00	75.64
ATOM	2569	C	HIS	B	266	51.638	31.431	44.752	1.00	75.85
ATOM	2570	O	HIS	B	266	52.799	31.224	44.398	1.00	75.74
ATOM	2571	N	SER	B	274	54.706	43.885	50.601	1.00	53.01
ATOM	2572	CA	SER	B	274	55.692	43.688	49.531	1.00	53.10
ATOM	2573	CB	SER	B	274	56.806	42.736	50.004	1.00	53.24
ATOM	2574	OG	SER	B	274	57.868	42.675	49.073	1.00	52.75
ATOM	2575	C	SER	B	274	55.063	43.211	48.200	1.00	53.06
ATOM	2576	O	SER	B	274	55.781	42.982	47.213	1.00	53.20
ATOM	2577	N	LYS	B	275	53.726	43.101	48.195	1.00	52.45
ATOM	2578	CA	LYS	B	275	52.920	42.592	47.082	1.00	52.02
ATOM	2579	CB	LYS	B	275	53.217	41.088	46.872	1.00	52.15
ATOM	2580	CG	LYS	B	275	52.138	40.219	46.187	1.00	50.97
ATOM	2581	CD	LYS	B	275	52.116	40.341	44.669	1.00	50.80
ATOM	2582	CE	LYS	B	275	51.144	41.427	44.208	1.00	48.45
ATOM	2583	NZ	LYS	B	275	51.704	42.140	42.974	1.00	48.17
ATOM	2584	C	LYS	B	275	51.438	42.861	47.421	1.00	51.75
ATOM	2585	O	LYS	B	275	50.852	42.152	48.243	1.00	52.24
ATOM	2586	N	GLU	B	276	50.839	43.881	46.793	1.00	50.97
ATOM	2587	CA	GLU	B	276	49.605	44.525	47.331	1.00	49.97
ATOM	2588	CB	GLU	B	276	49.584	46.027	47.010	1.00	50.32
ATOM	2589	CG	GLU	B	276	50.450	46.893	47.929	1.00	51.37
ATOM	2590	CD	GLU	B	276	49.949	46.962	49.386	1.00	52.60
ATOM	2591	OE1	GLU	B	276	48.780	46.587	49.670	1.00	52.69
ATOM	2592	OE2	GLU	B	276	50.746	47.398	50.248	1.00	50.82
ATOM	2593	C	GLU	B	276	48.218	43.919	47.044	1.00	48.77
ATOM	2594	O	GLU	B	276	47.865	43.636	45.904	1.00	48.74
ATOM	2595	N	VAL	B	277	47.438	43.788	48.117	1.00	47.23
ATOM	2596	CA	VAL	B	277	46.117	43.125	48.156	1.00	45.71
ATOM	2597	CB	VAL	B	277	45.308	43.586	49.403	1.00	45.76
ATOM	2598	CG1	VAL	B	277	43.928	42.921	49.448	1.00	45.19
ATOM	2599	CG2	VAL	B	277	46.082	43.298	50.677	1.00	45.91
ATOM	2600	C	VAL	B	277	45.211	43.194	46.909	1.00	44.74
ATOM	2601	O	VAL	B	277	44.843	42.154	46.361	1.00	44.70
ATOM	2602	N	ALA	B	278	44.833	44.396	46.476	1.00	43.40
ATOM	2603	CA	ALA	B	278	43.867	44.530	45.378	1.00	42.14
ATOM	2604	CB	ALA	B	278	43.517	45.976	45.138	1.00	41.98
ATOM	2605	C	ALA	B	278	44.330	43.861	44.083	1.00	41.48
ATOM	2606	O	ALA	B	278	43.503	43.370	43.288	1.00	41.15
ATOM	2607	N	ILE	B	279	45.649	43.842	43.897	1.00	40.88
ATOM	2608	CA	ILE	B	279	46.285	43.210	42.749	1.00	40.42

47/75

ATOM	2609	CB	ILE	B	279	47.786	43.617	42.585	1.00	40.33
ATOM	2610	CG1	ILE	B	279	48.049	45.027	43.116	1.00	40.61
ATOM	2611	CD1	ILE	B	279	49.523	45.295	43.456	1.00	40.83
ATOM	2612	CG2	ILE	B	279	48.223	43.498	41.117	1.00	40.73
ATOM	2613	C	ILE	B	279	46.203	41.692	42.836	1.00	39.62
ATOM	2614	O	ILE	B	279	45.882	41.053	41.855	1.00	40.43
ATOM	2615	N	ARG	B	280	46.498	41.117	43.998	1.00	39.17
ATOM	2616	CA	ARG	B	280	46.487	39.670	44.138	1.00	38.40
ATOM	2617	CB	ARG	B	280	47.017	39.225	45.491	1.00	39.06
ATOM	2618	CG	ARG	B	280	48.536	39.234	45.643	1.00	40.22
ATOM	2619	CD	ARG	B	280	48.935	39.818	47.001	1.00	43.76
ATOM	2620	NE	ARG	B	280	48.200	39.258	48.147	1.00	45.10
ATOM	2621	CZ	ARG	B	280	48.157	39.807	49.364	1.00	45.35
ATOM	2622	NH1	ARG	B	280	48.801	40.947	49.612	1.00	44.85
ATOM	2623	NH2	ARG	B	280	47.463	39.216	50.337	1.00	44.62
ATOM	2624	C	ARG	B	280	45.091	39.135	43.957	1.00	37.92
ATOM	2625	O	ARG	B	280	44.939	38.088	43.352	1.00	37.56
ATOM	2626	N	ILE	B	281	44.089	39.850	44.474	1.00	37.76
ATOM	2627	CA	ILE	B	281	42.662	39.481	44.304	1.00	37.56
ATOM	2628	CB	ILE	B	281	41.708	40.389	45.146	1.00	36.98
ATOM	2629	CG1	ILE	B	281	41.880	40.118	46.633	1.00	37.26
ATOM	2630	CD1	ILE	B	281	41.152	41.117	47.542	1.00	37.51
ATOM	2631	CG2	ILE	B	281	40.263	40.119	44.840	1.00	37.06
ATOM	2632	C	ILE	B	281	42.270	39.511	42.821	1.00	38.23
ATOM	2633	O	ILE	B	281	41.657	38.577	42.307	1.00	37.99
ATOM	2634	N	PHE	B	282	42.642	40.587	42.137	1.00	38.95
ATOM	2635	CA	PHE	B	282	42.379	40.732	40.713	1.00	39.86
ATOM	2636	CB	PHE	B	282	42.820	42.125	40.253	1.00	40.45
ATOM	2637	CG	PHE	B	282	42.825	42.309	38.755	1.00	42.46
ATOM	2638	CD1	PHE	B	282	41.764	42.934	38.117	1.00	43.63
ATOM	2639	CE1	PHE	B	282	41.776	43.105	36.749	1.00	43.92
ATOM	2640	CZ	PHE	B	282	42.846	42.652	36.002	1.00	43.86
ATOM	2641	CE2	PHE	B	282	43.919	42.035	36.616	1.00	43.78
ATOM	2642	CD2	PHE	B	282	43.909	41.871	37.984	1.00	44.11
ATOM	2643	C	PHE	B	282	43.050	39.622	39.885	1.00	39.83
ATOM	2644	O	PHE	B	282	42.414	39.029	39.007	1.00	39.35
ATOM	2645	N	GLN	B	283	44.325	39.350	40.167	1.00	40.51
ATOM	2646	CA	GLN	B	283	45.064	38.275	39.504	1.00	40.86
ATOM	2647	CB	GLN	B	283	46.504	38.264	39.972	1.00	41.56
ATOM	2648	CG	GLN	B	283	47.357	39.414	39.447	1.00	41.98
ATOM	2649	CD	GLN	B	283	48.665	39.565	40.200	1.00	41.38
ATOM	2650	OE1	GLN	B	283	48.852	39.011	41.299	1.00	41.16
ATOM	2651	NE2	GLN	B	283	49.585	40.312	39.611	1.00	41.02
ATOM	2652	C	GLN	B	283	44.441	36.907	39.753	1.00	41.48
ATOM	2653	O	GLN	B	283	44.430	36.042	38.870	1.00	41.67
ATOM	2654	N	GLY	B	284	43.915	36.714	40.958	1.00	42.02
ATOM	2655	CA	GLY	B	284	43.174	35.507	41.297	1.00	42.04
ATOM	2656	C	GLY	B	284	41.930	35.386	40.449	1.00	42.39
ATOM	2657	O	GLY	B	284	41.631	34.310	39.942	1.00	42.54
ATOM	2658	N	CYS	B	285	41.194	36.477	40.263	1.00	42.88
ATOM	2659	CA	CYS	B	285	39.998	36.386	39.407	1.00	43.69
ATOM	2660	CB	CYS	B	285	39.056	37.589	39.562	1.00	44.35
ATOM	2661	SG	CYS	B	285	38.141	37.560	41.184	1.00	49.94
ATOM	2662	C	CYS	B	285	40.379	36.118	37.961	1.00	42.98
ATOM	2663	O	CYS	B	285	39.609	35.533	37.238	1.00	43.23
ATOM	2664	N	GLN	B	286	41.586	36.529	37.575	1.00	42.95
ATOM	2665	CA	GLN	B	286	42.171	36.214	36.279	1.00	42.38
ATOM	2666	CB	GLN	B	286	43.541	36.908	36.106	1.00	43.27

48/75

ATOM	2667	CG	GLN	B	286	43.540	38.360	35.611	1.00	43.78
ATOM	2668	CD	GLN	B	286	42.177	38.857	35.185	1.00	44.85
ATOM	2669	OE1	GLN	B	286	41.854	38.900	33.994	1.00	48.29
ATOM	2670	NE2	GLN	B	286	41.357	39.219	36.158	1.00	45.17
ATOM	2671	C	GLN	B	286	42.334	34.719	36.104	1.00	41.38
ATOM	2672	O	GLN	B	286	41.814	34.151	35.146	1.00	41.88
ATOM	2673	N	PHE	B	287	43.069	34.104	37.028	1.00	40.67
ATOM	2674	CA	PHE	B	287	43.330	32.658	37.053	1.00	39.99
ATOM	2675	CB	PHE	B	287	44.003	32.233	38.371	1.00	39.36
ATOM	2676	CG	PHE	B	287	44.463	30.778	38.396	1.00	38.55
ATOM	2677	CD1	PHE	B	287	43.581	29.749	38.743	1.00	38.17
ATOM	2678	CE1	PHE	B	287	44.013	28.406	38.748	1.00	36.93
ATOM	2679	CZ	PHE	B	287	45.357	28.096	38.432	1.00	36.38
ATOM	2680	CE2	PHE	B	287	46.235	29.113	38.095	1.00	36.10
ATOM	2681	CD2	PHE	B	287	45.790	30.442	38.085	1.00	37.41
ATOM	2682	C	PHE	B	287	42.058	31.850	36.902	1.00	40.29
ATOM	2683	O	PHE	B	287	42.012	30.910	36.105	1.00	39.51
ATOM	2684	N	ARG	B	288	41.043	32.206	37.697	1.00	40.34
ATOM	2685	CA	ARG	B	288	39.817	31.435	37.768	1.00	40.39
ATOM	2686	CB	ARG	B	288	39.047	31.715	39.080	1.00	41.51
ATOM	2687	CG	ARG	B	288	39.845	31.547	40.405	1.00	45.39
ATOM	2688	CD	ARG	B	288	39.790	30.139	41.098	1.00	51.17
ATOM	2689	NE	ARG	B	288	38.491	29.948	41.775	1.00	57.12
ATOM	2690	CZ	ARG	B	288	37.837	28.786	41.893	1.00	57.18
ATOM	2691	NH1	ARG	B	288	38.347	27.658	41.401	1.00	60.12
ATOM	2692	NH2	ARG	B	288	36.663	28.754	42.499	1.00	54.82
ATOM	2693	C	ARG	B	288	38.976	31.689	36.518	1.00	40.27
ATOM	2694	O	ARG	B	288	38.203	30.822	36.084	1.00	39.55
ATOM	2695	N	SER	B	289	39.124	32.856	35.899	1.00	39.54
ATOM	2696	CA	SER	B	289	38.306	33.082	34.711	1.00	39.99
ATOM	2697	CB	SER	B	289	37.979	34.565	34.467	1.00	40.02
ATOM	2698	OG	SER	B	289	39.147	35.267	34.159	1.00	43.49
ATOM	2699	C	SER	B	289	38.902	32.349	33.508	1.00	38.62
ATOM	2700	O	SER	B	289	38.171	31.838	32.687	1.00	38.66
ATOM	2701	N	VAL	B	290	40.225	32.264	33.453	1.00	37.85
ATOM	2702	CA	VAL	B	290	40.929	31.430	32.468	1.00	36.48
ATOM	2703	CB	VAL	B	290	42.436	31.709	32.522	1.00	36.43
ATOM	2704	CG1	VAL	B	290	43.251	30.631	31.803	1.00	35.47
ATOM	2705	CG2	VAL	B	290	42.717	33.054	31.888	1.00	36.26
ATOM	2706	C	VAL	B	290	40.630	29.930	32.645	1.00	35.99
ATOM	2707	O	VAL	B	290	40.542	29.209	31.674	1.00	35.63
ATOM	2708	N	GLU	B	291	40.502	29.465	33.883	1.00	35.37
ATOM	2709	CA	GLU	B	291	39.992	28.127	34.154	1.00	35.47
ATOM	2710	CB	GLU	B	291	39.966	27.862	35.644	1.00	35.80
ATOM	2711	CG	GLU	B	291	41.325	27.439	36.257	1.00	32.83
ATOM	2712	CD	GLU	B	291	41.182	27.063	37.714	1.00	34.62
ATOM	2713	OE1	GLU	B	291	40.568	27.830	38.482	1.00	33.58
ATOM	2714	OE2	GLU	B	291	41.730	26.016	38.110	1.00	35.01
ATOM	2715	C	GLU	B	291	38.561	27.992	33.618	1.00	37.38
ATOM	2716	O	GLU	B	291	38.265	27.059	32.894	1.00	38.83
ATOM	2717	N	ALA	B	292	37.677	28.927	33.944	1.00	37.84
ATOM	2718	CA	ALA	B	292	36.301	28.879	33.383	1.00	39.47
ATOM	2719	CB	ALA	B	292	35.445	30.009	33.958	1.00	38.27
ATOM	2720	C	ALA	B	292	36.256	28.873	31.827	1.00	40.00
ATOM	2721	O	ALA	B	292	35.452	28.165	31.223	1.00	41.81
ATOM	2722	N	VAL	B	293	37.127	29.629	31.161	1.00	41.18
ATOM	2723	CA	VAL	B	293	37.158	29.596	29.695	1.00	41.92
ATOM	2724	CB	VAL	B	293	38.341	30.422	29.106	1.00	42.55

49/75

ATOM	2725	CG1	VAL	B	293	38.656	29.991	27.654	1.00	40.08
ATOM	2726	CG2	VAL	B	293	38.032	31.920	29.210	1.00	41.23
ATOM	2727	C	VAL	B	293	37.211	28.164	29.190	1.00	42.50
ATOM	2728	O	VAL	B	293	36.497	27.825	28.250	1.00	43.54
ATOM	2729	N	GLN	B	294	38.056	27.338	29.810	1.00	42.73
ATOM	2730	CA	GLN	B	294	38.323	25.974	29.319	1.00	42.43
ATOM	2731	CB	GLN	B	294	39.666	25.423	29.831	1.00	42.59
ATOM	2732	CG	GLN	B	294	40.009	23.913	29.482	1.00	45.24
ATOM	2733	CD	GLN	B	294	40.320	23.556	27.979	1.00	50.26
ATOM	2734	OE1	GLN	B	294	40.737	22.418	27.694	1.00	46.34
ATOM	2735	NE2	GLN	B	294	40.096	24.507	27.038	1.00	48.41
ATOM	2736	C	GLN	B	294	37.153	25.031	29.571	1.00	41.18
ATOM	2737	O	GLN	B	294	36.899	24.147	28.770	1.00	40.85
ATOM	2738	N	GLU	B	295	36.411	25.272	30.646	1.00	39.70
ATOM	2739	CA	GLU	B	295	35.223	24.511	30.957	1.00	38.10
ATOM	2740	CB	GLU	B	295	34.725	24.913	32.337	1.00	37.85
ATOM	2741	CG	GLU	B	295	35.576	24.400	33.500	1.00	37.31
ATOM	2742	CD	GLU	B	295	35.142	24.981	34.848	1.00	39.55
ATOM	2743	OE1	GLU	B	295	34.410	25.991	34.877	1.00	41.86
ATOM	2744	OE2	GLU	B	295	35.513	24.417	35.904	1.00	44.62
ATOM	2745	C	GLU	B	295	34.132	24.761	29.908	1.00	38.63
ATOM	2746	O	GLU	B	295	33.438	23.809	29.491	1.00	38.63
ATOM	2747	N	ILE	B	296	34.002	26.038	29.499	1.00	37.11
ATOM	2748	CA	ILE	B	296	32.956	26.535	28.568	1.00	37.40
ATOM	2749	CB	ILE	B	296	32.875	28.057	28.610	1.00	35.99
ATOM	2750	CG1	ILE	B	296	32.476	28.515	30.019	1.00	37.72
ATOM	2751	CD1	ILE	B	296	32.842	29.975	30.349	1.00	37.73
ATOM	2752	CG2	ILE	B	296	31.848	28.637	27.576	1.00	37.71
ATOM	2753	C	ILE	B	296	33.229	26.032	27.149	1.00	37.85
ATOM	2754	O	ILE	B	296	32.304	25.651	26.433	1.00	38.37
ATOM	2755	N	THR	B	297	34.518	26.009	26.792	1.00	38.45
ATOM	2756	CA	THR	B	297	35.039	25.512	25.533	1.00	38.85
ATOM	2757	CB	THR	B	297	36.560	25.726	25.505	1.00	38.98
ATOM	2758	OG1	THR	B	297	36.811	27.136	25.458	1.00	36.52
ATOM	2759	CG2	THR	B	297	37.225	25.036	24.289	1.00	39.82
ATOM	2760	C	THR	B	297	34.669	24.048	25.359	1.00	40.13
ATOM	2761	O	THR	B	297	34.232	23.641	24.290	1.00	40.55
ATOM	2762	N	GLU	B	298	34.822	23.286	26.436	1.00	41.16
ATOM	2763	CA	GLU	B	298	34.569	21.858	26.472	1.00	42.24
ATOM	2764	CB	GLU	B	298	35.051	21.273	27.799	1.00	42.55
ATOM	2765	CG	GLU	B	298	35.303	19.754	27.761	1.00	46.91
ATOM	2766	CD	GLU	B	298	34.794	18.998	28.996	1.00	51.31
ATOM	2767	OE1	GLU	B	298	34.791	19.553	30.116	1.00	52.93
ATOM	2768	OE2	GLU	B	298	34.395	17.818	28.840	1.00	54.93
ATOM	2769	C	GLU	B	298	33.067	21.690	26.379	1.00	42.04
ATOM	2770	O	GLU	B	298	32.575	20.844	25.637	1.00	41.50
ATOM	2771	N	TYR	B	299	32.348	22.503	27.150	1.00	41.99
ATOM	2772	CA	TYR	B	299	30.883	22.481	27.121	1.00	41.51
ATOM	2773	CB	TYR	B	299	30.281	23.536	28.040	1.00	41.72
ATOM	2774	CG	TYR	B	299	28.781	23.575	27.972	1.00	37.38
ATOM	2775	CD1	TYR	B	299	28.059	22.476	28.298	1.00	33.44
ATOM	2776	CE1	TYR	B	299	26.707	22.447	28.245	1.00	34.60
ATOM	2777	CZ	TYR	B	299	26.037	23.529	27.816	1.00	37.97
ATOM	2778	OH	TYR	B	299	24.651	23.452	27.783	1.00	40.81
ATOM	2779	CE2	TYR	B	299	26.732	24.683	27.505	1.00	35.01
ATOM	2780	CD2	TYR	B	299	28.109	24.691	27.557	1.00	37.46
ATOM	2781	C	TYR	B	299	30.424	22.650	25.682	1.00	42.25
ATOM	2782	O	TYR	B	299	29.751	21.752	25.145	1.00	42.66

50/75

ATOM	2783	N	ALA	B	300	30.875	23.737	25.035	1.00	41.52
ATOM	2784	CA	ALA	B	300	30.367	24.142	23.711	1.00	41.49
ATOM	2785	CB	ALA	B	300	31.049	25.389	23.218	1.00	40.07
ATOM	2786	C	ALA	B	300	30.509	23.042	22.682	1.00	41.56
ATOM	2787	O	ALA	B	300	29.616	22.810	21.890	1.00	41.75
ATOM	2788	N	LYS	B	301	31.646	22.371	22.702	1.00	41.18
ATOM	2789	CA	LYS	B	301	31.934	21.329	21.742	1.00	41.86
ATOM	2790	CB	LYS	B	301	33.343	20.724	21.959	1.00	41.35
ATOM	2791	CG	LYS	B	301	34.534	21.663	21.616	1.00	40.64
ATOM	2792	CD	LYS	B	301	35.914	20.916	21.892	1.00	42.80
ATOM	2793	CE	LYS	B	301	37.172	21.827	21.663	1.00	43.53
ATOM	2794	NZ	LYS	B	301	38.294	21.259	20.829	1.00	49.34
ATOM	2795	C	LYS	B	301	30.855	20.266	21.785	1.00	41.74
ATOM	2796	O	LYS	B	301	30.625	19.577	20.788	1.00	43.01
ATOM	2797	N	SER	B	302	30.178	20.162	22.925	1.00	42.43
ATOM	2798	CA	SER	B	302	29.160	19.155	23.133	1.00	42.05
ATOM	2799	CB	SER	B	302	29.010	18.868	24.602	1.00	42.41
ATOM	2800	OG	SER	B	302	28.027	19.718	25.146	1.00	44.68
ATOM	2801	C	SER	B	302	27.797	19.579	22.625	1.00	42.02
ATOM	2802	O	SER	B	302	26.875	18.807	22.687	1.00	41.13
ATOM	2803	N	ILE	B	303	27.668	20.813	22.149	1.00	42.29
ATOM	2804	CA	ILE	B	303	26.390	21.329	21.642	1.00	42.05
ATOM	2805	CB	ILE	B	303	26.334	22.857	21.710	1.00	42.00
ATOM	2806	CG1	ILE	B	303	26.487	23.352	23.155	1.00	39.73
ATOM	2807	CD1	ILE	B	303	26.892	24.827	23.242	1.00	39.60
ATOM	2808	CG2	ILE	B	303	25.006	23.397	21.108	1.00	39.86
ATOM	2809	C	ILE	B	303	26.171	20.897	20.186	1.00	42.45
ATOM	2810	O	ILE	B	303	26.993	21.194	19.309	1.00	42.02
ATOM	2811	N	PRO	B	304	25.062	20.192	19.918	1.00	42.91
ATOM	2812	CA	PRO	B	304	24.967	19.565	18.583	1.00	42.85
ATOM	2813	CB	PRO	B	304	23.634	18.807	18.651	1.00	43.41
ATOM	2814	CG	PRO	B	304	23.470	18.535	20.177	1.00	43.22
ATOM	2815	CD	PRO	B	304	23.890	19.864	20.749	1.00	42.52
ATOM	2816	C	PRO	B	304	25.066	20.515	17.399	1.00	42.45
ATOM	2817	O	PRO	B	304	24.355	21.517	17.329	1.00	42.16
ATOM	2818	N	GLY	B	305	25.971	20.198	16.481	1.00	42.27
ATOM	2819	CA	GLY	B	305	26.260	21.081	15.360	1.00	42.13
ATOM	2820	C	GLY	B	305	27.448	22.027	15.531	1.00	41.57
ATOM	2821	O	GLY	B	305	28.039	22.418	14.539	1.00	41.11
ATOM	2822	N	PHE	B	306	27.816	22.360	16.774	1.00	40.91
ATOM	2823	CA	PHE	B	306	28.872	23.376	17.066	1.00	39.51
ATOM	2824	CB	PHE	B	306	29.051	23.604	18.598	1.00	39.22
ATOM	2825	CG	PHE	B	306	30.115	24.648	18.931	1.00	39.04
ATOM	2826	CD1	PHE	B	306	29.831	25.987	18.890	1.00	37.29
ATOM	2827	CE1	PHE	B	306	30.833	26.938	19.114	1.00	35.88
ATOM	2828	CZ	PHE	B	306	32.120	26.541	19.396	1.00	37.51
ATOM	2829	CE2	PHE	B	306	32.403	25.219	19.429	1.00	33.80
ATOM	2830	CD2	PHE	B	306	31.416	24.282	19.195	1.00	35.91
ATOM	2831	C	PHE	B	306	30.199	23.032	16.396	1.00	39.08
ATOM	2832	O	PHE	B	306	30.772	23.848	15.658	1.00	39.28
ATOM	2833	N	VAL	B	307	30.651	21.794	16.590	1.00	38.71
ATOM	2834	CA	VAL	B	307	31.891	21.293	15.964	1.00	39.04
ATOM	2835	CB	VAL	B	307	32.386	19.994	16.649	1.00	38.92
ATOM	2836	CG1	VAL	B	307	32.511	20.232	18.162	1.00	42.00
ATOM	2837	CG2	VAL	B	307	31.480	18.830	16.376	1.00	38.92
ATOM	2838	C	VAL	B	307	31.848	21.085	14.450	1.00	39.10
ATOM	2839	O	VAL	B	307	32.879	21.004	13.801	1.00	39.28
ATOM	2840	N	ASN	B	308	30.650	21.035	13.882	1.00	39.96

51/75

ATOM	2841	CA	ASN	B	308	30.487	20.980	12.435	1.00	38.69
ATOM	2842	CB	ASN	B	308	29.147	20.357	12.102	1.00	39.44
ATOM	2843	CG	ASN	B	308	29.088	18.933	12.543	1.00	40.51
ATOM	2844	OD1	ASN	B	308	28.205	18.548	13.291	1.00	49.78
ATOM	2845	ND2	ASN	B	308	30.062	18.158	12.138	1.00	38.76
ATOM	2846	C	ASN	B	308	30.645	22.313	11.759	1.00	38.50
ATOM	2847	O	ASN	B	308	30.810	22.400	10.536	1.00	37.40
ATOM	2848	N	LEU	B	309	30.630	23.361	12.564	1.00	37.66
ATOM	2849	CA	LEU	B	309	30.748	24.711	12.041	1.00	36.31
ATOM	2850	CB	LEU	B	309	30.420	25.682	13.164	1.00	35.96
ATOM	2851	CG	LEU	B	309	29.034	25.791	13.779	1.00	35.65
ATOM	2852	CD1	LEU	B	309	29.166	26.807	15.021	1.00	30.87
ATOM	2853	CD2	LEU	B	309	27.850	26.191	12.744	1.00	35.54
ATOM	2854	C	LEU	B	309	32.179	24.937	11.591	1.00	36.69
ATOM	2855	O	LEU	B	309	33.087	24.325	12.118	1.00	36.91
ATOM	2856	N	ASP	B	310	32.370	25.789	10.597	1.00	37.55
ATOM	2857	CA	ASP	B	310	33.679	26.312	10.208	1.00	38.15
ATOM	2858	CB	ASP	B	310	33.437	27.535	9.316	1.00	38.21
ATOM	2859	CG	ASP	B	310	34.645	28.421	9.146	1.00	39.19
ATOM	2860	OD1	ASP	B	310	35.187	28.444	8.050	1.00	39.65
ATOM	2861	OD2	ASP	B	310	34.998	29.168	10.066	1.00	42.19
ATOM	2862	C	ASP	B	310	34.519	26.649	11.454	1.00	38.14
ATOM	2863	O	ASP	B	310	34.026	27.225	12.414	1.00	38.60
ATOM	2864	N	LEU	B	311	35.788	26.282	11.447	1.00	39.15
ATOM	2865	CA	LEU	B	311	36.576	26.387	12.677	1.00	39.17
ATOM	2866	CB	LEU	B	311	37.908	25.640	12.534	1.00	39.78
ATOM	2867	CG	LEU	B	311	37.974	24.262	13.209	1.00	38.37
ATOM	2868	CD1	LEU	B	311	37.581	23.225	12.215	1.00	41.93
ATOM	2869	CD2	LEU	B	311	39.416	23.966	13.666	1.00	42.14
ATOM	2870	C	LEU	B	311	36.792	27.836	13.121	1.00	39.15
ATOM	2871	O	LEU	B	311	36.777	28.118	14.294	1.00	38.54
ATOM	2872	N	ASN	B	312	37.004	28.747	12.173	1.00	39.23
ATOM	2873	CA	ASN	B	312	37.159	30.165	12.496	1.00	38.86
ATOM	2874	CB	ASN	B	312	37.460	30.995	11.257	1.00	38.24
ATOM	2875	CG	ASN	B	312	38.887	30.785	10.741	1.00	37.52
ATOM	2876	OD1	ASN	B	312	39.855	31.112	11.418	1.00	39.43
ATOM	2877	ND2	ASN	B	312	39.012	30.258	9.540	1.00	35.12
ATOM	2878	C	ASN	B	312	35.930	30.677	13.219	1.00	39.59
ATOM	2879	O	ASN	B	312	36.054	31.385	14.219	1.00	39.50
ATOM	2880	N	ASP	B	313	34.749	30.255	12.765	1.00	39.83
ATOM	2881	CA	ASP	B	313	33.509	30.593	13.447	1.00	39.53
ATOM	2882	CB	ASP	B	313	32.309	30.174	12.624	1.00	39.83
ATOM	2883	CG	ASP	B	313	32.098	31.078	11.457	1.00	40.82
ATOM	2884	OD1	ASP	B	313	32.890	32.051	11.314	1.00	36.88
ATOM	2885	OD2	ASP	B	313	31.142	30.827	10.698	1.00	38.11
ATOM	2886	C	ASP	B	313	33.367	30.094	14.865	1.00	39.05
ATOM	2887	O	ASP	B	313	32.938	30.846	15.726	1.00	38.51
ATOM	2888	N	GLN	B	314	33.710	28.829	15.112	1.00	39.10
ATOM	2889	CA	GLN	B	314	33.792	28.290	16.486	1.00	37.11
ATOM	2890	CB	GLN	B	314	34.421	26.902	16.440	1.00	38.05
ATOM	2891	CG	GLN	B	314	33.590	25.835	15.766	1.00	35.84
ATOM	2892	CD	GLN	B	314	34.316	24.496	15.811	1.00	37.26
ATOM	2893	OE1	GLN	B	314	34.808	24.094	16.860	1.00	32.58
ATOM	2894	NE2	GLN	B	314	34.388	23.819	14.691	1.00	37.62
ATOM	2895	C	GLN	B	314	34.655	29.182	17.391	1.00	36.33
ATOM	2896	O	GLN	B	314	34.275	29.482	18.523	1.00	34.89
ATOM	2897	N	VAL	B	315	35.830	29.566	16.891	1.00	37.39
ATOM	2898	CA	VAL	B	315	36.751	30.426	17.648	1.00	38.19

52/75

ATOM	2899	CB	VAL	B	315	38.072	30.643	16.924	1.00	39.13
ATOM	2900	CG1	VAL	B	315	38.911	31.763	17.637	1.00	39.50
ATOM	2901	CG2	VAL	B	315	38.872	29.351	16.875	1.00	39.57
ATOM	2902	C	VAL	B	315	36.085	31.769	17.956	1.00	38.35
ATOM	2903	O	VAL	B	315	35.989	32.165	19.134	1.00	38.12
ATOM	2904	N	THR	B	316	35.583	32.427	16.906	1.00	38.07
ATOM	2905	CA	THR	B	316	34.786	33.663	17.038	1.00	38.02
ATOM	2906	CB	THR	B	316	34.235	34.125	15.684	1.00	37.35
ATOM	2907	OG1	THR	B	316	35.321	34.442	14.829	1.00	35.64
ATOM	2908	CG2	THR	B	316	33.371	35.348	15.822	1.00	37.13
ATOM	2909	C	THR	B	316	33.673	33.555	18.065	1.00	38.35
ATOM	2910	O	THR	B	316	33.654	34.335	18.995	1.00	38.55
ATOM	2911	N	LEU	B	317	32.776	32.568	17.947	1.00	38.64
ATOM	2912	CA	LEU	B	317	31.681	32.391	18.928	1.00	38.09
ATOM	2913	CB	LEU	B	317	30.772	31.191	18.557	1.00	38.49
ATOM	2914	CG	LEU	B	317	30.056	31.244	17.204	1.00	37.74
ATOM	2915	CD1	LEU	B	317	29.478	29.869	16.924	1.00	36.71
ATOM	2916	CD2	LEU	B	317	28.969	32.365	17.145	1.00	33.14
ATOM	2917	C	LEU	B	317	32.154	32.263	20.390	1.00	38.39
ATOM	2918	O	LEU	B	317	31.511	32.789	21.314	1.00	37.37
ATOM	2919	N	LEU	B	318	33.283	31.576	20.585	1.00	37.19
ATOM	2920	CA	LEU	B	318	33.837	31.418	21.912	1.00	37.57
ATOM	2921	CB	LEU	B	318	34.790	30.226	21.907	1.00	37.42
ATOM	2922	CG	LEU	B	318	34.430	28.873	22.588	1.00	39.13
ATOM	2923	CD1	LEU	B	318	33.010	28.656	23.074	1.00	40.58
ATOM	2924	CD2	LEU	B	318	34.929	27.710	21.785	1.00	37.92
ATOM	2925	C	LEU	B	318	34.512	32.729	22.391	1.00	36.81
ATOM	2926	O	LEU	B	318	34.271	33.184	23.501	1.00	36.07
ATOM	2927	N	LYS	B	319	35.303	33.340	21.518	1.00	37.15
ATOM	2928	CA	LYS	B	319	35.964	34.608	21.789	1.00	39.69
ATOM	2929	CB	LYS	B	319	36.520	35.216	20.512	1.00	39.48
ATOM	2930	CG	LYS	B	319	37.211	36.515	20.764	1.00	41.29
ATOM	2931	CD	LYS	B	319	37.744	37.098	19.477	1.00	46.26
ATOM	2932	CE	LYS	B	319	38.784	38.183	19.737	1.00	49.52
ATOM	2933	NZ	LYS	B	319	38.497	39.017	20.943	1.00	50.98
ATOM	2934	C	LYS	B	319	35.051	35.636	22.416	1.00	39.90
ATOM	2935	O	LYS	B	319	35.371	36.192	23.455	1.00	38.33
ATOM	2936	N	TYR	B	320	33.914	35.859	21.749	1.00	41.91
ATOM	2937	CA	TYR	B	320	32.884	36.807	22.174	1.00	42.50
ATOM	2938	CB	TYR	B	320	32.158	37.336	20.951	1.00	42.98
ATOM	2939	CG	TYR	B	320	33.039	38.251	20.156	1.00	44.91
ATOM	2940	CD1	TYR	B	320	33.702	37.804	19.013	1.00	44.98
ATOM	2941	CE1	TYR	B	320	34.555	38.645	18.320	1.00	45.34
ATOM	2942	CZ	TYR	B	320	34.748	39.956	18.766	1.00	45.17
ATOM	2943	OH	TYR	B	320	35.571	40.824	18.079	1.00	46.48
ATOM	2944	CE2	TYR	B	320	34.124	40.413	19.887	1.00	44.46
ATOM	2945	CD2	TYR	B	320	33.281	39.558	20.592	1.00	45.62
ATOM	2946	C	TYR	B	320	31.899	36.250	23.182	1.00	42.66
ATOM	2947	O	TYR	B	320	31.241	37.023	23.843	1.00	45.03
ATOM	2948	N	GLY	B	321	31.799	34.931	23.335	1.00	42.16
ATOM	2949	CA	GLY	B	321	30.706	34.345	24.121	1.00	41.46
ATOM	2950	C	GLY	B	321	31.069	34.040	25.569	1.00	41.97
ATOM	2951	O	GLY	B	321	30.225	34.101	26.449	1.00	41.17
ATOM	2952	N	VAL	B	322	32.355	33.741	25.781	1.00	41.03
ATOM	2953	CA	VAL	B	322	32.949	33.274	27.034	1.00	40.87
ATOM	2954	CB	VAL	B	322	34.466	32.914	26.797	1.00	40.71
ATOM	2955	CG1	VAL	B	322	35.378	34.114	26.986	1.00	41.62
ATOM	2956	CG2	VAL	B	322	34.892	31.835	27.650	1.00	41.67

53/75

ATOM	2957	C	VAL	B	322	32.757	34.294	28.155	1.00	40.57
ATOM	2958	O	VAL	B	322	32.534	33.906	29.305	1.00	40.03
ATOM	2959	N	HIS	B	323	32.784	35.586	27.819	1.00	40.42
ATOM	2960	CA	HIS	B	323	32.619	36.627	28.824	1.00	40.71
ATOM	2961	CB	HIS	B	323	32.973	37.987	28.237	1.00	42.95
ATOM	2962	CG	HIS	B	323	34.361	38.442	28.544	1.00	45.96
ATOM	2963	ND1	HIS	B	323	35.450	38.084	27.772	1.00	49.99
ATOM	2964	CE1	HIS	B	323	36.536	38.648	28.268	1.00	51.20
ATOM	2965	NE2	HIS	B	323	36.191	39.349	29.341	1.00	52.92
ATOM	2966	CD2	HIS	B	323	34.836	39.237	29.533	1.00	49.82
ATOM	2967	C	HIS	B	323	31.199	36.663	29.361	1.00	40.34
ATOM	2968	O	HIS	B	323	30.982	36.840	30.558	1.00	42.46
ATOM	2969	N	GLU	B	324	30.219	36.506	28.482	1.00	39.02
ATOM	2970	CA	GLU	B	324	28.823	36.532	28.889	1.00	37.67
ATOM	2971	CB	GLU	B	324	27.909	36.655	27.665	1.00	36.84
ATOM	2972	CG	GLU	B	324	28.025	37.981	26.917	1.00	37.51
ATOM	2973	CD	GLU	B	324	27.422	37.926	25.511	1.00	38.41
ATOM	2974	OE1	GLU	B	324	26.524	37.095	25.251	1.00	37.92
ATOM	2975	OE2	GLU	B	324	27.822	38.732	24.680	1.00	40.88
ATOM	2976	C	GLU	B	324	28.487	35.297	29.685	1.00	37.07
ATOM	2977	O	GLU	B	324	27.768	35.385	30.674	1.00	38.89
ATOM	2978	N	ILE	B	325	28.990	34.141	29.254	1.00	36.00
ATOM	2979	CA	ILE	B	325	28.876	32.894	30.055	1.00	35.28
ATOM	2980	CB	ILE	B	325	29.458	31.677	29.357	1.00	33.69
ATOM	2981	CG1	ILE	B	325	28.895	31.511	27.943	1.00	36.52
ATOM	2982	CD1	ILE	B	325	27.467	31.946	27.829	1.00	35.15
ATOM	2983	CG2	ILE	B	325	29.237	30.372	30.204	1.00	34.59
ATOM	2984	C	ILE	B	325	29.522	33.031	31.442	1.00	35.02
ATOM	2985	O	ILE	B	325	28.909	32.680	32.418	1.00	34.74
ATOM	2986	N	ILE	B	326	30.735	33.575	31.538	1.00	35.72
ATOM	2987	CA	ILE	B	326	31.367	33.762	32.841	1.00	36.01
ATOM	2988	CB	ILE	B	326	32.793	34.423	32.709	1.00	36.21
ATOM	2989	CG1	ILE	B	326	33.802	33.392	32.180	1.00	35.48
ATOM	2990	CD1	ILE	B	326	35.070	34.028	31.615	1.00	35.27
ATOM	2991	CG2	ILE	B	326	33.248	35.036	34.028	1.00	33.82
ATOM	2992	C	ILE	B	326	30.503	34.483	33.859	1.00	37.21
ATOM	2993	O	ILE	B	326	30.274	33.967	34.973	1.00	38.37
ATOM	2994	N	TYR	B	327	29.990	35.657	33.482	1.00	38.62
ATOM	2995	CA	TYR	B	327	29.152	36.441	34.379	1.00	39.38
ATOM	2996	CB	TYR	B	327	29.028	37.890	33.892	1.00	40.75
ATOM	2997	CG	TYR	B	327	30.397	38.513	33.707	1.00	41.97
ATOM	2998	CD1	TYR	B	327	31.350	38.458	34.725	1.00	45.34
ATOM	2999	CE1	TYR	B	327	32.623	38.992	34.546	1.00	46.63
ATOM	3000	CZ	TYR	B	327	32.937	39.594	33.334	1.00	44.96
ATOM	3001	OH	TYR	B	327	34.196	40.155	33.133	1.00	46.45
ATOM	3002	CE2	TYR	B	327	32.007	39.650	32.317	1.00	44.05
ATOM	3003	CD2	TYR	B	327	30.757	39.101	32.502	1.00	42.70
ATOM	3004	C	TYR	B	327	27.798	35.813	34.678	1.00	40.51
ATOM	3005	O	TYR	B	327	27.227	36.047	35.754	1.00	41.42
ATOM	3006	N	THR	B	328	27.310	34.990	33.759	1.00	40.57
ATOM	3007	CA	THR	B	328	26.107	34.209	33.973	1.00	41.70
ATOM	3008	CB	THR	B	328	25.636	33.542	32.642	1.00	41.87
ATOM	3009	OG1	THR	B	328	25.081	34.549	31.776	1.00	43.78
ATOM	3010	CG2	THR	B	328	24.568	32.494	32.912	1.00	40.81
ATOM	3011	C	THR	B	328	26.368	33.125	35.036	1.00	42.11
ATOM	3012	O	THR	B	328	25.559	32.902	35.936	1.00	42.61
ATOM	3013	N	MET	B	329	27.497	32.446	34.931	1.00	41.91
ATOM	3014	CA	MET	B	329	27.749	31.370	35.858	1.00	42.97

54/75

ATOM	3015	CB	MET	B	329	28.627	30.305	35.215	1.00	42.63
ATOM	3016	CG	MET	B	329	28.094	29.814	33.890	1.00	41.92
ATOM	3017	SD	MET	B	329	28.948	28.350	33.261	1.00	48.91
ATOM	3018	CE	MET	B	329	28.265	27.174	34.450	1.00	40.62
ATOM	3019	C	MET	B	329	28.306	31.867	37.181	1.00	41.62
ATOM	3020	O	MET	B	329	28.184	31.195	38.193	1.00	42.28
ATOM	3021	N	LEU	B	330	28.921	33.049	37.165	1.00	40.90
ATOM	3022	CA	LEU	B	330	29.351	33.744	38.380	1.00	38.64
ATOM	3023	CB	LEU	B	330	29.950	35.119	38.043	1.00	39.25
ATOM	3024	CG	LEU	B	330	31.261	35.694	38.644	1.00	40.12
ATOM	3025	CD1	LEU	B	330	31.304	37.251	38.654	1.00	37.50
ATOM	3026	CD2	LEU	B	330	31.617	35.145	40.020	1.00	39.10
ATOM	3027	C	LEU	B	330	28.142	33.971	39.265	1.00	38.26
ATOM	3028	O	LEU	B	330	28.245	33.934	40.483	1.00	37.76
ATOM	3029	N	ALA	B	331	26.998	34.248	38.646	1.00	38.08
ATOM	3030	CA	ALA	B	331	25.793	34.576	39.403	1.00	38.56
ATOM	3031	CB	ALA	B	331	24.700	35.202	38.523	1.00	38.73
ATOM	3032	C	ALA	B	331	25.301	33.387	40.206	1.00	39.08
ATOM	3033	O	ALA	B	331	24.802	33.552	41.317	1.00	39.91
ATOM	3034	N	SER	B	332	25.484	32.181	39.681	1.00	39.58
ATOM	3035	CA	SER	B	332	25.196	30.972	40.447	1.00	40.11
ATOM	3036	CB	SER	B	332	25.489	29.746	39.614	1.00	39.81
ATOM	3037	OG	SER	B	332	24.713	29.798	38.451	1.00	40.48
ATOM	3038	C	SER	B	332	25.982	30.858	41.759	1.00	40.71
ATOM	3039	O	SER	B	332	25.540	30.166	42.659	1.00	40.91
ATOM	3040	N	LEU	B	333	27.140	31.519	41.854	1.00	41.87
ATOM	3041	CA	LEU	B	333	27.964	31.514	43.071	1.00	41.84
ATOM	3042	CB	LEU	B	333	29.460	31.395	42.714	1.00	42.09
ATOM	3043	CG	LEU	B	333	29.952	30.487	41.595	1.00	42.67
ATOM	3044	CD1	LEU	B	333	31.396	30.838	41.250	1.00	40.65
ATOM	3045	CD2	LEU	B	333	29.778	29.027	41.934	1.00	44.22
ATOM	3046	C	LEU	B	333	27.764	32.768	43.936	1.00	42.29
ATOM	3047	O	LEU	B	333	28.424	32.936	44.980	1.00	43.29
ATOM	3048	N	MET	B	334	26.876	33.664	43.505	1.00	41.65
ATOM	3049	CA	MET	B	334	26.603	34.891	44.247	1.00	39.94
ATOM	3050	CB	MET	B	334	26.678	36.080	43.309	1.00	39.93
ATOM	3051	CG	MET	B	334	28.084	36.481	42.979	1.00	39.47
ATOM	3052	SD	MET	B	334	28.075	37.664	41.644	1.00	36.58
ATOM	3053	CE	MET	B	334	29.699	38.399	41.838	1.00	36.75
ATOM	3054	C	MET	B	334	25.245	34.916	44.934	1.00	40.20
ATOM	3055	O	MET	B	334	24.260	34.344	44.425	1.00	40.41
ATOM	3056	N	ASN	B	335	25.227	35.535	46.109	1.00	38.54
ATOM	3057	CA	ASN	B	335	24.039	36.148	46.679	1.00	38.94
ATOM	3058	CB	ASN	B	335	23.593	35.425	47.965	1.00	38.82
ATOM	3059	CG	ASN	B	335	24.599	35.507	49.076	1.00	39.48
ATOM	3060	OD1	ASN	B	335	24.647	34.647	49.953	1.00	38.65
ATOM	3061	ND2	ASN	B	335	25.395	36.552	49.067	1.00	39.66
ATOM	3062	C	ASN	B	335	24.308	37.652	46.891	1.00	37.98
ATOM	3063	O	ASN	B	335	25.406	38.103	46.614	1.00	36.80
ATOM	3064	N	LYS	B	336	23.332	38.410	47.403	1.00	38.54
ATOM	3065	CA	LYS	B	336	23.486	39.861	47.665	1.00	38.41
ATOM	3066	CB	LYS	B	336	22.176	40.472	48.246	1.00	38.84
ATOM	3067	CG	LYS	B	336	21.602	39.748	49.488	1.00	40.06
ATOM	3068	CD	LYS	B	336	20.550	40.529	50.363	1.00	42.06
ATOM	3069	CE	LYS	B	336	19.411	41.328	49.628	1.00	48.11
ATOM	3070	NZ	LYS	B	336	18.883	40.842	48.292	1.00	49.61
ATOM	3071	C	LYS	B	336	24.662	40.243	48.584	1.00	37.46
ATOM	3072	O	LYS	B	336	24.985	41.428	48.710	1.00	37.59

55/75

ATOM	3073	N	ASP	B	337	25.282	39.259	49.237	1.00	36.01
ATOM	3074	CA	ASP	B	337	26.283	39.531	50.291	1.00	35.23
ATOM	3075	CB	ASP	B	337	25.881	38.896	51.620	1.00	34.26
ATOM	3076	CG	ASP	B	337	24.652	39.545	52.241	1.00	35.98
ATOM	3077	OD1	ASP	B	337	24.680	40.747	52.588	1.00	30.49
ATOM	3078	OD2	ASP	B	337	23.656	38.827	52.412	1.00	37.23
ATOM	3079	C	ASP	B	337	27.675	39.026	49.954	1.00	34.66
ATOM	3080	O	ASP	B	337	28.609	39.355	50.648	1.00	33.86
ATOM	3081	N	GLY	B	338	27.831	38.202	48.924	1.00	33.80
ATOM	3082	CA	GLY	B	338	29.176	37.778	48.569	1.00	34.05
ATOM	3083	C	GLY	B	338	29.201	36.740	47.487	1.00	34.61
ATOM	3084	O	GLY	B	338	28.191	36.464	46.900	1.00	33.35
ATOM	3085	N	VAL	B	339	30.377	36.165	47.241	1.00	34.91
ATOM	3086	CA	VAL	B	339	30.573	35.230	46.156	1.00	34.55
ATOM	3087	CB	VAL	B	339	31.248	35.926	44.924	1.00	33.97
ATOM	3088	CG1	VAL	B	339	32.650	36.462	45.288	1.00	34.90
ATOM	3089	CG2	VAL	B	339	31.360	35.001	43.767	1.00	32.12
ATOM	3090	C	VAL	B	339	31.426	34.070	46.676	1.00	35.44
ATOM	3091	O	VAL	B	339	32.398	34.274	47.408	1.00	35.03
ATOM	3092	N	LEU	B	340	31.040	32.856	46.314	1.00	36.11
ATOM	3093	CA	LEU	B	340	31.806	31.687	46.639	1.00	37.39
ATOM	3094	CB	LEU	B	340	31.055	30.422	46.234	1.00	37.21
ATOM	3095	CG	LEU	B	340	29.945	29.953	47.148	1.00	37.61
ATOM	3096	CD1	LEU	B	340	29.183	28.888	46.449	1.00	39.05
ATOM	3097	CD2	LEU	B	340	30.505	29.456	48.530	1.00	37.62
ATOM	3098	C	LEU	B	340	33.125	31.744	45.902	1.00	39.24
ATOM	3099	O	LEU	B	340	33.205	32.247	44.771	1.00	39.14
ATOM	3100	N	ILE	B	341	34.148	31.196	46.548	1.00	40.65
ATOM	3101	CA	ILE	B	341	35.515	31.240	46.069	1.00	42.31
ATOM	3102	CB	ILE	B	341	36.277	32.354	46.861	1.00	42.76
ATOM	3103	CG1	ILE	B	341	36.730	33.461	45.923	1.00	42.62
ATOM	3104	CD1	ILE	B	341	35.581	34.353	45.529	1.00	43.57
ATOM	3105	CG2	ILE	B	341	37.361	31.823	47.870	1.00	40.78
ATOM	3106	C	ILE	B	341	36.116	29.839	46.253	1.00	43.90
ATOM	3107	O	ILE	B	341	35.751	29.118	47.187	1.00	43.99
ATOM	3108	N	SER	B	342	36.973	29.433	45.323	1.00	45.59
ATOM	3109	CA	SER	B	342	37.821	28.254	45.486	1.00	47.33
ATOM	3110	CB	SER	B	342	38.691	28.458	46.723	1.00	47.13
ATOM	3111	OG	SER	B	342	39.871	27.682	46.661	1.00	50.03
ATOM	3112	C	SER	B	342	37.054	26.923	45.562	1.00	48.01
ATOM	3113	O	SER	B	342	37.075	26.261	46.587	1.00	48.32
ATOM	3114	N	GLU	B	343	36.370	26.535	44.489	1.00	49.45
ATOM	3115	CA	GLU	B	343	35.515	25.329	44.502	1.00	50.04
ATOM	3116	CB	GLU	B	343	36.369	24.034	44.680	1.00	51.17
ATOM	3117	CG	GLU	B	343	35.644	22.624	44.489	1.00	52.47
ATOM	3118	CD	GLU	B	343	34.900	22.426	43.116	1.00	56.70
ATOM	3119	OE1	GLU	B	343	35.350	22.961	42.058	1.00	55.15
ATOM	3120	OE2	GLU	B	343	33.854	21.712	43.116	1.00	56.89
ATOM	3121	C	GLU	B	343	34.447	25.498	45.583	1.00	49.95
ATOM	3122	O	GLU	B	343	33.833	24.525	46.062	1.00	50.47
ATOM	3123	N	GLY	B	344	34.225	26.761	45.960	1.00	49.01
ATOM	3124	CA	GLY	B	344	33.267	27.098	46.995	1.00	47.77
ATOM	3125	C	GLY	B	344	33.702	26.731	48.398	1.00	46.58
ATOM	3126	O	GLY	B	344	32.842	26.559	49.266	1.00	46.80
ATOM	3127	N	GLN	B	345	35.022	26.618	48.618	1.00	45.53
ATOM	3128	CA	GLN	B	345	35.598	26.383	49.954	1.00	44.46
ATOM	3129	CB	GLN	B	345	36.983	25.708	49.905	1.00	44.79
ATOM	3130	CG	GLN	B	345	37.213	24.583	48.885	1.00	48.47

56/75

ATOM	3131	CD	GLN	B	345	36.381	23.313	49.109	1.00	52.42
ATOM	3132	OE1	GLN	B	345	35.730	23.132	50.146	1.00	54.54
ATOM	3133	NE2	GLN	B	345	36.413	22.418	48.118	1.00	53.95
ATOM	3134	C	GLN	B	345	35.748	27.692	50.738	1.00	43.01
ATOM	3135	O	GLN	B	345	36.030	27.682	51.945	1.00	42.33
ATOM	3136	N	GLY	B	346	35.608	28.810	50.031	1.00	41.06
ATOM	3137	CA	GLY	B	346	35.638	30.118	50.641	1.00	38.91
ATOM	3138	C	GLY	B	346	34.467	30.948	50.166	1.00	37.56
ATOM	3139	O	GLY	B	346	33.851	30.621	49.179	1.00	37.09
ATOM	3140	N	PHE	B	347	34.189	32.028	50.884	1.00	36.79
ATOM	3141	CA	PHE	B	347	33.192	33.026	50.519	1.00	36.50
ATOM	3142	CB	PHE	B	347	31.976	32.858	51.437	1.00	36.48
ATOM	3143	CG	PHE	B	347	30.870	33.853	51.221	1.00	36.22
ATOM	3144	CD1	PHE	B	347	29.897	33.646	50.242	1.00	36.33
ATOM	3145	CE1	PHE	B	347	28.854	34.562	50.082	1.00	33.47
ATOM	3146	CZ	PHE	B	347	28.764	35.668	50.919	1.00	34.61
ATOM	3147	CE2	PHE	B	347	29.709	35.872	51.893	1.00	33.22
ATOM	3148	CD2	PHE	B	347	30.744	34.955	52.059	1.00	35.88
ATOM	3149	C	PHE	B	347	33.836	34.387	50.729	1.00	36.04
ATOM	3150	O	PHE	B	347	34.303	34.690	51.799	1.00	36.19
ATOM	3151	N	MET	B	348	33.870	35.209	49.702	1.00	36.78
ATOM	3152	CA	MET	B	348	34.415	36.548	49.837	1.00	36.85
ATOM	3153	CB	MET	B	348	35.354	36.856	48.661	1.00	36.82
ATOM	3154	CG	MET	B	348	36.234	38.106	48.873	1.00	37.24
ATOM	3155	SD	MET	B	348	37.464	38.341	47.575	1.00	39.28
ATOM	3156	CE	MET	B	348	38.843	37.343	48.125	1.00	39.56
ATOM	3157	C	MET	B	348	33.240	37.514	49.875	1.00	35.73
ATOM	3158	O	MET	B	348	32.368	37.421	49.039	1.00	35.93
ATOM	3159	N	THR	B	349	33.214	38.433	50.834	1.00	35.47
ATOM	3160	CA	THR	B	349	32.061	39.313	51.003	1.00	34.73
ATOM	3161	CB	THR	B	349	31.965	39.955	52.432	1.00	35.15
ATOM	3162	OG1	THR	B	349	32.929	41.003	52.575	1.00	31.87
ATOM	3163	CG2	THR	B	349	32.148	38.923	53.513	1.00	34.04
ATOM	3164	C	THR	B	349	32.015	40.413	49.967	1.00	35.36
ATOM	3165	O	THR	B	349	33.055	40.895	49.503	1.00	34.89
ATOM	3166	N	ARG	B	350	30.792	40.798	49.607	1.00	35.84
ATOM	3167	CA	ARG	B	350	30.521	41.950	48.756	1.00	36.18
ATOM	3168	CB	ARG	B	350	29.004	42.125	48.614	1.00	36.26
ATOM	3169	CG	ARG	B	350	28.550	43.261	47.726	1.00	36.40
ATOM	3170	CD	ARG	B	350	27.096	43.069	47.340	1.00	39.53
ATOM	3171	NE	ARG	B	350	26.667	44.049	46.346	1.00	40.55
ATOM	3172	CZ	ARG	B	350	25.419	44.187	45.908	1.00	40.78
ATOM	3173	NH1	ARG	B	350	24.455	43.378	46.340	1.00	40.91
ATOM	3174	NH2	ARG	B	350	25.143	45.129	45.025	1.00	38.84
ATOM	3175	C	ARG	B	350	31.158	43.221	49.325	1.00	37.06
ATOM	3176	O	ARG	B	350	31.800	43.961	48.587	1.00	36.84
ATOM	3177	N	GLU	B	351	30.968	43.457	50.632	1.00	38.00
ATOM	3178	CA	GLU	B	351	31.524	44.625	51.373	1.00	39.01
ATOM	3179	CB	GLU	B	351	31.087	44.574	52.862	1.00	39.42
ATOM	3180	CG	GLU	B	351	32.049	45.227	53.927	1.00	45.15
ATOM	3181	CD	GLU	B	351	33.149	44.265	54.526	1.00	50.37
ATOM	3182	OE1	GLU	B	351	32.920	42.965	54.447	1.00	51.16
ATOM	3183	OE2	GLU	B	351	34.239	44.835	55.100	1.00	47.65
ATOM	3184	C	GLU	B	351	33.041	44.724	51.280	1.00	38.11
ATOM	3185	O	GLU	B	351	33.592	45.818	51.159	1.00	38.87
ATOM	3186	N	PHE	B	352	33.707	43.578	51.385	1.00	37.21
ATOM	3187	CA	PHE	B	352	35.151	43.535	51.335	1.00	36.23
ATOM	3188	CB	PHE	B	352	35.695	42.178	51.762	1.00	35.50

57/75

ATOM	3189	CG	PHE	B	352	37.177	42.074	51.613	1.00	35.41
ATOM	3190	CD1	PHE	B	352	38.015	42.970	52.264	1.00	33.86
ATOM	3191	CE1	PHE	B	352	39.393	42.899	52.115	1.00	34.60
ATOM	3192	CZ	PHE	B	352	39.936	41.944	51.292	1.00	34.09
ATOM	3193	CE2	PHE	B	352	39.113	41.059	50.625	1.00	33.66
ATOM	3194	CD2	PHE	B	352	37.738	41.127	50.780	1.00	35.23
ATOM	3195	C	PHE	B	352	35.674	43.896	49.955	1.00	36.33
ATOM	3196	O	PHE	B	352	36.626	44.646	49.847	1.00	35.85
ATOM	3197	N	LEU	B	353	35.047	43.359	48.910	1.00	36.54
ATOM	3198	CA	LEU	B	353	35.445	43.615	47.530	1.00	37.53
ATOM	3199	CB	LEU	B	353	34.635	42.725	46.572	1.00	37.22
ATOM	3200	CG	LEU	B	353	35.211	41.319	46.501	1.00	36.67
ATOM	3201	CD1	LEU	B	353	34.231	40.295	45.900	1.00	34.01
ATOM	3202	CD2	LEU	B	353	36.555	41.388	45.735	1.00	35.33
ATOM	3203	C	LEU	B	353	35.278	45.082	47.158	1.00	38.55
ATOM	3204	O	LEU	B	353	36.128	45.675	46.481	1.00	38.78
ATOM	3205	N	LYS	B	354	34.182	45.657	47.632	1.00	39.24
ATOM	3206	CA	LYS	B	354	33.795	47.008	47.320	1.00	40.36
ATOM	3207	CB	LYS	B	354	32.281	47.172	47.589	1.00	40.34
ATOM	3208	CG	LYS	B	354	31.724	48.600	47.667	1.00	41.18
ATOM	3209	CD	LYS	B	354	30.209	48.667	47.395	1.00	41.63
ATOM	3210	CE	LYS	B	354	29.353	47.988	48.456	1.00	43.83
ATOM	3211	NZ	LYS	B	354	28.044	47.503	47.872	1.00	47.84
ATOM	3212	C	LYS	B	354	34.678	47.955	48.123	1.00	40.59
ATOM	3213	O	LYS	B	354	34.859	49.101	47.736	1.00	41.55
ATOM	3214	N	SER	B	355	35.274	47.452	49.205	1.00	40.91
ATOM	3215	CA	SER	B	355	36.233	48.210	50.025	1.00	40.71
ATOM	3216	CB	SER	B	355	36.409	47.548	51.403	1.00	40.54
ATOM	3217	OG	SER	B	355	37.463	46.603	51.414	1.00	38.25
ATOM	3218	C	SER	B	355	37.617	48.433	49.376	1.00	41.41
ATOM	3219	O	SER	B	355	38.340	49.341	49.770	1.00	41.57
ATOM	3220	N	LEU	B	356	37.976	47.612	48.394	1.00	41.74
ATOM	3221	CA	LEU	B	356	39.314	47.629	47.795	1.00	42.37
ATOM	3222	CB	LEU	B	356	39.443	46.512	46.749	1.00	41.63
ATOM	3223	CG	LEU	B	356	39.332	45.067	47.243	1.00	40.70
ATOM	3224	CD1	LEU	B	356	39.220	44.094	46.096	1.00	39.90
ATOM	3225	CD2	LEU	B	356	40.524	44.718	48.098	1.00	40.07
ATOM	3226	C	LEU	B	356	39.707	48.975	47.171	1.00	43.40
ATOM	3227	O	LEU	B	356	38.839	49.741	46.737	1.00	43.57
ATOM	3228	N	ARG	B	357	41.021	49.232	47.150	1.00	44.57
ATOM	3229	CA	ARG	B	357	41.675	50.391	46.505	1.00	45.50
ATOM	3230	CB	ARG	B	357	43.096	49.999	46.073	1.00	45.74
ATOM	3231	CG	ARG	B	357	44.159	51.157	46.179	1.00	45.41
ATOM	3232	CD	ARG	B	357	45.255	51.044	45.051	1.00	45.54
ATOM	3233	NE	ARG	B	357	45.705	49.499	44.903	1.00	46.27
ATOM	3234	CZ	ARG	B	357	46.759	48.824	45.682	1.00	46.35
ATOM	3235	NH1	ARG	B	357	47.475	49.681	46.667	1.00	46.98
ATOM	3236	NH2	ARG	B	357	47.057	47.503	45.523	1.00	44.35
ATOM	3237	C	ARG	B	357	40.948	50.981	45.290	1.00	46.12
ATOM	3238	O	ARG	B	357	40.320	50.262	44.514	1.00	46.15
ATOM	3239	N	LYS	B	358	41.144	52.284	45.110	1.00	46.89
ATOM	3240	CA	LYS	B	358	40.361	53.179	44.243	1.00	47.41
ATOM	3241	CB	LYS	B	358	40.865	54.625	44.416	1.00	48.00
ATOM	3242	CG	LYS	B	358	40.174	55.452	45.541	1.00	48.68
ATOM	3243	CD	LYS	B	358	40.213	54.809	46.946	1.00	49.85
ATOM	3244	CE	LYS	B	358	38.862	54.136	47.310	1.00	50.43
ATOM	3245	NZ	LYS	B	358	38.850	53.687	48.781	1.00	49.49
ATOM	3246	C	LYS	B	358	40.129	52.878	42.752	1.00	47.49

58/75

ATOM	3247	O	LYS	B	358	39.263	53.519	42.164	1.00	47.85
ATOM	3248	N	PRO	B	359	40.931	51.994	42.109	1.00	47.45
ATOM	3249	CA	PRO	B	359	40.401	51.349	40.879	1.00	47.46
ATOM	3250	CB	PRO	B	359	41.641	51.202	39.993	1.00	47.37
ATOM	3251	CG	PRO	B	359	42.821	51.215	40.961	1.00	47.43
ATOM	3252	CD	PRO	B	359	42.352	51.663	42.331	1.00	47.37
ATOM	3253	C	PRO	B	359	39.683	49.981	41.048	1.00	47.40
ATOM	3254	O	PRO	B	359	38.694	49.714	40.360	1.00	47.53
ATOM	3255	N	PHE	B	360	40.165	49.128	41.956	1.00	47.22
ATOM	3256	CA	PHE	B	360	39.706	47.730	42.032	1.00	46.34
ATOM	3257	CB	PHE	B	360	40.808	46.816	42.586	1.00	45.56
ATOM	3258	CG	PHE	B	360	42.039	46.739	41.731	1.00	44.42
ATOM	3259	CD1	PHE	B	360	42.164	45.763	40.759	1.00	42.46
ATOM	3260	CE1	PHE	B	360	43.309	45.686	39.982	1.00	42.79
ATOM	3261	CZ	PHE	B	360	44.356	46.583	40.185	1.00	42.74
ATOM	3262	CE2	PHE	B	360	44.246	47.554	41.154	1.00	42.67
ATOM	3263	CD2	PHE	B	360	43.096	47.624	41.927	1.00	43.40
ATOM	3264	C	PHE	B	360	38.439	47.513	42.858	1.00	46.67
ATOM	3265	O	PHE	B	360	37.966	46.383	42.977	1.00	46.62
ATOM	3266	N	GLY	B	361	37.896	48.582	43.424	1.00	47.13
ATOM	3267	CA	GLY	B	361	36.753	48.474	44.318	1.00	48.34
ATOM	3268	C	GLY	B	361	35.391	48.528	43.645	1.00	49.32
ATOM	3269	O	GLY	B	361	34.370	48.612	44.320	1.00	49.83
ATOM	3270	N	ASP	B	362	35.364	48.488	42.318	1.00	50.12
ATOM	3271	CA	ASP	B	362	34.097	48.506	41.573	1.00	51.02
ATOM	3272	CB	ASP	B	362	33.712	49.946	41.195	1.00	51.30
ATOM	3273	CG	ASP	B	362	34.910	50.783	40.812	1.00	51.40
ATOM	3274	OD1	ASP	B	362	35.622	50.357	39.879	1.00	51.11
ATOM	3275	OD2	ASP	B	362	35.148	51.849	41.448	1.00	51.80
ATOM	3276	C	ASP	B	362	34.153	47.577	40.357	1.00	51.20
ATOM	3277	O	ASP	B	362	33.334	47.672	39.440	1.00	51.97
ATOM	3278	N	PHE	B	363	35.139	46.679	40.395	1.00	51.04
ATOM	3279	CA	PHE	B	363	35.344	45.558	39.471	1.00	50.58
ATOM	3280	CB	PHE	B	363	36.722	44.922	39.822	1.00	51.48
ATOM	3281	CG	PHE	B	363	37.183	43.781	38.918	1.00	53.53
ATOM	3282	CD1	PHE	B	363	38.030	44.027	37.825	1.00	55.98
ATOM	3283	CE1	PHE	B	363	38.489	42.951	37.003	1.00	55.80
ATOM	3284	CZ	PHE	B	363	38.120	41.617	37.309	1.00	53.61
ATOM	3285	CE2	PHE	B	363	37.316	41.370	38.420	1.00	53.95
ATOM	3286	CD2	PHE	B	363	36.869	42.442	39.227	1.00	53.79
ATOM	3287	C	PHE	B	363	34.185	44.546	39.596	1.00	49.72
ATOM	3288	O	PHE	B	363	33.731	44.022	38.585	1.00	50.21
ATOM	3289	N	MET	B	364	33.701	44.289	40.819	1.00	48.10
ATOM	3290	CA	MET	B	364	32.705	43.228	41.058	1.00	47.26
ATOM	3291	CB	MET	B	364	33.175	42.245	42.151	1.00	47.43
ATOM	3292	CG	MET	B	364	34.291	41.297	41.755	1.00	47.33
ATOM	3293	SD	MET	B	364	33.744	40.005	40.633	1.00	49.28
ATOM	3294	CE	MET	B	364	32.766	39.027	41.734	1.00	48.14
ATOM	3295	C	MET	B	364	31.279	43.693	41.379	1.00	46.42
ATOM	3296	O	MET	B	364	30.336	42.912	41.277	1.00	45.77
ATOM	3297	N	GLU	B	365	31.124	44.954	41.762	1.00	46.15
ATOM	3298	CA	GLU	B	365	29.816	45.491	42.133	1.00	46.17
ATOM	3299	CB	GLU	B	365	29.905	46.959	42.581	1.00	46.53
ATOM	3300	CG	GLU	B	365	29.905	47.142	44.064	1.00	46.25
ATOM	3301	CD	GLU	B	365	28.749	46.442	44.753	1.00	46.94
ATOM	3302	OE1	GLU	B	365	27.584	46.894	44.628	1.00	47.47
ATOM	3303	OE2	GLU	B	365	29.022	45.444	45.446	1.00	45.24
ATOM	3304	C	GLU	B	365	28.761	45.328	41.051	1.00	46.44

59/75

ATOM	3305	O	GLU	B	365	27.654	44.872	41.357	1.00	46.42
ATOM	3306	N	PRO	B	366	29.087	45.703	39.791	1.00	46.31
ATOM	3307	CA	PRO	B	366	28.221	45.421	38.635	1.00	45.88
ATOM	3308	CB	PRO	B	366	29.069	45.891	37.441	1.00	46.00
ATOM	3309	CG	PRO	B	366	29.963	46.931	37.987	1.00	46.20
ATOM	3310	CD	PRO	B	366	30.271	46.497	39.397	1.00	46.28
ATOM	3311	C	PRO	B	366	27.821	43.958	38.430	1.00	45.58
ATOM	3312	O	PRO	B	366	26.704	43.693	37.959	1.00	46.27
ATOM	3313	N	LYS	B	367	28.727	43.023	38.717	1.00	44.47
ATOM	3314	CA	LYS	B	367	28.393	41.595	38.657	1.00	43.52
ATOM	3315	CB	LYS	B	367	29.619	40.692	38.769	1.00	43.41
ATOM	3316	CG	LYS	B	367	30.928	41.283	38.354	1.00	45.59
ATOM	3317	CD	LYS	B	367	30.979	41.831	36.933	1.00	45.36
ATOM	3318	CE	LYS	B	367	32.430	41.973	36.490	1.00	45.44
ATOM	3319	NZ	LYS	B	367	32.614	43.218	35.688	1.00	47.24
ATOM	3320	C	LYS	B	367	27.396	41.252	39.763	1.00	42.89
ATOM	3321	O	LYS	B	367	26.468	40.468	39.527	1.00	42.05
ATOM	3322	N	PHE	B	368	27.575	41.872	40.946	1.00	41.79
ATOM	3323	CA	PHE	B	368	26.650	41.680	42.055	1.00	41.88
ATOM	3324	CB	PHE	B	368	27.149	42.290	43.375	1.00	40.78
ATOM	3325	CG	PHE	B	368	28.134	41.421	44.094	1.00	39.28
ATOM	3326	CD1	PHE	B	368	27.701	40.299	44.783	1.00	37.53
ATOM	3327	CE1	PHE	B	368	28.608	39.489	45.426	1.00	36.01
ATOM	3328	CZ	PHE	B	368	29.971	39.800	45.370	1.00	37.49
ATOM	3329	CE2	PHE	B	368	30.415	40.917	44.678	1.00	37.06
ATOM	3330	CD2	PHE	B	368	29.499	41.712	44.048	1.00	37.62
ATOM	3331	C	PHE	B	368	25.274	42.191	41.739	1.00	42.45
ATOM	3332	O	PHE	B	368	24.288	41.509	42.034	1.00	42.68
ATOM	3333	N	GLU	B	369	25.209	43.377	41.137	1.00	43.03
ATOM	3334	CA	GLU	B	369	23.933	43.990	40.785	1.00	44.09
ATOM	3335	CB	GLU	B	369	24.118	45.412	40.225	1.00	44.23
ATOM	3336	CG	GLU	B	369	24.583	46.424	41.266	1.00	44.47
ATOM	3337	CD	GLU	B	369	24.857	47.798	40.694	1.00	46.42
ATOM	3338	OE1	GLU	B	369	25.888	47.969	40.013	1.00	49.54
ATOM	3339	OE2	GLU	B	369	24.062	48.735	40.951	1.00	51.61
ATOM	3340	C	GLU	B	369	23.190	43.084	39.817	1.00	43.94
ATOM	3341	O	GLU	B	369	22.026	42.795	40.038	1.00	44.29
ATOM	3342	N	PHE	B	370	23.883	42.604	38.784	1.00	43.79
ATOM	3343	CA	PHE	B	370	23.315	41.678	37.797	1.00	43.74
ATOM	3344	CB	PHE	B	370	24.307	41.421	36.642	1.00	43.91
ATOM	3345	CG	PHE	B	370	23.969	40.210	35.793	1.00	44.74
ATOM	3346	CD1	PHE	B	370	22.980	40.277	34.807	1.00	44.32
ATOM	3347	CE1	PHE	B	370	22.650	39.163	34.026	1.00	44.52
ATOM	3348	CZ	PHE	B	370	23.312	37.975	34.224	1.00	43.03
ATOM	3349	CE2	PHE	B	370	24.313	37.893	35.206	1.00	42.72
ATOM	3350	CD2	PHE	B	370	24.644	39.006	35.978	1.00	43.08
ATOM	3351	C	PHE	B	370	22.877	40.366	38.408	1.00	44.13
ATOM	3352	O	PHE	B	370	21.734	39.924	38.175	1.00	44.30
ATOM	3353	N	ALA	B	371	23.775	39.731	39.180	1.00	44.39
ATOM	3354	CA	ALA	B	371	23.493	38.433	39.820	1.00	44.17
ATOM	3355	CB	ALA	B	371	24.669	38.001	40.678	1.00	44.10
ATOM	3356	C	ALA	B	371	22.218	38.441	40.656	1.00	44.87
ATOM	3357	O	ALA	B	371	21.432	37.490	40.640	1.00	44.67
ATOM	3358	N	VAL	B	372	22.032	39.522	41.410	1.00	44.91
ATOM	3359	CA	VAL	B	372	20.878	39.698	42.259	1.00	45.14
ATOM	3360	CB	VAL	B	372	21.058	40.961	43.143	1.00	44.70
ATOM	3361	CG1	VAL	B	372	19.742	41.432	43.701	1.00	46.17
ATOM	3362	CG2	VAL	B	372	22.095	40.696	44.267	1.00	43.30

60/75

ATOM	3363	C	VAL	B	372	19.593	39.742	41.416	1.00	45.75
ATOM	3364	O	VAL	B	372	18.601	39.092	41.743	1.00	46.91
ATOM	3365	N	LYS	B	373	19.633	40.504	40.332	1.00	46.35
ATOM	3366	CA	LYS	B	373	18.535	40.623	39.390	1.00	47.16
ATOM	3367	CB	LYS	B	373	18.794	41.771	38.381	1.00	47.34
ATOM	3368	CG	LYS	B	373	18.833	43.181	39.005	1.00	49.45
ATOM	3369	CD	LYS	B	373	18.674	44.353	37.993	1.00	49.57
ATOM	3370	CE	LYS	B	373	19.878	44.539	37.033	1.00	52.90
ATOM	3371	NZ	LYS	B	373	19.848	45.871	36.309	1.00	52.78
ATOM	3372	C	LYS	B	373	18.299	39.294	38.666	1.00	46.47
ATOM	3373	O	LYS	B	373	17.148	38.840	38.592	1.00	47.11
ATOM	3374	N	PHE	B	374	19.378	38.675	38.175	1.00	44.54
ATOM	3375	CA	PHE	B	374	19.307	37.390	37.431	1.00	44.14
ATOM	3376	CB	PHE	B	374	20.675	37.095	36.794	1.00	43.79
ATOM	3377	CG	PHE	B	374	20.716	35.877	35.877	1.00	42.81
ATOM	3378	CD1	PHE	B	374	20.322	35.968	34.534	1.00	42.87
ATOM	3379	CE1	PHE	B	374	20.406	34.851	33.654	1.00	41.35
ATOM	3380	CZ	PHE	B	374	20.900	33.651	34.140	1.00	41.20
ATOM	3381	CE2	PHE	B	374	21.325	33.561	35.485	1.00	41.54
ATOM	3382	CD2	PHE	B	374	21.244	34.674	36.333	1.00	43.30
ATOM	3383	C	PHE	B	374	18.848	36.213	38.295	1.00	43.92
ATOM	3384	O	PHE	B	374	18.060	35.360	37.839	1.00	44.21
ATOM	3385	N	ASN	B	375	19.316	36.182	39.548	1.00	42.77
ATOM	3386	CA	ASN	B	375	19.049	35.040	40.428	1.00	42.04
ATOM	3387	CB	ASN	B	375	19.989	35.026	41.629	1.00	41.73
ATOM	3388	CG	ASN	B	375	21.363	34.466	41.293	1.00	41.87
ATOM	3389	OD1	ASN	B	375	21.583	33.903	40.224	1.00	39.91
ATOM	3390	ND2	ASN	B	375	22.294	34.617	42.217	1.00	44.23
ATOM	3391	C	ASN	B	375	17.606	34.989	40.861	1.00	41.75
ATOM	3392	O	ASN	B	375	17.085	33.929	41.193	1.00	41.25
ATOM	3393	N	ALA	B	376	16.967	36.157	40.814	1.00	42.01
ATOM	3394	CA	ALA	B	376	15.565	36.341	41.158	1.00	41.81
ATOM	3395	CB	ALA	B	376	15.264	37.818	41.240	1.00	41.68
ATOM	3396	C	ALA	B	376	14.611	35.640	40.171	1.00	41.66
ATOM	3397	O	ALA	B	376	13.396	35.689	40.350	1.00	41.78
ATOM	3398	N	LEU	B	377	15.172	34.993	39.150	1.00	41.38
ATOM	3399	CA	LEU	B	377	14.401	34.212	38.203	1.00	41.37
ATOM	3400	CB	LEU	B	377	14.959	34.369	36.787	1.00	41.30
ATOM	3401	CG	LEU	B	377	15.030	35.742	36.102	1.00	41.30
ATOM	3402	CD1	LEU	B	377	15.782	35.637	34.793	1.00	39.76
ATOM	3403	CD2	LEU	B	377	13.653	36.383	35.857	1.00	41.91
ATOM	3404	C	LEU	B	377	14.394	32.734	38.598	1.00	41.58
ATOM	3405	O	LEU	B	377	13.643	31.923	38.036	1.00	40.97
ATOM	3406	N	GLU	B	378	15.244	32.385	39.558	1.00	41.12
ATOM	3407	CA	GLU	B	378	15.209	31.052	40.181	1.00	41.17
ATOM	3408	CB	GLU	B	378	13.930	30.904	40.988	1.00	41.20
ATOM	3409	CG	GLU	B	378	13.839	32.017	42.029	1.00	43.05
ATOM	3410	CD	GLU	B	378	12.621	31.923	42.945	1.00	45.48
ATOM	3411	OE1	GLU	B	378	12.749	32.301	44.121	1.00	46.78
ATOM	3412	OE2	GLU	B	378	11.537	31.494	42.496	1.00	49.74
ATOM	3413	C	GLU	B	378	15.347	30.001	39.105	1.00	40.98
ATOM	3414	O	GLU	B	378	14.618	29.042	39.033	1.00	41.53
ATOM	3415	N	LEU	B	379	16.276	30.258	38.204	1.00	41.67
ATOM	3416	CA	LEU	B	379	16.604	29.327	37.160	1.00	41.14
ATOM	3417	CB	LEU	B	379	17.471	30.057	36.167	1.00	41.61
ATOM	3418	CG	LEU	B	379	16.988	30.468	34.793	1.00	41.36
ATOM	3419	CD1	LEU	B	379	15.661	31.138	34.821	1.00	37.01
ATOM	3420	CD2	LEU	B	379	18.043	31.344	34.226	1.00	41.46

61/75

ATOM	3421	C	LEU	B	379	17.419	28.247	37.831	1.00	41.60
ATOM	3422	O	LEU	B	379	18.054	28.483	38.859	1.00	40.85
ATOM	3423	N	ASP	B	380	17.401	27.051	37.268	1.00	42.33
ATOM	3424	CA	ASP	B	380	18.257	26.002	37.800	1.00	42.36
ATOM	3425	CB	ASP	B	380	17.438	24.855	38.421	1.00	43.32
ATOM	3426	CG	ASP	B	380	16.494	24.216	37.450	1.00	44.46
ATOM	3427	OD1	ASP	B	380	16.860	24.110	36.266	1.00	43.99
ATOM	3428	OD2	ASP	B	380	15.367	23.850	37.878	1.00	48.64
ATOM	3429	C	ASP	B	380	19.224	25.556	36.721	1.00	41.60
ATOM	3430	O	ASP	B	380	19.256	26.126	35.625	1.00	42.00
ATOM	3431	N	ASP	B	381	20.052	24.580	37.052	1.00	41.01
ATOM	3432	CA	ASP	B	381	21.091	24.088	36.157	1.00	39.94
ATOM	3433	CB	ASP	B	381	21.839	22.927	36.859	1.00	40.43
ATOM	3434	CG	ASP	B	381	22.673	23.404	38.027	1.00	40.36
ATOM	3435	OD1	ASP	B	381	22.422	22.950	39.144	1.00	40.39
ATOM	3436	OD2	ASP	B	381	23.545	24.281	37.827	1.00	40.61
ATOM	3437	C	ASP	B	381	20.590	23.588	34.813	1.00	38.82
ATOM	3438	O	ASP	B	381	21.266	23.738	33.817	1.00	37.90
ATOM	3439	N	SER	B	382	19.447	22.912	34.788	1.00	39.95
ATOM	3440	CA	SER	B	382	18.943	22.346	33.531	1.00	41.58
ATOM	3441	CB	SER	B	382	17.806	21.343	33.799	1.00	42.16
ATOM	3442	OG	SER	B	382	16.812	21.935	34.656	1.00	45.29
ATOM	3443	C	SER	B	382	18.476	23.487	32.625	1.00	41.51
ATOM	3444	O	SER	B	382	18.533	23.375	31.398	1.00	42.37
ATOM	3445	N	ASP	B	383	18.012	24.573	33.259	1.00	41.81
ATOM	3446	CA	ASP	B	383	17.617	25.841	32.590	1.00	40.93
ATOM	3447	CB	ASP	B	383	16.944	26.811	33.552	1.00	40.34
ATOM	3448	CG	ASP	B	383	15.637	26.274	34.144	1.00	41.50
ATOM	3449	OD1	ASP	B	383	14.915	25.503	33.494	1.00	41.14
ATOM	3450	OD2	ASP	B	383	15.303	26.633	35.278	1.00	40.09
ATOM	3451	C	ASP	B	383	18.901	26.479	32.052	1.00	40.70
ATOM	3452	O	ASP	B	383	19.041	26.646	30.855	1.00	40.33
ATOM	3453	N	LEU	B	384	19.849	26.797	32.937	1.00	40.80
ATOM	3454	CA	LEU	B	384	21.155	27.366	32.520	1.00	40.23
ATOM	3455	CB	LEU	B	384	22.048	27.615	33.753	1.00	40.07
ATOM	3456	CG	LEU	B	384	21.387	28.655	34.661	1.00	39.46
ATOM	3457	CD1	LEU	B	384	21.816	28.537	36.132	1.00	39.28
ATOM	3458	CD2	LEU	B	384	21.527	30.055	34.086	1.00	39.15
ATOM	3459	C	LEU	B	384	21.902	26.593	31.450	1.00	38.75
ATOM	3460	O	LEU	B	384	22.447	27.184	30.564	1.00	40.35
ATOM	3461	N	ALA	B	385	21.930	25.268	31.510	1.00	38.57
ATOM	3462	CA	ALA	B	385	22.579	24.492	30.445	1.00	38.37
ATOM	3463	CB	ALA	B	385	22.318	22.967	30.635	1.00	38.60
ATOM	3464	C	ALA	B	385	22.149	24.947	29.046	1.00	38.68
ATOM	3465	O	ALA	B	385	22.977	25.087	28.149	1.00	39.17
ATOM	3466	N	ILE	B	386	20.852	25.225	28.874	1.00	38.09
ATOM	3467	CA	ILE	B	386	20.320	25.622	27.579	1.00	37.44
ATOM	3468	CB	ILE	B	386	18.827	25.284	27.380	1.00	37.48
ATOM	3469	CG1	ILE	B	386	18.517	23.822	27.717	1.00	35.33
ATOM	3470	CD1	ILE	B	386	16.998	23.565	27.972	1.00	35.72
ATOM	3471	CG2	ILE	B	386	18.438	25.618	25.895	1.00	36.06
ATOM	3472	C	ILE	B	386	20.477	27.095	27.328	1.00	36.86
ATOM	3473	O	ILE	B	386	20.849	27.498	26.244	1.00	36.36
ATOM	3474	N	PHE	B	387	20.253	27.905	28.342	1.00	38.41
ATOM	3475	CA	PHE	B	387	20.553	29.314	28.204	1.00	40.18
ATOM	3476	CB	PHE	B	387	20.328	30.015	29.540	1.00	40.93
ATOM	3477	CG	PHE	B	387	20.605	31.495	29.499	1.00	43.46
ATOM	3478	CD1	PHE	B	387	19.917	32.327	28.612	1.00	44.18

62/75

ATOM	3479	CE1	PHE	B	387	20.162	33.680	28.591	1.00	45.29
ATOM	3480	CZ	PHE	B	387	21.093	34.207	29.444	1.00	41.09
ATOM	3481	CE2	PHE	B	387	21.763	33.402	30.320	1.00	42.51
ATOM	3482	CD2	PHE	B	387	21.536	32.065	30.360	1.00	41.74
ATOM	3483	C	PHE	B	387	21.979	29.552	27.721	1.00	39.79
ATOM	3484	O	PHE	B	387	22.242	30.340	26.809	1.00	41.64
ATOM	3485	N	ILE	B	388	22.922	28.889	28.343	1.00	40.37
ATOM	3486	CA	ILE	B	388	24.323	29.134	28.041	1.00	38.90
ATOM	3487	CB	ILE	B	388	25.209	28.425	29.116	1.00	41.31
ATOM	3488	CG1	ILE	B	388	25.363	29.360	30.340	1.00	41.15
ATOM	3489	CD1	ILE	B	388	25.447	28.595	31.625	1.00	48.53
ATOM	3490	CG2	ILE	B	388	26.521	27.862	28.573	1.00	39.04
ATOM	3491	C	ILE	B	388	24.610	28.800	26.588	1.00	38.72
ATOM	3492	O	ILE	B	388	25.330	29.530	25.918	1.00	39.25
ATOM	3493	N	ALA	B	389	23.993	27.731	26.074	1.00	36.93
ATOM	3494	CA	ALA	B	389	24.222	27.270	24.725	1.00	35.47
ATOM	3495	CB	ALA	B	389	23.642	25.896	24.543	1.00	34.27
ATOM	3496	C	ALA	B	389	23.626	28.236	23.743	1.00	36.57
ATOM	3497	O	ALA	B	389	24.203	28.449	22.706	1.00	37.58
ATOM	3498	N	VAL	B	390	22.483	28.850	24.096	1.00	37.82
ATOM	3499	CA	VAL	B	390	21.859	29.927	23.266	1.00	38.40
ATOM	3500	CB	VAL	B	390	20.558	30.427	23.867	1.00	38.38
ATOM	3501	CG1	VAL	B	390	20.068	31.720	23.159	1.00	39.19
ATOM	3502	CG2	VAL	B	390	19.521	29.352	23.737	1.00	40.52
ATOM	3503	C	VAL	B	390	22.818	31.061	23.125	1.00	38.16
ATOM	3504	O	VAL	B	390	23.050	31.518	22.010	1.00	38.83
ATOM	3505	N	ILE	B	391	23.378	31.533	24.247	1.00	38.81
ATOM	3506	CA	ILE	B	391	24.431	32.602	24.236	1.00	36.86
ATOM	3507	CB	ILE	B	391	25.013	32.943	25.667	1.00	37.79
ATOM	3508	CG1	ILE	B	391	23.983	33.566	26.610	1.00	37.28
ATOM	3509	CD1	ILE	B	391	24.473	33.616	28.093	1.00	33.49
ATOM	3510	CG2	ILE	B	391	26.169	33.957	25.561	1.00	38.20
ATOM	3511	C	ILE	B	391	25.632	32.269	23.333	1.00	37.44
ATOM	3512	O	ILE	B	391	26.150	33.159	22.650	1.00	35.88
ATOM	3513	N	ILE	B	392	26.123	31.010	23.338	1.00	37.18
ATOM	3514	CA	ILE	B	392	27.270	30.713	22.507	1.00	36.95
ATOM	3515	CB	ILE	B	392	27.947	29.338	22.821	1.00	38.50
ATOM	3516	CG1	ILE	B	392	28.463	29.311	24.269	1.00	36.98
ATOM	3517	CD1	ILE	B	392	28.552	27.861	24.959	1.00	37.83
ATOM	3518	CG2	ILE	B	392	29.051	29.059	21.785	1.00	36.86
ATOM	3519	C	ILE	B	392	26.887	30.778	21.033	1.00	39.20
ATOM	3520	O	ILE	B	392	27.663	31.252	20.202	1.00	37.87
ATOM	3521	N	LEU	B	393	25.695	30.289	20.692	1.00	39.80
ATOM	3522	CA	LEU	B	393	25.353	30.266	19.264	1.00	40.95
ATOM	3523	CB	LEU	B	393	24.430	29.093	18.901	1.00	40.86
ATOM	3524	CG	LEU	B	393	25.063	27.724	18.708	1.00	38.40
ATOM	3525	CD1	LEU	B	393	26.002	27.638	17.479	1.00	38.15
ATOM	3526	CD2	LEU	B	393	25.748	27.275	19.971	1.00	38.57
ATOM	3527	C	LEU	B	393	24.731	31.574	18.827	1.00	41.30
ATOM	3528	O	LEU	B	393	23.670	31.596	18.228	1.00	42.84
ATOM	3529	N	SER	B	394	25.409	32.673	19.079	1.00	42.64
ATOM	3530	CA	SER	B	394	24.787	33.975	18.770	1.00	43.30
ATOM	3531	CB	SER	B	394	25.248	35.086	19.723	1.00	41.97
ATOM	3532	OG	SER	B	394	24.762	34.830	21.057	1.00	43.04
ATOM	3533	C	SER	B	394	24.778	34.360	17.279	1.00	45.03
ATOM	3534	O	SER	B	394	23.702	34.492	16.658	1.00	47.21
ATOM	3535	N	GLY	B	395	25.892	34.557	16.624	1.00	44.71
ATOM	3536	CA	GLY	B	395	25.618	34.867	15.180	1.00	45.03

63/75

ATOM	3537	C	GLY	B	395	25.538	36.335	14.793	1.00	44.79
ATOM	3538	O	GLY	B	395	25.652	36.711	13.608	1.00	42.67
ATOM	3539	N	ASP	B	396	25.398	37.183	15.797	1.00	44.32
ATOM	3540	CA	ASP	B	396	25.652	38.563	15.578	1.00	44.65
ATOM	3541	CB	ASP	B	396	24.632	39.410	16.320	1.00	45.52
ATOM	3542	CG	ASP	B	396	24.769	39.275	17.815	1.00	48.07
ATOM	3543	OD1	ASP	B	396	24.864	40.309	18.510	1.00	49.31
ATOM	3544	OD2	ASP	B	396	24.791	38.125	18.291	1.00	47.08
ATOM	3545	C	ASP	B	396	27.069	38.912	16.013	1.00	43.94
ATOM	3546	O	ASP	B	396	27.420	40.100	16.089	1.00	44.21
ATOM	3547	N	ARG	B	397	27.900	37.909	16.294	1.00	41.95
ATOM	3548	CA	ARG	B	397	29.278	38.199	16.677	1.00	40.75
ATOM	3549	CB	ARG	B	397	30.015	36.929	17.138	1.00	40.22
ATOM	3550	CG	ARG	B	397	29.292	36.143	18.183	1.00	37.80
ATOM	3551	CD	ARG	B	397	28.932	37.002	19.373	1.00	37.85
ATOM	3552	NE	ARG	B	397	28.471	36.145	20.467	1.00	35.45
ATOM	3553	CZ	ARG	B	397	28.165	36.543	21.687	1.00	34.57
ATOM	3554	NH1	ARG	B	397	28.266	37.809	22.032	1.00	33.20
ATOM	3555	NH2	ARG	B	397	27.750	35.658	22.574	1.00	37.46
ATOM	3556	C	ARG	B	397	30.006	38.784	15.488	1.00	40.62
ATOM	3557	O	ARG	B	397	29.805	38.301	14.373	1.00	42.22
ATOM	3558	N	PRO	B	398	30.909	39.768	15.713	1.00	40.11
ATOM	3559	CA	PRO	B	398	31.629	40.295	14.549	1.00	39.72
ATOM	3560	CB	PRO	B	398	32.452	41.477	15.095	1.00	39.49
ATOM	3561	CG	PRO	B	398	32.071	41.612	16.581	1.00	39.51
ATOM	3562	CD	PRO	B	398	31.319	40.391	16.993	1.00	40.16
ATOM	3563	C	PRO	B	398	32.546	39.262	13.980	1.00	39.66
ATOM	3564	O	PRO	B	398	33.105	38.475	14.725	1.00	40.27
ATOM	3565	N	GLY	B	399	32.651	39.251	12.654	1.00	39.27
ATOM	3566	CA	GLY	B	399	33.607	38.447	11.911	1.00	37.46
ATOM	3567	C	GLY	B	399	33.187	37.030	11.568	1.00	37.13
ATOM	3568	O	GLY	B	399	34.010	36.262	11.106	1.00	36.59
ATOM	3569	N	LEU	B	400	31.924	36.676	11.791	1.00	36.44
ATOM	3570	CA	LEU	B	400	31.435	35.355	11.395	1.00	36.70
ATOM	3571	CB	LEU	B	400	30.124	34.952	12.102	1.00	35.37
ATOM	3572	CG	LEU	B	400	30.206	34.727	13.596	1.00	34.44
ATOM	3573	CD1	LEU	B	400	28.872	34.843	14.207	1.00	29.03
ATOM	3574	CD2	LEU	B	400	30.896	33.379	13.992	1.00	30.20
ATOM	3575	C	LEU	B	400	31.308	35.248	9.885	1.00	36.81
ATOM	3576	O	LEU	B	400	30.909	36.196	9.208	1.00	37.66
ATOM	3577	N	LEU	B	401	31.699	34.089	9.382	1.00	37.66
ATOM	3578	CA	LEU	B	401	31.752	33.806	7.966	1.00	37.70
ATOM	3579	CB	LEU	B	401	32.943	32.882	7.690	1.00	38.42
ATOM	3580	CG	LEU	B	401	34.303	33.503	8.014	1.00	37.75
ATOM	3581	CD1	LEU	B	401	35.358	32.426	8.037	1.00	36.50
ATOM	3582	CD2	LEU	B	401	34.602	34.587	6.995	1.00	33.86
ATOM	3583	C	LEU	B	401	30.489	33.119	7.438	1.00	38.64
ATOM	3584	O	LEU	B	401	30.116	33.318	6.279	1.00	38.67
ATOM	3585	N	ASN	B	402	29.843	32.290	8.256	1.00	38.58
ATOM	3586	CA	ASN	B	402	28.616	31.592	7.820	1.00	38.91
ATOM	3587	CB	ASN	B	402	28.932	30.142	7.393	1.00	38.50
ATOM	3588	CG	ASN	B	402	27.710	29.398	6.824	1.00	38.76
ATOM	3589	OD1	ASN	B	402	26.659	29.992	6.625	1.00	32.92
ATOM	3590	ND2	ASN	B	402	27.855	28.074	6.579	1.00	36.71
ATOM	3591	C	ASN	B	402	27.575	31.613	8.942	1.00	39.13
ATOM	3592	O	ASN	B	402	27.579	30.737	9.821	1.00	39.11
ATOM	3593	N	VAL	B	403	26.697	32.613	8.909	1.00	39.28
ATOM	3594	CA	VAL	B	403	25.733	32.830	9.977	1.00	39.78

64/75

ATOM	3595	CB	VAL	B	403	25.283	34.336	10.020	1.00	41.00
ATOM	3596	CG1	VAL	B	403	24.105	34.574	10.991	1.00	39.14
ATOM	3597	CG2	VAL	B	403	26.481	35.253	10.336	1.00	41.12
ATOM	3598	C	VAL	B	403	24.527	31.864	9.921	1.00	40.45
ATOM	3599	O	VAL	B	403	23.869	31.622	10.910	1.00	39.63
ATOM	3600	N	LYS	B	404	24.250	31.257	8.786	1.00	41.65
ATOM	3601	CA	LYS	B	404	23.044	30.443	8.726	1.00	42.96
ATOM	3602	CB	LYS	B	404	22.734	29.978	7.303	1.00	42.33
ATOM	3603	CG	LYS	B	404	21.369	29.341	7.153	1.00	42.87
ATOM	3604	CD	LYS	B	404	21.240	28.685	5.750	1.00	44.32
ATOM	3605	CE	LYS	B	404	20.165	27.589	5.697	1.00	45.68
ATOM	3606	NZ	LYS	B	404	18.965	27.899	6.529	1.00	47.34
ATOM	3607	C	LYS	B	404	23.005	29.274	9.724	1.00	43.30
ATOM	3608	O	LYS	B	404	22.058	29.215	10.510	1.00	43.17
ATOM	3609	N	PRO	B	405	24.018	28.356	9.719	1.00	43.78
ATOM	3610	CA	PRO	B	405	23.798	27.218	10.597	1.00	44.13
ATOM	3611	CB	PRO	B	405	24.906	26.204	10.199	1.00	44.54
ATOM	3612	CG	PRO	B	405	25.973	27.006	9.574	1.00	43.46
ATOM	3613	CD	PRO	B	405	25.316	28.258	9.008	1.00	44.54
ATOM	3614	C	PRO	B	405	23.911	27.656	12.053	1.00	44.60
ATOM	3615	O	PRO	B	405	23.240	27.083	12.903	1.00	46.32
ATOM	3616	N	ILE	B	406	24.675	28.709	12.338	1.00	44.38
ATOM	3617	CA	ILE	B	406	24.742	29.203	13.705	1.00	43.69
ATOM	3618	CB	ILE	B	406	25.683	30.414	13.848	1.00	43.59
ATOM	3619	CG1	ILE	B	406	27.119	29.991	13.527	1.00	42.32
ATOM	3620	CD1	ILE	B	406	28.065	31.106	13.191	1.00	40.12
ATOM	3621	CG2	ILE	B	406	25.653	30.874	15.287	1.00	43.39
ATOM	3622	C	ILE	B	406	23.341	29.540	14.221	1.00	44.02
ATOM	3623	O	ILE	B	406	22.941	29.064	15.277	1.00	43.65
ATOM	3624	N	GLU	B	407	22.590	30.350	13.462	1.00	44.37
ATOM	3625	CA	GLU	B	407	21.235	30.727	13.826	1.00	44.97
ATOM	3626	CB	GLU	B	407	20.783	31.935	12.999	1.00	44.95
ATOM	3627	CG	GLU	B	407	21.497	33.221	13.418	1.00	46.68
ATOM	3628	CD	GLU	B	407	20.969	34.466	12.713	1.00	47.60
ATOM	3629	OE1	GLU	B	407	20.341	34.292	11.649	1.00	48.54
ATOM	3630	OE2	GLU	B	407	21.186	35.604	13.240	1.00	49.55
ATOM	3631	C	GLU	B	407	20.250	29.560	13.704	1.00	44.69
ATOM	3632	O	GLU	B	407	19.245	29.507	14.417	1.00	45.10
ATOM	3633	N	ASP	B	408	20.537	28.621	12.810	1.00	44.91
ATOM	3634	CA	ASP	B	408	19.729	27.383	12.696	1.00	44.25
ATOM	3635	CB	ASP	B	408	20.229	26.492	11.558	1.00	44.38
ATOM	3636	CG	ASP	B	408	19.727	26.920	10.188	1.00	46.27
ATOM	3637	OD1	ASP	B	408	19.194	28.050	10.037	1.00	43.93
ATOM	3638	OD2	ASP	B	408	19.871	26.083	9.257	1.00	47.12
ATOM	3639	C	ASP	B	408	19.807	26.603	13.994	1.00	43.13
ATOM	3640	O	ASP	B	408	18.810	26.222	14.562	1.00	43.51
ATOM	3641	N	ILE	B	409	21.012	26.380	14.470	1.00	42.54
ATOM	3642	CA	ILE	B	409	21.223	25.744	15.786	1.00	41.42
ATOM	3643	CB	ILE	B	409	22.693	25.560	16.049	1.00	41.32
ATOM	3644	CG1	ILE	B	409	23.305	24.632	14.984	1.00	42.13
ATOM	3645	CD1	ILE	B	409	24.815	24.502	15.090	1.00	38.71
ATOM	3646	CG2	ILE	B	409	22.926	25.001	17.482	1.00	40.92
ATOM	3647	C	ILE	B	409	20.670	26.551	16.968	1.00	40.84
ATOM	3648	O	ILE	B	409	20.142	25.989	17.913	1.00	41.14
ATOM	3649	N	GLN	B	410	20.815	27.860	16.935	1.00	39.48
ATOM	3650	CA	GLN	B	410	20.333	28.693	18.029	1.00	39.91
ATOM	3651	CB	GLN	B	410	20.758	30.154	17.871	1.00	39.79
ATOM	3652	CG	GLN	B	410	20.664	30.820	19.241	1.00	41.11

65/75

ATOM	3653	CD	GLN	B	410	20.747	32.302	19.272	1.00	42.44
ATOM	3654	OE1	GLN	B	410	21.337	32.854	20.208	1.00	43.23
ATOM	3655	NE2	GLN	B	410	20.087	32.985	18.310	1.00	41.04
ATOM	3656	C	GLN	B	410	18.838	28.688	18.104	1.00	40.48
ATOM	3657	O	GLN	B	410	18.279	28.653	19.190	1.00	40.62
ATOM	3658	N	ASP	B	411	18.162	28.785	16.951	1.00	42.66
ATOM	3659	CA	ASP	B	411	16.679	28.649	16.912	1.00	43.10
ATOM	3660	CB	ASP	B	411	16.156	28.798	15.483	1.00	44.33
ATOM	3661	CG	ASP	B	411	16.407	30.186	14.926	1.00	47.85
ATOM	3662	OD1	ASP	B	411	16.738	31.095	15.733	1.00	50.10
ATOM	3663	OD2	ASP	B	411	16.261	30.374	13.691	1.00	51.10
ATOM	3664	C	ASP	B	411	16.173	27.355	17.543	1.00	42.52
ATOM	3665	O	ASP	B	411	15.249	27.367	18.366	1.00	42.70
ATOM	3666	N	ASN	B	412	16.796	26.245	17.172	1.00	43.25
ATOM	3667	CA	ASN	B	412	16.575	24.942	17.856	1.00	43.20
ATOM	3668	CB	ASN	B	412	17.545	23.930	17.306	1.00	44.23
ATOM	3669	CG	ASN	B	412	16.946	22.556	17.166	1.00	48.18
ATOM	3670	OD1	ASN	B	412	17.476	21.748	16.415	1.00	55.38
ATOM	3671	OD2	ASN	B	412	15.844	22.278	17.872	1.00	50.05
ATOM	3672	C	ASN	B	412	16.761	25.002	19.384	1.00	41.88
ATOM	3673	O	ASN	B	412	15.962	24.446	20.147	1.00	41.34
ATOM	3674	N	LEU	B	413	17.833	25.666	19.817	1.00	40.48
ATOM	3675	CA	LEU	B	413	18.170	25.810	21.253	1.00	38.81
ATOM	3676	CB	LEU	B	413	19.573	26.376	21.404	1.00	37.82
ATOM	3677	CG	LEU	B	413	20.697	25.442	21.005	1.00	35.80
ATOM	3678	CD1	LEU	B	413	21.950	26.286	20.951	1.00	34.94
ATOM	3679	CD2	LEU	B	413	20.787	24.300	22.005	1.00	34.77
ATOM	3680	C	LEU	B	413	17.197	26.710	22.017	1.00	38.21
ATOM	3681	O	LEU	B	413	16.878	26.446	23.163	1.00	38.10
ATOM	3682	N	LEU	B	414	16.758	27.778	21.369	1.00	37.82
ATOM	3683	CA	LEU	B	414	15.702	28.640	21.888	1.00	37.46
ATOM	3684	CB	LEU	B	414	15.547	29.891	20.990	1.00	38.04
ATOM	3685	CG	LEU	B	414	16.729	30.879	21.008	1.00	38.46
ATOM	3686	CD1	LEU	B	414	16.667	31.709	19.745	1.00	36.60
ATOM	3687	CD2	LEU	B	414	16.672	31.744	22.293	1.00	40.66
ATOM	3688	C	LEU	B	414	14.370	27.906	22.002	1.00	36.88
ATOM	3689	O	LEU	B	414	13.649	28.093	23.001	1.00	37.28
ATOM	3690	N	GLN	B	415	14.022	27.077	21.012	1.00	36.07
ATOM	3691	CA	GLN	B	415	12.767	26.297	21.142	1.00	37.72
ATOM	3692	CB	GLN	B	415	12.449	25.470	19.906	1.00	38.01
ATOM	3693	CG	GLN	B	415	12.460	26.206	18.629	1.00	42.95
ATOM	3694	CD	GLN	B	415	12.040	25.326	17.515	1.00	48.11
ATOM	3695	OE1	GLN	B	415	10.909	24.837	17.515	1.00	53.99
ATOM	3696	NE2	GLN	B	415	12.936	25.092	16.557	1.00	48.57
ATOM	3697	C	GLN	B	415	12.840	25.344	22.323	1.00	37.47
ATOM	3698	O	GLN	B	415	11.834	25.072	22.989	1.00	37.99
ATOM	3699	N	ALA	B	416	14.039	24.815	22.543	1.00	36.63
ATOM	3700	CA	ALA	B	416	14.306	23.898	23.630	1.00	36.73
ATOM	3701	CB	ALA	B	416	15.669	23.219	23.414	1.00	35.55
ATOM	3702	C	ALA	B	416	14.249	24.568	24.985	1.00	37.65
ATOM	3703	O	ALA	B	416	13.723	23.992	25.917	1.00	38.13
ATOM	3704	N	LEU	B	417	14.812	25.775	25.106	1.00	37.60
ATOM	3705	CA	LEU	B	417	14.749	26.558	26.339	1.00	38.06
ATOM	3706	CB	LEU	B	417	15.686	27.753	26.196	1.00	37.74
ATOM	3707	CG	LEU	B	417	15.779	28.781	27.334	1.00	39.69
ATOM	3708	CD1	LEU	B	417	16.378	28.156	28.579	1.00	34.04
ATOM	3709	CD2	LEU	B	417	16.576	29.971	26.878	1.00	36.88
ATOM	3710	C	LEU	B	417	13.314	27.041	26.608	1.00	39.40

66/75

ATOM	3711	O	LEU	B	417	12.803	26.974	27.732	1.00	40.74
ATOM	3712	N	GLU	B	418	12.660	27.541	25.571	1.00	39.84
ATOM	3713	CA	GLU	B	418	11.220	27.775	25.631	1.00	40.59
ATOM	3714	CB	GLU	B	418	10.664	28.066	24.226	1.00	41.18
ATOM	3715	CG	GLU	B	418	9.374	28.827	24.255	1.00	41.69
ATOM	3716	CD	GLU	B	418	8.938	29.271	22.879	1.00	43.09
ATOM	3717	OE1	GLU	B	418	9.646	29.052	21.863	1.00	43.58
ATOM	3718	OE2	GLU	B	418	7.846	29.834	22.827	1.00	48.45
ATOM	3719	C	GLU	B	418	10.443	26.604	26.294	1.00	39.93
ATOM	3720	O	GLU	B	418	9.837	26.793	27.326	1.00	40.13
ATOM	3721	N	LEU	B	419	10.479	25.406	25.713	1.00	39.54
ATOM	3722	CA	LEU	B	419	9.753	24.276	26.287	1.00	38.57
ATOM	3723	CB	LEU	B	419	9.889	23.031	25.404	1.00	39.25
ATOM	3724	CG	LEU	B	419	9.111	21.753	25.739	1.00	38.30
ATOM	3725	CD1	LEU	B	419	7.619	21.988	25.774	1.00	40.35
ATOM	3726	CD2	LEU	B	419	9.468	20.651	24.746	1.00	37.73
ATOM	3727	C	LEU	B	419	10.195	23.967	27.719	1.00	38.79
ATOM	3728	O	LEU	B	419	9.365	23.610	28.556	1.00	37.68
ATOM	3729	N	GLN	B	420	11.499	24.124	27.987	1.00	38.36
ATOM	3730	CA	GLN	B	420	12.083	23.852	29.300	1.00	37.99
ATOM	3731	CB	GLN	B	420	13.622	23.882	29.217	1.00	37.72
ATOM	3732	CG	GLN	B	420	14.329	23.877	30.582	1.00	36.21
ATOM	3733	CD	GLN	B	420	14.308	22.520	31.271	1.00	37.11
ATOM	3734	OE1	GLN	B	420	14.183	21.477	30.615	1.00	35.51
ATOM	3735	NE2	GLN	B	420	14.440	22.525	32.598	1.00	34.54
ATOM	3736	C	GLN	B	420	11.560	24.770	30.417	1.00	38.69
ATOM	3737	O	GLN	B	420	11.099	24.288	31.445	1.00	39.38
ATOM	3738	N	LEU	B	421	11.613	26.091	30.221	1.00	38.82
ATOM	3739	CA	LEU	B	421	11.023	27.045	31.162	1.00	38.38
ATOM	3740	CB	LEU	B	421	11.292	28.472	30.666	1.00	38.73
ATOM	3741	CG	LEU	B	421	12.797	28.652	30.394	1.00	37.63
ATOM	3742	CD1	LEU	B	421	13.126	30.024	29.812	1.00	35.55
ATOM	3743	CD2	LEU	B	421	13.621	28.366	31.650	1.00	36.86
ATOM	3744	C	LEU	B	421	9.521	26.825	31.349	1.00	38.81
ATOM	3745	O	LEU	B	421	8.969	27.023	32.421	1.00	38.34
ATOM	3746	N	LYS	B	422	8.848	26.403	30.303	1.00	39.81
ATOM	3747	CA	LYS	B	422	7.394	26.206	30.421	1.00	41.09
ATOM	3748	CB	LYS	B	422	6.729	26.186	29.054	1.00	41.48
ATOM	3749	CG	LYS	B	422	6.699	27.566	28.385	1.00	44.79
ATOM	3750	CD	LYS	B	422	6.085	27.496	27.004	1.00	49.08
ATOM	3751	CE	LYS	B	422	5.457	28.816	26.582	1.00	51.04
ATOM	3752	NZ	LYS	B	422	4.815	28.578	25.264	1.00	53.36
ATOM	3753	C	LYS	B	422	7.043	24.970	31.243	1.00	40.82
ATOM	3754	O	LYS	B	422	6.183	25.041	32.101	1.00	41.01
ATOM	3755	N	LEU	B	423	7.755	23.861	31.017	1.00	41.18
ATOM	3756	CA	LEU	B	423	7.609	22.660	31.869	1.00	40.91
ATOM	3757	CB	LEU	B	423	8.201	21.439	31.172	1.00	40.04
ATOM	3758	CG	LEU	B	423	7.593	21.184	29.793	1.00	39.40
ATOM	3759	CD1	LEU	B	423	8.418	20.189	29.040	1.00	39.88
ATOM	3760	CD2	LEU	B	423	6.126	20.761	29.902	1.00	38.01
ATOM	3761	C	LEU	B	423	8.195	22.796	33.263	1.00	41.19
ATOM	3762	O	LEU	B	423	7.565	22.447	34.248	1.00	42.23
ATOM	3763	N	ASN	B	424	9.415	23.300	33.339	1.00	42.37
ATOM	3764	CA	ASN	B	424	10.102	23.538	34.597	1.00	42.39
ATOM	3765	CB	ASN	B	424	11.561	23.898	34.304	1.00	43.08
ATOM	3766	CG	ASN	B	424	12.505	23.508	35.418	1.00	46.09
ATOM	3767	OD1	ASN	B	424	12.153	22.746	36.331	1.00	45.06
ATOM	3768	ND2	ASN	B	424	13.737	24.017	35.340	1.00	50.38

67/75

ATOM	3769	C	ASN	B	424	9.439	24.608	35.471	1.00	42.53
ATOM	3770	O	ASN	B	424	9.444	24.482	36.688	1.00	41.89
ATOM	3771	N	HIS	B	425	8.865	25.652	34.855	1.00	41.96
ATOM	3772	CA	HIS	B	425	8.282	26.786	35.592	1.00	41.80
ATOM	3773	CB	HIS	B	425	9.219	28.020	35.570	1.00	41.23
ATOM	3774	CG	HIS	B	425	10.651	27.705	35.880	1.00	42.07
ATOM	3775	ND1	HIS	B	425	11.155	27.713	37.161	1.00	43.17
ATOM	3776	CE1	HIS	B	425	12.431	27.376	37.134	1.00	42.86
ATOM	3777	NE2	HIS	B	425	12.775	27.160	35.880	1.00	41.89
ATOM	3778	CD2	HIS	B	425	11.683	27.368	35.075	1.00	41.28
ATOM	3779	C	HIS	B	425	6.929	27.177	35.002	1.00	42.06
ATOM	3780	O	HIS	B	425	6.792	28.261	34.426	1.00	43.07
ATOM	3781	N	PRO	B	426	5.908	26.311	35.139	1.00	42.14
ATOM	3782	CA	PRO	B	426	4.621	26.660	34.507	1.00	41.80
ATOM	3783	CB	PRO	B	426	3.744	25.415	34.750	1.00	41.30
ATOM	3784	CG	PRO	B	426	4.387	24.673	35.881	1.00	41.50
ATOM	3785	CD	PRO	B	426	5.858	25.014	35.853	1.00	41.81
ATOM	3786	C	PRO	B	426	3.957	27.918	35.074	1.00	41.71
ATOM	3787	O	PRO	B	426	3.168	28.566	34.384	1.00	40.95
ATOM	3788	N	GLU	B	427	4.284	28.271	36.312	1.00	42.47
ATOM	3789	CA	GLU	B	427	3.600	29.379	36.998	1.00	42.71
ATOM	3790	CB	GLU	B	427	3.324	29.025	38.471	1.00	43.04
ATOM	3791	CG	GLU	B	427	2.357	27.843	38.666	1.00	45.13
ATOM	3792	CD	GLU	B	427	0.908	28.189	38.303	1.00	48.97
ATOM	3793	OE1	GLU	B	427	0.483	27.909	37.143	1.00	48.60
ATOM	3794	OE2	GLU	B	427	0.206	28.758	39.182	1.00	50.14
ATOM	3795	C	GLU	B	427	4.318	30.720	36.883	1.00	42.57
ATOM	3796	O	GLU	B	427	3.889	31.707	37.486	1.00	42.47
ATOM	3797	N	SER	B	428	5.413	30.735	36.109	1.00	42.88
ATOM	3798	CA	SER	B	428	6.297	31.899	35.932	1.00	42.58
ATOM	3799	CB	SER	B	428	7.758	31.443	36.147	1.00	42.98
ATOM	3800	OG	SER	B	428	8.735	32.482	36.187	1.00	43.06
ATOM	3801	C	SER	B	428	6.048	32.469	34.526	1.00	42.52
ATOM	3802	O	SER	B	428	6.670	32.038	33.562	1.00	42.65
ATOM	3803	N	SER	B	429	5.086	33.394	34.397	1.00	43.14
ATOM	3804	CA	SER	B	429	4.686	33.880	33.071	1.00	42.92
ATOM	3805	CB	SER	B	429	3.405	34.744	33.107	1.00	44.06
ATOM	3806	OG	SER	B	429	3.667	36.144	33.201	1.00	46.56
ATOM	3807	C	SER	B	429	5.837	34.627	32.430	1.00	42.11
ATOM	3808	O	SER	B	429	6.537	35.421	33.094	1.00	42.63
ATOM	3809	N	GLN	B	430	6.053	34.350	31.150	1.00	40.03
ATOM	3810	CA	GLN	B	430	6.981	35.136	30.373	1.00	40.03
ATOM	3811	CB	GLN	B	430	6.530	36.609	30.260	1.00	40.41
ATOM	3812	CG	GLN	B	430	5.356	36.825	29.305	1.00	40.23
ATOM	3813	CD	GLN	B	430	5.614	36.165	27.957	1.00	42.19
ATOM	3814	OE1	GLN	B	430	4.911	35.228	27.547	1.00	46.06
ATOM	3815	NE2	GLN	B	430	6.637	36.626	27.276	1.00	39.78
ATOM	3816	C	GLN	B	430	8.378	35.058	30.957	1.00	39.42
ATOM	3817	O	GLN	B	430	9.202	35.917	30.706	1.00	40.45
ATOM	3818	N	LEU	B	431	8.671	34.016	31.721	1.00	38.57
ATOM	3819	CA	LEU	B	431	10.058	33.803	32.111	1.00	37.05
ATOM	3820	CB	LEU	B	431	10.198	32.532	32.956	1.00	37.92
ATOM	3821	CG	LEU	B	431	11.605	32.291	33.493	1.00	36.73
ATOM	3822	CD1	LEU	B	431	11.961	33.374	34.528	1.00	39.05
ATOM	3823	CD2	LEU	B	431	11.722	30.868	34.101	1.00	37.49
ATOM	3824	C	LEU	B	431	11.010	33.722	30.919	1.00	37.07
ATOM	3825	O	LEU	B	431	12.195	34.137	31.013	1.00	37.69
ATOM	3826	N	PHE	B	432	10.564	33.108	29.827	1.00	35.75

68/75

ATOM	3827	CA	PHE	B	432	11.429	32.972	28.667	1.00	35.81
ATOM	3828	CB	PHE	B	432	10.728	32.085	27.619	1.00	36.27
ATOM	3829	CG	PHE	B	432	11.383	32.042	26.269	1.00	35.95
ATOM	3830	CD1	PHE	B	432	12.541	31.279	26.055	1.00	37.92
ATOM	3831	CE1	PHE	B	432	13.106	31.199	24.783	1.00	40.13
ATOM	3832	CZ	PHE	B	432	12.479	31.887	23.690	1.00	38.48
ATOM	3833	CE2	PHE	B	432	11.307	32.594	23.907	1.00	36.42
ATOM	3834	CD2	PHE	B	432	10.773	32.659	25.185	1.00	35.86
ATOM	3835	C	PHE	B	432	11.844	34.355	28.133	1.00	36.36
ATOM	3836	O	PHE	B	432	13.027	34.574	27.866	1.00	38.46
ATOM	3837	N	ALA	B	433	10.883	35.278	27.995	1.00	36.37
ATOM	3838	CA	ALA	B	433	11.170	36.677	27.607	1.00	36.75
ATOM	3839	CB	ALA	B	433	9.901	37.424	27.455	1.00	35.83
ATOM	3840	C	ALA	B	433	12.050	37.440	28.604	1.00	37.47
ATOM	3841	O	ALA	B	433	12.921	38.171	28.192	1.00	37.06
ATOM	3842	N	LYS	B	434	11.778	37.329	29.906	1.00	38.74
ATOM	3843	CA	LYS	B	434	12.654	37.945	30.910	1.00	40.15
ATOM	3844	CB	LYS	B	434	12.081	37.809	32.330	1.00	40.53
ATOM	3845	CG	LYS	B	434	10.660	38.317	32.544	1.00	42.28
ATOM	3846	CD	LYS	B	434	10.197	37.803	33.927	1.00	44.12
ATOM	3847	CE	LYS	B	434	8.726	38.057	34.206	1.00	48.84
ATOM	3848	NZ	LYS	B	434	8.475	39.331	34.964	1.00	48.83
ATOM	3849	C	LYS	B	434	14.093	37.371	30.901	1.00	40.28
ATOM	3850	O	LYS	B	434	15.030	38.080	31.242	1.00	40.34
ATOM	3851	N	LEU	B	435	14.268	36.097	30.558	1.00	41.24
ATOM	3852	CA	LEU	B	435	15.606	35.531	30.454	1.00	41.50
ATOM	3853	CB	LEU	B	435	15.559	33.984	30.445	1.00	42.39
ATOM	3854	CG	LEU	B	435	16.852	33.129	30.485	1.00	42.01
ATOM	3855	CD1	LEU	B	435	17.895	33.663	31.493	1.00	43.33
ATOM	3856	CD2	LEU	B	435	16.636	31.618	30.729	1.00	40.67
ATOM	3857	C	LEU	B	435	16.344	36.166	29.240	1.00	42.83
ATOM	3858	O	LEU	B	435	17.499	36.657	29.355	1.00	41.69
ATOM	3859	N	LEU	B	436	15.660	36.231	28.099	1.00	42.64
ATOM	3860	CA	LEU	B	436	16.229	36.901	26.916	1.00	43.19
ATOM	3861	CB	LEU	B	436	15.295	36.790	25.689	1.00	43.02
ATOM	3862	CG	LEU	B	436	14.880	35.375	25.264	1.00	43.19
ATOM	3863	CD1	LEU	B	436	13.771	35.386	24.207	1.00	43.76
ATOM	3864	CD2	LEU	B	436	16.073	34.490	24.828	1.00	42.13
ATOM	3865	C	LEU	B	436	16.637	38.372	27.160	1.00	42.30
ATOM	3866	O	LEU	B	436	17.696	38.795	26.736	1.00	41.68
ATOM	3867	N	GLN	B	437	15.792	39.138	27.837	1.00	43.04
ATOM	3868	CA	GLN	B	437	16.077	40.548	28.186	1.00	43.31
ATOM	3869	CB	GLN	B	437	14.970	41.084	29.027	1.00	42.50
ATOM	3870	CG	GLN	B	437	13.615	41.088	28.379	1.00	41.90
ATOM	3871	CD	GLN	B	437	12.631	41.890	29.193	1.00	40.35
ATOM	3872	OE1	GLN	B	437	12.101	42.889	28.710	1.00	42.12
ATOM	3873	NE2	GLN	B	437	12.405	41.489	30.445	1.00	38.23
ATOM	3874	C	GLN	B	437	17.351	40.727	29.019	1.00	44.77
ATOM	3875	O	GLN	B	437	17.903	41.813	29.058	1.00	44.46
ATOM	3876	N	LYS	B	438	17.744	39.673	29.723	1.00	44.24
ATOM	3877	CA	LYS	B	438	18.950	39.630	30.539	1.00	46.70
ATOM	3878	CB	LYS	B	438	18.834	38.526	31.610	1.00	45.82
ATOM	3879	CG	LYS	B	438	18.504	39.051	33.026	1.00	47.44
ATOM	3880	CD	LYS	B	438	17.040	39.000	33.342	1.00	53.87
ATOM	3881	CE	LYS	B	438	16.731	39.813	34.552	1.00	55.25
ATOM	3882	NZ	LYS	B	438	17.718	40.939	34.586	1.00	60.37
ATOM	3883	C	LYS	B	438	20.229	39.428	29.724	1.00	47.89
ATOM	3884	O	LYS	B	438	21.323	39.749	30.191	1.00	46.56

69/75

ATOM	3885	N	MET	B	439	20.082	38.925	28.497	1.00	50.22
ATOM	3886	CA	MET	B	439	21.203	38.806	27.562	1.00	53.99
ATOM	3887	CB	MET	B	439	20.797	38.103	26.275	1.00	52.90
ATOM	3888	CG	MET	B	439	20.571	36.643	26.513	1.00	55.97
ATOM	3889	SD	MET	B	439	19.915	35.827	25.068	1.00	59.31
ATOM	3890	CE	MET	B	439	21.457	35.313	24.273	1.00	56.65
ATOM	3891	C	MET	B	439	21.816	40.129	27.234	1.00	54.13
ATOM	3892	O	MET	B	439	22.993	40.186	26.892	1.00	55.30
ATOM	3893	N	THR	B	440	21.021	41.186	27.362	1.00	54.97
ATOM	3894	CA	THR	B	440	21.476	42.525	27.071	1.00	55.63
ATOM	3895	CB	THR	B	440	20.355	43.389	26.288	1.00	56.69
ATOM	3896	OG1	THR	B	440	19.566	44.196	27.179	1.00	56.68
ATOM	3897	CG2	THR	B	440	19.441	42.493	25.366	1.00	55.92
ATOM	3898	C	THR	B	440	22.064	43.229	28.309	1.00	55.57
ATOM	3899	O	THR	B	440	22.867	44.161	28.180	1.00	56.74
ATOM	3900	N	ASP	B	441	21.647	42.803	29.495	1.00	54.68
ATOM	3901	CA	ASP	B	441	22.280	43.198	30.753	1.00	54.17
ATOM	3902	CB	ASP	B	441	21.469	42.657	31.926	1.00	54.79
ATOM	3903	CG	ASP	B	441	20.029	43.139	31.930	1.00	55.86
ATOM	3904	OD1	ASP	B	441	19.591	43.753	30.925	1.00	56.31
ATOM	3905	OD2	ASP	B	441	19.354	42.915	32.966	1.00	57.14
ATOM	3906	C	ASP	B	441	23.715	42.650	30.895	1.00	53.58
ATOM	3907	O	ASP	B	441	24.564	43.280	31.524	1.00	53.85
ATOM	3908	N	LEU	B	442	23.930	41.454	30.359	1.00	51.94
ATOM	3909	CA	LEU	B	442	25.223	40.760	30.276	1.00	51.65
ATOM	3910	CB	LEU	B	442	25.000	39.363	29.709	1.00	49.88
ATOM	3911	CG	LEU	B	442	24.679	38.185	30.598	1.00	50.74
ATOM	3912	CD1	LEU	B	442	24.429	36.973	29.666	1.00	45.66
ATOM	3913	CD2	LEU	B	442	25.829	37.923	31.609	1.00	48.34
ATOM	3914	C	LEU	B	442	26.208	41.397	29.327	1.00	51.57
ATOM	3915	O	LEU	B	442	27.415	41.306	29.532	1.00	51.90
ATOM	3916	N	ARG	B	443	25.665	41.969	28.248	1.00	51.34
ATOM	3917	CA	ARG	B	443	26.403	42.578	27.173	1.00	50.63
ATOM	3918	CB	ARG	B	443	25.463	42.780	25.989	1.00	50.77
ATOM	3919	CG	ARG	B	443	25.969	42.285	24.659	1.00	52.30
ATOM	3920	CD	ARG	B	443	25.531	40.853	24.327	1.00	56.19
ATOM	3921	NE	ARG	B	443	25.497	40.646	22.872	1.00	55.68
ATOM	3922	CZ	ARG	B	443	25.245	39.493	22.251	1.00	56.98
ATOM	3923	NH1	ARG	B	443	25.026	38.360	22.938	1.00	60.30
ATOM	3924	NH2	ARG	B	443	25.230	39.468	20.928	1.00	50.48
ATOM	3925	C	ARG	B	443	26.937	43.909	27.679	1.00	50.45
ATOM	3926	O	ARG	B	443	28.063	44.288	27.352	1.00	50.16
ATOM	3927	N	GLN	B	444	26.122	44.597	28.483	1.00	49.68
ATOM	3928	CA	GLN	B	444	26.516	45.763	29.258	1.00	49.84
ATOM	3929	CB	GLN	B	444	25.271	46.408	29.886	1.00	50.61
ATOM	3930	CG	GLN	B	444	24.493	47.378	28.949	1.00	53.91
ATOM	3931	CD	GLN	B	444	25.226	48.709	28.668	1.00	57.85
ATOM	3932	OE1	GLN	B	444	25.142	49.264	27.554	1.00	58.58
ATOM	3933	NE2	GLN	B	444	25.943	49.220	29.675	1.00	57.64
ATOM	3934	C	GLN	B	444	27.594	45.509	30.341	1.00	49.12
ATOM	3935	O	GLN	B	444	28.536	46.295	30.462	1.00	49.92
ATOM	3936	N	ILE	B	445	27.468	44.431	31.120	1.00	48.37
ATOM	3937	CA	ILE	B	445	28.507	44.038	32.089	1.00	47.79
ATOM	3938	CB	ILE	B	445	28.241	42.662	32.791	1.00	48.14
ATOM	3939	CG1	ILE	B	445	26.942	42.667	33.581	1.00	50.36
ATOM	3940	CD1	ILE	B	445	26.732	43.929	34.426	1.00	48.48
ATOM	3941	CG2	ILE	B	445	29.368	42.311	33.758	1.00	49.36
ATOM	3942	C	ILE	B	445	29.817	43.896	31.360	1.00	46.31

70/75

ATOM	3943	O	ILE	B	445	30.822	44.414	31.800	1.00	46.00
ATOM	3944	N	VAL	B	446	29.780	43.166	30.253	1.00	45.26
ATOM	3945	CA	VAL	B	446	30.959	42.856	29.445	1.00	44.60
ATOM	3946	CB	VAL	B	446	30.629	41.835	28.333	1.00	44.09
ATOM	3947	CG1	VAL	B	446	31.826	41.587	27.458	1.00	43.10
ATOM	3948	CG2	VAL	B	446	30.205	40.558	28.955	1.00	41.53
ATOM	3949	C	VAL	B	446	31.567	44.131	28.877	1.00	45.18
ATOM	3950	O	VAL	B	446	32.778	44.337	28.982	1.00	45.61
ATOM	3951	N	THR	B	447	30.720	44.991	28.307	1.00	45.65
ATOM	3952	CA	THR	B	447	31.137	46.298	27.796	1.00	46.16
ATOM	3953	CB	THR	B	447	29.970	47.027	27.118	1.00	46.04
ATOM	3954	OG1	THR	B	447	29.637	46.335	25.921	1.00	45.11
ATOM	3955	CG2	THR	B	447	30.360	48.464	26.729	1.00	46.47
ATOM	3956	C	THR	B	447	31.751	47.193	28.873	1.00	47.05
ATOM	3957	O	THR	B	447	32.769	47.840	28.636	1.00	47.35
ATOM	3958	N	GLU	B	448	31.127	47.221	30.046	1.00	47.86
ATOM	3959	CA	GLU	B	448	31.606	47.992	31.198	1.00	48.94
ATOM	3960	CB	GLU	B	448	30.523	47.968	32.296	1.00	48.98
ATOM	3961	CG	GLU	B	448	30.734	48.923	33.485	1.00	50.83
ATOM	3962	CD	GLU	B	448	29.642	48.817	34.570	1.00	50.26
ATOM	3963	OE1	GLU	B	448	28.779	47.917	34.491	1.00	50.45
ATOM	3964	OE2	GLU	B	448	29.658	49.651	35.516	1.00	51.37
ATOM	3965	C	GLU	B	448	32.937	47.421	31.730	1.00	48.93
ATOM	3966	O	GLU	B	448	33.863	48.164	32.060	1.00	48.63
ATOM	3967	N	HIS	B	449	33.010	46.097	31.810	1.00	49.54
ATOM	3968	CA	HIS	B	449	34.191	45.382	32.280	1.00	50.46
ATOM	3969	CB	HIS	B	449	33.935	43.873	32.302	1.00	50.88
ATOM	3970	CG	HIS	B	449	34.980	43.089	33.037	1.00	53.65
ATOM	3971	ND1	HIS	B	449	36.021	42.447	32.397	1.00	54.72
ATOM	3972	CE1	HIS	B	449	36.773	41.827	33.291	1.00	56.89
ATOM	3973	NE2	HIS	B	449	36.262	42.050	34.490	1.00	57.07
ATOM	3974	CD2	HIS	B	449	35.140	42.835	34.360	1.00	55.38
ATOM	3975	C	HIS	B	449	35.427	45.716	31.445	1.00	50.52
ATOM	3976	O	HIS	B	449	36.449	46.123	31.994	1.00	50.03
ATOM	3977	N	VAL	B	450	35.330	45.562	30.123	1.00	50.58
ATOM	3978	CA	VAL	B	450	36.444	45.915	29.237	1.00	50.59
ATOM	3979	CB	VAL	B	450	36.171	45.492	27.761	1.00	50.96
ATOM	3980	CG1	VAL	B	450	35.616	44.051	27.715	1.00	50.28
ATOM	3981	CG2	VAL	B	450	35.237	46.486	27.032	1.00	51.43
ATOM	3982	C	VAL	B	450	36.974	47.370	29.379	1.00	50.82
ATOM	3983	O	VAL	B	450	38.168	47.604	29.194	1.00	50.69
ATOM	3984	N	GLN	B	451	36.110	48.336	29.709	1.00	51.06
ATOM	3985	CA	GLN	B	451	36.568	49.696	30.050	1.00	51.21
ATOM	3986	CB	GLN	B	451	35.421	50.736	30.048	1.00	51.38
ATOM	3987	CG	GLN	B	451	35.440	51.787	28.868	1.00	52.10
ATOM	3988	CD	GLN	B	451	36.327	53.078	29.113	1.00	53.17
ATOM	3989	OE1	GLN	B	451	36.910	53.628	28.168	1.00	51.41
ATOM	3990	NE2	GLN	B	451	36.403	53.548	30.370	1.00	52.53
ATOM	3991	C	GLN	B	451	37.286	49.704	31.401	1.00	51.70
ATOM	3992	O	GLN	B	451	38.114	50.576	31.677	1.00	51.38
ATOM	3993	N	LEU	B	452	36.970	48.732	32.248	1.00	52.11
ATOM	3994	CA	LEU	B	452	37.685	48.582	33.506	1.00	53.08
ATOM	3995	CB	LEU	B	452	36.971	47.596	34.427	1.00	52.97
ATOM	3996	CG	LEU	B	452	36.515	48.293	35.700	1.00	53.95
ATOM	3997	CD1	LEU	B	452	35.135	47.765	36.153	1.00	55.33
ATOM	3998	CD2	LEU	B	452	37.588	48.104	36.753	1.00	53.43
ATOM	3999	C	LEU	B	452	39.137	48.172	33.295	1.00	53.25
ATOM	4000	O	LEU	B	452	40.047	48.789	33.837	1.00	53.09

71/75

ATOM	4001	N	LEU	B	453	39.332	47.129	32.500	1.00	54.01
ATOM	4002	CA	LEU	B	453	40.659	46.659	32.140	1.00	54.94
ATOM	4003	CB	LEU	B	453	40.541	45.449	31.220	1.00	54.89
ATOM	4004	CG	LEU	B	453	40.167	44.064	31.754	1.00	54.78
ATOM	4005	CD1	LEU	B	453	39.849	44.003	33.255	1.00	55.33
ATOM	4006	CD2	LEU	B	453	39.033	43.493	30.933	1.00	55.14
ATOM	4007	C	LEU	B	453	41.488	47.757	31.470	1.00	55.45
ATOM	4008	O	LEU	B	453	42.684	47.879	31.741	1.00	55.80
ATOM	4009	N	GLN	B	454	40.856	48.568	30.619	1.00	56.10
ATOM	4010	CA	GLN	B	454	41.571	49.654	29.950	1.00	56.88
ATOM	4011	CB	GLN	B	454	40.702	50.384	28.902	1.00	57.06
ATOM	4012	CG	GLN	B	454	39.858	51.556	29.443	1.00	58.00
ATOM	4013	CD	GLN	B	454	39.981	52.845	28.625	1.00	58.94
ATOM	4014	OE1	GLN	B	454	39.841	52.840	27.398	1.00	59.75
ATOM	4015	NE2	GLN	B	454	40.233	53.960	29.313	1.00	58.40
ATOM	4016	C	GLN	B	454	42.179	50.609	30.982	1.00	57.05
ATOM	4017	O	GLN	B	454	43.358	50.944	30.884	1.00	57.00
ATOM	4018	N	VAL	B	455	41.393	51.011	31.983	1.00	57.85
ATOM	4019	CA	VAL	B	455	41.896	51.857	33.092	1.00	58.42
ATOM	4020	CB	VAL	B	455	40.782	52.239	34.119	1.00	58.08
ATOM	4021	CG1	VAL	B	455	41.289	53.294	35.093	1.00	58.18
ATOM	4022	CG2	VAL	B	455	39.536	52.750	33.420	1.00	57.25
ATOM	4023	C	VAL	B	455	43.065	51.165	33.812	1.00	59.23
ATOM	4024	O	VAL	B	455	44.093	51.794	34.074	1.00	59.19
ATOM	4025	N	ILE	B	456	42.886	49.872	34.110	1.00	60.56
ATOM	4026	CA	ILE	B	456	43.931	48.982	34.655	1.00	61.57
ATOM	4027	CB	ILE	B	456	43.404	47.514	34.899	1.00	61.53
ATOM	4028	CG1	ILE	B	456	42.285	47.472	35.953	1.00	61.13
ATOM	4029	CD1	ILE	B	456	42.542	48.315	37.195	1.00	61.23
ATOM	4030	CG2	ILE	B	456	44.533	46.560	35.299	1.00	61.50
ATOM	4031	C	ILE	B	456	45.234	48.956	33.825	1.00	62.54
ATOM	4032	O	ILE	B	456	46.298	49.234	34.375	1.00	62.75
ATOM	4033	N	LYS	B	457	45.162	48.635	32.526	1.00	63.55
ATOM	4034	CA	LYS	B	457	46.366	48.628	31.662	1.00	64.55
ATOM	4035	CB	LYS	B	457	46.048	48.086	30.253	1.00	64.55
ATOM	4036	CG	LYS	B	457	47.134	48.317	29.172	1.00	64.23
ATOM	4037	CD	LYS	B	457	48.513	47.723	29.533	1.00	64.84
ATOM	4038	CE	LYS	B	457	49.657	48.458	28.800	1.00	64.24
ATOM	4039	NZ	LYS	B	457	51.016	48.014	29.236	1.00	62.89
ATOM	4040	C	LYS	B	457	47.112	49.991	31.633	1.00	65.42
ATOM	4041	O	LYS	B	457	48.330	50.048	31.420	1.00	65.51
ATOM	4042	N	LYS	B	458	46.384	51.078	31.877	1.00	66.53
ATOM	4043	CA	LYS	B	458	47.007	52.366	32.180	1.00	67.55
ATOM	4044	CB	LYS	B	458	46.133	53.532	31.689	1.00	67.54
ATOM	4045	CG	LYS	B	458	45.193	53.194	30.519	1.00	67.17
ATOM	4046	CD	LYS	B	458	44.827	54.406	29.662	1.00	67.51
ATOM	4047	CE	LYS	B	458	44.178	55.540	30.462	1.00	67.36
ATOM	4048	NZ	LYS	B	458	44.376	56.857	29.778	1.00	66.25
ATOM	4049	C	LYS	B	458	47.250	52.451	33.701	1.00	68.45
ATOM	4050	O	LYS	B	458	46.829	53.414	34.356	1.00	68.41
ATOM	4051	N	THR	B	459	47.908	51.415	34.241	1.00	69.70
ATOM	4052	CA	THR	B	459	48.287	51.277	35.674	1.00	70.76
ATOM	4053	CB	THR	B	459	47.058	51.445	36.640	1.00	70.86
ATOM	4054	OG1	THR	B	459	46.857	52.842	36.894	1.00	71.23
ATOM	4055	CG2	THR	B	459	47.235	50.699	37.983	1.00	71.02
ATOM	4056	C	THR	B	459	49.103	49.986	35.934	1.00	71.33
ATOM	4057	O	THR	B	459	50.297	50.057	36.246	1.00	71.49
ATOM	4058	N	GLU	B	460	48.468	48.821	35.778	1.00	72.19

72/75

ATOM	4059	CA	GLU	B	460	49.134	47.516	35.934	1.00	72.89
ATOM	4060	CB	GLU	B	460	48.099	46.388	36.115	1.00	73.00
ATOM	4061	CG	GLU	B	460	48.475	45.290	37.142	1.00	73.16
ATOM	4062	CD	GLU	B	460	49.648	44.397	36.708	1.00	73.40
ATOM	4063	OE1	GLU	B	460	49.827	44.162	35.489	1.00	73.80
ATOM	4064	OE2	GLU	B	460	50.389	43.921	37.596	1.00	72.86
ATOM	4065	C	GLU	B	460	50.014	47.272	34.705	1.00	73.19
ATOM	4066	O	GLU	B	460	49.589	46.627	33.728	1.00	73.30
ATOM	4067	N	THR	B	461	51.245	47.779	34.779	1.00	73.45
ATOM	4068	CA	THR	B	461	52.042	48.045	33.582	1.00	73.79
ATOM	4069	CB	THR	B	461	52.338	49.551	33.472	1.00	73.61
ATOM	4070	OG1	THR	B	461	52.658	50.059	34.771	1.00	74.03
ATOM	4071	CG2	THR	B	461	51.119	50.284	32.972	1.00	73.55
ATOM	4072	C	THR	B	461	53.326	47.207	33.412	1.00	74.05
ATOM	4073	O	THR	B	461	53.262	45.979	33.277	1.00	74.16
ATOM	4074	N	ASP	B	462	54.479	47.880	33.421	1.00	74.29
ATOM	4075	CA	ASP	B	462	55.744	47.284	32.965	1.00	74.38
ATOM	4076	CB	ASP	B	462	56.535	48.273	32.083	1.00	74.31
ATOM	4077	CG	ASP	B	462	56.848	49.606	32.777	1.00	73.94
ATOM	4078	OD1	ASP	B	462	56.258	49.924	33.834	1.00	73.37
ATOM	4079	OD2	ASP	B	462	57.694	50.349	32.234	1.00	73.13
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ATOM	4081	O	ASP	B	462	57.308	47.287	34.825	1.00	74.48
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ATOM	4083	CA	MET	B	463	57.596	44.461	34.766	1.00	74.43
ATOM	4084	CB	MET	B	463	56.918	43.900	36.025	1.00	74.48
ATOM	4085	CG	MET	B	463	56.194	44.947	36.894	1.00	74.73
ATOM	4086	SD	MET	B	463	54.863	44.281	37.926	1.00	74.43
ATOM	4087	CE	MET	B	463	55.796	43.746	39.368	1.00	74.62
ATOM	4088	C	MET	B	463	58.082	43.324	33.849	1.00	74.21
ATOM	4089	O	MET	B	463	57.286	42.758	33.087	1.00	74.04
ATOM	4090	N	SER	B	464	59.381	43.009	33.913	1.00	73.83
ATOM	4091	CA	SER	B	464	60.007	42.000	33.024	1.00	73.18
ATOM	4092	CB	SER	B	464	61.305	42.540	32.398	1.00	73.17
ATOM	4093	OG	SER	B	464	61.096	42.899	31.042	1.00	73.02
ATOM	4094	C	SER	B	464	60.227	40.581	33.610	1.00	72.66
ATOM	4095	O	SER	B	464	61.091	39.832	33.123	1.00	72.71
ATOM	4096	N	LEU	B	465	59.454	40.227	34.646	1.00	71.79
ATOM	4097	CA	LEU	B	465	59.265	38.819	35.051	1.00	70.62
ATOM	4098	CB	LEU	B	465	59.659	38.575	36.517	1.00	70.70
ATOM	4099	CG	LEU	B	465	60.577	37.369	36.801	1.00	70.56
ATOM	4100	CD1	LEU	B	465	62.049	37.737	36.656	1.00	70.02
ATOM	4101	CD2	LEU	B	465	60.333	36.789	38.185	1.00	70.70
ATOM	4102	C	LEU	B	465	57.808	38.411	34.765	1.00	69.67
ATOM	4103	O	LEU	B	465	57.435	37.236	34.865	1.00	69.69
ATOM	4104	N	HIS	B	466	57.003	39.405	34.388	1.00	68.33
ATOM	4105	CA	HIS	B	466	55.665	39.190	33.853	1.00	67.05
ATOM	4106	CB	HIS	B	466	55.015	40.524	33.453	1.00	67.31
ATOM	4107	CG	HIS	B	466	54.140	41.127	34.509	1.00	67.81
ATOM	4108	ND1	HIS	B	466	52.780	41.287	34.345	1.00	68.07
ATOM	4109	CE1	HIS	B	466	52.271	41.847	35.429	1.00	68.42
ATOM	4110	NE2	HIS	B	466	53.252	42.062	36.287	1.00	68.35
ATOM	4111	CD2	HIS	B	466	54.432	41.621	35.736	1.00	68.00
ATOM	4112	C	HIS	B	466	55.665	38.243	32.650	1.00	65.82
ATOM	4113	O	HIS	B	466	54.996	37.216	32.710	1.00	65.61
ATOM	4114	N	PRO	B	467	56.454	38.562	31.583	1.00	64.66
ATOM	4115	CA	PRO	B	467	56.344	38.073	30.206	1.00	63.60
ATOM	4116	CB	PRO	B	467	57.802	37.821	29.832	1.00	63.57

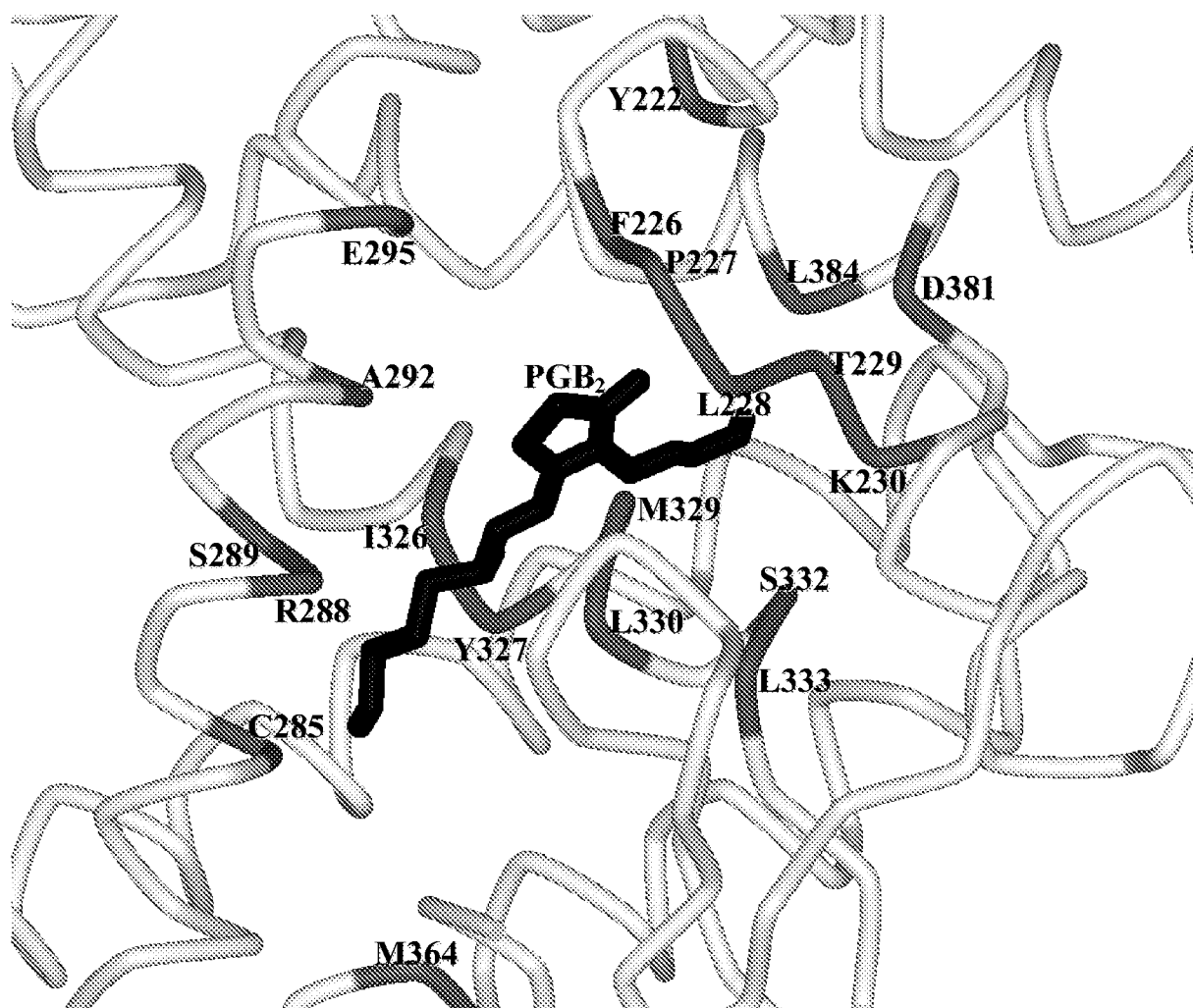
73/75

ATOM	4117	CG	PRO	B	467	58.574	38.856	30.629	1.00	63.99
ATOM	4118	CD	PRO	B	467	57.633	39.442	31.665	1.00	64.60
ATOM	4119	C	PRO	B	467	55.472	36.847	29.930	1.00	62.63
ATOM	4120	O	PRO	B	467	54.578	36.907	29.084	1.00	62.24
ATOM	4121	N	LEU	B	468	55.734	35.748	30.629	1.00	61.70
ATOM	4122	CA	LEU	B	468	55.052	34.496	30.353	1.00	60.53
ATOM	4123	CB	LEU	B	468	55.920	33.318	30.783	1.00	60.29
ATOM	4124	CG	LEU	B	468	56.207	32.167	29.818	1.00	59.26
ATOM	4125	CD1	LEU	B	468	56.073	32.549	28.348	1.00	58.25
ATOM	4126	CD2	LEU	B	468	57.601	31.662	30.110	1.00	56.48
ATOM	4127	C	LEU	B	468	53.680	34.444	31.020	1.00	60.50
ATOM	4128	O	LEU	B	468	52.821	33.683	30.585	1.00	60.31
ATOM	4129	N	LEU	B	469	53.485	35.245	32.072	1.00	60.17
ATOM	4130	CA	LEU	B	469	52.164	35.423	32.700	1.00	60.08
ATOM	4131	CB	LEU	B	469	52.305	35.898	34.150	1.00	60.21
ATOM	4132	CG	LEU	B	469	52.527	34.856	35.248	1.00	60.07
ATOM	4133	CD1	LEU	B	469	53.190	35.471	36.501	1.00	60.51
ATOM	4134	CD2	LEU	B	469	51.215	34.187	35.573	1.00	59.33
ATOM	4135	C	LEU	B	469	51.325	36.425	31.915	1.00	59.92
ATOM	4136	O	LEU	B	469	50.109	36.277	31.805	1.00	59.68
ATOM	4137	N	GLN	B	470	52.002	37.448	31.388	1.00	60.08
ATOM	4138	CA	GLN	B	470	51.420	38.431	30.470	1.00	60.07
ATOM	4139	CB	GLN	B	470	52.528	39.355	29.936	1.00	60.00
ATOM	4140	CG	GLN	B	470	52.141	40.827	29.771	1.00	60.15
ATOM	4141	CD	GLN	B	470	52.469	41.393	28.379	1.00	59.96
ATOM	4142	OE1	GLN	B	470	51.612	42.011	27.741	1.00	58.83
ATOM	4143	NE2	GLN	B	470	53.706	41.179	27.908	1.00	59.37
ATOM	4144	C	GLN	B	470	50.734	37.700	29.312	1.00	59.89
ATOM	4145	O	GLN	B	470	49.638	38.062	28.900	1.00	60.04
ATOM	4146	N	GLU	B	471	51.402	36.660	28.816	1.00	60.01
ATOM	4147	CA	GLU	B	471	50.914	35.786	27.747	1.00	59.99
ATOM	4148	CB	GLU	B	471	52.041	34.850	27.276	1.00	59.93
ATOM	4149	CG	GLU	B	471	52.531	35.088	25.861	1.00	58.98
ATOM	4150	CD	GLU	B	471	52.954	36.525	25.609	1.00	58.24
ATOM	4151	OE1	GLU	B	471	54.077	36.907	26.012	1.00	58.25
ATOM	4152	OE2	GLU	B	471	52.157	37.274	25.004	1.00	56.56
ATOM	4153	C	GLU	B	471	49.709	34.950	28.148	1.00	60.27
ATOM	4154	O	GLU	B	471	48.755	34.829	27.379	1.00	60.20
ATOM	4155	N	ILE	B	472	49.758	34.363	29.341	1.00	60.83
ATOM	4156	CA	ILE	B	472	48.684	33.475	29.800	1.00	61.57
ATOM	4157	CB	ILE	B	472	49.054	32.717	31.122	1.00	61.34
ATOM	4158	CG1	ILE	B	472	50.322	31.883	30.921	1.00	60.74
ATOM	4159	CD1	ILE	B	472	50.739	31.035	32.110	1.00	60.96
ATOM	4160	CG2	ILE	B	472	47.937	31.765	31.548	1.00	61.80
ATOM	4161	C	ILE	B	472	47.361	34.235	29.893	1.00	62.57
ATOM	4162	O	ILE	B	472	46.307	33.710	29.527	1.00	62.96
ATOM	4163	N	TYR	B	473	47.419	35.492	30.317	1.00	64.02
ATOM	4164	CA	TYR	B	473	46.189	36.268	30.504	1.00	65.58
ATOM	4165	CB	TYR	B	473	46.176	36.909	31.895	1.00	65.47
ATOM	4166	CG	TYR	B	473	46.382	35.864	32.964	1.00	65.21
ATOM	4167	CD1	TYR	B	473	45.489	34.808	33.088	1.00	64.61
ATOM	4168	CE1	TYR	B	473	45.663	33.822	34.035	1.00	65.01
ATOM	4169	CZ	TYR	B	473	46.745	33.876	34.883	1.00	64.87
ATOM	4170	OH	TYR	B	473	46.877	32.881	35.811	1.00	64.95
ATOM	4171	CE2	TYR	B	473	47.668	34.914	34.791	1.00	64.77
ATOM	4172	CD2	TYR	B	473	47.484	35.904	33.824	1.00	65.02
ATOM	4173	C	TYR	B	473	45.804	37.248	29.382	1.00	66.80
ATOM	4174	O	TYR	B	473	44.862	38.023	29.543	1.00	67.02

74/75

ATOM	4175	N	LYS	B	474	46.538	37.189	28.266	1.00	68.22
ATOM	4176	CA	LYS	B	474	46.138	37.730	26.945	1.00	69.93
ATOM	4177	CB	LYS	B	474	45.706	36.567	26.032	1.00	70.19
ATOM	4178	CG	LYS	B	474	45.758	36.822	24.498	1.00	70.49
ATOM	4179	CD	LYS	B	474	44.634	36.076	23.718	1.00	70.53
ATOM	4180	CE	LYS	B	474	44.301	34.667	24.272	1.00	71.57
ATOM	4181	NZ	LYS	B	474	45.436	33.679	24.156	1.00	72.57
ATOM	4182	C	LYS	B	474	45.051	38.827	26.929	1.00	70.74
ATOM	4183	O	LYS	B	474	45.361	40.008	26.745	1.00	70.79
ATOM	4184	N	ASP	B	475	43.786	38.415	27.085	1.00	71.75
ATOM	4185	CA	ASP	B	475	42.610	39.314	27.124	1.00	72.64
ATOM	4186	CB	ASP	B	475	42.574	40.272	25.913	1.00	72.78
ATOM	4187	CG	ASP	B	475	42.414	41.747	26.315	1.00	72.99
ATOM	4188	OD1	ASP	B	475	41.525	42.066	27.145	1.00	72.07
ATOM	4189	OD2	ASP	B	475	43.186	42.591	25.789	1.00	72.77
ATOM	4190	C	ASP	B	475	41.311	38.481	27.173	1.00	73.27
ATOM	4191	O	ASP	B	475	40.291	38.938	27.713	1.00	73.17
ATOM	4192	N	LEU	B	476	41.363	37.270	26.602	1.00	73.78
ATOM	4193	CA	LEU	B	476	40.231	36.323	26.622	1.00	74.30
ATOM	4194	CB	LEU	B	476	39.820	35.871	25.188	1.00	74.74
ATOM	4195	CG	LEU	B	476	40.753	35.806	23.948	1.00	75.27
ATOM	4196	CD1	LEU	B	476	40.211	34.816	22.891	1.00	74.82
ATOM	4197	CD2	LEU	B	476	41.034	37.186	23.305	1.00	75.44
ATOM	4198	C	LEU	B	476	40.407	35.128	27.608	1.00	74.14
ATOM	4199	O	LEU	B	476	40.153	35.250	28.815	1.00	74.17
ATOM	4200	OXT	LEU	B	476	40.792	34.009	27.261	1.00	73.89
ATOM	4225	C1	E2P	P	3	35.348	37.117	36.457	1.00	47.90
ATOM	4226	C2	E2P	P	3	35.670	36.175	37.647	1.00	47.37
ATOM	4227	C3	E2P	P	3	35.972	34.723	37.196	1.00	44.09
ATOM	4228	C4	E2P	P	3	35.078	33.688	37.862	1.00	42.82
ATOM	4229	C5	E2P	P	3	34.713	32.543	36.915	1.00	42.83
ATOM	4230	C6	E2P	P	3	33.468	31.765	37.408	1.00	44.53
ATOM	4231	O6	E2P	P	3	32.421	31.858	36.506	1.00	44.01
ATOM	4232	C7	E2P	P	3	33.711	30.285	37.452	1.00	45.26
ATOM	4233	C8	E2P	P	3	32.560	29.576	37.688	1.00	44.93
ATOM	4234	C9	E2P	P	3	32.557	28.203	37.779	1.00	45.97
ATOM	4235	C10	E2P	P	3	33.737	27.217	37.616	1.00	45.45
ATOM	4236	C11	E2P	P	3	33.080	25.841	37.826	1.00	44.05
ATOM	4237	C12	E2P	P	3	31.605	26.197	38.078	1.00	44.93
ATOM	4238	O12	E2P	P	3	30.743	25.356	38.279	1.00	46.16
ATOM	4239	C13	E2P	P	3	31.363	27.570	38.031	1.00	44.63
ATOM	4240	C14	E2P	P	3	30.097	28.368	38.221	1.00	43.91
ATOM	4241	C15	E2P	P	3	28.998	27.545	38.257	1.00	41.39
ATOM	4242	C16	E2P	P	3	27.874	28.040	37.659	1.00	36.40
ATOM	4243	C17	E2P	P	3	26.757	27.215	37.672	1.00	37.50
ATOM	4244	C18	E2P	P	3	25.660	27.865	36.865	1.00	23.95

Fig. 2/3

**Fig. 3/3**

INTERNATIONAL SEARCH REPORT

International application No

PCT/EP2007/058076

A. CLASSIFICATION OF SUBJECT MATTER
 INV. C07K14/705 G06F19/00

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
 G06F C07K

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

EPO-Internal, BIOSIS, EMBASE, WPI Data

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	LU I-LIN ET AL: "Structure-based drug design of a novel family of PPARGgamma partial agonists: virtual screening, X-ray crystallography, and in vitro/in vivo biological activities." JOURNAL OF MEDICINAL CHEMISTRY 4 MAY 2006, vol. 49, no. 9, 4 May 2006 (2006-05-04), pages 2703-2712, XP002455932 ISSN: 0022-2623	1-14
Y	page 2704, column 2, paragraph 2 - page 2705, column 2, paragraph 1 page 2709, column 1, paragraph 2 page 2709, column 2, paragraph 2 - paragraph 3 page 2711, column 1, paragraph 3 - paragraph 4 figures 5-7 abstract ----- -/--	15

☒ Further documents are listed in the continuation of Box C.

☒ See patent family annex.

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- *Z* document member of the same patent family

Date of the actual completion of the international search

22 October 2007

Date of mailing of the international search report

06/11/2007

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Schlegel, Birgit

INTERNATIONAL SEARCH REPORT

International application No

PCT/EP2007/058076

C(Continuation). DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	LAMBERT ET AL: "1K74: THE 2.3 ANGSTROM RESOLUTION CRYSTAL STRUCTURE OF THE HETERODIMER OF THE HUMAN PPARGAMMA AND RXRALPHA LIGAND BINDING DOMAINS RESPECTIVELY BOUND WITH GW409544 AND 9-CIS RETINOIC ACID AND CO-ACTIVATOR PEPTIDES." [Online] 18 October 2001 (2001-10-18), pages 1-75, XP002455933 Protein Database (PDB) PDB Retrieved from the Internet: URL: http://www.pdb.org/pdb/files/1k74.pdb [retrieved on 2007-10-22] page 1 page 35 - page 67	1-15
Y	SAWAI HIROZUMI ET AL: "Activation of peroxisome proliferator-activated receptor-gamma decreases pancreatic cancer cell invasion through modulation of the plasminogen activator system." MOLECULAR CANCER RESEARCH : MCR MAR 2006, vol. 4, no. 3, March 2006 (2006-03), pages 159-167, XP002455934 ISSN: 1541-7786 cited in the application the whole document	15
A	US 2004/137518 A1 (LAMBERT MILLARD HURST [US] ET AL) 15 July 2004 (2004-07-15) the whole document	1-15
A	FYFFE STEWART A ET AL: "Recombinant human PPAR-beta/delta ligand-binding domain is locked in an activated conformation by endogenous fatty acids" JOURNAL OF MOLECULAR BIOLOGY, vol. 356, no. 4, March 2006 (2006-03), pages 1005-1013, XP005265686 ISSN: 0022-2836 page 1005 - page 1011, column 1, paragraph 2; figures 3-5; table 1	1-15

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INTERNATIONAL SEARCH REPORT

International application No

PCT/EP2007/058076

C(Continuation). DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	SHIRAKI TAKUMA ET AL: "Alpha,beta-unsaturated ketone is a core moiety of natural ligands for covalent binding to peroxisome proliferator-activated receptor gamma." THE JOURNAL OF BIOLOGICAL CHEMISTRY. 8 APR 2005, vol. 280, no. 14, 8 April 2005 (2005-04-08), pages 14145-14153, XP002367917 ISSN: 0021-9258 the whole document -----	1-15
A	SHEU SHU-HSIEN ET AL: "Exploring the binding site structure of the PPAR gamma ligand-binding domain by computational solvent mapping." BIOCHEMISTRY. 1 FEB 2005, vol. 44, no. 4, 1 February 2005 (2005-02-01), pages 1193-1209, XP002408942 ISSN: 0006-2960 page 1193, column 1, paragraph 1 - page 1194, column 2, paragraph 1; tables 1,2 abstract -----	1-15

Information on patent family members

PCT/EP2007/058076

Form PCT/ISA/210 (patent family annex) (April 2005)