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(54) **Title**: AMYLOID-BETA PEPTIDE CRYSTAL STRUCTURE

(57) **Abstract**: The invention relates provides a novel crystal structure of the fibrillogenic part of amyloid β-peptide (Aβ). More specifically the crystal structure is Aβ-IgNAR and, accordingly the present invention also relates to selecting and/or designing compounds that modulate amyloid β-peptide (Aβ) activity using techniques such as in silico screening and crystal soaking experiments. The invention further relates to compounds and methods for inhibiting interaction between amyloid β-peptide (Aβ) monomers, more particularly, inhibiting or disrupting amyloid β-peptide (Aβ) oligomer formation and toxic activity.

AMYLOID-BETA PEPTIDE CRYSTAL STRUCTURE

FILING DATA

[0001] This application is associated with and claims priority from Australian patent application no. 2008905174 filed on 6 October 2008 and Australian patent application no. 2008905176 filed on 6 October 2008, the entire contents of each of these applications are incorporated herein by reference.

FIELD

[0002] The invention relates generally to a novel crystal structure of the fibrillogenic part of amyloid β-peptide (Aβ). More specifically the crystal structure is Aβ-IgNAR and, accordingly the present invention also relates to selecting and/or designing compounds that modulate amyloid β-peptide (Aβ) activity using techniques such as in silico screening and crystal soaking experiments. The invention further relates to compounds and methods for inhibiting interaction between amyloid β-peptide (Aβ) monomers, more particularly, inhibiting or disrupting amyloid β-peptide (Aβ) oligomer formation and toxic activity

BACKGROUND

[0003] Bibliographic details of the publications referred to by author in this specification are collected alphabetically at the end of the description. The disclosure of each reference referred to in this application is incorporated herein by reference.

[0004] Reference to any prior art in this specification is not, and should not be taken as, an acknowledgment or any form of suggestion that this prior art forms part of the common general knowledge in any country.

[0005] Alzheimer's disease (AD) is a progressive neurodegenerative disorder characterized by the presence of misfolded protein depositions or amyloid plaques Crouch, P. J., S.-M. E. Harding, et al. (2008). "Mechanisms of Aβ mediated neurodegeneration in Alzheimer's disease." Int J Biochem Cell Biol 40(2): 181-198. Plaques consist predominantly of amyloid β-peptide (Aβ), which is produced by cleavage from the membrane-bound amyloid precursor protein (APP) via the β/γ secretase pathway. (The sequence of Aβ is set out in SEQ ID NO 1). However, the current view suggests that soluble Aβ oligomer intermediates, and not the plaque burden, may be the major drivers of Aβ-mediated neuronal dysfunction Walsh, D. M. and D. J. Selkoe (2007). "Aβ oligomers - a decade of discovery." J. Neurochem. 101(5): 1172-1184. Shankar, G. M., S. Li, et al. (2008). "Amyloid-beta protein dimers isolated directly from Alzheimer's brains impair synaptic plasticity and memory." Nat Med. Frustratingly, obtaining atomic resolution information for Aβ and such oligomers has been a

major challenge Kajava, A. V., J. M. Squire, et al. (2006). "β-structures in fibrous proteins." Adv Protein Chem 73: 1-15. Nelson, R. and D. Eisenberg (2006). "Recent atomic models of amyloid fibril structure." Curr Opin Struct Biol 16(2): 260-265. Nelson, R. and D. Eisenberg (2006). "Structural models of amyloid-like fibrils." Adv Protein Chem 73: 235-282, due in part to the propensity of the peptide to form amyloidal fibrils and aggregates rather than form crystallographic lattices.

[0006] The present inventors have obtained a 2.2 Å resolution crystal structure of residues 18-41 of Aβ peptide constrained within the CDR3 loop region of a shark IgNAR single variable domain antibody Henderson, K. A., V. A. Streltsov, et al. (2007). "Structure of an IgNAR-AMA1 complex: targeting a conserved hydrophobic cleft broadens malarial strain recognition." Structure 15(11): 1452-66. The predominant oligomeric species is a tightly-associated Aβ dimer, with paired dimers forming a tetramer which is caged within four IgNAR domains, preventing further uncontrolled amyloid formation. The results reveal unusual Aβ loop topologies and inter-peptide interactions, strikingly different from fibrillar models based on solid state NMR spectroscopy data Petkova, A. T., Y. Ishii, et al. (2002). "A structural model for Alzheimer's b-amyloid fibrils based on experimental constraints from solid state NMR." Proc Natl Acad Sci U S A 99(26): 16742-16747. Luhrs, T., C. Ritter, et al. (2005). "3D structure of Alzheimer's amyloid-β(1-42) fibrils." Proc Natl Acad Sci U S A 102(48): 17342-17347. Petkova, A. T., W. M. Yau, et al. (2006). "Experimental constraints on quaternary structure in Alzheimer's β-amyloid fibrils." Biochemistry 45(2): 498-512. Sato, T., P. Kienlen-Campard, et al. (2006). "Inhibitors of amyloid toxicity based on β-sheet packing of Aβ40 and Aβ42." Biochemistry 45(17): 5503-5516, that describe Aβ residues 18–42 as forming parallel, in-register β-sheets. Notwithstanding, conserved elements can be identified within the structure consistent with residues and motifs previously identified as critical in Aβ peptide folding and neurotoxicity. This crystallographic model suggests a novel paradigm for Aβ oligomer formation, and potentially provides a system for the testing of Aβ oligomer imaging reagents and Alzheimer's disease drug candidates.

SUMMARY OF THE INVENTION

[0007] In a first aspect the present invention provides a crystal of amyloid β-peptide (Aβ(18-41) as a fusion with IgNAR (Aβ-IgNAR). In a preferred embodiment the Aβ-IgNAR crystal substantially conforms to the atomic co-ordinates of Appendix I. Preferably at least 75% of the structure has the recited RMSD value, more preferably at least 90% of the structure has the recited RMSD value and most preferably about 100% of the structure has the recited RMSD value.

[0008] In a second aspect the present invention provides an Aβ-IgNAR molecule having the amino acid sequence of SEQ ID Nos 15 to 24.

[0009] In a third aspect the present invention provides a method of assessing the interaction of a compound with Aβ, the method comprising contacting the crystal of the present invention with the compound and measuring the level of binding of the compound to the Aβ crystal.

[0010] In a fourth aspect the present invention provides a method of selecting or designing a compound that interacts with Aβ protein, the method comprising (a) assessing the stereochemical complementarity between a compound and a topographic region of Aβ protein, wherein the protein comprises: (i) amino acids 18-41 of the Aβ protein positioned at atomic coordinates as shown in Appendix I, or structural coordinates having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å ; or (ii) one or more subsets of said amino acids related to the coordinates shown in Appendix I by whole body translations and/or rotations; (b) obtaining a compound which possesses stereochemical complementarity to a topographic region of the Aβ protein; and (c) testing the compound for its ability to modulate an activity associated with the Aβ protein.

[0011] In a fifth aspect the present invention provides a method for identifying a potential modulator compound for Aβ protein which method comprises: (a) providing a three-dimensional structure of amino acids 18-41 of Aβ protein as defined by the atomic coordinates shown in Appendix I, or atomic coordinates having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, or one or more subsets of said amino acids, or one or more subsets of said amino acids related to the coordinates shown in Appendix I by whole body translations and/or rotations; (b) providing the three-dimensional structure of a candidate compound; and (c) assessing the stereochemical complementarity between the three- dimensional structure of step (b) and a topographic region of the three-dimensional structure of step (a).

[0012] In a sixth aspect the present invention provides a computer-assisted method for identifying potential compounds able to interact with Aβ protein and thereby modulate an activity mediated by Aβ protein, using a programmed computer comprising a processor, an input device, and an output device, comprising the steps of: (a) inputting into the programmed computer, through the input device, data comprising the atomic coordinates of amino acids 18-41 of Aβ protein as shown in Appendix I, or structural coordinates having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, or one or more subsets of said amino acids, or one or more subsets of said amino acids related to the coordinates shown in Appendix I by whole body translations and/or rotations; (b) generating, using computer methods, a set of atomic coordinates of a structure that possesses stereochemical complementarity to the atomic coordinates of amino acids 18-41 of the Aβ protein as shown in Appendix I, or structural coordinates having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, or one or more subsets

of said amino acids, or one or more subsets of said amino acids related to the coordinates shown in Appendix I by whole body translations and/or rotations, thereby generating a criteria data set; (c) comparing, using the processor, the criteria data set to a computer database of chemical structures; (d) selecting from the database, using computer methods, chemical structures which are similar to a portion of said criteria data set; and (e) outputting, to the output device, the selected chemical structures which are complementary to or similar to a portion of the criteria data set.

[0013] In a seventh aspect the present invention provides a method for evaluating the ability of a chemical entity to interact with Aβ protein, said method comprising the steps of: (a) creating a computer model of amino acids 18-41 of Aβ protein using structure coordinates wherein the root mean square deviation between said structure coordinates and the structure coordinates of amino acids 18-41 of Aβ protein as set forth in Appendix I is not more than about 1.5 Å ; (b) employing computational means to perform a fitting operation between the chemical entity and said computer model of the binding surface; and (c) analysing the results of said fitting operation to quantify the association between the chemical entity and the Aβ protein model.

[0014] In an eighth aspect the present invention provides a computer for producing a three-dimensional representation of a molecule or molecular complex, wherein the computer comprises: (a) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein the machine readable data comprise the atomic coordinates of amino acids 18-41 of Aβ protein as shown in Appendix I, or structural coordinates having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, or one or more subsets of said amino acids, or one or more subsets of said amino acids related to the coordinates shown in Appendix I by whole body translations and/or rotations; (b) a working memory for storing instructions for processing the machine-readable data; (c) a central-processing unit coupled to the working memory and to the machine-readable data storage medium, for processing the machine- readable data into the three dimensional representation; and (d) an output hardware coupled to the central processing unit, for receiving the three-dimensional representation.

[0015] In a ninth aspect the present invention provides a method of assessing the ability of a compound to affect the ability of Aβ to form dimers or tetramers, the method comprising assessing the level Aβ-IgNAR dimerisation or tetramerisation in the presence or absence of the compound.

[0016] In an embodiment of this aspect of the invention the Aβ-IgNAR has the amino acid sequence of any one of SEQ ID NOs: 2, 4-13, 15-24. In another embodiment the assessment of dimerisation or tetramerisation is made by SDS-PAGE or western blot.

[0017] In a tenth aspect the present invention provides a method of assessing the affect of a mutation in Aβ to affect the ability of Aβ to form dimers or tetramers, the method comprising assessing the level of dimerisation or tetramerisation of Aβ-IgNAR including the mutation, assessing the level of dimerisation or tetramerisation of Aβ-IgNAR without the mutation and comparing the two levels.

[0018] In an embodiment of this aspect of the invention the Aβ-IgNAR not including the mutation has the amino acid sequence of any one of SEQ ID NOs: 2, 4-6, 15-18. In another embodiment the assessment of dimerisation or tetramerisation is made by SDS-PAGE or western blot.

[0019] In a eleventh aspect the present invention provides a compound for inhibiting or disrupting amyloid β-peptide oligomer formation or toxic activity, wherein the compound interacts with the region of Aβ-peptide defined by N27, K28, I31 and L34 of Aβ-peptide wherein amino acids 18-41 of the Aβ protein are positioned at atomic coordinates as shown in Appendix I, or structural coordinates having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

[0020] In an twelfth aspect the present invention provides a compound for inhibiting or disrupting amyloid β-peptide oligomer formation or toxic activity, wherein the compound interacts with the region of Aβ-peptide defined by G33, L34, M35 and V36 of Aβ-peptide wherein amino acids 18-41 of the Aβ protein are positioned at atomic coordinates as shown in Appendix I, or structural coordinates having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

[0021] In a thirteenth aspect the present invention provides a compound for inhibiting or disrupting amyloid β-peptide oligomer formation or toxic activity, wherein the compound interacts with the region of Aβ-peptide defined by V18, F20, S26, K28, G29, I32, M35, V39 and I41 of Aβ-peptide wherein amino acids 18-41 of the Aβ protein are positioned at atomic coordinates as shown in Appendix I, or structural coordinates having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

[0022] In a fourteenth aspect the present invention provides a compound for decreasing metal binding by amyloid β-peptide oligomers, wherein the compound interacts with the aligned E22 of the Aβ monomers in the Aβ oligomer.

[0023] In a fifteenth aspect the present invention provides the use of an Aβ-IgNAR molecule of any one SEQ ID NOs 2, 4, 5, 6, 13, 15, 16, 17 or 18 to raise antibodies against Aβ wherein the antibodies bind to residues 18 to 41 of SEQ ID NO 1 when presented in the

Aβ-IgNAR molecule of any one of SEQ ID NOs 2, 4, 5, 6, 13, 15, 16, 17 or 18 but not to an isolated linear peptide having a sequence of residues 18 to 41 of SEQ ID NO 1.

[0024] In a sixteenth aspect the present invention provides an antibody which specifically binds to residues 18 to 41 of SEQ ID NO 1 when presented in the Aβ-IgNAR molecule of any one of SEQ ID NOs 2, 4, 5, 6, 13, 15, 16, 17 or 18 but not to an isolated linear peptide having the sequence of residues 18 to 41 of SEQ ID NO 1.

BRIEF DESCRIPTION OF THE FIGURES

[0025] **Figure 1** shows a schematic representation Aβ-IgNAR dimer, illustrating dimer (1), tetramer (2), and amyloid (3) interfaces.

[0026] **Figure 2 Aβ-IgNAR fusions form a stable dimer. a,** Affinity purified Aβ-IgNAR-G1 elutes as a dimer by gel filtration (solid line) in comparison to 12Y-2 IgNAR monomer (dotted line), **b,** SDS-PAGE of affinity-purified Aβ-IgNAR-G1 under reducing (R) and non-reducing (U) conditions, illustrating formation of tetrameric (arrowed) species in the absence of heating/reducing agent.

[0027] **Figure 3 Representative electron density for Aβ-IgNAR-G1.** Electron density $2F_0$-F_c for residues 18-41 of Aβ-IgNAR-G1 chain A. The map is contoured at 1.0σ.

[0028] **Figure 4 Aβ-IgNAR-G1 tetramer.** Three aspects of the Aβ-IgNAR-G1 tetramer are shown, illustrating the axis of approximate symmetry through dimeric and tetrameric forms.

[0029] **Figure 5 Models of amyloid fibril formation. a,** Construction of Aβ oligomer model based on the Aβ-IgNAR-G1 tetramer, incorporating six Aβ (1-41) metal-binding tetramers. The cartoon representation is overlayed with surfaces shaded by chains. Black spheres represent metals (Zn, Cu etc). **b,** As for a, represented as solubility surface (dark - hydrophilic; light – hydrophobic) **c,** View along the oligomer axis.

[0030] **Figure 6** In silico docking of ChemBridge 9124833 to the Aβ-IgNAR-G1 structure. The compound 3-methoxy-4-[2-(4-morpholinyl)-2-oxoethoxy]aniline (dark shading) docked within the Aβ-IgNAR-G1 structure (wireframe).

[0031] **Figure 7** In silico docking of ChemBridge 7996209 to the Aβ-IgNAR-G1 structure. The compound N-[2-(4-methylphenyl)-2-oxoethyl]-1-oxo-3,4-dihydro-1H-isochromene-3-carboxamide (dark shading) docked within the Aβ-IgNAR-G1 structure (wireframe).

[0032] **Figure 8** In silico docking of ChemBridge 7949851 to the Aβ-IgNAR-G1 structure. The compound methyl [3-(phenoxyacetyl)-1H-indol-1-yl]acetate (dark shading) docked

within the Aβ-IgNAR-G1 structure (wireframe).

[0033] Figure 9 In silico docking of ChemBridge 7780327 to the Aβ–IgNAR-G1 structure. The compound 2-methyl-3-{[(3-methylphenoxy)acetyl]amino}benzoic acid (dark shading) docked within the Aβ–IgNAR-G1 structure (wireframe).

[0034] Figure 10 In silico docking of ChemBridge 7302096 to the Aβ-IgNAR-G1 structure. The compound 3-{[(2,5-dimethoxyphenyl)amino]carbonyl}-7-oxabicyclo[2.2.1]hept-5-ene-2-carboxylic acid (dark shading) docked within the Aβ-IgNAR-G1 structure (wireframe).

[0035] Figure 11 In silico docking of ChemBridge 5785027 to the Aβ-IgNAR-G1 structure. The compound 2-{2-[(2-hydroxyethyl)amino]-1H-benzimidazol-1-yl}-1-(1-naphthyl)ethanone hydrobromide (dark shading) docked within the Aβ-IgNAR-G1 structure (wireframe).

[0036] Figure 12 In silico docking of fenofibrate to the Aβ-IgNAR-G1 structure. Fenofibrate (dark shading) docked within the Aβ-IgNAR-G1 structure (wireframe).

DETAILED DESCRIPTION OF THE INVENTION

Definitions

[0037] The reference to residue numbers in respect of Aβ is to number residue as in the sequence of Aβ as provided in SEQ ID NO: 1. The residue number is not the number of the residue as it appears in the Aβ-IgNAR molecule.

[0038] As used herein, the term "atomic coordinates" refer to a set of values which define the position of one or more atoms with reference to a system of axes.

[0039] A structure that "substantially conforms" to a given set of atomic coordinates is a structure wherein at least about 50% of such structure has an RMSD of less than about 1.5 Å for the backbone atoms in secondary structure elements in each domain, and more preferably, less than about 1.3 Å for the backbone atoms in secondary structure elements in each domain, and, in increasing preference, less than about 1.0 Å, less than about 0.7 Å, less than about 0.5 Å, and most preferably, less than about 0.3 Å for the backbone atoms in secondary structure elements in each domain.

[0040] Preferably a structure that substantially conforms to a given set of atomic co-ordinates is a structure wherein at least about 75% of such structure has the recited RMSD value, more preferably at least about 90% of such structure has the recited RMSD value, and most preferably, about 100% of such structure has the recited RMSD value.

[0041] The above definition of "substantially conforms" can be extended to include atoms of amino acid side chains. As used herein, the phrase "common amino acid side chains" refers to amino acid side chains that are common to both the structure which substantially conforms to a given set of atomic coordinates and the structure that is actually represented by such atomic coordinates.

[0042] By the terms "modulate" or "modulating" it is meant that the compound changes an Aβ monomer, dimer, or tetramer by at least 10%. Suitably, a compound modulates Aβ monomer, dimer, or tetramer by decreasing oligomerization or toxicity.

[0043] By using the terms "inhibition"/"inhibiting" and/or "disruption"/"disrupting" it is intended to include the concept of "modulate" or "modulating."

[0044] The phrase "decrease oligomerization or toxicity" is intended to encompass partial or complete inhibition of oligomerization or toxicity. The ability of a compound to increase or decrease activity can be assessed by any one of the Aβ oligomerization or toxicity assays described herein.

[0045] The term "antibody", as used herein, broadly refers to any immunoglobulin (Ig) molecule comprised of four polypeptide chains, two heavy (H) chains and two light (L) chains, or any functional fragment, mutant, variant, or derivation thereof, which retains the essential epitope binding features of an Ig molecule. Such mutant, variant, or derivative antibody formats are known in the art. Non-limiting embodiments of which are discussed below.

[0046] In a full-length antibody, each heavy chain is comprised of a heavy chain variable region (abbreviated herein as HCVR or VH) and a heavy chain constant region. The heavy chain constant region is comprised of three domains, CHl, CH2 and CH3. Each light chain is comprised of a light chain variable region (abbreviated herein as LCVR or VL) and a light chain constant region. The light chain constant region is comprised of one domain, CL. The VH and VL regions can be further subdivided into regions of hypervariability, termed complementarity determining regions (CDR), interspersed with regions that are more conserved, termed framework regions (FR). Each VH and VL is composed of three CDRs and four FRs, arranged from amino-terminus to carboxy-terminus in the following order: FRl, CDRl, FR2, CDR2, FR3, CDR3, FR4. Immunoglobulin molecules can be of any type (e.g., IgG, IgE, IgM, IgD, IgA and IgY), class (e.g., IgG1, IgG2, IgG 3, IgG4, IgAl and IgA2) or subclass.

[0047] The term "antigen binding domain" or “antigen binding portion” of an antibody, as used herein, refers to one or more fragments of an antibody or protein that retain the ability to

specifically bind to an antigen (e.g., IL-12). It has been shown that the antigen-binding function of an antibody can be performed by fragments of a full-length antibody. Such antibody embodiments may also be bispecific, dual specific, or multi-specific formats; specifically binding to two or more different antigens. Examples of binding fragments encompassed within the term "antigen- binding portion" of an antibody include (i) a Fab fragment, a monovalent fragment consisting of the VL, VH, CL and CHl domains; (ii) a F(ab')2 fragment, a bivalent fragment comprising two Fab fragments linked by a disulfide bridge at the hinge region; (iii) a Fd fragment consisting of the VH and CHl domains; (iv) a Fv fragment consisting of the VL and VH domains of a single arm of an antibody , (v) a dAb fragment (Ward et al. 1989 Nature 341 544-6, Winter et al., PCT publication WO 90/05144 Al herein incorporated by reference), which comprises a single variable domain; and (vi) an isolated complementarity determining region (CDR). Furthermore, although the two domains of the Fv fragment, VL and VH, are coded for by separate genes, they can be joined, using recombinant methods, by a synthetic linker that enables them to be made as a single protein chain in which the VL and VH regions pair to form monovalent molecules (known as single chain Fv (scFv); (see e.g.,Bird et al. 1988 Science 242 423-6; Huston et al. 1988 Proc Natl Acad Sci U S A 85 5879-83). Such single chain antibodies are also intended to be encompassed within the term "antigen-binding portion" of an antibody. Other forms of single chain antibodies, such as diabodies are also encompassed. Diabodies are bivalent, bispecific antibodies in which VH and VL domains are expressed on a single polypeptide chain, but using a linker that is too short to allow for pairing between the two domains on the same chain, thereby forcing the domains to pair with complementary domains of another chain and creating two antigen binding sites (see e.g., Holliger, P., et al., 1993, Proc. Natl. Acad. Sci. USA 90:6444-6448; Poljak, R. J., et al., 1994, Structure 2:1121-1123). Such antibody binding portions are known in the art (Kontermann and Dubel eds., Antibody Engineering 2001 Springer-Verlag. New York. 790 pp., ISBN 3-540-41354-5).

[0048] In a first aspect the present invention provides a crystal of amyloid β-peptide Aβ(18-41) as a fusion with IgNAR (Aβ-IgNAR). In a preferred embodiment the Aβ-IgNAR crystal substantially conforms to the atomic co-ordinates of Appendix I. Preferably at least 75% of the structure has the recited RMSD value, more preferably at least 90% of the structure has the recited RMSD value and most preferably about 100% of the structure has the recited RMSD value.

[0049] In a second aspect the present invention provides an Aβ-IgNAR molecule having the amino acid sequence of SEQ ID Nos 15 to 24.

[0050] In a third aspect the present invention provides a method of assessing the interaction of a compound with Aβ, the method comprising contacting the crystal of the present invention

with the compound and measuring the level of binding of the compound to the Aβ crystal.

[0051] In a fourth aspect the present invention provides a method of selecting or designing a compound that interacts with Aβ protein, the method comprising (a) assessing the stereochemical complementarity between a compound and a topographic region of Aβ protein, wherein the protein comprises: (i) amino acids 18-41 of the Aβ protein positioned at atomic coordinates as shown in Appendix I, or structural coordinates having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å; or (ii) one or more subsets of said amino acids related to the coordinates shown in Appendix I by whole body translations and/or rotations; (b) obtaining a compound which possesses stereochemical complementarity to a topographic region of the Aβ protein; and (c) testing the compound for its ability to modulate an activity associated with the Aβ protein.

[0052] In a fifth aspect the present invention provides a method for identifying a potential modulator compound for Aβ protein which method comprises: (a) providing a three-dimensional structure of amino acids 18-41 of Aβ protein as defined by the atomic coordinates shown in Appendix I, or atomic coordinates having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, or one or more subsets of said amino acids, or one or more subsets of said amino acids related to the coordinates shown in Appendix I by whole body translations and/or rotations; (b) providing the three-dimensional structure of a candidate compound; and (c) assessing the stereochemical complementarity between the three- dimensional structure of step (b) and a topographical region of the three-dimensional structure of step (a).

[0053] In a sixth aspect the present invention provides a computer-assisted method for identifying potential compounds able to interact with Aβ protein and thereby modulate an activity mediated by Aβ protein, using a programmed computer comprising a processor, an input device, and an output device, comprising the steps of: (a) inputting into the programmed computer, through the input device, data comprising the atomic coordinates of amino acids 18-41 of Aβ protein as shown in Appendix I, or structural coordinates having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, or one or more subsets of said amino acids, or one or more subsets of said amino acids related to the coordinates shown in Appendix I by whole body translations and/or rotations; (b) generating, using computer methods, a set of atomic coordinates of a structure that possesses stereochemical complementarity to the atomic coordinates of amino acids 18-41 of the Aβ protein as shown in Appendix I, or structural coordinates having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, or one or more subsets of said amino acids, or one or more subsets of said amino acids related to the coordinates shown in Appendix I by whole body translations and/or rotations, thereby generating a criteria

data set; (c) comparing, using the processor, the criteria data set to a computer database of chemical structures; (d) selecting from the database, using computer methods, chemical structures which are similar to a portion of said criteria data set; and (e) outputting, to the output device, the selected chemical structures which are complementary to or similar to a portion of the criteria data set.

[0054] In a seventh aspect the present invention provides a method for evaluating the ability of a chemical entity to interact with Aβ protein, said method comprising the steps of: (a) creating a computer model of amino acids 18-41 of Aβ protein using structure coordinates wherein the root mean square deviation between said structure coordinates and the structure coordinates of amino acids 18-41 of Aβ protein as set forth in Appendix I is not more than about 1.5 Å ; (b) employing computational means to perform a fitting operation between the chemical entity and said computer model of the binding surface; and (c) analysing the results of said fitting operation to quantify the association between the chemical entity and the Aβ protein model.

[0055] In an eighth aspect the present invention provides a computer for producing a three-dimensional representation of a molecule or molecular complex, wherein the computer comprises: (a) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein the machine readable data comprise the atomic coordinates of amino acids 18-41 of Aβ protein as shown in Appendix I, or structural coordinates having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, or one or more subsets of said amino acids, or one or more subsets of said amino acids related to the coordinates shown in Appendix I by whole body translations and/or rotations; (b) a working memory for storing instructions for processing the machine-readable data; (c) a central-processing unit coupled to the working memory and to the machine-readable data storage medium, for processing the machine- readable data into the three dimensional representation; and (d) an output hardware coupled to the central processing unit, for receiving the three-dimensional representation.

[0056] The Aβ-IgNAR crystal may comprises an Aβ-IgNAR monomer, dimer or tetramer as described in more detail below.

[0057] In a preferred embodiment, an Aβ-IgNAR crystal of the invention has the atomic coordinates set forth in Appendix I. It will be understood by those skilled in the art that atomic coordinates may be varied, without affecting significantly the accuracy of models derived therefrom; thus, although the invention provides a very precise definition of a preferred atomic structure, it will be understood that minor variations are envisaged and the claims are intended to encompass such variations. Preferred are variants in which the root mean square deviation (RMSD) of the x, y and z co-ordinates for all backbone atoms other

than hydrogen is less than 1.5 Å (preferably less than 1 Å, 0.7 Å or less than 0. 3 Å) compared with the coordinates given in Appendix I. It will be readily appreciated by those skilled in the art that a 3D rigid body rotation and/or translation of the atomic coordinates does not alter the structure of the molecule concerned.

[0058] In a highly preferred embodiment, the crystal has the atomic coordinates as shown in Appendix I.

[0059] As used herein, the term "atomic coordinates" refer to a set of values which define the position of one or more atoms with reference to a system of axes.

[0060] The present invention also provides a crystal structure of an Aβ(18-41) polypeptide (monomer, dimer and tetramer), or a region thereof.

[0061] The atomic coordinates obtained experimentally for amino acids 18 to 41 of Aβ-IgNAR are shown in Appendix I. However, a person skilled in the art will appreciate that a set of atomic coordinates determined by X-ray crystallography is not without standard error. Accordingly, any set of structure coordinates for an Aβ-IgNAR polypeptide that has a root mean square deviation of protein backbone atoms of less than 1.5 Å when superimposed (using backbone atoms) on the atomic coordinates listed in Appendix I shall be considered identical.

[0062] The present invention also comprises the atomic coordinates of Aβ(18-41) polypeptide (monomer, dimer and tetramer) that substantially conform to the atomic coordinates listed in Appendix I.

[0063] A structure that "substantially conforms" to a given set of atomic coordinates is a structure wherein at least about 50% of such structure has an RMSD of less than about 1.5 Å for the backbone atoms in secondary structure elements in each domain, and more preferably, less than about 1.3 Å for the backbone atoms in secondary structure elements in each domain, and, in increasing preference, less than about 1.0 Å, less than about 0.7 Å, less than about 0.5 Å, and most preferably, less than about 0.3 Å for the backbone atoms in secondary structure elements in each domain.

[0064] In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of such structure has the recited RMSD value, and more preferably, at least about 90% of such structure has the recited RMSD value, and most preferably, about 100% of such structure has the recited RMSD value.

[0065] In an even more preferred embodiment, the above definition of "substantially conforms" can be extended to include atoms of amino acid side chains. As used herein, the

phrase "common amino acid side chains" refers to amino acid side chains that are common to both the structure which substantially conforms to a given set of atomic coordinates and the structure that is actually represented by such atomic coordinates.

[0066] The variations in coordinates may be generated due to mathematical manipulations of the structure coordinates. For example, the structure coordinates set forth in Appendix I could be manipulated by crystallographic permutations of the structure coordinates, fractionalisation of the structure coordinates, integer additions or subtractions to sets of the structure coordinates, inversion of the structure coordinates, or any combination thereof.

[0067] Alternatively, modification in the crystal structure due to mutations, additions, substitutions, and/or deletions of amino acids, or other changes in any of the components that make up the crystal could also account for variations in structure coordinates.

[0068] Various computational analyses are used to determine whether a molecular complex or a portion thereof is sufficiently similar to all or parts of the structure of Aβ-IgNAR and Aβ monomer, dimer and tetramer described above. Such analyses may be carried out in current software applications, such as the Molecular Similarity program of QUANTA (Molecular Simulations Inc., San Diego, CA) version 4.1.

[0069] The Molecular Similarity program permits comparisons between different structures, different conformations of the same structure, and different parts of the same structure.

[0070] Comparisons typically involve calculation of the optimum translations and rotations required such that the root mean square difference of the fit over the specified pairs of equivalent atoms is an absolute minimum. This number is given in angstroms.

[0071] Accordingly, structural coordinates of Aβ-IgNAR or Aβ monomer, dimer or tetramer within the scope of the present invention include structural coordinates related to the atomic coordinates listed in Appendix I by whole body translations and/or rotations. Accordingly, RMSD values listed above assume that at least the backbone atoms of the structures are optimally superimposed which may require translation and/or rotation to achieve the required optimal fit from which to calculate the RMSD value.

[0072] A three dimensional structure of Aβ-IgNAR or Aβ monomer, dimer or tetramer or region thereof which substantially conforms to a specified set of atomic coordinates can be modelled by a suitable modeling computer program such as MODELER (Sali & Blundell, 1993), as implemented in the Insight II Homology software package (Insight II (97.0), MSI, San Diego), using information, for example, derived from the following data: (1) the amino acid sequence of the Aβ-IgNAR or Aβ monomer, dimer or tetramer polypeptide; (2) the amino acid sequence of the related portion(s) of the protein represented by the specified set of

atomic coordinates having a three dimensional configuration; and, (3) the atomic coordinates of the specified three dimensional configuration. A three dimensional structure of Aβ-IgNAR or Aβ monomer, dimer or tetramer polypeptide which substantially conforms to a specified set of atomic coordinates can also be calculated by a method such as molecular replacement, which is described in detail below.

[0073] Structure coordinates/atomic coordinates are typically loaded onto a machine readable-medium for subsequent computational manipulation. Thus models and/or atomic coordinates are advantageously stored on machine-readable media, such as magnetic or optical media and random-access or read-only memory, including tapes, diskettes, hard disks, CD-ROMs and DVDs, flash memory cards or chips, servers and the internet. The machine is typically a computer.

[0074] The structure coordinates/atomic coordinates may be used in a computer to generate a representation, e.g. an image, of the three-dimensional structure of the Aβ-IgNAR or Aβ monomer, dimer or tetramer crystal which can be displayed by the computer and/or represented in an electronic file.

[0075] The structure coordinates/atomic coordinates and models derived therefrom may also be used for a variety of purposes such as drug discovery, biological reagent (binding protein) selection and X-ray crystallographic analysis of other protein crystals.

[0076] The three-dimensional structure of Aβ-IgNAR or Aβ monomer, dimer or tetramer provided by the present invention can be used to identify potential target binding sites on Aβ monomer, dimer or tetramers, or derived higher order multimers (i.e. to identify those regions of Aβ involved in oligomerization and/or toxicity and/or disease) as well as in methods for identifying or designing compounds which interact with potential target binding sites of Aβ, e.g. potential modulators/inhibitors of Aβ.

[0077] In one embodiment, the target binding site is a region of Aβ involved in oligermisation. Preferred target binding sites comprise one or more of the following domains: the dimerisation domain, the tetramerisation domain, the amyloid formation domain.

[0078] In a ninth aspect the present invention provides a method of assessing the ability of a compound to affect the ability of Aβ to form dimers or tetramers, the method comprising assessing the level Aβ-IgNAR dimerisation or tetramerisation in the presence or absence of the compound.

[0079] In an embodiment of this aspect of the invention the Aβ-IgNAR has the amino acid sequence of any one of SEQ ID NOs: 2, 4-13, 15-24. In another embodiment the assessment of dimerisation or tetramerisation is made by SDS-PAGE or western blot.

[0080] In a tenth aspect the present invention provides a method of assessing the affect of a mutation in Aβ to affect the ability of Aβ to form dimers or tetramers, the method comprising assessing the level of dimerisation or tetramerisation of Aβ-IgNAR including the mutation, assessing the level of dimerisation or tetramerisation of Aβ-IgNAR without the mutation and comparing the two levels.

[0081] In a eleventh aspect the present invention provides a compound for inhibiting or disrupting amyloid β-peptide oligomer formation or toxic activity, wherein the compound interacts with the region of Aβ-peptide defined by N27, K28, I31 and L34 of Aβ-peptide wherein amino acids 18-41 of the Aβ protein are positioned at atomic coordinates as shown in Appendix I, or structural coordinates having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

[0082] In an embodiment of this aspect the region of Aβ-peptide is defined by F19, A21, G25, N27, K28, I31 and L34.

[0083] In an embodiment of this aspect of the invention the compound is the peptide 27-NKGAI-31 to compete with formation of the dimer.

[0084] In another embodiment of this aspect of the invention the compound is the peptide 27-NKxxIxxL-34 (wherein x is any amino acid) to compete with formation of the dimer with or with out flanking residues.

[0085] In another embodiment the compound is an antibody or an antigen binding region thereof which binds Aβ-peptide in the region defined by N27, K28, I31 and L34. The antibody or antigen binding region may bind the Aβ-peptide in the region defined by F19, A21, G25, N27, K28, I31 and L34.

[0086] In an twelfth aspect the present invention provides a compound for inhibiting or disrupting amyloid β-peptide oligomer formation or toxic activity, wherein the compound interacts with the region of Aβ-peptide defined by G33, L34, M35 and V36 of Aβ-peptide wherein amino acids 18-41 of the Aβ protein are positioned at atomic coordinates as shown in Appendix I, or structural coordinates having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

[0087] In an embodiment of this aspect the region of Aβ-peptide is defined by I32, G33, L34, M35 and V36.

[0088] In an embodiment of this aspect of the invention the compound is the peptide 33-GLMV-36 to compete for tetramer with or without flanking residues

[0089] In another embodiment of this aspect of the invention the compound is the peptide 31-IIGLxV-36 (wherein x is any amino acid) to compete with the formation of the tetramer.

[0090] In another embodiment the compound is an antibody or an antigen binding region thereof which binds Aβ-peptide in the region defined by G33, L34, M35 and V36. The antibody or antigen binding region may bind the Aβ-peptide in the region defined by I32, G33, L34, M35 and V36.

[0091] In a thirteenth aspect the present invention provides a compound for inhibiting or disrupting amyloid β-peptide oligomer formation or toxic activity, wherein the compound interacts with the region of Aβ-peptide defined by V18, F20, S26, K28, G29, I32, M35, V39 and I41 of Aβ-peptide wherein amino acids 18-41 of the Aβ protein are positioned at atomic coordinates as shown in Appendix I, or structural coordinates having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

[0092] In an embodiment of this aspect the region of Aβ-peptide is defined by V18, F20, D23, S26, K28, G29, A30, I32, M35, G37, V39 and I41.

[0093] In an embodiment of this aspect of the invention the compound is the peptide selected from the group consisting of the peptides 26-SxKG-29, 18-VxF-20, 32-IxxM-35, and 39-VxI-41 each with or without flanking sequences; wherein the peptide competes for formation of amyloid.

[0094] In another embodiment the compound is an antibody or an antigen binding region thereof which binds Aβ-peptide in the region defined by V18, F20, S26, K28, G29, I32, M35, V39 and I41.. The antibody or antigen binding region may bind the Aβ-peptide in the region defined by V18, F20, D23, S26, K28, G29, A30, I32, M35, G37, V39 and I41.

[0095] In a fourteenth aspect the present invention provides a compound for decreasing metal binding by amyloid β-peptide oligomers, wherein the compound interacts with the aligned E22 of the Aβ monomers in the Aβ oligomer.

[0096] The compounds of the present invention may also be foldamers or peptidomimetics including peptidomimetics based on β-peptides. More information these classes of compounds can be found in the following references, the disclosure of which is incorporated herein by reference.

Ripka, Amy Sa; Rich, Daniel Ha. Peptidomimetic design. Current Opinion in Chemical Biology. Vol: 2, Issue: 4, 1998 441-452.
Robinson JA, Demarco S, Gombert F, Moehle K, Obrecht D. The design, structures and therapeutic potential of protein epitope mimetics. Drug Discov Today. 2008 Sep

10.
Robinson JA. beta-Hairpin Peptidomimetics: Design, Structures and Biological Activities. Acc Chem Res. 2008 Apr 16.
Appella, D. H.; Christianson, L. A.; Karle, I. L.; Powell, D. R.; Gellman, S. H. β-Peptide Foldamers: Robust Helix Formation in a New Family of -Amino Acid Oligomers J. Am. Chem. Soc.; (Communication); 1996; 118(51); 13071-13072.
Gellman, S.H., "Foldamers: a manifesto", Acc. Chem. Res 1998, 31(4): 173–180.
Hill DJ, Mio MJ, Prince RB, Hughes TS, Moore JS, "A field guide to foldamers", Chem. Rev. 2001, 101(12): 3893–4012.

[0097] In another aspect the present invention provides a method of inhibiting or disrupting amyloid β-peptide oligomer formation or toxic activity, the method comprising contacting the Aβ-peptide with a compound according to the present invention.

[0098] In another embodiment of the present invention the peptides have the same or a similar conformation as they do in the Aβ-peptide. This confirmation is provided by the coordinates amino acids 18-41 of the Aβ protein as shown in Appendix I, or structural coordinates having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

[0099] The target or binding site is a region of Aβ involved in oligermisation. Preferred target or binding sites comprise one or more of the following domains: the dimerisation domain, the tetramerisation domain, the amyloid formation domain.

[00100] A schematic representation of Aβ-IgNAR dimer is shown in Figure 1. The interfaces which may be targeted include:

The dimer interface (1)
The tetramer interface (2) and
The amyloid interface (3)

[00101] Alternatively, the target binding site may comprise one or more amino acids from one or more of the following amino acid sequences:

(i) amino acids V18 – I41;
(ii) amino acids F19, A21, G25, N27, K28, G29, I31, L34 (dimer interface)
(iii) amino acids I32, G33, L34, M35, V36 (tetramer interface)
(iv) amino acids V18, F20, D23, S26, K28, G29, A30, I32, M35, G37, V39, I41 (amyloid interface)

[00102] A compound may interact with a specified region of Aβ-IgNAR and Aβ monomer, dimer, or tetramer (e.g. an interface) by binding either directly or indirectly to that region. A

compound which binds directly, binds to the specified region. A compound which binds indirectly, binds to a region in close proximity to or adjacent to the specified region with the result that it interferes with the ability of the specified region to oligomerise, either antagonistically or agonistically. Such interference may be steric, electrostatic, or allosteric. Preferably, a compound interacts with a specified region of the Aβ-IgNAR and Aβ monomer, dimer, or tetramer by binding directly to the specified region.

[0100] Binding can be either by covalent or non-covalent interactions, or both. Examples of non-covalent interactions include electrostatic interactions, van der Waals interactions, hydrophobic interactions and hydrophilic interactions.

[0101] When a compound interacts with Aβ-IgNAR and Aβ monomer, dimer, or tetramer, it preferably "modulates" Aβ-IgNAR and Aβ monomer, dimer, or tetramer activity respectively. By "modulate" we mean that the compound changes an activity of Aβ-IgNAR and Aβ monomer, dimer, or tetramer by at least 10%. Suitably, a compound modulates Aβ-IgNAR and Aβ monomer, dimer, or tetramer by decreasing oligomerization or toxicity. The phrase "decrease oligomerization or toxicity " is intended to encompass partial or complete inhibition of oligomerization or toxicity. The ability of a candidate compound to increase or decrease activity can be assessed by any one of the Aβ oligomerization or toxicity assays described herein.

[0102] As mentioned above one of the assay protocols involves assessment of binding using the actual crystal. Binding of chemical fragments/compounds is assessed by soaking or co-crystallizing such fragments/compounds into crystals provided by the invention and then subjecting these to an X-ray beam and obtaining diffraction data. Difference Fourier techniques are readily applied by those skilled in the art to determine the location within the Aβ-IgNAR and Aβ monomer, dimer, or tetramer structure at which these fragments/compounds bind.

[0103] Typically compounds derived from the various screening protocols described herein are subjected to biological testing. There are a number of such test and a useful review is provided in Rahimi, F., Shanmugam, A. & Bitan, G.; Structure-function relationships of pre-fibrillar protein assemblies in Alzheimer's disease and related disorders. Current Alzheimer research 5, 319-341 (2008) The disclosure of which is incorporated herein by reference.

[0104] Other methods involving the use of the crystal or Aβ-IgNAR protein include:

Assays utilising the Aβ-IgNAR protein and crystals/structure:

Recombinant protein production and SDS-PAGE/Western blot

- Assessment of dimerisation and tetramerisation of recombinant Aβ-IgNAR proteins.
- Analysis of affect of familial/in vitro determined/structurally predicted/experimentally derived mutations on Aβ-IgNAR folding, oligomerization, and toxicity.
- Analysis of action of peptides/compounds/fragments/metals/antibodies on oligomerization of Aβ peptide.

[0105] An example of this method is shown in Fig 2a where the monomer-dimer ratio is used an assay tool ie using ability of compounds to disrupt formation of dimer, and assaying by SDS-PAGE and western blot.

[0106] Size exclusion chromatography

- Assessment of dimerisation and tetramerisation of recombinant Aβ-IgNAR proteins.
- Analysis of affect of familial/in vitro determined/ structurally predicted /experimentally derived mutations on Aβ-IgNAR folding, oligomerization, and toxicity.
- Analysis of action of peptides/compounds/fragments/antibodies on dimerisation and tetramerisation of Aβ-IgNAR.
- Analysis of action of peptides/compounds/fragments/metals/antibodies on oligomerization of Aβ-IgNAR.

[0107] BIAcore biosensor

- Determination of binding affinities for peptides/compounds/fragments/antibodies targeting the Aβ-IgNAR structure.

[0108] Protein crystallography

- Analysis of affect of familial/in vitro determined/ structurally predicted /experimentally derived mutations on Aβ-IgNAR structure and oligomerization.
- Determination of binding site of peptides/compounds/fragments/metals/antibodies in the Aβ-IgNAR structure.

[0109] X-ray absorption spectrometry

- Determination of binding sites of metals, stoichiometry and oxidation state in the Aβ-IgNAR structure using X-ray Absorption Near-Edge Spectroscopy (XANES) and Extended X-ray Absorption Fine Structure (EXAFS) methods.

Assaying derived/selected peptides/compounds/fragments/antibodies for activity

[0110] Electron microscopy

- Analysis of action of peptides/compounds/fragments/metals/antibodies on oligomerization of Aβ peptide.

[0111] Yeast cell toxicity assays

- Analysis of affect of peptides/compounds/fragments/antibodies on oligomerization of Aβ peptide in yeast systems.
- Analysis of action of peptides/compounds/fragments/metals/antibodies in reducing Aβ-mediated cellular toxicity in yeast systems.

[0112] Neuronal cell toxicity assays

- Analysis of action of peptides/compounds/fragments/metals/antibodies in reducing Aβ-mediated cellular toxicity in neuronal cell lines.
- In vitro neuroprotection (MTT) assay against oligomer-mediated toxicity

[0113] Animal studies

- Analysis of action of peptides/compounds/fragments/metals/antibodies in reducing Aβ-mediated cellular toxicity in animal model systems.

[0114] Further information regarding these and other methods which may be usefully applied in the present invention is provided in the following references the disclosures of which is incorporated herein by reference

Streltsov, V. A. (2008). "X-ray absorption and diffraction studies of the metal binding sites in amyloid β-peptide." Eur Biophys J **37**(3): 257-263.
Streltsov, V. A. and J. N. Varghese (2008). "Substrate mediated reduction of copper-amyloid-β complex in Alzheimer's disease." Chem Commun (Camb)(27): 3169-3171.
Streltsov, V. A. Titmuss, S.J., Epa, V. C., Barnham, K. J., Masters, C. L., Varghese,

J. N. (2008). "The structure of the Amyloid β-peptide high affinity Copper II binding site in Alzheimer's Disease." Biophysical Journal. (2008) 95 (7) 3447-3456
Caine, J., et al. Alzheimer's Ab fused to green fluorescent protein induces growth stress and a heat shock response. FEMS Yeast Res 7, 1230-1236 (2007).
Bharadwaj, P., Waddington, L., Varghese, J. & Macreadie, I.G. A new method to measure cellular toxicity of non-fibrillar and fibrillar Alzheimer's Abeta using yeast. J Alzheimers Dis 13, 147-150 (2008).
Mosmann, T. Rapid colorimetric assay for cellular growth and survival: application to proliferation and cytotoxicity assays. *Journal of immunological methods* **65**, 55-63 (1983).
Maynard CJ, Cappai R, Volitakis I, Cherny RA, Masters CL, Li QX, Bush AI.Gender and genetic background effects on brain metal levels in APP transgenic and normal mice: implications for Alzheimer beta-amyloid pathology.J Inorg Biochem. 2006 May;100(5-6):952-62.
Gotz, J., *et al.* A decade of tau transgenic animal models and beyond. *Brain pathology (Zurich, Switzerland)* **17**, 91-103 (2007).

[0115] Direct binding of compounds to Aβ-IgNAR and Aβ monomer, dimer, or tetramer can also be assessed by Surface Plasmon Resonance (BIAcore) (reviewed in Morton & Myszka, 1998). Here Aβ-IgNAR and Aβ monomer, dimer, or tetramer is immobilized on a CM5 or other sensor chip by either direct chemical coupling using amine or thiol-disulphide exchange coupling (Nice & Catimel, 1999) or by capturing as a fusion protein to an appropriately derivatised sensor surface (Morten & Myszka, 1998). The potential binding molecule (called an analyte) is passed over the sensor surface at an appropriate flow rate and a range of concentrations. The classical method of analysis is to collect responses for a wide range of analyte concentrations. A range of concentrations provides sufficient information about the reaction, and by using a fitting algorithm such as CLAMP (see Morton & Myszka, 1998), rate constants can be determined (Morton & Myszka, 1998; Nice & Catimel, 1999). Normally, the ligand surface is regenerated at the end of each analyte binding cycle. Surface regeneration ensures that the same number of ligand binding sites is accessible to the analyte at the beginning of each cycle.

[0116] Incubation periods are selected for optimum activity, but may also be optimized to facilitate rapid high-throughput screening. Normally, between 0.1 and 1 hour will be sufficient. In general, a plurality of assay mixtures is run in parallel with different test agent concentrations to obtain a differential response to these concentrations. Typically, one of these concentrations serves as a negative control, i.e. at zero concentration or below the level of detection.

[0117] The basic format of oligomerization and toxicity assays are as follows:

- (i) gel filtration; and western blot/SDS-PAGE
- (ii) cellular assays
- (iii) electron microscopy and oligomerization
- (iv) yeast assays
- (v) animal studies

[0118] The compounds/chemical entities of the present invention may be used to modulate Aβ oligomerization and/or toxicity in cells, by direct binding of the chemical entity to an interface or region of Aβ-IgNAR and Aβ monomer, dimer, or tetramer and/or by an allosteric interaction elsewhere.

[0119] Given that Aβ monomer, dimer, or tetramer or oligomerization activity and toxicity is implicated in neuronal disfunction and a range of disorders, the compounds of the present invention may also be used to treat, ameliorate or prevent disorders associated with Alzheimer's disease and/or other amyloidogenic neuropathies.

[0120] The compounds which interact with Aβ-IgNAR and Aβ monomer, dimer, or tetramer and in particular to interact with the target interfaces, are useful as agonists or antagonists against the action of Aβ on other yet to be identified ligands. The compounds are useful as assay reagents for identifying other useful ligands by, for example as research tools for further analysis of Aβ oligomerization and as potential therapeutics in pharmaceutical compositions.

[0121] Aβ-IgNAR and Aβ monomer, dimer, or tetramer antagonists provided by this invention are potentially useful as therapeutics. For example, compounds are potentially useful as treatments for Alzheimers disease. These antagonists may also be used to detect the presence of Ab dimers in biological samples in particular blood and CSF. In this regard the biological sample is contacted with the compound and the level of binding assessed.

[0122] As will be evident to the skilled person, the crystal structures presented herein have enabled, for the first time, the identification of critical regions and conformations of Aβ involved in folding, dimerisation, tetramerisation, and oligermisation leading to fibril formation and toxicity.

[0123] Using a variety of known modelling techniques, the crystal structure of the present invention can be used to produce a model for at least part of Aβ monomer, dimer, or tetramer, and higher order oligomers.

[0124] As used herein, the term "modelling" includes the quantitative and qualitative analysis of molecular structure and/or function based on atomic structural information and interaction models. The term "modelling" includes conventional numeric-based molecular dynamic and energy minimisation models, interactive computer graphic models, modified molecular mechanics models, distance geometry and other structure-based constraint models.

[0125] Molecular modelling techniques can be applied to the atomic coordinates of the Aβ-IgNAR and Aβ monomer, dimer, or tetramer or a region thereof to derive a range of 3D models and to investigate the structure of interfaces and binding sites, such as the binding sites of monoclonal antibodies, nonimmunoglobulin binding proteins and inhibitory peptides.

[0126] These techniques may also be used to screen for or design small and large chemical entities which are capable of binding Aβ-IgNAR and Aβ monomer, dimer, or tetramer, their respective interfaces, and affecting oligomerization and toxicity. The screen may employ a solid 3D screening system or a computational screening system.

[0127] Such modelling methods are to design or select chemical entities that possess stereochemical complementary to particular regions of Aβ-IgNAR and Aβ monomer, dimer, or tetramer. By "stereochemical complementarity" we mean that the compound or a portion thereof makes a sufficient number of energetically favourable contacts with Aβ as to have a net reduction of free energy on binding.

[0128] Such stereochemical complementarity is characteristic of a molecule that matches intra-site surface residues located at

- (i) amino acids V18 – I41;
- (ii) amino acids N27, K28, I31, L34, (dimer interface)
- (iii) amino acids G33, L34, M35, V36; (tetramer interface)
- (iv) amino acids V18, F20, S26, K28, G29, I32, M35, V39, I41 (amyloid interface),
- Or combinations thereof.

[0129] Additional intra-site residues include:

amino acids F19, A21, G25, N27, K28, G29, I31, L34 (dimer interface)
amino acids I32, G33, L34, M35, V36 (tetramer interface)
amino acids V18, F20, D23, S26, K28, A30, I32, M35, G37, V39, I41 (amyloid interface)

[0130] By "match" we mean that the identified portions interact with the surface residues, for example, via hydrogen bonding or by non-covalent Van der Waals and Coulomb interactions (with surface or residue) which promote desolvation of the molecule within the site, in such a way that retention of the molecule at the binding site is favoured energetically.

[0131] It is preferred that the stereochemical complementarity is such that the compound has a K_d for the site of less than 10^{-4}M, more preferably less than 10^{-5}M and more preferably 10^{-6}M. In a most preferred embodiment, the K_d value is less than 10^{-8}M and more preferably less than 10^{-9}M.

[0132] Chemical entities which are complementary to the shape and electrostatics or chemistry of the sites characterised by amino acids positioned at atomic coordinates set out in Appendix I will be able to bind to the regions given above, either independently or in combination and when the binding is sufficiently strong, substantially inhibit oligomerization and/or toxicity.

[0133] It will be appreciated that it is not necessary that the complementarity between chemical entities and the site(s) extend over all residues of the site(s) in order to inhibit oligomerization and/or toxicity.

[0134] A number of methods may be used to identify chemical entities possessing stereo-complementarity to a region of the Aβ-IgNAR and Aβ monomer, dimer, or tetramer. For instance, the process may begin by visual inspection of potential interface sites, on the computer screen based on the Aβ-IgNAR and Aβ monomer, dimer, or tetramer structures, or region thereof, coordinates in Appendix I generated from the machine-readable storage medium. Alternatively, selected fragments or chemical entities may then be positioned in a variety of orientations, or docked, within an individual binding site of Aβ-IgNAR and Aβ monomer, dimer, or tetramer, as defined supra. Modelling software that is well known and available in the art may be used (Guida, 1994). These include QUANTA and InsightII [Molecular Simulations, Inc., San Diego, Calif., a division of Pharmacopiea, Inc., Princeton, N.J., 1992], SYBYL [Molecular Modeling Software, Tripos Associates, Inc., St. Louis, Mo., 1992]. This modelling step may be followed by energy minimization with standard molecular mechanics force fields such as AMBER (Weiner *et al.*, 1984), and CHARMM (Brooks *et al.*, 1983). In addition, there are a number of more specialized computer programs to assist in the process of selecting the binding moieties of this invention.

[0135] Specialised computer programs may also assist in the process of selecting fragments or chemical entities. These include, inter alia:

1. GRID (Goodford, 1985). GRID is available from Oxford University, Oxford, UK.

2. MCSS (MXXXanker & Karplus, 1991). MCSS is available from Molecular Simulations, Burlington, MA.

3. AUTODOCK (Goodsell & Olsen, 1990). AUTODOCK is available from Scripps Research Institute, La Jolla, CA.

4. DOCK (Kuntz *et al.*, 1982). DOCK is available from University of California, San Francisco, CA.

[0136] Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound. In one embodiment, assembly may proceed 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 Aβ-IgNAR and Aβ monomer, dimer, or tetramer. This is followed by manual model building using software such as Quanta or Sybyl. Alternatively, fragments may be joined to additional atoms using standard chemical geometry.

[0137] The above-described evaluation process for chemical entities may be performed in a similar fashion for chemical compounds.

[0138] Useful programs to aid one skilled in the art in connecting the individual chemical entities or fragments include:

1. CAVEAT (Bartlett *et al.*, 1989). CAVEAT is available from the University of California, Berkeley, CA.

2. 3D Database systems such as MACCS-3D (MDL Information Systems, San Leandro, CA). This area is reviewed in Martin (1992).

3. HOOK (available from Molecular Simulations, Burlington, MA).

[0139] Other molecular modeling techniques may also be employed in accordance with this invention, see, e.g., Cohen *et al.* (1990) and Navia & Murcko (1992).

[0140] There are two preferred approaches to designing a molecule, according to the present invention, that complement the stereochemistry of Aβ-IgNAR and Aβ monomer, dimer, or tetramer. The first approach is to in silico directly dock molecules from a three-dimensional structural database, to the interface site(s), using mostly, but not exclusively, geometric criteria to assess the goodness-of-fit of a particular molecule to the site. In this approach, the number of internal degrees of freedom (and the corresponding local minima in the molecular conformation space) is reduced by considering only the geometric (hard-sphere) interactions of two rigid bodies, where one body (the active site) contains "pockets" or "grooves" that

form binding sites for the second body (the complementing molecule).

[0141] This approach is illustrated by Kuntz *et al.* (1982) and Ewing *et al.* (2001), the contents of which are hereby incorporated by reference, whose algorithm for ligand design is implemented in a commercial software package, DOCK version 4.0, distributed by the Regents of the University of California and further described in a document, provided by the distributor, which is entitled "Overview of the DOCK program suite" the contents of which are hereby incorporated by reference. Pursuant to the Kuntz algorithm, the shape of the interface represented by a site on the Aβ-IgNAR and Aβ monomer, dimer, or tetramer is defined as a series of overlapping spheres of different radii. One or more extant databases of crystallographic data, such as the Cambridge Structural Database System maintained by Cambridge University (University Chemical Laboratory, Lensfield Road, Cambridge, U.K.), the Protein Data Bank maintained by the Research Collaboratory for Structural Bioinformatics (Rutgers University, N.J., U.S.A.), LeadQuest (Tripos Associates, Inc., St. Louis, MO), Available Chemicals DXXXectory (Molecular Design Ltd., San Leandro, CA), and the NCI database (National Cancer Institute, U.S.A) is then searched for molecules which approximate the shape thus defined.

[0142] Molecules identified on the basis of geometric parameters, can then be modified to satisfy criteria associated with chemical complementarity, such as hydrogen bonding, ionic interactions and Van der Waals interactions. Different scoring functions can be employed to rank and select the best molecule from a database. See for example Bohm & Stahl (1999). The software package FlexX, marketed by Tripos Associates, Inc. (St. Louis, MO) is another program that can be used in this direct docking approach (see Rarey *et al.*, 1996).

[0143] The second preferred approach entails an assessment of the interaction of respective chemical groups ("probes") with the active site at sample positions within and around the site, resulting in an array of energy values from which three-dimensional contour surfaces at selected energy levels can be generated. The chemical-probe approach to ligand design is described, for example, by Goodford, (1985), the contents of which are hereby incorporated by reference, and is implemented in several commercial software packages, such as GRID (product of Molecular Discovery Ltd., West Way House, Elms Parade, Oxford OX2 9LL, U.K.).

[0144] Pursuant to this approach, the chemical prerequisites for a site-complementing molecule are identified at the outset, by probing the active site with different chemical probes, e.g., water, a methyl group, an amine nitrogen, a carboxyl oxygen, or a hydroxyl. Favoured sites for interaction between the active site and each probe are thus determined, and from the resulting three-dimensional pattern of such sites a putative complementary molecule can be generated. This may be done either by programs that can search three-dimensional databases

to identify molecules incorporating desired pharmacophore patterns or by programs which use the favoured sites and probes as input to perform de novo design. Suitable programs for determining and designing pharmacophores include CATALYST (including HypoGen or HipHop) (Molecular Simulations, Inc), and CERIUS2, DISCO (Abbott Laboratories, Abbott Park, IL) and ChemDBS-3D (Chemical Design Ltd., Oxford, U.K.).

[0145] The pharmacophore can be used to screen in silico compound libraries/ three-dimensional databases, using a program such as CATALYST (Molecular Simulations, Inc); MACCS-3D and ISIS/3D (Molecular Design Ltd., San Leandro, CA), ChemDBS-3D (Chemical Design Ltd., Oxford, U.K.), and Sybyl/3DB Unity (Tripos Associates, Inc., St. Louis, MO).

[0146] Databases of chemical structures are available from a number of sources including Cambridge Crystallographic Data Centre (Cambridge, U.K.), Molecular Design, Ltd., (San Leandro, CA), Tripos Associates, Inc. (St. Louis, MO), Chemical Abstracts Service (Columbus, OH), the Available Chemical DXXXectory (MDL Inc), the Derwent World Drug Index (WDI), BioByteMasterFile, the National Cancer Institute database (NCI), and the Maybridge catalogue.

[0147] De novo design programs include LUDI (Biosym Technologies Inc., San Diego, CA), Leapfrog (Tripos Associates, Inc.), Aladdin (Daylight Chemical Information Systems, Irvine, CA), and LigBuilder (Peking University, China).

[0148] Once an entity or compound has been designed or selected by the above methods, the efficiency with which that entity or compound may bind to Aβ-IgNAR and Aβ monomer, dimer, or tetramer can be tested and optimised by computational evaluation. An effective Aβ-IgNAR and Aβ monomer, dimer, or tetramer binding compound 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 Aβ-IgNAR and Aβ monomer, dimer, or tetramer binding compound should preferably be designed with a deformation energy of binding of not greater than about 10 kcal/mole, preferably, not greater than 7 kcal/mole. Binding compounds may interact with Aβ-IgNAR and Aβ monomer, dimer, or tetramer in more than one conformation that are 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 compound and the average energy of the conformations observed when the compound binds to the protein.

[0149] A compound designed or selected as binding to Aβ-IgNAR and Aβ monomer, dimer, or tetramer may be further computationally optimised so that in its bound state it would preferably lack repulsive electrostatic interaction with the target protein. Such non-

complementary (e.g., electrostatic) interactions include repulsive charge-charge, dipole-dipole and charge-dipole interactions. Specifically, the sum of all electrostatic interactions between the compound and the protein when the compound is bound to Aβ-IgNAR and Aβ monomer, dimer, or tetramer, preferably make a neutral or favourable contribution to the enthalpy of binding.

[0150] Once an Aβ-IgNAR and Aβ monomer, dimer, or tetramer -binding compound has been optimally selected or designed, as described above, substitutions may then be made in some of its atoms or side groups to improve or modify its binding properties. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. It should, of course, be understood that components known in the art to alter conformation should be avoided. Such substituted chemical compounds may then be analysed for efficiency of fit to Aβ-IgNAR and Aβ monomer, dimer, or tetramer by the same computer methods described in detail above.

[0151] Specific computer software is available in the art to evaluate compound deformation energy and electrostatic interaction. Examples of programs designed for such uses include: Gaussian 92, revision C (Frisch, Gaussian, Inc., Pittsburgh, PA); AMBER, version 4.0 (Kollman, University of California at San Francisco); QUANTA/CHARMM (Molecular Simulations, Inc., Burlington, MA); and Insight II/Discover (Biosysm Technologies Inc., San Diego, CA).

[0152] The screening/design methods may be implemented in hardware or software, or a combination of both. However, preferably, the methods are implemented in computer programs executing on programmable computers each comprising a processor, a data storage system (including volatile and non-volatile memory and/or storage elements), at least one input device, and at least one output device. Program code is applied to input data to perform the functions described above and generate output information. The output information is applied to one or more output devices, in known fashion. The computer may be, for example, a personal computer, microcomputer, or workstation of conventional design.

[0153] Each program is preferably implemented in a high level procedural or object-oriented programming language to communicate with a computer system. However, the programs can be implemented in assembly or machine language, if desired. In any case, the language may be compiled or interpreted language.

[0154] Each such computer program is preferably stored on a storage medium or device (e.g., ROM or magnetic diskette) readable by a general or special purpose programmable computer, for configuring and operating the computer when the storage media or device is read by the computer to perform the procedures described herein. The system may also be

considered to be implemented as a computer-readable storage medium, configured with a computer program, where the storage medium so configured causes a computer to operate in a specific and predefined manner to perform the functions described herein.

Screening assays and confirmation of binding and biological activity

[0155] Compounds selected or designed in accordance with the in silico methods of the invention may be subjected to further confirmation of binding to Aβ-IgNAR and Aβ monomer, dimer, or tetramer by cocrystallization of the compound with Aβ-IgNAR and Aβ monomer, dimer, or tetramer and structural determination, as described herein.

[0156] Libraries may be screened in solution by methods generally known in the art for determining whether ligands competitively bind at a common site. Such methods may include screening libraries in solution (e.g., Houghten, 1992), or on beads (Lam, 1991), chips (Fodor, 1993), bacteria or spores (U.S. 5,223,409: Lardner), plasmids (Cull *et al.*, 1992), or on phage (Scott & Smith, 1990; Devlin, 1990; CwXXXla *et al.*, 1990; Felici, 1991; U.S. 5,223,409: Lardner).

[0157] Where the screening assay is a binding assay, Aβ-IgNAR and Aβ monomer, dimer, or tetramer may be joined to a label, where the label can directly or indirectly provide a detectable signal. Various labels include radioisotopes, fluorescent molecules, chemiluminescent molecules, enzymes, specific binding molecules, particles, e.g., magnetic particles, and the like. Specific binding molecules include pairs, such as biotin and streptavidin, digoxin and antidigoxin, etc. For the specific binding members, the complementary member would normally be labeled with a molecule that provides for detection, in accordance with known procedures.

[0158] A variety of other reagents may be included in the screening assay. These include reagents like salts, neutral proteins, e.g., albumin, detergents, etc., which are used to facilitate optimal protein-protein binding and/or reduce non-specific or background interactions. Reagents that improve the efficiency of the assay, such as protease inhibitors, nuclease inhibitors, antimicrobial agents, etc., may be used. The components are added in any order that produces the requisite binding. Incubations are performed at any temperature that facilitates optimal activity, typically between 4 and 40 °C.

[0159] The Aβ-IgNAR molecule may be used in its own right as a sink or tool to mop up oligomers both in vivo and in vitro ie as a therapeutic.

[0160] The Aβ-IgNAR molecule of the present invention may also be used as an antigen to raise antibodies against Aβ.

[0161] In a fifteenth aspect the present invention provides the use of an Aβ-IgNAR molecule of any one SEQ ID NOs 2, 4, 5, 6, 13, 15, 16, 17 or 18 to raise antibodies against Aβ wherein the antibodies bind to residues 18 to 41 of SEQ ID NO 1 when presented in the Aβ-IgNAR molecule of any one of SEQ ID NOs 2, 4, 5, 6, 15, 16, 17 or 18 but not to an isolated linear peptide having a sequence of residues 18 to 41 of SEQ ID NO 1.

[0162] In a sixteenth aspect the present invention provides an antibody which specifically binds to residues antibodies bind to residues 18 to 41 of SEQ ID NO 1 when presented in the Aβ-IgNAR molecule of any one of SEQ ID NOs 2, 4, 5, 6, 13, 15, 16, 17 or 18 but not to an isolated linear peptide having a sequence of residues 18 to 41 of SEQ ID NO 1.

[0163] In a preferred embodiment the antibody is a monoclonal antibody.

[0164] As will be understood by persons skilled in the art the antibodies of the present invention are directed to conformational epitopes of 18-41 of Aβ which are presented when Aβ 18-41 is positioned within the Aβ-IgNAR molecule. Such conformational epitopes will not be present in the isolated linear Aβ 18-41 peptide.

[0165] In addition to therapeutic uses the antibodies of the present invention may also be used in diagnostic assays to detect the presence of Aβ dimers in biological samples in particular blood and CSF. In this regard the biological sample is contacted with the antibody and the level of binding assessed.

[0166] Throughout this specification the word "comprise", or variations such as "comprises" or "comprising", will be understood to imply the inclusion of a stated element, integer or step, or group of elements, integers or steps, but not the exclusion of any other element, integer or step, or group of elements, integers or steps.

[0167] All publications mentioned in this specification are herein incorporated by reference. Any discussion of documents, acts, materials, devices, articles or the like which has been included in the present specification is solely for the purpose of providing a context for the present invention. It is not to be taken as an admission that any or all of these matters form part of the prior art base or were common general knowledge in the field relevant to the present invention as it existed in Australia or elsewhere before the priority date of each claim of this application.

[0168] In order that the nature of the present invention may be more clearly understood, preferred forms thereof will now be described with reference to the following non-limiting examples.

EXAMPLE 1

METHODS SUMMARY

[0169] Construction of Aβ-IgNAR chimeras. Aβ-IgNAR-G1/G3/G6 and G1-Leu^{34}Pro coding sequences were constructed by splice-overlap PCR using IgNAR 12Y-2 DNA template(Nuttall, Humberstone et al. 2004), cloned into *E. coli* periplasmic expression vector pGC, and verified by DNA sequencing.

[0170] Protein purification and crystallization. Recombinant proteins were expressed into the *E. coli* periplasmic space, purified by affinity chromatography through an anti-FLAG Ig/Sepharose column equilibrated in TBS, and collected as single peaks by gel filtration. Proteins (~4 - 5 mg/ml in 20 mM Tris.HCl, pH 8.0) were set up as 0.4 µl sitting drops. Aβ-IgNAR-G1 (SEQ ID NO: 2) crystallised under a wide range of conditions (biased towards PEG 6000; PEG 3350; and PEG MME 2000 at neutral pH). Final crystallisation conditions were 0.2 M ammonium chloride, 20% polyethylene glycol (PEG) 6000, 0.1 M MES pH 6, with diffraction quality crystals (Space Group $P3_2$ and cell parameters a=b=79.40, c= 84.89Å) obtained after 9 days. No crystals were obtained for Aβ-IgNAR-G3 (SEQ ID NO: 4) or Aβ-IgNAR-G6 (SEQ ID NO: 5).

[0171] Structure determination. A full data set (93% completeness) was collected at the Australian Synchrotron 3-BM1 beam line to 2.2 Å resolution. Data were collected at -160°C and processed using the HKL2000 suite(Otwinowski and Minor 1997). Diffraction data statistics are summarized in **Table 1.** The structure was solved by molecular replacement MOLREP(Vagin and Teplyakov 1997) using IgNAR 12Y-2 (PDB 1VES) minus CDR3 region as search template. Four independent molecules (A, B, C and D) were found in the asymmetric unit. The final refinement converged to R/R_{free} values of 0.164/0.246. In total, 97.8% residues are in the most favoured regions of the Ramachandran plot, with 1.6% residues in the additionally allowed regions.

Table 1 X-ray refinement statistics

Resolution (Å)	26.17-2.20
R_{work}/R_{free}	16.4 / 24.6
Number of	
Protein amino acids	503
Water	394
B-factors	
Overall	46.5
Protein	46.0
Water	51.7
R.m.s deviations	
Bond lengths (Å)	0.019
Bond angles (°)	1. 958

RESULTS

[0172] The crystallographic structures of the IgNAR single variable domain antibody 12Y-2(Streltsov, Varghese et al. 2004) (PDB: 1VES) reveal self-stabilized extended β-hairpin CDR3 loop regions. We hypothesized that engineering the amyloidogenic component of Aβ peptide (residues Val^{17}-Ala^{42}) within this loop would (1) allow formation of an amyloid protofilament structure; while (2) preventing uncontrolled fibril formation and polymerisation by trapping the amyloid moiety in a cage of IgNAR domains that are amenable to crystallization. Three chimeric proteins were modelled based on existing NMR β-hairpin models of amyloid plaques(Luhrs, Ritter et al. 2005), incorporating variable N- and C-terminal glycine linkers to allow in-register transition from the immunoglobulin framework β-sheets to the Aβ peptide. These constructs, designated Aβ-IgNAR-G1 (SEQ ID NO. 2); Aβ-IgNAR-G3 (SEQ ID NO. 4); and Aβ-IgNAR-G6 (SEQ ID NO. 5), were expressed as recombinant proteins in *E. coli* and tested for oligomer formation. SDS and β-mercaptoethanol-stable dimers were observed in the bacterial periplasmic space by Western blot for all three chimeric proteins but not the unmodified IgNAR. The greater conformational flexibility for the glycine-3 and glycine-6 versions appeared to allow more rapid dimer formation, and protein induction at higher temperature tended to promote a higher dimer:monomer ratio. Upon affinity purification all 3 variants behaved as dimers, rather than the monomer observed for the wild type IgNAR, and tetrameric species were also apparent. (**Figures 2a and 2b**). Trigonal crystals of Aβ-IgNAR-G1 (SEQ ID NO: 2), but not the other two chimeric proteins, grew under a variety of conditions and diffracted to 2.2 Å resolution. The structure was solved by molecular replacement using IgNAR 12Y-2 (SEQ ID NO: 3) with removed CDR3 region as the search model, and refinement completed with R/R_{free} factors of 16.4/24.6% (**Table 1**). Representative regions of electron density are shown in **Fig. 3**.

[0173] The Aβ-IgNAR-G1 (SEQ ID NO: 2)quaternary structure consists of four independent molecules (A, B, C and D) in the asymmetric unit (**Fig. 4**), which form a tight tetramer (dimer of dimers) through interactions predominantly mediated by the Aβ peptide component. The inter-chain association for each dimer (A-C and B-D) is extremely robust, as indicated by an average surface of interaction (buried surface) of 580 $Å^2$ and an average shape correlation statistic(Lawrence and Colman 1993) (S_c) = 0.64 (**Tables 2 & 3**). The dimer-dimer interaction (AC – BD) which forms the crystallographic tetramer is somewhat less extensive (buried surface of 546 $Å^2$). The underlying IgNAR scaffold monomers are very closely overlaid with each-other and with the previously described 12Y-2 structure.

Table 2: Aβ-IgNAR-G1 buried surface areas[1].

Chain	A	B	C	D	**Total[2]**

A	-	215.7	589.0	290.8	1095.5
B	215.7	-	254.9	563.8	1034.4
C	578.2	250.2	-	215.8	1044.2
D	296.5	569.6	221.5	-	1087.6
Average					1065.4

[1] For Aβ regions only.

[2] Area excluded on first molecule due to interaction with second (in Angstroms squared). Calculated using point density = 10 points/square Å; Probe sphere radius = 1.7 Å.

Table 3: Aβ-IgNAR-G1 shape complementarity statistics [1].

Sc	A	B	C	D
A	1	0.590	0.709	0.786
B		1	0.742	0.567
C			1	0.717
D				1

[1] Calculated using the Sc program with a 1.7Å probe radius.

[0174] The Aβ-IgNAR-G1 structure reveals the Aβ peptide region (Val^{18}-Ile^{41}) as comprising two adjacent and connected loop motifs, rather than the expected extended β-hairpin structure. The first motif consists of residues Val^{18}-Ile^{31} which adopt a 10-11 Å wide β-α structure, stabilised by intra-molecular and inter-molecular contacts and consisting of one β strand (Val^{18}-Ala^{21}) plus a 3_{10}- helical turn (Val^{24}-Ser^{26})(chains A) and similar but distorted helix in chain B or an extended loop (chains C and D). The second motif consists of residues Ile^{32}-Ile^{41} and is a β-hairpin consisting of two anti-parallel β-strands which form a 3-strand β-sheet with the parallel β-strand of the first loop motif. The overlaid Aβ loops have an average r.m.s.d. = 1.19 $Å^2$, and as can be seen from figure 2d the greatest divergence occurs between residues Val^{24}-Asn^{27}, where chains A and B adopt a different conformation from chains C and D. Consequently, for the A/B chain conformations the Lys^{28} side-chain is directed out of the plane of the loop and forms intramolecular contacts with Val^{24} (2.6 Å) and Asn^{27} (3.6 Å) (chain A) and helps maintain the helical conformation of Val^{24}-Ser^{26}. In contrast, for the C/D chains the Lys^{28} side chain is now directed internally and forms two intra-molecular contacts with the carbonyl oxygens of Asp^{23} (3.0 and 3.5 Å) and Ser^{26} (4.0 and 3.0 Å) and two inter-molecular contacts with carbonyl oxygens of chain A/B: Gly^{29} (2.6 and 3.3 Å) and Asn^{27} (2.8 and 3.6 Å). The transition between the two states for Lys^{28} appears pivotal to crystallisation, and may represent a vital mechanism (and energy minimum) for Aβ oligomer formation. In NMR-based structures of amyloid plaques, residues Leu^{17} - Ala^{42} form parallel, in-register β-sheets(Petkova, Ishii et al. 2002; Luhrs, Ritter et al. 2005; Sato,

Kienlen-Campard et al. 2006), with Lys^{28} facing outward in the first Aβ chain of the adjacently stacked peptides, while subsequent Aβ peptides have the Lys^{28} side-chain directed internally and forming intermolecular contacts (salt bridges) with residue Asp^{23} (Luhrs, Ritter et al. 2005; Petkova, Yau et al. 2006; Sato, Kienlen-Campard et al. 2006). Thus our structure is consistent with NMR data for this position.

[0175] Overall, the dimers (AC and BD), each related by an pseudo 2-fold axis running through the long axis of the tetramer, are stabilized around the Asp^{23} - Ala^{30} loop by the carbonyl oxygen charges neutralizing the buried Lys^{28} amide group and by the amide group of Asp^{27} forming a hydrogen bonding network with the neighbouring dimer's carbonyl oxygen of Gly^{29} and carboxy oxygen of Asp^{27}. The surface towards the tetramer interface is stabilized by the hydrophobic residues Ile^{31}, Val^{40}, and Leu^{34}. The tetramer interface is stabilized by two 3-stranded β-sheets of the monomer forming a single 6-stranded β-sheet with a pseudo-2-fold axis running perpendicular to and through the centroid of the extended β-sheets. The Leu^{34} side-chains face each other: two from each side of the tetramer, rotated by ~90° (see later). Similarly, the respective Met^{35} side-chains are surrounded by hydrophobic residues Ile^{32}, Val^{39} and Ile^{41}. Intermolecular contacts seen by NMR such as Ala^{21}/Val^{36} (Luhrs, Ritter et al. 2005) and Ile^{32}/Leu^{34}/Val^{36} (Petkova, Yau et al. 2006) are also observed for this motif. An earlier crystallographic structure of Aβ(28-42) fused C-terminally to Tk-RNase HII(Takano, Endo et al. 2006) also suggested formation of a limited β-hairpin conformation which partially overlaps with the Aβ-IgNAR-G1 β-hairpin motif (r.m.s.d. = 1.9 Å for 13 atoms).

[0176] The tetrameric structure displays features described for various models of both aβ protofilaments(Malinchik, Inouye et al. 1998; Losic, Martin et al. 2006) and soluble globulomers(Barghorn, Nimmrich et al. 2005) and shows strong correlation with other independently obtained structural data for Aβ fragments and fibrils(Rahimi, Shanmugam et al. 2008). The top and bottom of the tetramer is covered by a contiguous hydrophobic surface with a girdle of hydrophilic residues (^{22}EDVGSNKGA^{30}) running along the sides. The wedged-shape interface visible in our structure also suggest a possible mechanism for membrane-spanning pore formation(Jang, Zheng et al. 2008). Thus, we hypothesised that the observed dimer or tetramer may be a common structural motif in Aβ oligomerization, and modelled the Aβ tetramers minus the IgNAR domain as a building block of high order oligomers. By aligning Aβ tetramers on top of each other along the polar axis, utilising the interaction pattern observed between parallel Aβ stacks by NMR structure(Petkova, Yau et al. 2006), a series of multimeric constructs were generated (**Fig. 5a-c**). Sequential tetramers in this model are rotated by ~30° along the oligomer axis creating a twisted (coiled) cylinder up to ~40 Å wide. While the N-terminal residue Val^{18} appears to be too close to the next tetramer in this configuration, this probably results from constraints imposed by the IgNAR scaffold, which would be absent in a soluble oligomeric form. Adding N-terminal Aβ peptides residues

Ala^{1}-Lys^{16}, as described by XAFS data(Streltsov 2008), onto the crystallographic tetramer results in a model whereby this unstructured metal-binding fragment is ideally oriented to mediate reactive oxygen species toxicity. Mechanistically, neighbouring tetramers as shown in figure 3a-c align Glu^{22} and Asp^{23} side chains (from different tetramers) to form a belt of 4 potential metal-binding sites (Glu^{22}-Glu^{22} = 10-12 Å; Asp^{23}-Asp^{23} = 5.5-7 Å). With contributions from oxygen and nitrogens atoms this may conceivably produce one additional low affinity binding site per Aβ monomer in the aggregate. Upon metal binding to the Aβ N-terminus (Asp^{1}; Glu^{11}; His^{6}; His^{13}; His^{14}), the adjacent Val^{18}-Ala^{21} fragment should be stabilized, facilitating tetramer-tetramer interactions and accelerating oligomer (fibril) growth.

[0177] Familial and *in vitro*-generated mutations represent valuable tools for dissecting Aβ peptide function. For example the major pathogenic familial AD mutations(Walsh 2005), i.e. Ala^{21}Gly (Flemish), Glu^{22}Gly (Arctic), Glu^{22}Lys (Italian) and Asp^{23}Asn (Iowa) are localized within a β-turn stabilized by hydrogen bonds between Asp^{23} (OD1) and Ser^{26} (OG) (2.8 Å), and Asp^{23} (OD2) and Gly^{25} (N) (3.4 Å). Interactions with Phe^{20} also appear important for loop stability: Asp^{23} (OD1) is at 2.6 Å from an intra-loop water molecule which is at 3.1 Å from Phe^{20} (N), an interaction which FAD mutation Asp^{23}Asn is predicted break. Similarly, the "Wurth" mutations(Wurth, Guimard et al. 2002), derived *in vitro* from studies of the folding of Aβ(1-42) - GFP fusions(Wurth, Guimard et al. 2002), signpost residues important in aggregation. These mutations map into the surface residues of the monomer that interfere with formation of the dimer or tetramer interfaces and the amylogenic surface. For example mutation Leu^{34}Pro is described to markedly decrease Aβ aggregation, both alone and in combination with other variants. Here, the four Leu^{34} side-chains form a universal type joint, leading to our prediction that a Leu^{34}Pro substitution would here (1) disrupts the central hydrophobic core of the tetramer; and (2) break the β-sheets formed by residues Ile^{32}-Val^{36} between adjacent dimers. To test this theory, we produced the variant Aβ-IgNAR-G1 (Leu^{34}Pro) (SEQ ID NO. 7) and assessed the affect of this change on dimerisation. We observed marked reversion to monomeric form, of similar magnitude (~30%) to that originally described for this mutation *in vitro*(Wurth, Guimard et al. 2002). Upon affinity purification, this variant tended toward dimerisation, but in contrast to the parental Aβ-IgNAR-G1 was not resistant to β-mercaptoethanol treatment and failed to crystallise, suggesting that the tetramer interface had indeed been compromised.

[0178] The mechanistic basis of Aβ-mediated toxicity remains controversial and unresolved. Currently popular candidate mechanisms include: neuronal damage mediated by reactive oxygen species (ROS)(Bush 2000; Streltsov 2008); membrane destabilisation and/or pore formation(Jang, Zheng et al. 2008); and activation or modification of the apotopic pathway(Culmsee and Landshamer 2006). Most probably the final disease aetiology will prove to be multi-factorial. By developing a crystallographic model for amyloidogenic Aβ,

we hoped to devise a system to test such hypotheses. Surprisingly, our structures revealed not the expected β-turn-β extended loop, but rather an unusual and compact four-lobed cloverleaf structure, which may prove to be the proto-oligomeric building block. To the best of our knowledge, this "cloverleaf" model is the first full x-ray crystallographic structure of the amyloidogenic component of the Aβ peptide.

[0179] Simplistically, our structure can be envisaged as presenting three aspects, which we describe as the dimer interface, the tetramer interface, and the amyloid-extension face. Each potentially represents a viable target for interventionist agents aimed at disrupting oligomer formation and toxic activity. Such moieties may extend beyond imaging agents to novel chemical and biological entities, including chemical compounds and peptidomimetic constructs. In this sense, we believe our structure represents a possible novel paradigm for Aβ folding, which will engender testable hypotheses for the protein folding and toxicity of this medically important peptide and its associated forms.

EXAMPLE 2

Familial Mutations

[0180] A series of variants for Aβ-IgNAR-G1 were produced (Table 4), with the aim of determining the affect of so-called "familial mutations" upon the Aβ-IgNAR-G1 structure. All these mutation map to residues 21-23. All variants displayed the characteristic Aβ dimerization predicted from the structure.

Table 4

Protein	Description	Mutation	MW (Da)	Tag	SEQ ID NO:
35A-1	Aβ-IgNAR	-	15,654	FLAG x 2	2
12Y-2	IgNAR wt	-	14,878	FLAG x 2	3
37A-1	Aβ-IgNAR	Gly3	15,953	FLAG x 2	4
37Q-6	Aβ-IgNAR	Gly6	16,123	FLAG x 2	5
37P-3	Aβ-IgNAR	Gly2	15,768	FLAG x 2	6
37D-4	Aβ-IgNAR	Leu34Pro	15,638	FLAG x 2	7
37F-2	Aβ-IgNAR	Asp23Asn	15,653	FLAG x 2	8
37K-1	Aβ-IgNAR	Glu22Gln	15,653	FLAG x 2	9
37L-2	Aβ-IgNAR	Ala21Gly	15,640	FLAG x 2	10
37R-1	Aβ-IgNAR	ΔGlu22	15,525	FLAG x 2	11
37M-4	Aβ-IgNAR	Ser26Cys	15,670	FLAG x 2	12
37V-2	Aβ-IgNAR	-	14,345	His	13
37Y-1	IgNAR wt	-	13,553	His	14

[0181] A Western blot showed the characteristic dimerization for the familial mutants

compared to wild type Aβ-IgNAR-G1 (35A-1) and the non-dimerizing wild type IgNAR (12Y-2) and "Wurth" mutant 37D-4. Familial mutants of Aβ-IgNAR-G1 reveal the presence of dimeric species at ~30 kDa, in contrast to the wild type IgNAR (12Y-2) and the mutant Leu34Pro (37D-4)

EXAMPLE 3

In silico screening

[0182] The crystallographic structure co-ordinates were taken and screened *in silico* against a database of compounds.

[0183] The crystal structure of the tetramer was examined disregarding the IgNAR domains. A site (cavity) on the 'amyloidogenic' surface, bounded by residues (chain B and chain C and Aβ amino acid residue number within these chains) B18, B32, B33, B34, B35, B41, C18, C32, C33, C34, C35, and C41 was selected as the target for docking molecules from the chemical database. The 'Clean lead-like' subset (approx. 1136000 compounds) from the ZINC database (http://zinc.docking.org; J.J. Irwin and B.K. Shoichet, J. Chem. Inf. Model,. (2005), 45, 177-182) was used for the virtual screening or docking.

[0184] First, the program DOCK v. 6.2 (Univ. of California at San Francisco, USA; T.J.A. Ewing et al., J. Comput.-Aided Molec. Design, (2001), 15, 411-428.) was used to dock a segment of approx. 25000 compounds (molecules) from the database to the selected docking site on the tetramer surface. The force-field grid energy (sum of van der Waals and Coulomb energies) was used as the primary scoring function while the Zou GB/SA score (H-Y. Liu et al., J. Phys. Chem. B, (2004), 108, 5453-5462)) was used as the secondary scoring function. The DOCK output .mol2 files for each compound, giving the scores (energies) and the docked poses, were then processed by the program Binding Response (S. Zhong and A.D. MacKerell, J. Chem. Inf. Model., (2007), 47, 2302-2315) to obtain n, the number of docked molecule atoms enclosed by the docking site. Sorting the output, a total of 361 compounds were chosen for the second stage of virtual screening on the basis of the highest grid score, GB/SA score, and n.

[0185] The second stage of virtual screening was done with the program Surflex-Dock v.2.3 (A.N. Jain, J. Comput.-Aided Mol. Design, (2007), 21, 281-306), within Sybyl v.8.1 (Tripos Inc., St. Louis, USA). In docking with this program, the GeomX docking option was used with the number of additional starting conformations per molecule increased to 10 and the soft grid treatment turned off. From the docked poses, the top scoring molecules (Total score greater than 4.0, 'Crash' component of the score greater than -1.0) were visually examined and 6 compounds available from ChemBridge Corp. (San Diego, USA) were selected for

purchase. These compounds are set out in Table 5.

Table 5

Compound ID	Molecular Name	Molecular Weight
7996209	N-[2-(4-methylphenyl)-2-oxoethyl]-1-oxo-3,4-dihydro-1H-isochromene-3-carboxamide	323.3
7780327	2-methyl-3-{[(3-methylphenoxy)acetyl]amino}benzoic acid	299.2
7302096	3-{[(2,5-dimethoxyphenyl)amino]carbonyl}-7-oxabicyclo[2.2.1]hept-5-ene-2-carboxylic acid	319.3
5785027	2-{2-[(2-hydroxyethyl)amino]-1H-benzimidazol-1-yl}-1-(1-naphthyl)ethanone hydrobromide	426.3
9124833	3-methoxy-4-[2-(4-morpholinyl)-2-oxoethoxy]aniline	266.3
7949851	methyl [3-(phenoxyacetyl)-1H-indol-1-yl]acetate	323.3

[0186] Illustrations of these compounds binding to Ab-IgNAR structure are shown in Figures 6 to 11.

[0187] These 6 compounds were purchased and tested for binding to the Aβ-IgNAR-G1 dimer and IgNAR alone by BIAcore biosensor. No binding definitively above background was observed, perhaps due to the interface targeted ie dimer immobilized, but the cavity targeted was formed by the dimer-tetramer interface.

[0188] By way of comparison, docking performed for the anti-inflammatory drug fenofibrate which has been shown to bind Aβ (Kukar et al. Nature 453, 925-929 (2008) Substrate-targeting -secretase modulators). Docking experiments performed using the structure and a possible modelled solution presented in Figure 12.

[0189] No biochemical data for fenofibrate as soaking into crystals cracked the protein crystals, and the insolubility of fenofibrate precluded definitive biosensor experimentation.

[0190] It will be appreciated by persons skilled in the art that numerous variations and/or

modifications may be made to the invention as shown in the specific embodiments without departing from the spirit or scope of the invention as broadly described. The present embodiments are, therefore, to be considered in all respects as illustrative and not restrictive.

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APPENDIX I

```
HEADER    Ab-IgNAR
REMARK   3
REMARK   3 REFINEMENT.
REMARK   3   PROGRAM     : REFMAC 5.3.0040
REMARK   3
REMARK   3    REFINEMENT TARGET : MAXIMUM LIKELIHOOD
REMARK   3
REMARK   3  DATA USED IN REFINEMENT.
REMARK   3   RESOLUTION RANGE HIGH (ANGSTROMS) :   2.20
REMARK   3   RESOLUTION RANGE LOW  (ANGSTROMS) :  68.84
REMARK   3   DATA CUTOFF        (SIGMA(F)) : NONE
REMARK   3   COMPLETENESS FOR RANGE        (%) :  93.45
REMARK   3   NUMBER OF REFLECTIONS         :   26860
REMARK   3
REMARK   3  FIT TO DATA USED IN REFINEMENT.
REMARK   3   CROSS-VALIDATION METHOD           : THROUGHOUT
REMARK   3   FREE R VALUE TEST SET SELECTION   : RANDOM
REMARK   3   R VALUE     (WORKING + TEST SET) : 0.16841
REMARK   3   R VALUE       (WORKING SET) :  0.16431
REMARK   3   FREE R VALUE                  :  0.24650
REMARK   3   FREE R VALUE TEST SET SIZE   (%) :  5.1
REMARK   3   FREE R VALUE TEST SET COUNT      :  1439
REMARK   3
REMARK   3  FIT IN THE HIGHEST RESOLUTION BIN.
REMARK   3   TOTAL NUMBER OF BINS USED      :      20
REMARK   3   BIN RESOLUTION RANGE HIGH      :   2.202
REMARK   3   BIN RESOLUTION RANGE LOW       :   2.260
REMARK   3   REFLECTION IN BIN     (WORKING SET) :     1219
REMARK   3   BIN COMPLETENESS (WORKING+TEST) (%) :    56.98
REMARK   3   BIN R VALUE      (WORKING SET) :    0.229
REMARK   3   BIN FREE R VALUE SET COUNT           :       55
REMARK   3   BIN FREE R VALUE                 :    0.307
REMARK   3
REMARK   3  NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK   3   ALL ATOMS           :     4173
REMARK   3
REMARK   3  B VALUES.
REMARK   3   FROM WILSON PLOT      (A**2) : NULL
REMARK   3   MEAN B VALUE      (OVERALL, A**2) :  46.544
REMARK   3   OVERALL ANISOTROPIC B VALUE.
REMARK   3    B11 (A**2) :     0.05
REMARK   3    B22 (A**2) :     0.05
REMARK   3    B33 (A**2) :    -0.08
REMARK   3    B12 (A**2) :     0.03
REMARK   3    B13 (A**2) :     0.00
REMARK   3    B23 (A**2) :     0.00
REMARK   3
REMARK   3  ESTIMATED OVERALL COORDINATE ERROR.
REMARK   3   ESU BASED ON R VALUE                    (A):   0.241
REMARK   3   ESU BASED ON FREE R VALUE               (A):   0.223
REMARK   3   ESU BASED ON MAXIMUM LIKELIHOOD              (A):   0.152
REMARK   3   ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2):  11.557
REMARK   3
REMARK   3 CORRELATION COEFFICIENTS.
REMARK   3   CORRELATION COEFFICIENT FO-FC      :   0.968
REMARK   3   CORRELATION COEFFICIENT FO-FC FREE :   0.930
REMARK   3
REMARK   3  RMS DEVIATIONS FROM IDEAL VALUES         COUNT    RMS    WEIGHT
REMARK   3   BOND LENGTHS REFINED ATOMS        (A):  3835 ; 0.022 ; 0.022
REMARK   3   BOND ANGLES REFINED ATOMS   (DEGREES):  5173 ; 1.994 ; 1.953
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REMARK   3   TORSION ANGLES, PERIOD 1    (DEGREES):   499 ; 7.067 ; 5.000
REMARK   3   TORSION ANGLES, PERIOD 2    (DEGREES):   152 ;35.901 ;23.947
REMARK   3   TORSION ANGLES, PERIOD 3    (DEGREES):   664 ;21.119 ;15.000
REMARK   3   TORSION ANGLES, PERIOD 4    (DEGREES):    24 ;14.991 ;15.000
REMARK   3   CHIRAL-CENTER RESTRAINTS       (A**3):   591 ; 0.179 ; 0.200
REMARK   3   GENERAL PLANES REFINED ATOMS      (A):  2832 ; 0.008 ; 0.020
REMARK   3   NON-BONDED CONTACTS REFINED ATOMS (A):  1537 ; 0.228 ; 0.200
REMARK   3   NON-BONDED TORSION REFINED ATOMS  (A):  2516 ; 0.311 ; 0.200
REMARK   3   H-BOND (X...Y) REFINED ATOMS      (A):   292 ; 0.240 ; 0.200
REMARK   3   SYMMETRY VDW REFINED ATOMS        (A):    52 ; 0.222 ; 0.200
REMARK   3   SYMMETRY H-BOND REFINED ATOMS     (A):    22 ; 0.298 ; 0.200
REMARK   3
REMARK   3  ISOTROPIC THERMAL FACTOR RESTRAINTS.      COUNT   RMS    WEIGHT
REMARK   3   MAIN-CHAIN BOND REFINED ATOMS  (A**2):  2501 ; 1.051 ; 1.500
REMARK   3   MAIN-CHAIN ANGLE REFINED ATOMS (A**2):  3921 ; 1.795 ; 2.000
REMARK   3   SIDE-CHAIN BOND REFINED ATOMS  (A**2):  1515 ; 3.032 ; 3.000
REMARK   3   SIDE-CHAIN ANGLE REFINED ATOMS (A**2):  1252 ; 4.656 ; 4.500
REMARK   3
REMARK   3  NCS RESTRAINTS STATISTICS
REMARK   3   NUMBER OF NCS GROUPS : NULL
REMARK   3
REMARK   3  TLS DETAILS
REMARK   3   NUMBER OF TLS GROUPS  :    4
REMARK   3   ATOM RECORD CONTAINS RESIDUAL B FACTORS ONLY
REMARK   3
REMARK   3   TLS GROUP :     1
REMARK   3    NUMBER OF COMPONENTS GROUP :    1
REMARK   3    COMPONENTS        C SSSEQI   TO  C SSSEQI
REMARK   3    RESIDUE RANGE :   A        1        A      126
REMARK   3    ORIGIN FOR THE GROUP (A):  63.8110   0.9650 -21.6740
REMARK   3    T TENSOR
REMARK   3      T11:  -0.1980 T22:  -0.2050
REMARK   3      T33:  -0.1620 T12:   0.0369
REMARK   3      T13:   0.0437 T23:   0.0680
REMARK   3    L TENSOR
REMARK   3      L11:   2.9649 L22:   2.1492
REMARK   3      L33:   5.5016 L12:   1.6240
REMARK   3      L13:  -3.1186 L23:  -1.7013
REMARK   3    S TENSOR
REMARK   3      S11:  -0.1563 S12:   0.1452 S13:  -0.2168
REMARK   3      S21:  -0.3866 S22:   0.0489 S23:  -0.3471
REMARK   3      S31:   0.2723 S32:  -0.1279 S33:   0.1075
REMARK   3
REMARK   3   TLS GROUP :     2
REMARK   3    NUMBER OF COMPONENTS GROUP :    1
REMARK   3    COMPONENTS        C SSSEQI   TO  C SSSEQI
REMARK   3    RESIDUE RANGE :   B        1        B      126
REMARK   3    ORIGIN FOR THE GROUP (A):  22.5770 -14.1900 -12.2800
REMARK   3    T TENSOR
REMARK   3      T11:  -0.0751 T22:  -0.1155
REMARK   3      T33:  -0.1816 T12:  -0.0421
REMARK   3      T13:  -0.0399 T23:  -0.0558
REMARK   3    L TENSOR
REMARK   3      L11:  10.1470 L22:   1.3573
REMARK   3      L33:   3.5880 L12:   1.6659
REMARK   3      L13:   3.8599 L23:   0.8640
REMARK   3    S TENSOR
REMARK   3      S11:   0.2336 S12:  -0.7625 S13:  -0.3980
REMARK   3      S21:   0.2329 S22:  -0.2032 S23:  -0.1926
REMARK   3      S31:   0.0115 S32:  -0.2069 S33:  -0.0305
REMARK   3
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REMARK   3   TLS GROUP :     3
REMARK   3    NUMBER OF COMPONENTS GROUP :    1
REMARK   3    COMPONENTS        C SSSEQI   TO  C SSSEQI
REMARK   3    RESIDUE RANGE :   C        1        C      126
REMARK   3    ORIGIN FOR THE GROUP (A):  35.8140   7.3450   5.8670
REMARK   3    T TENSOR
REMARK   3      T11:  -0.1853 T22:  -0.1041
REMARK   3      T33:  -0.2449 T12:   0.0111
REMARK   3      T13:  -0.0203 T23:  -0.0062
REMARK   3    L TENSOR
REMARK   3      L11:   2.6982 L22:   1.5248
REMARK   3      L33:   3.8494 L12:  -1.7131
REMARK   3      L13:  -3.2164 L23:   2.1240
REMARK   3    S TENSOR
REMARK   3      S11:  -0.1201 S12:  -0.0335 S13:   0.0035
REMARK   3      S21:   0.0881 S22:  -0.0407 S23:   0.0913
REMARK   3      S31:   0.1124 S32:   0.0662 S33:   0.1608
REMARK   3
REMARK   3   TLS GROUP :     4
REMARK   3    NUMBER OF COMPONENTS GROUP :    1
REMARK   3    COMPONENTS        C SSSEQI   TO  C SSSEQI
REMARK   3    RESIDUE RANGE :   D        1        D      125
REMARK   3    ORIGIN FOR THE GROUP (A):  59.5290 -29.2800  -4.2380
REMARK   3    T TENSOR
REMARK   3      T11:   0.0220 T22:  -0.0010
REMARK   3      T33:  -0.1489 T12:   0.0046
REMARK   3      T13:   0.0795 T23:   0.0694
REMARK   3    L TENSOR
REMARK   3      L11:   2.7989 L22:   9.7864
REMARK   3      L33:   4.7502 L12:  -4.5612
REMARK   3      L13:   2.9365 L23:  -5.7275
REMARK   3    S TENSOR
REMARK   3      S11:   0.4188 S12:   0.4905 S13:   0.0482
REMARK   3      S21:  -0.7846 S22:  -0.4194 S23:   0.2228
REMARK   3      S31:   0.4959 S32:   0.5328 S33:   0.0006
REMARK   3
REMARK   3  BULK SOLVENT MODELLING.
REMARK   3   METHOD USED :  MASK
REMARK   3   PARAMETERS FOR MASK CALCULATION
REMARK   3   VDW PROBE RADIUS   :   1.20
REMARK   3   ION PROBE RADIUS   :   0.80
REMARK   3   SHRINKAGE RADIUS   :   0.80
REMARK   3
REMARK   3  OTHER REFINEMENT REMARKS:
REMARK   3  HYDROGENS HAVE BEEN ADDED IN THE RIDING POSITIONS
REMARK   3
SSBOND   1 CYS A   22    CYS A   83
SSBOND   2 CYS B   22    CYS B   83
SSBOND   3 CYS C   22    CYS C   83
SSBOND   4 CYS D   22    CYS D   83
CISPEP   1 THR A    6    PRO A    7               0.00
CISPEP   2 THR D    6    PRO D    7               0.00
CISPEP   3 THR B    6    PRO B    7               0.00
CISPEP   4 THR C    6    PRO C    7               0.00
CRYST1   79.399   79.399   84.890  90.00  90.00 120.00 P 32
SCALE1      0.012595  0.007272  0.000000        0.00000
SCALE2      0.000000  0.014543  0.000000        0.00000
SCALE3      0.000000  0.000000  0.011780        0.00000
ATOM      1  N   ALA A   1      61.749   8.643  -7.895  1.00 40.15      N
ATOM      2  CA  ALA A   1      62.634   7.902  -8.884  1.00 40.18      C
ATOM      3  CB  ALA A   1      62.339   6.518  -8.853  1.00 39.79      C
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ATOM      4  C   ALA A   1      62.285   8.403 -10.269  1.00 40.24      C
ATOM      5  O   ALA A   1      61.183   8.874 -10.490  1.00 40.36      O
ATOM      6  N   TRP A   2      63.195   8.273 -11.213  1.00 39.60      N
ATOM      7  CA  TRP A   2      62.842   8.487 -12.631  1.00 39.57      C
ATOM      8  CB  TRP A   2      62.870   9.972 -12.978  1.00 38.16      C
ATOM      9  CG  TRP A   2      64.196  10.736 -12.660  1.00 37.18      C
ATOM     10  CD1 TRP A   2      64.695  11.043 -11.419  1.00 36.93      C
ATOM     11  NE1 TRP A   2      65.878  11.763 -11.534  1.00 39.31      N
ATOM     12  CE2 TRP A   2      66.153  11.943 -12.869  1.00 37.67      C
ATOM     13  CD2 TRP A   2      65.132  11.298 -13.609  1.00 36.59      C
ATOM     14  CE3 TRP A   2      65.173  11.364 -15.011  1.00 37.43      C
ATOM     15  CZ3 TRP A   2      66.223  12.030 -15.622  1.00 37.01      C
ATOM     16  CH2 TRP A   2      67.259  12.614 -14.864  1.00 37.70      C
ATOM     17  CZ2 TRP A   2      67.247  12.571 -13.485  1.00 38.75      C
ATOM     18  C   TRP A   2      63.930   7.731 -13.337  1.00 40.62      C
ATOM     19  O   TRP A   2      64.970   7.444 -12.740  1.00 41.17      O
ATOM     20  N   VAL A   3      63.713   7.420 -14.598  1.00 41.79      N
ATOM     21  CA  VAL A   3      64.712   6.737 -15.393  1.00 41.23      C
ATOM     22  CB  VAL A   3      64.067   5.575 -16.107  1.00 42.49      C
ATOM     23  CG1 VAL A   3      65.010   5.042 -17.208  1.00 41.14      C
ATOM     24  CG2 VAL A   3      63.708   4.417 -15.072  1.00 42.49      C
ATOM     25  C   VAL A   3      65.240   7.752 -16.400  1.00 42.26      C
ATOM     26  O   VAL A   3      64.461   8.371 -17.135  1.00 39.69      O
ATOM     27  N   ASP A   4      66.560   7.946 -16.388  1.00 42.27      N
ATOM     28  CA  ASP A   4      67.259   8.833 -17.277  1.00 42.47      C
ATOM     29  CB  ASP A   4      68.484   9.335 -16.509  1.00 44.28      C
ATOM     30  CG  ASP A   4      69.123  10.573 -17.112  1.00 43.29      C
ATOM     31  OD1 ASP A   4      68.608  11.128 -18.127  1.00 41.54      O
ATOM     32  OD2 ASP A   4      70.150  10.991 -16.507  1.00 47.28      O
ATOM     33  C   ASP A   4      67.725   8.103 -18.544  1.00 42.79      C
ATOM     34  O   ASP A   4      68.709   7.350 -18.523  1.00 43.97      O
ATOM     35  N   GLN A   5      67.048   8.361 -19.639  1.00 42.16      N
ATOM     36  CA  GLN A   5      67.299   7.703 -20.903  1.00 43.25      C
ATOM     37  CB  GLN A   5      65.983   7.258 -21.571  1.00 42.36      C
ATOM     38  CG  GLN A   5      66.230   6.429 -22.844  1.00 43.49      C
ATOM     39  CD  GLN A   5      64.959   5.836 -23.412  1.00 43.79      C
ATOM     40  OE1 GLN A   5      63.975   5.772 -22.714  1.00 45.41      O
ATOM     41  NE2 GLN A   5      64.976   5.402 -24.693  1.00 41.11      N
ATOM     42  C   GLN A   5      68.052   8.629 -21.864  1.00 42.68      C
ATOM     43  O   GLN A   5      67.584   9.724 -22.191  1.00 41.82      O
ATOM     44  N   THR A   6      69.198   8.157 -22.354  1.00 42.97      N
ATOM     45  CA  THR A   6      69.971   8.908 -23.364  1.00 42.86      C
ATOM     46  CB  THR A   6      71.203   9.619 -22.713  1.00 43.54      C
ATOM     47  OG1 THR A   6      71.985   8.617 -22.080  1.00 44.91      O
ATOM     48  CG2 THR A   6      70.801  10.670 -21.649  1.00 41.18      C
ATOM     49  C   THR A   6      70.442   8.007 -24.507  1.00 43.00      C
ATOM     50  O   THR A   6      70.734   6.818 -24.262  1.00 44.11      O
ATOM     51  N   PRO A   7      70.571   8.561 -25.757  1.00 42.63      N
ATOM     52  CA  PRO A   7      70.323   9.961 -26.145  1.00 42.77      C
ATOM     53  CB  PRO A   7      71.057  10.081 -27.477  1.00 41.46      C
ATOM     54  CG  PRO A   7      70.903   8.752 -28.078  1.00 41.46      C
ATOM     55  CD  PRO A   7      71.052   7.779 -26.918  1.00 43.08      C
ATOM     56  C   PRO A   7      68.835  10.178 -26.359  1.00 43.23      C
ATOM     57  O   PRO A   7      68.177   9.198 -26.651  1.00 44.91      O
ATOM     58  N   ARG A   8      68.302  11.392 -26.222  1.00 43.41      N
ATOM     59  CA  ARG A   8      66.868  11.625 -26.493  1.00 44.08      C
ATOM     60  CB  ARG A   8      66.349  12.944 -25.869  1.00 43.76      C
ATOM     61  CG  ARG A   8      64.763  13.006 -25.738  1.00 46.28      C
ATOM     62  CD  ARG A   8      64.248  13.844 -24.561  1.00 48.21      C
ATOM     63  NE  ARG A   8      64.530  13.270 -23.235  1.00 51.99      N
ATOM     64  CZ  ARG A   8      64.574  13.982 -22.102  1.00 49.58      C
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ATOM	65	NH1	ARG	A	8	64.388	15.306	-22.123	1.00	45.49	N
ATOM	66	NH2	ARG	A	8	64.817	13.367	-20.953	1.00	50.31	N
ATOM	67	C	ARG	A	8	66.538	11.587	-27.988	1.00	43.51	C
ATOM	68	O	ARG	A	8	65.418	11.284	-28.370	1.00	43.05	O
ATOM	69	N	THR	A	9	67.498	11.929	-28.846	1.00	42.86	N
ATOM	70	CA	THR	A	9	67.285	11.777	-30.274	1.00	43.57	C
ATOM	71	CB	THR	A	9	66.814	13.095	-30.939	1.00	43.56	C
ATOM	72	OG1	THR	A	9	67.858	14.036	-30.821	1.00	48.77	O
ATOM	73	CG2	THR	A	9	65.563	13.731	-30.225	1.00	43.75	C
ATOM	74	C	THR	A	9	68.564	11.279	-30.904	1.00	42.93	C
ATOM	75	O	THR	A	9	69.650	11.556	-30.398	1.00	43.89	O
ATOM	76	N	ALA	A	10	68.453	10.511	-31.978	1.00	42.78	N
ATOM	77	CA	ALA	A	10	69.619	9.970	-32.667	1.00	42.32	C
ATOM	78	CB	ALA	A	10	69.994	8.627	-32.086	1.00	42.83	C
ATOM	79	C	ALA	A	10	69.314	9.859	-34.149	1.00	43.20	C
ATOM	80	O	ALA	A	10	68.155	9.623	-34.518	1.00	43.17	O
ATOM	81	N	THR	A	11	70.318	10.143	-34.992	1.00	42.97	N
ATOM	82	CA	THR	A	11	70.225	9.915	-36.444	1.00	43.50	C
ATOM	83	CB	THR	A	11	70.189	11.203	-37.289	1.00	43.99	C
ATOM	84	OG1	THR	A	11	69.173	12.071	-36.792	1.00	46.81	O
ATOM	85	CG2	THR	A	11	69.888	10.919	-38.782	1.00	44.63	C
ATOM	86	C	THR	A	11	71.394	9.035	-36.818	1.00	42.68	C
ATOM	87	O	THR	A	11	72.527	9.265	-36.405	1.00	42.50	O
ATOM	88	N	LYS	A	12	71.095	7.988	-37.565	1.00	42.11	N
ATOM	89	CA	LYS	A	12	72.062	6.984	-37.863	1.00	41.61	C
ATOM	90	CB	LYS	A	12	71.742	5.752	-37.024	1.00	42.20	C
ATOM	91	CG	LYS	A	12	72.682	5.566	-35.832	1.00	42.69	C
ATOM	92	CD	LYS	A	12	72.462	6.488	-34.722	1.00	42.75	C
ATOM	93	CE	LYS	A	12	73.785	6.938	-34.193	1.00	45.64	C
ATOM	94	NZ	LYS	A	12	74.413	5.947	-33.372	1.00	45.06	N
ATOM	95	C	LYS	A	12	72.005	6.639	-39.319	1.00	41.13	C
ATOM	96	O	LYS	A	12	70.939	6.763	-39.917	1.00	40.78	O
ATOM	97	N	GLU	A	13	73.148	6.221	-39.886	1.00	41.13	N
ATOM	98	CA	GLU	A	13	73.217	5.639	-41.224	1.00	41.27	C
ATOM	99	CB	GLU	A	13	74.632	5.698	-41.828	1.00	42.20	C
ATOM	100	CG	GLU	A	13	75.229	7.083	-41.972	1.00	45.88	C
ATOM	101	CD	GLU	A	13	74.375	8.034	-42.822	1.00	46.51	C
ATOM	102	OE1	GLU	A	13	74.450	9.257	-42.598	1.00	46.46	O
ATOM	103	OE2	GLU	A	13	73.643	7.546	-43.710	1.00	49.37	O
ATOM	104	C	GLU	A	13	72.800	4.187	-41.192	1.00	40.83	C
ATOM	105	O	GLU	A	13	72.992	3.508	-40.169	1.00	41.54	O
ATOM	106	N	THR	A	14	72.215	3.721	-42.301	1.00	40.03	N
ATOM	107	CA	THR	A	14	71.940	2.318	-42.489	1.00	39.84	C
ATOM	108	CB	THR	A	14	71.377	2.042	-43.909	1.00	40.21	C
ATOM	109	OG1	THR	A	14	69.983	2.377	-43.955	1.00	37.92	O
ATOM	110	CG2	THR	A	14	71.526	0.563	-44.299	1.00	39.74	C
ATOM	111	C	THR	A	14	73.270	1.599	-42.243	1.00	40.13	C
ATOM	112	O	THR	A	14	74.324	2.000	-42.791	1.00	39.27	O
ATOM	113	N	GLY	A	15	73.233	0.613	-41.342	1.00	40.34	N
ATOM	114	CA	GLY	A	15	74.396	-0.218	-41.032	1.00	40.42	C
ATOM	115	C	GLY	A	15	75.117	0.128	-39.748	1.00	40.96	C
ATOM	116	O	GLY	A	15	75.788	-0.709	-39.224	1.00	41.04	O
ATOM	117	N	GLU	A	16	74.989	1.365	-39.256	1.00	41.99	N
ATOM	118	CA	GLU	A	16	75.598	1.850	-38.014	1.00	43.51	C
ATOM	119	CB	GLU	A	16	75.343	3.359	-37.860	1.00	43.93	C
ATOM	120	CG	GLU	A	16	76.304	4.377	-38.538	1.00	45.03	C
ATOM	121	CD	GLU	A	16	76.197	5.807	-37.839	1.00	46.94	C
ATOM	122	OE1	GLU	A	16	75.428	6.678	-38.323	1.00	43.22	O
ATOM	123	OE2	GLU	A	16	76.837	6.036	-36.754	1.00	52.94	O
ATOM	124	C	GLU	A	16	74.854	1.177	-36.872	1.00	43.56	C
ATOM	125	O	GLU	A	16	73.865	0.509	-37.092	1.00	43.77	O

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ATOM    126  N   SER A  17      75.282   1.388 -35.641  1.00 43.74      N
ATOM    127  CA  SER A  17      74.492   0.923 -34.544  1.00 44.40      C
ATOM    128  CB  SER A  17      75.215  -0.229 -33.873  1.00 44.97      C
ATOM    129  OG  SER A  17      76.123   0.270 -32.945  1.00 50.00      O
ATOM    130  C   SER A  17      74.111   2.054 -33.578  1.00 44.40      C
ATOM    131  O   SER A  17      74.564   3.183 -33.740  1.00 43.42      O
ATOM    132  N   LEU A  18      73.218   1.768 -32.623  1.00 44.29      N
ATOM    133  CA  LEU A  18      72.750   2.743 -31.631  1.00 43.42      C
ATOM    134  CB  LEU A  18      71.264   3.018 -31.857  1.00 44.02      C
ATOM    135  CG  LEU A  18      70.458   4.188 -31.246  1.00 45.03      C
ATOM    136  CD1 LEU A  18      69.189   3.777 -30.570  1.00 43.77      C
ATOM    137  CD2 LEU A  18      71.201   5.339 -30.494  1.00 43.20      C
ATOM    138  C   LEU A  18      72.893   2.116 -30.251  1.00 43.15      C
ATOM    139  O   LEU A  18      72.533   0.967 -30.042  1.00 42.50      O
ATOM    140  N   THR A  19      73.396   2.881 -29.305  1.00 42.18      N
ATOM    141  CA  THR A  19      73.367   2.460 -27.919  1.00 42.94      C
ATOM    142  CB  THR A  19      74.762   2.333 -27.352  1.00 41.91      C
ATOM    143  OG1 THR A  19      75.459   1.366 -28.144  1.00 46.16      O
ATOM    144  CG2 THR A  19      74.690   1.835 -25.920  1.00 43.14      C
ATOM    145  C   THR A  19      72.566   3.445 -27.107  1.00 42.46      C
ATOM    146  O   THR A  19      72.838   4.656 -27.120  1.00 42.53      O
ATOM    147  N   ILE A  20      71.548   2.927 -26.451  1.00 42.31      N
ATOM    148  CA  ILE A  20      70.689   3.706 -25.552  1.00 43.03      C
ATOM    149  CB  ILE A  20      69.201   3.335 -25.767  1.00 43.33      C
ATOM    150  CG1 ILE A  20      68.800   3.502 -27.256  1.00 44.11      C
ATOM    151  CD1 ILE A  20      67.399   2.948 -27.600  1.00 44.88      C
ATOM    152  CG2 ILE A  20      68.302   4.141 -24.822  1.00 42.84      C
ATOM    153  C   ILE A  20      71.077   3.333 -24.134  1.00 42.61      C
ATOM    154  O   ILE A  20      71.157   2.147 -23.843  1.00 41.82      O
ATOM    155  N   ASN A  21      71.379   4.327 -23.294  1.00 43.17      N
ATOM    156  CA  ASN A  21      71.708   4.102 -21.860  1.00 44.83      C
ATOM    157  CB  ASN A  21      72.990   4.831 -21.455  1.00 44.74      C
ATOM    158  CG  ASN A  21      74.197   4.409 -22.296  1.00 50.81      C
ATOM    159  OD1 ASN A  21      74.786   3.335 -22.070  1.00 57.38      O
ATOM    160  ND2 ASN A  21      74.594   5.257 -23.256  1.00 52.86      N
ATOM    161  C   ASN A  21      70.569   4.588 -20.961  1.00 45.00      C
ATOM    162  O   ASN A  21      70.033   5.670 -21.182  1.00 44.50      O
ATOM    163  N   CYS A  22      70.208   3.816 -19.949  1.00 44.60      N
ATOM    164  CA  CYS A  22      69.167   4.237 -19.029  1.00 45.32      C
ATOM    165  CB  CYS A  22      67.909   3.372 -19.165  1.00 45.74      C
ATOM    166  SG  CYS A  22      66.995   3.746 -20.639  1.00 54.23      S
ATOM    167  C   CYS A  22      69.658   4.101 -17.624  1.00 44.15      C
ATOM    168  O   CYS A  22      70.236   3.107 -17.289  1.00 43.54      O
ATOM    169  N   VAL A  23      69.395   5.085 -16.785  1.00 43.49      N
ATOM    170  CA  VAL A  23      69.643   4.909 -15.365  1.00 42.35      C
ATOM    171  CB  VAL A  23      71.085   5.352 -14.883  1.00 43.00      C
ATOM    172  CG1 VAL A  23      71.963   6.041 -15.953  1.00 41.73      C
ATOM    173  CG2 VAL A  23      71.199   5.917 -13.413  1.00 42.45      C
ATOM    174  C   VAL A  23      68.417   5.249 -14.481  1.00 42.71      C
ATOM    175  O   VAL A  23      67.709   6.260 -14.671  1.00 41.74      O
ATOM    176  N   LEU A  24      68.123   4.344 -13.563  1.00 42.36      N
ATOM    177  CA  LEU A  24      67.057   4.563 -12.645  1.00 43.14      C
ATOM    178  CB  LEU A  24      66.608   3.213 -12.068  1.00 43.10      C
ATOM    179  CG  LEU A  24      65.662   3.260 -10.863  1.00 44.67      C
ATOM    180  CD1 LEU A  24      64.281   3.811 -11.337  1.00 42.56      C
ATOM    181  CD2 LEU A  24      65.508   1.885 -10.150  1.00 44.14      C
ATOM    182  C   LEU A  24      67.691   5.476 -11.592  1.00 42.20      C
ATOM    183  O   LEU A  24      68.575   5.053 -10.877  1.00 42.62      O
ATOM    184  N   ARG A  25      67.261   6.734 -11.531  1.00 41.75      N
ATOM    185  CA  ARG A  25      67.859   7.731 -10.598  1.00 40.94      C
ATOM    186  CB  ARG A  25      68.196   9.032 -11.327  1.00 39.67      C
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ATOM	187	CG	ARG	A	25	69.067	8.832	-12.554	1.00	39.63	C
ATOM	188	CD	ARG	A	25	69.891	10.080	-12.859	1.00	38.88	C
ATOM	189	NE	ARG	A	25	70.828	9.833	-13.950	1.00	44.89	N
ATOM	190	CZ	ARG	A	25	72.121	9.535	-13.783	1.00	47.29	C
ATOM	191	NH1	ARG	A	25	72.620	9.447	-12.539	1.00	46.01	N
ATOM	192	NH2	ARG	A	25	72.924	9.391	-14.850	1.00	43.92	N
ATOM	193	C	ARG	A	25	66.903	8.056	-9.468	1.00	41.31	C
ATOM	194	O	ARG	A	25	65.691	7.828	-9.600	1.00	39.67	O
ATOM	195	N	ASP	A	26	67.466	8.586	-8.375	1.00	41.32	N
ATOM	196	CA	ASP	A	26	66.756	8.989	-7.190	1.00	43.62	C
ATOM	197	CB	ASP	A	26	66.179	10.401	-7.349	1.00	45.00	C
ATOM	198	CG	ASP	A	26	67.224	11.395	-7.953	1.00	52.91	C
ATOM	199	OD1	ASP	A	26	66.854	12.215	-8.853	1.00	59.13	O
ATOM	200	OD2	ASP	A	26	68.436	11.347	-7.556	1.00	60.06	O
ATOM	201	C	ASP	A	26	65.732	7.986	-6.674	1.00	43.23	C
ATOM	202	O	ASP	A	26	64.635	8.350	-6.232	1.00	43.09	O
ATOM	203	N	ALA	A	27	66.114	6.708	-6.710	1.00	43.21	N
ATOM	204	CA	ALA	A	27	65.231	5.600	-6.311	1.00	42.66	C
ATOM	205	CB	ALA	A	27	65.081	4.609	-7.466	1.00	40.95	C
ATOM	206	C	ALA	A	27	65.800	4.898	-5.058	1.00	43.66	C
ATOM	207	O	ALA	A	27	66.997	4.563	-4.986	1.00	43.64	O
ATOM	208	N	SER	A	28	64.929	4.643	-4.097	1.00	44.63	N
ATOM	209	CA	SER	A	28	65.301	3.945	-2.860	1.00	46.25	C
ATOM	210	CB	SER	A	28	64.306	4.340	-1.793	1.00	46.62	C
ATOM	211	OG	SER	A	28	62.989	4.076	-2.343	1.00	51.66	O
ATOM	212	C	SER	A	28	65.244	2.424	-3.024	1.00	45.27	C
ATOM	213	O	SER	A	28	65.753	1.699	-2.204	1.00	45.50	O
ATOM	214	N	PHE	A	29	64.597	1.951	-4.080	1.00	44.65	N
ATOM	215	CA	PHE	A	29	64.428	0.515	-4.320	1.00	44.66	C
ATOM	216	CB	PHE	A	29	63.026	0.206	-4.853	1.00	44.20	C
ATOM	217	CG	PHE	A	29	62.491	1.236	-5.821	1.00	43.80	C
ATOM	218	CD1	PHE	A	29	61.557	2.181	-5.392	1.00	42.75	C
ATOM	219	CE1	PHE	A	29	61.055	3.155	-6.275	1.00	42.50	C
ATOM	220	CZ	PHE	A	29	61.457	3.156	-7.641	1.00	42.43	C
ATOM	221	CE2	PHE	A	29	62.376	2.202	-8.074	1.00	43.56	C
ATOM	222	CD2	PHE	A	29	62.895	1.243	-7.168	1.00	40.83	C
ATOM	223	C	PHE	A	29	65.444	0.022	-5.324	1.00	44.85	C
ATOM	224	O	PHE	A	29	66.046	0.816	-6.017	1.00	45.13	O
ATOM	225	N	GLU	A	30	65.606	-1.292	-5.428	1.00	44.65	N
ATOM	226	CA	GLU	A	30	66.616	-1.829	-6.302	1.00	45.34	C
ATOM	227	CB	GLU	A	30	67.141	-3.148	-5.719	1.00	46.03	C
ATOM	228	CG	GLU	A	30	67.484	-3.139	-4.182	1.00	51.87	C
ATOM	229	CD	GLU	A	30	68.905	-2.718	-3.833	1.00	61.36	C
ATOM	230	OE1	GLU	A	30	69.655	-3.533	-3.218	1.00	64.71	O
ATOM	231	OE2	GLU	A	30	69.283	-1.554	-4.132	1.00	66.90	O
ATOM	232	C	GLU	A	30	66.040	-2.045	-7.710	1.00	44.87	C
ATOM	233	O	GLU	A	30	64.804	-2.206	-7.902	1.00	43.77	O
ATOM	234	N	LEU	A	31	66.933	-2.100	-8.692	1.00	44.05	N
ATOM	235	CA	LEU	A	31	66.527	-2.480	-10.022	1.00	44.47	C
ATOM	236	CB	LEU	A	31	67.529	-1.966	-11.057	1.00	44.35	C
ATOM	237	CG	LEU	A	31	67.302	-2.279	-12.541	1.00	44.08	C
ATOM	238	CD1	LEU	A	31	68.569	-2.051	-13.351	1.00	41.58	C
ATOM	239	CD2	LEU	A	31	66.136	-1.523	-13.132	1.00	41.76	C
ATOM	240	C	LEU	A	31	66.373	-4.001	-10.047	1.00	45.45	C
ATOM	241	O	LEU	A	31	67.337	-4.736	-9.819	1.00	46.74	O
ATOM	242	N	LYS	A	32	65.139	-4.478	-10.238	1.00	45.05	N
ATOM	243	CA	LYS	A	32	64.876	-5.919	-10.271	1.00	44.49	C
ATOM	244	CB	LYS	A	32	63.509	-6.221	-9.649	1.00	44.92	C
ATOM	245	CG	LYS	A	32	63.393	-5.867	-8.121	1.00	46.76	C
ATOM	246	CD	LYS	A	32	64.441	-6.598	-7.239	1.00	46.19	C
ATOM	247	CE	LYS	A	32	63.953	-6.546	-5.816	1.00	50.58	C

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ATOM    248  NZ  LYS A  32      64.928  -7.103  -4.883  1.00 53.68      N
ATOM    249  C   LYS A  32      64.934  -6.509 -11.676  1.00 44.11      C
ATOM    250  O   LYS A  32      65.328  -7.643 -11.858  1.00 42.45      O
ATOM    251  N   ASP A  33      64.509  -5.743 -12.676  1.00 44.84      N
ATOM    252  CA  ASP A  33      64.436  -6.261 -14.076  1.00 44.80      C
ATOM    253  CB  ASP A  33      63.261  -7.211 -14.233  1.00 45.40      C
ATOM    254  CG  ASP A  33      63.419  -8.179 -15.400  1.00 49.24      C
ATOM    255  OD1 ASP A  33      64.455  -8.192 -16.141  1.00 47.77      O
ATOM    256  OD2 ASP A  33      62.433  -8.933 -15.577  1.00 55.63      O
ATOM    257  C   ASP A  33      64.293  -5.127 -15.063  1.00 44.19      C
ATOM    258  O   ASP A  33      64.063  -3.981 -14.671  1.00 42.88      O
ATOM    259  N   THR A  34      64.481  -5.431 -16.348  1.00 43.32      N
ATOM    260  CA  THR A  34      64.513  -4.362 -17.365  1.00 42.96      C
ATOM    261  CB  THR A  34      65.977  -4.082 -17.816  1.00 43.35      C
ATOM    262  OG1 THR A  34      66.616  -5.313 -18.245  1.00 46.20      O
ATOM    263  CG2 THR A  34      66.799  -3.582 -16.631  1.00 42.87      C
ATOM    264  C   THR A  34      63.634  -4.801 -18.566  1.00 42.17      C
ATOM    265  O   THR A  34      63.395  -6.018 -18.771  1.00 40.33      O
ATOM    266  N   GLY A  35      63.143  -3.820 -19.318  1.00 40.76      N
ATOM    267  CA  GLY A  35      62.446  -4.100 -20.554  1.00 40.48      C
ATOM    268  C   GLY A  35      62.659  -2.980 -21.531  1.00 40.71      C
ATOM    269  O   GLY A  35      63.001  -1.868 -21.139  1.00 41.72      O
ATOM    270  N   TRP A  36      62.465  -3.294 -22.815  1.00 40.28      N
ATOM    271  CA  TRP A  36      62.674  -2.399 -23.935  1.00 40.14      C
ATOM    272  CB  TRP A  36      63.993  -2.767 -24.656  1.00 38.78      C
ATOM    273  CG  TRP A  36      65.201  -2.495 -23.763  1.00 37.14      C
ATOM    274  CD1 TRP A  36      65.778  -3.349 -22.867  1.00 36.99      C
ATOM    275  NE1 TRP A  36      66.846  -2.715 -22.216  1.00 37.64      N
ATOM    276  CE2 TRP A  36      66.915  -1.410 -22.659  1.00 37.73      C
ATOM    277  CD2 TRP A  36      65.912  -1.233 -23.632  1.00 35.75      C
ATOM    278  CE3 TRP A  36      65.771   0.021 -24.231  1.00 38.30      C
ATOM    279  CZ3 TRP A  36      66.662   1.028 -23.895  1.00 38.55      C
ATOM    280  CH2 TRP A  36      67.669   0.808 -22.922  1.00 38.11      C
ATOM    281  CZ2 TRP A  36      67.803  -0.388 -22.308  1.00 39.69      C
ATOM    282  C   TRP A  36      61.462  -2.494 -24.882  1.00 40.45      C
ATOM    283  O   TRP A  36      60.900  -3.575 -25.086  1.00 37.84      O
ATOM    284  N   TYR A  37      61.082  -1.350 -25.466  1.00 40.70      N
ATOM    285  CA  TYR A  37      59.866  -1.236 -26.308  1.00 41.93      C
ATOM    286  CB  TYR A  37      58.685  -0.707 -25.468  1.00 42.76      C
ATOM    287  CG  TYR A  37      58.563  -1.427 -24.194  1.00 42.14      C
ATOM    288  CD1 TYR A  37      57.719  -2.520 -24.075  1.00 40.34      C
ATOM    289  CE1 TYR A  37      57.646  -3.242 -22.868  1.00 41.85      C
ATOM    290  CZ  TYR A  37      58.426  -2.826 -21.801  1.00 42.69      C
ATOM    291  OH  TYR A  37      58.379  -3.479 -20.599  1.00 47.21      O
ATOM    292  CE2 TYR A  37      59.238  -1.728 -21.895  1.00 42.12      C
ATOM    293  CD2 TYR A  37      59.307  -1.027 -23.098  1.00 41.52      C
ATOM    294  C   TYR A  37      60.081  -0.257 -27.427  1.00 42.18      C
ATOM    295  O   TYR A  37      60.936   0.595 -27.346  1.00 41.61      O
ATOM    296  N   ARG A  38      59.267  -0.357 -28.453  1.00 43.78      N
ATOM    297  CA  ARG A  38      59.532   0.406 -29.648  1.00 46.16      C
ATOM    298  CB  ARG A  38      60.599  -0.320 -30.467  1.00 45.76      C
ATOM    299  CG  ARG A  38      60.521  -0.353 -31.940  1.00 49.53      C
ATOM    300  CD  ARG A  38      61.333  -1.543 -32.436  1.00 50.13      C
ATOM    301  NE  ARG A  38      60.989  -1.847 -33.794  1.00 52.73      N
ATOM    302  CZ  ARG A  38      61.856  -1.891 -34.805  1.00 60.11      C
ATOM    303  NH1 ARG A  38      61.402  -2.162 -36.023  1.00 59.27      N
ATOM    304  NH2 ARG A  38      63.172  -1.662 -34.620  1.00 60.83      N
ATOM    305  C   ARG A  38      58.216   0.686 -30.345  1.00 46.60      C
ATOM    306  O   ARG A  38      57.320  -0.172 -30.373  1.00 46.42      O
ATOM    307  N   THR A  39      58.077   1.929 -30.802  1.00 46.84      N
ATOM    308  CA  THR A  39      56.980   2.339 -31.664  1.00 47.57      C
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ATOM	309	CB	THR	A	39	56.261	3.586	-31.110	1.00	47.10	C
ATOM	310	OG1	THR	A	39	55.916	3.378	-29.750	1.00	50.61	O
ATOM	311	CG2	THR	A	39	54.999	3.839	-31.858	1.00	49.14	C
ATOM	312	C	THR	A	39	57.637	2.703	-32.961	1.00	47.84	C
ATOM	313	O	THR	A	39	58.482	3.618	-32.983	1.00	46.61	O
ATOM	314	N	LYS	A	40	57.283	1.980	-34.034	1.00	49.00	N
ATOM	315	CA	LYS	A	40	57.849	2.253	-35.349	1.00	51.32	C
ATOM	316	CB	LYS	A	40	57.656	1.095	-36.329	1.00	51.60	C
ATOM	317	CG	LYS	A	40	58.368	-0.180	-35.877	1.00	54.32	C
ATOM	318	CD	LYS	A	40	58.208	-1.327	-36.858	1.00	55.56	C
ATOM	319	CE	LYS	A	40	59.149	-1.119	-38.039	1.00	55.54	C
ATOM	320	NZ	LYS	A	40	59.491	-2.440	-38.640	1.00	58.58	N
ATOM	321	C	LYS	A	40	57.310	3.555	-35.909	1.00	51.81	C
ATOM	322	O	LYS	A	40	56.245	4.013	-35.513	1.00	51.60	O
ATOM	323	N	LEU	A	41	58.073	4.166	-36.805	1.00	53.16	N
ATOM	324	CA	LEU	A	41	57.623	5.383	-37.454	1.00	54.73	C
ATOM	325	CB	LEU	A	41	58.735	5.951	-38.319	1.00	55.27	C
ATOM	326	CG	LEU	A	41	58.569	7.373	-38.833	1.00	56.10	C
ATOM	327	CD1	LEU	A	41	59.828	7.743	-39.616	1.00	54.91	C
ATOM	328	CD2	LEU	A	41	58.320	8.338	-37.636	1.00	58.13	C
ATOM	329	C	LEU	A	41	56.385	5.086	-38.311	1.00	55.70	C
ATOM	330	O	LEU	A	41	56.424	4.238	-39.228	1.00	55.38	O
ATOM	331	N	GLY	A	42	55.290	5.778	-38.001	1.00	56.61	N
ATOM	332	CA	GLY	A	42	54.043	5.583	-38.715	1.00	57.83	C
ATOM	333	C	GLY	A	42	53.064	4.709	-37.968	1.00	59.16	C
ATOM	334	O	GLY	A	42	51.849	4.803	-38.199	1.00	59.45	O
ATOM	335	N	SER	A	43	53.587	3.873	-37.060	1.00	60.41	N
ATOM	336	CA	SER	A	43	52.775	2.988	-36.198	1.00	61.00	C
ATOM	337	CB	SER	A	43	53.550	1.722	-35.781	1.00	60.84	C
ATOM	338	OG	SER	A	43	53.706	0.833	-36.880	1.00	61.59	O
ATOM	339	C	SER	A	43	52.239	3.671	-34.956	1.00	61.22	C
ATOM	340	O	SER	A	43	52.845	4.581	-34.387	1.00	61.91	O
ATOM	341	N	THR	A	44	51.092	3.206	-34.507	1.00	61.44	N
ATOM	342	CA	THR	A	44	50.502	3.811	-33.352	1.00	61.38	C
ATOM	343	CB	THR	A	44	48.964	3.869	-33.493	1.00	61.80	C
ATOM	344	OG1	THR	A	44	48.650	4.479	-34.762	1.00	60.23	O
ATOM	345	CG2	THR	A	44	48.307	4.653	-32.316	1.00	59.36	C
ATOM	346	C	THR	A	44	50.973	3.105	-32.083	1.00	61.97	C
ATOM	347	O	THR	A	44	51.440	3.773	-31.146	1.00	62.38	O
ATOM	348	N	ASN	A	45	50.885	1.770	-32.064	1.00	61.54	N
ATOM	349	CA	ASN	A	45	51.100	1.020	-30.825	1.00	61.43	C
ATOM	350	CB	ASN	A	45	50.127	-0.173	-30.705	1.00	61.50	C
ATOM	351	CG	ASN	A	45	48.642	0.221	-30.958	1.00	62.37	C
ATOM	352	OD1	ASN	A	45	48.185	1.305	-30.582	1.00	62.72	O
ATOM	353	ND2	ASN	A	45	47.896	-0.683	-31.590	1.00	61.46	N
ATOM	354	C	ASN	A	45	52.560	0.609	-30.523	1.00	60.98	C
ATOM	355	O	ASN	A	45	53.299	0.149	-31.394	1.00	61.08	O
ATOM	356	N	GLU	A	46	52.938	0.823	-29.265	1.00	60.78	N
ATOM	357	CA	GLU	A	46	54.210	0.400	-28.672	1.00	60.71	C
ATOM	358	CB	GLU	A	46	54.284	0.954	-27.266	1.00	60.85	C
ATOM	359	CG	GLU	A	46	55.575	0.708	-26.576	1.00	63.83	C
ATOM	360	CD	GLU	A	46	55.497	1.029	-25.103	1.00	70.18	C
ATOM	361	OE1	GLU	A	46	54.694	0.349	-24.389	1.00	72.55	O
ATOM	362	OE2	GLU	A	46	56.254	1.940	-24.657	1.00	73.06	O
ATOM	363	C	GLU	A	46	54.333	-1.121	-28.614	1.00	59.83	C
ATOM	364	O	GLU	A	46	53.389	-1.791	-28.220	1.00	60.32	O
ATOM	365	N	GLN	A	47	55.485	-1.669	-29.007	1.00	58.86	N
ATOM	366	CA	GLN	A	47	55.685	-3.121	-28.999	1.00	57.92	C
ATOM	367	CB	GLN	A	47	55.601	-3.679	-30.411	1.00	58.34	C
ATOM	368	CG	GLN	A	47	56.948	-3.889	-31.081	1.00	61.68	C
ATOM	369	CD	GLN	A	47	56.886	-3.720	-32.595	1.00	68.07	C

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ATOM    370  OE1 GLN A  47      57.774  -3.090 -33.219  1.00 69.58      O
ATOM    371  NE2 GLN A  47      55.838  -4.288 -33.204  1.00 69.32      N
ATOM    372  C   GLN A  47      56.991  -3.546 -28.291  1.00 56.40      C
ATOM    373  O   GLN A  47      57.991  -2.855 -28.403  1.00 56.16      O
ATOM    374  N   SER A  48      56.973  -4.691 -27.599  1.00 53.86      N
ATOM    375  CA  SER A  48      58.112  -5.136 -26.806  1.00 53.14      C
ATOM    376  CB  SER A  48      57.759  -6.239 -25.793  1.00 52.59      C
ATOM    377  OG  SER A  48      56.373  -6.331 -25.659  1.00 55.97      O
ATOM    378  C   SER A  48      59.210  -5.658 -27.672  1.00 51.60      C
ATOM    379  O   SER A  48      58.968  -6.329 -28.679  1.00 51.19      O
ATOM    380  N   ILE A  49      60.433  -5.380 -27.229  1.00 50.47      N
ATOM    381  CA  ILE A  49      61.627  -5.856 -27.920  1.00 49.33      C
ATOM    382  CB  ILE A  49      62.710  -4.755 -28.005  1.00 48.45      C
ATOM    383  CG1 ILE A  49      62.251  -3.636 -28.919  1.00 48.57      C
ATOM    384  CD1 ILE A  49      62.995  -2.348 -28.670  1.00 47.03      C
ATOM    385  CG2 ILE A  49      64.064  -5.362 -28.492  1.00 47.35      C
ATOM    386  C   ILE A  49      62.198  -7.054 -27.160  1.00 48.70      C
ATOM    387  O   ILE A  49      62.555  -6.911 -25.986  1.00 48.29      O
ATOM    388  N   SER A  50      62.293  -8.198 -27.849  1.00 49.00      N
ATOM    389  CA  SER A  50      62.998  -9.436 -27.400  1.00 49.52      C
ATOM    390  CB  SER A  50      62.551 -10.647 -28.223  1.00 49.72      C
ATOM    391  OG  SER A  50      61.213 -10.968 -27.948  1.00 52.50      O
ATOM    392  C   SER A  50      64.507  -9.299 -27.621  1.00 48.65      C
ATOM    393  O   SER A  50      64.944  -9.131 -28.735  1.00 48.05      O
ATOM    394  N   ILE A  51      65.270  -9.397 -26.540  1.00 47.94      N
ATOM    395  CA  ILE A  51      66.706  -9.224 -26.516  1.00 47.34      C
ATOM    396  CB  ILE A  51      67.134  -9.131 -25.012  1.00 47.28      C
ATOM    397  CG1 ILE A  51      66.616  -7.835 -24.342  1.00 47.48      C
ATOM    398  CD1 ILE A  51      66.759  -6.511 -25.185  1.00 46.22      C
ATOM    399  CG2 ILE A  51      68.618  -9.405 -24.815  1.00 49.45      C
ATOM    400  C   ILE A  51      67.332 -10.427 -27.229  1.00 46.82      C
ATOM    401  O   ILE A  51      66.976 -11.538 -26.927  1.00 46.57      O
ATOM    402  N   GLY A  52      68.227 -10.219 -28.197  1.00 46.54      N
ATOM    403  CA  GLY A  52      68.790 -11.324 -28.979  1.00 45.30      C
ATOM    404  C   GLY A  52      69.129 -10.786 -30.354  1.00 46.43      C
ATOM    405  O   GLY A  52      68.603  -9.736 -30.754  1.00 47.18      O
ATOM    406  N   GLY A  53      70.047 -11.446 -31.054  1.00 45.33      N
ATOM    407  CA  GLY A  53      70.408 -11.065 -32.399  1.00 45.72      C
ATOM    408  C   GLY A  53      71.007  -9.680 -32.446  1.00 45.66      C
ATOM    409  O   GLY A  53      72.039  -9.435 -31.823  1.00 46.03      O
ATOM    410  N   ARG A  54      70.359  -8.794 -33.207  1.00 45.46      N
ATOM    411  CA  ARG A  54      70.681  -7.360 -33.292  1.00 45.57      C
ATOM    412  CB  ARG A  54      69.802  -6.697 -34.364  1.00 45.77      C
ATOM    413  CG  ARG A  54      70.428  -6.723 -35.756  1.00 47.80      C
ATOM    414  CD  ARG A  54      69.460  -6.515 -36.962  1.00 47.13      C
ATOM    415  NE  ARG A  54      68.139  -5.901 -36.699  1.00 48.21      N
ATOM    416  CZ  ARG A  54      67.854  -4.597 -36.739  1.00 48.23      C
ATOM    417  NH1 ARG A  54      68.788  -3.680 -36.949  1.00 47.12      N
ATOM    418  NH2 ARG A  54      66.614  -4.205 -36.539  1.00 47.74      N
ATOM    419  C   ARG A  54      70.538  -6.549 -31.994  1.00 44.48      C
ATOM    420  O   ARG A  54      71.102  -5.455 -31.899  1.00 45.01      O
ATOM    421  N   TYR A  55      69.760  -7.042 -31.028  1.00 43.84      N
ATOM    422  CA  TYR A  55      69.450  -6.305 -29.788  1.00 43.35      C
ATOM    423  CB  TYR A  55      67.958  -6.426 -29.448  1.00 44.35      C
ATOM    424  CG  TYR A  55      67.074  -5.915 -30.548  1.00 46.48      C
ATOM    425  CD1 TYR A  55      66.572  -6.774 -31.512  1.00 49.83      C
ATOM    426  CE1 TYR A  55      65.784  -6.314 -32.555  1.00 49.58      C
ATOM    427  CZ  TYR A  55      65.477  -4.973 -32.627  1.00 50.34      C
ATOM    428  OH  TYR A  55      64.687  -4.523 -33.663  1.00 50.81      O
ATOM    429  CE2 TYR A  55      65.965  -4.079 -31.681  1.00 48.69      C
ATOM    430  CD2 TYR A  55      66.772  -4.557 -30.655  1.00 48.63      C
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ATOM    431  C   TYR A  55      70.266  -6.876 -28.651  1.00 42.80      C
ATOM    432  O   TYR A  55      69.952  -7.955 -28.191  1.00 42.93      O
ATOM    433  N   VAL A  56      71.355  -6.232 -28.240  1.00 41.64      N
ATOM    434  CA  VAL A  56      72.001  -6.733 -27.046  1.00 40.80      C
ATOM    435  CB  VAL A  56      73.464  -7.357 -27.245  1.00 42.17      C
ATOM    436  CG1 VAL A  56      73.841  -7.600 -28.748  1.00 38.54      C
ATOM    437  CG2 VAL A  56      74.538  -6.558 -26.522  1.00 43.83      C
ATOM    438  C   VAL A  56      71.827  -5.785 -25.862  1.00 41.18      C
ATOM    439  O   VAL A  56      71.910  -4.546 -25.990  1.00 39.41      O
ATOM    440  N   GLU A  57      71.512  -6.367 -24.712  1.00 40.70      N
ATOM    441  CA  GLU A  57      71.286  -5.580 -23.520  1.00 41.90      C
ATOM    442  CB  GLU A  57      69.900  -5.898 -22.929  1.00 42.24      C
ATOM    443  CG  GLU A  57      69.600  -5.062 -21.704  1.00 42.95      C
ATOM    444  CD  GLU A  57      68.308  -5.403 -20.974  1.00 42.25      C
ATOM    445  OE1 GLU A  57      67.949  -6.577 -20.900  1.00 38.99      O
ATOM    446  OE2 GLU A  57      67.670  -4.457 -20.460  1.00 44.79      O
ATOM    447  C   GLU A  57      72.384  -5.881 -22.492  1.00 42.34      C
ATOM    448  O   GLU A  57      72.798  -7.042 -22.344  1.00 42.11      O
ATOM    449  N   THR A  58      72.877  -4.831 -21.831  1.00 42.68      N
ATOM    450  CA  THR A  58      73.858  -4.957 -20.757  1.00 43.59      C
ATOM    451  CB  THR A  58      75.189  -4.212 -21.077  1.00 43.40      C
ATOM    452  OG1 THR A  58      75.624  -4.579 -22.385  1.00 46.66      O
ATOM    453  CG2 THR A  58      76.359  -4.628 -20.109  1.00 43.34      C
ATOM    454  C   THR A  58      73.158  -4.367 -19.552  1.00 44.00      C
ATOM    455  O   THR A  58      72.617  -3.287 -19.658  1.00 44.75      O
ATOM    456  N   VAL A  59      73.085  -5.096 -18.435  1.00 45.31      N
ATOM    457  CA  VAL A  59      72.445  -4.573 -17.188  1.00 46.32      C
ATOM    458  CB  VAL A  59      71.193  -5.433 -16.756  1.00 46.73      C
ATOM    459  CG1 VAL A  59      70.611  -4.939 -15.416  1.00 45.96      C
ATOM    460  CG2 VAL A  59      70.109  -5.392 -17.855  1.00 46.73      C
ATOM    461  C   VAL A  59      73.470  -4.509 -16.019  1.00 46.15      C
ATOM    462  O   VAL A  59      74.107  -5.492 -15.742  1.00 45.02      O
ATOM    463  N   ASN A  60      73.646  -3.357 -15.368  1.00 46.21      N
ATOM    464  CA  ASN A  60      74.410  -3.289 -14.091  1.00 47.08      C
ATOM    465  CB  ASN A  60      75.582  -2.282 -14.177  1.00 46.82      C
ATOM    466  CG  ASN A  60      76.468  -2.280 -12.923  1.00 49.00      C
ATOM    467  OD1 ASN A  60      75.999  -2.345 -11.785  1.00 52.76      O
ATOM    468  ND2 ASN A  60      77.757  -2.224 -13.138  1.00 49.31      N
ATOM    469  C   ASN A  60      73.440  -2.923 -12.955  1.00 47.32      C
ATOM    470  O   ASN A  60      73.134  -1.773 -12.726  1.00 46.07      O
ATOM    471  N   LYS A  61      72.939  -3.925 -12.255  1.00 48.72      N
ATOM    472  CA  LYS A  61      71.962  -3.707 -11.182  1.00 49.59      C
ATOM    473  CB  LYS A  61      71.378  -5.055 -10.716  1.00 49.75      C
ATOM    474  CG  LYS A  61      70.215  -5.564 -11.593  1.00 50.68      C
ATOM    475  CD  LYS A  61      69.812  -6.983 -11.174  1.00 50.86      C
ATOM    476  CE  LYS A  61      68.695  -7.504 -12.055  1.00 54.11      C
ATOM    477  NZ  LYS A  61      68.044  -8.687 -11.416  1.00 56.87      N
ATOM    478  C   LYS A  61      72.560  -2.919 -10.000  1.00 49.82      C
ATOM    479  O   LYS A  61      71.854  -2.143  -9.371  1.00 50.15      O
ATOM    480  N   GLY A  62      73.848  -3.134  -9.718  1.00 49.68      N
ATOM    481  CA  GLY A  62      74.606  -2.382  -8.706  1.00 49.85      C
ATOM    482  C   GLY A  62      74.552  -0.878  -8.922  1.00 49.84      C
ATOM    483  O   GLY A  62      74.322  -0.121  -7.980  1.00 50.26      O
ATOM    484  N   SER A  63      74.731  -0.433 -10.169  1.00 48.77      N
ATOM    485  CA  SER A  63      74.577   0.986 -10.490  1.00 47.70      C
ATOM    486  CB  SER A  63      75.754   1.436 -11.342  1.00 47.84      C
ATOM    487  OG  SER A  63      75.593   0.909 -12.632  1.00 51.09      O
ATOM    488  C   SER A  63      73.200   1.385 -11.111  1.00 46.97      C
ATOM    489  O   SER A  63      73.043   2.490 -11.649  1.00 47.21      O
ATOM    490  N   LYS A  64      72.209   0.497 -11.007  1.00 44.94      N
ATOM    491  CA  LYS A  64      70.843   0.715 -11.475  1.00 44.84      C
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ATOM	492	CB	LYS	A	64	70.057	1.625	-10.509	1.00	43.86	C
ATOM	493	CG	LYS	A	64	70.033	1.170	-9.029	1.00	47.25	C
ATOM	494	CD	LYS	A	64	69.005	2.001	-8.219	1.00	44.70	C
ATOM	495	CE	LYS	A	64	69.247	1.819	-6.729	1.00	44.99	C
ATOM	496	NZ	LYS	A	64	68.112	2.477	-6.068	1.00	44.40	N
ATOM	497	C	LYS	A	64	70.804	1.247	-12.917	1.00	44.07	C
ATOM	498	O	LYS	A	64	70.049	2.146	-13.280	1.00	43.97	O
ATOM	499	N	SER	A	65	71.587	0.626	-13.752	1.00	43.50	N
ATOM	500	CA	SER	A	65	71.940	1.168	-15.069	1.00	44.29	C
ATOM	501	CB	SER	A	65	73.362	1.691	-14.968	1.00	44.32	C
ATOM	502	OG	SER	A	65	73.875	1.947	-16.238	1.00	50.36	O
ATOM	503	C	SER	A	65	71.865	0.026	-16.097	1.00	43.54	C
ATOM	504	O	SER	A	65	72.276	-1.068	-15.818	1.00	44.78	O
ATOM	505	N	PHE	A	66	71.310	0.273	-17.268	1.00	43.55	N
ATOM	506	CA	PHE	A	66	71.086	-0.763	-18.282	1.00	42.34	C
ATOM	507	CB	PHE	A	66	69.779	-1.568	-18.040	1.00	41.29	C
ATOM	508	CG	PHE	A	66	68.550	-0.738	-17.764	1.00	43.12	C
ATOM	509	CD1	PHE	A	66	68.427	0.051	-16.599	1.00	42.71	C
ATOM	510	CE1	PHE	A	66	67.241	0.790	-16.358	1.00	44.02	C
ATOM	511	CZ	PHE	A	66	66.195	0.688	-17.257	1.00	45.56	C
ATOM	512	CE2	PHE	A	66	66.300	-0.135	-18.391	1.00	43.21	C
ATOM	513	CD2	PHE	A	66	67.444	-0.813	-18.639	1.00	43.36	C
ATOM	514	C	PHE	A	66	71.113	-0.110	-19.662	1.00	42.27	C
ATOM	515	O	PHE	A	66	70.725	1.063	-19.818	1.00	40.59	O
ATOM	516	N	SER	A	67	71.578	-0.848	-20.661	1.00	42.12	N
ATOM	517	CA	SER	A	67	71.575	-0.287	-22.008	1.00	42.94	C
ATOM	518	CB	SER	A	67	72.871	0.482	-22.245	1.00	44.09	C
ATOM	519	OG	SER	A	67	73.943	-0.414	-22.195	1.00	46.13	O
ATOM	520	C	SER	A	67	71.318	-1.326	-23.109	1.00	42.30	C
ATOM	521	O	SER	A	67	71.475	-2.518	-22.887	1.00	41.64	O
ATOM	522	N	LEU	A	68	70.843	-0.857	-24.259	1.00	42.72	N
ATOM	523	CA	LEU	A	68	70.479	-1.706	-25.376	1.00	42.24	C
ATOM	524	CB	LEU	A	68	69.032	-1.415	-25.795	1.00	42.06	C
ATOM	525	CG	LEU	A	68	68.062	-2.356	-26.561	1.00	42.82	C
ATOM	526	CD1	LEU	A	68	67.123	-1.619	-27.518	1.00	37.15	C
ATOM	527	CD2	LEU	A	68	68.630	-3.617	-27.193	1.00	45.54	C
ATOM	528	C	LEU	A	68	71.342	-1.215	-26.521	1.00	42.90	C
ATOM	529	O	LEU	A	68	71.347	-0.010	-26.820	1.00	41.46	O
ATOM	530	N	ARG	A	69	72.031	-2.141	-27.196	1.00	42.96	N
ATOM	531	CA	ARG	A	69	72.635	-1.810	-28.465	1.00	43.33	C
ATOM	532	CB	ARG	A	69	74.071	-2.295	-28.521	1.00	44.06	C
ATOM	533	CG	ARG	A	69	74.908	-1.467	-29.419	1.00	44.93	C
ATOM	534	CD	ARG	A	69	76.347	-1.648	-29.074	1.00	51.01	C
ATOM	535	NE	ARG	A	69	77.032	-2.495	-30.046	1.00	55.03	N
ATOM	536	CZ	ARG	A	69	77.938	-2.041	-30.924	1.00	59.47	C
ATOM	537	NH1	ARG	A	69	78.259	-0.733	-30.942	1.00	59.92	N
ATOM	538	NH2	ARG	A	69	78.520	-2.876	-31.794	1.00	52.94	N
ATOM	539	C	ARG	A	69	71.867	-2.458	-29.589	1.00	43.41	C
ATOM	540	O	ARG	A	69	71.684	-3.661	-29.590	1.00	42.37	O
ATOM	541	N	ILE	A	70	71.416	-1.646	-30.545	1.00	43.65	N
ATOM	542	CA	ILE	A	70	70.858	-2.153	-31.779	1.00	44.23	C
ATOM	543	CB	ILE	A	70	69.492	-1.515	-32.157	1.00	44.17	C
ATOM	544	CG1	ILE	A	70	68.603	-1.333	-30.942	1.00	45.74	C
ATOM	545	CD1	ILE	A	70	67.758	-0.131	-31.117	1.00	46.30	C
ATOM	546	CG2	ILE	A	70	68.756	-2.351	-33.172	1.00	43.47	C
ATOM	547	C	ILE	A	70	71.856	-1.934	-32.893	1.00	44.58	C
ATOM	548	O	ILE	A	70	72.153	-0.792	-33.282	1.00	45.70	O
ATOM	549	N	SER	A	71	72.376	-3.022	-33.425	1.00	45.40	N
ATOM	550	CA	SER	A	71	73.387	-2.879	-34.435	1.00	46.26	C
ATOM	551	CB	SER	A	71	74.597	-3.736	-34.104	1.00	46.66	C
ATOM	552	OG	SER	A	71	74.223	-5.080	-34.154	1.00	46.90	O

ATOM	553	C	SER	A	71	72.788	-3.238	-35.776	1.00	46.26	C
ATOM	554	O	SER	A	71	71.702	-3.811	-35.833	1.00	45.27	O
ATOM	555	N	ASP	A	72	73.491	-2.855	-36.845	1.00	47.04	N
ATOM	556	CA	ASP	A	72	73.083	-3.164	-38.220	1.00	47.40	C
ATOM	557	CB	ASP	A	72	73.125	-4.671	-38.470	1.00	47.74	C
ATOM	558	CG	ASP	A	72	73.180	-5.019	-39.934	1.00	51.59	C
ATOM	559	OD1	ASP	A	72	73.693	-4.202	-40.771	1.00	53.46	O
ATOM	560	OD2	ASP	A	72	72.705	-6.140	-40.238	1.00	56.93	O
ATOM	561	C	ASP	A	72	71.704	-2.556	-38.534	1.00	46.75	C
ATOM	562	O	ASP	A	72	70.796	-3.217	-39.079	1.00	46.48	O
ATOM	563	N	LEU	A	73	71.601	-1.275	-38.183	1.00	46.13	N
ATOM	564	CA	LEU	A	73	70.406	-0.467	-38.296	1.00	45.96	C
ATOM	565	CB	LEU	A	73	70.745	0.931	-37.780	1.00	45.33	C
ATOM	566	CG	LEU	A	73	70.287	1.479	-36.425	1.00	48.34	C
ATOM	567	CD1	LEU	A	73	69.586	0.448	-35.493	1.00	42.67	C
ATOM	568	CD2	LEU	A	73	71.423	2.297	-35.755	1.00	49.05	C
ATOM	569	C	LEU	A	73	69.946	-0.366	-39.742	1.00	46.10	C
ATOM	570	O	LEU	A	73	70.764	-0.352	-40.660	1.00	44.78	O
ATOM	571	N	ARG	A	74	68.631	-0.281	-39.934	1.00	46.57	N
ATOM	572	CA	ARG	A	74	68.040	-0.106	-41.264	1.00	47.37	C
ATOM	573	CB	ARG	A	74	67.637	-1.474	-41.849	1.00	46.77	C
ATOM	574	CG	ARG	A	74	66.719	-2.239	-40.899	1.00	49.24	C
ATOM	575	CD	ARG	A	74	66.663	-3.759	-41.079	1.00	50.32	C
ATOM	576	NE	ARG	A	74	67.971	-4.409	-40.931	1.00	53.80	N
ATOM	577	CZ	ARG	A	74	68.136	-5.671	-40.534	1.00	55.17	C
ATOM	578	NH1	ARG	A	74	67.079	-6.433	-40.214	1.00	53.89	N
ATOM	579	NH2	ARG	A	74	69.367	-6.169	-40.440	1.00	55.31	N
ATOM	580	C	ARG	A	74	66.851	0.854	-41.114	1.00	46.54	C
ATOM	581	O	ARG	A	74	66.367	1.069	-39.989	1.00	46.24	O
ATOM	582	N	VAL	A	75	66.407	1.456	-42.221	1.00	46.74	N
ATOM	583	CA	VAL	A	75	65.304	2.453	-42.211	1.00	47.37	C
ATOM	584	CB	VAL	A	75	64.850	2.870	-43.638	1.00	47.20	C
ATOM	585	CG1	VAL	A	75	63.727	3.897	-43.563	1.00	48.39	C
ATOM	586	CG2	VAL	A	75	65.979	3.477	-44.373	1.00	45.91	C
ATOM	587	C	VAL	A	75	64.073	2.053	-41.387	1.00	47.49	C
ATOM	588	O	VAL	A	75	63.434	2.919	-40.786	1.00	48.41	O
ATOM	589	N	GLU	A	76	63.774	0.748	-41.340	1.00	47.38	N
ATOM	590	CA	GLU	A	76	62.578	0.186	-40.682	1.00	47.03	C
ATOM	591	CB	GLU	A	76	62.327	-1.264	-41.122	1.00	46.90	C
ATOM	592	CG	GLU	A	76	62.075	-1.440	-42.631	1.00	50.85	C
ATOM	593	CD	GLU	A	76	63.370	-1.574	-43.459	1.00	56.49	C
ATOM	594	OE1	GLU	A	76	64.438	-1.844	-42.855	1.00	56.84	O
ATOM	595	OE2	GLU	A	76	63.321	-1.414	-44.721	1.00	60.06	O
ATOM	596	C	GLU	A	76	62.681	0.239	-39.173	1.00	46.09	C
ATOM	597	O	GLU	A	76	61.694	0.020	-38.485	1.00	46.19	O
ATOM	598	N	ASP	A	77	63.880	0.526	-38.662	1.00	45.73	N
ATOM	599	CA	ASP	A	77	64.123	0.677	-37.224	1.00	44.49	C
ATOM	600	CB	ASP	A	77	65.557	0.277	-36.855	1.00	44.34	C
ATOM	601	CG	ASP	A	77	65.839	-1.207	-37.086	1.00	47.06	C
ATOM	602	OD1	ASP	A	77	64.964	-2.086	-36.810	1.00	51.98	O
ATOM	603	OD2	ASP	A	77	66.959	-1.515	-37.546	1.00	50.67	O
ATOM	604	C	ASP	A	77	63.820	2.086	-36.705	1.00	44.17	C
ATOM	605	O	ASP	A	77	63.795	2.288	-35.501	1.00	43.66	O
ATOM	606	N	SER	A	78	63.606	3.056	-37.601	1.00	43.76	N
ATOM	607	CA	SER	A	78	63.254	4.403	-37.176	1.00	43.69	C
ATOM	608	CB	SER	A	78	62.975	5.334	-38.352	1.00	43.43	C
ATOM	609	OG	SER	A	78	64.074	5.409	-39.232	1.00	42.84	O
ATOM	610	C	SER	A	78	62.026	4.342	-36.304	1.00	44.36	C
ATOM	611	O	SER	A	78	61.112	3.604	-36.591	1.00	45.78	O
ATOM	612	N	GLY	A	79	62.009	5.134	-35.239	1.00	44.36	N
ATOM	613	CA	GLY	A	79	60.931	5.138	-34.284	1.00	43.30	C

ATOM	614	C	GLY	A	79	61.435	5.586	-32.936	1.00	43.00	C
ATOM	615	O	GLY	A	79	62.541	6.110	-32.830	1.00	43.25	O
ATOM	616	N	THR	A	80	60.585	5.415	-31.929	1.00	42.21	N
ATOM	617	CA	THR	A	80	60.837	5.861	-30.587	1.00	42.60	C
ATOM	618	CB	THR	A	80	59.658	6.697	-30.047	1.00	43.53	C
ATOM	619	OG1	THR	A	80	59.501	7.860	-30.873	1.00	45.61	O
ATOM	620	CG2	THR	A	80	59.869	7.123	-28.565	1.00	44.78	C
ATOM	621	C	THR	A	80	61.047	4.587	-29.775	1.00	42.21	C
ATOM	622	O	THR	A	80	60.308	3.637	-29.924	1.00	41.06	O
ATOM	623	N	TYR	A	81	62.115	4.578	-28.973	1.00	41.77	N
ATOM	624	CA	TYR	A	81	62.463	3.459	-28.122	1.00	40.78	C
ATOM	625	CB	TYR	A	81	63.891	2.998	-28.407	1.00	39.74	C
ATOM	626	CG	TYR	A	81	64.031	2.350	-29.774	1.00	40.54	C
ATOM	627	CD1	TYR	A	81	64.286	0.993	-29.909	1.00	38.77	C
ATOM	628	CE1	TYR	A	81	64.400	0.414	-31.226	1.00	42.36	C
ATOM	629	CZ	TYR	A	81	64.245	1.208	-32.347	1.00	37.03	C
ATOM	630	OH	TYR	A	81	64.353	0.685	-33.633	1.00	39.33	O
ATOM	631	CE2	TYR	A	81	63.975	2.523	-32.218	1.00	38.69	C
ATOM	632	CD2	TYR	A	81	63.891	3.106	-30.932	1.00	40.06	C
ATOM	633	C	TYR	A	81	62.382	3.935	-26.715	1.00	40.90	C
ATOM	634	O	TYR	A	81	62.766	5.033	-26.462	1.00	40.58	O
ATOM	635	N	LYS	A	82	61.896	3.088	-25.819	1.00	41.29	N
ATOM	636	CA	LYS	A	82	61.850	3.350	-24.388	1.00	42.71	C
ATOM	637	CB	LYS	A	82	60.422	3.634	-23.944	1.00	42.24	C
ATOM	638	CG	LYS	A	82	59.994	4.963	-24.379	1.00	44.27	C
ATOM	639	CD	LYS	A	82	58.731	5.424	-23.596	1.00	45.18	C
ATOM	640	CE	LYS	A	82	58.202	6.727	-24.265	1.00	46.00	C
ATOM	641	NZ	LYS	A	82	57.117	7.194	-23.357	1.00	56.94	N
ATOM	642	C	LYS	A	82	62.315	2.107	-23.650	1.00	42.18	C
ATOM	643	O	LYS	A	82	62.061	1.027	-24.094	1.00	40.76	O
ATOM	644	N	CYS	A	83	63.042	2.318	-22.560	1.00	43.46	N
ATOM	645	CA	CYS	A	83	63.439	1.309	-21.629	1.00	44.61	C
ATOM	646	CB	CYS	A	83	64.761	1.693	-20.986	1.00	45.96	C
ATOM	647	SG	CYS	A	83	64.973	3.375	-20.311	1.00	48.94	S
ATOM	648	C	CYS	A	83	62.409	1.325	-20.534	1.00	45.71	C
ATOM	649	O	CYS	A	83	61.631	2.271	-20.456	1.00	46.30	O
ATOM	650	N	GLN	A	84	62.385	0.287	-19.692	1.00	43.77	N
ATOM	651	CA	GLN	A	84	61.568	0.350	-18.534	1.00	42.92	C
ATOM	652	CB	GLN	A	84	60.203	-0.292	-18.790	1.00	42.16	C
ATOM	653	CG	GLN	A	84	59.330	-0.191	-17.551	1.00	43.09	C
ATOM	654	CD	GLN	A	84	57.821	-0.376	-17.766	1.00	46.36	C
ATOM	655	OE1	GLN	A	84	57.016	0.257	-17.094	1.00	50.63	O
ATOM	656	NE2	GLN	A	84	57.443	-1.260	-18.660	1.00	44.97	N
ATOM	657	C	GLN	A	84	62.286	-0.351	-17.413	1.00	42.33	C
ATOM	658	O	GLN	A	84	62.766	-1.454	-17.614	1.00	40.11	O
ATOM	659	N	ALA	A	85	62.403	0.310	-16.256	1.00	42.76	N
ATOM	660	CA	ALA	A	85	62.992	-0.323	-15.027	1.00	43.66	C
ATOM	661	CB	ALA	A	85	63.803	0.674	-14.213	1.00	42.44	C
ATOM	662	C	ALA	A	85	61.854	-0.875	-14.159	1.00	43.77	C
ATOM	663	O	ALA	A	85	60.904	-0.143	-13.877	1.00	42.85	O
ATOM	664	N	PHE	A	86	61.986	-2.140	-13.760	1.00	42.59	N
ATOM	665	CA	PHE	A	86	61.015	-2.843	-12.918	1.00	43.37	C
ATOM	666	CB	PHE	A	86	60.674	-4.222	-13.484	1.00	41.48	C
ATOM	667	CG	PHE	A	86	60.048	-4.178	-14.879	1.00	43.52	C
ATOM	668	CD1	PHE	A	86	58.751	-3.695	-15.063	1.00	40.20	C
ATOM	669	CE1	PHE	A	86	58.158	-3.672	-16.327	1.00	38.57	C
ATOM	670	CZ	PHE	A	86	58.871	-4.088	-17.428	1.00	42.08	C
ATOM	671	CE2	PHE	A	86	60.178	-4.538	-17.273	1.00	43.63	C
ATOM	672	CD2	PHE	A	86	60.765	-4.568	-15.998	1.00	42.39	C
ATOM	673	C	PHE	A	86	61.564	-2.990	-11.487	1.00	44.25	C
ATOM	674	O	PHE	A	86	62.745	-3.227	-11.275	1.00	45.17	O

ATOM	675	N	TYR	A	87	60.673	-2.891	-10.514	1.00	44.26	N
ATOM	676	CA	TYR	A	87	61.056	-2.955	-9.127	1.00	42.81	C
ATOM	677	CB	TYR	A	87	61.591	-1.595	-8.705	1.00	42.95	C
ATOM	678	CG	TYR	A	87	60.589	-0.506	-9.034	1.00	44.84	C
ATOM	679	CD1	TYR	A	87	60.593	0.094	-10.300	1.00	44.05	C
ATOM	680	CE1	TYR	A	87	59.685	1.047	-10.640	1.00	46.61	C
ATOM	681	CZ	TYR	A	87	58.730	1.425	-9.702	1.00	45.72	C
ATOM	682	OH	TYR	A	87	57.877	2.355	-10.081	1.00	48.88	O
ATOM	683	CE2	TYR	A	87	58.659	0.878	-8.442	1.00	45.57	C
ATOM	684	CD2	TYR	A	87	59.622	-0.126	-8.110	1.00	45.85	C
ATOM	685	C	TYR	A	87	59.820	-3.359	-8.308	1.00	42.27	C
ATOM	686	O	TYR	A	87	58.694	-3.482	-8.832	1.00	42.84	O
ATOM	687	N	VAL	A	88	60.017	-3.599	-7.022	1.00	41.80	N
ATOM	688	CA	VAL	A	88	58.912	-3.966	-6.147	1.00	40.05	C
ATOM	689	CB	VAL	A	88	59.180	-5.357	-5.568	1.00	40.65	C
ATOM	690	CG1	VAL	A	88	60.622	-5.432	-4.904	1.00	34.41	C
ATOM	691	CG2	VAL	A	88	59.093	-6.416	-6.658	1.00	36.97	C
ATOM	692	C	VAL	A	88	58.720	-2.893	-5.015	1.00	41.14	C
ATOM	693	O	VAL	A	88	59.646	-2.140	-4.619	1.00	42.19	O
ATOM	694	N	PHE	A	89	57.529	-2.846	-4.472	1.00	40.69	N
ATOM	695	CA	PHE	A	89	57.239	-1.957	-3.367	1.00	38.05	C
ATOM	696	CB	PHE	A	89	57.064	-0.483	-3.841	1.00	37.66	C
ATOM	697	CG	PHE	A	89	55.841	-0.218	-4.771	1.00	35.47	C
ATOM	698	CD1	PHE	A	89	55.948	-0.343	-6.141	1.00	34.15	C
ATOM	699	CE1	PHE	A	89	54.868	-0.074	-6.984	1.00	30.34	C
ATOM	700	CZ	PHE	A	89	53.716	0.379	-6.408	1.00	38.20	C
ATOM	701	CE2	PHE	A	89	53.627	0.586	-4.999	1.00	30.74	C
ATOM	702	CD2	PHE	A	89	54.662	0.290	-4.241	1.00	36.54	C
ATOM	703	C	PHE	A	89	56.012	-2.518	-2.694	1.00	39.07	C
ATOM	704	O	PHE	A	89	55.218	-3.234	-3.341	1.00	35.78	O
ATOM	705	N	PHE	A	90	55.886	-2.215	-1.394	1.00	38.51	N
ATOM	706	CA	PHE	A	90	54.693	-2.576	-0.621	1.00	39.88	C
ATOM	707	CB	PHE	A	90	54.993	-2.528	0.874	1.00	37.98	C
ATOM	708	CG	PHE	A	90	55.700	-3.740	1.386	1.00	37.62	C
ATOM	709	CD1	PHE	A	90	55.078	-5.003	1.336	1.00	35.79	C
ATOM	710	CE1	PHE	A	90	55.688	-6.126	1.895	1.00	37.83	C
ATOM	711	CZ	PHE	A	90	56.950	-6.030	2.476	1.00	38.12	C
ATOM	712	CE2	PHE	A	90	57.601	-4.739	2.526	1.00	38.60	C
ATOM	713	CD2	PHE	A	90	56.922	-3.620	1.998	1.00	37.29	C
ATOM	714	C	PHE	A	90	53.467	-1.698	-0.981	1.00	40.53	C
ATOM	715	O	PHE	A	90	53.605	-0.502	-1.196	1.00	40.32	O
ATOM	716	N	ALA	A	91	52.277	-2.306	-0.985	1.00	41.27	N
ATOM	717	CA	ALA	A	91	51.067	-1.617	-1.372	1.00	41.84	C
ATOM	718	CB	ALA	A	91	49.892	-2.513	-1.182	1.00	42.15	C
ATOM	719	C	ALA	A	91	50.860	-0.249	-0.668	1.00	43.70	C
ATOM	720	O	ALA	A	91	50.328	0.664	-1.280	1.00	43.35	O
ATOM	721	N	GLU	A	92	51.321	-0.091	0.581	1.00	44.95	N
ATOM	722	CA	GLU	A	92	51.195	1.188	1.293	1.00	45.93	C
ATOM	723	CB	GLU	A	92	50.780	0.942	2.711	1.00	46.65	C
ATOM	724	CG	GLU	A	92	49.555	0.079	2.779	1.00	48.11	C
ATOM	725	CD	GLU	A	92	48.913	0.127	4.131	1.00	57.18	C
ATOM	726	OE1	GLU	A	92	48.562	1.252	4.563	1.00	59.80	O
ATOM	727	OE2	GLU	A	92	48.750	-0.953	4.764	1.00	56.56	O
ATOM	728	C	GLU	A	92	52.446	2.067	1.252	1.00	47.30	C
ATOM	729	O	GLU	A	92	52.450	3.195	1.756	1.00	48.77	O
ATOM	730	N	ASP	A	93	53.503	1.616	0.598	1.00	46.55	N
ATOM	731	CA	ASP	A	93	54.636	2.501	0.483	1.00	46.41	C
ATOM	732	CB	ASP	A	93	55.884	1.692	0.182	1.00	45.51	C
ATOM	733	CG	ASP	A	93	57.082	2.561	-0.131	1.00	44.76	C
ATOM	734	OD1	ASP	A	93	58.026	2.046	-0.789	1.00	42.86	O
ATOM	735	OD2	ASP	A	93	57.072	3.754	0.253	1.00	42.99	O

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ATOM    736  C   ASP A  93      54.344   3.551  -0.605  1.00 46.69      C
ATOM    737  O   ASP A  93      54.653   3.334  -1.774  1.00 46.46      O
ATOM    738  N   VAL A  94      53.716   4.660  -0.218  1.00 46.68      N
ATOM    739  CA  VAL A  94      53.276   5.672  -1.199  1.00 47.78      C
ATOM    740  CB  VAL A  94      52.240   6.690  -0.629  1.00 47.50      C
ATOM    741  CG1 VAL A  94      52.844   7.591   0.471  1.00 48.03      C
ATOM    742  CG2 VAL A  94      51.023   5.941  -0.088  1.00 48.45      C
ATOM    743  C   VAL A  94      54.439   6.375  -1.893  1.00 47.62      C
ATOM    744  O   VAL A  94      54.323   6.822  -3.039  1.00 48.80      O
ATOM    745  N   GLY A  95      55.577   6.444  -1.228  1.00 47.46      N
ATOM    746  CA  GLY A  95      56.743   7.084  -1.829  1.00 46.54      C
ATOM    747  C   GLY A  95      57.216   6.371  -3.077  1.00 46.80      C
ATOM    748  O   GLY A  95      57.971   6.944  -3.858  1.00 48.77      O
ATOM    749  N   SER A  96      56.789   5.125  -3.282  1.00 45.12      N
ATOM    750  CA  SER A  96      57.316   4.299  -4.367  1.00 43.91      C
ATOM    751  CB  SER A  96      57.806   2.951  -3.774  1.00 43.86      C
ATOM    752  OG  SER A  96      59.082   3.050  -3.170  1.00 45.47      O
ATOM    753  C   SER A  96      56.280   3.976  -5.464  1.00 43.04      C
ATOM    754  O   SER A  96      56.556   3.141  -6.333  1.00 41.97      O
ATOM    755  N   ASN A  97      55.083   4.582  -5.411  1.00 42.62      N
ATOM    756  CA  ASN A  97      53.955   4.125  -6.262  1.00 41.42      C
ATOM    757  CB  ASN A  97      52.664   3.995  -5.411  1.00 41.08      C
ATOM    758  CG  ASN A  97      52.129   5.344  -4.941  1.00 42.94      C
ATOM    759  OD1 ASN A  97      52.503   6.365  -5.465  1.00 46.83      O
ATOM    760  ND2 ASN A  97      51.255   5.342  -3.965  1.00 40.83      N
ATOM    761  C   ASN A  97      53.666   4.932  -7.525  1.00 42.28      C
ATOM    762  O   ASN A  97      52.585   4.750  -8.141  1.00 41.82      O
ATOM    763  N   LYS A  98      54.573   5.850  -7.915  1.00 42.02      N
ATOM    764  CA  LYS A  98      54.248   6.732  -9.041  1.00 43.43      C
ATOM    765  CB  LYS A  98      54.942   8.098  -8.900  1.00 44.23      C
ATOM    766  CG  LYS A  98      55.210   8.508  -7.418  1.00 46.17      C
ATOM    767  CD  LYS A  98      54.021   9.049  -6.764  1.00 48.50      C
ATOM    768  CE  LYS A  98      54.408   9.875  -5.559  1.00 45.50      C
ATOM    769  NZ  LYS A  98      54.697   8.979  -4.390  1.00 48.43      N
ATOM    770  C   LYS A  98      54.460   6.112 -10.439  1.00 43.17      C
ATOM    771  O   LYS A  98      54.025   6.663 -11.415  1.00 42.52      O
ATOM    772  N   GLY A  99      55.057   4.929 -10.498  1.00 43.81      N
ATOM    773  CA  GLY A  99      55.295   4.242 -11.742  1.00 43.60      C
ATOM    774  C   GLY A  99      54.052   3.507 -12.181  1.00 42.19      C
ATOM    775  O   GLY A  99      53.008   3.607 -11.544  1.00 42.85      O
ATOM    776  N   ALA A 100      54.151   2.775 -13.283  1.00 40.39      N
ATOM    777  CA  ALA A 100      53.014   1.974 -13.753  1.00 39.22      C
ATOM    778  CB  ALA A 100      53.278   1.513 -15.205  1.00 36.47      C
ATOM    779  C   ALA A 100      52.932   0.751 -12.819  1.00 38.50      C
ATOM    780  O   ALA A 100      53.913   0.368 -12.262  1.00 38.16      O
ATOM    781  N   ILE A 101      51.772   0.140 -12.652  1.00 38.62      N
ATOM    782  CA  ILE A 101      51.638  -1.134 -11.945  1.00 38.55      C
ATOM    783  CB  ILE A 101      50.190  -1.269 -11.405  1.00 40.06      C
ATOM    784  CG1 ILE A 101      49.797   0.015 -10.598  1.00 42.79      C
ATOM    785  CD1 ILE A 101      50.554   0.261  -9.310  1.00 39.48      C
ATOM    786  CG2 ILE A 101      49.959  -2.667 -10.762  1.00 36.33      C
ATOM    787  C   ILE A 101      51.767  -2.274 -12.951  1.00 39.19      C
ATOM    788  O   ILE A 101      50.995  -2.357 -13.950  1.00 36.64      O
ATOM    789  N   ILE A 102      52.677  -3.191 -12.663  1.00 39.81      N
ATOM    790  CA  ILE A 102      52.909  -4.348 -13.578  1.00 39.64      C
ATOM    791  CB  ILE A 102      54.454  -4.487 -13.734  1.00 39.59      C
ATOM    792  CG1 ILE A 102      55.089  -3.117 -14.157  1.00 38.41      C
ATOM    793  CD1 ILE A 102      54.460  -2.524 -15.511  1.00 33.86      C
ATOM    794  CG2 ILE A 102      54.819  -5.583 -14.725  1.00 40.76      C
ATOM    795  C   ILE A 102      52.195  -5.647 -13.073  1.00 39.13      C
ATOM    796  O   ILE A 102      51.854  -6.530 -13.816  1.00 39.94      O
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ATOM	797	N	GLY	A	103	52.050	-5.776	-11.775	1.00	39.01	N
ATOM	798	CA	GLY	A	103	51.334	-6.885	-11.213	1.00	38.49	C
ATOM	799	C	GLY	A	103	51.324	-6.752	-9.716	1.00	37.24	C
ATOM	800	O	GLY	A	103	51.882	-5.833	-9.130	1.00	36.17	O
ATOM	801	N	LEU	A	104	50.749	-7.742	-9.089	1.00	37.99	N
ATOM	802	CA	LEU	A	104	50.493	-7.683	-7.688	1.00	39.66	C
ATOM	803	CB	LEU	A	104	49.031	-7.210	-7.355	1.00	37.53	C
ATOM	804	CG	LEU	A	104	48.649	-7.290	-5.842	1.00	40.70	C
ATOM	805	CD1	LEU	A	104	47.171	-7.118	-5.505	1.00	39.27	C
ATOM	806	CD2	LEU	A	104	49.430	-6.275	-4.991	1.00	38.45	C
ATOM	807	C	LEU	A	104	50.744	-9.080	-7.236	1.00	40.91	C
ATOM	808	O	LEU	A	104	50.123	-10.019	-7.747	1.00	40.88	O
ATOM	809	N	MET	A	105	51.687	-9.213	-6.306	1.00	43.27	N
ATOM	810	CA	MET	A	105	51.982	-10.471	-5.649	1.00	45.57	C
ATOM	811	CB	MET	A	105	53.480	-10.581	-5.502	1.00	47.53	C
ATOM	812	CG	MET	A	105	54.143	-11.586	-6.445	1.00	56.01	C
ATOM	813	SD	MET	A	105	53.858	-11.477	-8.250	1.00	66.51	S
ATOM	814	CE	MET	A	105	54.839	-12.860	-8.841	1.00	57.93	C
ATOM	815	C	MET	A	105	51.291	-10.529	-4.289	1.00	44.27	C
ATOM	816	O	MET	A	105	51.143	-9.509	-3.650	1.00	43.68	O
ATOM	817	N	VAL	A	106	50.826	-11.700	-3.870	1.00	44.78	N
ATOM	818	CA	VAL	A	106	50.387	-11.916	-2.462	1.00	46.00	C
ATOM	819	CB	VAL	A	106	50.185	-13.396	-2.124	1.00	46.66	C
ATOM	820	CG1	VAL	A	106	51.551	-14.154	-2.328	1.00	47.69	C
ATOM	821	CG2	VAL	A	106	49.015	-13.959	-2.921	1.00	45.00	C
ATOM	822	C	VAL	A	106	51.431	-11.451	-1.442	1.00	46.49	C
ATOM	823	O	VAL	A	106	52.639	-11.733	-1.590	1.00	46.05	O
ATOM	824	N	GLY	A	107	50.942	-10.795	-0.390	1.00	45.74	N
ATOM	825	CA	GLY	A	107	51.799	-10.227	0.629	1.00	44.85	C
ATOM	826	C	GLY	A	107	51.784	-8.730	0.425	1.00	44.68	C
ATOM	827	O	GLY	A	107	52.526	-8.029	1.054	1.00	45.42	O
ATOM	828	N	GLY	A	108	50.939	-8.247	-0.480	1.00	43.98	N
ATOM	829	CA	GLY	A	108	50.840	-6.821	-0.790	1.00	43.08	C
ATOM	830	C	GLY	A	108	52.084	-6.255	-1.442	1.00	42.91	C
ATOM	831	O	GLY	A	108	52.434	-5.089	-1.242	1.00	42.44	O
ATOM	832	N	VAL	A	109	52.719	-7.046	-2.291	1.00	43.26	N
ATOM	833	CA	VAL	A	109	53.948	-6.599	-2.957	1.00	42.66	C
ATOM	834	CB	VAL	A	109	55.000	-7.751	-2.883	1.00	43.69	C
ATOM	835	CG1	VAL	A	109	56.193	-7.522	-3.854	1.00	42.19	C
ATOM	836	CG2	VAL	A	109	55.408	-8.004	-1.423	1.00	42.91	C
ATOM	837	C	VAL	A	109	53.554	-6.242	-4.387	1.00	42.97	C
ATOM	838	O	VAL	A	109	53.096	-7.113	-5.167	1.00	42.03	O
ATOM	839	N	VAL	A	110	53.665	-4.958	-4.723	1.00	42.17	N
ATOM	840	CA	VAL	A	110	53.415	-4.541	-6.054	1.00	40.80	C
ATOM	841	CB	VAL	A	110	52.310	-3.424	-6.153	1.00	44.02	C
ATOM	842	CG1	VAL	A	110	52.372	-2.549	-7.365	1.00	42.03	C
ATOM	843	CG2	VAL	A	110	51.848	-2.769	-4.779	1.00	41.33	C
ATOM	844	C	VAL	A	110	54.630	-4.554	-6.979	1.00	41.32	C
ATOM	845	O	VAL	A	110	55.745	-4.275	-6.542	1.00	41.11	O
ATOM	846	N	ILE	A	111	54.454	-4.937	-8.242	1.00	40.50	N
ATOM	847	CA	ILE	A	111	55.520	-4.758	-9.218	1.00	39.74	C
ATOM	848	CB	ILE	A	111	55.693	-6.002	-10.151	1.00	42.13	C
ATOM	849	CG1	ILE	A	111	55.947	-7.264	-9.286	1.00	44.65	C
ATOM	850	CD1	ILE	A	111	55.492	-8.577	-9.969	1.00	51.14	C
ATOM	851	CG2	ILE	A	111	56.814	-5.793	-11.241	1.00	39.84	C
ATOM	852	C	ILE	A	111	55.308	-3.462	-9.981	1.00	38.67	C
ATOM	853	O	ILE	A	111	54.231	-3.209	-10.519	1.00	39.08	O
ATOM	854	N	GLY	A	112	56.314	-2.594	-9.989	1.00	37.53	N
ATOM	855	CA	GLY	A	112	56.135	-1.251	-10.626	1.00	36.49	C
ATOM	856	C	GLY	A	112	57.100	-1.138	-11.758	1.00	37.46	C
ATOM	857	O	GLY	A	112	58.065	-1.929	-11.859	1.00	37.41	O

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ATOM    858  N   GLY A 113      56.787  -0.246 -12.688  1.00 38.41      N
ATOM    859  CA  GLY A 113      57.674   0.011 -13.832  1.00 39.24      C
ATOM    860  C   GLY A 113      57.818   1.473 -14.008  1.00 38.63      C
ATOM    861  O   GLY A 113      56.810   2.152 -13.932  1.00 40.39      O
ATOM    862  N   GLU A 114      59.046   1.981 -14.149  1.00 40.63      N
ATOM    863  CA  GLU A 114      59.293   3.395 -14.613  1.00 42.64      C
ATOM    864  CB  GLU A 114      60.340   4.176 -13.800  1.00 42.87      C
ATOM    865  CG  GLU A 114      59.955   4.975 -12.595  1.00 50.17      C
ATOM    866  CD  GLU A 114      58.981   6.134 -12.814  1.00 55.34      C
ATOM    867  OE1 GLU A 114      59.160   6.926 -13.769  1.00 61.09      O
ATOM    868  OE2 GLU A 114      58.080   6.310 -11.959  1.00 57.31      O
ATOM    869  C   GLU A 114      59.949   3.324 -15.964  1.00 42.42      C
ATOM    870  O   GLU A 114      60.953   2.626 -16.132  1.00 43.93      O
ATOM    871  N   LYS A 115      59.503   4.152 -16.876  1.00 42.38      N
ATOM    872  CA  LYS A 115      60.016   4.192 -18.240  1.00 42.73      C
ATOM    873  CB  LYS A 115      58.829   4.219 -19.234  1.00 44.06      C
ATOM    874  CG  LYS A 115      58.069   2.975 -19.365  1.00 47.53      C
ATOM    875  CD  LYS A 115      57.203   3.006 -20.629  1.00 53.24      C
ATOM    876  CE  LYS A 115      56.289   1.786 -20.589  1.00 54.45      C
ATOM    877  NZ  LYS A 115      55.402   1.783 -21.803  1.00 61.37      N
ATOM    878  C   LYS A 115      60.796   5.484 -18.507  1.00 41.16      C
ATOM    879  O   LYS A 115      60.463   6.586 -18.007  1.00 40.33      O
ATOM    880  N   GLY A 116      61.804   5.356 -19.341  1.00 40.59      N
ATOM    881  CA  GLY A 116      62.579   6.518 -19.817  1.00 39.49      C
ATOM    882  C   GLY A 116      61.717   7.400 -20.692  1.00 40.21      C
ATOM    883  O   GLY A 116      60.615   6.997 -21.112  1.00 38.64      O
ATOM    884  N   ALA A 117      62.212   8.605 -20.987  1.00 41.52      N
ATOM    885  CA  ALA A 117      61.472   9.547 -21.817  1.00 42.80      C
ATOM    886  CB  ALA A 117      62.048  10.974 -21.662  1.00 44.34      C
ATOM    887  C   ALA A 117      61.451   9.187 -23.295  1.00 43.54      C
ATOM    888  O   ALA A 117      60.687   9.767 -24.039  1.00 44.55      O
ATOM    889  N   GLY A 118      62.303   8.280 -23.760  1.00 43.70      N
ATOM    890  CA  GLY A 118      62.260   7.966 -25.184  1.00 41.16      C
ATOM    891  C   GLY A 118      63.528   8.367 -25.883  1.00 41.11      C
ATOM    892  O   GLY A 118      64.195   9.321 -25.473  1.00 41.17      O
ATOM    893  N   THR A 119      63.870   7.617 -26.927  1.00 40.36      N
ATOM    894  CA  THR A 119      64.921   7.982 -27.896  1.00 39.93      C
ATOM    895  CB  THR A 119      66.082   6.926 -27.933  1.00 39.67      C
ATOM    896  OG1 THR A 119      66.775   6.941 -26.682  1.00 36.77      O
ATOM    897  CG2 THR A 119      67.130   7.237 -29.078  1.00 37.93      C
ATOM    898  C   THR A 119      64.168   7.915 -29.198  1.00 40.54      C
ATOM    899  O   THR A 119      63.610   6.841 -29.510  1.00 41.01      O
ATOM    900  N   ALA A 120      64.042   9.058 -29.886  1.00 39.18      N
ATOM    901  CA  ALA A 120      63.474   9.123 -31.240  1.00 39.16      C
ATOM    902  CB  ALA A 120      62.887  10.544 -31.521  1.00 39.16      C
ATOM    903  C   ALA A 120      64.617   8.819 -32.234  1.00 38.85      C
ATOM    904  O   ALA A 120      65.576   9.562 -32.300  1.00 37.63      O
ATOM    905  N   LEU A 121      64.560   7.680 -32.925  1.00 39.42      N
ATOM    906  CA  LEU A 121      65.634   7.279 -33.798  1.00 39.83      C
ATOM    907  CB  LEU A 121      66.049   5.819 -33.513  1.00 40.42      C
ATOM    908  CG  LEU A 121      66.974   5.144 -34.569  1.00 40.59      C
ATOM    909  CD1 LEU A 121      68.396   5.751 -34.587  1.00 38.95      C
ATOM    910  CD2 LEU A 121      67.007   3.604 -34.288  1.00 41.03      C
ATOM    911  C   LEU A 121      65.256   7.492 -35.280  1.00 40.22      C
ATOM    912  O   LEU A 121      64.147   7.165 -35.705  1.00 39.00      O
ATOM    913  N   THR A 122      66.171   8.081 -36.057  1.00 40.54      N
ATOM    914  CA  THR A 122      65.968   8.199 -37.476  1.00 40.45      C
ATOM    915  CB  THR A 122      65.896   9.701 -37.936  1.00 41.48      C
ATOM    916  OG1 THR A 122      64.702  10.294 -37.406  1.00 44.87      O
ATOM    917  CG2 THR A 122      65.878   9.852 -39.480  1.00 39.71      C
ATOM    918  C   THR A 122      67.138   7.487 -38.092  1.00 40.29      C
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ATOM    919  O   THR A 122      68.279   7.874 -37.877  1.00 39.60      O
ATOM    920  N   VAL A 123      66.875   6.408 -38.818  1.00 40.92      N
ATOM    921  CA  VAL A 123      67.930   5.869 -39.707  1.00 41.20      C
ATOM    922  CB  VAL A 123      68.359   4.405 -39.388  1.00 41.03      C
ATOM    923  CG1 VAL A 123      67.511   3.799 -38.233  1.00 39.09      C
ATOM    924  CG2 VAL A 123      68.518   3.549 -40.620  1.00 40.22      C
ATOM    925  C   VAL A 123      67.788   6.260 -41.186  1.00 42.10      C
ATOM    926  O   VAL A 123      66.767   6.047 -41.842  1.00 42.13      O
ATOM    927  N   LYS A 124      68.836   6.892 -41.677  1.00 43.39      N
ATOM    928  CA  LYS A 124      68.864   7.415 -43.030  1.00 44.97      C
ATOM    929  CB  LYS A 124      70.047   8.388 -43.187  1.00 44.33      C
ATOM    930  CG  LYS A 124      69.902   9.697 -42.471  1.00 43.86      C
ATOM    931  CD  LYS A 124      71.265  10.355 -42.186  1.00 42.06      C
ATOM    932  CE  LYS A 124      71.842  11.023 -43.404  1.00 46.07      C
ATOM    933  NZ  LYS A 124      73.312  11.366 -43.269  1.00 46.30      N
ATOM    934  C   LYS A 124      68.989   6.198 -43.984  1.00 45.36      C
ATOM    935  O   LYS A 124      69.693   5.235 -43.663  1.00 45.33      O
ATOM    936  N   ALA A 125      68.274   6.214 -45.110  1.00 46.08      N
ATOM    937  CA  ALA A 125      68.489   5.175 -46.141  1.00 47.11      C
ATOM    938  CB  ALA A 125      67.648   5.451 -47.384  1.00 46.76      C
ATOM    939  C   ALA A 125      69.972   5.123 -46.500  1.00 47.33      C
ATOM    940  O   ALA A 125      70.618   6.175 -46.508  1.00 47.44      O
ATOM    941  N   ALA A 126      70.528   3.890 -46.738  1.00 48.74      N
ATOM    942  CA  ALA A 126      71.863   3.817 -47.444  1.00 49.81      C
ATOM    943  CB  ALA A 126      72.337   2.362 -47.714  1.00 49.59      C
ATOM    944  C   ALA A 126      71.800   4.577 -48.758  1.00 49.59      C
ATOM    945  O   ALA A 126      70.772   4.531 -49.478  1.00 51.31      O
ATOM    946  OXT ALA A 126      72.764   5.235 -49.161  1.00 51.16      O
ATOM    947  N   ALA B   1      32.574 -25.808  -7.345  1.00 54.95      N
ATOM    948  CA  ALA B   1      31.899 -24.453  -7.214  1.00 54.95      C
ATOM    949  CB  ALA B   1      32.851 -23.438  -6.634  1.00 55.01      C
ATOM    950  C   ALA B   1      31.283 -23.899  -8.498  1.00 54.51      C
ATOM    951  O   ALA B   1      31.993 -23.349  -9.338  1.00 55.95      O
ATOM    952  N   TRP B   2      29.963 -23.999  -8.630  1.00 53.08      N
ATOM    953  CA  TRP B   2      29.268 -23.472  -9.820  1.00 50.94      C
ATOM    954  CB  TRP B   2      29.049 -24.605 -10.808  1.00 51.28      C
ATOM    955  CG  TRP B   2      28.244 -25.758 -10.275  1.00 51.82      C
ATOM    956  CD1 TRP B   2      28.645 -26.700  -9.352  1.00 52.56      C
ATOM    957  NE1 TRP B   2      27.625 -27.612  -9.141  1.00 53.31      N
ATOM    958  CE2 TRP B   2      26.550 -27.281  -9.932  1.00 51.80      C
ATOM    959  CD2 TRP B   2      26.903 -26.123 -10.670  1.00 51.84      C
ATOM    960  CE3 TRP B   2      25.970 -25.573 -11.562  1.00 51.22      C
ATOM    961  CZ3 TRP B   2      24.719 -26.207 -11.705  1.00 52.11      C
ATOM    962  CH2 TRP B   2      24.404 -27.365 -10.954  1.00 52.45      C
ATOM    963  CZ2 TRP B   2      25.303 -27.907 -10.064  1.00 51.92      C
ATOM    964  C   TRP B   2      27.938 -22.763  -9.508  1.00 49.34      C
ATOM    965  O   TRP B   2      27.440 -22.864  -8.388  1.00 48.53      O
ATOM    966  N   VAL B   3      27.368 -22.056 -10.497  1.00 47.43      N
ATOM    967  CA  VAL B   3      26.076 -21.354 -10.319  1.00 45.64      C
ATOM    968  CB  VAL B   3      26.099 -19.865 -10.731  1.00 45.32      C
ATOM    969  CG1 VAL B   3      24.721 -19.227 -10.539  1.00 42.93      C
ATOM    970  CG2 VAL B   3      27.168 -19.097  -9.887  1.00 45.26      C
ATOM    971  C   VAL B   3      24.945 -22.081 -11.021  1.00 45.65      C
ATOM    972  O   VAL B   3      24.996 -22.334 -12.239  1.00 45.33      O
ATOM    973  N   ASP B   4      23.951 -22.435 -10.211  1.00 44.65      N
ATOM    974  CA  ASP B   4      22.792 -23.198 -10.608  1.00 44.39      C
ATOM    975  CB  ASP B   4      22.440 -24.131  -9.458  1.00 44.31      C
ATOM    976  CG  ASP B   4      21.422 -25.186  -9.834  1.00 48.07      C
ATOM    977  OD1 ASP B   4      20.972 -25.212 -11.005  1.00 48.90      O
ATOM    978  OD2 ASP B   4      21.052 -25.997  -8.932  1.00 51.27      O
ATOM    979  C   ASP B   4      21.621 -22.242 -10.868  1.00 44.17      C
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ATOM	980	O	ASP	B	4	20.926	-21.829	-9.913	1.00	45.13	O
ATOM	981	N	GLN	B	5	21.411	-21.881	-12.140	1.00	41.99	N
ATOM	982	CA	GLN	B	5	20.330	-20.945	-12.536	1.00	40.63	C
ATOM	983	CB	GLN	B	5	20.776	-20.017	-13.679	1.00	38.50	C
ATOM	984	CG	GLN	B	5	19.743	-18.908	-14.001	1.00	38.32	C
ATOM	985	CD	GLN	B	5	20.265	-17.971	-15.026	1.00	40.18	C
ATOM	986	OE1	GLN	B	5	21.484	-17.928	-15.203	1.00	40.72	O
ATOM	987	NE2	GLN	B	5	19.367	-17.207	-15.738	1.00	32.03	N
ATOM	988	C	GLN	B	5	19.078	-21.717	-12.978	1.00	40.31	C
ATOM	989	O	GLN	B	5	19.183	-22.575	-13.867	1.00	40.15	O
ATOM	990	N	THR	B	6	17.928	-21.407	-12.360	1.00	40.19	N
ATOM	991	CA	THR	B	6	16.597	-21.960	-12.747	1.00	41.32	C
ATOM	992	CB	THR	B	6	16.104	-23.106	-11.802	1.00	42.19	C
ATOM	993	OG1	THR	B	6	16.242	-22.695	-10.438	1.00	45.35	O
ATOM	994	CG2	THR	B	6	16.930	-24.421	-11.980	1.00	42.80	C
ATOM	995	C	THR	B	6	15.521	-20.844	-12.901	1.00	40.56	C
ATOM	996	O	THR	B	6	15.543	-19.855	-12.194	1.00	41.21	O
ATOM	997	N	PRO	B	7	14.605	-20.982	-13.859	1.00	40.24	N
ATOM	998	CA	PRO	B	7	14.476	-22.120	-14.793	1.00	39.70	C
ATOM	999	CB	PRO	B	7	13.018	-22.018	-15.237	1.00	38.51	C
ATOM	1000	CG	PRO	B	7	12.763	-20.573	-15.267	1.00	37.58	C
ATOM	1001	CD	PRO	B	7	13.570	-19.975	-14.102	1.00	39.88	C
ATOM	1002	C	PRO	B	7	15.428	-21.915	-15.952	1.00	39.21	C
ATOM	1003	O	PRO	B	7	15.772	-20.760	-16.237	1.00	40.93	O
ATOM	1004	N	ARG	B	8	15.863	-22.985	-16.598	1.00	39.22	N
ATOM	1005	CA	ARG	B	8	16.691	-22.864	-17.793	1.00	41.90	C
ATOM	1006	CB	ARG	B	8	17.582	-24.141	-17.979	1.00	40.92	C
ATOM	1007	CG	ARG	B	8	19.021	-23.843	-17.244	1.00	46.48	C
ATOM	1008	CD	ARG	B	8	20.003	-25.051	-17.078	1.00	49.30	C
ATOM	1009	NE	ARG	B	8	20.903	-25.344	-18.231	1.00	58.14	N
ATOM	1010	CZ	ARG	B	8	21.129	-24.550	-19.298	1.00	60.29	C
ATOM	1011	NH1	ARG	B	8	21.970	-24.991	-20.239	1.00	62.88	N
ATOM	1012	NH2	ARG	B	8	20.541	-23.343	-19.446	1.00	55.02	N
ATOM	1013	C	ARG	B	8	15.916	-22.266	-19.062	1.00	41.20	C
ATOM	1014	O	ARG	B	8	16.488	-21.531	-19.915	1.00	39.59	O
ATOM	1015	N	THR	B	9	14.594	-22.472	-19.057	1.00	40.29	N
ATOM	1016	CA	THR	B	9	13.687	-22.185	-20.154	1.00	41.50	C
ATOM	1017	CB	THR	B	9	13.369	-23.496	-20.870	1.00	41.08	C
ATOM	1018	OG1	THR	B	9	14.478	-23.831	-21.716	1.00	44.54	O
ATOM	1019	CG2	THR	B	9	12.186	-23.397	-21.691	1.00	44.46	C
ATOM	1020	C	THR	B	9	12.420	-21.625	-19.532	1.00	41.17	C
ATOM	1021	O	THR	B	9	11.988	-22.105	-18.486	1.00	42.29	O
ATOM	1022	N	ALA	B	10	11.863	-20.577	-20.120	1.00	39.83	N
ATOM	1023	CA	ALA	B	10	10.527	-20.109	-19.709	1.00	39.81	C
ATOM	1024	CB	ALA	B	10	10.636	-19.150	-18.520	1.00	39.10	C
ATOM	1025	C	ALA	B	10	9.708	-19.486	-20.865	1.00	39.00	C
ATOM	1026	O	ALA	B	10	10.218	-18.783	-21.709	1.00	37.05	O
ATOM	1027	N	THR	B	11	8.433	-19.807	-20.926	1.00	41.44	N
ATOM	1028	CA	THR	B	11	7.504	-19.035	-21.763	1.00	42.21	C
ATOM	1029	CB	THR	B	11	7.116	-19.744	-23.092	1.00	43.19	C
ATOM	1030	OG1	THR	B	11	5.708	-19.620	-23.359	1.00	45.57	O
ATOM	1031	CG2	THR	B	11	7.568	-21.172	-23.089	1.00	43.44	C
ATOM	1032	C	THR	B	11	6.410	-18.391	-20.904	1.00	43.25	C
ATOM	1033	O	THR	B	11	5.846	-19.026	-20.001	1.00	42.68	O
ATOM	1034	N	LYS	B	12	6.255	-17.074	-21.067	1.00	43.20	N
ATOM	1035	CA	LYS	B	12	5.257	-16.353	-20.305	1.00	43.24	C
ATOM	1036	CB	LYS	B	12	5.922	-15.425	-19.313	1.00	43.55	C
ATOM	1037	CG	LYS	B	12	6.850	-16.125	-18.282	1.00	43.71	C
ATOM	1038	CD	LYS	B	12	6.045	-16.918	-17.255	1.00	46.08	C
ATOM	1039	CE	LYS	B	12	6.956	-17.432	-16.177	1.00	46.77	C
ATOM	1040	NZ	LYS	B	12	6.207	-18.212	-15.178	1.00	48.14	N

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ATOM   1041  C   LYS B  12       4.323 -15.587 -21.224  1.00 43.67      C
ATOM   1042  O   LYS B  12       4.603 -15.377 -22.399  1.00 43.55      O
ATOM   1043  N   GLU B  13       3.196 -15.198 -20.670  1.00 44.88      N
ATOM   1044  CA  GLU B  13       2.183 -14.407 -21.349  1.00 45.97      C
ATOM   1045  CB  GLU B  13       0.819 -14.763 -20.763  1.00 45.50      C
ATOM   1046  CG  GLU B  13      -0.252 -14.954 -21.805  1.00 51.14      C
ATOM   1047  CD  GLU B  13      -1.672 -15.025 -21.223  1.00 52.49      C
ATOM   1048  OE1 GLU B  13      -2.214 -13.977 -20.736  1.00 56.84      O
ATOM   1049  OE2 GLU B  13      -2.268 -16.136 -21.318  1.00 61.96      O
ATOM   1050  C   GLU B  13       2.512 -12.959 -21.020  1.00 43.04      C
ATOM   1051  O   GLU B  13       3.028 -12.701 -19.945  1.00 41.31      O
ATOM   1052  N   THR B  14       2.223 -12.015 -21.916  1.00 41.79      N
ATOM   1053  CA  THR B  14       2.424 -10.600 -21.549  1.00 41.84      C
ATOM   1054  CB  THR B  14       2.091  -9.590 -22.653  1.00 41.46      C
ATOM   1055  OG1 THR B  14       0.695  -9.668 -22.914  1.00 46.96      O
ATOM   1056  CG2 THR B  14       2.850  -9.885 -23.954  1.00 39.14      C
ATOM   1057  C   THR B  14       1.601 -10.261 -20.284  1.00 41.06      C
ATOM   1058  O   THR B  14       0.519 -10.798 -20.082  1.00 39.53      O
ATOM   1059  N   GLY B  15       2.167  -9.424 -19.419  1.00 39.95      N
ATOM   1060  CA  GLY B  15       1.531  -9.033 -18.178  1.00 39.59      C
ATOM   1061  C   GLY B  15       1.928  -9.927 -17.032  1.00 39.94      C
ATOM   1062  O   GLY B  15       1.745  -9.553 -15.861  1.00 40.01      O
ATOM   1063  N   GLU B  16       2.448 -11.112 -17.347  1.00 40.07      N
ATOM   1064  CA  GLU B  16       2.963 -12.013 -16.311  1.00 41.17      C
ATOM   1065  CB  GLU B  16       3.024 -13.455 -16.850  1.00 40.57      C
ATOM   1066  CG  GLU B  16       1.656 -14.146 -16.761  1.00 41.94      C
ATOM   1067  CD  GLU B  16       1.562 -15.517 -17.442  1.00 43.73      C
ATOM   1068  OE1 GLU B  16       2.530 -16.134 -17.948  1.00 43.61      O
ATOM   1069  OE2 GLU B  16       0.432 -16.009 -17.477  1.00 54.01      O
ATOM   1070  C   GLU B  16       4.321 -11.577 -15.715  1.00 40.58      C
ATOM   1071  O   GLU B  16       4.936 -10.595 -16.140  1.00 41.16      O
ATOM   1072  N   SER B  17       4.803 -12.311 -14.732  1.00 40.31      N
ATOM   1073  CA  SER B  17       6.133 -12.054 -14.205  1.00 39.94      C
ATOM   1074  CB  SER B  17       5.987 -11.519 -12.797  1.00 40.72      C
ATOM   1075  OG  SER B  17       5.762 -12.588 -11.942  1.00 41.64      O
ATOM   1076  C   SER B  17       7.004 -13.346 -14.277  1.00 39.37      C
ATOM   1077  O   SER B  17       6.488 -14.426 -14.552  1.00 39.99      O
ATOM   1078  N   LEU B  18       8.320 -13.220 -14.120  1.00 39.17      N
ATOM   1079  CA  LEU B  18       9.270 -14.346 -14.176  1.00 39.40      C
ATOM   1080  CB  LEU B  18      10.217 -14.269 -15.412  1.00 39.88      C
ATOM   1081  CG  LEU B  18      10.975 -15.464 -16.093  1.00 39.25      C
ATOM   1082  CD1 LEU B  18      12.361 -15.081 -16.621  1.00 36.41      C
ATOM   1083  CD2 LEU B  18      11.031 -16.801 -15.375  1.00 36.79      C
ATOM   1084  C   LEU B  18      10.151 -14.217 -12.952  1.00 39.21      C
ATOM   1085  O   LEU B  18      10.648 -13.131 -12.684  1.00 38.56      O
ATOM   1086  N   THR B  19      10.350 -15.309 -12.208  1.00 39.51      N
ATOM   1087  CA  THR B  19      11.356 -15.331 -11.145  1.00 38.61      C
ATOM   1088  CB  THR B  19      10.745 -15.681  -9.777  1.00 39.40      C
ATOM   1089  OG1 THR B  19       9.596 -14.859  -9.569  1.00 40.21      O
ATOM   1090  CG2 THR B  19      11.734 -15.391  -8.613  1.00 37.97      C
ATOM   1091  C   THR B  19      12.481 -16.291 -11.544  1.00 39.08      C
ATOM   1092  O   THR B  19      12.242 -17.425 -11.918  1.00 38.36      O
ATOM   1093  N   ILE B  20      13.713 -15.795 -11.510  1.00 39.84      N
ATOM   1094  CA  ILE B  20      14.881 -16.577 -11.832  1.00 40.37      C
ATOM   1095  CB  ILE B  20      15.752 -15.886 -12.869  1.00 41.04      C
ATOM   1096  CG1 ILE B  20      14.963 -15.656 -14.189  1.00 41.04      C
ATOM   1097  CD1 ILE B  20      15.801 -14.744 -15.167  1.00 40.82      C
ATOM   1098  CG2 ILE B  20      17.039 -16.690 -13.157  1.00 37.32      C
ATOM   1099  C   ILE B  20      15.653 -16.721 -10.544  1.00 42.32      C
ATOM   1100  O   ILE B  20      15.910 -15.743  -9.821  1.00 42.02      O
ATOM   1101  N   ASN B  21      16.009 -17.959 -10.235  1.00 43.42      N
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ATOM   1102  CA  ASN B  21      16.750 -18.232  -9.028  1.00 44.99      C
ATOM   1103  CB  ASN B  21      15.975 -19.274  -8.234  1.00 45.42      C
ATOM   1104  CG  ASN B  21      14.760 -18.676  -7.544  1.00 49.78      C
ATOM   1105  OD1 ASN B  21      14.911 -17.898  -6.575  1.00 55.43      O
ATOM   1106  ND2 ASN B  21      13.546 -19.031  -8.021  1.00 48.66      N
ATOM   1107  C   ASN B  21      18.162 -18.714  -9.316  1.00 45.15      C
ATOM   1108  O   ASN B  21      18.355 -19.604 -10.139  1.00 46.04      O
ATOM   1109  N   CYS B  22      19.145 -18.141  -8.642  1.00 45.51      N
ATOM   1110  CA  CYS B  22      20.512 -18.645  -8.738  1.00 46.56      C
ATOM   1111  CB  CYS B  22      21.398 -17.616  -9.407  1.00 46.01      C
ATOM   1112  SG  CYS B  22      20.937 -17.240 -11.134  1.00 54.66      S
ATOM   1113  C   CYS B  22      21.094 -19.006  -7.382  1.00 46.14      C
ATOM   1114  O   CYS B  22      20.802 -18.342  -6.400  1.00 45.68      O
ATOM   1115  N   VAL B  23      21.914 -20.064  -7.348  1.00 46.34      N
ATOM   1116  CA  VAL B  23      22.574 -20.552  -6.137  1.00 45.67      C
ATOM   1117  CB  VAL B  23      21.951 -21.906  -5.581  1.00 45.26      C
ATOM   1118  CG1 VAL B  23      22.335 -22.151  -4.112  1.00 44.69      C
ATOM   1119  CG2 VAL B  23      20.461 -21.936  -5.697  1.00 46.49      C
ATOM   1120  C   VAL B  23      24.018 -20.856  -6.513  1.00 46.67      C
ATOM   1121  O   VAL B  23      24.255 -21.594  -7.477  1.00 46.49      O
ATOM   1122  N   LEU B  24      24.964 -20.275  -5.775  1.00 47.05      N
ATOM   1123  CA  LEU B  24      26.379 -20.661  -5.783  1.00 49.11      C
ATOM   1124  CB  LEU B  24      27.194 -19.589  -5.042  1.00 48.19      C
ATOM   1125  CG  LEU B  24      28.539 -19.018  -5.483  1.00 50.04      C
ATOM   1126  CD1 LEU B  24      29.178 -18.189  -4.317  1.00 47.71      C
ATOM   1127  CD2 LEU B  24      29.500 -20.085  -5.957  1.00 51.22      C
ATOM   1128  C   LEU B  24      26.508 -21.967  -4.994  1.00 50.50      C
ATOM   1129  O   LEU B  24      26.243 -21.987  -3.785  1.00 50.47      O
ATOM   1130  N   ARG B  25      26.902 -23.047  -5.670  1.00 52.28      N
ATOM   1131  CA  ARG B  25      27.026 -24.372  -5.044  1.00 53.42      C
ATOM   1132  CB  ARG B  25      26.429 -25.461  -5.933  1.00 53.07      C
ATOM   1133  CG  ARG B  25      25.046 -25.141  -6.419  1.00 51.09      C
ATOM   1134  CD  ARG B  25      24.139 -26.318  -6.287  1.00 51.67      C
ATOM   1135  NE  ARG B  25      22.742 -25.901  -6.377  1.00 52.28      N
ATOM   1136  CZ  ARG B  25      21.895 -25.907  -5.354  1.00 51.59      C
ATOM   1137  NH1 ARG B  25      22.299 -26.334  -4.157  1.00 51.61      N
ATOM   1138  NH2 ARG B  25      20.644 -25.498  -5.532  1.00 50.56      N
ATOM   1139  C   ARG B  25      28.483 -24.685  -4.733  1.00 55.51      C
ATOM   1140  O   ARG B  25      29.364 -23.827  -4.909  1.00 55.95      O
ATOM   1141  N   ASP B  26      28.724 -25.902  -4.238  1.00 57.67      N
ATOM   1142  CA  ASP B  26      30.064 -26.414  -3.891  1.00 59.47      C
ATOM   1143  CB  ASP B  26      30.592 -27.321  -5.009  1.00 59.83      C
ATOM   1144  CG  ASP B  26      29.669 -28.511  -5.285  1.00 61.62      C
ATOM   1145  OD1 ASP B  26      28.795 -28.416  -6.198  1.00 62.14      O
ATOM   1146  OD2 ASP B  26      29.814 -29.530  -4.572  1.00 62.86      O
ATOM   1147  C   ASP B  26      31.052 -25.293  -3.599  1.00 60.27      C
ATOM   1148  O   ASP B  26      32.103 -25.207  -4.225  1.00 60.76      O
ATOM   1149  N   ALA B  27      30.693 -24.433  -2.646  1.00 61.28      N
ATOM   1150  CA  ALA B  27      31.493 -23.273  -2.307  1.00 61.93      C
ATOM   1151  CB  ALA B  27      30.784 -22.014  -2.708  1.00 61.89      C
ATOM   1152  C   ALA B  27      31.863 -23.212  -0.829  1.00 62.84      C
ATOM   1153  O   ALA B  27      30.991 -23.186   0.053  1.00 63.36      O
ATOM   1154  N   SER B  28      33.171 -23.214  -0.581  1.00 63.10      N
ATOM   1155  CA  SER B  28      33.737 -22.641   0.624  1.00 63.63      C
ATOM   1156  CB  SER B  28      35.224 -22.968   0.718  1.00 63.90      C
ATOM   1157  OG  SER B  28      35.570 -24.105  -0.058  1.00 64.95      O
ATOM   1158  C   SER B  28      33.601 -21.129   0.427  1.00 63.77      C
ATOM   1159  O   SER B  28      33.495 -20.363   1.393  1.00 64.47      O
ATOM   1160  N   PHE B  29      33.625 -20.737  -0.852  1.00 63.20      N
ATOM   1161  CA  PHE B  29      33.530 -19.355  -1.334  1.00 62.45      C
ATOM   1162  CB  PHE B  29      33.358 -19.335  -2.872  1.00 62.20      C
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ATOM	1163	CG	PHE	B	29	34.395	-20.140	-3.656	1.00	60.55	C
ATOM	1164	CD1	PHE	B	29	35.699	-20.308	-3.201	1.00	60.68	C
ATOM	1165	CE1	PHE	B	29	36.646	-21.025	-3.950	1.00	60.56	C
ATOM	1166	CZ	PHE	B	29	36.304	-21.564	-5.173	1.00	60.35	C
ATOM	1167	CE2	PHE	B	29	35.014	-21.392	-5.648	1.00	62.60	C
ATOM	1168	CD2	PHE	B	29	34.066	-20.671	-4.891	1.00	61.14	C
ATOM	1169	C	PHE	B	29	32.352	-18.604	-0.706	1.00	62.55	C
ATOM	1170	O	PHE	B	29	31.268	-19.188	-0.504	1.00	62.53	O
ATOM	1171	N	GLU	B	30	32.545	-17.315	-0.411	1.00	61.80	N
ATOM	1172	CA	GLU	B	30	31.445	-16.518	0.143	1.00	61.37	C
ATOM	1173	CB	GLU	B	30	31.797	-15.884	1.497	1.00	61.71	C
ATOM	1174	CG	GLU	B	30	32.680	-14.633	1.411	1.00	64.15	C
ATOM	1175	CD	GLU	B	30	32.153	-13.451	2.233	1.00	65.74	C
ATOM	1176	OE1	GLU	B	30	32.866	-13.015	3.168	1.00	63.81	O
ATOM	1177	OE2	GLU	B	30	31.033	-12.963	1.925	1.00	66.59	O
ATOM	1178	C	GLU	B	30	30.920	-15.470	-0.836	1.00	59.86	C
ATOM	1179	O	GLU	B	30	31.681	-14.655	-1.343	1.00	59.82	O
ATOM	1180	N	LEU	B	31	29.606	-15.497	-1.069	1.00	58.15	N
ATOM	1181	CA	LEU	B	31	28.946	-14.572	-1.982	1.00	56.44	C
ATOM	1182	CB	LEU	B	31	27.444	-14.831	-1.998	1.00	56.25	C
ATOM	1183	CG	LEU	B	31	26.669	-14.204	-3.148	1.00	54.16	C
ATOM	1184	CD1	LEU	B	31	27.090	-14.868	-4.401	1.00	51.33	C
ATOM	1185	CD2	LEU	B	31	25.183	-14.389	-2.910	1.00	53.29	C
ATOM	1186	C	LEU	B	31	29.187	-13.136	-1.575	1.00	55.70	C
ATOM	1187	O	LEU	B	31	28.791	-12.748	-0.489	1.00	55.50	O
ATOM	1188	N	LYS	B	32	29.831	-12.354	-2.436	1.00	54.55	N
ATOM	1189	CA	LYS	B	32	30.081	-10.963	-2.096	1.00	54.28	C
ATOM	1190	CB	LYS	B	32	31.576	-10.589	-2.202	1.00	54.33	C
ATOM	1191	CG	LYS	B	32	31.918	-9.629	-3.367	1.00	56.46	C
ATOM	1192	CD	LYS	B	32	33.271	-8.944	-3.278	1.00	55.97	C
ATOM	1193	CE	LYS	B	32	33.233	-7.762	-2.288	1.00	63.91	C
ATOM	1194	NZ	LYS	B	32	32.451	-6.536	-2.708	1.00	64.90	N
ATOM	1195	C	LYS	B	32	29.216	-10.009	-2.902	1.00	52.81	C
ATOM	1196	O	LYS	B	32	28.927	-8.898	-2.450	1.00	52.61	O
ATOM	1197	N	ASP	B	33	28.818	-10.438	-4.093	1.00	51.52	N
ATOM	1198	CA	ASP	B	33	28.077	-9.585	-5.000	1.00	50.34	C
ATOM	1199	CB	ASP	B	33	29.020	-8.581	-5.653	1.00	51.45	C
ATOM	1200	CG	ASP	B	33	28.458	-7.192	-5.654	1.00	54.79	C
ATOM	1201	OD1	ASP	B	33	29.150	-6.290	-5.130	1.00	60.70	O
ATOM	1202	OD2	ASP	B	33	27.308	-6.997	-6.126	1.00	60.01	O
ATOM	1203	C	ASP	B	33	27.349	-10.349	-6.103	1.00	48.37	C
ATOM	1204	O	ASP	B	33	27.618	-11.514	-6.338	1.00	47.51	O
ATOM	1205	N	THR	B	34	26.435	-9.656	-6.783	1.00	46.63	N
ATOM	1206	CA	THR	B	34	25.607	-10.230	-7.812	1.00	45.52	C
ATOM	1207	CB	THR	B	34	24.228	-10.594	-7.311	1.00	45.26	C
ATOM	1208	OG1	THR	B	34	23.507	-9.400	-7.005	1.00	44.94	O
ATOM	1209	CG2	THR	B	34	24.280	-11.520	-6.066	1.00	46.07	C
ATOM	1210	C	THR	B	34	25.396	-9.238	-8.924	1.00	45.83	C
ATOM	1211	O	THR	B	34	25.372	-8.017	-8.702	1.00	45.11	O
ATOM	1212	N	GLY	B	35	25.201	-9.773	-10.125	1.00	45.83	N
ATOM	1213	CA	GLY	B	35	24.725	-8.972	-11.249	1.00	44.82	C
ATOM	1214	C	GLY	B	35	23.816	-9.785	-12.153	1.00	43.28	C
ATOM	1215	O	GLY	B	35	23.801	-11.019	-12.111	1.00	42.32	O
ATOM	1216	N	TRP	B	36	23.074	-9.070	-12.992	1.00	42.69	N
ATOM	1217	CA	TRP	B	36	22.094	-9.665	-13.876	1.00	42.22	C
ATOM	1218	CB	TRP	B	36	20.695	-9.393	-13.321	1.00	41.99	C
ATOM	1219	CG	TRP	B	36	20.426	-10.204	-12.070	1.00	42.02	C
ATOM	1220	CD1	TRP	B	36	20.606	-9.809	-10.785	1.00	39.92	C
ATOM	1221	NE1	TRP	B	36	20.263	-10.839	-9.929	1.00	42.86	N
ATOM	1222	CE2	TRP	B	36	19.869	-11.931	-10.660	1.00	41.27	C
ATOM	1223	CD2	TRP	B	36	19.955	-11.571	-12.021	1.00	41.39	C

ATOM	1224	CE3	TRP	B	36	19.601	-12.520	-13.014	1.00	42.24	C
ATOM	1225	CZ3	TRP	B	36	19.161	-13.779	-12.616	1.00	42.06	C
ATOM	1226	CH2	TRP	B	36	19.077	-14.117	-11.226	1.00	42.99	C
ATOM	1227	CZ2	TRP	B	36	19.428	-13.199	-10.235	1.00	42.30	C
ATOM	1228	C	TRP	B	36	22.263	-9.062	-15.251	1.00	42.47	C
ATOM	1229	O	TRP	B	36	22.527	-7.848	-15.372	1.00	43.87	O
ATOM	1230	N	TYR	B	37	22.124	-9.884	-16.284	1.00	42.85	N
ATOM	1231	CA	TYR	B	37	22.396	-9.464	-17.688	1.00	44.60	C
ATOM	1232	CB	TYR	B	37	23.771	-9.983	-18.167	1.00	45.76	C
ATOM	1233	CG	TYR	B	37	24.857	-9.689	-17.146	1.00	47.71	C
ATOM	1234	CD1	TYR	B	37	25.524	-8.464	-17.117	1.00	50.27	C
ATOM	1235	CE1	TYR	B	37	26.524	-8.179	-16.125	1.00	51.99	C
ATOM	1236	CZ	TYR	B	37	26.825	-9.195	-15.183	1.00	53.06	C
ATOM	1237	OH	TYR	B	37	27.770	-9.042	-14.172	1.00	54.16	O
ATOM	1238	CE2	TYR	B	37	26.137	-10.395	-15.213	1.00	54.10	C
ATOM	1239	CD2	TYR	B	37	25.163	-10.627	-16.175	1.00	51.46	C
ATOM	1240	C	TYR	B	37	21.332	-10.026	-18.555	1.00	44.88	C
ATOM	1241	O	TYR	B	37	20.705	-11.043	-18.209	1.00	45.77	O
ATOM	1242	N	ARG	B	38	21.135	-9.388	-19.698	1.00	45.01	N
ATOM	1243	CA	ARG	B	38	20.136	-9.799	-20.689	1.00	44.85	C
ATOM	1244	CB	ARG	B	38	18.859	-8.971	-20.449	1.00	44.48	C
ATOM	1245	CG	ARG	B	38	17.818	-8.990	-21.512	1.00	49.57	C
ATOM	1246	CD	ARG	B	38	16.572	-8.154	-21.096	1.00	50.80	C
ATOM	1247	NE	ARG	B	38	16.808	-6.728	-20.931	1.00	59.29	N
ATOM	1248	CZ	ARG	B	38	16.791	-5.849	-21.929	1.00	65.43	C
ATOM	1249	NH1	ARG	B	38	16.570	-6.250	-23.196	1.00	68.18	N
ATOM	1250	NH2	ARG	B	38	17.020	-4.560	-21.670	1.00	66.70	N
ATOM	1251	C	ARG	B	38	20.678	-9.588	-22.100	1.00	43.70	C
ATOM	1252	O	ARG	B	38	21.291	-8.573	-22.413	1.00	43.08	O
ATOM	1253	N	THR	B	39	20.399	-10.551	-22.970	1.00	43.10	N
ATOM	1254	CA	THR	B	39	20.574	-10.401	-24.392	1.00	41.41	C
ATOM	1255	CB	THR	B	39	21.561	-11.463	-24.921	1.00	40.29	C
ATOM	1256	OG1	THR	B	39	22.780	-11.325	-24.192	1.00	44.60	O
ATOM	1257	CG2	THR	B	39	21.830	-11.278	-26.361	1.00	38.65	C
ATOM	1258	C	THR	B	39	19.209	-10.611	-25.023	1.00	40.66	C
ATOM	1259	O	THR	B	39	18.632	-11.718	-24.960	1.00	40.48	O
ATOM	1260	N	LYS	B	40	18.696	-9.575	-25.658	1.00	38.27	N
ATOM	1261	CA	LYS	B	40	17.420	-9.673	-26.286	1.00	40.05	C
ATOM	1262	CB	LYS	B	40	16.985	-8.329	-26.866	1.00	40.66	C
ATOM	1263	CG	LYS	B	40	18.180	-7.401	-27.336	1.00	46.79	C
ATOM	1264	CD	LYS	B	40	19.495	-7.235	-26.337	1.00	45.68	C
ATOM	1265	CE	LYS	B	40	20.177	-5.941	-26.663	1.00	47.93	C
ATOM	1266	NZ	LYS	B	40	19.625	-5.348	-28.020	1.00	50.16	N
ATOM	1267	C	LYS	B	40	17.399	-10.781	-27.346	1.00	39.05	C
ATOM	1268	O	LYS	B	40	18.428	-11.090	-27.963	1.00	38.47	O
ATOM	1269	N	LEU	B	41	16.231	-11.387	-27.526	1.00	37.38	N
ATOM	1270	CA	LEU	B	41	16.110	-12.482	-28.447	1.00	36.97	C
ATOM	1271	CB	LEU	B	41	14.693	-13.025	-28.410	1.00	35.93	C
ATOM	1272	CG	LEU	B	41	14.361	-14.498	-28.751	1.00	38.03	C
ATOM	1273	CD1	LEU	B	41	15.260	-15.201	-29.688	1.00	29.12	C
ATOM	1274	CD2	LEU	B	41	12.935	-14.628	-29.245	1.00	34.95	C
ATOM	1275	C	LEU	B	41	16.456	-12.015	-29.853	1.00	37.90	C
ATOM	1276	O	LEU	B	41	15.750	-11.171	-30.429	1.00	38.11	O
ATOM	1277	N	GLY	B	42	17.516	-12.596	-30.428	1.00	38.84	N
ATOM	1278	CA	GLY	B	42	17.894	-12.309	-31.828	1.00	39.84	C
ATOM	1279	C	GLY	B	42	19.138	-11.426	-31.882	1.00	41.12	C
ATOM	1280	O	GLY	B	42	19.889	-11.451	-32.845	1.00	40.47	O
ATOM	1281	N	SER	B	43	19.398	-10.703	-30.795	1.00	42.54	N
ATOM	1282	CA	SER	B	43	20.505	-9.752	-30.700	1.00	43.80	C
ATOM	1283	CB	SER	B	43	20.102	-8.627	-29.733	1.00	43.55	C
ATOM	1284	OG	SER	B	43	21.263	-8.058	-29.131	1.00	47.40	O

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ATOM   1285  C   SER B  43      21.837 -10.389 -30.246  1.00 44.08      C
ATOM   1286  O   SER B  43      21.850 -11.442 -29.639  1.00 43.11      O
ATOM   1287  N   THR B  44      22.950  -9.730 -30.556  1.00 46.01      N
ATOM   1288  CA  THR B  44      24.284 -10.132 -30.088  1.00 49.08      C
ATOM   1289  CB  THR B  44      25.386  -9.746 -31.113  1.00 49.56      C
ATOM   1290  OG1 THR B  44      24.825  -8.862 -32.111  1.00 50.26      O
ATOM   1291  CG2 THR B  44      25.951 -10.982 -31.782  1.00 51.25      C
ATOM   1292  C   THR B  44      24.609  -9.414 -28.788  1.00 50.25      C
ATOM   1293  O   THR B  44      25.441  -9.865 -27.991  1.00 51.27      O
ATOM   1294  N   ASN B  45      23.915  -8.304 -28.560  1.00 51.11      N
ATOM   1295  CA  ASN B  45      24.288  -7.373 -27.522  1.00 51.61      C
ATOM   1296  CB  ASN B  45      23.900  -5.973 -27.975  1.00 51.54      C
ATOM   1297  CG  ASN B  45      24.666  -5.532 -29.257  1.00 52.45      C
ATOM   1298  OD1 ASN B  45      24.146  -4.760 -30.070  1.00 52.60      O
ATOM   1299  ND2 ASN B  45      25.895  -6.033 -29.433  1.00 53.59      N
ATOM   1300  C   ASN B  45      23.809  -7.699 -26.105  1.00 51.58      C
ATOM   1301  O   ASN B  45      22.632  -7.837 -25.840  1.00 52.48      O
ATOM   1302  N   GLU B  46      24.750  -7.844 -25.189  1.00 51.92      N
ATOM   1303  CA  GLU B  46      24.414  -8.133 -23.821  1.00 52.44      C
ATOM   1304  CB  GLU B  46      25.368  -9.161 -23.221  1.00 52.91      C
ATOM   1305  CG  GLU B  46      24.884  -9.678 -21.894  1.00 58.15      C
ATOM   1306  CD  GLU B  46      25.957 -10.405 -21.123  1.00 66.36      C
ATOM   1307  OE1 GLU B  46      25.706 -11.582 -20.727  1.00 70.62      O
ATOM   1308  OE2 GLU B  46      27.039  -9.793 -20.894  1.00 69.30      O
ATOM   1309  C   GLU B  46      24.380  -6.860 -22.976  1.00 51.53      C
ATOM   1310  O   GLU B  46      25.327  -6.088 -22.964  1.00 53.42      O
ATOM   1311  N   GLN B  47      23.278  -6.642 -22.286  1.00 49.40      N
ATOM   1312  CA  GLN B  47      23.107  -5.475 -21.450  1.00 48.39      C
ATOM   1313  CB  GLN B  47      21.867  -4.713 -21.877  1.00 48.97      C
ATOM   1314  CG  GLN B  47      21.851  -4.315 -23.390  1.00 54.17      C
ATOM   1315  CD  GLN B  47      22.859  -3.187 -23.733  1.00 58.95      C
ATOM   1316  OE1 GLN B  47      22.457  -2.123 -24.216  1.00 59.67      O
ATOM   1317  NE2 GLN B  47      24.167  -3.430 -23.488  1.00 56.36      N
ATOM   1318  C   GLN B  47      22.954  -5.913 -20.012  1.00 46.93      C
ATOM   1319  O   GLN B  47      22.368  -6.955 -19.731  1.00 45.54      O
ATOM   1320  N   SER B  48      23.510  -5.138 -19.103  1.00 45.48      N
ATOM   1321  CA  SER B  48      23.310  -5.430 -17.703  1.00 45.97      C
ATOM   1322  CB  SER B  48      24.518  -5.024 -16.823  1.00 44.83      C
ATOM   1323  OG  SER B  48      24.567  -3.634 -16.677  1.00 48.28      O
ATOM   1324  C   SER B  48      21.996  -4.775 -17.260  1.00 45.25      C
ATOM   1325  O   SER B  48      21.625  -3.706 -17.747  1.00 44.79      O
ATOM   1326  N   ILE B  49      21.310  -5.440 -16.336  1.00 44.46      N
ATOM   1327  CA  ILE B  49      19.994  -5.034 -15.879  1.00 43.57      C
ATOM   1328  CB  ILE B  49      19.191  -6.343 -15.528  1.00 43.55      C
ATOM   1329  CG1 ILE B  49      18.786  -7.071 -16.799  1.00 41.77      C
ATOM   1330  CD1 ILE B  49      18.315  -8.465 -16.522  1.00 45.18      C
ATOM   1331  CG2 ILE B  49      17.998  -6.077 -14.627  1.00 42.15      C
ATOM   1332  C   ILE B  49      20.202  -4.130 -14.678  1.00 43.36      C
ATOM   1333  O   ILE B  49      20.937  -4.516 -13.800  1.00 43.25      O
ATOM   1334  N   SER B  50      19.619  -2.910 -14.657  1.00 44.45      N
ATOM   1335  CA  SER B  50      19.533  -2.085 -13.399  1.00 44.63      C
ATOM   1336  CB  SER B  50      19.444  -0.561 -13.621  1.00 44.94      C
ATOM   1337  OG  SER B  50      19.832  -0.190 -14.927  1.00 49.21      O
ATOM   1338  C   SER B  50      18.328  -2.500 -12.603  1.00 43.86      C
ATOM   1339  O   SER B  50      17.189  -2.461 -13.099  1.00 43.03      O
ATOM   1340  N   ILE B  51      18.603  -2.881 -11.369  1.00 43.39      N
ATOM   1341  CA  ILE B  51      17.624  -3.379 -10.447  1.00 43.30      C
ATOM   1342  CB  ILE B  51      18.340  -3.979  -9.224  1.00 43.57      C
ATOM   1343  CG1 ILE B  51      19.287  -5.151  -9.618  1.00 44.05      C
ATOM   1344  CD1 ILE B  51      18.667  -6.326 -10.418  1.00 35.96      C
ATOM   1345  CG2 ILE B  51      17.357  -4.242  -8.073  1.00 43.78      C
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ATOM   1346  C   ILE B  51      16.771  -2.224   -9.993  1.00 44.13      C
ATOM   1347  O   ILE B  51      17.287  -1.167   -9.601  1.00 45.28      O
ATOM   1348  N   GLY B  52      15.456  -2.413  -10.016  1.00 44.21      N
ATOM   1349  CA  GLY B  52      14.540  -1.395   -9.504  1.00 43.63      C
ATOM   1350  C   GLY B  52      13.381  -1.293  -10.469  1.00 43.28      C
ATOM   1351  O   GLY B  52      13.460  -1.784  -11.585  1.00 43.58      O
ATOM   1352  N   GLY B  53      12.310  -0.656  -10.035  1.00 43.27      N
ATOM   1353  CA  GLY B  53      11.083  -0.560  -10.850  1.00 42.78      C
ATOM   1354  C   GLY B  53      10.462  -2.015  -10.752  1.00 43.77      C
ATOM   1355  O   GLY B  53       9.995  -2.673   -9.640  1.00 43.34      O
ATOM   1356  N   ARG B  54      10.551  -2.654  -12.075  1.00 43.61      N
ATOM   1357  CA  ARG B  54       9.886  -3.914  -12.251  1.00 42.86      C
ATOM   1358  CB  ARG B  54       9.068  -3.913  -13.539  1.00 44.13      C
ATOM   1359  CG  ARG B  54       9.889  -3.906  -14.830  1.00 42.33      C
ATOM   1360  CD  ARG B  54       8.906  -3.835  -15.998  1.00 45.56      C
ATOM   1361  NE  ARG B  54       9.580  -3.821  -17.288  1.00 47.32      N
ATOM   1362  CZ  ARG B  54       9.650  -4.835  -18.148  1.00 47.04      C
ATOM   1363  NH1 ARG B  54       9.064  -6.010  -17.908  1.00 50.81      N
ATOM   1364  NH2 ARG B  54      10.306  -4.664  -19.280  1.00 46.49      N
ATOM   1365  C   ARG B  54      10.892  -5.077  -12.274  1.00 44.33      C
ATOM   1366  O   ARG B  54      10.498  -6.291  -12.483  1.00 44.77      O
ATOM   1367  N   TYR B  55      12.186  -4.751  -12.152  1.00 43.57      N
ATOM   1368  CA  TYR B  55      13.228  -5.749  -11.905  1.00 43.62      C
ATOM   1369  CB  TYR B  55      14.498  -5.407  -12.673  1.00 44.46      C
ATOM   1370  CG  TYR B  55      14.287  -5.318  -14.171  1.00 46.09      C
ATOM   1371  CD1 TYR B  55      14.032  -4.088  -14.784  1.00 48.85      C
ATOM   1372  CE1 TYR B  55      13.812  -3.998  -16.152  1.00 48.27      C
ATOM   1373  CZ  TYR B  55      13.865  -5.144  -16.918  1.00 48.69      C
ATOM   1374  OH  TYR B  55      13.655  -5.041  -18.268  1.00 47.96      O
ATOM   1375  CE2 TYR B  55      14.087  -6.373  -16.336  1.00 48.31      C
ATOM   1376  CD2 TYR B  55      14.296  -6.448  -14.959  1.00 45.72      C
ATOM   1377  C   TYR B  55      13.511  -5.706  -10.398  1.00 43.55      C
ATOM   1378  O   TYR B  55      14.064  -4.715   -9.878  1.00 42.28      O
ATOM   1379  N   VAL B  56      13.071  -6.744   -9.689  1.00 43.19      N
ATOM   1380  CA  VAL B  56      13.348  -6.837   -8.260  1.00 42.73      C
ATOM   1381  CB  VAL B  56      12.127  -6.516   -7.293  1.00 42.21      C
ATOM   1382  CG1 VAL B  56      10.841  -6.421   -7.968  1.00 44.06      C
ATOM   1383  CG2 VAL B  56      12.051  -7.448   -6.048  1.00 45.27      C
ATOM   1384  C   VAL B  56      14.263  -8.013   -7.898  1.00 42.60      C
ATOM   1385  O   VAL B  56      13.991  -9.173   -8.224  1.00 41.88      O
ATOM   1386  N   GLU B  57      15.388  -7.664   -7.277  1.00 42.73      N
ATOM   1387  CA  GLU B  57      16.395  -8.617   -6.875  1.00 44.06      C
ATOM   1388  CB  GLU B  57      17.815  -8.148   -7.214  1.00 42.94      C
ATOM   1389  CG  GLU B  57      18.805  -9.083   -6.512  1.00 44.58      C
ATOM   1390  CD  GLU B  57      20.228  -9.094   -7.028  1.00 48.71      C
ATOM   1391  OE1 GLU B  57      20.904  -8.036   -7.062  1.00 49.40      O
ATOM   1392  OE2 GLU B  57      20.704 -10.204   -7.334  1.00 49.94      O
ATOM   1393  C   GLU B  57      16.271  -8.867   -5.374  1.00 44.37      C
ATOM   1394  O   GLU B  57      16.096  -7.910   -4.621  1.00 43.80      O
ATOM   1395  N   THR B  58      16.326 -10.154   -4.985  1.00 45.59      N
ATOM   1396  CA  THR B  58      16.372 -10.633   -3.584  1.00 47.38      C
ATOM   1397  CB  THR B  58      15.228 -11.630   -3.244  1.00 47.57      C
ATOM   1398  OG1 THR B  58      13.968 -11.157   -3.752  1.00 48.77      O
ATOM   1399  CG2 THR B  58      15.109 -11.859   -1.738  1.00 46.75      C
ATOM   1400  C   THR B  58      17.694 -11.404   -3.420  1.00 48.37      C
ATOM   1401  O   THR B  58      18.014 -12.246   -4.263  1.00 48.05      O
ATOM   1402  N   VAL B  59      18.443 -11.121   -2.353  1.00 48.84      N
ATOM   1403  CA  VAL B  59      19.708 -11.814   -2.089  1.00 50.27      C
ATOM   1404  CB  VAL B  59      20.942 -10.858   -2.229  1.00 49.98      C
ATOM   1405  CG1 VAL B  59      22.241 -11.607   -1.987  1.00 48.98      C
ATOM   1406  CG2 VAL B  59      20.971 -10.233   -3.605  1.00 49.50      C
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ATOM   1407  C   VAL B  59      19.732 -12.503  -0.708  1.00 51.31      C
ATOM   1408  O   VAL B  59      19.396 -11.889   0.306  1.00 51.41      O
ATOM   1409  N   ASN B  60      20.110 -13.784  -0.692  1.00 52.16      N
ATOM   1410  CA  ASN B  60      20.417 -14.503   0.550  1.00 52.82      C
ATOM   1411  CB  ASN B  60      19.494 -15.713   0.703  1.00 52.46      C
ATOM   1412  CG  ASN B  60      19.190 -16.052   2.165  1.00 53.85      C
ATOM   1413  OD1 ASN B  60      18.162 -16.662   2.452  1.00 55.75      O
ATOM   1414  ND2 ASN B  60      20.069 -15.657   3.083  1.00 51.06      N
ATOM   1415  C   ASN B  60      21.917 -14.916   0.621  1.00 53.15      C
ATOM   1416  O   ASN B  60      22.307 -16.018   0.189  1.00 53.51      O
ATOM   1417  N   LYS B  61      22.758 -14.024   1.159  1.00 53.07      N
ATOM   1418  CA  LYS B  61      24.188 -14.318   1.304  1.00 52.63      C
ATOM   1419  CB  LYS B  61      24.962 -13.086   1.789  1.00 52.57      C
ATOM   1420  CG  LYS B  61      25.168 -12.025   0.708  1.00 53.36      C
ATOM   1421  CD  LYS B  61      25.866 -10.798   1.240  1.00 53.65      C
ATOM   1422  CE  LYS B  61      26.365  -9.877   0.126  1.00 53.16      C
ATOM   1423  NZ  LYS B  61      27.560  -9.116   0.657  1.00 54.11      N
ATOM   1424  C   LYS B  61      24.443 -15.537   2.211  1.00 52.22      C
ATOM   1425  O   LYS B  61      25.476 -16.199   2.070  1.00 52.39      O
ATOM   1426  N   GLY B  62      23.489 -15.827   3.105  1.00 51.07      N
ATOM   1427  CA  GLY B  62      23.513 -17.025   3.955  1.00 50.34      C
ATOM   1428  C   GLY B  62      23.572 -18.280   3.105  1.00 49.30      C
ATOM   1429  O   GLY B  62      24.571 -19.021   3.116  1.00 49.51      O
ATOM   1430  N   SER B  63      22.498 -18.488   2.327  1.00 48.43      N
ATOM   1431  CA  SER B  63      22.370 -19.683   1.482  1.00 47.02      C
ATOM   1432  CB  SER B  63      20.884 -19.978   1.224  1.00 46.83      C
ATOM   1433  OG  SER B  63      20.078 -19.136   2.232  1.00 47.96      O
ATOM   1434  C   SER B  63      23.105 -19.552   0.135  1.00 45.91      C
ATOM   1435  O   SER B  63      23.128 -20.499  -0.652  1.00 45.61      O
ATOM   1436  N   LYS B  64      23.718 -18.402  -0.122  1.00 44.87      N
ATOM   1437  CA  LYS B  64      24.410 -18.152  -1.417  1.00 44.92      C
ATOM   1438  CB  LYS B  64      25.586 -19.115  -1.651  1.00 44.61      C
ATOM   1439  CG  LYS B  64      26.660 -19.099  -0.554  1.00 45.05      C
ATOM   1440  CD  LYS B  64      27.665 -20.213  -0.805  1.00 44.56      C
ATOM   1441  CE  LYS B  64      28.244 -20.755   0.486  1.00 42.89      C
ATOM   1442  NZ  LYS B  64      29.561 -20.185   0.780  1.00 41.38      N
ATOM   1443  C   LYS B  64      23.429 -18.180  -2.601  1.00 44.11      C
ATOM   1444  O   LYS B  64      23.754 -18.623  -3.704  1.00 44.27      O
ATOM   1445  N   SER B  65      22.219 -17.710  -2.358  1.00 43.78      N
ATOM   1446  CA  SER B  65      21.231 -17.677  -3.417  1.00 45.07      C
ATOM   1447  CB  SER B  65      20.157 -18.737  -3.220  1.00 45.06      C
ATOM   1448  OG  SER B  65      19.602 -18.635  -1.939  1.00 46.48      O
ATOM   1449  C   SER B  65      20.654 -16.282  -3.598  1.00 44.87      C
ATOM   1450  O   SER B  65      20.725 -15.444  -2.695  1.00 46.30      O
ATOM   1451  N   PHE B  66      20.165 -16.024  -4.795  1.00 43.98      N
ATOM   1452  CA  PHE B  66      19.662 -14.717  -5.174  1.00 43.45      C
ATOM   1453  CB  PHE B  66      20.794 -13.716  -5.484  1.00 43.22      C
ATOM   1454  CG  PHE B  66      21.805 -14.199  -6.486  1.00 42.41      C
ATOM   1455  CD1 PHE B  66      22.667 -15.256  -6.188  1.00 41.96      C
ATOM   1456  CE1 PHE B  66      23.629 -15.678  -7.083  1.00 40.78      C
ATOM   1457  CZ  PHE B  66      23.745 -15.037  -8.303  1.00 43.25      C
ATOM   1458  CE2 PHE B  66      22.909 -13.946  -8.609  1.00 42.43      C
ATOM   1459  CD2 PHE B  66      21.955 -13.537  -7.693  1.00 42.09      C
ATOM   1460  C   PHE B  66      18.748 -14.890  -6.362  1.00 43.59      C
ATOM   1461  O   PHE B  66      18.876 -15.857  -7.112  1.00 43.27      O
ATOM   1462  N   SER B  67      17.813 -13.966  -6.521  1.00 43.46      N
ATOM   1463  CA  SER B  67      16.872 -14.080  -7.599  1.00 43.95      C
ATOM   1464  CB  SER B  67      15.647 -14.891  -7.177  1.00 44.17      C
ATOM   1465  OG  SER B  67      14.969 -14.198  -6.173  1.00 47.70      O
ATOM   1466  C   SER B  67      16.442 -12.745  -8.140  1.00 43.18      C
ATOM   1467  O   SER B  67      16.571 -11.715  -7.497  1.00 42.89      O
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ATOM   1529  CA  VAL B  75       7.276  -9.328 -26.006  1.00 45.62      C
ATOM   1530  CB  VAL B  75       6.624  -9.140 -27.368  1.00 45.40      C
ATOM   1531  CG1 VAL B  75       5.223  -9.671 -27.324  1.00 46.53      C
ATOM   1532  CG2 VAL B  75       7.440  -9.851 -28.447  1.00 45.91      C
ATOM   1533  C   VAL B  75       8.765  -9.030 -26.108  1.00 44.93      C
ATOM   1534  O   VAL B  75       9.578  -9.937 -26.234  1.00 45.36      O
ATOM   1535  N   GLU B  76       9.105  -7.760 -25.986  1.00 44.44      N
ATOM   1536  CA  GLU B  76      10.458  -7.282 -26.127  1.00 44.58      C
ATOM   1537  CB  GLU B  76      10.449  -5.771 -26.372  1.00 45.85      C
ATOM   1538  CG  GLU B  76       9.328  -5.317 -27.417  1.00 51.77      C
ATOM   1539  CD  GLU B  76       7.931  -5.030 -26.766  1.00 59.07      C
ATOM   1540  OE1 GLU B  76       6.879  -5.154 -27.462  1.00 60.29      O
ATOM   1541  OE2 GLU B  76       7.898  -4.661 -25.557  1.00 62.06      O
ATOM   1542  C   GLU B  76      11.389  -7.671 -24.957  1.00 43.89      C
ATOM   1543  O   GLU B  76      12.627  -7.513 -25.082  1.00 42.88      O
ATOM   1544  N   ASP B  77      10.817  -8.202 -23.859  1.00 42.42      N
ATOM   1545  CA  ASP B  77      11.618  -8.761 -22.766  1.00 41.98      C
ATOM   1546  CB  ASP B  77      10.833  -8.835 -21.468  1.00 42.23      C
ATOM   1547  CG  ASP B  77      10.458  -7.483 -20.905  1.00 44.50      C
ATOM   1548  OD1 ASP B  77      11.179  -6.460 -21.084  1.00 48.11      O
ATOM   1549  OD2 ASP B  77       9.417  -7.454 -20.227  1.00 47.95      O
ATOM   1550  C   ASP B  77      12.117 -10.205 -23.101  1.00 42.26      C
ATOM   1551  O   ASP B  77      12.839 -10.816 -22.314  1.00 42.73      O
ATOM   1552  N   SER B  78      11.679 -10.742 -24.230  1.00 40.74      N
ATOM   1553  CA  SER B  78      12.145 -12.007 -24.758  1.00 40.45      C
ATOM   1554  CB  SER B  78      11.467 -12.307 -26.105  1.00 37.71      C
ATOM   1555  OG  SER B  78      10.070 -12.574 -25.878  1.00 37.58      O
ATOM   1556  C   SER B  78      13.660 -11.964 -24.910  1.00 40.32      C
ATOM   1557  O   SER B  78      14.208 -11.100 -25.589  1.00 40.12      O
ATOM   1558  N   GLY B  79      14.328 -12.910 -24.280  1.00 39.35      N
ATOM   1559  CA  GLY B  79      15.758 -13.031 -24.490  1.00 39.80      C
ATOM   1560  C   GLY B  79      16.392 -13.943 -23.466  1.00 38.99      C
ATOM   1561  O   GLY B  79      15.697 -14.690 -22.788  1.00 39.42      O
ATOM   1562  N   THR B  80      17.706 -13.880 -23.381  1.00 38.30      N
ATOM   1563  CA  THR B  80      18.493 -14.660 -22.436  1.00 39.61      C
ATOM   1564  CB  THR B  80      19.765 -15.195 -23.148  1.00 39.70      C
ATOM   1565  OG1 THR B  80      19.339 -16.052 -24.190  1.00 38.59      O
ATOM   1566  CG2 THR B  80      20.688 -15.994 -22.197  1.00 37.90      C
ATOM   1567  C   THR B  80      18.929 -13.821 -21.246  1.00 40.30      C
ATOM   1568  O   THR B  80      19.531 -12.776 -21.414  1.00 39.92      O
ATOM   1569  N   TYR B  81      18.642 -14.329 -20.060  1.00 41.21      N
ATOM   1570  CA  TYR B  81      18.921 -13.698 -18.817  1.00 41.29      C
ATOM   1571  CB  TYR B  81      17.654 -13.633 -17.949  1.00 41.37      C
ATOM   1572  CG  TYR B  81      16.647 -12.664 -18.510  1.00 41.48      C
ATOM   1573  CD1 TYR B  81      16.562 -11.381 -18.023  1.00 40.06      C
ATOM   1574  CE1 TYR B  81      15.644 -10.454 -18.583  1.00 44.06      C
ATOM   1575  CZ  TYR B  81      14.846 -10.857 -19.675  1.00 43.01      C
ATOM   1576  OH  TYR B  81      13.959  -9.992 -20.249  1.00 42.85      O
ATOM   1577  CE2 TYR B  81      14.913 -12.137 -20.160  1.00 37.03      C
ATOM   1578  CD2 TYR B  81      15.798 -13.043 -19.604  1.00 38.04      C
ATOM   1579  C   TYR B  81      19.940 -14.563 -18.132  1.00 43.06      C
ATOM   1580  O   TYR B  81      19.798 -15.785 -18.103  1.00 43.90      O
ATOM   1581  N   LYS B  82      20.990 -13.924 -17.631  1.00 43.98      N
ATOM   1582  CA  LYS B  82      22.054 -14.585 -16.866  1.00 45.48      C
ATOM   1583  CB  LYS B  82      23.331 -14.667 -17.693  1.00 46.06      C
ATOM   1584  CG  LYS B  82      23.440 -16.011 -18.369  1.00 48.70      C
ATOM   1585  CD  LYS B  82      24.530 -16.006 -19.412  1.00 54.28      C
ATOM   1586  CE  LYS B  82      24.476 -17.315 -20.209  1.00 53.81      C
ATOM   1587  NZ  LYS B  82      25.735 -17.388 -20.957  1.00 57.58      N
ATOM   1588  C   LYS B  82      22.308 -13.867 -15.552  1.00 44.33      C
ATOM   1589  O   LYS B  82      22.201 -12.664 -15.484  1.00 44.79      O
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ATOM	1468	N	LEU	B	68	15.918	-12.787	-9.347	1.00	42.60	N
ATOM	1469	CA	LEU	B	68	15.432	-11.612	-10.012	1.00	42.76	C
ATOM	1470	CB	LEU	B	68	16.174	-11.461	-11.336	1.00	41.93	C
ATOM	1471	CG	LEU	B	68	16.515	-10.118	-11.984	1.00	45.17	C
ATOM	1472	CD1	LEU	B	68	16.440	-10.205	-13.537	1.00	43.08	C
ATOM	1473	CD2	LEU	B	68	15.823	-8.866	-11.437	1.00	43.46	C
ATOM	1474	C	LEU	B	68	13.988	-11.907	-10.355	1.00	42.62	C
ATOM	1475	O	LEU	B	68	13.711	-12.896	-11.018	1.00	42.63	O
ATOM	1476	N	ARG	B	69	13.075	-11.045	-9.973	1.00	42.71	N
ATOM	1477	CA	ARG	B	69	11.746	-11.161	-10.528	1.00	44.20	C
ATOM	1478	CB	ARG	B	69	10.715	-11.157	-9.418	1.00	43.82	C
ATOM	1479	CG	ARG	B	69	9.300	-11.193	-9.930	1.00	44.98	C
ATOM	1480	CD	ARG	B	69	8.390	-11.421	-8.752	1.00	50.13	C
ATOM	1481	NE	ARG	B	69	7.015	-11.124	-9.113	1.00	58.36	N
ATOM	1482	CZ	ARG	B	69	6.457	-9.914	-9.010	1.00	61.11	C
ATOM	1483	NH1	ARG	B	69	7.188	-8.871	-8.565	1.00	61.04	N
ATOM	1484	NH2	ARG	B	69	5.170	-9.750	-9.367	1.00	59.12	N
ATOM	1485	C	ARG	B	69	11.485	-10.025	-11.500	1.00	43.87	C
ATOM	1486	O	ARG	B	69	11.692	-8.876	-11.157	1.00	45.00	O
ATOM	1487	N	ILE	B	70	11.026	-10.355	-12.699	1.00	43.46	N
ATOM	1488	CA	ILE	B	70	10.727	-9.370	-13.697	1.00	43.63	C
ATOM	1489	CB	ILE	B	70	11.407	-9.689	-15.035	1.00	45.10	C
ATOM	1490	CG1	ILE	B	70	12.912	-9.941	-14.806	1.00	43.18	C
ATOM	1491	CD1	ILE	B	70	13.478	-10.890	-15.730	1.00	45.17	C
ATOM	1492	CG2	ILE	B	70	11.137	-8.524	-16.012	1.00	44.11	C
ATOM	1493	C	ILE	B	70	9.209	-9.326	-13.860	1.00	43.63	C
ATOM	1494	O	ILE	B	70	8.592	-10.314	-14.166	1.00	43.43	O
ATOM	1495	N	SER	B	71	8.610	-8.175	-13.579	1.00	44.13	N
ATOM	1496	CA	SER	B	71	7.177	-8.025	-13.678	1.00	44.47	C
ATOM	1497	CB	SER	B	71	6.659	-7.217	-12.519	1.00	43.71	C
ATOM	1498	OG	SER	B	71	6.974	-7.938	-11.370	1.00	45.34	O
ATOM	1499	C	SER	B	71	6.729	-7.397	-14.962	1.00	44.92	C
ATOM	1500	O	SER	B	71	7.546	-6.909	-15.731	1.00	43.62	O
ATOM	1501	N	ASP	B	72	5.398	-7.295	-15.068	1.00	46.93	N
ATOM	1502	CA	ASP	B	72	4.640	-7.266	-16.317	1.00	47.72	C
ATOM	1503	CB	ASP	B	72	3.574	-6.195	-16.338	1.00	49.50	C
ATOM	1504	CG	ASP	B	72	4.135	-4.834	-16.302	1.00	54.38	C
ATOM	1505	OD1	ASP	B	72	4.521	-4.403	-15.190	1.00	60.99	O
ATOM	1506	OD2	ASP	B	72	4.146	-4.186	-17.381	1.00	60.20	O
ATOM	1507	C	ASP	B	72	5.411	-7.335	-17.615	1.00	46.39	C
ATOM	1508	O	ASP	B	72	5.706	-6.316	-18.250	1.00	46.34	O
ATOM	1509	N	LEU	B	73	5.653	-8.569	-18.014	1.00	45.38	N
ATOM	1510	CA	LEU	B	73	6.476	-8.921	-19.147	1.00	44.12	C
ATOM	1511	CB	LEU	B	73	6.686	-10.447	-19.152	1.00	43.05	C
ATOM	1512	CG	LEU	B	73	7.513	-11.022	-17.984	1.00	42.55	C
ATOM	1513	CD1	LEU	B	73	7.264	-12.505	-17.805	1.00	37.65	C
ATOM	1514	CD2	LEU	B	73	9.037	-10.729	-18.116	1.00	40.53	C
ATOM	1515	C	LEU	B	73	5.861	-8.430	-20.443	1.00	44.58	C
ATOM	1516	O	LEU	B	73	4.637	-8.415	-20.594	1.00	44.57	O
ATOM	1517	N	ARG	B	74	6.712	-8.006	-21.370	1.00	44.91	N
ATOM	1518	CA	ARG	B	74	6.279	-7.680	-22.737	1.00	45.45	C
ATOM	1519	CB	ARG	B	74	6.565	-6.224	-23.047	1.00	45.64	C
ATOM	1520	CG	ARG	B	74	6.164	-5.286	-22.019	1.00	49.91	C
ATOM	1521	CD	ARG	B	74	7.106	-4.109	-22.126	1.00	57.66	C
ATOM	1522	NE	ARG	B	74	7.462	-3.603	-20.811	1.00	60.89	N
ATOM	1523	CZ	ARG	B	74	6.724	-2.746	-20.101	1.00	64.00	C
ATOM	1524	NH1	ARG	B	74	5.571	-2.278	-20.587	1.00	65.92	N
ATOM	1525	NH2	ARG	B	74	7.155	-2.334	-18.909	1.00	64.22	N
ATOM	1526	C	ARG	B	74	7.067	-8.497	-23.727	1.00	44.79	C
ATOM	1527	O	ARG	B	74	8.042	-9.136	-23.365	1.00	45.02	O
ATOM	1528	N	VAL	B	75	6.666	-8.466	-24.983	1.00	45.42	N

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ATOM   1590  N   CYS B  83      22.566 -14.626 -14.507  1.00 43.87      N
ATOM   1591  CA  CYS B  83      22.995 -14.054 -13.266  1.00 44.81      C
ATOM   1592  CB  CYS B  83      22.327 -14.739 -12.098  1.00 44.27      C
ATOM   1593  SG  CYS B  83      22.696 -16.465 -11.941  1.00 45.41      S
ATOM   1594  C   CYS B  83      24.497 -14.258 -13.210  1.00 46.24      C
ATOM   1595  O   CYS B  83      25.008 -15.105 -13.936  1.00 46.71      O
ATOM   1596  N   GLN B  84      25.197 -13.440 -12.415  1.00 46.76      N
ATOM   1597  CA  GLN B  84      26.617 -13.650 -12.077  1.00 46.51      C
ATOM   1598  CB  GLN B  84      27.526 -12.679 -12.810  1.00 47.55      C
ATOM   1599  CG  GLN B  84      29.032 -12.902 -12.495  1.00 50.71      C
ATOM   1600  CD  GLN B  84      29.953 -12.348 -13.563  1.00 54.90      C
ATOM   1601  OE1 GLN B  84      30.999 -12.943 -13.851  1.00 61.33      O
ATOM   1602  NE2 GLN B  84      29.584 -11.212 -14.160  1.00 54.98      N
ATOM   1603  C   GLN B  84      26.829 -13.518 -10.569  1.00 45.81      C
ATOM   1604  O   GLN B  84      26.324 -12.604  -9.944  1.00 44.81      O
ATOM   1605  N   ALA B  85      27.532 -14.488  -9.993  1.00 44.59      N
ATOM   1606  CA  ALA B  85      27.840 -14.484  -8.590  1.00 43.83      C
ATOM   1607  CB  ALA B  85      27.646 -15.884  -8.031  1.00 43.38      C
ATOM   1608  C   ALA B  85      29.316 -14.014  -8.479  1.00 43.84      C
ATOM   1609  O   ALA B  85      30.172 -14.539  -9.175  1.00 45.10      O
ATOM   1610  N   PHE B  86      29.603 -12.990  -7.689  1.00 43.41      N
ATOM   1611  CA  PHE B  86      30.985 -12.634  -7.399  1.00 43.48      C
ATOM   1612  CB  PHE B  86      31.195 -11.139  -7.499  1.00 43.25      C
ATOM   1613  CG  PHE B  86      30.922 -10.598  -8.863  1.00 45.60      C
ATOM   1614  CD1 PHE B  86      29.695  -9.993  -9.153  1.00 46.99      C
ATOM   1615  CE1 PHE B  86      29.434  -9.498 -10.461  1.00 49.94      C
ATOM   1616  CZ  PHE B  86      30.427  -9.610 -11.452  1.00 47.51      C
ATOM   1617  CE2 PHE B  86      31.649 -10.207 -11.143  1.00 46.33      C
ATOM   1618  CD2 PHE B  86      31.874 -10.723  -9.877  1.00 43.78      C
ATOM   1619  C   PHE B  86      31.291 -13.124  -6.015  1.00 44.35      C
ATOM   1620  O   PHE B  86      30.508 -12.925  -5.066  1.00 44.86      O
ATOM   1621  N   TYR B  87      32.427 -13.779  -5.866  1.00 43.59      N
ATOM   1622  CA  TYR B  87      32.679 -14.421  -4.604  1.00 43.44      C
ATOM   1623  CB  TYR B  87      32.251 -15.913  -4.633  1.00 43.50      C
ATOM   1624  CG  TYR B  87      32.810 -16.691  -5.817  1.00 44.45      C
ATOM   1625  CD1 TYR B  87      34.022 -17.351  -5.704  1.00 46.50      C
ATOM   1626  CE1 TYR B  87      34.574 -18.044  -6.759  1.00 45.78      C
ATOM   1627  CZ  TYR B  87      33.918 -18.111  -7.953  1.00 46.91      C
ATOM   1628  OH  TYR B  87      34.547 -18.831  -8.957  1.00 48.61      O
ATOM   1629  CE2 TYR B  87      32.684 -17.477  -8.120  1.00 45.59      C
ATOM   1630  CD2 TYR B  87      32.130 -16.777  -7.031  1.00 43.90      C
ATOM   1631  C   TYR B  87      34.139 -14.221  -4.248  1.00 42.55      C
ATOM   1632  O   TYR B  87      34.935 -13.761  -5.046  1.00 42.89      O
ATOM   1633  N   VAL B  88      34.468 -14.599  -3.037  1.00 41.90      N
ATOM   1634  CA  VAL B  88      35.747 -14.320  -2.484  1.00 40.38      C
ATOM   1635  CB  VAL B  88      35.563 -13.113  -1.524  1.00 41.09      C
ATOM   1636  CG1 VAL B  88      36.089 -13.331  -0.157  1.00 39.39      C
ATOM   1637  CG2 VAL B  88      36.117 -11.869  -2.206  1.00 41.64      C
ATOM   1638  C   VAL B  88      36.321 -15.611  -1.910  1.00 39.32      C
ATOM   1639  O   VAL B  88      35.617 -16.392  -1.274  1.00 39.48      O
ATOM   1640  N   PHE B  89      37.584 -15.880  -2.214  1.00 38.33      N
ATOM   1641  CA  PHE B  89      38.325 -16.946  -1.527  1.00 36.70      C
ATOM   1642  CB  PHE B  89      38.362 -18.233  -2.346  1.00 35.81      C
ATOM   1643  CG  PHE B  89      38.830 -18.069  -3.773  1.00 33.80      C
ATOM   1644  CD1 PHE B  89      40.156 -18.343  -4.112  1.00 33.47      C
ATOM   1645  CE1 PHE B  89      40.606 -18.225  -5.403  1.00 30.77      C
ATOM   1646  CZ  PHE B  89      39.726 -17.835  -6.426  1.00 31.68      C
ATOM   1647  CE2 PHE B  89      38.387 -17.583  -6.134  1.00 33.87      C
ATOM   1648  CD2 PHE B  89      37.946 -17.711  -4.782  1.00 36.04      C
ATOM   1649  C   PHE B  89      39.704 -16.451  -1.269  1.00 37.19      C
ATOM   1650  O   PHE B  89      40.059 -15.356  -1.701  1.00 36.81      O
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ATOM	1651	N	PHE	B	90	40.484	-17.258	-0.565	1.00	38.03	N
ATOM	1652	CA	PHE	B	90	41.842	-16.928	-0.180	1.00	38.04	C
ATOM	1653	CB	PHE	B	90	42.075	-17.297	1.280	1.00	39.75	C
ATOM	1654	CG	PHE	B	90	41.328	-16.416	2.209	1.00	43.37	C
ATOM	1655	CD1	PHE	B	90	39.930	-16.435	2.223	1.00	47.99	C
ATOM	1656	CE1	PHE	B	90	39.208	-15.584	3.055	1.00	50.22	C
ATOM	1657	CZ	PHE	B	90	39.893	-14.691	3.875	1.00	46.73	C
ATOM	1658	CE2	PHE	B	90	41.285	-14.653	3.848	1.00	49.56	C
ATOM	1659	CD2	PHE	B	90	41.992	-15.504	2.998	1.00	47.02	C
ATOM	1660	C	PHE	B	90	42.831	-17.568	-1.103	1.00	37.73	C
ATOM	1661	O	PHE	B	90	42.675	-18.723	-1.455	1.00	35.86	O
ATOM	1662	N	ALA	B	91	43.808	-16.766	-1.541	1.00	38.81	N
ATOM	1663	CA	ALA	B	91	44.880	-17.186	-2.450	1.00	41.01	C
ATOM	1664	CB	ALA	B	91	45.887	-16.050	-2.613	1.00	41.04	C
ATOM	1665	C	ALA	B	91	45.610	-18.459	-1.997	1.00	42.55	C
ATOM	1666	O	ALA	B	91	46.126	-19.208	-2.826	1.00	41.40	O
ATOM	1667	N	GLU	B	92	45.643	-18.675	-0.677	1.00	45.64	N
ATOM	1668	CA	GLU	B	92	46.278	-19.854	-0.067	1.00	49.34	C
ATOM	1669	CB	GLU	B	92	46.339	-19.765	1.468	1.00	49.34	C
ATOM	1670	CG	GLU	B	92	47.103	-18.578	2.047	1.00	53.21	C
ATOM	1671	CD	GLU	B	92	46.215	-17.331	2.266	1.00	57.21	C
ATOM	1672	OE1	GLU	B	92	45.848	-17.086	3.448	1.00	59.01	O
ATOM	1673	OE2	GLU	B	92	45.901	-16.599	1.280	1.00	55.91	O
ATOM	1674	C	GLU	B	92	45.529	-21.121	-0.433	1.00	50.92	C
ATOM	1675	O	GLU	B	92	46.163	-22.112	-0.803	1.00	51.36	O
ATOM	1676	N	ASP	B	93	44.198	-21.098	-0.315	1.00	52.93	N
ATOM	1677	CA	ASP	B	93	43.454	-22.356	-0.337	1.00	55.69	C
ATOM	1678	CB	ASP	B	93	41.992	-22.280	0.238	1.00	55.85	C
ATOM	1679	CG	ASP	B	93	40.982	-21.501	-0.651	1.00	58.02	C
ATOM	1680	OD1	ASP	B	93	40.972	-21.667	-1.896	1.00	60.03	O
ATOM	1681	OD2	ASP	B	93	40.134	-20.749	-0.080	1.00	58.21	O
ATOM	1682	C	ASP	B	93	43.647	-23.117	-1.659	1.00	57.09	C
ATOM	1683	O	ASP	B	93	43.222	-22.670	-2.731	1.00	56.60	O
ATOM	1684	N	VAL	B	94	44.381	-24.231	-1.542	1.00	59.08	N
ATOM	1685	CA	VAL	B	94	44.863	-25.029	-2.673	1.00	61.07	C
ATOM	1686	CB	VAL	B	94	46.088	-25.913	-2.271	1.00	61.32	C
ATOM	1687	CG1	VAL	B	94	46.489	-26.881	-3.404	1.00	61.77	C
ATOM	1688	CG2	VAL	B	94	47.300	-25.062	-1.795	1.00	61.40	C
ATOM	1689	C	VAL	B	94	43.755	-25.952	-3.125	1.00	62.29	C
ATOM	1690	O	VAL	B	94	42.925	-26.361	-2.312	1.00	62.77	O
ATOM	1691	N	GLY	B	95	43.738	-26.286	-4.410	1.00	63.72	N
ATOM	1692	CA	GLY	B	95	42.849	-27.341	-4.889	1.00	65.63	C
ATOM	1693	C	GLY	B	95	41.366	-26.996	-4.820	1.00	66.94	C
ATOM	1694	O	GLY	B	95	40.503	-27.897	-4.790	1.00	67.35	O
ATOM	1695	N	SER	B	96	41.082	-25.693	-4.764	1.00	67.66	N
ATOM	1696	CA	SER	B	96	39.752	-25.126	-5.019	1.00	68.33	C
ATOM	1697	CB	SER	B	96	38.719	-25.490	-3.934	1.00	68.30	C
ATOM	1698	OG	SER	B	96	39.096	-25.003	-2.655	1.00	69.15	O
ATOM	1699	C	SER	B	96	39.951	-23.610	-5.149	1.00	68.57	C
ATOM	1700	O	SER	B	96	40.232	-22.909	-4.161	1.00	68.47	O
ATOM	1701	N	ASN	B	97	39.872	-23.144	-6.399	1.00	68.54	N
ATOM	1702	CA	ASN	B	97	40.063	-21.737	-6.798	1.00	67.90	C
ATOM	1703	CB	ASN	B	97	41.539	-21.450	-7.190	1.00	67.64	C
ATOM	1704	CG	ASN	B	97	42.549	-21.839	-6.102	1.00	67.80	C
ATOM	1705	OD1	ASN	B	97	43.346	-21.010	-5.642	1.00	68.17	O
ATOM	1706	ND2	ASN	B	97	42.535	-23.103	-5.706	1.00	67.46	N
ATOM	1707	C	ASN	B	97	39.164	-21.548	-8.020	1.00	67.37	C
ATOM	1708	O	ASN	B	97	39.474	-20.763	-8.918	1.00	67.83	O
ATOM	1709	N	LYS	B	98	38.028	-22.246	-8.012	1.00	66.43	N
ATOM	1710	CA	LYS	B	98	37.501	-22.902	-9.221	1.00	65.41	C
ATOM	1711	CB	LYS	B	98	36.489	-24.003	-8.837	1.00	65.75	C

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ATOM   1712  CG  LYS B  98      37.167 -25.283  -8.285  1.00 67.70      C
ATOM   1713  CD  LYS B  98      36.292 -26.019  -7.266  1.00 70.57      C
ATOM   1714  CE  LYS B  98      36.108 -25.188  -5.992  1.00 71.50      C
ATOM   1715  NZ  LYS B  98      35.816 -26.004  -4.778  1.00 71.51      N
ATOM   1716  C   LYS B  98      37.036 -22.104 -10.467  1.00 64.00      C
ATOM   1717  O   LYS B  98      37.100 -22.642 -11.587  1.00 64.50      O
ATOM   1718  N   GLY B  99      36.583 -20.861 -10.313  1.00 61.92      N
ATOM   1719  CA  GLY B  99      35.934 -20.173 -11.453  1.00 58.65      C
ATOM   1720  C   GLY B  99      36.850 -19.277 -12.268  1.00 56.59      C
ATOM   1721  O   GLY B  99      38.048 -19.538 -12.374  1.00 56.84      O
ATOM   1722  N   ALA B 100      36.282 -18.223 -12.849  1.00 53.87      N
ATOM   1723  CA  ALA B 100      37.065 -17.133 -13.429  1.00 51.62      C
ATOM   1724  CB  ALA B 100      36.164 -16.245 -14.269  1.00 51.17      C
ATOM   1725  C   ALA B 100      37.690 -16.294 -12.312  1.00 49.55      C
ATOM   1726  O   ALA B 100      36.987 -15.896 -11.373  1.00 49.34      O
ATOM   1727  N   ILE B 101      38.985 -16.005 -12.395  1.00 47.31      N
ATOM   1728  CA  ILE B 101      39.533 -14.981 -11.484  1.00 45.25      C
ATOM   1729  CB  ILE B 101      40.904 -15.345 -10.756  1.00 45.80      C
ATOM   1730  CG1 ILE B 101      42.016 -14.358 -11.079  1.00 46.05      C
ATOM   1731  CD1 ILE B 101      42.324 -13.495  -9.928  1.00 46.13      C
ATOM   1732  CG2 ILE B 101      41.319 -16.849 -10.843  1.00 44.18      C
ATOM   1733  C   ILE B 101      39.355 -13.542 -12.031  1.00 44.02      C
ATOM   1734  O   ILE B 101      39.651 -13.227 -13.209  1.00 43.07      O
ATOM   1735  N   ILE B 102      38.734 -12.724 -11.185  1.00 41.55      N
ATOM   1736  CA  ILE B 102      38.307 -11.368 -11.482  1.00 40.42      C
ATOM   1737  CB  ILE B 102      36.935 -11.028 -10.777  1.00 41.20      C
ATOM   1738  CG1 ILE B 102      35.748 -11.863 -11.308  1.00 43.88      C
ATOM   1739  CD1 ILE B 102      35.773 -12.274 -12.825  1.00 43.26      C
ATOM   1740  CG2 ILE B 102      36.582  -9.531 -10.871  1.00 44.23      C
ATOM   1741  C   ILE B 102      39.378 -10.376 -10.971  1.00 39.32      C
ATOM   1742  O   ILE B 102      39.623  -9.342 -11.614  1.00 39.71      O
ATOM   1743  N   GLY B 103      40.002 -10.670  -9.810  1.00 36.32      N
ATOM   1744  CA  GLY B 103      41.079  -9.842  -9.312  1.00 32.38      C
ATOM   1745  C   GLY B 103      41.673 -10.369  -8.038  1.00 31.16      C
ATOM   1746  O   GLY B 103      41.199 -11.372  -7.457  1.00 31.39      O
ATOM   1747  N   LEU B 104      42.706  -9.670  -7.578  1.00 29.03      N
ATOM   1748  CA  LEU B 104      43.424 -10.049  -6.423  1.00 27.58      C
ATOM   1749  CB  LEU B 104      44.839 -10.544  -6.818  1.00 26.53      C
ATOM   1750  CG  LEU B 104      45.829 -10.943  -5.733  1.00 26.78      C
ATOM   1751  CD1 LEU B 104      47.232 -11.015  -6.252  1.00 30.47      C
ATOM   1752  CD2 LEU B 104      45.473 -12.251  -5.078  1.00 27.53      C
ATOM   1753  C   LEU B 104      43.459  -8.841  -5.496  1.00 28.83      C
ATOM   1754  O   LEU B 104      43.870  -7.752  -5.901  1.00 27.59      O
ATOM   1755  N   MET B 105      43.067  -9.055  -4.233  1.00 29.96      N
ATOM   1756  CA  MET B 105      43.136  -8.031  -3.177  1.00 31.39      C
ATOM   1757  CB  MET B 105      41.918  -8.182  -2.270  1.00 33.00      C
ATOM   1758  CG  MET B 105      41.063  -6.942  -2.145  1.00 38.80      C
ATOM   1759  SD  MET B 105      40.356  -6.594  -3.753  1.00 41.80      S
ATOM   1760  CE  MET B 105      39.143  -7.874  -3.693  1.00 49.56      C
ATOM   1761  C   MET B 105      44.336  -8.189  -2.319  1.00 31.71      C
ATOM   1762  O   MET B 105      44.667  -9.305  -1.911  1.00 31.15      O
ATOM   1763  N   VAL B 106      44.991  -7.075  -2.006  1.00 31.47      N
ATOM   1764  CA  VAL B 106      45.960  -7.056  -0.929  1.00 33.12      C
ATOM   1765  CB  VAL B 106      46.528  -5.649  -0.736  1.00 32.05      C
ATOM   1766  CG1 VAL B 106      47.526  -5.649   0.323  1.00 32.12      C
ATOM   1767  CG2 VAL B 106      47.164  -5.186  -2.013  1.00 31.80      C
ATOM   1768  C   VAL B 106      45.287  -7.601   0.368  1.00 34.62      C
ATOM   1769  O   VAL B 106      44.032  -7.384   0.577  1.00 34.28      O
ATOM   1770  N   GLY B 107      46.126  -8.309   1.212  1.00 34.95      N
ATOM   1771  CA  GLY B 107      45.566  -9.209   2.267  1.00 34.64      C
ATOM   1772  C   GLY B 107      45.048 -10.613   1.825  1.00 35.04      C
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ATOM   1773  O   GLY B 107      44.566 -11.404   2.676  1.00 36.55      O
ATOM   1774  N   GLY B 108      45.122 -10.929   0.525  1.00 32.55      N
ATOM   1775  CA  GLY B 108      45.225 -12.307   0.075  1.00 30.81      C
ATOM   1776  C   GLY B 108      43.925 -12.886  -0.359  1.00 30.73      C
ATOM   1777  O   GLY B 108      43.812 -14.091  -0.489  1.00 31.42      O
ATOM   1778  N   VAL B 109      42.963 -12.006  -0.622  1.00 30.06      N
ATOM   1779  CA  VAL B 109      41.610 -12.332  -1.113  1.00 29.98      C
ATOM   1780  CB  VAL B 109      40.595 -11.330  -0.447  1.00 29.82      C
ATOM   1781  CG1 VAL B 109      39.238 -11.415  -0.954  1.00 27.30      C
ATOM   1782  CG2 VAL B 109      40.579 -11.519   1.073  1.00 31.58      C
ATOM   1783  C   VAL B 109      41.576 -12.271  -2.652  1.00 30.22      C
ATOM   1784  O   VAL B 109      41.988 -11.285  -3.280  1.00 29.55      O
ATOM   1785  N   VAL B 110      41.103 -13.354  -3.257  1.00 31.00      N
ATOM   1786  CA  VAL B 110      40.832 -13.376  -4.656  1.00 30.34      C
ATOM   1787  CB  VAL B 110      41.760 -14.318  -5.501  1.00 30.78      C
ATOM   1788  CG1 VAL B 110      41.079 -14.939  -6.663  1.00 27.57      C
ATOM   1789  CG2 VAL B 110      42.605 -15.240  -4.676  1.00 28.92      C
ATOM   1790  C   VAL B 110      39.376 -13.342  -4.934  1.00 32.42      C
ATOM   1791  O   VAL B 110      38.617 -13.904  -4.193  1.00 32.63      O
ATOM   1792  N   ILE B 111      38.986 -12.596  -5.962  1.00 34.25      N
ATOM   1793  CA  ILE B 111      37.608 -12.418  -6.360  1.00 36.25      C
ATOM   1794  CB  ILE B 111      37.377 -10.966  -6.834  1.00 37.63      C
ATOM   1795  CG1 ILE B 111      38.177  -9.980  -5.960  1.00 39.86      C
ATOM   1796  CD1 ILE B 111      37.582  -9.749  -4.568  1.00 44.15      C
ATOM   1797  CG2 ILE B 111      35.871 -10.598  -6.970  1.00 35.86      C
ATOM   1798  C   ILE B 111      37.401 -13.299  -7.581  1.00 37.45      C
ATOM   1799  O   ILE B 111      38.116 -13.150  -8.569  1.00 38.10      O
ATOM   1800  N   GLY B 112      36.478 -14.244  -7.487  1.00 37.85      N
ATOM   1801  CA  GLY B 112      36.044 -15.026  -8.625  1.00 39.55      C
ATOM   1802  C   GLY B 112      34.660 -14.536  -9.031  1.00 40.92      C
ATOM   1803  O   GLY B 112      33.991 -13.833  -8.279  1.00 40.69      O
ATOM   1804  N   GLY B 113      34.240 -14.877 -10.241  1.00 41.72      N
ATOM   1805  CA  GLY B 113      32.878 -14.675 -10.631  1.00 42.68      C
ATOM   1806  C   GLY B 113      32.526 -15.932 -11.369  1.00 44.53      C
ATOM   1807  O   GLY B 113      33.385 -16.523 -12.033  1.00 45.28      O
ATOM   1808  N   GLU B 114      31.281 -16.352 -11.230  1.00 45.00      N
ATOM   1809  CA  GLU B 114      30.721 -17.475 -11.954  1.00 46.79      C
ATOM   1810  CB  GLU B 114      30.486 -18.650 -11.003  1.00 47.57      C
ATOM   1811  CG  GLU B 114      31.481 -19.777 -11.016  1.00 54.05      C
ATOM   1812  CD  GLU B 114      31.681 -20.428 -12.384  1.00 60.74      C
ATOM   1813  OE1 GLU B 114      32.730 -21.116 -12.540  1.00 65.24      O
ATOM   1814  OE2 GLU B 114      30.834 -20.241 -13.294  1.00 62.06      O
ATOM   1815  C   GLU B 114      29.349 -16.990 -12.451  1.00 46.24      C
ATOM   1816  O   GLU B 114      28.600 -16.427 -11.683  1.00 45.45      O
ATOM   1817  N   LYS B 115      29.048 -17.210 -13.730  1.00 47.57      N
ATOM   1818  CA  LYS B 115      27.705 -16.986 -14.306  1.00 47.63      C
ATOM   1819  CB  LYS B 115      27.868 -16.442 -15.716  1.00 49.05      C
ATOM   1820  CG  LYS B 115      28.285 -14.990 -15.769  1.00 49.49      C
ATOM   1821  CD  LYS B 115      28.457 -14.608 -17.209  1.00 58.06      C
ATOM   1822  CE  LYS B 115      28.325 -13.100 -17.425  1.00 62.98      C
ATOM   1823  NZ  LYS B 115      29.569 -12.371 -16.971  1.00 67.39      N
ATOM   1824  C   LYS B 115      26.831 -18.235 -14.341  1.00 46.96      C
ATOM   1825  O   LYS B 115      27.328 -19.359 -14.475  1.00 46.33      O
ATOM   1826  N   GLY B 116      25.522 -18.055 -14.202  1.00 46.82      N
ATOM   1827  CA  GLY B 116      24.551 -19.156 -14.429  1.00 45.94      C
ATOM   1828  C   GLY B 116      24.477 -19.549 -15.896  1.00 46.06      C
ATOM   1829  O   GLY B 116      24.948 -18.798 -16.764  1.00 46.74      O
ATOM   1830  N   ALA B 117      23.929 -20.732 -16.203  1.00 44.78      N
ATOM   1831  CA  ALA B 117      23.856 -21.181 -17.602  1.00 43.54      C
ATOM   1832  CB  ALA B 117      23.609 -22.733 -17.710  1.00 42.15      C
ATOM   1833  C   ALA B 117      22.804 -20.377 -18.395  1.00 43.36      C
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ATOM   1834  O   ALA B 117      22.765 -20.473 -19.619  1.00 44.57      O
ATOM   1835  N   GLY B 118      22.009 -19.543 -17.711  1.00 42.01      N
ATOM   1836  CA  GLY B 118      21.041 -18.672 -18.374  1.00 40.50      C
ATOM   1837  C   GLY B 118      19.638 -19.226 -18.447  1.00 40.45      C
ATOM   1838  O   GLY B 118      19.440 -20.454 -18.385  1.00 39.63      O
ATOM   1839  N   THR B 119      18.689 -18.293 -18.609  1.00 39.73      N
ATOM   1840  CA  THR B 119      17.267 -18.517 -18.728  1.00 39.06      C
ATOM   1841  CB  THR B 119      16.494 -17.767 -17.648  1.00 39.37      C
ATOM   1842  OG1 THR B 119      16.867 -18.298 -16.359  1.00 42.58      O
ATOM   1843  CG2 THR B 119      14.985 -17.926 -17.817  1.00 36.37      C
ATOM   1844  C   THR B 119      16.846 -18.000 -20.086  1.00 40.30      C
ATOM   1845  O   THR B 119      17.046 -16.827 -20.386  1.00 40.23      O
ATOM   1846  N   ALA B 120      16.306 -18.881 -20.930  1.00 40.46      N
ATOM   1847  CA  ALA B 120      15.808 -18.450 -22.232  1.00 39.96      C
ATOM   1848  CB  ALA B 120      16.032 -19.546 -23.327  1.00 38.10      C
ATOM   1849  C   ALA B 120      14.333 -18.107 -22.056  1.00 39.39      C
ATOM   1850  O   ALA B 120      13.514 -18.995 -21.874  1.00 39.29      O
ATOM   1851  N   LEU B 121      14.018 -16.811 -22.058  1.00 38.26      N
ATOM   1852  CA  LEU B 121      12.655 -16.366 -21.893  1.00 38.37      C
ATOM   1853  CB  LEU B 121      12.552 -15.321 -20.816  1.00 37.24      C
ATOM   1854  CG  LEU B 121      11.223 -14.563 -20.800  1.00 39.25      C
ATOM   1855  CD1 LEU B 121      10.056 -15.389 -20.199  1.00 38.60      C
ATOM   1856  CD2 LEU B 121      11.327 -13.202 -20.149  1.00 34.33      C
ATOM   1857  C   LEU B 121      11.955 -15.883 -23.237  1.00 39.04      C
ATOM   1858  O   LEU B 121      12.473 -15.020 -23.955  1.00 40.91      O
ATOM   1859  N   THR B 122      10.811 -16.491 -23.548  1.00 38.34      N
ATOM   1860  CA  THR B 122       9.930 -16.055 -24.614  1.00 39.43      C
ATOM   1861  CB  THR B 122       9.552 -17.214 -25.559  1.00 39.02      C
ATOM   1862  OG1 THR B 122      10.738 -17.917 -25.949  1.00 39.58      O
ATOM   1863  CG2 THR B 122       8.846 -16.654 -26.785  1.00 40.51      C
ATOM   1864  C   THR B 122       8.660 -15.512 -23.988  1.00 38.05      C
ATOM   1865  O   THR B 122       8.034 -16.192 -23.186  1.00 38.30      O
ATOM   1866  N   VAL B 123       8.343 -14.258 -24.283  1.00 38.09      N
ATOM   1867  CA  VAL B 123       7.093 -13.650 -23.812  1.00 38.38      C
ATOM   1868  CB  VAL B 123       7.274 -12.260 -23.225  1.00 37.30      C
ATOM   1869  CG1 VAL B 123       5.940 -11.665 -22.754  1.00 38.24      C
ATOM   1870  CG2 VAL B 123       8.307 -12.240 -22.120  1.00 35.68      C
ATOM   1871  C   VAL B 123       6.172 -13.609 -25.055  1.00 40.09      C
ATOM   1872  O   VAL B 123       6.580 -13.168 -26.152  1.00 38.15      O
ATOM   1873  N   LYS B 124       4.948 -14.096 -24.870  1.00 42.46      N
ATOM   1874  CA  LYS B 124       3.962 -14.184 -25.947  1.00 45.11      C
ATOM   1875  CB  LYS B 124       3.596 -15.645 -26.162  1.00 44.65      C
ATOM   1876  CG  LYS B 124       4.855 -16.487 -26.597  1.00 44.00      C
ATOM   1877  CD  LYS B 124       4.562 -17.860 -27.095  1.00 41.77      C
ATOM   1878  CE  LYS B 124       5.855 -18.519 -27.544  1.00 40.51      C
ATOM   1879  NZ  LYS B 124       5.576 -19.819 -28.207  1.00 47.63      N
ATOM   1880  C   LYS B 124       2.734 -13.382 -25.557  1.00 47.91      C
ATOM   1881  O   LYS B 124       2.298 -13.441 -24.407  1.00 48.54      O
ATOM   1882  N   ALA B 125       2.192 -12.603 -26.488  1.00 50.80      N
ATOM   1883  CA  ALA B 125       0.849 -12.034 -26.276  1.00 53.80      C
ATOM   1884  CB  ALA B 125       0.556 -10.903 -27.275  1.00 53.63      C
ATOM   1885  C   ALA B 125      -0.163 -13.137 -26.440  1.00 55.22      C
ATOM   1886  O   ALA B 125      -0.164 -13.791 -27.472  1.00 56.23      O
ATOM   1887  N   ALA B 126      -1.002 -13.379 -25.438  1.00 57.49      N
ATOM   1888  CA  ALA B 126      -2.254 -14.133 -25.698  1.00 59.24      C
ATOM   1889  CB  ALA B 126      -3.063 -14.300 -24.393  1.00 59.45      C
ATOM   1890  C   ALA B 126      -3.111 -13.414 -26.810  1.00 60.27      C
ATOM   1891  O   ALA B 126      -3.505 -13.983 -27.865  1.00 59.50      O
ATOM   1892  OXT ALA B 126      -3.391 -12.183 -26.675  1.00 60.56      O
ATOM   1893  N   ALA C   1      47.894  12.704  -2.969  1.00 49.41      N
ATOM   1894  CA  ALA C   1      46.483  12.845  -2.525  1.00 48.69      C
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ATOM   1895  CB  ALA C   1      45.612  11.926  -3.320  1.00 49.22      C
ATOM   1896  C   ALA C   1      46.345  12.555  -1.040  1.00 49.03      C
ATOM   1897  O   ALA C   1      47.219  11.950  -0.422  1.00 48.45      O
ATOM   1898  N   TRP C   2      45.241  12.989  -0.442  1.00 48.83      N
ATOM   1899  CA  TRP C   2      45.029  12.703   0.970  1.00 47.92      C
ATOM   1900  CB  TRP C   2      45.920  13.592   1.858  1.00 46.22      C
ATOM   1901  CG  TRP C   2      45.728  15.092   1.734  1.00 46.85      C
ATOM   1902  CD1 TRP C   2      46.068  15.895   0.653  1.00 46.02      C
ATOM   1903  NE1 TRP C   2      45.753  17.216   0.924  1.00 45.63      N
ATOM   1904  CE2 TRP C   2      45.233  17.303   2.191  1.00 46.81      C
ATOM   1905  CD2 TRP C   2      45.200  15.983   2.737  1.00 47.63      C
ATOM   1906  CE3 TRP C   2      44.719  15.802   4.053  1.00 46.87      C
ATOM   1907  CZ3 TRP C   2      44.289  16.918   4.769  1.00 46.19      C
ATOM   1908  CH2 TRP C   2      44.326  18.226   4.185  1.00 45.94      C
ATOM   1909  CZ2 TRP C   2      44.781  18.428   2.907  1.00 46.39      C
ATOM   1910  C   TRP C   2      43.560  12.862   1.314  1.00 48.15      C
ATOM   1911  O   TRP C   2      42.877  13.673   0.702  1.00 47.92      O
ATOM   1912  N   VAL C   3      43.077  12.104   2.304  1.00 48.14      N
ATOM   1913  CA  VAL C   3      41.713  12.343   2.793  1.00 47.09      C
ATOM   1914  CB  VAL C   3      40.905  11.060   3.039  1.00 46.72      C
ATOM   1915  CG1 VAL C   3      39.538  11.402   3.680  1.00 44.65      C
ATOM   1916  CG2 VAL C   3      40.706  10.367   1.753  1.00 46.02      C
ATOM   1917  C   VAL C   3      41.738  13.261   3.993  1.00 46.31      C
ATOM   1918  O   VAL C   3      42.494  13.073   4.925  1.00 48.10      O
ATOM   1919  N   ASP C   4      40.937  14.303   3.930  1.00 46.31      N
ATOM   1920  CA  ASP C   4      40.908  15.306   4.965  1.00 45.27      C
ATOM   1921  CB  ASP C   4      40.916  16.681   4.312  1.00 45.16      C
ATOM   1922  CG  ASP C   4      40.888  17.815   5.312  1.00 46.64      C
ATOM   1923  OD1 ASP C   4      41.135  17.640   6.526  1.00 52.47      O
ATOM   1924  OD2 ASP C   4      40.594  18.933   4.886  1.00 48.46      O
ATOM   1925  C   ASP C   4      39.615  15.025   5.728  1.00 44.41      C
ATOM   1926  O   ASP C   4      38.534  15.276   5.260  1.00 43.86      O
ATOM   1927  N   GLN C   5      39.777  14.424   6.883  1.00 43.38      N
ATOM   1928  CA  GLN C   5      38.699  14.020   7.725  1.00 42.49      C
ATOM   1929  CB  GLN C   5      38.951  12.585   8.184  1.00 43.25      C
ATOM   1930  CG  GLN C   5      37.964  12.087   9.266  1.00 42.78      C
ATOM   1931  CD  GLN C   5      38.117  10.629   9.568  1.00 43.36      C
ATOM   1932  OE1 GLN C   5      38.975   9.911   8.977  1.00 44.25      O
ATOM   1933  NE2 GLN C   5      37.341  10.171  10.522  1.00 41.48      N
ATOM   1934  C   GLN C   5      38.612  14.947   8.919  1.00 41.74      C
ATOM   1935  O   GLN C   5      39.573  15.107   9.659  1.00 41.18      O
ATOM   1936  N   THR C   6      37.434  15.557   9.077  1.00 42.37      N
ATOM   1937  CA  THR C   6      37.127  16.448  10.187  1.00 42.38      C
ATOM   1938  CB  THR C   6      37.134  17.922   9.730  1.00 43.81      C
ATOM   1939  OG1 THR C   6      36.323  18.087   8.567  1.00 42.52      O
ATOM   1940  CG2 THR C   6      38.614  18.342   9.375  1.00 41.50      C
ATOM   1941  C   THR C   6      35.801  16.006  10.801  1.00 42.03      C
ATOM   1942  O   THR C   6      34.967  15.469  10.102  1.00 42.87      O
ATOM   1943  N   PRO C   7      35.654  16.121  12.134  1.00 41.26      N
ATOM   1944  CA  PRO C   7      36.674  16.605  13.095  1.00 39.68      C
ATOM   1945  CB  PRO C   7      35.847  17.012  14.318  1.00 38.19      C
ATOM   1946  CG  PRO C   7      34.571  16.163  14.235  1.00 39.85      C
ATOM   1947  CD  PRO C   7      34.370  15.774  12.795  1.00 41.08      C
ATOM   1948  C   PRO C   7      37.674  15.539  13.526  1.00 40.17      C
ATOM   1949  O   PRO C   7      37.376  14.341  13.492  1.00 40.26      O
ATOM   1950  N   ARG C   8      38.833  15.968  14.000  1.00 39.86      N
ATOM   1951  CA  ARG C   8      39.787  15.015  14.450  1.00 42.27      C
ATOM   1952  CB  ARG C   8      41.170  15.678  14.495  1.00 43.98      C
ATOM   1953  CG  ARG C   8      42.321  14.715  14.708  1.00 50.28      C
ATOM   1954  CD  ARG C   8      42.501  13.799  13.469  1.00 56.99      C
ATOM   1955  NE  ARG C   8      43.131  14.492  12.357  1.00 59.34      N
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ATOM	1956	CZ	ARG	C	8	44.447	14.636	12.274	1.00	64.10	C
ATOM	1957	NH1	ARG	C	8	45.012	15.284	11.252	1.00	65.07	N
ATOM	1958	NH2	ARG	C	8	45.200	14.117	13.239	1.00	67.46	N
ATOM	1959	C	ARG	C	8	39.357	14.418	15.816	1.00	41.81	C
ATOM	1960	O	ARG	C	8	39.638	13.250	16.123	1.00	41.61	O
ATOM	1961	N	THR	C	9	38.647	15.208	16.622	1.00	41.23	N
ATOM	1962	CA	THR	C	9	38.189	14.769	17.918	1.00	41.41	C
ATOM	1963	CB	THR	C	9	39.112	15.257	19.097	1.00	42.45	C
ATOM	1964	OG1	THR	C	9	39.108	16.701	19.180	1.00	45.56	O
ATOM	1965	CG2	THR	C	9	40.515	14.757	18.961	1.00	40.73	C
ATOM	1966	C	THR	C	9	36.847	15.389	18.127	1.00	41.08	C
ATOM	1967	O	THR	C	9	36.648	16.543	17.778	1.00	42.09	O
ATOM	1968	N	ALA	C	10	35.932	14.635	18.707	1.00	40.39	N
ATOM	1969	CA	ALA	C	10	34.587	15.110	19.081	1.00	40.33	C
ATOM	1970	CB	ALA	C	10	33.522	14.620	18.072	1.00	38.32	C
ATOM	1971	C	ALA	C	10	34.259	14.568	20.473	1.00	41.20	C
ATOM	1972	O	ALA	C	10	34.525	13.384	20.784	1.00	40.94	O
ATOM	1973	N	THR	C	11	33.736	15.455	21.324	1.00	42.57	N
ATOM	1974	CA	THR	C	11	33.123	15.099	22.616	1.00	42.23	C
ATOM	1975	CB	THR	C	11	33.759	15.861	23.749	1.00	42.79	C
ATOM	1976	OG1	THR	C	11	35.145	15.491	23.827	1.00	46.26	O
ATOM	1977	CG2	THR	C	11	33.078	15.537	25.097	1.00	40.59	C
ATOM	1978	C	THR	C	11	31.633	15.460	22.493	1.00	42.65	C
ATOM	1979	O	THR	C	11	31.325	16.618	22.223	1.00	43.18	O
ATOM	1980	N	LYS	C	12	30.743	14.467	22.657	1.00	41.78	N
ATOM	1981	CA	LYS	C	12	29.339	14.597	22.369	1.00	41.37	C
ATOM	1982	CB	LYS	C	12	28.928	13.733	21.191	1.00	41.59	C
ATOM	1983	CG	LYS	C	12	29.465	14.167	19.826	1.00	41.91	C
ATOM	1984	CD	LYS	C	12	29.346	15.654	19.576	1.00	43.02	C
ATOM	1985	CE	LYS	C	12	28.977	15.936	18.151	1.00	46.80	C
ATOM	1986	NZ	LYS	C	12	29.307	17.320	17.716	1.00	49.30	N
ATOM	1987	C	LYS	C	12	28.579	14.096	23.536	1.00	42.56	C
ATOM	1988	O	LYS	C	12	29.097	13.230	24.256	1.00	43.65	O
ATOM	1989	N	GLU	C	13	27.341	14.602	23.726	1.00	41.23	N
ATOM	1990	CA	GLU	C	13	26.474	14.080	24.762	1.00	41.54	C
ATOM	1991	CB	GLU	C	13	25.675	15.232	25.379	1.00	41.00	C
ATOM	1992	CG	GLU	C	13	26.562	16.359	25.900	1.00	42.17	C
ATOM	1993	CD	GLU	C	13	25.723	17.635	26.233	1.00	46.00	C
ATOM	1994	OE1	GLU	C	13	26.311	18.695	26.591	1.00	47.15	O
ATOM	1995	OE2	GLU	C	13	24.466	17.550	26.116	1.00	48.60	O
ATOM	1996	C	GLU	C	13	25.563	13.073	24.149	1.00	40.75	C
ATOM	1997	O	GLU	C	13	25.335	13.105	22.910	1.00	42.27	O
ATOM	1998	N	THR	C	14	25.002	12.167	24.938	1.00	40.94	N
ATOM	1999	CA	THR	C	14	24.042	11.239	24.328	1.00	42.25	C
ATOM	2000	CB	THR	C	14	23.544	10.101	25.272	1.00	42.73	C
ATOM	2001	OG1	THR	C	14	22.715	10.665	26.243	1.00	48.01	O
ATOM	2002	CG2	THR	C	14	24.705	9.386	25.975	1.00	42.04	C
ATOM	2003	C	THR	C	14	22.861	12.015	23.700	1.00	40.89	C
ATOM	2004	O	THR	C	14	22.487	13.053	24.202	1.00	41.70	O
ATOM	2005	N	GLY	C	15	22.308	11.538	22.591	1.00	39.88	N
ATOM	2006	CA	GLY	C	15	21.224	12.239	21.898	1.00	38.62	C
ATOM	2007	C	GLY	C	15	21.690	13.211	20.812	1.00	38.27	C
ATOM	2008	O	GLY	C	15	20.912	13.537	19.886	1.00	39.29	O
ATOM	2009	N	GLU	C	16	22.921	13.685	20.902	1.00	36.77	N
ATOM	2010	CA	GLU	C	16	23.522	14.515	19.858	1.00	38.21	C
ATOM	2011	CB	GLU	C	16	24.766	15.286	20.373	1.00	37.37	C
ATOM	2012	CG	GLU	C	16	24.448	16.420	21.495	1.00	38.40	C
ATOM	2013	CD	GLU	C	16	25.627	17.359	21.780	1.00	38.50	C
ATOM	2014	OE1	GLU	C	16	26.733	16.846	21.984	1.00	40.44	O
ATOM	2015	OE2	GLU	C	16	25.489	18.609	21.757	1.00	38.88	O
ATOM	2016	C	GLU	C	16	23.874	13.652	18.635	1.00	40.24	C

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ATOM   2017  O   GLU C  16      23.852  12.414  18.745  1.00 42.05      O
ATOM   2018  N   SER C  17      24.137  14.306  17.494  1.00 39.57      N
ATOM   2019  CA  SER C  17      24.621  13.722  16.264  1.00 40.14      C
ATOM   2020  CB  SER C  17      23.844  14.317  15.073  1.00 39.97      C
ATOM   2021  OG  SER C  17      22.451  13.972  15.174  1.00 42.60      O
ATOM   2022  C   SER C  17      26.094  14.113  16.057  1.00 40.75      C
ATOM   2023  O   SER C  17      26.547  15.102  16.557  1.00 40.20      O
ATOM   2024  N   LEU C  18      26.823  13.314  15.288  1.00 40.85      N
ATOM   2025  CA  LEU C  18      28.139  13.643  14.874  1.00 41.38      C
ATOM   2026  CB  LEU C  18      29.061  12.561  15.427  1.00 41.14      C
ATOM   2027  CG  LEU C  18      30.600  12.596  15.451  1.00 44.10      C
ATOM   2028  CD1 LEU C  18      31.251  11.259  14.907  1.00 38.99      C
ATOM   2029  CD2 LEU C  18      31.291  13.933  15.015  1.00 41.87      C
ATOM   2030  C   LEU C  18      28.102  13.544  13.321  1.00 41.20      C
ATOM   2031  O   LEU C  18      27.616  12.564  12.803  1.00 39.57      O
ATOM   2032  N   THR C  19      28.624  14.567  12.624  1.00 41.23      N
ATOM   2033  CA  THR C  19      28.945  14.495  11.209  1.00 41.67      C
ATOM   2034  CB  THR C  19      28.303  15.664  10.371  1.00 41.81      C
ATOM   2035  OG1 THR C  19      26.939  15.741  10.732  1.00 41.36      O
ATOM   2036  CG2 THR C  19      28.390  15.426   8.826  1.00 41.66      C
ATOM   2037  C   THR C  19      30.442  14.493  11.061  1.00 41.89      C
ATOM   2038  O   THR C  19      31.144  15.426  11.504  1.00 41.70      O
ATOM   2039  N   ILE C  20      30.930  13.399  10.473  1.00 41.66      N
ATOM   2040  CA  ILE C  20      32.321  13.291  10.062  1.00 42.12      C
ATOM   2041  CB  ILE C  20      32.855  11.887  10.306  1.00 41.88      C
ATOM   2042  CG1 ILE C  20      32.758  11.550  11.820  1.00 41.13      C
ATOM   2043  CD1 ILE C  20      32.960  10.088  12.166  1.00 40.95      C
ATOM   2044  CG2 ILE C  20      34.363  11.820   9.859  1.00 42.36      C
ATOM   2045  C   ILE C  20      32.348  13.605   8.568  1.00 42.26      C
ATOM   2046  O   ILE C  20      31.661  12.949   7.823  1.00 41.71      O
ATOM   2047  N   ASN C  21      33.104  14.624   8.159  1.00 43.04      N
ATOM   2048  CA  ASN C  21      33.313  14.925   6.762  1.00 45.16      C
ATOM   2049  CB  ASN C  21      33.189  16.438   6.512  1.00 46.62      C
ATOM   2050  CG  ASN C  21      31.762  16.957   6.721  1.00 49.24      C
ATOM   2051  OD1 ASN C  21      30.831  16.593   5.972  1.00 56.70      O
ATOM   2052  ND2 ASN C  21      31.582  17.830   7.730  1.00 49.52      N
ATOM   2053  C   ASN C  21      34.686  14.471   6.266  1.00 45.75      C
ATOM   2054  O   ASN C  21      35.684  14.670   6.944  1.00 46.28      O
ATOM   2055  N   CYS C  22      34.723  13.897   5.073  1.00 46.82      N
ATOM   2056  CA  CYS C  22      35.959  13.487   4.390  1.00 48.35      C
ATOM   2057  CB  CYS C  22      36.085  11.967   4.403  1.00 49.01      C
ATOM   2058  SG  CYS C  22      36.404  11.250   6.007  1.00 54.40      S
ATOM   2059  C   CYS C  22      35.984  13.967   2.918  1.00 47.56      C
ATOM   2060  O   CYS C  22      34.978  13.866   2.185  1.00 47.67      O
ATOM   2061  N   VAL C  23      37.123  14.505   2.496  1.00 46.77      N
ATOM   2062  CA  VAL C  23      37.304  14.992   1.118  1.00 44.55      C
ATOM   2063  CB  VAL C  23      37.150  16.531   1.002  1.00 44.60      C
ATOM   2064  CG1 VAL C  23      37.928  17.212   2.000  1.00 46.21      C
ATOM   2065  CG2 VAL C  23      37.482  17.046  -0.374  1.00 41.80      C
ATOM   2066  C   VAL C  23      38.626  14.498   0.625  1.00 44.64      C
ATOM   2067  O   VAL C  23      39.675  14.683   1.266  1.00 43.95      O
ATOM   2068  N   LEU C  24      38.574  13.824  -0.512  1.00 44.47      N
ATOM   2069  CA  LEU C  24      39.784  13.393  -1.220  1.00 44.52      C
ATOM   2070  CB  LEU C  24      39.348  12.419  -2.293  1.00 44.25      C
ATOM   2071  CG  LEU C  24      40.109  11.175  -2.724  1.00 44.73      C
ATOM   2072  CD1 LEU C  24      39.957  11.047  -4.204  1.00 40.23      C
ATOM   2073  CD2 LEU C  24      41.538  11.066  -2.237  1.00 39.12      C
ATOM   2074  C   LEU C  24      40.400  14.631  -1.912  1.00 44.53      C
ATOM   2075  O   LEU C  24      39.900  15.064  -2.955  1.00 44.70      O
ATOM   2076  N   ARG C  25      41.478  15.178  -1.362  1.00 44.03      N
ATOM   2077  CA  ARG C  25      42.084  16.424  -1.857  1.00 44.69      C
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ATOM	2078	CB	ARG	C	25	42.553	17.314	-0.692	1.00	44.52	C
ATOM	2079	CG	ARG	C	25	41.525	17.578	0.303	1.00	48.32	C
ATOM	2080	CD	ARG	C	25	41.769	18.944	0.893	1.00	55.19	C
ATOM	2081	NE	ARG	C	25	40.566	19.723	0.675	1.00	61.48	N
ATOM	2082	CZ	ARG	C	25	39.708	19.984	1.631	1.00	63.06	C
ATOM	2083	NH1	ARG	C	25	39.998	19.570	2.840	1.00	64.66	N
ATOM	2084	NH2	ARG	C	25	38.597	20.665	1.395	1.00	64.06	N
ATOM	2085	C	ARG	C	25	43.299	16.116	-2.694	1.00	44.89	C
ATOM	2086	O	ARG	C	25	43.971	15.093	-2.441	1.00	45.00	O
ATOM	2087	N	ASP	C	26	43.593	17.013	-3.647	1.00	44.78	N
ATOM	2088	CA	ASP	C	26	44.661	16.859	-4.650	1.00	45.57	C
ATOM	2089	CB	ASP	C	26	46.044	17.275	-4.103	1.00	46.72	C
ATOM	2090	CG	ASP	C	26	45.991	18.501	-3.221	1.00	50.19	C
ATOM	2091	OD1	ASP	C	26	45.405	19.537	-3.629	1.00	53.01	O
ATOM	2092	OD2	ASP	C	26	46.552	18.429	-2.099	1.00	56.34	O
ATOM	2093	C	ASP	C	26	44.784	15.464	-5.185	1.00	44.38	C
ATOM	2094	O	ASP	C	26	45.871	14.927	-5.215	1.00	43.71	O
ATOM	2095	N	ALA	C	27	43.679	14.845	-5.567	1.00	44.56	N
ATOM	2096	CA	ALA	C	27	43.757	13.530	-6.180	1.00	44.95	C
ATOM	2097	CB	ALA	C	27	42.740	12.552	-5.573	1.00	43.12	C
ATOM	2098	C	ALA	C	27	43.581	13.633	-7.690	1.00	46.25	C
ATOM	2099	O	ALA	C	27	42.797	14.464	-8.174	1.00	46.95	O
ATOM	2100	N	SER	C	28	44.294	12.777	-8.432	1.00	46.99	N
ATOM	2101	CA	SER	C	28	44.153	12.779	-9.869	1.00	48.62	C
ATOM	2102	CB	SER	C	28	45.480	12.479	-10.560	1.00	48.58	C
ATOM	2103	OG	SER	C	28	46.044	11.353	-9.990	1.00	52.33	O
ATOM	2104	C	SER	C	28	43.026	11.836	-10.303	1.00	48.24	C
ATOM	2105	O	SER	C	28	42.716	11.733	-11.473	1.00	49.15	O
ATOM	2106	N	PHE	C	29	42.370	11.220	-9.334	1.00	47.44	N
ATOM	2107	CA	PHE	C	29	41.340	10.221	-9.612	1.00	46.65	C
ATOM	2108	CB	PHE	C	29	41.726	8.894	-8.920	1.00	45.70	C
ATOM	2109	CG	PHE	C	29	43.158	8.502	-9.180	1.00	42.81	C
ATOM	2110	CD1	PHE	C	29	43.538	8.066	-10.448	1.00	36.25	C
ATOM	2111	CE1	PHE	C	29	44.850	7.768	-10.742	1.00	40.99	C
ATOM	2112	CZ	PHE	C	29	45.820	7.884	-9.731	1.00	43.75	C
ATOM	2113	CE2	PHE	C	29	45.441	8.337	-8.441	1.00	40.55	C
ATOM	2114	CD2	PHE	C	29	44.116	8.649	-8.189	1.00	40.78	C
ATOM	2115	C	PHE	C	29	39.958	10.697	-9.171	1.00	46.58	C
ATOM	2116	O	PHE	C	29	39.831	11.601	-8.317	1.00	46.70	O
ATOM	2117	N	GLU	C	30	38.942	10.067	-9.750	1.00	45.81	N
ATOM	2118	CA	GLU	C	30	37.563	10.269	-9.351	1.00	46.83	C
ATOM	2119	CB	GLU	C	30	36.632	9.980	-10.536	1.00	47.06	C
ATOM	2120	CG	GLU	C	30	36.882	10.950	-11.687	1.00	49.84	C
ATOM	2121	CD	GLU	C	30	36.469	12.382	-11.319	1.00	57.62	C
ATOM	2122	OE1	GLU	C	30	37.291	13.328	-11.489	1.00	60.20	O
ATOM	2123	OE2	GLU	C	30	35.322	12.553	-10.835	1.00	58.67	O
ATOM	2124	C	GLU	C	30	37.257	9.401	-8.127	1.00	46.19	C
ATOM	2125	O	GLU	C	30	37.833	8.321	-7.956	1.00	47.70	O
ATOM	2126	N	LEU	C	31	36.387	9.880	-7.259	1.00	45.21	N
ATOM	2127	CA	LEU	C	31	35.899	9.053	-6.142	1.00	44.93	C
ATOM	2128	CB	LEU	C	31	35.102	9.934	-5.217	1.00	43.15	C
ATOM	2129	CG	LEU	C	31	35.111	9.885	-3.699	1.00	44.69	C
ATOM	2130	CD1	LEU	C	31	33.683	10.296	-3.177	1.00	36.97	C
ATOM	2131	CD2	LEU	C	31	35.711	8.615	-3.022	1.00	38.29	C
ATOM	2132	C	LEU	C	31	34.937	7.956	-6.652	1.00	45.16	C
ATOM	2133	O	LEU	C	31	33.860	8.246	-7.196	1.00	44.80	O
ATOM	2134	N	LYS	C	32	35.286	6.701	-6.434	1.00	46.15	N
ATOM	2135	CA	LYS	C	32	34.505	5.608	-6.991	1.00	46.54	C
ATOM	2136	CB	LYS	C	32	35.461	4.506	-7.478	1.00	46.96	C
ATOM	2137	CG	LYS	C	32	34.801	3.264	-8.090	1.00	50.13	C
ATOM	2138	CD	LYS	C	32	33.911	3.610	-9.290	1.00	57.71	C

ATOM	2139	CE	LYS	C	32	33.263	2.363	-9.882	1.00	61.56	C
ATOM	2140	NZ	LYS	C	32	33.432	1.172	-8.953	1.00	64.12	N
ATOM	2141	C	LYS	C	32	33.606	5.063	-5.905	1.00	46.00	C
ATOM	2142	O	LYS	C	32	32.462	4.730	-6.158	1.00	46.13	O
ATOM	2143	N	ASP	C	33	34.149	4.969	-4.698	1.00	44.66	N
ATOM	2144	CA	ASP	C	33	33.519	4.229	-3.609	1.00	44.59	C
ATOM	2145	CB	ASP	C	33	33.969	2.787	-3.714	1.00	45.73	C
ATOM	2146	CG	ASP	C	33	32.854	1.826	-3.570	1.00	53.17	C
ATOM	2147	OD1	ASP	C	33	32.322	1.737	-2.442	1.00	60.90	O
ATOM	2148	OD2	ASP	C	33	32.510	1.158	-4.597	1.00	61.93	O
ATOM	2149	C	ASP	C	33	34.007	4.777	-2.272	1.00	42.39	C
ATOM	2150	O	ASP	C	33	35.028	5.440	-2.230	1.00	39.76	O
ATOM	2151	N	THR	C	34	33.338	4.398	-1.181	1.00	42.58	N
ATOM	2152	CA	THR	C	34	33.698	4.850	0.198	1.00	43.04	C
ATOM	2153	CB	THR	C	34	32.810	6.031	0.681	1.00	43.33	C
ATOM	2154	OG1	THR	C	34	31.451	5.618	0.749	1.00	45.15	O
ATOM	2155	CG2	THR	C	34	32.867	7.227	-0.263	1.00	43.17	C
ATOM	2156	C	THR	C	34	33.529	3.715	1.235	1.00	43.65	C
ATOM	2157	O	THR	C	34	32.668	2.867	1.082	1.00	44.87	O
ATOM	2158	N	GLY	C	35	34.384	3.686	2.256	1.00	43.02	N
ATOM	2159	CA	GLY	C	35	34.214	2.825	3.400	1.00	40.60	C
ATOM	2160	C	GLY	C	35	34.387	3.562	4.711	1.00	40.55	C
ATOM	2161	O	GLY	C	35	35.086	4.603	4.784	1.00	40.16	O
ATOM	2162	N	TRP	C	36	33.817	2.969	5.766	1.00	39.56	N
ATOM	2163	CA	TRP	C	36	33.800	3.546	7.094	1.00	39.04	C
ATOM	2164	CB	TRP	C	36	32.434	4.191	7.420	1.00	37.69	C
ATOM	2165	CG	TRP	C	36	32.204	5.462	6.649	1.00	36.88	C
ATOM	2166	CD1	TRP	C	36	31.534	5.601	5.445	1.00	37.03	C
ATOM	2167	NE1	TRP	C	36	31.582	6.905	5.028	1.00	39.08	N
ATOM	2168	CE2	TRP	C	36	32.299	7.641	5.951	1.00	36.41	C
ATOM	2169	CD2	TRP	C	36	32.682	6.771	6.993	1.00	35.39	C
ATOM	2170	CE3	TRP	C	36	33.372	7.289	8.105	1.00	39.61	C
ATOM	2171	CZ3	TRP	C	36	33.629	8.658	8.149	1.00	41.57	C
ATOM	2172	CH2	TRP	C	36	33.200	9.514	7.090	1.00	39.46	C
ATOM	2173	CZ2	TRP	C	36	32.533	9.007	5.998	1.00	38.02	C
ATOM	2174	C	TRP	C	36	34.152	2.464	8.081	1.00	39.80	C
ATOM	2175	O	TRP	C	36	33.630	1.365	7.971	1.00	39.62	O
ATOM	2176	N	TYR	C	37	35.047	2.780	9.028	1.00	39.72	N
ATOM	2177	CA	TYR	C	37	35.586	1.769	9.988	1.00	42.18	C
ATOM	2178	CB	TYR	C	37	37.003	1.298	9.614	1.00	42.50	C
ATOM	2179	CG	TYR	C	37	37.114	0.995	8.128	1.00	46.10	C
ATOM	2180	CD1	TYR	C	37	36.832	-0.275	7.647	1.00	46.08	C
ATOM	2181	CE1	TYR	C	37	36.869	-0.558	6.267	1.00	49.05	C
ATOM	2182	CZ	TYR	C	37	37.246	0.447	5.381	1.00	48.62	C
ATOM	2183	OH	TYR	C	37	37.305	0.146	4.032	1.00	51.96	O
ATOM	2184	CE2	TYR	C	37	37.562	1.732	5.836	1.00	48.05	C
ATOM	2185	CD2	TYR	C	37	37.495	2.009	7.191	1.00	46.46	C
ATOM	2186	C	TYR	C	37	35.599	2.413	11.358	1.00	41.82	C
ATOM	2187	O	TYR	C	37	35.694	3.624	11.464	1.00	41.95	O
ATOM	2188	N	ARG	C	38	35.544	1.586	12.381	1.00	42.36	N
ATOM	2189	CA	ARG	C	38	35.573	2.021	13.729	1.00	44.49	C
ATOM	2190	CB	ARG	C	38	34.144	2.242	14.237	1.00	43.43	C
ATOM	2191	CG	ARG	C	38	34.110	2.406	15.718	1.00	47.74	C
ATOM	2192	CD	ARG	C	38	32.742	2.530	16.225	1.00	51.14	C
ATOM	2193	NE	ARG	C	38	31.885	1.427	15.821	1.00	52.19	N
ATOM	2194	CZ	ARG	C	38	30.571	1.409	16.035	1.00	57.68	C
ATOM	2195	NH1	ARG	C	38	29.942	2.452	16.614	1.00	59.02	N
ATOM	2196	NH2	ARG	C	38	29.868	0.353	15.673	1.00	59.82	N
ATOM	2197	C	ARG	C	38	36.288	0.991	14.613	1.00	45.46	C
ATOM	2198	O	ARG	C	38	36.115	-0.222	14.456	1.00	46.19	O
ATOM	2199	N	THR	C	39	37.083	1.516	15.543	1.00	46.20	N

ATOM	2200	CA	THR	C	39	37.717	0.800	16.641	1.00	46.40	C
ATOM	2201	CB	THR	C	39	39.209	1.155	16.699	1.00	45.51	C
ATOM	2202	OG1	THR	C	39	39.825	0.817	15.455	1.00	49.49	O
ATOM	2203	CG2	THR	C	39	39.937	0.406	17.866	1.00	48.80	C
ATOM	2204	C	THR	C	39	36.992	1.338	17.885	1.00	47.15	C
ATOM	2205	O	THR	C	39	37.109	2.523	18.232	1.00	45.10	O
ATOM	2206	N	LYS	C	40	36.167	0.482	18.484	1.00	49.20	N
ATOM	2207	CA	LYS	C	40	35.389	0.844	19.650	1.00	51.33	C
ATOM	2208	CB	LYS	C	40	34.355	-0.221	19.990	1.00	51.30	C
ATOM	2209	CG	LYS	C	40	32.952	0.226	19.595	1.00	55.88	C
ATOM	2210	CD	LYS	C	40	31.926	-0.887	19.626	1.00	59.21	C
ATOM	2211	CE	LYS	C	40	31.099	-0.803	20.895	1.00	63.11	C
ATOM	2212	NZ	LYS	C	40	31.075	-2.176	21.526	1.00	61.59	N
ATOM	2213	C	LYS	C	40	36.333	1.157	20.816	1.00	52.57	C
ATOM	2214	O	LYS	C	40	37.423	0.611	20.886	1.00	50.99	O
ATOM	2215	N	LEU	C	41	35.938	2.114	21.659	1.00	54.39	N
ATOM	2216	CA	LEU	C	41	36.802	2.622	22.737	1.00	57.08	C
ATOM	2217	CB	LEU	C	41	36.066	3.736	23.533	1.00	57.10	C
ATOM	2218	CG	LEU	C	41	36.543	4.136	24.933	1.00	59.84	C
ATOM	2219	CD1	LEU	C	41	35.549	5.096	25.662	1.00	61.21	C
ATOM	2220	CD2	LEU	C	41	37.964	4.735	24.863	1.00	62.80	C
ATOM	2221	C	LEU	C	41	37.302	1.465	23.642	1.00	58.11	C
ATOM	2222	O	LEU	C	41	36.505	0.742	24.266	1.00	58.05	O
ATOM	2223	N	GLY	C	42	38.616	1.264	23.669	1.00	59.71	N
ATOM	2224	CA	GLY	C	42	39.187	0.174	24.457	1.00	61.51	C
ATOM	2225	C	GLY	C	42	39.653	-1.023	23.643	1.00	62.72	C
ATOM	2226	O	GLY	C	42	40.460	-1.830	24.139	1.00	63.71	O
ATOM	2227	N	SER	C	43	39.164	-1.138	22.404	1.00	62.76	N
ATOM	2228	CA	SER	C	43	39.511	-2.239	21.519	1.00	62.79	C
ATOM	2229	CB	SER	C	43	38.328	-2.559	20.602	1.00	62.63	C
ATOM	2230	OG	SER	C	43	38.301	-3.927	20.271	1.00	61.87	O
ATOM	2231	C	SER	C	43	40.742	-1.897	20.689	1.00	63.37	C
ATOM	2232	O	SER	C	43	41.116	-0.728	20.557	1.00	63.84	O
ATOM	2233	N	THR	C	44	41.394	-2.912	20.139	1.00	63.50	N
ATOM	2234	CA	THR	C	44	42.377	-2.657	19.070	1.00	64.33	C
ATOM	2235	CB	THR	C	44	43.793	-3.127	19.469	1.00	64.45	C
ATOM	2236	OG1	THR	C	44	43.781	-4.544	19.687	1.00	66.10	O
ATOM	2237	CG2	THR	C	44	44.238	-2.424	20.769	1.00	63.59	C
ATOM	2238	C	THR	C	44	41.890	-3.251	17.729	1.00	63.70	C
ATOM	2239	O	THR	C	44	42.568	-3.185	16.695	1.00	64.39	O
ATOM	2240	N	ASN	C	45	40.675	-3.793	17.782	1.00	63.29	N
ATOM	2241	CA	ASN	C	45	39.968	-4.421	16.665	1.00	63.06	C
ATOM	2242	CB	ASN	C	45	38.963	-5.407	17.285	1.00	63.41	C
ATOM	2243	CG	ASN	C	45	38.299	-6.286	16.258	1.00	64.24	C
ATOM	2244	OD1	ASN	C	45	38.944	-6.744	15.312	1.00	64.63	O
ATOM	2245	ND2	ASN	C	45	36.996	-6.530	16.436	1.00	64.01	N
ATOM	2246	C	ASN	C	45	39.202	-3.426	15.744	1.00	62.52	C
ATOM	2247	O	ASN	C	45	38.108	-2.951	16.115	1.00	62.14	O
ATOM	2248	N	GLU	C	46	39.763	-3.111	14.573	1.00	61.57	N
ATOM	2249	CA	GLU	C	46	39.080	-2.251	13.572	1.00	61.38	C
ATOM	2250	CB	GLU	C	46	40.062	-1.708	12.530	1.00	61.16	C
ATOM	2251	CG	GLU	C	46	39.403	-1.084	11.308	1.00	63.74	C
ATOM	2252	CD	GLU	C	46	40.014	0.267	10.932	1.00	66.98	C
ATOM	2253	OE1	GLU	C	46	39.729	1.274	11.635	1.00	69.02	O
ATOM	2254	OE2	GLU	C	46	40.770	0.320	9.935	1.00	67.74	O
ATOM	2255	C	GLU	C	46	37.917	-2.948	12.868	1.00	60.84	C
ATOM	2256	O	GLU	C	46	38.086	-4.018	12.322	1.00	61.63	O
ATOM	2257	N	GLN	C	47	36.748	-2.322	12.856	1.00	60.18	N
ATOM	2258	CA	GLN	C	47	35.542	-2.929	12.279	1.00	59.69	C
ATOM	2259	CB	GLN	C	47	34.492	-3.142	13.364	1.00	60.04	C
ATOM	2260	CG	GLN	C	47	34.685	-4.423	14.153	1.00	63.45	C

ATOM	2261	CD	GLN	C	47	33.988	-4.364	15.502	1.00	67.03	C
ATOM	2262	OE1	GLN	C	47	33.722	-5.409	16.101	1.00	69.04	O
ATOM	2263	NE2	GLN	C	47	33.687	-3.134	15.992	1.00	65.48	N
ATOM	2264	C	GLN	C	47	34.882	-2.103	11.188	1.00	57.90	C
ATOM	2265	O	GLN	C	47	34.807	-0.893	11.276	1.00	56.91	O
ATOM	2266	N	SER	C	48	34.333	-2.792	10.205	1.00	57.17	N
ATOM	2267	CA	SER	C	48	33.545	-2.155	9.151	1.00	57.02	C
ATOM	2268	CB	SER	C	48	33.367	-3.095	7.949	1.00	57.30	C
ATOM	2269	OG	SER	C	48	33.469	-2.341	6.749	1.00	59.39	O
ATOM	2270	C	SER	C	48	32.203	-1.664	9.682	1.00	55.73	C
ATOM	2271	O	SER	C	48	31.564	-2.325	10.497	1.00	55.50	O
ATOM	2272	N	ILE	C	49	31.823	-0.460	9.257	1.00	55.13	N
ATOM	2273	CA	ILE	C	49	30.555	0.176	9.651	1.00	54.08	C
ATOM	2274	CB	ILE	C	49	30.701	1.702	9.867	1.00	53.11	C
ATOM	2275	CG1	ILE	C	49	31.364	2.013	11.191	1.00	54.19	C
ATOM	2276	CD1	ILE	C	49	31.747	3.486	11.251	1.00	50.86	C
ATOM	2277	CG2	ILE	C	49	29.335	2.437	9.866	1.00	53.88	C
ATOM	2278	C	ILE	C	49	29.495	-0.094	8.577	1.00	53.70	C
ATOM	2279	O	ILE	C	49	29.695	0.176	7.389	1.00	54.09	O
ATOM	2280	N	SER	C	50	28.372	-0.637	9.027	1.00	53.80	N
ATOM	2281	CA	SER	C	50	27.170	-0.832	8.215	1.00	53.15	C
ATOM	2282	CB	SER	C	50	26.378	-2.049	8.731	1.00	53.47	C
ATOM	2283	OG	SER	C	50	27.216	-3.191	8.674	1.00	55.46	O
ATOM	2284	C	SER	C	50	26.299	0.421	8.248	1.00	51.25	C
ATOM	2285	O	SER	C	50	25.876	0.861	9.314	1.00	50.95	O
ATOM	2286	N	ILE	C	51	26.055	0.964	7.058	1.00	49.62	N
ATOM	2287	CA	ILE	C	51	25.252	2.177	6.854	1.00	47.96	C
ATOM	2288	CB	ILE	C	51	25.704	2.918	5.527	1.00	47.87	C
ATOM	2289	CG1	ILE	C	51	27.198	3.362	5.611	1.00	47.14	C
ATOM	2290	CD1	ILE	C	51	27.596	4.066	6.953	1.00	42.36	C
ATOM	2291	CG2	ILE	C	51	24.764	4.088	5.185	1.00	47.30	C
ATOM	2292	C	ILE	C	51	23.750	1.837	6.844	1.00	46.21	C
ATOM	2293	O	ILE	C	51	23.318	0.974	6.084	1.00	47.08	O
ATOM	2294	N	GLY	C	52	22.958	2.488	7.697	1.00	44.14	N
ATOM	2295	CA	GLY	C	52	21.505	2.239	7.784	1.00	41.65	C
ATOM	2296	C	GLY	C	52	21.099	2.653	9.184	1.00	40.74	C
ATOM	2297	O	GLY	C	52	21.943	2.713	10.069	1.00	40.48	O
ATOM	2298	N	GLY	C	53	19.822	2.961	9.391	1.00	38.99	N
ATOM	2299	CA	GLY	C	53	19.345	3.387	10.677	1.00	37.19	C
ATOM	2300	C	GLY	C	53	19.888	4.738	11.055	1.00	37.85	C
ATOM	2301	O	GLY	C	53	19.829	5.692	10.269	1.00	37.66	O
ATOM	2302	N	ARG	C	54	20.424	4.812	12.277	1.00	38.16	N
ATOM	2303	CA	ARG	C	54	21.107	5.990	12.806	1.00	36.67	C
ATOM	2304	CB	ARG	C	54	21.487	5.783	14.286	1.00	37.09	C
ATOM	2305	CG	ARG	C	54	20.294	5.610	15.167	1.00	36.01	C
ATOM	2306	CD	ARG	C	54	20.611	5.607	16.667	1.00	37.36	C
ATOM	2307	NE	ARG	C	54	21.596	4.563	16.963	1.00	39.11	N
ATOM	2308	CZ	ARG	C	54	22.885	4.774	17.227	1.00	39.90	C
ATOM	2309	NH1	ARG	C	54	23.418	6.002	17.263	1.00	35.96	N
ATOM	2310	NH2	ARG	C	54	23.645	3.734	17.490	1.00	38.73	N
ATOM	2311	C	ARG	C	54	22.310	6.430	12.016	1.00	37.64	C
ATOM	2312	O	ARG	C	54	22.696	7.611	12.105	1.00	38.33	O
ATOM	2313	N	TYR	C	55	22.927	5.527	11.242	1.00	38.47	N
ATOM	2314	CA	TYR	C	55	24.111	5.852	10.435	1.00	38.95	C
ATOM	2315	CB	TYR	C	55	25.104	4.647	10.444	1.00	41.10	C
ATOM	2316	CG	TYR	C	55	25.676	4.328	11.842	1.00	43.73	C
ATOM	2317	CD1	TYR	C	55	24.897	3.737	12.850	1.00	45.50	C
ATOM	2318	CE1	TYR	C	55	25.432	3.473	14.108	1.00	47.29	C
ATOM	2319	CZ	TYR	C	55	26.778	3.788	14.349	1.00	47.61	C
ATOM	2320	OH	TYR	C	55	27.392	3.558	15.581	1.00	49.34	O
ATOM	2321	CE2	TYR	C	55	27.541	4.359	13.367	1.00	44.66	C

ATOM	2322	CD2	TYR	C	55	27.001	4.622	12.141	1.00	44.65	C
ATOM	2323	C	TYR	C	55	23.703	6.228	8.973	1.00	38.22	C
ATOM	2324	O	TYR	C	55	23.137	5.426	8.270	1.00	38.89	O
ATOM	2325	N	VAL	C	56	24.009	7.436	8.522	1.00	37.84	N
ATOM	2326	CA	VAL	C	56	23.618	7.965	7.202	1.00	37.02	C
ATOM	2327	CB	VAL	C	56	22.603	9.173	7.358	1.00	37.86	C
ATOM	2328	CG1	VAL	C	56	22.116	9.728	5.981	1.00	36.06	C
ATOM	2329	CG2	VAL	C	56	21.430	8.757	8.169	1.00	36.23	C
ATOM	2330	C	VAL	C	56	24.901	8.476	6.531	1.00	38.69	C
ATOM	2331	O	VAL	C	56	25.605	9.334	7.094	1.00	37.27	O
ATOM	2332	N	GLU	C	57	25.230	7.898	5.369	1.00	39.95	N
ATOM	2333	CA	GLU	C	57	26.318	8.383	4.518	1.00	41.91	C
ATOM	2334	CB	GLU	C	57	27.001	7.223	3.793	1.00	42.73	C
ATOM	2335	CG	GLU	C	57	28.243	7.712	3.058	1.00	44.86	C
ATOM	2336	CD	GLU	C	57	29.213	6.641	2.626	1.00	46.27	C
ATOM	2337	OE1	GLU	C	57	30.406	6.928	2.665	1.00	51.32	O
ATOM	2338	OE2	GLU	C	57	28.819	5.529	2.281	1.00	45.88	O
ATOM	2339	C	GLU	C	57	25.772	9.321	3.461	1.00	42.24	C
ATOM	2340	O	GLU	C	57	24.679	9.095	2.933	1.00	42.46	O
ATOM	2341	N	THR	C	58	26.505	10.370	3.128	1.00	42.56	N
ATOM	2342	CA	THR	C	58	26.114	11.189	1.984	1.00	44.27	C
ATOM	2343	CB	THR	C	58	25.754	12.622	2.431	1.00	45.63	C
ATOM	2344	OG1	THR	C	58	24.690	12.556	3.388	1.00	44.93	O
ATOM	2345	CG2	THR	C	58	25.232	13.504	1.208	1.00	46.97	C
ATOM	2346	C	THR	C	58	27.348	11.189	1.130	1.00	44.50	C
ATOM	2347	O	THR	C	58	28.413	11.350	1.666	1.00	43.33	O
ATOM	2348	N	VAL	C	59	27.230	10.942	-0.176	1.00	45.04	N
ATOM	2349	CA	VAL	C	59	28.406	10.977	-1.063	1.00	45.53	C
ATOM	2350	CB	VAL	C	59	28.708	9.588	-1.708	1.00	46.05	C
ATOM	2351	CG1	VAL	C	59	29.915	9.649	-2.706	1.00	47.53	C
ATOM	2352	CG2	VAL	C	59	29.006	8.579	-0.643	1.00	45.51	C
ATOM	2353	C	VAL	C	59	28.206	12.053	-2.134	1.00	45.35	C
ATOM	2354	O	VAL	C	59	27.147	12.120	-2.743	1.00	44.02	O
ATOM	2355	N	ASN	C	60	29.203	12.919	-2.317	1.00	44.36	N
ATOM	2356	CA	ASN	C	60	29.194	13.869	-3.435	1.00	44.75	C
ATOM	2357	CB	ASN	C	60	29.177	15.316	-2.912	1.00	45.64	C
ATOM	2358	CG	ASN	C	60	28.884	16.325	-4.015	1.00	47.39	C
ATOM	2359	OD1	ASN	C	60	29.294	16.141	-5.154	1.00	49.89	O
ATOM	2360	ND2	ASN	C	60	28.148	17.385	-3.681	1.00	49.11	N
ATOM	2361	C	ASN	C	60	30.404	13.658	-4.329	1.00	44.46	C
ATOM	2362	O	ASN	C	60	31.482	14.175	-4.051	1.00	44.94	O
ATOM	2363	N	LYS	C	61	30.277	12.837	-5.357	1.00	43.78	N
ATOM	2364	CA	LYS	C	61	31.416	12.530	-6.207	1.00	43.85	C
ATOM	2365	CB	LYS	C	61	31.024	11.439	-7.200	1.00	45.23	C
ATOM	2366	CG	LYS	C	61	30.890	10.014	-6.579	1.00	46.82	C
ATOM	2367	CD	LYS	C	61	30.106	9.171	-7.582	1.00	50.75	C
ATOM	2368	CE	LYS	C	61	29.705	7.801	-7.064	1.00	54.46	C
ATOM	2369	NZ	LYS	C	61	30.794	6.802	-7.151	1.00	54.88	N
ATOM	2370	C	LYS	C	61	31.910	13.801	-6.932	1.00	43.81	C
ATOM	2371	O	LYS	C	61	33.080	13.971	-7.175	1.00	42.45	O
ATOM	2372	N	GLY	C	62	31.000	14.714	-7.249	1.00	44.61	N
ATOM	2373	CA	GLY	C	62	31.383	15.991	-7.859	1.00	45.46	C
ATOM	2374	C	GLY	C	62	32.487	16.728	-7.119	1.00	45.37	C
ATOM	2375	O	GLY	C	62	33.376	17.295	-7.727	1.00	45.73	O
ATOM	2376	N	SER	C	63	32.450	16.704	-5.792	1.00	45.46	N
ATOM	2377	CA	SER	C	63	33.420	17.441	-5.008	1.00	44.70	C
ATOM	2378	CB	SER	C	63	32.688	18.416	-4.091	1.00	45.19	C
ATOM	2379	OG	SER	C	63	31.893	17.677	-3.181	1.00	47.62	O
ATOM	2380	C	SER	C	63	34.264	16.451	-4.232	1.00	44.60	C
ATOM	2381	O	SER	C	63	34.979	16.823	-3.314	1.00	45.58	O
ATOM	2382	N	LYS	C	64	34.200	15.185	-4.631	1.00	43.31	N

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ATOM   2383  CA  LYS C  64      34.998  14.106  -4.028  1.00 42.72      C
ATOM   2384  CB  LYS C  64      36.477  14.180  -4.442  1.00 43.43      C
ATOM   2385  CG  LYS C  64      36.775  14.385  -5.937  1.00 42.33      C
ATOM   2386  CD  LYS C  64      38.280  14.079  -6.230  1.00 41.50      C
ATOM   2387  CE  LYS C  64      38.590  14.577  -7.695  1.00 39.78      C
ATOM   2388  NZ  LYS C  64      39.915  14.109  -8.180  1.00 42.69      N
ATOM   2389  C   LYS C  64      34.886  14.092  -2.496  1.00 43.21      C
ATOM   2390  O   LYS C  64      35.878  13.779  -1.795  1.00 42.92      O
ATOM   2391  N   SER C  65      33.699  14.441  -1.992  1.00 41.43      N
ATOM   2392  CA  SER C  65      33.469  14.458  -0.580  1.00 42.62      C
ATOM   2393  CB  SER C  65      33.231  15.866  -0.083  1.00 43.83      C
ATOM   2394  OG  SER C  65      32.354  16.529  -0.959  1.00 45.50      O
ATOM   2395  C   SER C  65      32.347  13.565  -0.135  1.00 42.45      C
ATOM   2396  O   SER C  65      31.421  13.224  -0.874  1.00 40.59      O
ATOM   2397  N   PHE C  66      32.466  13.139   1.103  1.00 42.45      N
ATOM   2398  CA  PHE C  66      31.473  12.198   1.636  1.00 43.16      C
ATOM   2399  CB  PHE C  66      31.730  10.756   1.181  1.00 42.27      C
ATOM   2400  CG  PHE C  66      33.099  10.222   1.510  1.00 44.09      C
ATOM   2401  CD1 PHE C  66      34.242  10.716   0.857  1.00 42.19      C
ATOM   2402  CE1 PHE C  66      35.517  10.219   1.123  1.00 44.28      C
ATOM   2403  CZ  PHE C  66      35.670   9.175   2.052  1.00 45.40      C
ATOM   2404  CE2 PHE C  66      34.513   8.620   2.721  1.00 43.80      C
ATOM   2405  CD2 PHE C  66      33.244   9.152   2.449  1.00 46.12      C
ATOM   2406  C   PHE C  66      31.421  12.354   3.123  1.00 43.16      C
ATOM   2407  O   PHE C  66      32.351  12.914   3.730  1.00 43.47      O
ATOM   2408  N   SER C  67      30.295  12.004   3.716  1.00 43.08      N
ATOM   2409  CA  SER C  67      30.192  12.283   5.145  1.00 43.78      C
ATOM   2410  CB  SER C  67      29.498  13.599   5.348  1.00 42.88      C
ATOM   2411  OG  SER C  67      28.148  13.307   5.122  1.00 50.83      O
ATOM   2412  C   SER C  67      29.420  11.172   5.783  1.00 42.30      C
ATOM   2413  O   SER C  67      28.653  10.502   5.119  1.00 42.27      O
ATOM   2414  N   LEU C  68      29.704  10.935   7.050  1.00 40.76      N
ATOM   2415  CA  LEU C  68      28.938  10.035   7.877  1.00 39.22      C
ATOM   2416  CB  LEU C  68      29.870   9.117   8.675  1.00 39.26      C
ATOM   2417  CG  LEU C  68      29.519   7.673   9.067  1.00 39.79      C
ATOM   2418  CD1 LEU C  68      30.187   7.273  10.332  1.00 36.92      C
ATOM   2419  CD2 LEU C  68      28.064   7.184   8.998  1.00 41.23      C
ATOM   2420  C   LEU C  68      28.281  10.919   8.932  1.00 38.92      C
ATOM   2421  O   LEU C  68      28.962  11.636   9.668  1.00 36.62      O
ATOM   2422  N   ARG C  69      26.988  10.734   9.088  1.00 38.05      N
ATOM   2423  CA  ARG C  69      26.216  11.297  10.182  1.00 38.81      C
ATOM   2424  CB  ARG C  69      24.957  12.018   9.603  1.00 37.83      C
ATOM   2425  CG  ARG C  69      24.394  12.996  10.666  1.00 42.79      C
ATOM   2426  CD  ARG C  69      23.175  13.730  10.200  1.00 53.15      C
ATOM   2427  NE  ARG C  69      23.050  14.889  11.076  1.00 60.64      N
ATOM   2428  CZ  ARG C  69      22.234  14.973  12.136  1.00 64.79      C
ATOM   2429  NH1 ARG C  69      21.415  13.954  12.452  1.00 64.71      N
ATOM   2430  NH2 ARG C  69      22.227  16.089  12.882  1.00 64.93      N
ATOM   2431  C   ARG C  69      25.714  10.174  11.063  1.00 38.49      C
ATOM   2432  O   ARG C  69      25.016   9.296  10.576  1.00 38.05      O
ATOM   2433  N   ILE C  70      26.036  10.204  12.355  1.00 38.71      N
ATOM   2434  CA  ILE C  70      25.420   9.290  13.321  1.00 38.97      C
ATOM   2435  CB  ILE C  70      26.478   8.582  14.218  1.00 39.33      C
ATOM   2436  CG1 ILE C  70      27.623   8.001  13.370  1.00 41.07      C
ATOM   2437  CD1 ILE C  70      28.826   7.749  14.203  1.00 42.56      C
ATOM   2438  CG2 ILE C  70      25.853   7.519  15.050  1.00 36.50      C
ATOM   2439  C   ILE C  70      24.425  10.106  14.188  1.00 38.51      C
ATOM   2440  O   ILE C  70      24.863  10.970  14.928  1.00 38.32      O
ATOM   2441  N   SER C  71      23.124   9.833  14.069  1.00 36.88      N
ATOM   2442  CA  SER C  71      22.084  10.437  14.955  1.00 38.63      C
ATOM   2443  CB  SER C  71      20.691  10.355  14.353  1.00 36.29      C
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ATOM	2444	OG	SER	C	71	20.721	10.830	13.058	1.00	42.47	O
ATOM	2445	C	SER	C	71	21.938	9.783	16.308	1.00	37.24	C
ATOM	2446	O	SER	C	71	22.280	8.640	16.509	1.00	39.57	O
ATOM	2447	N	ASP	C	72	21.394	10.530	17.218	1.00	37.94	N
ATOM	2448	CA	ASP	C	72	21.064	10.056	18.525	1.00	38.88	C
ATOM	2449	CB	ASP	C	72	19.761	9.261	18.465	1.00	38.48	C
ATOM	2450	CG	ASP	C	72	19.127	9.150	19.805	1.00	40.88	C
ATOM	2451	OD1	ASP	C	72	19.397	10.036	20.649	1.00	41.95	O
ATOM	2452	OD2	ASP	C	72	18.355	8.204	20.029	1.00	46.35	O
ATOM	2453	C	ASP	C	72	22.192	9.248	19.194	1.00	39.02	C
ATOM	2454	O	ASP	C	72	21.996	8.088	19.548	1.00	40.28	O
ATOM	2455	N	LEU	C	73	23.354	9.857	19.369	1.00	38.81	N
ATOM	2456	CA	LEU	C	73	24.525	9.137	19.900	1.00	39.26	C
ATOM	2457	CB	LEU	C	73	25.754	10.076	20.004	1.00	38.40	C
ATOM	2458	CG	LEU	C	73	26.271	10.505	18.635	1.00	37.52	C
ATOM	2459	CD1	LEU	C	73	27.086	11.766	18.820	1.00	36.13	C
ATOM	2460	CD2	LEU	C	73	27.118	9.367	18.077	1.00	35.66	C
ATOM	2461	C	LEU	C	73	24.290	8.464	21.258	1.00	38.78	C
ATOM	2462	O	LEU	C	73	23.600	9.018	22.132	1.00	38.58	O
ATOM	2463	N	ARG	C	74	24.851	7.275	21.430	1.00	38.74	N
ATOM	2464	CA	ARG	C	74	24.881	6.575	22.744	1.00	40.73	C
ATOM	2465	CB	ARG	C	74	24.123	5.247	22.684	1.00	40.63	C
ATOM	2466	CG	ARG	C	74	23.674	4.750	21.330	1.00	44.45	C
ATOM	2467	CD	ARG	C	74	22.291	5.411	21.028	1.00	52.00	C
ATOM	2468	NE	ARG	C	74	21.296	4.424	20.582	1.00	57.73	N
ATOM	2469	CZ	ARG	C	74	20.034	4.701	20.272	1.00	54.39	C
ATOM	2470	NH1	ARG	C	74	19.236	3.719	19.917	1.00	55.75	N
ATOM	2471	NH2	ARG	C	74	19.588	5.942	20.292	1.00	49.28	N
ATOM	2472	C	ARG	C	74	26.351	6.305	23.159	1.00	41.08	C
ATOM	2473	O	ARG	C	74	27.223	6.297	22.283	1.00	39.54	O
ATOM	2474	N	VAL	C	75	26.629	6.061	24.453	1.00	41.83	N
ATOM	2475	CA	VAL	C	75	28.019	5.793	24.874	1.00	42.82	C
ATOM	2476	CB	VAL	C	75	28.167	5.434	26.383	1.00	42.84	C
ATOM	2477	CG1	VAL	C	75	27.517	6.484	27.263	1.00	42.05	C
ATOM	2478	CG2	VAL	C	75	27.552	4.094	26.683	1.00	44.76	C
ATOM	2479	C	VAL	C	75	28.658	4.705	24.017	1.00	43.85	C
ATOM	2480	O	VAL	C	75	29.833	4.797	23.665	1.00	44.32	O
ATOM	2481	N	GLU	C	76	27.888	3.668	23.662	1.00	44.43	N
ATOM	2482	CA	GLU	C	76	28.437	2.562	22.865	1.00	45.15	C
ATOM	2483	CB	GLU	C	76	27.474	1.346	22.799	1.00	46.21	C
ATOM	2484	CG	GLU	C	76	25.983	1.699	22.474	1.00	51.67	C
ATOM	2485	CD	GLU	C	76	25.070	1.966	23.696	1.00	56.22	C
ATOM	2486	OE1	GLU	C	76	23.911	1.494	23.654	1.00	60.97	O
ATOM	2487	OE2	GLU	C	76	25.456	2.651	24.684	1.00	58.26	O
ATOM	2488	C	GLU	C	76	28.927	3.022	21.474	1.00	44.53	C
ATOM	2489	O	GLU	C	76	29.708	2.291	20.812	1.00	43.93	O
ATOM	2490	N	ASP	C	77	28.535	4.236	21.040	1.00	42.84	N
ATOM	2491	CA	ASP	C	77	29.055	4.766	19.743	1.00	41.95	C
ATOM	2492	CB	ASP	C	77	28.118	5.832	19.168	1.00	42.62	C
ATOM	2493	CG	ASP	C	77	26.752	5.282	18.781	1.00	45.69	C
ATOM	2494	OD1	ASP	C	77	26.657	4.110	18.318	1.00	43.73	O
ATOM	2495	OD2	ASP	C	77	25.773	6.049	18.913	1.00	44.99	O
ATOM	2496	C	ASP	C	77	30.508	5.313	19.846	1.00	40.76	C
ATOM	2497	O	ASP	C	77	31.127	5.640	18.846	1.00	40.30	O
ATOM	2498	N	SER	C	78	31.024	5.464	21.061	1.00	40.14	N
ATOM	2499	CA	SER	C	78	32.383	5.978	21.240	1.00	40.43	C
ATOM	2500	CB	SER	C	78	32.751	6.039	22.716	1.00	38.77	C
ATOM	2501	OG	SER	C	78	31.800	6.795	23.385	1.00	40.31	O
ATOM	2502	C	SER	C	78	33.411	5.118	20.519	1.00	40.44	C
ATOM	2503	O	SER	C	78	33.259	3.898	20.413	1.00	41.58	O
ATOM	2504	N	GLY	C	79	34.456	5.763	20.014	1.00	39.91	N

ATOM	2505	CA	GLY	C	79	35.569	5.065	19.403	1.00	39.20	C
ATOM	2506	C	GLY	C	79	36.243	5.931	18.378	1.00	39.12	C
ATOM	2507	O	GLY	C	79	35.911	7.103	18.272	1.00	38.52	O
ATOM	2508	N	THR	C	80	37.125	5.335	17.584	1.00	39.32	N
ATOM	2509	CA	THR	C	80	37.814	6.062	16.539	1.00	40.74	C
ATOM	2510	CB	THR	C	80	39.345	5.858	16.627	1.00	40.22	C
ATOM	2511	OG1	THR	C	80	39.806	6.345	17.896	1.00	41.93	O
ATOM	2512	CG2	THR	C	80	40.088	6.585	15.475	1.00	39.67	C
ATOM	2513	C	THR	C	80	37.331	5.592	15.192	1.00	41.67	C
ATOM	2514	O	THR	C	80	37.464	4.406	14.867	1.00	42.93	O
ATOM	2515	N	TYR	C	81	36.797	6.532	14.413	1.00	41.16	N
ATOM	2516	CA	TYR	C	81	36.235	6.302	13.098	1.00	41.38	C
ATOM	2517	CB	TYR	C	81	34.934	7.118	12.928	1.00	41.71	C
ATOM	2518	CG	TYR	C	81	33.832	6.627	13.831	1.00	41.50	C
ATOM	2519	CD1	TYR	C	81	32.840	5.753	13.343	1.00	42.16	C
ATOM	2520	CE1	TYR	C	81	31.777	5.275	14.208	1.00	37.37	C
ATOM	2521	CZ	TYR	C	81	31.752	5.716	15.516	1.00	42.71	C
ATOM	2522	OH	TYR	C	81	30.763	5.238	16.353	1.00	44.53	O
ATOM	2523	CE2	TYR	C	81	32.747	6.575	16.023	1.00	41.06	C
ATOM	2524	CD2	TYR	C	81	33.763	7.031	15.181	1.00	40.89	C
ATOM	2525	C	TYR	C	81	37.221	6.760	12.031	1.00	41.95	C
ATOM	2526	O	TYR	C	81	37.878	7.771	12.247	1.00	42.20	O
ATOM	2527	N	LYS	C	82	37.373	5.968	10.947	1.00	41.37	N
ATOM	2528	CA	LYS	C	82	38.121	6.382	9.764	1.00	42.18	C
ATOM	2529	CB	LYS	C	82	39.448	5.632	9.579	1.00	41.37	C
ATOM	2530	CG	LYS	C	82	40.368	5.886	10.712	1.00	46.60	C
ATOM	2531	CD	LYS	C	82	41.821	5.742	10.339	1.00	52.93	C
ATOM	2532	CE	LYS	C	82	42.613	5.556	11.625	1.00	55.71	C
ATOM	2533	NZ	LYS	C	82	44.075	5.483	11.354	1.00	61.02	N
ATOM	2534	C	LYS	C	82	37.281	6.164	8.540	1.00	41.18	C
ATOM	2535	O	LYS	C	82	36.568	5.188	8.473	1.00	40.69	O
ATOM	2536	N	CYS	C	83	37.420	7.065	7.587	1.00	40.93	N
ATOM	2537	CA	CYS	C	83	36.864	6.904	6.294	1.00	44.17	C
ATOM	2538	CB	CYS	C	83	36.274	8.199	5.799	1.00	43.61	C
ATOM	2539	SG	CYS	C	83	37.465	9.490	5.676	1.00	48.89	S
ATOM	2540	C	CYS	C	83	37.964	6.491	5.319	1.00	45.48	C
ATOM	2541	O	CYS	C	83	39.145	6.776	5.525	1.00	46.68	O
ATOM	2542	N	GLN	C	84	37.567	5.801	4.258	1.00	45.72	N
ATOM	2543	CA	GLN	C	84	38.485	5.529	3.193	1.00	44.76	C
ATOM	2544	CB	GLN	C	84	38.975	4.074	3.282	1.00	44.52	C
ATOM	2545	CG	GLN	C	84	39.885	3.726	2.122	1.00	45.70	C
ATOM	2546	CD	GLN	C	84	40.912	2.652	2.388	1.00	49.09	C
ATOM	2547	OE1	GLN	C	84	42.083	2.752	1.918	1.00	52.22	O
ATOM	2548	NE2	GLN	C	84	40.512	1.628	3.106	1.00	43.81	N
ATOM	2549	C	GLN	C	84	37.809	5.818	1.886	1.00	44.70	C
ATOM	2550	O	GLN	C	84	36.677	5.362	1.628	1.00	45.18	O
ATOM	2551	N	ALA	C	85	38.503	6.588	1.058	1.00	44.54	N
ATOM	2552	CA	ALA	C	85	38.073	6.857	-0.324	1.00	43.12	C
ATOM	2553	CB	ALA	C	85	38.450	8.228	-0.717	1.00	41.23	C
ATOM	2554	C	ALA	C	85	38.750	5.826	-1.261	1.00	43.54	C
ATOM	2555	O	ALA	C	85	40.001	5.667	-1.262	1.00	42.69	O
ATOM	2556	N	PHE	C	86	37.919	5.123	-2.014	1.00	42.31	N
ATOM	2557	CA	PHE	C	86	38.354	4.226	-3.079	1.00	42.97	C
ATOM	2558	CB	PHE	C	86	37.549	2.932	-3.061	1.00	43.29	C
ATOM	2559	CG	PHE	C	86	37.713	2.185	-1.762	1.00	45.80	C
ATOM	2560	CD1	PHE	C	86	36.695	2.201	-0.782	1.00	42.22	C
ATOM	2561	CE1	PHE	C	86	36.905	1.563	0.421	1.00	42.36	C
ATOM	2562	CZ	PHE	C	86	38.101	0.899	0.668	1.00	42.36	C
ATOM	2563	CE2	PHE	C	86	39.105	0.869	-0.301	1.00	42.11	C
ATOM	2564	CD2	PHE	C	86	38.913	1.529	-1.489	1.00	43.32	C
ATOM	2565	C	PHE	C	86	38.206	4.860	-4.425	1.00	42.06	C

ATOM	2566	O	PHE	C	86	37.274	5.618	-4.692	1.00	41.81	O
ATOM	2567	N	TYR	C	87	39.169	4.558	-5.277	1.00	42.72	N
ATOM	2568	CA	TYR	C	87	39.184	5.052	-6.646	1.00	42.08	C
ATOM	2569	CB	TYR	C	87	39.938	6.398	-6.719	1.00	43.64	C
ATOM	2570	CG	TYR	C	87	41.182	6.458	-5.859	1.00	44.34	C
ATOM	2571	CD1	TYR	C	87	41.161	7.043	-4.589	1.00	46.58	C
ATOM	2572	CE1	TYR	C	87	42.332	7.098	-3.787	1.00	46.11	C
ATOM	2573	CZ	TYR	C	87	43.502	6.541	-4.268	1.00	47.59	C
ATOM	2574	OH	TYR	C	87	44.668	6.553	-3.504	1.00	48.00	O
ATOM	2575	CE2	TYR	C	87	43.538	5.961	-5.531	1.00	47.66	C
ATOM	2576	CD2	TYR	C	87	42.385	5.926	-6.320	1.00	48.34	C
ATOM	2577	C	TYR	C	87	39.850	3.971	-7.494	1.00	41.63	C
ATOM	2578	O	TYR	C	87	40.505	3.080	-6.962	1.00	40.18	O
ATOM	2579	N	VAL	C	88	39.649	4.060	-8.807	1.00	40.58	N
ATOM	2580	CA	VAL	C	88	40.190	3.116	-9.791	1.00	38.74	C
ATOM	2581	CB	VAL	C	88	39.090	2.177	-10.417	1.00	38.40	C
ATOM	2582	CG1	VAL	C	88	38.522	1.217	-9.367	1.00	35.07	C
ATOM	2583	CG2	VAL	C	88	37.906	2.991	-11.012	1.00	37.81	C
ATOM	2584	C	VAL	C	88	40.912	3.876	-10.888	1.00	38.92	C
ATOM	2585	O	VAL	C	88	40.597	5.063	-11.145	1.00	38.50	O
ATOM	2586	N	PHE	C	89	41.883	3.200	-11.534	1.00	37.31	N
ATOM	2587	CA	PHE	C	89	42.656	3.790	-12.610	1.00	36.15	C
ATOM	2588	CB	PHE	C	89	43.787	4.711	-12.062	1.00	36.75	C
ATOM	2589	CG	PHE	C	89	44.555	4.132	-10.846	1.00	36.77	C
ATOM	2590	CD1	PHE	C	89	44.066	4.284	-9.550	1.00	38.64	C
ATOM	2591	CE1	PHE	C	89	44.743	3.751	-8.429	1.00	36.48	C
ATOM	2592	CZ	PHE	C	89	45.932	3.067	-8.631	1.00	39.07	C
ATOM	2593	CE2	PHE	C	89	46.401	2.894	-9.914	1.00	37.47	C
ATOM	2594	CD2	PHE	C	89	45.720	3.431	-11.009	1.00	35.24	C
ATOM	2595	C	PHE	C	89	43.291	2.637	-13.345	1.00	37.04	C
ATOM	2596	O	PHE	C	89	43.464	1.544	-12.808	1.00	34.79	O
ATOM	2597	N	PHE	C	90	43.645	2.885	-14.591	1.00	36.52	N
ATOM	2598	CA	PHE	C	90	44.378	1.903	-15.331	1.00	37.25	C
ATOM	2599	CB	PHE	C	90	44.357	2.209	-16.812	1.00	36.55	C
ATOM	2600	CG	PHE	C	90	43.017	1.968	-17.458	1.00	35.98	C
ATOM	2601	CD1	PHE	C	90	42.555	0.662	-17.653	1.00	37.27	C
ATOM	2602	CE1	PHE	C	90	41.365	0.403	-18.313	1.00	35.06	C
ATOM	2603	CZ	PHE	C	90	40.588	1.508	-18.772	1.00	40.72	C
ATOM	2604	CE2	PHE	C	90	41.050	2.842	-18.572	1.00	35.96	C
ATOM	2605	CD2	PHE	C	90	42.266	3.045	-17.941	1.00	30.26	C
ATOM	2606	C	PHE	C	90	45.793	1.765	-14.824	1.00	38.44	C
ATOM	2607	O	PHE	C	90	46.373	2.754	-14.304	1.00	37.09	O
ATOM	2608	N	ALA	C	91	46.305	0.523	-14.949	1.00	38.72	N
ATOM	2609	CA	ALA	C	91	47.654	0.146	-14.505	1.00	40.42	C
ATOM	2610	CB	ALA	C	91	47.942	-1.248	-14.918	1.00	39.03	C
ATOM	2611	C	ALA	C	91	48.790	1.067	-14.986	1.00	41.68	C
ATOM	2612	O	ALA	C	91	49.730	1.312	-14.221	1.00	42.62	O
ATOM	2613	N	GLU	C	92	48.683	1.578	-16.211	1.00	42.40	N
ATOM	2614	CA	GLU	C	92	49.667	2.488	-16.825	1.00	45.96	C
ATOM	2615	CB	GLU	C	92	49.609	2.365	-18.350	1.00	46.83	C
ATOM	2616	CG	GLU	C	92	49.960	0.958	-18.882	1.00	54.78	C
ATOM	2617	CD	GLU	C	92	51.461	0.705	-19.228	1.00	65.73	C
ATOM	2618	OE1	GLU	C	92	51.753	0.838	-20.455	1.00	68.70	O
ATOM	2619	OE2	GLU	C	92	52.324	0.333	-18.328	1.00	67.00	O
ATOM	2620	C	GLU	C	92	49.561	3.991	-16.450	1.00	46.75	C
ATOM	2621	O	GLU	C	92	50.310	4.807	-16.965	1.00	47.85	O
ATOM	2622	N	ASP	C	93	48.622	4.360	-15.586	1.00	46.84	N
ATOM	2623	CA	ASP	C	93	48.578	5.692	-14.997	1.00	47.98	C
ATOM	2624	CB	ASP	C	93	47.402	5.780	-14.024	1.00	48.91	C
ATOM	2625	CG	ASP	C	93	47.048	7.201	-13.702	1.00	53.37	C
ATOM	2626	OD1	ASP	C	93	47.669	7.763	-12.756	1.00	59.02	O

ATOM	2627	OD2	ASP	C	93	46.171	7.745	-14.411	1.00	52.66	O
ATOM	2628	C	ASP	C	93	49.855	5.869	-14.185	1.00	46.99	C
ATOM	2629	O	ASP	C	93	50.113	5.046	-13.293	1.00	48.62	O
ATOM	2630	N	VAL	C	94	50.638	6.908	-14.499	1.00	43.77	N
ATOM	2631	CA	VAL	C	94	51.934	7.192	-13.906	1.00	40.69	C
ATOM	2632	CB	VAL	C	94	53.120	6.915	-14.893	1.00	40.79	C
ATOM	2633	CG1	VAL	C	94	52.921	7.686	-16.247	1.00	38.04	C
ATOM	2634	CG2	VAL	C	94	53.260	5.446	-15.184	1.00	38.24	C
ATOM	2635	C	VAL	C	94	51.966	8.674	-13.471	1.00	40.53	C
ATOM	2636	O	VAL	C	94	51.209	9.479	-13.973	1.00	39.56	O
ATOM	2637	N	GLY	C	95	52.867	9.022	-12.553	1.00	40.49	N
ATOM	2638	CA	GLY	C	95	53.050	10.415	-12.093	1.00	38.78	C
ATOM	2639	C	GLY	C	95	52.272	10.847	-10.852	1.00	38.81	C
ATOM	2640	O	GLY	C	95	52.535	11.890	-10.335	1.00	40.05	O
ATOM	2641	N	SER	C	96	51.312	10.069	-10.362	1.00	37.58	N
ATOM	2642	CA	SER	C	96	50.546	10.497	-9.227	1.00	39.65	C
ATOM	2643	CB	SER	C	96	49.053	10.780	-9.608	1.00	39.56	C
ATOM	2644	OG	SER	C	96	49.035	11.894	-10.504	1.00	43.48	O
ATOM	2645	C	SER	C	96	50.567	9.465	-8.136	1.00	39.35	C
ATOM	2646	O	SER	C	96	50.517	8.279	-8.401	1.00	39.38	O
ATOM	2647	N	ASN	C	97	50.640	9.963	-6.915	1.00	39.49	N
ATOM	2648	CA	ASN	C	97	50.421	9.178	-5.740	1.00	40.25	C
ATOM	2649	CB	ASN	C	97	50.339	10.076	-4.528	1.00	38.65	C
ATOM	2650	CG	ASN	C	97	50.340	9.274	-3.160	1.00	44.04	C
ATOM	2651	OD1	ASN	C	97	50.540	9.865	-2.086	1.00	43.90	O
ATOM	2652	ND2	ASN	C	97	50.135	7.962	-3.221	1.00	43.78	N
ATOM	2653	C	ASN	C	97	49.107	8.442	-5.898	1.00	38.81	C
ATOM	2654	O	ASN	C	97	48.018	9.028	-5.895	1.00	39.38	O
ATOM	2655	N	LYS	C	98	49.235	7.141	-5.999	1.00	38.34	N
ATOM	2656	CA	LYS	C	98	48.109	6.210	-6.077	1.00	37.85	C
ATOM	2657	CB	LYS	C	98	48.641	4.910	-6.704	1.00	37.89	C
ATOM	2658	CG	LYS	C	98	49.077	5.156	-8.197	1.00	34.79	C
ATOM	2659	CD	LYS	C	98	49.488	3.865	-8.838	1.00	40.63	C
ATOM	2660	CE	LYS	C	98	49.867	4.054	-10.316	1.00	40.81	C
ATOM	2661	NZ	LYS	C	98	51.073	4.918	-10.448	1.00	38.45	N
ATOM	2662	C	LYS	C	98	47.375	5.892	-4.755	1.00	39.19	C
ATOM	2663	O	LYS	C	98	46.408	5.154	-4.777	1.00	38.96	O
ATOM	2664	N	GLY	C	99	47.858	6.420	-3.636	1.00	38.59	N
ATOM	2665	CA	GLY	C	99	47.449	5.964	-2.296	1.00	40.76	C
ATOM	2666	C	GLY	C	99	47.880	4.530	-2.081	1.00	41.30	C
ATOM	2667	O	GLY	C	99	48.795	4.036	-2.767	1.00	43.80	O
ATOM	2668	N	ALA	C	100	47.248	3.856	-1.143	1.00	40.11	N
ATOM	2669	CA	ALA	C	100	47.560	2.475	-0.883	1.00	39.38	C
ATOM	2670	CB	ALA	C	100	46.860	2.024	0.434	1.00	39.23	C
ATOM	2671	C	ALA	C	100	46.989	1.713	-2.025	1.00	39.51	C
ATOM	2672	O	ALA	C	100	45.893	2.022	-2.468	1.00	39.92	O
ATOM	2673	N	ILE	C	101	47.710	0.705	-2.490	1.00	39.69	N
ATOM	2674	CA	ILE	C	101	47.214	-0.164	-3.542	1.00	39.24	C
ATOM	2675	CB	ILE	C	101	48.382	-0.869	-4.334	1.00	39.71	C
ATOM	2676	CG1	ILE	C	101	49.331	0.190	-5.017	1.00	39.84	C
ATOM	2677	CD1	ILE	C	101	48.627	1.159	-5.924	1.00	36.72	C
ATOM	2678	CG2	ILE	C	101	47.804	-1.860	-5.378	1.00	35.43	C
ATOM	2679	C	ILE	C	101	46.322	-1.192	-2.832	1.00	40.48	C
ATOM	2680	O	ILE	C	101	46.747	-1.835	-1.875	1.00	39.46	O
ATOM	2681	N	ILE	C	102	45.077	-1.290	-3.277	1.00	41.20	N
ATOM	2682	CA	ILE	C	102	44.077	-2.062	-2.594	1.00	42.13	C
ATOM	2683	CB	ILE	C	102	42.722	-1.275	-2.453	1.00	42.58	C
ATOM	2684	CG1	ILE	C	102	42.912	-0.020	-1.630	1.00	42.57	C
ATOM	2685	CD1	ILE	C	102	43.084	-0.204	-0.096	1.00	41.89	C
ATOM	2686	CG2	ILE	C	102	41.542	-2.148	-1.947	1.00	42.41	C
ATOM	2687	C	ILE	C	102	43.887	-3.331	-3.396	1.00	41.41	C

ATOM	2688	O	ILE	C	102	43.698	-4.376	-2.821	1.00	42.57	O
ATOM	2689	N	GLY	C	103	43.942	-3.261	-4.715	1.00	40.57	N
ATOM	2690	CA	GLY	C	103	43.742	-4.479	-5.498	1.00	38.60	C
ATOM	2691	C	GLY	C	103	44.033	-4.305	-6.974	1.00	37.22	C
ATOM	2692	O	GLY	C	103	44.253	-3.238	-7.441	1.00	37.08	O
ATOM	2693	N	LEU	C	104	44.060	-5.393	-7.704	1.00	38.36	N
ATOM	2694	CA	LEU	C	104	44.255	-5.381	-9.148	1.00	39.71	C
ATOM	2695	CB	LEU	C	104	45.653	-5.917	-9.493	1.00	39.02	C
ATOM	2696	CG	LEU	C	104	46.002	-6.069	-10.973	1.00	40.16	C
ATOM	2697	CD1	LEU	C	104	45.968	-4.664	-11.690	1.00	34.76	C
ATOM	2698	CD2	LEU	C	104	47.334	-6.727	-11.161	1.00	38.01	C
ATOM	2699	C	LEU	C	104	43.142	-6.283	-9.728	1.00	41.24	C
ATOM	2700	O	LEU	C	104	42.985	-7.408	-9.276	1.00	38.88	O
ATOM	2701	N	MET	C	105	42.368	-5.743	-10.678	1.00	43.67	N
ATOM	2702	CA	MET	C	105	41.297	-6.447	-11.366	1.00	47.58	C
ATOM	2703	CB	MET	C	105	40.101	-5.568	-11.687	1.00	47.39	C
ATOM	2704	CG	MET	C	105	39.496	-4.652	-10.666	1.00	50.10	C
ATOM	2705	SD	MET	C	105	37.752	-4.217	-11.239	1.00	57.87	S
ATOM	2706	CE	MET	C	105	37.532	-4.959	-12.846	1.00	54.27	C
ATOM	2707	C	MET	C	105	41.835	-6.794	-12.704	1.00	47.26	C
ATOM	2708	O	MET	C	105	42.684	-6.094	-13.231	1.00	47.11	O
ATOM	2709	N	VAL	C	106	41.329	-7.879	-13.266	1.00	48.20	N
ATOM	2710	CA	VAL	C	106	41.630	-8.250	-14.630	1.00	49.68	C
ATOM	2711	CB	VAL	C	106	41.031	-9.665	-14.914	1.00	50.52	C
ATOM	2712	CG1	VAL	C	106	41.298	-10.144	-16.355	1.00	51.88	C
ATOM	2713	CG2	VAL	C	106	41.664	-10.679	-13.916	1.00	51.57	C
ATOM	2714	C	VAL	C	106	41.214	-7.095	-15.602	1.00	48.70	C
ATOM	2715	O	VAL	C	106	40.269	-6.361	-15.355	1.00	49.46	O
ATOM	2716	N	GLY	C	107	42.012	-6.859	-16.629	1.00	48.36	N
ATOM	2717	CA	GLY	C	107	41.763	-5.713	-17.516	1.00	47.26	C
ATOM	2718	C	GLY	C	107	42.676	-4.536	-17.234	1.00	45.75	C
ATOM	2719	O	GLY	C	107	42.501	-3.459	-17.799	1.00	46.81	O
ATOM	2720	N	GLY	C	108	43.627	-4.736	-16.328	1.00	43.80	N
ATOM	2721	CA	GLY	C	108	44.597	-3.735	-15.974	1.00	42.42	C
ATOM	2722	C	GLY	C	108	44.050	-2.585	-15.171	1.00	41.50	C
ATOM	2723	O	GLY	C	108	44.487	-1.448	-15.371	1.00	43.12	O
ATOM	2724	N	VAL	C	109	43.083	-2.852	-14.304	1.00	39.69	N
ATOM	2725	CA	VAL	C	109	42.387	-1.806	-13.556	1.00	37.50	C
ATOM	2726	CB	VAL	C	109	40.845	-1.962	-13.644	1.00	37.78	C
ATOM	2727	CG1	VAL	C	109	40.292	-1.715	-15.041	1.00	32.98	C
ATOM	2728	CG2	VAL	C	109	40.105	-1.033	-12.610	1.00	35.07	C
ATOM	2729	C	VAL	C	109	42.802	-1.942	-12.103	1.00	38.36	C
ATOM	2730	O	VAL	C	109	42.639	-3.027	-11.512	1.00	36.60	O
ATOM	2731	N	VAL	C	110	43.336	-0.870	-11.513	1.00	37.27	N
ATOM	2732	CA	VAL	C	110	43.845	-0.955	-10.160	1.00	37.80	C
ATOM	2733	CB	VAL	C	110	45.245	-0.371	-10.070	1.00	38.39	C
ATOM	2734	CG1	VAL	C	110	46.115	-1.019	-11.123	1.00	35.91	C
ATOM	2735	CG2	VAL	C	110	45.851	-0.565	-8.672	1.00	34.68	C
ATOM	2736	C	VAL	C	110	42.897	-0.237	-9.248	1.00	39.02	C
ATOM	2737	O	VAL	C	110	42.247	0.697	-9.695	1.00	38.55	O
ATOM	2738	N	ILE	C	111	42.743	-0.718	-8.010	1.00	39.64	N
ATOM	2739	CA	ILE	C	111	41.985	-0.007	-6.976	1.00	40.38	C
ATOM	2740	CB	ILE	C	111	41.039	-0.966	-6.233	1.00	40.84	C
ATOM	2741	CG1	ILE	C	111	40.202	-1.806	-7.257	1.00	43.74	C
ATOM	2742	CD1	ILE	C	111	39.645	-3.116	-6.586	1.00	44.34	C
ATOM	2743	CG2	ILE	C	111	40.111	-0.240	-5.264	1.00	40.12	C
ATOM	2744	C	ILE	C	111	42.995	0.553	-6.005	1.00	40.90	C
ATOM	2745	O	ILE	C	111	43.911	-0.155	-5.522	1.00	40.15	O
ATOM	2746	N	GLY	C	112	42.870	1.839	-5.722	1.00	41.79	N
ATOM	2747	CA	GLY	C	112	43.727	2.465	-4.695	1.00	41.67	C
ATOM	2748	C	GLY	C	112	42.804	3.024	-3.631	1.00	42.53	C

ATOM	2749	O	GLY	C	112	41.599	3.097	-3.837	1.00	42.69	O
ATOM	2750	N	GLY	C	113	43.352	3.378	-2.479	1.00	42.32	N
ATOM	2751	CA	GLY	C	113	42.544	3.983	-1.444	1.00	42.68	C
ATOM	2752	C	GLY	C	113	43.431	4.872	-0.602	1.00	43.14	C
ATOM	2753	O	GLY	C	113	44.645	4.595	-0.482	1.00	42.77	O
ATOM	2754	N	GLU	C	114	42.829	5.961	-0.105	1.00	43.84	N
ATOM	2755	CA	GLU	C	114	43.389	6.874	0.895	1.00	45.57	C
ATOM	2756	CB	GLU	C	114	43.530	8.314	0.328	1.00	46.12	C
ATOM	2757	CG	GLU	C	114	44.677	8.540	-0.659	1.00	48.41	C
ATOM	2758	CD	GLU	C	114	46.012	8.648	0.104	1.00	53.32	C
ATOM	2759	OE1	GLU	C	114	45.961	8.894	1.318	1.00	54.08	O
ATOM	2760	OE2	GLU	C	114	47.105	8.460	-0.484	1.00	53.74	O
ATOM	2761	C	GLU	C	114	42.434	6.922	2.110	1.00	45.53	C
ATOM	2762	O	GLU	C	114	41.258	7.185	1.933	1.00	44.18	O
ATOM	2763	N	LYS	C	115	42.973	6.750	3.330	1.00	45.32	N
ATOM	2764	CA	LYS	C	115	42.202	6.844	4.591	1.00	44.84	C
ATOM	2765	CB	LYS	C	115	42.676	5.771	5.567	1.00	46.12	C
ATOM	2766	CG	LYS	C	115	42.435	4.362	5.125	1.00	51.00	C
ATOM	2767	CD	LYS	C	115	42.795	3.392	6.277	1.00	58.28	C
ATOM	2768	CE	LYS	C	115	41.567	2.885	7.055	1.00	57.90	C
ATOM	2769	NZ	LYS	C	115	41.949	1.742	8.016	1.00	54.76	N
ATOM	2770	C	LYS	C	115	42.365	8.197	5.290	1.00	44.22	C
ATOM	2771	O	LYS	C	115	43.431	8.823	5.252	1.00	43.62	O
ATOM	2772	N	GLY	C	116	41.305	8.645	5.954	1.00	43.05	N
ATOM	2773	CA	GLY	C	116	41.356	9.864	6.689	1.00	42.05	C
ATOM	2774	C	GLY	C	116	42.174	9.631	7.930	1.00	42.35	C
ATOM	2775	O	GLY	C	116	42.452	8.484	8.287	1.00	42.05	O
ATOM	2776	N	ALA	C	117	42.571	10.708	8.596	1.00	42.37	N
ATOM	2777	CA	ALA	C	117	43.399	10.550	9.757	1.00	43.05	C
ATOM	2778	CB	ALA	C	117	44.260	11.829	10.014	1.00	42.67	C
ATOM	2779	C	ALA	C	117	42.634	10.084	11.023	1.00	43.56	C
ATOM	2780	O	ALA	C	117	43.246	9.826	12.055	1.00	43.65	O
ATOM	2781	N	GLY	C	118	41.314	9.951	10.965	1.00	43.66	N
ATOM	2782	CA	GLY	C	118	40.611	9.472	12.152	1.00	42.79	C
ATOM	2783	C	GLY	C	118	39.896	10.562	12.934	1.00	41.73	C
ATOM	2784	O	GLY	C	118	40.354	11.701	12.976	1.00	40.92	O
ATOM	2785	N	THR	C	119	38.743	10.194	13.496	1.00	39.98	N
ATOM	2786	CA	THR	C	119	37.946	11.020	14.384	1.00	38.58	C
ATOM	2787	CB	THR	C	119	36.488	11.253	13.783	1.00	39.57	C
ATOM	2788	OG1	THR	C	119	36.588	12.076	12.602	1.00	38.54	O
ATOM	2789	CG2	THR	C	119	35.520	11.976	14.801	1.00	36.85	C
ATOM	2790	C	THR	C	119	37.848	10.245	15.679	1.00	38.20	C
ATOM	2791	O	THR	C	119	37.235	9.181	15.707	1.00	38.00	O
ATOM	2792	N	ALA	C	120	38.444	10.762	16.760	1.00	39.02	N
ATOM	2793	CA	ALA	C	120	38.267	10.190	18.104	1.00	38.01	C
ATOM	2794	CB	ALA	C	120	39.460	10.554	19.000	1.00	37.67	C
ATOM	2795	C	ALA	C	120	36.956	10.710	18.698	1.00	38.14	C
ATOM	2796	O	ALA	C	120	36.900	11.849	19.022	1.00	38.99	O
ATOM	2797	N	LEU	C	121	35.904	9.888	18.786	1.00	37.88	N
ATOM	2798	CA	LEU	C	121	34.606	10.267	19.338	1.00	37.54	C
ATOM	2799	CB	LEU	C	121	33.405	9.771	18.456	1.00	37.32	C
ATOM	2800	CG	LEU	C	121	32.005	9.892	19.096	1.00	36.95	C
ATOM	2801	CD1	LEU	C	121	31.645	11.412	19.345	1.00	30.48	C
ATOM	2802	CD2	LEU	C	121	30.953	9.178	18.323	1.00	36.88	C
ATOM	2803	C	LEU	C	121	34.449	9.684	20.736	1.00	39.77	C
ATOM	2804	O	LEU	C	121	34.550	8.474	20.921	1.00	39.94	O
ATOM	2805	N	THR	C	122	34.231	10.558	21.715	1.00	39.58	N
ATOM	2806	CA	THR	C	122	33.743	10.128	23.012	1.00	42.41	C
ATOM	2807	CB	THR	C	122	34.744	10.283	24.221	1.00	42.49	C
ATOM	2808	OG1	THR	C	122	34.066	10.807	25.351	1.00	47.39	O
ATOM	2809	CG2	THR	C	122	35.975	11.103	23.923	1.00	44.50	C

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ATOM   2810  C   THR C 122      32.368  10.695  23.269  1.00 41.60      C
ATOM   2811  O   THR C 122      32.115  11.879  22.992  1.00 40.70      O
ATOM   2812  N   VAL C 123      31.465   9.800  23.664  1.00 41.20      N
ATOM   2813  CA  VAL C 123      30.065  10.141  23.928  1.00 41.97      C
ATOM   2814  CB  VAL C 123      29.040   9.174  23.218  1.00 41.64      C
ATOM   2815  CG1 VAL C 123      27.572   9.521  23.597  1.00 38.86      C
ATOM   2816  CG2 VAL C 123      29.222   9.177  21.701  1.00 36.97      C
ATOM   2817  C   VAL C 123      29.901  10.060  25.442  1.00 43.60      C
ATOM   2818  O   VAL C 123      30.189   9.036  26.029  1.00 43.27      O
ATOM   2819  N   LYS C 124      29.459  11.137  26.070  1.00 46.27      N
ATOM   2820  CA  LYS C 124      29.335  11.162  27.519  1.00 50.07      C
ATOM   2821  CB  LYS C 124      29.566  12.574  28.019  1.00 51.04      C
ATOM   2822  CG  LYS C 124      30.992  13.088  27.721  1.00 55.46      C
ATOM   2823  CD  LYS C 124      31.184  14.509  28.264  1.00 62.63      C
ATOM   2824  CE  LYS C 124      30.287  15.512  27.491  1.00 64.83      C
ATOM   2825  NZ  LYS C 124      30.202  16.850  28.169  1.00 67.51      N
ATOM   2826  C   LYS C 124      27.960  10.729  27.900  1.00 51.41      C
ATOM   2827  O   LYS C 124      27.006  11.094  27.223  1.00 53.12      O
ATOM   2828  N   ALA C 125      27.857   9.965  28.982  1.00 53.39      N
ATOM   2829  CA  ALA C 125      26.584   9.427  29.504  1.00 55.35      C
ATOM   2830  CB  ALA C 125      26.828   8.627  30.778  1.00 54.28      C
ATOM   2831  C   ALA C 125      25.485  10.460  29.739  1.00 57.36      C
ATOM   2832  O   ALA C 125      25.745  11.656  29.989  1.00 56.29      O
ATOM   2833  N   ALA C 126      24.240   9.987  29.654  1.00 60.08      N
ATOM   2834  CA  ALA C 126      23.084  10.865  29.877  1.00 62.33      C
ATOM   2835  CB  ALA C 126      21.766  10.076  29.780  1.00 62.64      C
ATOM   2836  C   ALA C 126      23.246  11.540  31.244  1.00 63.68      C
ATOM   2837  O   ALA C 126      23.436  10.871  32.272  1.00 64.15      O
ATOM   2838  OXT ALA C 126      23.253  12.783  31.350  1.00 65.04      O
ATOM   2839  N   ALA D   1      46.173 -30.720 -12.181  1.00 52.41      N
ATOM   2840  CA  ALA D   1      47.352 -29.997 -11.635  1.00 52.38      C
ATOM   2841  CB  ALA D   1      47.073 -28.463 -11.586  1.00 52.73      C
ATOM   2842  C   ALA D   1      47.756 -30.484 -10.247  1.00 52.06      C
ATOM   2843  O   ALA D   1      47.324 -29.889  -9.245  1.00 52.92      O
ATOM   2844  N   TRP D   2      48.618 -31.503 -10.174  1.00 50.77      N
ATOM   2845  CA  TRP D   2      49.207 -31.901  -8.886  1.00 49.15      C
ATOM   2846  CB  TRP D   2      48.379 -33.027  -8.243  1.00 49.04      C
ATOM   2847  CG  TRP D   2      48.455 -34.342  -8.948  1.00 48.39      C
ATOM   2848  CD1 TRP D   2      47.909 -34.665 -10.162  1.00 48.80      C
ATOM   2849  NE1 TRP D   2      48.181 -35.993 -10.473  1.00 47.88      N
ATOM   2850  CE2 TRP D   2      48.915 -36.540  -9.456  1.00 48.78      C
ATOM   2851  CD2 TRP D   2      49.105 -35.532  -8.474  1.00 48.50      C
ATOM   2852  CE3 TRP D   2      49.816 -35.851  -7.312  1.00 49.44      C
ATOM   2853  CZ3 TRP D   2      50.318 -37.152  -7.169  1.00 48.14      C
ATOM   2854  CH2 TRP D   2      50.130 -38.111  -8.167  1.00 48.46      C
ATOM   2855  CZ2 TRP D   2      49.430 -37.833  -9.311  1.00 48.68      C
ATOM   2856  C   TRP D   2      50.692 -32.283  -8.969  1.00 48.37      C
ATOM   2857  O   TRP D   2      51.129 -32.808  -9.982  1.00 47.97      O
ATOM   2858  N   VAL D   3      51.447 -32.014  -7.892  1.00 47.21      N
ATOM   2859  CA  VAL D   3      52.880 -32.359  -7.783  1.00 46.09      C
ATOM   2860  CB  VAL D   3      53.713 -31.248  -7.051  1.00 45.63      C
ATOM   2861  CG1 VAL D   3      55.086 -31.739  -6.681  1.00 45.70      C
ATOM   2862  CG2 VAL D   3      53.857 -30.036  -7.931  1.00 45.94      C
ATOM   2863  C   VAL D   3      53.042 -33.724  -7.090  1.00 45.51      C
ATOM   2864  O   VAL D   3      52.541 -33.953  -5.995  1.00 45.34      O
ATOM   2865  N   ASP D   4      53.726 -34.629  -7.766  1.00 44.30      N
ATOM   2866  CA  ASP D   4      53.861 -36.002  -7.344  1.00 43.85      C
ATOM   2867  CB  ASP D   4      53.638 -36.897  -8.574  1.00 43.56      C
ATOM   2868  CG  ASP D   4      53.731 -38.385  -8.283  1.00 46.38      C
ATOM   2869  OD1 ASP D   4      53.456 -39.152  -9.224  1.00 48.84      O
ATOM   2870  OD2 ASP D   4      54.085 -38.824  -7.165  1.00 49.73      O
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ATOM	2871	C	ASP	D	4	55.282	-36.096	-6.773	1.00	42.85	C
ATOM	2872	O	ASP	D	4	56.260	-36.173	-7.527	1.00	43.36	O
ATOM	2873	N	GLN	D	5	55.399	-36.044	-5.450	1.00	40.53	N
ATOM	2874	CA	GLN	D	5	56.695	-36.068	-4.816	1.00	39.40	C
ATOM	2875	CB	GLN	D	5	56.769	-34.988	-3.723	1.00	38.84	C
ATOM	2876	CG	GLN	D	5	58.080	-34.973	-2.919	1.00	37.60	C
ATOM	2877	CD	GLN	D	5	58.067	-33.903	-1.836	1.00	40.37	C
ATOM	2878	OE1	GLN	D	5	57.169	-33.053	-1.805	1.00	39.68	O
ATOM	2879	NE2	GLN	D	5	59.067	-33.928	-0.944	1.00	37.57	N
ATOM	2880	C	GLN	D	5	56.978	-37.445	-4.208	1.00	39.58	C
ATOM	2881	O	GLN	D	5	56.165	-37.959	-3.443	1.00	39.26	O
ATOM	2882	N	THR	D	6	58.153	-37.997	-4.531	1.00	39.50	N
ATOM	2883	CA	THR	D	6	58.650	-39.281	-4.032	1.00	39.81	C
ATOM	2884	CB	THR	D	6	58.637	-40.379	-5.152	1.00	39.82	C
ATOM	2885	OG1	THR	D	6	59.280	-39.861	-6.318	1.00	41.35	O
ATOM	2886	CG2	THR	D	6	57.202	-40.812	-5.536	1.00	41.10	C
ATOM	2887	C	THR	D	6	60.103	-39.129	-3.536	1.00	39.11	C
ATOM	2888	O	THR	D	6	60.846	-38.306	-4.047	1.00	38.91	O
ATOM	2889	N	PRO	D	7	60.509	-39.925	-2.532	1.00	38.82	N
ATOM	2890	CA	PRO	D	7	59.674	-40.854	-1.771	1.00	38.84	C
ATOM	2891	CB	PRO	D	7	60.708	-41.859	-1.250	1.00	39.29	C
ATOM	2892	CG	PRO	D	7	61.982	-40.990	-1.047	1.00	38.10	C
ATOM	2893	CD	PRO	D	7	61.918	-39.932	-2.080	1.00	38.51	C
ATOM	2894	C	PRO	D	7	58.938	-40.128	-0.616	1.00	38.96	C
ATOM	2895	O	PRO	D	7	59.364	-39.093	-0.218	1.00	38.31	O
ATOM	2896	N	ARG	D	8	57.835	-40.664	-0.098	1.00	40.27	N
ATOM	2897	CA	ARG	D	8	57.128	-40.039	1.046	1.00	40.80	C
ATOM	2898	CB	ARG	D	8	55.743	-40.686	1.236	1.00	40.70	C
ATOM	2899	CG	ARG	D	8	54.775	-40.011	2.223	1.00	45.33	C
ATOM	2900	CD	ARG	D	8	54.283	-38.614	1.746	1.00	52.07	C
ATOM	2901	NE	ARG	D	8	54.080	-38.557	0.289	1.00	54.98	N
ATOM	2902	CZ	ARG	D	8	52.900	-38.616	-0.330	1.00	57.24	C
ATOM	2903	NH1	ARG	D	8	51.758	-38.714	0.359	1.00	56.56	N
ATOM	2904	NH2	ARG	D	8	52.862	-38.549	-1.658	1.00	58.04	N
ATOM	2905	C	ARG	D	8	57.977	-40.100	2.331	1.00	40.53	C
ATOM	2906	O	ARG	D	8	57.929	-39.207	3.158	1.00	40.81	O
ATOM	2907	N	THR	D	9	58.770	-41.153	2.475	1.00	40.47	N
ATOM	2908	CA	THR	D	9	59.629	-41.350	3.634	1.00	40.91	C
ATOM	2909	CB	THR	D	9	58.994	-42.340	4.695	1.00	41.45	C
ATOM	2910	OG1	THR	D	9	58.726	-43.600	4.084	1.00	41.04	O
ATOM	2911	CG2	THR	D	9	57.639	-41.805	5.351	1.00	41.38	C
ATOM	2912	C	THR	D	9	60.999	-41.914	3.169	1.00	41.67	C
ATOM	2913	O	THR	D	9	61.083	-42.696	2.225	1.00	40.23	O
ATOM	2914	N	ALA	D	10	62.064	-41.522	3.868	1.00	42.06	N
ATOM	2915	CA	ALA	D	10	63.392	-42.065	3.635	1.00	41.77	C
ATOM	2916	CB	ALA	D	10	64.160	-41.142	2.735	1.00	42.21	C
ATOM	2917	C	ALA	D	10	64.086	-42.181	4.998	1.00	42.56	C
ATOM	2918	O	ALA	D	10	63.811	-41.387	5.903	1.00	40.53	O
ATOM	2919	N	THR	D	11	64.914	-43.211	5.161	1.00	43.58	N
ATOM	2920	CA	THR	D	11	65.800	-43.354	6.320	1.00	45.06	C
ATOM	2921	CB	THR	D	11	65.427	-44.561	7.235	1.00	45.98	C
ATOM	2922	OG1	THR	D	11	64.100	-44.386	7.754	1.00	48.35	O
ATOM	2923	CG2	THR	D	11	66.423	-44.712	8.442	1.00	45.10	C
ATOM	2924	C	THR	D	11	67.177	-43.562	5.723	1.00	46.01	C
ATOM	2925	O	THR	D	11	67.379	-44.392	4.825	1.00	46.79	O
ATOM	2926	N	LYS	D	12	68.118	-42.766	6.193	1.00	46.59	N
ATOM	2927	CA	LYS	D	12	69.488	-42.806	5.725	1.00	46.11	C
ATOM	2928	CB	LYS	D	12	69.766	-41.586	4.863	1.00	45.49	C
ATOM	2929	CG	LYS	D	12	68.877	-41.544	3.598	1.00	44.78	C
ATOM	2930	CD	LYS	D	12	69.231	-42.666	2.588	1.00	40.67	C
ATOM	2931	CE	LYS	D	12	68.264	-42.658	1.445	1.00	42.32	C

ATOM	2932	NZ	LYS	D	12	68.712	-43.565	0.374	1.00	41.82	N
ATOM	2933	C	LYS	D	12	70.441	-42.847	6.903	1.00	47.39	C
ATOM	2934	O	LYS	D	12	70.080	-42.564	8.065	1.00	46.27	O
ATOM	2935	N	GLU	D	13	71.669	-43.213	6.583	1.00	48.57	N
ATOM	2936	CA	GLU	D	13	72.742	-43.190	7.538	1.00	49.48	C
ATOM	2937	CB	GLU	D	13	73.578	-44.461	7.335	1.00	50.69	C
ATOM	2938	CG	GLU	D	13	73.899	-45.243	8.610	1.00	53.61	C
ATOM	2939	CD	GLU	D	13	75.339	-45.752	8.601	1.00	59.15	C
ATOM	2940	OE1	GLU	D	13	75.609	-46.771	9.288	1.00	59.36	O
ATOM	2941	OE2	GLU	D	13	76.200	-45.139	7.892	1.00	59.86	O
ATOM	2942	C	GLU	D	13	73.534	-41.911	7.193	1.00	48.81	C
ATOM	2943	O	GLU	D	13	73.480	-41.453	6.043	1.00	48.11	O
ATOM	2944	N	THR	D	14	74.259	-41.324	8.155	1.00	48.09	N
ATOM	2945	CA	THR	D	14	75.143	-40.192	7.810	1.00	47.65	C
ATOM	2946	CB	THR	D	14	75.925	-39.621	9.031	1.00	47.59	C
ATOM	2947	OG1	THR	D	14	76.628	-40.678	9.687	1.00	48.03	O
ATOM	2948	CG2	THR	D	14	74.987	-38.998	10.048	1.00	47.29	C
ATOM	2949	C	THR	D	14	76.117	-40.593	6.681	1.00	47.56	C
ATOM	2950	O	THR	D	14	76.583	-41.748	6.620	1.00	47.03	O
ATOM	2951	N	GLY	D	15	76.414	-39.648	5.793	1.00	46.77	N
ATOM	2952	CA	GLY	D	15	77.304	-39.915	4.667	1.00	46.69	C
ATOM	2953	C	GLY	D	15	76.607	-40.296	3.367	1.00	46.34	C
ATOM	2954	O	GLY	D	15	77.083	-39.969	2.293	1.00	46.24	O
ATOM	2955	N	GLU	D	16	75.484	-40.998	3.474	1.00	46.52	N
ATOM	2956	CA	GLU	D	16	74.670	-41.389	2.327	1.00	46.87	C
ATOM	2957	CB	GLU	D	16	73.574	-42.384	2.757	1.00	46.63	C
ATOM	2958	CG	GLU	D	16	74.023	-43.586	3.578	1.00	46.69	C
ATOM	2959	CD	GLU	D	16	72.979	-44.733	3.575	1.00	48.35	C
ATOM	2960	OE1	GLU	D	16	73.193	-45.693	2.807	1.00	53.70	O
ATOM	2961	OE2	GLU	D	16	71.954	-44.705	4.299	1.00	48.55	O
ATOM	2962	C	GLU	D	16	74.003	-40.187	1.632	1.00	46.94	C
ATOM	2963	O	GLU	D	16	74.209	-39.019	1.977	1.00	46.67	O
ATOM	2964	N	SER	D	17	73.174	-40.471	0.637	1.00	47.38	N
ATOM	2965	CA	SER	D	17	72.518	-39.376	-0.056	1.00	47.46	C
ATOM	2966	CB	SER	D	17	73.184	-39.131	-1.410	1.00	48.28	C
ATOM	2967	OG	SER	D	17	72.749	-40.047	-2.416	1.00	52.49	O
ATOM	2968	C	SER	D	17	71.029	-39.642	-0.196	1.00	46.61	C
ATOM	2969	O	SER	D	17	70.588	-40.785	0.001	1.00	46.62	O
ATOM	2970	N	LEU	D	18	70.263	-38.583	-0.477	1.00	44.97	N
ATOM	2971	CA	LEU	D	18	68.829	-38.674	-0.742	1.00	43.88	C
ATOM	2972	CB	LEU	D	18	68.010	-37.924	0.319	1.00	44.17	C
ATOM	2973	CG	LEU	D	18	66.612	-38.336	0.802	1.00	44.22	C
ATOM	2974	CD1	LEU	D	18	65.730	-37.114	0.965	1.00	44.33	C
ATOM	2975	CD2	LEU	D	18	65.950	-39.375	-0.033	1.00	43.22	C
ATOM	2976	C	LEU	D	18	68.614	-37.943	-2.049	1.00	43.24	C
ATOM	2977	O	LEU	D	18	69.159	-36.865	-2.231	1.00	42.98	O
ATOM	2978	N	THR	D	19	67.817	-38.528	-2.936	1.00	42.05	N
ATOM	2979	CA	THR	D	19	67.259	-37.821	-4.062	1.00	41.13	C
ATOM	2980	CB	THR	D	19	67.673	-38.509	-5.373	1.00	41.27	C
ATOM	2981	OG1	THR	D	19	68.982	-39.032	-5.185	1.00	42.63	O
ATOM	2982	CG2	THR	D	19	67.703	-37.531	-6.542	1.00	39.59	C
ATOM	2983	C	THR	D	19	65.731	-37.751	-3.892	1.00	40.45	C
ATOM	2984	O	THR	D	19	65.055	-38.763	-3.753	1.00	40.58	O
ATOM	2985	N	ILE	D	20	65.207	-36.542	-3.859	1.00	39.89	N
ATOM	2986	CA	ILE	D	20	63.766	-36.329	-3.894	1.00	40.16	C
ATOM	2987	CB	ILE	D	20	63.326	-35.181	-2.940	1.00	40.54	C
ATOM	2988	CG1	ILE	D	20	63.757	-35.493	-1.505	1.00	41.28	C
ATOM	2989	CD1	ILE	D	20	63.883	-34.280	-0.649	1.00	41.55	C
ATOM	2990	CG2	ILE	D	20	61.799	-34.926	-3.043	1.00	39.20	C
ATOM	2991	C	ILE	D	20	63.383	-35.979	-5.323	1.00	39.22	C
ATOM	2992	O	ILE	D	20	64.012	-35.141	-5.904	1.00	38.55	O

ATOM	2993	N	ASN	D	21	62.358	-36.632	-5.859	1.00 39.57	N
ATOM	2994	CA	ASN	D	21	61.852	-36.370	-7.213	1.00 41.08	C
ATOM	2995	CB	ASN	D	21	61.773	-37.676	-7.967	1.00 41.24	C
ATOM	2996	CG	ASN	D	21	63.008	-37.956	-8.759	1.00 43.85	C
ATOM	2997	OD1	ASN	D	21	63.215	-37.323	-9.793	1.00 48.63	O
ATOM	2998	ND2	ASN	D	21	63.814	-38.942	-8.325	1.00 43.95	N
ATOM	2999	C	ASN	D	21	60.453	-35.779	-7.184	1.00 41.77	C
ATOM	3000	O	ASN	D	21	59.636	-36.200	-6.375	1.00 41.70	O
ATOM	3001	N	CYS	D	22	60.180	-34.794	-8.039	1.00 42.41	N
ATOM	3002	CA	CYS	D	22	58.840	-34.207	-8.137	1.00 43.48	C
ATOM	3003	CB	CYS	D	22	58.774	-32.833	-7.476	1.00 42.75	C
ATOM	3004	SG	CYS	D	22	59.105	-32.836	-5.677	1.00 49.46	S
ATOM	3005	C	CYS	D	22	58.428	-34.062	-9.580	1.00 43.16	C
ATOM	3006	O	CYS	D	22	59.168	-33.495	-10.359	1.00 43.59	O
ATOM	3007	N	VAL	D	23	57.228	-34.523	-9.918	1.00 43.81	N
ATOM	3008	CA	VAL	D	23	56.647	-34.300	-11.241	1.00 44.50	C
ATOM	3009	CB	VAL	D	23	56.382	-35.665	-11.979	1.00 44.28	C
ATOM	3010	CG1	VAL	D	23	55.931	-35.444	-13.468	1.00 44.41	C
ATOM	3011	CG2	VAL	D	23	57.614	-36.588	-11.902	1.00 42.56	C
ATOM	3012	C	VAL	D	23	55.358	-33.477	-11.126	1.00 45.73	C
ATOM	3013	O	VAL	D	23	54.510	-33.746	-10.265	1.00 45.32	O
ATOM	3014	N	LEU	D	24	55.224	-32.460	-11.986	1.00 47.64	N
ATOM	3015	CA	LEU	D	24	53.951	-31.724	-12.179	1.00 48.97	C
ATOM	3016	CB	LEU	D	24	54.214	-30.344	-12.795	1.00 48.56	C
ATOM	3017	CG	LEU	D	24	53.466	-29.079	-12.328	1.00 49.30	C
ATOM	3018	CD1	LEU	D	24	53.669	-27.924	-13.368	1.00 46.03	C
ATOM	3019	CD2	LEU	D	24	51.974	-29.319	-11.999	1.00 48.04	C
ATOM	3020	C	LEU	D	24	52.983	-32.521	-13.083	1.00 49.95	C
ATOM	3021	O	LEU	D	24	53.134	-32.529	-14.313	1.00 50.57	O
ATOM	3022	N	ARG	D	25	52.001	-33.195	-12.471	1.00 51.10	N
ATOM	3023	CA	ARG	D	25	51.019	-34.050	-13.192	1.00 51.64	C
ATOM	3024	CB	ARG	D	25	50.696	-35.313	-12.386	1.00 51.32	C
ATOM	3025	CG	ARG	D	25	51.863	-36.063	-11.871	1.00 49.97	C
ATOM	3026	CD	ARG	D	25	52.204	-37.166	-12.794	1.00 47.93	C
ATOM	3027	NE	ARG	D	25	53.274	-37.967	-12.225	1.00 47.52	N
ATOM	3028	CZ	ARG	D	25	53.981	-38.861	-12.909	1.00 47.68	C
ATOM	3029	NH1	ARG	D	25	53.741	-39.083	-14.202	1.00 46.46	N
ATOM	3030	NH2	ARG	D	25	54.941	-39.536	-12.298	1.00 48.61	N
ATOM	3031	C	ARG	D	25	49.699	-33.318	-13.473	1.00 52.55	C
ATOM	3032	O	ARG	D	25	49.412	-32.286	-12.847	1.00 52.60	O
ATOM	3033	N	ASP	D	26	48.891	-33.884	-14.386	1.00 53.55	N
ATOM	3034	CA	ASP	D	26	47.619	-33.276	-14.857	1.00 54.33	C
ATOM	3035	CB	ASP	D	26	46.477	-33.475	-13.843	1.00 54.58	C
ATOM	3036	CG	ASP	D	26	45.374	-34.384	-14.368	1.00 55.93	C
ATOM	3037	OD1	ASP	D	26	44.789	-34.090	-15.443	1.00 57.14	O
ATOM	3038	OD2	ASP	D	26	45.089	-35.398	-13.694	1.00 57.19	O
ATOM	3039	C	ASP	D	26	47.694	-31.801	-15.233	1.00 54.37	C
ATOM	3040	O	ASP	D	26	46.708	-31.085	-15.092	1.00 54.79	O
ATOM	3041	N	ALA	D	27	48.845	-31.346	-15.719	1.00 54.73	N
ATOM	3042	CA	ALA	D	27	49.050	-29.918	-15.985	1.00 54.79	C
ATOM	3043	CB	ALA	D	27	50.415	-29.475	-15.472	1.00 54.57	C
ATOM	3044	C	ALA	D	27	48.897	-29.583	-17.469	1.00 54.93	C
ATOM	3045	O	ALA	D	27	49.543	-30.202	-18.321	1.00 55.09	O
ATOM	3046	N	SER	D	28	48.038	-28.617	-17.781	1.00 54.75	N
ATOM	3047	CA	SER	D	28	47.935	-28.133	-19.152	1.00 54.93	C
ATOM	3048	CB	SER	D	28	46.488	-27.753	-19.510	1.00 55.22	C
ATOM	3049	OG	SER	D	28	46.074	-26.557	-18.862	1.00 55.13	O
ATOM	3050	C	SER	D	28	48.892	-26.952	-19.338	1.00 54.84	C
ATOM	3051	O	SER	D	28	49.138	-26.492	-20.463	1.00 54.36	O
ATOM	3052	N	PHE	D	29	49.413	-26.472	-18.209	1.00 54.77	N
ATOM	3053	CA	PHE	D	29	50.460	-25.448	-18.167	1.00 54.65	C

ATOM	3054	CB	PHE	D	29	50.152	-24.392	-17.096	1.00	55.22	C
ATOM	3055	CG	PHE	D	29	49.499	-24.951	-15.847	1.00	56.31	C
ATOM	3056	CD1	PHE	D	29	50.206	-25.806	-14.988	1.00	56.26	C
ATOM	3057	CE1	PHE	D	29	49.596	-26.332	-13.834	1.00	57.52	C
ATOM	3058	CZ	PHE	D	29	48.269	-25.993	-13.528	1.00	57.03	C
ATOM	3059	CE2	PHE	D	29	47.554	-25.124	-14.385	1.00	58.39	C
ATOM	3060	CD2	PHE	D	29	48.174	-24.614	-15.534	1.00	56.93	C
ATOM	3061	C	PHE	D	29	51.867	-26.058	-17.966	1.00	54.11	C
ATOM	3062	O	PHE	D	29	52.019	-27.269	-17.723	1.00	53.85	O
ATOM	3063	N	GLU	D	30	52.884	-25.210	-18.091	1.00	53.36	N
ATOM	3064	CA	GLU	D	30	54.270	-25.660	-18.088	1.00	52.94	C
ATOM	3065	CB	GLU	D	30	55.046	-25.061	-19.275	1.00	53.22	C
ATOM	3066	CG	GLU	D	30	54.424	-25.259	-20.663	1.00	54.41	C
ATOM	3067	CD	GLU	D	30	54.848	-26.554	-21.333	1.00	56.12	C
ATOM	3068	OE1	GLU	D	30	55.997	-27.002	-21.121	1.00	57.05	O
ATOM	3069	OE2	GLU	D	30	54.028	-27.124	-22.079	1.00	56.87	O
ATOM	3070	C	GLU	D	30	54.947	-25.262	-16.778	1.00	51.85	C
ATOM	3071	O	GLU	D	30	54.501	-24.352	-16.081	1.00	51.46	O
ATOM	3072	N	LEU	D	31	56.045	-25.942	-16.474	1.00	51.22	N
ATOM	3073	CA	LEU	D	31	56.825	-25.688	-15.275	1.00	49.86	C
ATOM	3074	CB	LEU	D	31	57.710	-26.901	-14.991	1.00	49.53	C
ATOM	3075	CG	LEU	D	31	58.340	-26.964	-13.595	1.00	48.63	C
ATOM	3076	CD1	LEU	D	31	57.315	-26.642	-12.490	1.00	43.48	C
ATOM	3077	CD2	LEU	D	31	58.957	-28.337	-13.398	1.00	46.35	C
ATOM	3078	C	LEU	D	31	57.695	-24.468	-15.489	1.00	49.34	C
ATOM	3079	O	LEU	D	31	58.652	-24.527	-16.250	1.00	49.11	O
ATOM	3080	N	LYS	D	32	57.362	-23.366	-14.838	1.00	49.24	N
ATOM	3081	CA	LYS	D	32	58.155	-22.156	-14.986	1.00	49.60	C
ATOM	3082	CB	LYS	D	32	57.325	-20.901	-14.692	1.00	49.77	C
ATOM	3083	CG	LYS	D	32	56.343	-20.516	-15.862	1.00	51.34	C
ATOM	3084	CD	LYS	D	32	56.909	-20.827	-17.265	1.00	50.23	C
ATOM	3085	CE	LYS	D	32	55.918	-20.497	-18.363	1.00	51.66	C
ATOM	3086	NZ	LYS	D	32	55.711	-21.653	-19.277	1.00	51.95	N
ATOM	3087	C	LYS	D	32	59.398	-22.205	-14.111	1.00	50.13	C
ATOM	3088	O	LYS	D	32	60.530	-22.068	-14.608	1.00	50.59	O
ATOM	3089	N	ASP	D	33	59.174	-22.422	-12.820	1.00	48.97	N
ATOM	3090	CA	ASP	D	33	60.207	-22.327	-11.799	1.00	49.30	C
ATOM	3091	CB	ASP	D	33	60.268	-20.869	-11.293	1.00	49.60	C
ATOM	3092	CG	ASP	D	33	61.514	-20.592	-10.464	1.00	54.11	C
ATOM	3093	OD1	ASP	D	33	62.644	-21.000	-10.869	1.00	55.49	O
ATOM	3094	OD2	ASP	D	33	61.356	-19.998	-9.367	1.00	59.32	O
ATOM	3095	C	ASP	D	33	59.965	-23.362	-10.629	1.00	47.92	C
ATOM	3096	O	ASP	D	33	58.887	-23.942	-10.506	1.00	47.18	O
ATOM	3097	N	THR	D	34	60.964	-23.576	-9.782	1.00	47.12	N
ATOM	3098	CA	THR	D	34	60.882	-24.571	-8.714	1.00	45.90	C
ATOM	3099	CB	THR	D	34	61.701	-25.848	-9.054	1.00	46.44	C
ATOM	3100	OG1	THR	D	34	63.095	-25.523	-9.217	1.00	43.45	O
ATOM	3101	CG2	THR	D	34	61.172	-26.526	-10.312	1.00	46.59	C
ATOM	3102	C	THR	D	34	61.449	-24.004	-7.427	1.00	46.20	C
ATOM	3103	O	THR	D	34	62.340	-23.122	-7.464	1.00	46.30	O
ATOM	3104	N	GLY	D	35	60.944	-24.509	-6.290	1.00	45.15	N
ATOM	3105	CA	GLY	D	35	61.530	-24.211	-4.995	1.00	44.20	C
ATOM	3106	C	GLY	D	35	61.560	-25.447	-4.130	1.00	44.10	C
ATOM	3107	O	GLY	D	35	60.734	-26.358	-4.309	1.00	43.01	O
ATOM	3108	N	TRP	D	36	62.497	-25.440	-3.172	1.00	43.91	N
ATOM	3109	CA	TRP	D	36	62.680	-26.524	-2.222	1.00	43.17	C
ATOM	3110	CB	TRP	D	36	63.989	-27.274	-2.505	1.00	42.16	C
ATOM	3111	CG	TRP	D	36	63.897	-28.084	-3.748	1.00	42.33	C
ATOM	3112	CD1	TRP	D	36	64.287	-27.709	-4.990	1.00	41.86	C
ATOM	3113	NE1	TRP	D	36	64.020	-28.710	-5.901	1.00	41.80	N
ATOM	3114	CE2	TRP	D	36	63.440	-29.761	-5.246	1.00	39.28	C

ATOM	3115	CD2	TRP	D	36	63.339	-29.404	-3.881	1.00	41.23	C
ATOM	3116	CE3	TRP	D	36	62.771	-30.315	-2.975	1.00	40.97	C
ATOM	3117	CZ3	TRP	D	36	62.320	-31.538	-3.462	1.00	41.67	C
ATOM	3118	CH2	TRP	D	36	62.442	-31.859	-4.835	1.00	42.09	C
ATOM	3119	CZ2	TRP	D	36	63.008	-30.988	-5.737	1.00	39.64	C
ATOM	3120	C	TRP	D	36	62.666	-25.949	-0.848	1.00	43.26	C
ATOM	3121	O	TRP	D	36	63.284	-24.931	-0.618	1.00	42.62	O
ATOM	3122	N	TYR	D	37	61.921	-26.603	0.042	1.00	43.77	N
ATOM	3123	CA	TYR	D	37	61.774	-26.215	1.445	1.00	44.44	C
ATOM	3124	CB	TYR	D	37	60.384	-25.667	1.724	1.00	45.80	C
ATOM	3125	CG	TYR	D	37	59.912	-24.825	0.615	1.00	50.24	C
ATOM	3126	CD1	TYR	D	37	60.243	-23.457	0.557	1.00	52.74	C
ATOM	3127	CE1	TYR	D	37	59.827	-22.661	-0.510	1.00	53.61	C
ATOM	3128	CZ	TYR	D	37	59.078	-23.238	-1.534	1.00	53.15	C
ATOM	3129	OH	TYR	D	37	58.677	-22.491	-2.597	1.00	53.11	O
ATOM	3130	CE2	TYR	D	37	58.744	-24.592	-1.499	1.00	53.55	C
ATOM	3131	CD2	TYR	D	37	59.167	-25.382	-0.419	1.00	51.12	C
ATOM	3132	C	TYR	D	37	61.987	-27.398	2.367	1.00	43.19	C
ATOM	3133	O	TYR	D	37	61.769	-28.539	1.964	1.00	41.62	O
ATOM	3134	N	ARG	D	38	62.305	-27.064	3.620	1.00	42.47	N
ATOM	3135	CA	ARG	D	38	62.552	-28.009	4.705	1.00	43.75	C
ATOM	3136	CB	ARG	D	38	64.045	-28.379	4.717	1.00	43.86	C
ATOM	3137	CG	ARG	D	38	64.576	-28.648	6.062	1.00	48.19	C
ATOM	3138	CD	ARG	D	38	65.373	-29.910	6.170	1.00	53.19	C
ATOM	3139	NE	ARG	D	38	66.808	-29.728	5.932	1.00	58.72	N
ATOM	3140	CZ	ARG	D	38	67.438	-28.558	5.839	1.00	57.26	C
ATOM	3141	NH1	ARG	D	38	66.768	-27.415	5.974	1.00	56.27	N
ATOM	3142	NH2	ARG	D	38	68.751	-28.546	5.624	1.00	57.23	N
ATOM	3143	C	ARG	D	38	62.090	-27.458	6.088	1.00	42.91	C
ATOM	3144	O	ARG	D	38	62.281	-26.267	6.405	1.00	42.55	O
ATOM	3145	N	THR	D	39	61.471	-28.341	6.874	1.00	42.58	N
ATOM	3146	CA	THR	D	39	61.179	-28.177	8.299	1.00	41.28	C
ATOM	3147	CB	THR	D	39	59.656	-28.312	8.600	1.00	41.27	C
ATOM	3148	OG1	THR	D	39	58.892	-27.440	7.743	1.00	43.39	O
ATOM	3149	CG2	THR	D	39	59.344	-27.965	10.027	1.00	42.59	C
ATOM	3150	C	THR	D	39	61.989	-29.229	9.060	1.00	41.19	C
ATOM	3151	O	THR	D	39	61.748	-30.449	8.968	1.00	40.45	O
ATOM	3152	N	LYS	D	40	62.968	-28.750	9.804	1.00	40.73	N
ATOM	3153	CA	LYS	D	40	63.868	-29.605	10.541	1.00	41.06	C
ATOM	3154	CB	LYS	D	40	64.893	-28.753	11.289	1.00	41.28	C
ATOM	3155	CG	LYS	D	40	66.298	-29.293	11.229	1.00	45.60	C
ATOM	3156	CD	LYS	D	40	67.141	-28.840	12.503	1.00	49.44	C
ATOM	3157	CE	LYS	D	40	68.173	-29.941	12.917	1.00	47.27	C
ATOM	3158	NZ	LYS	D	40	68.965	-29.678	14.177	1.00	50.09	N
ATOM	3159	C	LYS	D	40	63.075	-30.457	11.539	1.00	41.44	C
ATOM	3160	O	LYS	D	40	62.069	-30.038	12.073	1.00	40.57	O
ATOM	3161	N	LEU	D	41	63.524	-31.676	11.782	1.00	41.67	N
ATOM	3162	CA	LEU	D	41	62.755	-32.533	12.643	1.00	42.41	C
ATOM	3163	CB	LEU	D	41	63.321	-33.947	12.570	1.00	41.48	C
ATOM	3164	CG	LEU	D	41	62.834	-34.954	13.562	1.00	42.23	C
ATOM	3165	CD1	LEU	D	41	63.555	-36.244	13.284	1.00	38.77	C
ATOM	3166	CD2	LEU	D	41	61.360	-35.124	13.379	1.00	42.31	C
ATOM	3167	C	LEU	D	41	62.723	-31.942	14.067	1.00	42.92	C
ATOM	3168	O	LEU	D	41	63.747	-31.819	14.744	1.00	42.91	O
ATOM	3169	N	GLY	D	42	61.531	-31.532	14.484	1.00	43.29	N
ATOM	3170	CA	GLY	D	42	61.306	-31.127	15.848	1.00	44.22	C
ATOM	3171	C	GLY	D	42	61.080	-29.639	15.878	1.00	45.23	C
ATOM	3172	O	GLY	D	42	60.854	-29.079	16.923	1.00	45.24	O
ATOM	3173	N	SER	D	43	61.155	-29.018	14.704	1.00	46.01	N
ATOM	3174	CA	SER	D	43	60.973	-27.595	14.531	1.00	47.24	C
ATOM	3175	CB	SER	D	43	62.214	-27.065	13.803	1.00	46.38	C

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ATOM   3176  OG  SER D  43      61.967 -25.912  13.064  1.00 48.60      O
ATOM   3177  C   SER D  43      59.635 -27.315  13.798  1.00 48.54      C
ATOM   3178  O   SER D  43      59.126 -28.181  13.090  1.00 48.74      O
ATOM   3179  N   THR D  44      59.057 -26.130  13.995  1.00 50.34      N
ATOM   3180  CA  THR D  44      57.829 -25.713  13.289  1.00 52.56      C
ATOM   3181  CB  THR D  44      56.759 -25.084  14.274  1.00 53.48      C
ATOM   3182  OG1 THR D  44      56.875 -25.640  15.613  1.00 52.17      O
ATOM   3183  CG2 THR D  44      55.331 -25.334  13.742  1.00 54.43      C
ATOM   3184  C   THR D  44      58.044 -24.766  12.057  1.00 54.01      C
ATOM   3185  O   THR D  44      57.128 -24.557  11.228  1.00 54.29      O
ATOM   3186  N   ASN D  45      59.246 -24.208  11.908  1.00 54.74      N
ATOM   3187  CA  ASN D  45      59.508 -23.303  10.784  1.00 55.53      C
ATOM   3188  CB  ASN D  45      60.529 -22.227  11.169  1.00 56.24      C
ATOM   3189  CG  ASN D  45      61.816 -22.827  11.744  1.00 59.18      C
ATOM   3190  OD1 ASN D  45      62.441 -23.684  11.108  1.00 63.33      O
ATOM   3191  ND2 ASN D  45      62.210 -22.391  12.954  1.00 59.01      N
ATOM   3192  C   ASN D  45      59.965 -24.043   9.524  1.00 55.48      C
ATOM   3193  O   ASN D  45      60.900 -24.875   9.572  1.00 55.04      O
ATOM   3194  N   GLU D  46      59.292 -23.739   8.413  1.00 55.16      N
ATOM   3195  CA  GLU D  46      59.654 -24.237   7.120  1.00 55.65      C
ATOM   3196  CB  GLU D  46      58.413 -24.405   6.238  1.00 56.04      C
ATOM   3197  CG  GLU D  46      58.708 -25.157   4.911  1.00 56.84      C
ATOM   3198  CD  GLU D  46      57.527 -25.197   3.937  1.00 58.64      C
ATOM   3199  OE1 GLU D  46      57.030 -26.309   3.624  1.00 64.99      O
ATOM   3200  OE2 GLU D  46      57.106 -24.115   3.448  1.00 64.43      O
ATOM   3201  C   GLU D  46      60.613 -23.246   6.494  1.00 54.79      C
ATOM   3202  O   GLU D  46      60.260 -22.103   6.253  1.00 55.34      O
ATOM   3203  N   GLN D  47      61.827 -23.695   6.233  1.00 53.79      N
ATOM   3204  CA  GLN D  47      62.853 -22.868   5.641  1.00 52.99      C
ATOM   3205  CB  GLN D  47      64.145 -23.017   6.442  1.00 53.28      C
ATOM   3206  CG  GLN D  47      64.900 -21.697   6.634  1.00 57.45      C
ATOM   3207  CD  GLN D  47      64.465 -20.874   7.888  1.00 59.69      C
ATOM   3208  OE1 GLN D  47      65.207 -19.989   8.343  1.00 58.09      O
ATOM   3209  NE2 GLN D  47      63.291 -21.193   8.452  1.00 61.05      N
ATOM   3210  C   GLN D  47      63.105 -23.262   4.184  1.00 51.77      C
ATOM   3211  O   GLN D  47      63.009 -24.438   3.832  1.00 50.62      O
ATOM   3212  N   SER D  48      63.439 -22.274   3.341  1.00 50.27      N
ATOM   3213  CA  SER D  48      63.767 -22.526   1.941  1.00 49.06      C
ATOM   3214  CB  SER D  48      63.715 -21.209   1.153  1.00 50.37      C
ATOM   3215  OG  SER D  48      62.799 -20.303   1.782  1.00 54.39      O
ATOM   3216  C   SER D  48      65.158 -23.135   1.844  1.00 46.80      C
ATOM   3217  O   SER D  48      66.000 -22.874   2.670  1.00 46.24      O
ATOM   3218  N   ILE D  49      65.401 -23.952   0.838  1.00 46.02      N
ATOM   3219  CA  ILE D  49      66.723 -24.566   0.630  1.00 45.76      C
ATOM   3220  CB  ILE D  49      66.583 -26.054   0.296  1.00 45.49      C
ATOM   3221  CG1 ILE D  49      66.175 -26.853   1.553  1.00 44.65      C
ATOM   3222  CD1 ILE D  49      65.438 -28.191   1.239  1.00 45.72      C
ATOM   3223  CG2 ILE D  49      67.837 -26.618  -0.311  1.00 45.66      C
ATOM   3224  C   ILE D  49      67.497 -23.813  -0.475  1.00 46.86      C
ATOM   3225  O   ILE D  49      66.993 -23.579  -1.580  1.00 46.20      O
ATOM   3226  N   SER D  50      68.714 -23.400  -0.154  1.00 48.31      N
ATOM   3227  CA  SER D  50      69.582 -22.795  -1.161  1.00 50.07      C
ATOM   3228  CB  SER D  50      70.610 -21.875  -0.521  1.00 49.69      C
ATOM   3229  OG  SER D  50      69.966 -20.656  -0.222  1.00 51.30      O
ATOM   3230  C   SER D  50      70.259 -23.905  -1.918  1.00 50.54      C
ATOM   3231  O   SER D  50      70.853 -24.804  -1.304  1.00 50.91      O
ATOM   3232  N   ILE D  51      70.136 -23.854  -3.247  1.00 51.03      N
ATOM   3233  CA  ILE D  51      70.803 -24.826  -4.120  1.00 50.47      C
ATOM   3234  CB  ILE D  51      70.134 -24.926  -5.529  1.00 50.18      C
ATOM   3235  CG1 ILE D  51      68.659 -25.348  -5.394  1.00 49.97      C
ATOM   3236  CD1 ILE D  51      68.424 -26.692  -4.703  1.00 47.26      C
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ATOM	3237	CG2	ILE	D	51	70.886	-25.890	-6.438	1.00	50.01	C
ATOM	3238	C	ILE	D	51	72.267	-24.464	-4.162	1.00	50.13	C
ATOM	3239	O	ILE	D	51	72.621	-23.304	-4.390	1.00	51.21	O
ATOM	3240	N	GLY	D	52	73.112	-25.450	-3.903	1.00	49.83	N
ATOM	3241	CA	GLY	D	52	74.537	-25.220	-3.804	1.00	49.62	C
ATOM	3242	C	GLY	D	52	75.198	-26.276	-2.957	1.00	49.66	C
ATOM	3243	O	GLY	D	52	74.639	-26.711	-1.948	1.00	50.36	O
ATOM	3244	N	GLY	D	53	76.371	-26.698	-3.407	1.00	49.38	N
ATOM	3245	CA	GLY	D	53	77.253	-27.612	-2.696	1.00	49.23	C
ATOM	3246	C	GLY	D	53	76.697	-29.008	-2.480	1.00	49.36	C
ATOM	3247	O	GLY	D	53	76.756	-29.935	-3.362	1.00	49.29	O
ATOM	3248	N	ARG	D	54	76.120	-29.151	-1.269	1.00	49.43	N
ATOM	3249	CA	ARG	D	54	75.465	-30.394	-0.907	1.00	49.74	C
ATOM	3250	CB	ARG	D	54	75.282	-30.480	0.624	1.00	49.32	C
ATOM	3251	CG	ARG	D	54	76.280	-31.418	1.274	1.00	50.69	C
ATOM	3252	CD	ARG	D	54	76.661	-31.101	2.722	1.00	50.07	C
ATOM	3253	NE	ARG	D	54	75.585	-30.643	3.597	1.00	48.37	N
ATOM	3254	CZ	ARG	D	54	74.591	-31.392	4.086	1.00	49.71	C
ATOM	3255	NH1	ARG	D	54	74.447	-32.683	3.773	1.00	49.71	N
ATOM	3256	NH2	ARG	D	54	73.710	-30.832	4.899	1.00	47.05	N
ATOM	3257	C	ARG	D	54	74.141	-30.581	-1.660	1.00	49.58	C
ATOM	3258	O	ARG	D	54	73.723	-31.708	-1.911	1.00	50.26	O
ATOM	3259	N	TYR	D	55	73.485	-29.486	-2.017	1.00	49.51	N
ATOM	3260	CA	TYR	D	55	72.126	-29.555	-2.579	1.00	49.79	C
ATOM	3261	CB	TYR	D	55	71.193	-28.546	-1.877	1.00	49.87	C
ATOM	3262	CG	TYR	D	55	71.207	-28.685	-0.366	1.00	50.16	C
ATOM	3263	CD1	TYR	D	55	72.286	-28.218	0.368	1.00	50.07	C
ATOM	3264	CE1	TYR	D	55	72.336	-28.353	1.725	1.00	51.90	C
ATOM	3265	CZ	TYR	D	55	71.290	-28.965	2.417	1.00	52.02	C
ATOM	3266	OH	TYR	D	55	71.409	-29.070	3.799	1.00	51.10	O
ATOM	3267	CE2	TYR	D	55	70.183	-29.449	1.720	1.00	50.23	C
ATOM	3268	CD2	TYR	D	55	70.158	-29.306	0.317	1.00	48.86	C
ATOM	3269	C	TYR	D	55	72.155	-29.335	-4.089	1.00	49.96	C
ATOM	3270	O	TYR	D	55	72.233	-28.193	-4.549	1.00	49.02	O
ATOM	3271	N	VAL	D	56	72.139	-30.445	-4.840	1.00	50.10	N
ATOM	3272	CA	VAL	D	56	72.158	-30.378	-6.319	1.00	50.02	C
ATOM	3273	CB	VAL	D	56	73.128	-31.484	-6.945	1.00	49.66	C
ATOM	3274	CG1	VAL	D	56	72.672	-31.803	-8.492	1.00	49.55	C
ATOM	3275	CG2	VAL	D	56	74.716	-31.073	-6.641	1.00	50.23	C
ATOM	3276	C	VAL	D	56	70.703	-30.509	-6.834	1.00	50.01	C
ATOM	3277	O	VAL	D	56	69.996	-31.474	-6.542	1.00	50.57	O
ATOM	3278	N	GLU	D	57	70.240	-29.514	-7.565	1.00	50.47	N
ATOM	3279	CA	GLU	D	57	68.959	-29.637	-8.261	1.00	50.96	C
ATOM	3280	CB	GLU	D	57	68.069	-28.432	-8.002	1.00	49.91	C
ATOM	3281	CG	GLU	D	57	66.785	-28.464	-8.792	1.00	48.91	C
ATOM	3282	CD	GLU	D	57	65.896	-27.281	-8.499	1.00	46.98	C
ATOM	3283	OE1	GLU	D	57	66.400	-26.213	-8.111	1.00	46.14	O
ATOM	3284	OE2	GLU	D	57	64.670	-27.425	-8.644	1.00	49.35	O
ATOM	3285	C	GLU	D	57	69.192	-29.777	-9.755	1.00	51.88	C
ATOM	3286	O	GLU	D	57	70.071	-29.125	-10.302	1.00	52.11	O
ATOM	3287	N	THR	D	58	68.414	-30.645	-10.396	1.00	53.11	N
ATOM	3288	CA	THR	D	58	68.383	-30.727	-11.854	1.00	54.42	C
ATOM	3289	CB	THR	D	58	69.137	-31.978	-12.403	1.00	54.38	C
ATOM	3290	OG1	THR	D	58	68.449	-33.205	-11.829	1.00	56.17	O
ATOM	3291	CG2	THR	D	58	70.734	-31.924	-12.037	1.00	55.32	C
ATOM	3292	C	THR	D	58	66.896	-30.691	-12.250	1.00	55.02	C
ATOM	3293	O	THR	D	58	66.072	-31.406	-11.670	1.00	55.11	O
ATOM	3294	N	VAL	D	59	66.577	-29.813	-13.219	1.00	55.68	N
ATOM	3295	CA	VAL	D	59	65.203	-29.468	-13.615	1.00	55.90	C
ATOM	3296	CB	VAL	D	59	64.926	-27.955	-13.378	1.00	55.61	C
ATOM	3297	CG1	VAL	D	59	64.629	-27.687	-11.961	1.00	55.58	C

ATOM	3298	CG2	VAL	D	59	66.144	-27.115	-13.745	1.00	57.13	C
ATOM	3299	C	VAL	D	59	64.991	-29.817	-15.100	1.00	56.39	C
ATOM	3300	O	VAL	D	59	65.863	-29.553	-15.950	1.00	55.93	O
ATOM	3301	N	ASN	D	60	63.840	-30.415	-15.410	1.00	56.80	N
ATOM	3302	CA	ASN	D	60	63.549	-30.882	-16.774	1.00	56.63	C
ATOM	3303	CB	ASN	D	60	63.691	-32.413	-16.873	1.00	56.38	C
ATOM	3304	CG	ASN	D	60	64.099	-32.854	-18.348	1.00	57.37	C
ATOM	3305	OD1	ASN	D	60	65.090	-33.646	-18.466	1.00	56.92	O
ATOM	3306	ND2	ASN	D	60	63.351	-32.354	-19.408	1.00	55.67	N
ATOM	3307	C	ASN	D	60	62.172	-30.461	-17.310	1.00	56.88	C
ATOM	3308	O	ASN	D	60	61.252	-31.423	-17.192	1.00	56.87	O
ATOM	3309	N	LYS	D	61	62.032	-28.997	-17.392	1.00	57.33	N
ATOM	3310	CA	LYS	D	61	60.747	-28.473	-17.883	1.00	57.81	C
ATOM	3311	CB	LYS	D	61	60.891	-26.968	-18.145	1.00	58.40	C
ATOM	3312	CG	LYS	D	61	59.597	-26.259	-18.597	1.00	59.54	C
ATOM	3313	CD	LYS	D	61	59.929	-25.060	-19.492	1.00	61.86	C
ATOM	3314	CE	LYS	D	61	58.690	-24.361	-20.096	1.00	61.96	C
ATOM	3315	NZ	LYS	D	61	58.446	-23.001	-19.525	1.00	62.65	N
ATOM	3316	C	LYS	D	61	60.212	-29.215	-19.141	1.00	57.89	C
ATOM	3317	O	LYS	D	61	58.997	-29.366	-19.309	1.00	58.21	O
ATOM	3318	N	GLY	D	62	61.122	-29.693	-20.002	1.00	57.58	N
ATOM	3319	CA	GLY	D	62	60.761	-30.486	-21.186	1.00	57.06	C
ATOM	3320	C	GLY	D	62	60.000	-31.791	-20.907	1.00	56.82	C
ATOM	3321	O	GLY	D	62	59.381	-32.386	-21.864	1.00	57.25	O
ATOM	3322	N	SER	D	63	60.060	-32.244	-19.594	1.00	55.97	N
ATOM	3323	CA	SER	D	63	59.302	-33.409	-19.125	1.00	54.90	C
ATOM	3324	CB	SER	D	63	60.272	-34.621	-18.908	1.00	55.09	C
ATOM	3325	OG	SER	D	63	60.645	-34.692	-17.338	1.00	54.74	O
ATOM	3326	C	SER	D	63	58.474	-33.104	-17.762	1.00	53.75	C
ATOM	3327	O	SER	D	63	57.786	-34.003	-17.034	1.00	53.64	O
ATOM	3328	N	LYS	D	64	58.533	-31.834	-17.394	1.00	52.95	N
ATOM	3329	CA	LYS	D	64	57.857	-31.310	-16.167	1.00	52.47	C
ATOM	3330	CB	LYS	D	64	56.344	-31.240	-16.372	1.00	52.40	C
ATOM	3331	CG	LYS	D	64	55.971	-29.890	-17.112	1.00	53.07	C
ATOM	3332	CD	LYS	D	64	54.977	-30.113	-18.294	1.00	53.84	C
ATOM	3333	CE	LYS	D	64	53.558	-30.322	-17.603	1.00	53.96	C
ATOM	3334	NZ	LYS	D	64	52.517	-30.001	-18.618	1.00	51.87	N
ATOM	3335	C	LYS	D	64	58.301	-31.907	-14.795	1.00	51.17	C
ATOM	3336	O	LYS	D	64	57.603	-31.826	-13.761	1.00	51.55	O
ATOM	3337	N	SER	D	65	59.517	-32.439	-14.827	1.00	49.79	N
ATOM	3338	CA	SER	D	65	60.167	-33.103	-13.708	1.00	49.92	C
ATOM	3339	CB	SER	D	65	60.834	-34.407	-14.213	1.00	49.55	C
ATOM	3340	OG	SER	D	65	61.759	-34.932	-13.248	1.00	53.24	O
ATOM	3341	C	SER	D	65	61.234	-32.168	-13.120	1.00	49.16	C
ATOM	3342	O	SER	D	65	61.838	-31.333	-13.866	1.00	48.96	O
ATOM	3343	N	PHE	D	66	61.437	-32.304	-11.802	1.00	47.24	N
ATOM	3344	CA	PHE	D	66	62.543	-31.670	-11.066	1.00	46.15	C
ATOM	3345	CB	PHE	D	66	62.277	-30.171	-10.826	1.00	44.90	C
ATOM	3346	CG	PHE	D	66	61.128	-29.867	-9.891	1.00	44.59	C
ATOM	3347	CD1	PHE	D	66	59.801	-29.989	-10.317	1.00	42.09	C
ATOM	3348	CE1	PHE	D	66	58.738	-29.686	-9.470	1.00	41.74	C
ATOM	3349	CZ	PHE	D	66	58.997	-29.224	-8.170	1.00	42.61	C
ATOM	3350	CE2	PHE	D	66	60.315	-29.087	-7.722	1.00	43.21	C
ATOM	3351	CD2	PHE	D	66	61.376	-29.410	-8.586	1.00	44.86	C
ATOM	3352	C	PHE	D	66	62.988	-32.439	-9.769	1.00	45.82	C
ATOM	3353	O	PHE	D	66	62.222	-33.197	-9.181	1.00	46.26	O
ATOM	3354	N	SER	D	67	64.238	-32.257	-9.351	1.00	45.70	N
ATOM	3355	CA	SER	D	67	64.862	-33.149	-8.367	1.00	45.45	C
ATOM	3356	CB	SER	D	67	65.603	-34.242	-9.113	1.00	45.90	C
ATOM	3357	OG	SER	D	67	64.734	-35.335	-9.256	1.00	47.19	O
ATOM	3358	C	SER	D	67	65.871	-32.497	-7.455	1.00	45.20	C

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ATOM   3359  O   SER D  67      66.655 -31.642  -7.902  1.00 46.01      O
ATOM   3360  N   LEU D  68      65.872 -32.930  -6.196  1.00 44.54      N
ATOM   3361  CA  LEU D  68      66.855 -32.507  -5.212  1.00 44.12      C
ATOM   3362  CB  LEU D  68      66.203 -31.902  -3.968  1.00 43.76      C
ATOM   3363  CG  LEU D  68      66.799 -30.640  -3.315  1.00 44.66      C
ATOM   3364  CD1 LEU D  68      66.693 -30.684  -1.812  1.00 45.00      C
ATOM   3365  CD2 LEU D  68      68.213 -30.336  -3.739  1.00 41.15      C
ATOM   3366  C   LEU D  68      67.653 -33.717  -4.766  1.00 43.76      C
ATOM   3367  O   LEU D  68      67.095 -34.701  -4.302  1.00 41.85      O
ATOM   3368  N   ARG D  69      68.966 -33.629  -4.920  1.00 44.26      N
ATOM   3369  CA  ARG D  69      69.873 -34.621  -4.383  1.00 45.51      C
ATOM   3370  CB  ARG D  69      70.817 -35.147  -5.493  1.00 44.78      C
ATOM   3371  CG  ARG D  69      71.578 -36.356  -5.011  1.00 47.38      C
ATOM   3372  CD  ARG D  69      72.519 -36.978  -6.039  1.00 50.01      C
ATOM   3373  NE  ARG D  69      73.038 -38.236  -5.447  1.00 64.56      N
ATOM   3374  CZ  ARG D  69      74.278 -38.371  -4.916  1.00 70.54      C
ATOM   3375  NH1 ARG D  69      75.200 -37.308  -4.958  1.00 70.65      N
ATOM   3376  NH2 ARG D  69      74.628 -39.585  -4.368  1.00 70.40      N
ATOM   3377  C   ARG D  69      70.647 -33.877  -3.316  1.00 44.18      C
ATOM   3378  O   ARG D  69      71.228 -32.821  -3.583  1.00 45.88      O
ATOM   3379  N   ILE D  70      70.611 -34.393  -2.100  1.00 44.15      N
ATOM   3380  CA  ILE D  70      71.400 -33.865  -1.004  1.00 43.11      C
ATOM   3381  CB  ILE D  70      70.560 -33.577   0.247  1.00 43.37      C
ATOM   3382  CG1 ILE D  70      69.343 -32.713  -0.092  1.00 40.96      C
ATOM   3383  CD1 ILE D  70      68.184 -33.028   0.730  1.00 43.95      C
ATOM   3384  CG2 ILE D  70      71.443 -32.879   1.306  1.00 43.28      C
ATOM   3385  C   ILE D  70      72.431 -34.947  -0.699  1.00 43.35      C
ATOM   3386  O   ILE D  70      72.072 -36.079  -0.404  1.00 42.77      O
ATOM   3387  N   SER D  71      73.707 -34.619  -0.851  1.00 43.10      N
ATOM   3388  CA  SER D  71      74.735 -35.597  -0.571  1.00 43.65      C
ATOM   3389  CB  SER D  71      75.794 -35.590  -1.669  1.00 43.42      C
ATOM   3390  OG  SER D  71      76.168 -34.259  -1.929  1.00 44.36      O
ATOM   3391  C   SER D  71      75.306 -35.317   0.817  1.00 43.63      C
ATOM   3392  O   SER D  71      74.923 -34.309   1.447  1.00 44.14      O
ATOM   3393  N   ASP D  72      76.156 -36.232   1.309  1.00 43.29      N
ATOM   3394  CA  ASP D  72      76.858 -36.065   2.582  1.00 42.35      C
ATOM   3395  CB  ASP D  72      77.912 -34.951   2.458  1.00 42.24      C
ATOM   3396  CG  ASP D  72      78.973 -35.012   3.572  1.00 44.75      C
ATOM   3397  OD1 ASP D  72      78.995 -36.012   4.344  1.00 42.13      O
ATOM   3398  OD2 ASP D  72      79.800 -34.057   3.659  1.00 47.88      O
ATOM   3399  C   ASP D  72      75.880 -35.777   3.746  1.00 41.01      C
ATOM   3400  O   ASP D  72      75.935 -34.731   4.394  1.00 40.46      O
ATOM   3401  N   LEU D  73      74.982 -36.713   4.003  1.00 40.43      N
ATOM   3402  CA  LEU D  73      73.915 -36.470   4.965  1.00 39.98      C
ATOM   3403  CB  LEU D  73      72.761 -37.447   4.752  1.00 40.03      C
ATOM   3404  CG  LEU D  73      71.891 -37.260   3.493  1.00 38.61      C
ATOM   3405  CD1 LEU D  73      70.971 -38.462   3.446  1.00 37.16      C
ATOM   3406  CD2 LEU D  73      71.094 -36.006   3.576  1.00 38.44      C
ATOM   3407  C   LEU D  73      74.409 -36.458   6.424  1.00 39.77      C
ATOM   3408  O   LEU D  73      75.344 -37.149   6.802  1.00 38.86      O
ATOM   3409  N   ARG D  74      73.784 -35.600   7.214  1.00 40.34      N
ATOM   3410  CA  ARG D  74      74.125 -35.418   8.616  1.00 40.91      C
ATOM   3411  CB  ARG D  74      74.711 -34.024   8.803  1.00 41.22      C
ATOM   3412  CG  ARG D  74      75.561 -33.574   7.623  1.00 44.83      C
ATOM   3413  CD  ARG D  74      76.259 -32.276   7.888  1.00 51.37      C
ATOM   3414  NE  ARG D  74      75.309 -31.193   8.146  1.00 55.28      N
ATOM   3415  CZ  ARG D  74      75.645 -30.008   8.662  1.00 56.79      C
ATOM   3416  NH1 ARG D  74      76.913 -29.758   8.987  1.00 55.96      N
ATOM   3417  NH2 ARG D  74      74.711 -29.079   8.868  1.00 56.56      N
ATOM   3418  C   ARG D  74      72.820 -35.563   9.406  1.00 40.45      C
ATOM   3419  O   ARG D  74      71.735 -35.292   8.851  1.00 40.13      O
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ATOM	3420	N	VAL	D	75	72.901	-36.003	10.663	1.00 39.63	N
ATOM	3421	CA	VAL	D	75	71.700	-36.030	11.512	1.00 40.06	C
ATOM	3422	CB	VAL	D	75	71.970	-36.527	12.963	1.00 39.68	C
ATOM	3423	CG1	VAL	D	75	72.504	-37.923	12.939	1.00 37.56	C
ATOM	3424	CG2	VAL	D	75	72.893	-35.615	13.685	1.00 41.38	C
ATOM	3425	C	VAL	D	75	70.872	-34.702	11.509	1.00 40.03	C
ATOM	3426	O	VAL	D	75	69.652	-34.750	11.502	1.00 40.31	O
ATOM	3427	N	GLU	D	76	71.516	-33.534	11.474	1.00 39.38	N
ATOM	3428	CA	GLU	D	76	70.783	-32.267	11.413	1.00 38.58	C
ATOM	3429	CB	GLU	D	76	71.704	-31.072	11.643	1.00 39.43	C
ATOM	3430	CG	GLU	D	76	73.155	-31.300	11.253	1.00 43.81	C
ATOM	3431	CD	GLU	D	76	73.899	-32.091	12.300	1.00 49.07	C
ATOM	3432	OE1	GLU	D	76	74.410	-33.201	12.002	1.00 50.38	O
ATOM	3433	OE2	GLU	D	76	73.963	-31.604	13.445	1.00 53.73	O
ATOM	3434	C	GLU	D	76	70.012	-32.038	10.113	1.00 37.13	C
ATOM	3435	O	GLU	D	76	69.328	-31.018	9.981	1.00 36.46	O
ATOM	3436	N	ASP	D	77	70.139	-32.955	9.156	1.00 35.88	N
ATOM	3437	CA	ASP	D	77	69.302	-32.934	7.896	1.00 35.98	C
ATOM	3438	CB	ASP	D	77	69.995	-33.640	6.719	1.00 35.29	C
ATOM	3439	CG	ASP	D	77	71.259	-32.944	6.258	1.00 36.12	C
ATOM	3440	OD1	ASP	D	77	71.314	-31.707	6.247	1.00 34.87	O
ATOM	3441	OD2	ASP	D	77	72.200	-33.674	5.890	1.00 39.60	O
ATOM	3442	C	ASP	D	77	67.933	-33.626	8.022	1.00 35.40	C
ATOM	3443	O	ASP	D	77	67.106	-33.451	7.146	1.00 35.70	O
ATOM	3444	N	SER	D	78	67.740	-34.480	9.027	1.00 34.77	N
ATOM	3445	CA	SER	D	78	66.422	-34.981	9.345	1.00 35.45	C
ATOM	3446	CB	SER	D	78	66.473	-35.750	10.659	1.00 35.78	C
ATOM	3447	OG	SER	D	78	67.436	-36.770	10.546	1.00 36.74	O
ATOM	3448	C	SER	D	78	65.321	-33.899	9.393	1.00 35.23	C
ATOM	3449	O	SER	D	78	65.471	-32.828	10.038	1.00 35.34	O
ATOM	3450	N	GLY	D	79	64.210	-34.192	8.716	1.00 33.82	N
ATOM	3451	CA	GLY	D	79	63.078	-33.271	8.649	1.00 34.33	C
ATOM	3452	C	GLY	D	79	62.191	-33.603	7.481	1.00 35.45	C
ATOM	3453	O	GLY	D	79	62.404	-34.627	6.767	1.00 36.59	O
ATOM	3454	N	THR	D	80	61.239	-32.707	7.242	1.00 36.95	N
ATOM	3455	CA	THR	D	80	60.265	-32.773	6.142	1.00 37.81	C
ATOM	3456	CB	THR	D	80	58.812	-32.455	6.589	1.00 37.21	C
ATOM	3457	OG1	THR	D	80	58.540	-33.092	7.845	1.00 42.51	O
ATOM	3458	CG2	THR	D	80	57.794	-32.957	5.599	1.00 36.93	C
ATOM	3459	C	THR	D	80	60.658	-31.822	5.030	1.00 39.38	C
ATOM	3460	O	THR	D	80	60.734	-30.616	5.253	1.00 39.45	O
ATOM	3461	N	TYR	D	81	60.882	-32.394	3.835	1.00 39.69	N
ATOM	3462	CA	TYR	D	81	61.244	-31.683	2.641	1.00 40.11	C
ATOM	3463	CB	TYR	D	81	62.433	-32.367	1.967	1.00 40.22	C
ATOM	3464	CG	TYR	D	81	63.719	-32.354	2.802	1.00 39.55	C
ATOM	3465	CD1	TYR	D	81	64.755	-31.515	2.468	1.00 39.29	C
ATOM	3466	CE1	TYR	D	81	65.935	-31.489	3.213	1.00 39.91	C
ATOM	3467	CZ	TYR	D	81	66.087	-32.315	4.305	1.00 40.52	C
ATOM	3468	OH	TYR	D	81	67.291	-32.242	5.010	1.00 39.06	O
ATOM	3469	CE2	TYR	D	81	65.066	-33.175	4.655	1.00 37.99	C
ATOM	3470	CD2	TYR	D	81	63.892	-33.194	3.897	1.00 38.47	C
ATOM	3471	C	TYR	D	81	60.064	-31.621	1.693	1.00 40.88	C
ATOM	3472	O	TYR	D	81	59.242	-32.572	1.577	1.00 42.06	O
ATOM	3473	N	LYS	D	82	59.925	-30.469	1.063	1.00 41.23	N
ATOM	3474	CA	LYS	D	82	58.819	-30.189	0.172	1.00 41.95	C
ATOM	3475	CB	LYS	D	82	57.779	-29.315	0.863	1.00 42.23	C
ATOM	3476	CG	LYS	D	82	56.447	-30.008	1.156	1.00 46.06	C
ATOM	3477	CD	LYS	D	82	55.949	-29.607	2.549	1.00 53.37	C
ATOM	3478	CE	LYS	D	82	54.875	-30.528	3.091	1.00 51.30	C
ATOM	3479	NZ	LYS	D	82	53.540	-30.122	2.613	1.00 50.40	N
ATOM	3480	C	LYS	D	82	59.381	-29.472	-1.028	1.00 42.24	C

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ATOM   3481  O   LYS D  82      60.236 -28.607  -0.899  1.00 41.51      O
ATOM   3482  N   CYS D  83      58.912 -29.863  -2.207  1.00 43.47      N
ATOM   3483  CA  CYS D  83      59.163 -29.117  -3.400  1.00 44.82      C
ATOM   3484  CB  CYS D  83      59.474 -30.038  -4.564  1.00 45.49      C
ATOM   3485  SG  CYS D  83      58.161 -31.141  -4.953  1.00 44.99      S
ATOM   3486  C   CYS D  83      57.923 -28.295  -3.711  1.00 45.88      C
ATOM   3487  O   CYS D  83      56.827 -28.610  -3.259  1.00 46.33      O
ATOM   3488  N   GLN D  84      58.132 -27.220  -4.465  1.00 46.29      N
ATOM   3489  CA  GLN D  84      57.058 -26.400  -5.007  1.00 45.80      C
ATOM   3490  CB  GLN D  84      56.949 -25.084  -4.280  1.00 46.07      C
ATOM   3491  CG  GLN D  84      55.811 -24.290  -4.826  1.00 47.89      C
ATOM   3492  CD  GLN D  84      55.202 -23.369  -3.835  1.00 50.52      C
ATOM   3493  OE1 GLN D  84      54.030 -23.056  -3.953  1.00 54.26      O
ATOM   3494  NE2 GLN D  84      55.991 -22.898  -2.861  1.00 50.71      N
ATOM   3495  C   GLN D  84      57.352 -26.107  -6.466  1.00 44.92      C
ATOM   3496  O   GLN D  84      58.466 -25.756  -6.822  1.00 44.76      O
ATOM   3497  N   ALA D  85      56.328 -26.309  -7.271  1.00 44.45      N
ATOM   3498  CA  ALA D  85      56.287 -26.074  -8.693  1.00 44.03      C
ATOM   3499  CB  ALA D  85      55.513 -27.178  -9.330  1.00 43.73      C
ATOM   3500  C   ALA D  85      55.581 -24.740  -8.953  1.00 44.64      C
ATOM   3501  O   ALA D  85      54.506 -24.480  -8.398  1.00 45.56      O
ATOM   3502  N   PHE D  86      56.179 -23.900  -9.797  1.00 44.70      N
ATOM   3503  CA  PHE D  86      55.646 -22.570 -10.110  1.00 43.77      C
ATOM   3504  CB  PHE D  86      56.662 -21.505  -9.755  1.00 43.68      C
ATOM   3505  CG  PHE D  86      56.899 -21.325  -8.234  1.00 43.64      C
ATOM   3506  CD1 PHE D  86      58.108 -21.734  -7.644  1.00 39.50      C
ATOM   3507  CE1 PHE D  86      58.352 -21.536  -6.258  1.00 41.98      C
ATOM   3508  CZ  PHE D  86      57.392 -20.906  -5.466  1.00 43.10      C
ATOM   3509  CE2 PHE D  86      56.164 -20.469  -6.060  1.00 42.82      C
ATOM   3510  CD2 PHE D  86      55.936 -20.693  -7.427  1.00 42.57      C
ATOM   3511  C   PHE D  86      55.284 -22.518 -11.581  1.00 43.35      C
ATOM   3512  O   PHE D  86      56.047 -22.948 -12.451  1.00 43.61      O
ATOM   3513  N   TYR D  87      54.071 -22.067 -11.860  1.00 43.20      N
ATOM   3514  CA  TYR D  87      53.528 -22.118 -13.225  1.00 42.85      C
ATOM   3515  CB  TYR D  87      52.706 -23.392 -13.419  1.00 42.88      C
ATOM   3516  CG  TYR D  87      51.616 -23.570 -12.381  1.00 43.24      C
ATOM   3517  CD1 TYR D  87      50.361 -23.023 -12.574  1.00 41.66      C
ATOM   3518  CE1 TYR D  87      49.378 -23.166 -11.626  1.00 43.81      C
ATOM   3519  CZ  TYR D  87      49.645 -23.855 -10.456  1.00 42.83      C
ATOM   3520  OH  TYR D  87      48.635 -23.981  -9.495  1.00 45.90      O
ATOM   3521  CE2 TYR D  87      50.879 -24.412 -10.260  1.00 40.71      C
ATOM   3522  CD2 TYR D  87      51.849 -24.270 -11.203  1.00 41.31      C
ATOM   3523  C   TYR D  87      52.678 -20.887 -13.442  1.00 42.38      C
ATOM   3524  O   TYR D  87      52.341 -20.184 -12.479  1.00 41.90      O
ATOM   3525  N   VAL D  88      52.328 -20.625 -14.690  1.00 42.33      N
ATOM   3526  CA  VAL D  88      51.484 -19.482 -15.014  1.00 42.91      C
ATOM   3527  CB  VAL D  88      52.241 -18.322 -15.725  1.00 42.23      C
ATOM   3528  CG1 VAL D  88      52.648 -18.693 -17.134  1.00 42.89      C
ATOM   3529  CG2 VAL D  88      53.461 -17.852 -14.923  1.00 42.15      C
ATOM   3530  C   VAL D  88      50.343 -20.009 -15.861  1.00 43.65      C
ATOM   3531  O   VAL D  88      50.483 -21.016 -16.523  1.00 44.60      O
ATOM   3532  N   PHE D  89      49.204 -19.351 -15.789  1.00 44.07      N
ATOM   3533  CA  PHE D  89      48.019 -19.716 -16.558  1.00 44.21      C
ATOM   3534  CB  PHE D  89      47.186 -20.807 -15.865  1.00 43.34      C
ATOM   3535  CG  PHE D  89      46.719 -20.466 -14.459  1.00 42.59      C
ATOM   3536  CD1 PHE D  89      45.427 -19.948 -14.236  1.00 42.34      C
ATOM   3537  CE1 PHE D  89      44.978 -19.651 -12.942  1.00 41.00      C
ATOM   3538  CZ  PHE D  89      45.828 -19.873 -11.839  1.00 41.21      C
ATOM   3539  CE2 PHE D  89      47.115 -20.389 -12.048  1.00 40.99      C
ATOM   3540  CD2 PHE D  89      47.547 -20.683 -13.358  1.00 39.83      C
ATOM   3541  C   PHE D  89      47.258 -18.419 -16.699  1.00 45.29      C
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ATOM   3542  O   PHE D  89      47.586 -17.446 -16.012  1.00 44.92      O
ATOM   3543  N   PHE D  90      46.278 -18.379 -17.594  1.00 46.60      N
ATOM   3544  CA  PHE D  90      45.525 -17.166 -17.790  1.00 47.84      C
ATOM   3545  CB  PHE D  90      45.113 -17.033 -19.229  1.00 49.12      C
ATOM   3546  CG  PHE D  90      46.217 -16.590 -20.135  1.00 52.21      C
ATOM   3547  CD1 PHE D  90      46.291 -15.259 -20.561  1.00 55.64      C
ATOM   3548  CE1 PHE D  90      47.315 -14.828 -21.443  1.00 57.08      C
ATOM   3549  CZ  PHE D  90      48.263 -15.751 -21.908  1.00 55.59      C
ATOM   3550  CE2 PHE D  90      48.194 -17.095 -21.480  1.00 57.82      C
ATOM   3551  CD2 PHE D  90      47.171 -17.503 -20.596  1.00 55.72      C
ATOM   3552  C   PHE D  90      44.331 -17.079 -16.865  1.00 47.66      C
ATOM   3553  O   PHE D  90      43.697 -18.071 -16.572  1.00 46.94      O
ATOM   3554  N   ALA D  91      44.053 -15.867 -16.398  1.00 48.49      N
ATOM   3555  CA  ALA D  91      42.982 -15.599 -15.447  1.00 49.73      C
ATOM   3556  CB  ALA D  91      42.942 -14.112 -15.129  1.00 48.83      C
ATOM   3557  C   ALA D  91      41.632 -16.093 -15.969  1.00 51.41      C
ATOM   3558  O   ALA D  91      40.799 -16.593 -15.209  1.00 51.12      O
ATOM   3559  N   GLU D  92      41.441 -15.964 -17.282  1.00 53.68      N
ATOM   3560  CA  GLU D  92      40.229 -16.427 -17.962  1.00 56.07      C
ATOM   3561  CB  GLU D  92      40.134 -15.798 -19.358  1.00 56.18      C
ATOM   3562  CG  GLU D  92      40.983 -16.517 -20.403  1.00 57.25      C
ATOM   3563  CD  GLU D  92      41.361 -15.626 -21.547  1.00 59.32      C
ATOM   3564  OE1 GLU D  92      42.579 -15.479 -21.797  1.00 59.13      O
ATOM   3565  OE2 GLU D  92      40.441 -15.065 -22.189  1.00 60.55      O
ATOM   3566  C   GLU D  92      40.105 -17.952 -18.095  1.00 57.18      C
ATOM   3567  O   GLU D  92      39.052 -18.416 -18.520  1.00 57.56      O
ATOM   3568  N   ASP D  93      41.171 -18.709 -17.789  1.00 58.82      N
ATOM   3569  CA  ASP D  93      41.110 -20.181 -17.684  1.00 60.41      C
ATOM   3570  CB  ASP D  93      42.458 -20.800 -17.271  1.00 60.06      C
ATOM   3571  CG  ASP D  93      42.370 -22.306 -16.993  1.00 62.32      C
ATOM   3572  OD1 ASP D  93      43.088 -22.798 -16.075  1.00 63.69      O
ATOM   3573  OD2 ASP D  93      41.580 -23.010 -17.680  1.00 63.08      O
ATOM   3574  C   ASP D  93      39.992 -20.523 -16.698  1.00 61.55      C
ATOM   3575  O   ASP D  93      40.234 -20.746 -15.495  1.00 61.84      O
ATOM   3576  N   VAL D  94      38.775 -20.549 -17.266  1.00 62.79      N
ATOM   3577  CA  VAL D  94      37.473 -20.563 -16.567  1.00 63.66      C
ATOM   3578  CB  VAL D  94      36.302 -20.047 -17.526  1.00 63.67      C
ATOM   3579  CG1 VAL D  94      35.125 -19.424 -16.748  1.00 63.68      C
ATOM   3580  CG2 VAL D  94      35.843 -21.115 -18.522  1.00 63.79      C
ATOM   3581  C   VAL D  94      37.238 -21.948 -15.970  1.00 64.13      C
ATOM   3582  O   VAL D  94      38.119 -22.810 -16.078  1.00 64.47      O
ATOM   3583  N   GLY D  95      36.089 -22.145 -15.317  1.00 64.40      N
ATOM   3584  CA  GLY D  95      35.774 -23.376 -14.568  1.00 64.71      C
ATOM   3585  C   GLY D  95      36.866 -24.412 -14.294  1.00 65.01      C
ATOM   3586  O   GLY D  95      36.569 -25.624 -14.258  1.00 65.10      O
ATOM   3587  N   SER D  96      38.110 -23.954 -14.083  1.00 65.03      N
ATOM   3588  CA  SER D  96      39.264 -24.858 -13.891  1.00 65.03      C
ATOM   3589  CB  SER D  96      40.390 -24.533 -14.887  1.00 65.25      C
ATOM   3590  OG  SER D  96      41.339 -25.594 -14.955  1.00 64.98      O
ATOM   3591  C   SER D  96      39.806 -24.852 -12.454  1.00 64.82      C
ATOM   3592  O   SER D  96      40.023 -23.779 -11.867  1.00 65.31      O
ATOM   3593  N   ASN D  97      40.052 -26.057 -11.928  1.00 63.87      N
ATOM   3594  CA  ASN D  97      40.392 -26.313 -10.521  1.00 62.98      C
ATOM   3595  CB  ASN D  97      39.702 -27.644 -10.104  1.00 63.42      C
ATOM   3596  CG  ASN D  97      39.953 -28.045  -8.633  1.00 65.04      C
ATOM   3597  OD1 ASN D  97      40.047 -27.190  -7.736  1.00 66.76      O
ATOM   3598  ND2 ASN D  97      40.030 -29.363  -8.387  1.00 63.43      N
ATOM   3599  C   ASN D  97      41.921 -26.317 -10.231  1.00 61.78      C
ATOM   3600  O   ASN D  97      42.552 -27.385 -10.142  1.00 61.83      O
ATOM   3601  N   LYS D  98      42.507 -25.129 -10.063  1.00 59.84      N
ATOM   3602  CA  LYS D  98      43.970 -24.994  -9.904  1.00 58.24      C
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ATOM   3603  CB  LYS D  98      44.446 -23.620 -10.431  1.00 58.64      C
ATOM   3604  CG  LYS D  98      44.251 -23.361 -11.938  1.00 57.61      C
ATOM   3605  CD  LYS D  98      42.829 -22.926 -12.285  1.00 57.73      C
ATOM   3606  CE  LYS D  98      42.248 -21.834 -11.301  1.00 59.29      C
ATOM   3607  NZ  LYS D  98      41.046 -20.972 -12.134  1.00 57.74      N
ATOM   3608  C   LYS D  98      44.493 -25.245  -8.461  1.00 57.13      C
ATOM   3609  O   LYS D  98      43.767 -25.784  -7.606  1.00 57.08      O
ATOM   3610  N   GLY D  99      45.767 -24.891  -8.225  1.00 55.60      N
ATOM   3611  CA  GLY D  99      46.378 -24.754  -6.872  1.00 52.95      C
ATOM   3612  C   GLY D  99      46.501 -23.279  -6.415  1.00 50.67      C
ATOM   3613  O   GLY D  99      45.678 -22.440  -6.801  1.00 51.24      O
ATOM   3614  N   ALA D 100      47.510 -22.956  -5.601  1.00 47.56      N
ATOM   3615  CA  ALA D 100      47.594 -21.643  -4.932  1.00 44.47      C
ATOM   3616  CB  ALA D 100      48.583 -21.700  -3.781  1.00 44.23      C
ATOM   3617  C   ALA D 100      47.948 -20.493  -5.881  1.00 42.73      C
ATOM   3618  O   ALA D 100      48.733 -20.692  -6.805  1.00 41.87      O
ATOM   3619  N   ILE D 101      47.368 -19.313  -5.635  1.00 40.81      N
ATOM   3620  CA  ILE D 101      47.614 -18.108  -6.395  1.00 40.35      C
ATOM   3621  CB  ILE D 101      46.370 -17.176  -6.453  1.00 40.67      C
ATOM   3622  CG1 ILE D 101      45.119 -17.901  -6.945  1.00 41.30      C
ATOM   3623  CD1 ILE D 101      45.229 -18.533  -8.316  1.00 44.91      C
ATOM   3624  CG2 ILE D 101      46.719 -15.835  -7.192  1.00 38.52      C
ATOM   3625  C   ILE D 101      48.703 -17.316  -5.677  1.00 40.37      C
ATOM   3626  O   ILE D 101      48.578 -17.042  -4.478  1.00 40.20      O
ATOM   3627  N   ILE D 102      49.757 -16.950  -6.405  1.00 39.73      N
ATOM   3628  CA  ILE D 102      50.891 -16.245  -5.850  1.00 38.51      C
ATOM   3629  CB  ILE D 102      52.225 -16.834  -6.388  1.00 39.69      C
ATOM   3630  CG1 ILE D 102      52.294 -18.341  -6.159  1.00 40.45      C
ATOM   3631  CD1 ILE D 102      52.156 -18.810  -4.677  1.00 39.56      C
ATOM   3632  CG2 ILE D 102      53.461 -16.084  -5.804  1.00 40.43      C
ATOM   3633  C   ILE D 102      50.816 -14.788  -6.296  1.00 37.28      C
ATOM   3634  O   ILE D 102      51.315 -13.893  -5.613  1.00 38.01      O
ATOM   3635  N   GLY D 103      50.181 -14.539  -7.424  1.00 35.03      N
ATOM   3636  CA  GLY D 103      50.172 -13.194  -7.991  1.00 33.31      C
ATOM   3637  C   GLY D 103      49.411 -13.068  -9.275  1.00 32.34      C
ATOM   3638  O   GLY D 103      49.072 -14.050  -9.924  1.00 31.10      O
ATOM   3639  N   LEU D 104      49.098 -11.840  -9.621  1.00 32.17      N
ATOM   3640  CA  LEU D 104      48.403 -11.557 -10.841  1.00 32.15      C
ATOM   3641  CB  LEU D 104      46.965 -11.134 -10.534  1.00 33.36      C
ATOM   3642  CG  LEU D 104      46.100 -10.577 -11.696  1.00 35.07      C
ATOM   3643  CD1 LEU D 104      44.837  -9.947 -11.110  1.00 35.43      C
ATOM   3644  CD2 LEU D 104      45.772 -11.706 -12.740  1.00 34.01      C
ATOM   3645  C   LEU D 104      49.131 -10.472 -11.532  1.00 32.05      C
ATOM   3646  O   LEU D 104      49.436  -9.462 -10.903  1.00 31.50      O
ATOM   3647  N   MET D 105      49.419 -10.679 -12.826  1.00 31.71      N
ATOM   3648  CA  MET D 105      50.112  -9.717 -13.682  1.00 31.42      C
ATOM   3649  CB  MET D 105      51.206 -10.403 -14.533  1.00 31.83      C
ATOM   3650  CG  MET D 105      52.155 -11.228 -13.703  1.00 36.87      C
ATOM   3651  SD  MET D 105      53.267 -10.213 -12.674  1.00 43.45      S
ATOM   3652  CE  MET D 105      54.104  -9.296 -13.942  1.00 32.92      C
ATOM   3653  C   MET D 105      49.131  -9.055 -14.624  1.00 30.41      C
ATOM   3654  O   MET D 105      48.154  -9.673 -15.072  1.00 29.25      O
ATOM   3655  N   VAL D 106      49.362  -7.789 -14.917  1.00 29.43      N
ATOM   3656  CA  VAL D 106      48.394  -7.148 -15.760  1.00 30.76      C
ATOM   3657  CB  VAL D 106      48.317  -5.542 -15.699  1.00 30.85      C
ATOM   3658  CG1 VAL D 106      48.876  -4.946 -14.421  1.00 28.68      C
ATOM   3659  CG2 VAL D 106      48.867  -4.937 -16.875  1.00 27.85      C
ATOM   3660  C   VAL D 106      48.670  -7.711 -17.170  1.00 31.76      C
ATOM   3661  O   VAL D 106      49.843  -7.941 -17.524  1.00 32.26      O
ATOM   3662  N   GLY D 107      47.590  -7.909 -17.944  1.00 31.86      N
ATOM   3663  CA  GLY D 107      47.602  -8.730 -19.149  1.00 31.60      C
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ATOM   3664  C   GLY D 107      46.937 -10.076 -18.867  1.00 31.76      C
ATOM   3665  O   GLY D 107      46.782 -10.884 -19.774  1.00 32.48      O
ATOM   3666  N   GLY D 108      46.594 -10.347 -17.602  1.00 31.73      N
ATOM   3667  CA  GLY D 108      45.845 -11.561 -17.219  1.00 30.76      C
ATOM   3668  C   GLY D 108      46.575 -12.837 -16.858  1.00 30.68      C
ATOM   3669  O   GLY D 108      45.940 -13.868 -16.709  1.00 31.60      O
ATOM   3670  N   VAL D 109      47.894 -12.799 -16.705  1.00 31.23      N
ATOM   3671  CA  VAL D 109      48.659 -14.009 -16.355  1.00 31.01      C
ATOM   3672  CB  VAL D 109      50.115 -13.935 -16.919  1.00 31.60      C
ATOM   3673  CG1 VAL D 109      50.128 -14.044 -18.453  1.00 30.53      C
ATOM   3674  CG2 VAL D 109      50.988 -14.970 -16.332  1.00 28.81      C
ATOM   3675  C   VAL D 109      48.653 -14.172 -14.835  1.00 32.20      C
ATOM   3676  O   VAL D 109      48.994 -13.258 -14.125  1.00 32.24      O
ATOM   3677  N   VAL D 110      48.207 -15.323 -14.332  1.00 33.52      N
ATOM   3678  CA  VAL D 110      48.274 -15.592 -12.911  1.00 34.03      C
ATOM   3679  CB  VAL D 110      46.863 -15.796 -12.233  1.00 34.35      C
ATOM   3680  CG1 VAL D 110      46.831 -16.818 -11.135  1.00 33.72      C
ATOM   3681  CG2 VAL D 110      45.754 -15.985 -13.234  1.00 34.18      C
ATOM   3682  C   VAL D 110      49.389 -16.575 -12.582  1.00 35.97      C
ATOM   3683  O   VAL D 110      49.627 -17.552 -13.306  1.00 35.08      O
ATOM   3684  N   ILE D 111      50.130 -16.253 -11.526  1.00 38.15      N
ATOM   3685  CA  ILE D 111      51.201 -17.117 -11.055  1.00 40.04      C
ATOM   3686  CB  ILE D 111      52.441 -16.328 -10.556  1.00 39.96      C
ATOM   3687  CG1 ILE D 111      53.021 -15.546 -11.706  1.00 40.77      C
ATOM   3688  CD1 ILE D 111      52.827 -14.083 -11.586  1.00 42.20      C
ATOM   3689  CG2 ILE D 111      53.550 -17.273 -10.029  1.00 40.87      C
ATOM   3690  C   ILE D 111      50.628 -18.015 -10.003  1.00 40.99      C
ATOM   3691  O   ILE D 111      50.059 -17.563  -8.987  1.00 41.58      O
ATOM   3692  N   GLY D 112      50.722 -19.313 -10.257  1.00 42.26      N
ATOM   3693  CA  GLY D 112      50.331 -20.269  -9.235  1.00 41.93      C
ATOM   3694  C   GLY D 112      51.500 -21.086  -8.715  1.00 43.09      C
ATOM   3695  O   GLY D 112      52.575 -21.142  -9.325  1.00 42.76      O
ATOM   3696  N   GLY D 113      51.266 -21.778  -7.598  1.00 44.33      N
ATOM   3697  CA  GLY D 113      52.260 -22.648  -7.011  1.00 45.49      C
ATOM   3698  C   GLY D 113      51.626 -23.882  -6.435  1.00 47.03      C
ATOM   3699  O   GLY D 113      50.533 -23.830  -5.852  1.00 47.41      O
ATOM   3700  N   GLU D 114      52.319 -25.001  -6.599  1.00 47.97      N
ATOM   3701  CA  GLU D 114      51.835 -26.273  -6.122  1.00 48.98      C
ATOM   3702  CB  GLU D 114      51.275 -27.062  -7.304  1.00 49.06      C
ATOM   3703  CG  GLU D 114      50.539 -28.280  -6.942  1.00 52.21      C
ATOM   3704  CD  GLU D 114      49.046 -28.083  -6.856  1.00 56.29      C
ATOM   3705  OE1 GLU D 114      48.457 -28.646  -5.897  1.00 58.05      O
ATOM   3706  OE2 GLU D 114      48.462 -27.412  -7.753  1.00 57.66      O
ATOM   3707  C   GLU D 114      52.968 -27.042  -5.375  1.00 49.12      C
ATOM   3708  O   GLU D 114      54.066 -27.250  -5.899  1.00 48.87      O
ATOM   3709  N   LYS D 115      52.678 -27.446  -4.147  1.00 48.78      N
ATOM   3710  CA  LYS D 115      53.615 -28.192  -3.317  1.00 48.72      C
ATOM   3711  CB  LYS D 115      53.481 -27.719  -1.866  1.00 49.82      C
ATOM   3712  CG  LYS D 115      54.298 -26.510  -1.509  1.00 51.17      C
ATOM   3713  CD  LYS D 115      54.010 -26.041  -0.090  1.00 56.06      C
ATOM   3714  CE  LYS D 115      55.030 -24.958   0.334  1.00 62.44      C
ATOM   3715  NZ  LYS D 115      54.544 -24.084   1.479  1.00 66.54      N
ATOM   3716  C   LYS D 115      53.450 -29.733  -3.408  1.00 47.04      C
ATOM   3717  O   LYS D 115      52.334 -30.258  -3.557  1.00 46.88      O
ATOM   3718  N   GLY D 116      54.576 -30.441  -3.346  1.00 46.00      N
ATOM   3719  CA  GLY D 116      54.576 -31.909  -3.157  1.00 44.67      C
ATOM   3720  C   GLY D 116      54.109 -32.255  -1.746  1.00 44.37      C
ATOM   3721  O   GLY D 116      54.088 -31.386  -0.850  1.00 44.53      O
ATOM   3722  N   ALA D 117      53.718 -33.515  -1.544  1.00 43.07      N
ATOM   3723  CA  ALA D 117      53.148 -33.918  -0.289  1.00 41.97      C
ATOM   3724  CB  ALA D 117      52.397 -35.199  -0.448  1.00 41.67      C
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ATOM	3725	C	ALA	D	117	54.208	-34.037	0.806	1.00	41.59	C
ATOM	3726	O	ALA	D	117	53.855	-34.218	1.958	1.00	42.73	O
ATOM	3727	N	GLY	D	118	55.487	-33.984	0.449	1.00	40.27	N
ATOM	3728	CA	GLY	D	118	56.542	-33.997	1.430	1.00	39.78	C
ATOM	3729	C	GLY	D	118	57.349	-35.274	1.452	1.00	41.03	C
ATOM	3730	O	GLY	D	118	56.891	-36.346	1.032	1.00	41.30	O
ATOM	3731	N	THR	D	119	58.575	-35.170	1.943	1.00	41.33	N
ATOM	3732	CA	THR	D	119	59.336	-36.361	2.271	1.00	41.15	C
ATOM	3733	CB	THR	D	119	60.404	-36.914	1.152	1.00	41.78	C
ATOM	3734	OG1	THR	D	119	61.763	-36.991	1.623	1.00	46.65	O
ATOM	3735	CG2	THR	D	119	60.283	-36.324	-0.201	1.00	36.84	C
ATOM	3736	C	THR	D	119	59.867	-36.263	3.698	1.00	40.96	C
ATOM	3737	O	THR	D	119	60.532	-35.282	4.053	1.00	40.91	O
ATOM	3738	N	ALA	D	120	59.514	-37.258	4.517	1.00	38.25	N
ATOM	3739	CA	ALA	D	120	60.005	-37.311	5.887	1.00	37.80	C
ATOM	3740	CB	ALA	D	120	58.969	-38.040	6.791	1.00	35.79	C
ATOM	3741	C	ALA	D	120	61.369	-38.034	5.933	1.00	37.39	C
ATOM	3742	O	ALA	D	120	61.421	-39.245	5.827	1.00	37.29	O
ATOM	3743	N	LEU	D	121	62.471	-37.298	6.048	1.00	37.88	N
ATOM	3744	CA	LEU	D	121	63.791	-37.950	6.023	1.00	37.30	C
ATOM	3745	CB	LEU	D	121	64.792	-37.133	5.216	1.00	37.16	C
ATOM	3746	CG	LEU	D	121	66.302	-37.438	5.387	1.00	36.66	C
ATOM	3747	CD1	LEU	D	121	66.766	-38.702	4.727	1.00	34.65	C
ATOM	3748	CD2	LEU	D	121	67.118	-36.308	4.863	1.00	34.00	C
ATOM	3749	C	LEU	D	121	64.286	-38.098	7.456	1.00	38.21	C
ATOM	3750	O	LEU	D	121	64.305	-37.112	8.182	1.00	37.52	O
ATOM	3751	N	THR	D	122	64.672	-39.322	7.853	1.00	39.39	N
ATOM	3752	CA	THR	D	122	65.420	-39.553	9.093	1.00	40.36	C
ATOM	3753	CB	THR	D	122	64.764	-40.661	9.897	1.00	41.03	C
ATOM	3754	OG1	THR	D	122	63.433	-40.254	10.264	1.00	40.03	O
ATOM	3755	CG2	THR	D	122	65.574	-41.056	11.168	1.00	41.88	C
ATOM	3756	C	THR	D	122	66.850	-39.909	8.706	1.00	41.03	C
ATOM	3757	O	THR	D	122	67.056	-40.848	7.985	1.00	40.84	O
ATOM	3758	N	VAL	D	123	67.835	-39.101	9.103	1.00	42.99	N
ATOM	3759	CA	VAL	D	123	69.234	-39.583	9.052	1.00	44.79	C
ATOM	3760	CB	VAL	D	123	70.202	-38.754	8.099	1.00	45.22	C
ATOM	3761	CG1	VAL	D	123	71.523	-38.462	8.713	1.00	44.87	C
ATOM	3762	CG2	VAL	D	123	69.528	-37.548	7.456	1.00	43.50	C
ATOM	3763	C	VAL	D	123	69.796	-40.080	10.409	1.00	46.99	C
ATOM	3764	O	VAL	D	123	69.848	-39.349	11.408	1.00	46.54	O
ATOM	3765	N	LYS	D	124	70.123	-41.378	10.437	1.00	49.38	N
ATOM	3766	CA	LYS	D	124	70.636	-42.039	11.647	1.00	50.47	C
ATOM	3767	CB	LYS	D	124	70.156	-43.525	11.743	1.00	49.98	C
ATOM	3768	CG	LYS	D	124	68.619	-43.748	12.007	1.00	50.05	C
ATOM	3769	CD	LYS	D	124	68.052	-43.043	13.279	1.00	49.05	C
ATOM	3770	CE	LYS	D	124	66.688	-43.609	13.767	1.00	48.44	C
ATOM	3771	NZ	LYS	D	124	65.834	-42.572	14.515	1.00	47.51	N
ATOM	3772	C	LYS	D	124	72.171	-41.904	11.655	1.00	50.68	C
ATOM	3773	O	LYS	D	124	72.808	-42.063	10.610	1.00	51.52	O
ATOM	3774	N	ALA	D	125	72.722	-41.535	12.816	1.00	51.34	N
ATOM	3775	CA	ALA	D	125	74.161	-41.416	13.055	1.00	52.01	C
ATOM	3776	CB	ALA	D	125	74.443	-41.064	14.528	1.00	51.75	C
ATOM	3777	C	ALA	D	125	74.834	-42.715	12.711	1.00	52.46	C
ATOM	3778	O	ALA	D	125	74.540	-43.751	13.329	1.00	52.80	O
ATOM	3779	OXT	ALA	D	125	75.650	-42.744	11.792	1.00	52.94	O
ATOM	3780	O	HOH	W	1	27.537	-6.895	-25.418	1.00	49.96	O
ATOM	3781	O	HOH	W	2	16.484	-15.501	-2.860	1.00	51.92	O
ATOM	3782	O	HOH	W	3	64.994	-13.128	-29.648	1.00	61.47	O
ATOM	3783	O	HOH	W	4	58.640	-8.263	-15.036	1.00	51.01	O
ATOM	3784	O	HOH	W	5	49.811	-21.870	-19.181	1.00	53.77	O
ATOM	3785	O	HOH	W	6	47.451	15.219	8.922	1.00	53.13	O

ATOM	3786	O	HOH	W	7	57.241	6.450	-33.199	1.00	67.49	O
ATOM	3787	O	HOH	W	8	55.602	-37.210	4.291	1.00	45.54	O
ATOM	3788	O	HOH	W	9	71.793	-8.853	-14.510	1.00	53.04	O
ATOM	3789	O	HOH	W	10	28.959	18.294	23.084	1.00	44.15	O
ATOM	3790	O	HOH	W	11	51.211	-1.996	-16.782	1.00	34.13	O
ATOM	3791	O	HOH	W	12	20.537	2.113	13.747	1.00	37.57	O
ATOM	3792	O	HOH	W	13	63.618	-7.963	-22.008	1.00	48.46	O
ATOM	3793	O	HOH	W	14	15.973	-5.480	-1.302	1.00	58.45	O
ATOM	3794	O	HOH	W	15	47.026	19.336	-8.349	1.00	45.60	O
ATOM	3795	O	HOH	W	16	38.870	18.600	16.145	1.00	48.41	O
ATOM	3796	O	HOH	W	17	55.643	-13.712	-15.385	1.00	53.69	O
ATOM	3797	O	HOH	W	18	29.523	17.221	14.352	1.00	33.22	O
ATOM	3798	O	HOH	W	19	74.183	-13.852	-32.153	1.00	45.21	O
ATOM	3799	O	HOH	W	20	51.603	5.048	-41.486	1.00	67.11	O
ATOM	3800	O	HOH	W	21	75.638	-22.627	9.738	1.00	66.50	O
ATOM	3801	O	HOH	W	22	16.178	1.770	-16.784	1.00	63.18	O
ATOM	3802	O	HOH	W	23	72.855	-27.072	5.746	1.00	46.62	O
ATOM	3803	O	HOH	W	24	28.469	17.946	-7.226	1.00	50.63	O
ATOM	3804	O	HOH	W	25	52.814	15.053	-42.546	1.00	68.81	O
ATOM	3805	O	HOH	W	26	54.094	10.191	-35.541	1.00	68.73	O
ATOM	3806	O	HOH	W	27	28.221	15.502	-7.510	1.00	61.71	O
ATOM	3807	O	HOH	W	28	29.651	-7.408	-0.031	1.00	77.42	O
ATOM	3808	O	HOH	W	29	55.208	-11.816	-1.694	1.00	65.92	O
ATOM	3809	O	HOH	W	30	65.842	-14.431	-7.424	1.00	62.18	O
ATOM	3810	O	HOH	W	31	86.092	-37.988	19.084	1.00	62.21	O
ATOM	3811	O	HOH	W	32	57.547	-17.020	-8.281	1.00	54.14	O
ATOM	3812	O	HOH	W	33	15.238	-25.319	-14.960	1.00	48.17	O
ATOM	3813	O	HOH	W	34	32.868	-10.730	-16.000	1.00	60.24	O
ATOM	3814	O	HOH	W	35	27.383	-23.747	-14.732	1.00	54.01	O
ATOM	3815	O	HOH	W	36	45.466	-36.429	-7.768	1.00	61.01	O
ATOM	3816	O	HOH	W	37	85.751	6.805	-23.803	1.00	63.72	O
ATOM	3817	O	HOH	W	38	64.003	-17.550	-25.097	1.00	52.50	O
ATOM	3818	O	HOH	W	39	18.054	10.470	11.460	1.00	31.24	O
ATOM	3819	O	HOH	W	40	3.495	-9.168	-13.711	1.00	46.96	O
ATOM	3820	O	HOH	W	41	41.882	-5.080	13.345	1.00	59.64	O
ATOM	3821	O	HOH	W	42	53.605	-40.677	-18.373	1.00	65.41	O
ATOM	3822	O	HOH	W	43	36.386	-1.428	-3.036	1.00	50.71	O
ATOM	3823	O	HOH	W	44	73.455	-43.317	-0.552	1.00	59.07	O
ATOM	3824	O	HOH	W	45	78.144	-43.753	12.847	1.00	65.80	O
ATOM	3825	O	HOH	W	46	57.888	-11.778	-11.462	1.00	57.52	O
ATOM	3826	O	HOH	W	47	45.202	-5.340	3.650	1.00	48.23	O
ATOM	3827	O	HOH	W	48	63.611	-10.382	-24.415	1.00	50.05	O
ATOM	3828	O	HOH	W	49	57.536	6.456	-7.141	1.00	28.46	O
ATOM	3829	O	HOH	W	50	58.272	-0.505	-0.424	1.00	30.38	O
ATOM	3830	O	HOH	W	51	46.690	-1.769	0.708	1.00	25.84	O
ATOM	3831	O	HOH	W	52	43.295	5.650	-15.284	1.00	31.89	O
ATOM	3832	O	HOH	W	53	64.526	9.634	-19.506	1.00	29.96	O
ATOM	3833	O	HOH	W	54	23.155	-22.622	-14.253	1.00	34.18	O
ATOM	3834	O	HOH	W	55	64.074	-2.755	-3.506	1.00	32.46	O
ATOM	3835	O	HOH	W	56	65.733	-39.979	14.780	1.00	50.48	O
ATOM	3836	O	HOH	W	57	25.603	12.096	6.016	1.00	29.23	O
ATOM	3837	O	HOH	W	58	16.263	-22.766	-25.732	1.00	37.53	O
ATOM	3838	O	HOH	W	59	51.239	2.681	-2.880	1.00	34.06	O
ATOM	3839	O	HOH	W	60	54.458	-2.187	-19.524	1.00	40.20	O
ATOM	3840	O	HOH	W	61	71.361	7.864	-19.372	1.00	37.66	O
ATOM	3841	O	HOH	W	62	56.520	7.752	-18.350	1.00	37.39	O
ATOM	3842	O	HOH	W	63	13.694	-9.946	-29.896	1.00	38.42	O
ATOM	3843	O	HOH	W	64	61.439	-41.245	8.021	1.00	41.37	O
ATOM	3844	O	HOH	W	65	39.971	3.043	13.470	1.00	51.30	O
ATOM	3845	O	HOH	W	66	28.958	15.268	1.059	1.00	43.67	O
ATOM	3846	O	HOH	W	67	30.104	2.750	2.608	1.00	40.29	O

ATOM	3847	O	HOH W	68	69.821	-2.267	-8.072	1.00	33.11	O
ATOM	3848	O	HOH W	69	52.286	-7.121	-16.541	1.00	38.11	O
ATOM	3849	O	HOH W	70	58.487	-28.442	5.036	1.00	37.01	O
ATOM	3850	O	HOH W	71	25.719	16.565	13.085	1.00	44.30	O
ATOM	3851	O	HOH W	72	52.822	-11.013	-17.837	1.00	45.81	O
ATOM	3852	O	HOH W	73	22.805	-12.848	-21.485	1.00	48.51	O
ATOM	3853	O	HOH W	74	36.702	17.554	5.981	1.00	37.50	O
ATOM	3854	O	HOH W	75	71.895	-9.443	-24.558	1.00	45.80	O
ATOM	3855	O	HOH W	76	41.108	15.717	-5.487	1.00	39.02	O
ATOM	3856	O	HOH W	77	18.799	8.481	10.303	1.00	46.57	O
ATOM	3857	O	HOH W	78	61.610	7.007	-4.915	1.00	50.08	O
ATOM	3858	O	HOH W	79	60.439	-0.706	-2.323	1.00	33.12	O
ATOM	3859	O	HOH W	80	58.416	5.614	-9.104	1.00	39.99	O
ATOM	3860	O	HOH W	81	55.764	-3.255	-35.605	1.00	54.28	O
ATOM	3861	O	HOH W	82	42.688	13.409	7.580	1.00	32.60	O
ATOM	3862	O	HOH W	83	56.203	7.504	-13.473	1.00	53.50	O
ATOM	3863	O	HOH W	84	49.392	-17.628	-1.745	1.00	48.43	O
ATOM	3864	O	HOH W	85	38.478	17.991	-4.303	1.00	51.79	O
ATOM	3865	O	HOH W	86	27.380	11.533	-6.035	1.00	43.44	O
ATOM	3866	O	HOH W	87	17.419	-2.527	-17.186	1.00	46.81	O
ATOM	3867	O	HOH W	88	65.605	11.412	-34.743	1.00	39.99	O
ATOM	3868	O	HOH W	89	22.567	-9.323	0.874	1.00	67.08	O
ATOM	3869	O	HOH W	90	60.466	-7.608	-10.787	1.00	44.79	O
ATOM	3870	O	HOH W	91	70.029	13.354	-25.195	1.00	48.65	O
ATOM	3871	O	HOH W	92	27.738	-0.724	12.598	1.00	46.67	O
ATOM	3872	O	HOH W	93	67.709	-9.736	-34.668	1.00	44.52	O
ATOM	3873	O	HOH W	94	66.469	-42.220	-2.677	1.00	50.32	O
ATOM	3874	O	HOH W	95	39.659	4.264	19.635	1.00	47.26	O
ATOM	3875	O	HOH W	96	33.798	-0.629	0.634	1.00	57.82	O
ATOM	3876	O	HOH W	97	68.516	5.533	-7.794	1.00	38.76	O
ATOM	3877	O	HOH W	98	57.378	4.251	-27.603	1.00	49.36	O
ATOM	3878	O	HOH W	99	45.738	12.067	6.077	1.00	40.86	O
ATOM	3879	O	HOH W	100	72.260	-27.692	-8.666	1.00	69.19	O
ATOM	3880	O	HOH W	101	74.870	5.332	-30.099	1.00	41.86	O
ATOM	3881	O	HOH W	102	19.884	-13.568	-28.826	1.00	38.32	O
ATOM	3882	O	HOH W	103	3.023	-14.597	-13.318	1.00	47.56	O
ATOM	3883	O	HOH W	104	44.498	-8.083	-17.403	1.00	48.70	O
ATOM	3884	O	HOH W	105	75.836	-5.431	-10.641	1.00	58.00	O
ATOM	3885	O	HOH W	106	60.710	7.924	-15.560	1.00	30.19	O
ATOM	3886	O	HOH W	107	40.439	-9.476	15.038	1.00	60.28	O
ATOM	3887	O	HOH W	108	56.235	-30.734	8.744	1.00	53.65	O
ATOM	3888	O	HOH W	109	63.101	-1.697	-1.511	1.00	31.65	O
ATOM	3889	O	HOH W	110	56.808	5.705	-16.251	1.00	33.23	O
ATOM	3890	O	HOH W	111	38.263	8.376	22.049	1.00	55.72	O
ATOM	3891	O	HOH W	112	64.897	-23.439	-3.286	1.00	46.93	O
ATOM	3892	O	HOH W	113	30.449	-20.129	-16.647	1.00	51.12	O
ATOM	3893	O	HOH W	114	24.716	-6.274	-13.423	1.00	48.87	O
ATOM	3894	O	HOH W	115	69.646	14.058	-27.887	1.00	43.33	O
ATOM	3895	O	HOH W	116	74.378	8.019	-23.439	1.00	42.12	O
ATOM	3896	O	HOH W	117	74.411	-6.755	-12.312	1.00	46.21	O
ATOM	3897	O	HOH W	118	80.776	-40.223	6.131	1.00	51.98	O
ATOM	3898	O	HOH W	119	16.271	-26.835	-20.387	1.00	53.48	O
ATOM	3899	O	HOH W	120	45.888	8.444	12.000	1.00	56.59	O
ATOM	3900	O	HOH W	121	69.004	-39.355	13.718	1.00	48.52	O
ATOM	3901	O	HOH W	122	44.628	1.826	3.253	1.00	55.53	O
ATOM	3902	O	HOH W	123	10.540	-21.289	-24.117	1.00	55.75	O
ATOM	3903	O	HOH W	124	39.519	7.553	-11.796	1.00	42.99	O
ATOM	3904	O	HOH W	125	17.953	2.631	6.934	1.00	46.87	O
ATOM	3905	O	HOH W	126	59.706	-42.276	8.568	1.00	49.22	O
ATOM	3906	O	HOH W	127	71.515	9.604	-9.652	1.00	51.76	O
ATOM	3907	O	HOH W	128	22.711	-2.131	7.099	1.00	56.06	O

ATOM	3908	O	HOH W 129	50.497	1.860	-26.962	1.00	48.49	O
ATOM	3909	O	HOH W 130	13.213	-25.189	-17.571	1.00	47.33	O
ATOM	3910	O	HOH W 131	36.422	-18.594	1.861	1.00	59.55	O
ATOM	3911	O	HOH W 132	67.824	-18.443	8.774	1.00	64.42	O
ATOM	3912	O	HOH W 133	38.702	9.149	25.860	1.00	63.04	O
ATOM	3913	O	HOH W 134	26.829	-19.030	-19.104	1.00	49.31	O
ATOM	3914	O	HOH W 135	59.736	-32.012	10.576	1.00	35.03	O
ATOM	3915	O	HOH W 136	64.103	0.614	-0.340	1.00	40.32	O
ATOM	3916	O	HOH W 137	68.933	-33.671	-8.563	1.00	47.24	O
ATOM	3917	O	HOH W 138	30.091	-18.545	3.715	1.00	65.55	O
ATOM	3918	O	HOH W 139	11.871	-19.774	-24.246	1.00	33.50	O
ATOM	3919	O	HOH W 140	54.104	-8.838	-17.264	1.00	43.66	O
ATOM	3920	O	HOH W 141	68.475	-6.296	-7.780	1.00	51.54	O
ATOM	3921	O	HOH W 142	61.319	8.970	-35.221	1.00	63.08	O
ATOM	3922	O	HOH W 143	5.216	-2.074	-13.989	1.00	53.77	O
ATOM	3923	O	HOH W 144	77.471	-7.485	-20.605	1.00	62.28	O
ATOM	3924	O	HOH W 145	22.942	-15.078	-26.211	1.00	45.04	O
ATOM	3925	O	HOH W 146	62.912	-3.121	-6.057	1.00	35.08	O
ATOM	3926	O	HOH W 147	60.466	-10.624	-21.327	1.00	50.25	O
ATOM	3927	O	HOH W 148	49.218	8.905	-16.800	1.00	51.16	O
ATOM	3928	O	HOH W 149	33.265	10.047	-10.678	1.00	48.18	O
ATOM	3929	O	HOH W 150	58.095	9.361	-4.575	1.00	50.70	O
ATOM	3930	O	HOH W 151	44.991	-5.664	-19.770	1.00	52.37	O
ATOM	3931	O	HOH W 152	46.997	-10.249	-1.900	1.00	46.25	O
ATOM	3932	O	HOH W 153	30.534	2.664	-1.760	1.00	51.90	O
ATOM	3933	O	HOH W 154	75.688	-26.530	1.235	1.00	61.29	O
ATOM	3934	O	HOH W 155	31.837	18.468	15.789	1.00	47.11	O
ATOM	3935	O	HOH W 156	22.573	-6.055	-12.416	1.00	40.78	O
ATOM	3936	O	HOH W 157	69.966	-24.619	2.582	1.00	51.01	O
ATOM	3937	O	HOH W 158	7.080	-14.929	-10.596	1.00	46.45	O
ATOM	3938	O	HOH W 159	30.087	19.609	-1.446	1.00	65.48	O
ATOM	3939	O	HOH W 160	35.321	18.508	20.566	1.00	53.81	O
ATOM	3940	O	HOH W 161	66.872	-33.922	14.718	1.00	52.80	O
ATOM	3941	O	HOH W 162	19.048	-21.457	-21.483	1.00	49.57	O
ATOM	3942	O	HOH W 163	55.940	2.690	-8.893	1.00	32.16	O
ATOM	3943	O	HOH W 164	73.832	-5.186	-31.071	1.00	44.92	O
ATOM	3944	O	HOH W 165	73.497	4.469	-51.566	1.00	49.98	O
ATOM	3945	O	HOH W 166	46.143	-24.184	2.265	1.00	65.14	O
ATOM	3946	O	HOH W 167	53.822	-6.318	-27.868	1.00	59.13	O
ATOM	3947	O	HOH W 168	22.273	-7.060	-32.842	1.00	55.91	O
ATOM	3948	O	HOH W 169	69.920	5.647	-54.927	1.00	52.38	O
ATOM	3949	O	HOH W 170	75.276	-0.500	-18.493	1.00	56.03	O
ATOM	3950	O	HOH W 171	74.355	-7.796	-18.378	1.00	51.15	O
ATOM	3951	O	HOH W 172	49.846	7.730	-10.950	1.00	26.02	O
ATOM	3952	O	HOH W 173	74.688	6.874	-18.930	1.00	59.05	O
ATOM	3953	O	HOH W 174	8.532	-17.930	-12.696	1.00	46.51	O
ATOM	3954	O	HOH W 175	65.329	10.399	-23.289	1.00	31.68	O
ATOM	3955	O	HOH W 176	62.448	-6.262	-23.487	1.00	45.41	O
ATOM	3956	O	HOH W 177	13.206	-11.211	-6.299	1.00	49.50	O
ATOM	3957	O	HOH W 178	61.714	2.022	-1.453	1.00	36.23	O
ATOM	3958	O	HOH W 179	46.778	11.434	-6.992	1.00	35.69	O
ATOM	3959	O	HOH W 180	27.754	6.719	-4.382	1.00	58.45	O
ATOM	3960	O	HOH W 181	15.241	-0.832	-13.316	1.00	42.58	O
ATOM	3961	O	HOH W 182	58.699	9.096	-7.863	1.00	34.47	O
ATOM	3962	O	HOH W 183	64.941	-16.861	0.001	1.00	64.80	O
ATOM	3963	O	HOH W 184	77.519	-7.298	-17.771	1.00	59.86	O
ATOM	3964	O	HOH W 185	61.404	-45.244	5.009	1.00	47.15	O
ATOM	3965	O	HOH W 186	21.672	-2.040	-10.318	1.00	50.64	O
ATOM	3966	O	HOH W 187	29.956	-0.092	-9.945	1.00	62.76	O
ATOM	3967	O	HOH W 188	36.410	15.705	-10.591	1.00	55.05	O
ATOM	3968	O	HOH W 189	77.269	-24.718	-6.307	1.00	58.93	O

ATOM	3969	O	HOH W 190	53.639	-41.684	4.960	1.00	46.88		O
ATOM	3970	O	HOH W 191	39.701	-8.194	-19.650	1.00	68.65		O
ATOM	3971	O	HOH W 192	72.960	11.333	-30.255	1.00	57.07		O
ATOM	3972	O	HOH W 193	69.245	-8.902	-20.463	1.00	59.91		O
ATOM	3973	O	HOH W 194	25.519	2.766	-5.298	1.00	62.24		O
ATOM	3974	O	HOH W 195	23.823	-18.240	-23.523	1.00	53.83		O
ATOM	3975	O	HOH W 196	76.411	-10.927	-28.761	1.00	57.41		O
ATOM	3976	O	HOH W 197	68.909	7.633	-3.751	1.00	54.97		O
ATOM	3977	O	HOH W 198	68.238	4.063	-57.802	1.00	60.28		O
ATOM	3978	O	HOH W 199	57.902	-43.905	0.785	1.00	47.08		O
ATOM	3979	O	HOH W 200	26.387	1.586	19.253	1.00	57.98		O
ATOM	3980	O	HOH W 201	37.729	12.225	22.176	1.00	36.41		O
ATOM	3981	O	HOH W 202	52.534	7.353	-41.886	1.00	66.91		O
ATOM	3982	O	HOH W 203	27.054	-0.735	4.862	1.00	51.36		O
ATOM	3983	O	HOH W 204	42.236	-8.736	1.239	1.00	49.54		O
ATOM	3984	O	HOH W 205	72.453	-49.755	2.535	1.00	57.88		O
ATOM	3985	O	HOH W 206	21.715	13.751	27.357	1.00	63.70		O
ATOM	3986	O	HOH W 207	72.850	11.054	-33.545	1.00	48.23		O
ATOM	3987	O	HOH W 208	72.490	9.599	-53.823	1.00	63.34		O
ATOM	3988	O	HOH W 209	62.543	16.639	-24.176	1.00	32.72		O
ATOM	3989	O	HOH W 210	45.124	-6.604	-14.457	1.00	40.86		O
ATOM	3990	O	HOH W 211	67.128	11.703	-20.217	1.00	33.12		O
ATOM	3991	O	HOH W 212	71.826	-45.136	14.739	1.00	57.74		O
ATOM	3992	O	HOH W 213	57.710	7.585	-21.003	1.00	45.04		O
ATOM	3993	O	HOH W 214	38.961	-13.213	-15.679	1.00	47.33		O
ATOM	3994	O	HOH W 215	44.800	6.821	8.691	1.00	43.90		O
ATOM	3995	O	HOH W 216	52.098	-22.105	-2.209	1.00	58.29		O
ATOM	3996	O	HOH W 217	59.838	-5.952	-22.966	1.00	42.78		O
ATOM	3997	O	HOH W 218	18.495	-22.454	-8.937	1.00	43.08		O
ATOM	3998	O	HOH W 219	41.438	-0.960	2.947	1.00	47.12		O
ATOM	3999	O	HOH W 220	28.357	-12.574	2.320	1.00	67.42		O
ATOM	4000	O	HOH W 221	31.534	1.142	5.187	1.00	52.28		O
ATOM	4001	O	HOH W 222	52.061	-0.982	-33.448	1.00	66.10		O
ATOM	4002	O	HOH W 223	70.684	-25.967	-10.607	1.00	59.78		O
ATOM	4003	O	HOH W 224	24.630	-22.237	-21.050	1.00	62.09		O
ATOM	4004	O	HOH W 225	42.829	-4.753	-0.058	1.00	47.47		O
ATOM	4005	O	HOH W 226	70.534	13.938	-33.309	1.00	57.59		O
ATOM	4006	O	HOH W 227	37.629	6.169	-9.632	1.00	35.87		O
ATOM	4007	O	HOH W 228	39.050	-3.195	8.473	1.00	56.47		O
ATOM	4008	O	HOH W 229	50.163	-25.989	-2.653	1.00	57.19		O
ATOM	4009	O	HOH W 230	66.728	8.298	-2.609	1.00	53.22		O
ATOM	4010	O	HOH W 231	46.144	4.981	2.915	1.00	49.44		O
ATOM	4011	O	HOH W 232	64.030	15.931	-27.869	1.00	50.25		O
ATOM	4012	O	HOH W 233	78.237	-11.718	-16.675	1.00	66.40		O
ATOM	4013	O	HOH W 234	3.812	-6.905	-25.561	1.00	46.71		O
ATOM	4014	O	HOH W 235	64.296	-9.563	-18.956	1.00	55.82		O
ATOM	4015	O	HOH W 236	57.040	10.985	-10.979	1.00	33.38		O
ATOM	4016	O	HOH W 237	68.114	0.724	-44.435	1.00	47.88		O
ATOM	4017	O	HOH W 238	77.812	2.986	-35.556	1.00	54.12		O
ATOM	4018	O	HOH W 239	68.542	13.125	-10.000	1.00	42.93		O
ATOM	4019	O	HOH W 240	70.815	11.906	-8.762	1.00	61.18		O
ATOM	4020	O	HOH W 241	59.743	-4.943	-32.625	1.00	68.83		O
ATOM	4021	O	HOH W 242	53.599	-2.593	-24.738	1.00	57.17		O
ATOM	4022	O	HOH W 243	28.804	-22.157	-13.530	1.00	66.00		O
ATOM	4023	O	HOH W 244	12.528	-20.034	-9.931	1.00	54.81		O
ATOM	4024	O	HOH W 245	18.999	-13.928	-26.454	1.00	37.34		O
ATOM	4025	O	HOH W 246	9.399	-7.555	-10.236	1.00	51.74		O
ATOM	4026	O	HOH W 247	9.422	-23.577	-21.883	1.00	51.71		O
ATOM	4027	O	HOH W 248	48.989	16.285	-2.427	1.00	52.11		O
ATOM	4028	O	HOH W 249	25.370	13.160	27.839	1.00	51.67		O
ATOM	4029	O	HOH W 250	34.924	12.483	-8.217	1.00	36.25		O

ATOM	4030	O	HOH W 251	55.418	-37.562	-1.079	1.00	39.90	O
ATOM	4031	O	HOH W 252	65.053	-34.377	-13.229	1.00	61.20	O
ATOM	4032	O	HOH W 253	65.103	-23.855	-7.015	1.00	61.09	O
ATOM	4033	O	HOH W 254	59.191	-30.854	12.930	1.00	31.05	O
ATOM	4034	O	HOH W 255	74.576	-21.281	-5.297	1.00	62.37	O
ATOM	4035	O	HOH W 256	77.566	-33.129	5.274	1.00	55.66	O
ATOM	4036	O	HOH W 257	53.903	-22.288	-17.014	1.00	50.27	O
ATOM	4037	O	HOH W 258	45.037	-8.754	-15.227	1.00	49.48	O
ATOM	4038	O	HOH W 259	22.148	10.033	10.947	1.00	39.41	O
ATOM	4039	O	HOH W 260	65.185	-7.017	-20.794	1.00	45.24	O
ATOM	4040	O	HOH W 261	35.881	-2.206	17.490	1.00	44.28	O
ATOM	4041	O	HOH W 262	51.882	0.389	-39.836	1.00	67.72	O
ATOM	4042	O	HOH W 263	31.840	18.088	10.972	1.00	46.55	O
ATOM	4043	O	HOH W 264	0.515	-17.290	-27.161	1.00	54.35	O
ATOM	4044	O	HOH W 265	69.618	-46.411	15.204	1.00	62.11	O
ATOM	4045	O	HOH W 266	30.859	7.314	28.270	1.00	50.41	O
ATOM	4046	O	HOH W 267	18.081	11.850	9.552	1.00	53.90	O
ATOM	4047	O	HOH W 268	59.391	-23.586	16.532	1.00	66.97	O
ATOM	4048	O	HOH W 269	35.395	5.989	-11.309	1.00	48.68	O
ATOM	4049	O	HOH W 270	16.271	1.278	9.498	1.00	66.12	O
ATOM	4050	O	HOH W 271	46.429	19.602	7.510	1.00	50.45	O
ATOM	4051	O	HOH W 272	41.687	0.016	6.150	1.00	48.74	O
ATOM	4052	O	HOH W 273	55.497	-10.087	2.040	1.00	52.80	O
ATOM	4053	O	HOH W 274	11.272	-9.479	-30.539	1.00	38.85	O
ATOM	4054	O	HOH W 275	54.397	-1.130	-21.031	1.00	54.26	O
ATOM	4055	O	HOH W 276	12.883	-21.707	-24.390	1.00	53.71	O
ATOM	4056	O	HOH W 277	18.287	-21.975	-25.586	1.00	45.47	O
ATOM	4057	O	HOH W 278	46.785	0.418	-18.533	1.00	32.22	O
ATOM	4058	O	HOH W 279	45.873	-0.317	-20.312	1.00	58.31	O
ATOM	4059	O	HOH W 280	46.094	-1.639	-18.715	1.00	40.18	O
ATOM	4060	O	HOH W 281	42.337	-11.592	-18.551	1.00	65.25	O
ATOM	4061	O	HOH W 282	39.890	13.264	-12.839	1.00	51.77	O
ATOM	4062	O	HOH W 283	44.794	10.396	3.595	1.00	40.28	O
ATOM	4063	O	HOH W 284	39.618	18.733	13.341	1.00	51.45	O
ATOM	4064	O	HOH W 285	53.173	-35.468	-3.845	1.00	38.36	O
ATOM	4065	O	HOH W 286	17.906	-8.860	-0.520	1.00	47.10	O
ATOM	4066	O	HOH W 287	67.074	-7.604	-16.718	1.00	36.14	O
ATOM	4067	O	HOH W 288	12.354	-4.311	-22.662	1.00	46.21	O
ATOM	4068	O	HOH W 289	74.559	-22.448	-0.574	1.00	63.95	O
ATOM	4069	O	HOH W 290	24.579	9.857	-1.018	1.00	42.40	O
ATOM	4070	O	HOH W 291	42.836	-14.137	-19.076	1.00	48.67	O
ATOM	4071	O	HOH W 292	42.577	-32.888	-9.222	1.00	58.27	O
ATOM	4072	O	HOH W 293	51.889	-30.288	0.706	1.00	47.73	O
ATOM	4073	O	HOH W 294	58.591	9.524	-11.965	1.00	64.46	O
ATOM	4074	O	HOH W 295	23.195	6.118	25.651	1.00	51.90	O
ATOM	4075	O	HOH W 296	62.053	-7.731	-30.991	1.00	49.35	O
ATOM	4076	O	HOH W 297	49.685	-0.059	-34.867	1.00	57.45	O
ATOM	4077	O	HOH W 298	27.481	15.626	30.011	1.00	62.52	O
ATOM	4078	O	HOH W 299	22.412	16.454	25.493	1.00	43.70	O
ATOM	4079	O	HOH W 300	63.991	-24.156	-11.886	1.00	44.37	O
ATOM	4080	O	HOH W 301	23.584	-2.108	-14.137	1.00	51.53	O
ATOM	4081	O	HOH W 302	16.320	-11.014	1.961	1.00	61.11	O
ATOM	4082	O	HOH W 303	21.217	-22.569	-24.840	1.00	58.72	O
ATOM	4083	O	HOH W 304	41.646	17.848	-7.228	1.00	65.03	O
ATOM	4084	O	HOH W 305	22.950	17.731	10.015	1.00	58.75	O
ATOM	4085	O	HOH W 306	56.767	7.202	2.006	1.00	62.33	O
ATOM	4086	O	HOH W 307	58.177	-38.332	-8.428	1.00	51.10	O
ATOM	4087	O	HOH W 308	36.859	6.714	22.042	1.00	67.48	O
ATOM	4088	O	HOH W 309	8.548	-9.082	-6.377	1.00	64.08	O
ATOM	4089	O	HOH W 310	77.441	6.499	-18.901	1.00	53.22	O
ATOM	4090	O	HOH W 311	50.214	-2.598	-28.240	1.00	65.39	O

ATOM	4091	O	HOH W 312	67.157	-32.383	12.563	1.00	52.04	O
ATOM	4092	O	HOH W 313	42.103	10.501	15.691	1.00	58.68	O
ATOM	4093	O	HOH W 314	32.134	-22.541	-14.797	1.00	64.57	O
ATOM	4094	O	HOH W 315	49.067	3.344	-37.222	1.00	67.11	O
ATOM	4095	O	HOH W 316	61.987	-46.753	3.536	1.00	61.36	O
ATOM	4096	O	HOH W 317	60.318	-9.489	-9.294	1.00	50.74	O
ATOM	4097	O	HOH W 318	48.190	-10.315	0.317	1.00	44.60	O
ATOM	4098	O	HOH W 319	50.098	-10.842	-18.057	1.00	53.04	O
ATOM	4099	O	HOH W 320	46.094	9.952	6.886	1.00	54.78	O
ATOM	4100	O	HOH W 321	74.455	7.920	-30.461	1.00	54.66	O
ATOM	4101	O	HOH W 322	73.297	-11.177	-30.246	1.00	54.61	O
ATOM	4102	O	HOH W 323	55.869	3.785	-16.712	1.00	47.04	O
ATOM	4103	O	HOH W 324	17.752	-20.654	-6.176	1.00	66.30	O
ATOM	4104	O	HOH W 325	19.223	-5.198	-23.515	1.00	66.40	O
ATOM	4105	O	HOH W 326	14.416	-5.443	-29.063	1.00	58.70	O
ATOM	4106	O	HOH W 327	20.794	-20.150	-22.576	1.00	47.38	O
ATOM	4107	O	HOH W 328	46.970	9.591	-3.000	1.00	61.77	O
ATOM	4108	O	HOH W 329	44.733	9.137	-4.905	1.00	58.82	O
ATOM	4109	O	HOH W 330	44.656	15.089	8.206	1.00	62.37	O
ATOM	4110	O	HOH W 331	41.354	13.880	11.375	1.00	49.54	O
ATOM	4111	O	HOH W 332	37.483	14.530	22.480	1.00	53.31	O
ATOM	4112	O	HOH W 333	41.722	19.379	-3.546	1.00	50.97	O
ATOM	4113	O	HOH W 334	42.731	13.993	-12.884	1.00	72.77	O
ATOM	4114	O	HOH W 335	23.790	0.599	10.614	1.00	45.38	O
ATOM	4115	O	HOH W 336	59.513	-7.372	-13.143	1.00	61.55	O
ATOM	4116	O	HOH W 337	56.314	9.708	-14.663	1.00	50.95	O
ATOM	4117	O	HOH W 338	31.978	-18.528	-15.554	1.00	67.33	O
ATOM	4118	O	HOH W 339	56.351	-11.784	-4.728	1.00	42.25	O
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ATOM	4121	O	HOH W 342	45.883	15.519	-9.499	1.00	60.90	O
ATOM	4122	O	HOH W 343	42.607	11.894	21.114	1.00	59.64	O
ATOM	4123	O	HOH W 344	64.897	-45.210	2.801	1.00	46.00	O
ATOM	4124	O	HOH W 345	62.414	-44.124	9.836	1.00	54.24	O
ATOM	4125	O	HOH W 346	66.607	-47.490	14.098	1.00	51.46	O
ATOM	4126	O	HOH W 347	33.184	9.901	29.054	1.00	54.19	O
ATOM	4127	O	HOH W 348	61.338	-8.260	-18.802	1.00	61.80	O
ATOM	4128	O	HOH W 349	58.915	10.462	-1.335	1.00	59.07	O
ATOM	4129	O	HOH W 350	72.985	11.119	-6.571	1.00	57.45	O
ATOM	4130	O	HOH W 351	52.715	-5.406	-30.681	1.00	76.01	O
ATOM	4131	O	HOH W 352	79.919	-27.316	-4.944	1.00	61.96	O
ATOM	4132	O	HOH W 353	71.264	8.651	-47.201	1.00	49.44	O
ATOM	4133	O	HOH W 354	22.664	12.842	33.813	1.00	49.23	O
ATOM	4134	O	HOH W 355	27.068	20.483	22.480	1.00	39.84	O
ATOM	4135	O	HOH W 356	31.821	-0.902	1.857	1.00	55.00	O
ATOM	4136	O	HOH W 357	35.021	-1.745	3.155	1.00	59.58	O
ATOM	4137	O	HOH W 358	39.467	2.391	21.237	1.00	73.05	O
ATOM	4138	O	HOH W 359	35.690	-6.904	-2.480	1.00	64.18	O
ATOM	4139	O	HOH W 360	38.038	-8.228	-14.500	1.00	64.77	O
ATOM	4140	O	HOH W 361	56.585	-29.520	5.841	1.00	60.72	O
ATOM	4141	O	HOH W 362	55.461	-35.538	5.382	1.00	54.96	O
ATOM	4142	O	HOH W 363	62.048	-20.002	-5.479	1.00	55.47	O
ATOM	4143	O	HOH W 364	65.219	-29.258	15.468	1.00	67.43	O
ATOM	4144	O	HOH W 365	15.338	-5.304	-5.505	1.00	54.06	O
ATOM	4145	O	HOH W 366	28.667	17.880	30.849	1.00	58.81	O
ATOM	4146	O	HOH W 367	7.490	-4.018	-9.949	1.00	49.82	O
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ATOM	4148	O	HOH W 369	23.205	-24.145	-0.987	1.00	49.15	O
ATOM	4149	O	HOH W 370	46.687	7.432	6.640	1.00	58.62	O
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ATOM	4151	O	HOH W 372	6.503	-2.107	-24.879	1.00	52.47	O

ATOM	4152	O	HOH W 373	47.592	-16.616	-26.050	1.00	54.23		O
ATOM	4153	O	HOH W 374	32.148	2.927	25.177	1.00	51.95		O
ATOM	4154	O	HOH W 375	70.869	13.479	-15.671	1.00	61.78		O
ATOM	4155	O	HOH W 376	32.233	-9.491	0.706	1.00	64.72		O
ATOM	4156	O	HOH W 377	43.162	-20.025	-20.830	1.00	61.56		O
ATOM	4157	O	HOH W 378	7.447	-21.877	-18.708	1.00	54.28		O
ATOM	4158	O	HOH W 379	64.478	-20.926	-14.628	1.00	56.28		O
ATOM	4159	O	HOH W 380	70.262	-45.646	1.731	1.00	65.26		O
ATOM	4160	O	HOH W 381	20.516	12.524	8.760	1.00	43.73		O
ATOM	4161	O	HOH W 382	74.928	8.949	-8.247	1.00	54.24		O
ATOM	4162	O	HOH W 383	18.257	-25.208	-7.910	1.00	50.96		O
ATOM	4163	O	HOH W 384	34.170	18.737	17.233	1.00	47.03		O
ATOM	4164	O	HOH W 385	21.137	2.084	3.808	1.00	65.70		O
ATOM	4165	O	HOH W 386	38.186	-4.444	-15.698	1.00	66.07		O
ATOM	4166	O	HOH W 387	38.985	-6.466	-8.831	1.00	51.93		O
ATOM	4167	O	HOH W 388	3.906	-16.558	-13.958	1.00	54.64		O
ATOM	4168	O	HOH W 389	33.087	-21.326	-9.095	1.00	66.75		O
ATOM	4169	O	HOH W 390	27.295	-14.177	5.542	1.00	58.06		O
ATOM	4170	O	HOH W 391	41.013	-5.818	20.816	1.00	60.46		O
ATOM	4171	O	HOH W 392	22.713	1.185	14.363	1.00	64.09		O
ATOM	4172	O	HOH W 393	48.064	6.165	1.998	1.00	61.05		O
ATOM	4173	O	HOH W 394	46.193	7.105	3.046	1.00	37.46		O

CLAIMS:-

1. An Aβ-IgNAR molecule having the amino acid sequence of any one of SEQ ID NOs: 15 to 24.

2. A crystal of amyloid β-peptide Aβ(18-41) as a fusion with IgNAR (Aβ-IgNAR).

3. The Aβ-IgNAR crystal as claimed in claim 2 in which the crystal comprises an Aβ - IgNAR monomer.

4. The Aβ-IgNAR crystal as claimed in claim 2 in which the crystal comprises an Aβ - IgNAR dimer.

5. The Aβ-IgNAR crystal as claimed in claim 2 in which the crystal comprises an Aβ - IgNAR tetramer.

6. An Aβ -IgNAR crystal as claimed in any one of claims 2 to 6 in which the Aβ-IgNAR crystal has the atomic coordinates set forth in Appendix I.

7. A method of assessing the interaction of a compound with Aβ, the method comprising contacting the crystal of the present invention with the compound and measuring the level of binding of the compound to the Aβ crystal.

8. A method of selecting or designing a compound that interacts with Aβ protein, the method comprising (a) assessing the stereochemical complementarity between a compound and a topographic region of Aβ protein, wherein the protein comprises: (i) amino acids 18-41 of the Aβ protein positioned at atomic coordinates as shown in Appendix I, or structural coordinates having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å; or (ii) one or more subsets of said amino acids related to the coordinates shown in Appendix I by whole body translations and/or rotations; (b) obtaining a compound which possesses stereochemical complementarity to a topographic region of the Aβ protein; and (c) testing the compound for its ability to modulate an activity associated with the Aβ protein.

9. A method for identifying a potential modulator compound for Aβ protein which method comprises: (a) providing a three-dimensional structure of amino acids 18-41 of Aβ protein as defined by the atomic coordinates shown in Appendix I, or atomic coordinates having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, or one or more subsets of said amino acids, or one or more subsets of said amino acids related to the coordinates shown in Appendix I by whole body translations and/or rotations; (b) providing the three-

dimensional structure of a candidate compound; and (c) assessing the stereochemical complementarity between the three- dimensional structure of step (b) and a topographic region of the three-dimensional structure of step (a).

10. A method as claimed in claim 8 or claim 9 in which the topographic region is a region of Aβ involved in oligermisation.

11. A method as claimed in claim 8 or claim 9 in which the topographic region is defined by amino acids V18 – I41.

12. A method as claimed in claim 8 or claim 9 in which the topographic region is defined by amino acids N27, K28, I31 and L34.

13. A method as claimed in claim 8 or claim 9 in which the topographic region is defined by amino acids G33, L34, M35 and V36.

14. A method as claimed in claim 8 or claim 9 in which the topographic region is defined by amino acids V18, F20, S26, K28, G29, I32, M35, V39 and I41.

15. A method as claimed in claim 8 or claim 9 in which the topographic region is defined by amino acids F19, A21, G25, N27, K28, G29, I31 and L34.

16. A method as claimed in claim 8 or claim 9 in which the topographic region is defined by amino acids I32, G33, L34, M35 and V36.

17. A method as claimed in claim 8 or claim 9 in which the topographic region is defined by amino acids V18, F20, D23, S26, K28, A30, I32, M35, G37, V39 and I41.

18. A method of assessing the ability of a compound to affect the ability of Aβ to form dimers or tetramers, the method comprising assessing the level Aβ-IgNAR dimerisation or tetramerisation in the presence or absence of the compound.

19. A method as claimed in claim 18 in which the Aβ-IgNAR has the amino acid sequence of SEQ ID NO: 2, 4 or 5.

20. A method as claimed in claim 18 or claim 19 in which the assessment of dimerisation or tetramerisation is made by SDS-PAGE or western blot.

21. A computer-assisted method for identifying potential compounds able to interact with Aβ protein and thereby modulate an activity mediated by Aβ protein, using a programmed computer comprising a processor, an input device, and an output device, comprising the steps of: (a) inputting into the programmed computer, through

the input device, data comprising the atomic coordinates of amino acids 18-41 of Aβ protein as shown in Appendix I, or structural coordinates having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, or one or more subsets of said amino acids, or one or more subsets of said amino acids related to the coordinates shown in Appendix I by whole body translations and/or rotations; (b) generating, using computer methods, a set of atomic coordinates of a structure that possesses stereochemical complementarity to the atomic coordinates of amino acids 18-41 of the Aβ protein as shown in Appendix I, or structural coordinates having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, or one or more subsets of said amino acids, or one or more subsets of said amino acids related to the coordinates shown in Appendix I by whole body translations and/or rotations, thereby generating a criteria data set; (c) comparing, using the processor, the criteria data set to a computer database of chemical structures; (d) selecting from the database, using computer methods, chemical structures which are similar to a portion of said criteria data set; and (e) outputting, to the output device, the selected chemical structures which are complementary to or similar to a portion of the criteria data set.

22. A method for evaluating the ability of a chemical entity to interact with Aβ protein, said method comprising the steps of: (a) creating a computer model of amino acids 18-41 of Aβ protein using structure coordinates wherein the root mean square deviation between said structure coordinates and the structure coordinates of amino acids 18-41 of Aβ protein as set forth in Appendix I is not more than about 1.5 Å ; (b) employing computational means to perform a fitting operation between the chemical entity and said computer model of the binding surface; and (c) analysing the results of said fitting operation to quantify the association between the chemical entity and the Aβ protein model.

23. A computer for producing a three-dimensional representation of a molecule or molecular complex, wherein the computer comprises: (a) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein the machine readable data comprise the atomic coordinates of amino acids 18-41 of Aβ protein as shown in Appendix I, or structural coordinates having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, or one or more subsets of said amino acids, or one or more subsets of said amino acids related to the coordinates shown in Appendix I by whole body translations and/or rotations; (b) a working memory for storing instructions for processing the machine- readable data; (c) a central-processing unit coupled to the working memory and to the machine-readable data storage medium, for processing

the machine- readable data into the three dimensional representation; and (d) an output hardware coupled to the central processing unit, for receiving the three-dimensional representation.

24. A compound for inhibiting, disrupting or detecting amyloid β-peptide oligomer formation or toxic activity, wherein the compound interacts with one or more amino acids 18-41 of the Aβ protein are positioned at atomic coordinates as shown in Appendix I, or structural coordinates having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å

25. A compound as claimed in claim 24 wherein the compound interacts with the region of Aβ-peptide defined by N27, K28, I31 and L34 of Aβ-peptide wherein amino acids 18-41 of the Aβ protein are positioned at atomic coordinates as shown in Appendix I, or structural coordinates having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

26. A compound as claimed in claim 24 wherein the compound interacts with the region of Aβ-peptide defined by F19, A21, G25, N27, K28, G29, I31, L34 of Aβ-peptide wherein amino acids 18-41 of the Aβ protein are positioned at atomic coordinates as shown in Appendix I, or structural coordinates having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

27. A compound as claimed in claim 25 or claim 26 in which the compound is the peptide 27-NKGAI-31 to compete with formation of the dimer.

28. A compound as claimed in claim 25 or claim 26 in which the compound is the peptide 27-NKxxIxxL-34 (wherein x is any amino acid).

29. A compound as claimed in claim 24 in which the compound is an antibody or an antigen binding region thereof which binds Aβ-peptide in the region defined by N27, K28, I31 and L34.

30. A compound as claimed in claim 24 in which the compound is an antibody or an antigen binding region thereof which binds Aβ-peptide in the region defined by F19, A21, G25, N27, K28, G29, I31, L34.

31. A compound as claimed in claim 24 wherein the compound interacts with the region of Aβ-peptide defined by G33, L34, M35 and V36 of Aβ-peptide wherein amino acids 18-41 of the Aβ protein are positioned at atomic coordinates as shown in Appendix I, or structural coordinates having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

32. A compound as claimed in claim 21 wherein the compound interacts with the region of Aβ-peptide defined by I32, G33, L34, M35, V36 of Aβ-peptide wherein amino acids 18-41 of the Aβ protein are positioned at atomic coordinates as shown in Appendix I, or structural coordinates having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

33. A compound as claimed in claim 31 or claim 32 in which the compound is the peptide 33-GLMV-36 to compete for tetramer with or without flanking residues

34. A compound as claimed in claim 31 or claim 32 in which the compound is the peptide 31-IIGLxV-36 (wherein x is any amino acid).

35. A compound as claimed in claim 31 in which the compound is an antibody or an antigen binding region thereof which binds Aβ-peptide in the region defined by G33, L34, M35 and V36.

36. A compound as claimed in claim 32 in which the compound is an antibody or an antigen binding region thereof which binds Aβ-peptide in the region defined by I32, G33, L34, M35, V36.

37. A compound as claimed in claim 24 wherein the compound interacts with the region of Aβ-peptide defined by V18, F20, S26, K28, G29, I32, M35, V39 and I41 of Aβ-peptide wherein amino acids 18-41 of the Aβ protein are positioned at atomic coordinates as shown in Appendix I, or structural coordinates having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

38. A compound as claimed in claim 24 wherein the compound interacts with the region of Aβ-peptide defined by V18, F20, D23, S26, K28, A30, I32, M35, G37, V39, I41 of Aβ-peptide wherein amino acids 18-41 of the Aβ protein are positioned at atomic coordinates as shown in Appendix I, or structural coordinates having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

39. A compound as claimed in claim 37 or claim 38 in which the compound is the peptide selected from the group consisting of the peptides 26-SxKG-29, 18-VxF-20, 32-IxxM-35, and 39-VxI-41 each with or without flanking sequences; wherein the peptide competes for formation of amyloid.

40. A compound as claimed in claim 37 in which the compound is an antibody or an antigen binding region thereof which binds Aβ-peptide in the region defined by V18, F20, S26, K28, G29, I32, M35, V39 and I41.

41. A compound as claimed in claim 38 in which the compound is an antibody or an antigen binding region thereof which binds Aβ-peptide in the region defined by V18, F20, D23, S26, K28, A30, I32, M35, G37, V39and I41.

42. A compound for decreasing metal binding by amyloid β-peptide oligomers, wherein the compound interacts with the aligned E22 of the Aβ monomers in the Aβ oligomer.

43. The use Aβ-IgNAR oligomer in which teach of the Aβ-IgNAR molecules has a sequence of any one SEQ ID NOs 2, 4, 5, 6, 13, 15, 16, 17 or 18 to raise antibodies against Aβ wherein the antibodies bind to residues 18 to 41 of SEQ ID NO 1 when presented in the Aβ-IgNAR oligimer of any one of SEQ ID NOs 2, 4, 5, 6, 13, 15, 16, 17 or 18 but not to an isolated linear peptide having a sequence of residues 18 to 41 of SEQ ID NO 1.

44. An antibody which specifically binds to residues 18 to 41 of SEQ ID NO 1 when presented in an Aβ-IgNAR dimer of Aβ-IgNAR molecules of any one of SEQ ID NOs 2, 4, 5, 6, 13, 15, 16, 17 or 18 but not to an isolated linear peptide having a sequence of residues 18 to 41 of SEQ ID NO 1.

45. An antibody as claimed in claim 44 in which the antibody is a monoclonal antibody.

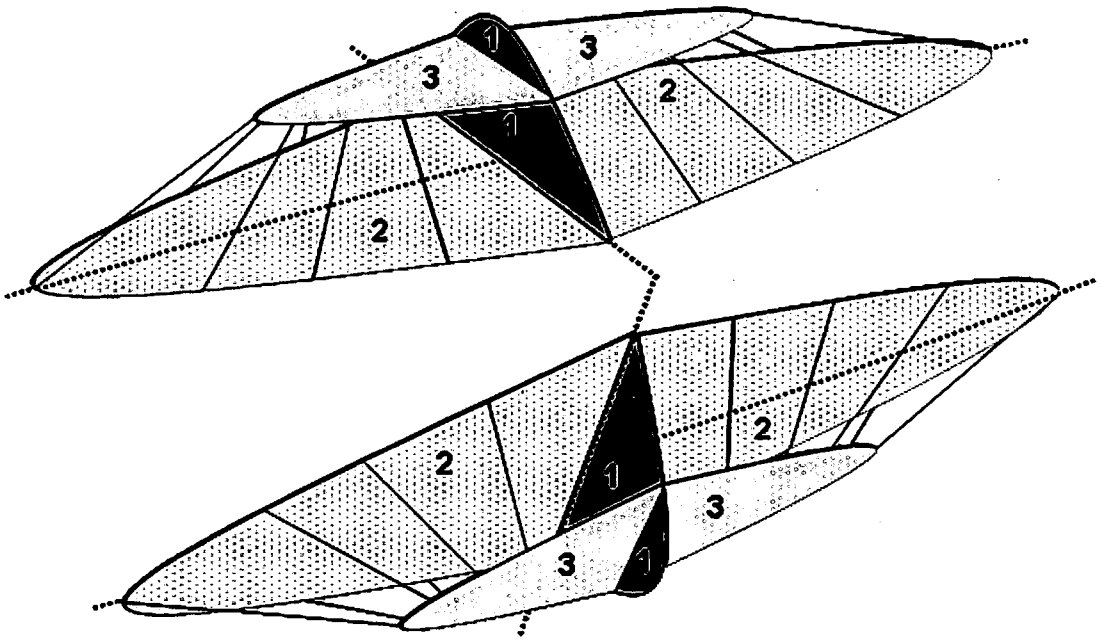
46. A method of detecting the presence of Aβ dimers in a biological sample, the method comprising contacting the biological sample with the antibody of claim 44 or claim 45 and assessing the level of binding of the antibody.

47. A method as claimed in claim 46 in which the biological sample is blood or CSF.

48. A method of detecting the presence of Aβ dimers in a biological sample, the method comprising contacting the biological sample with the compound as claimed in any one of claims 24 to 41 and assessing the level of binding of the compound.

49. A method as claimed in claim 48 in which the biological sample is blood or CSF.

Figure 1



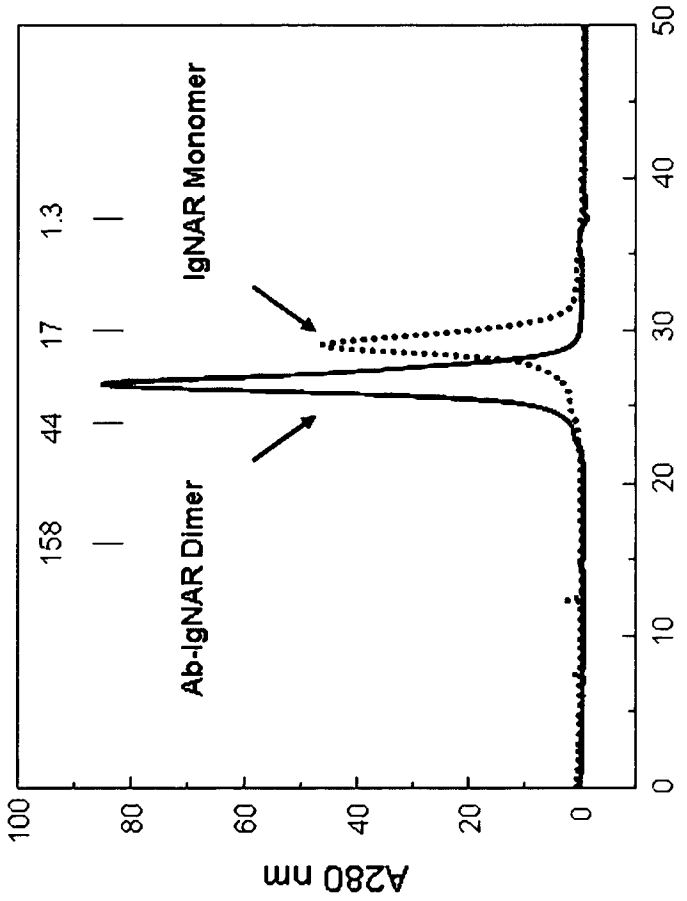

A280 nm
100
80
60
40
20
0
0
10
20
30
40
50
Time (min)
158
44
17
1.3
Ab-IgNAR Dimer
IgNAR Monomer

Figure 2a

Figure 2b

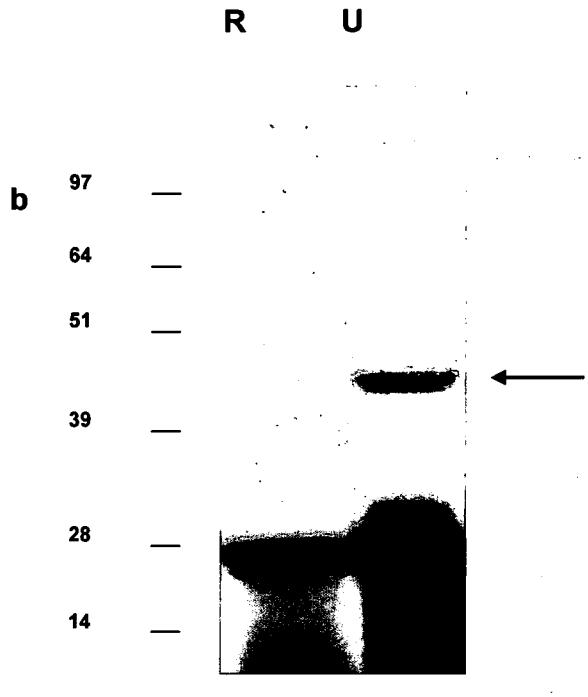


Figure 3

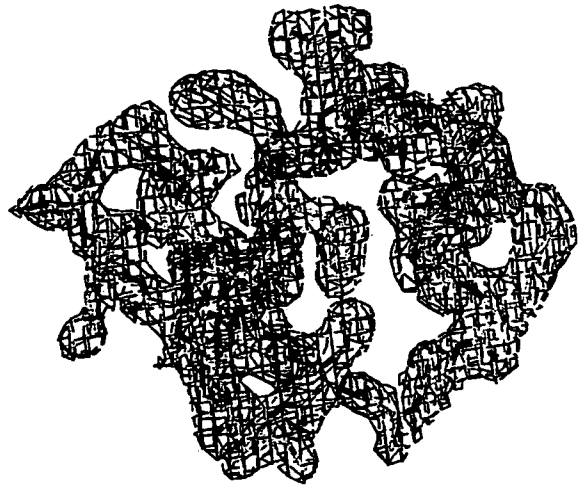
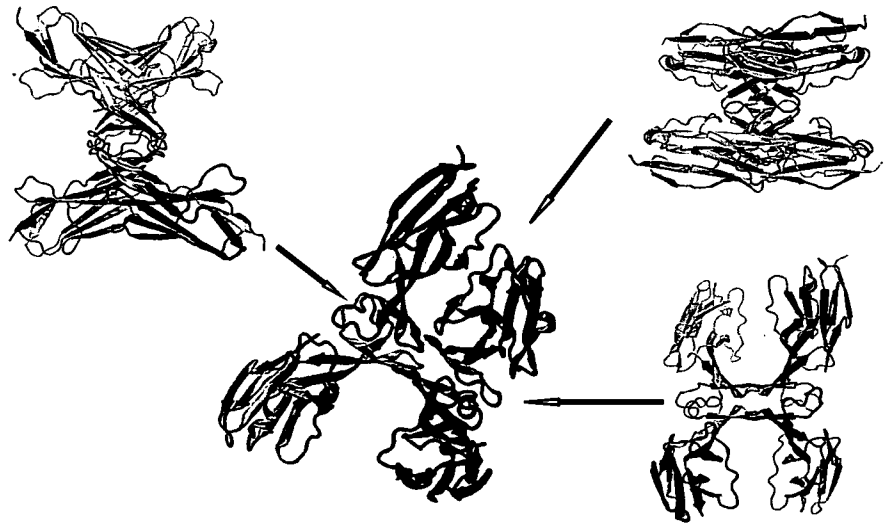


Figure 4



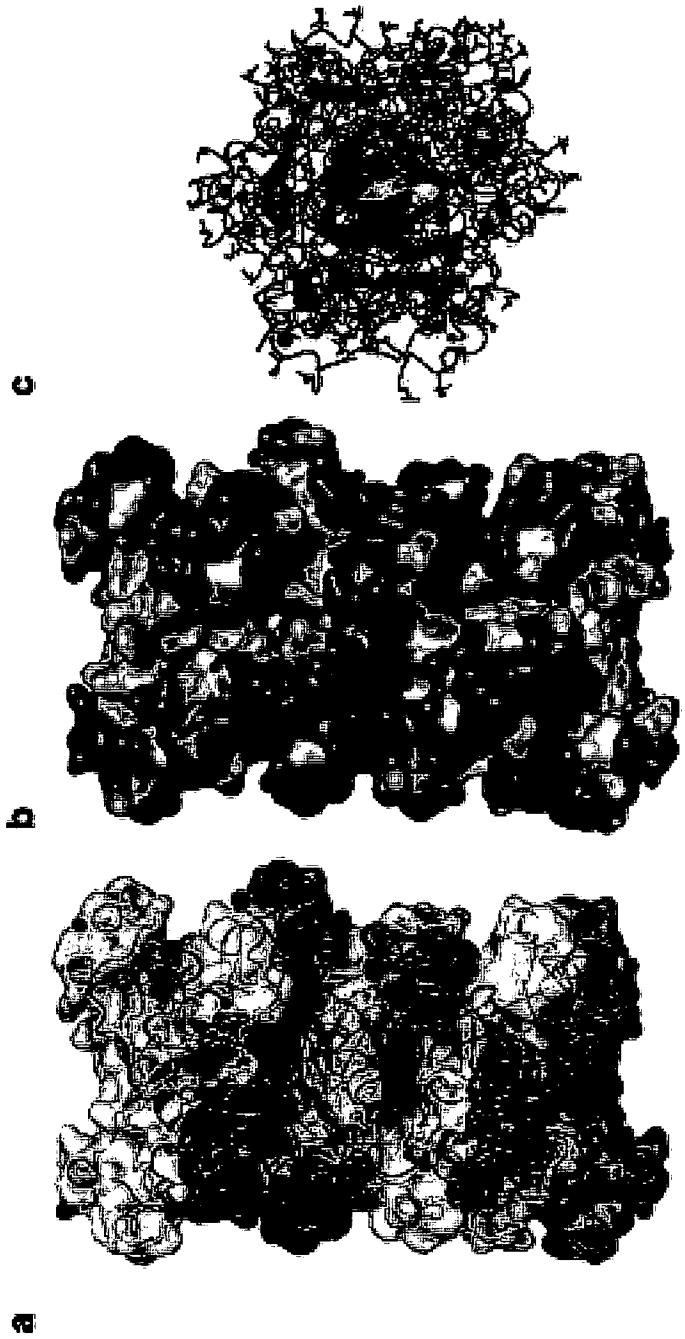


Figure 5

Figure 6

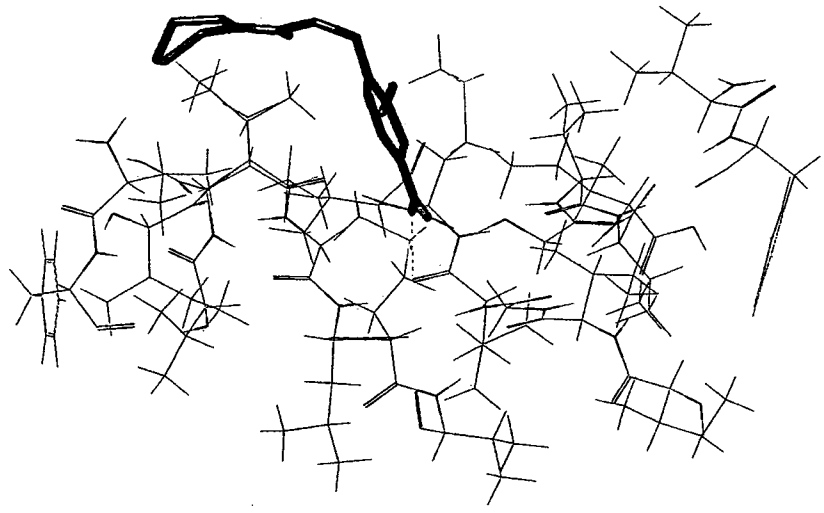


Figure 7

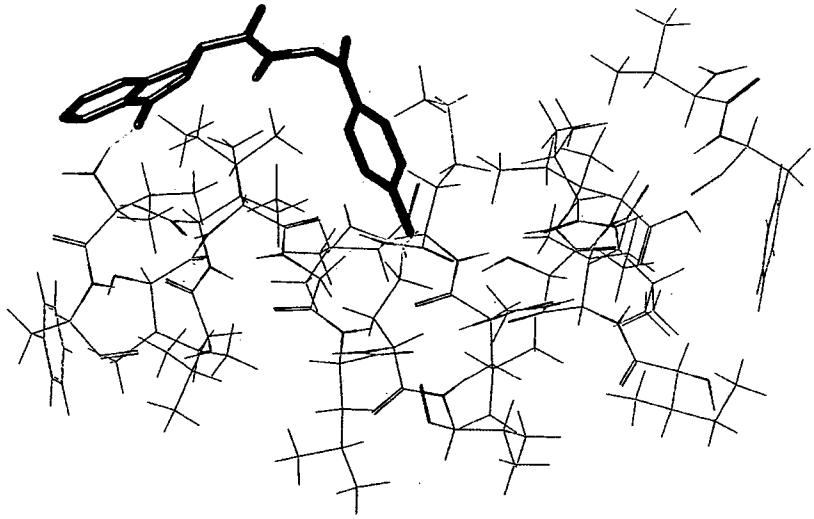


Figure 8

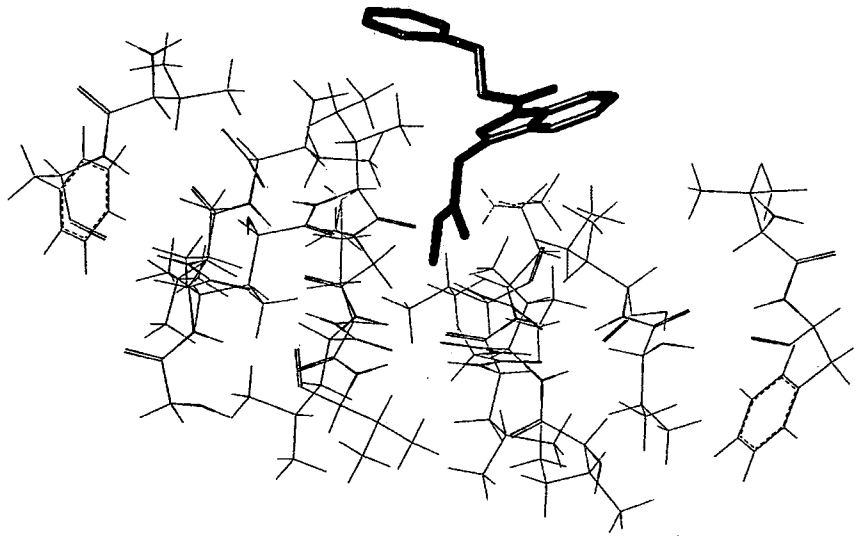


Figure 9

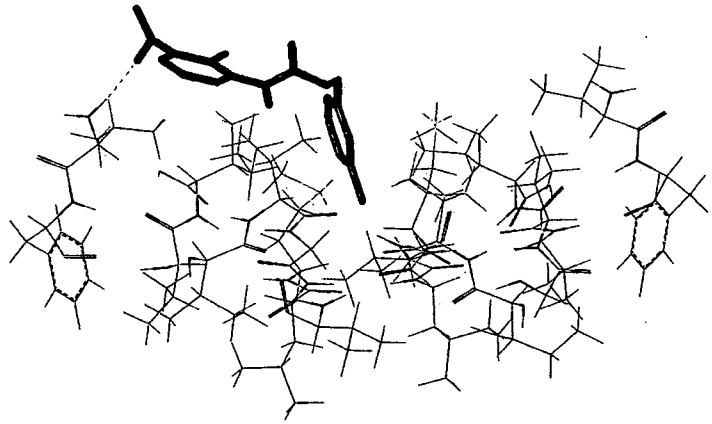


Figure 10

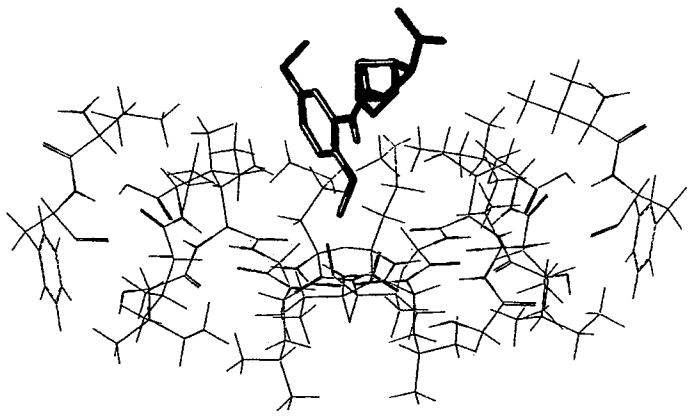


Figure 11

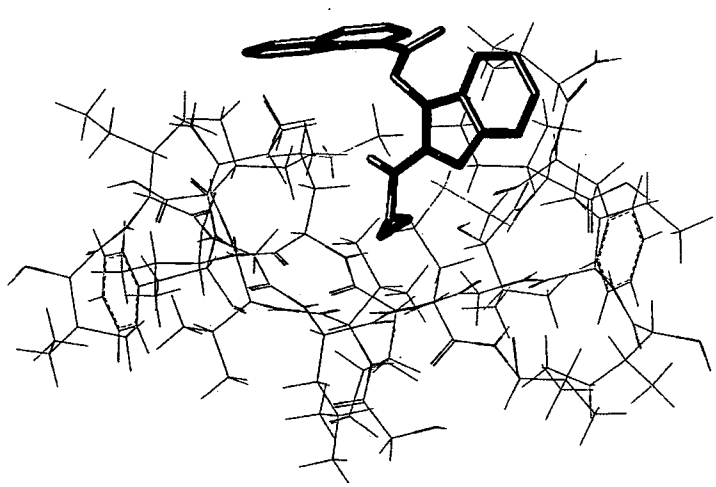
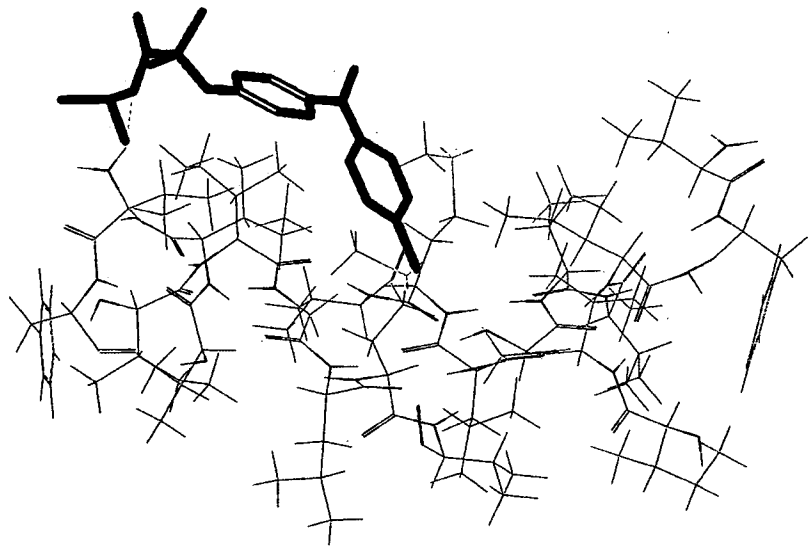


Figure 12



INTERNATIONAL SEARCH REPORT

International application No.
PCT/AU2009/001327

A. CLASSIFICATION OF SUBJECT MATTER

C07K 19/00 (2006.01) *C07K 16/18* (2006.01)

G06F 19/00 (2006.01) *G06F 17/50* (2006.01)

According to International Patent Classification (IPC)

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

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 practicable, search terms used)
GenomeQuest: Sequence search of amino acid SEQ ID NOs: 2, 4-6, 13, 15-24.
Keyword Search in MEDLINE, BIOSIS, WPIDS, CA: (IgNAR or new antigen receptor), (immunoglobulin or antibody), (amyloid beta, or aβ), (crystal or X-ray).
Keyword search in EPOQUE: (IgNAR or new antigen receptor), (immunoglobulin or antibody), (shark or ray or marine), (amyloid d beta).

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	WO 2005/118629 A1 (DIATECH PTY LTD) 15 December 2005 (see SEQ ID NO: 11)	
A	WO 2004/056318 A2 (NEW YORK UNIVERSITY) 08 July 2004 (see SEQ ID NO: 2 and pages 19-21)	
A	WO 2006/066089 A1 (NEURALAB LIMITED ET AL.) 22 June 2006 (see page 36, lines 11-13)	

[X] Further documents are listed in the continuation of Box C [X] See patent family annex

* Special categories of cited documents:
"A" document defining the general state of the art which is not considered to be of particular relevance
"E" earlier application or patent but published on or after the international filing date
"L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)
"O" document referring to an oral disclosure, use, exhibition or other means
"P" document published prior to the international filing date but later than the priority date claimed
"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention
"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone
"Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art
"&" document member of the same patent family

Date of the actual completion of the international search	Date of mailing of the international search report
15 January 2010	21 JAN 2010
Name and mailing address of the ISA/AU AUSTRALIAN PATENT OFFICE PO BOX 200, WODEN ACT 2606, AUSTRALIA E-mail address: pct@ipaustralia.gov.au Facsimile No. +61 2 6283 7999	Authorized officer **VANESSA WILLIAMS** AUSTRALIAN PATENT OFFICE (ISO 9001 Quality Certified Service) Telephone No : +61 2 6283 2939

INTERNATIONAL SEARCH REPORT

International application No.
PCT/AU2009/001327

C (Continuation). DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	Lührs, T. *et al.*, 3D Structure of Alzheimer's Amyloid-β(1-42) Fibrils. *PNAS.* **2005**, 102(48), 17342-17347. (see whole document)	

INTERNATIONAL SEARCH REPORT

International application No.
PCT/AU2009/001327

Box No. II Observations where certain claims were found unsearchable (Continuation of item 2 of first sheet)

This international search report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. [X] Claims No.: **23**

because they relate to subject matter not required to be searched by this Authority, namely:

Claim 23 is directed to a computer for producing a 3-D representation of a molecule. Such a storage medium is not considered to be a patentable invention; it merely specifies the atomic coordinates of a single protein molecule in space, without any direct technical character; the data merely encode cognitive content in a standard manner. As such, claim 23 represents a mere presentation of information and has not been the subject of an international search.

2. [ ] Claims Nos.:

because they relate to parts of the international application that do not comply with the prescribed requirements to such an extent that no meaningful international search can be carried out, specifically:

3. [ ] Claims Nos.:

because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a)

Box No. III Observations where unity of invention is lacking (Continuation of item 3 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:

See Separate Sheet.

1. [ ] As all required additional search fees were timely paid by the applicant, this international search report covers all searchable claims.

2. [ ] As all searchable claims could be searched without effort justifying additional fees, this Authority did not invite payment of additional fees.

3. [ ] As only some of the required additional search fees were timely paid by the applicant, this international search report covers only those claims for which fees were paid, specifically claims Nos.:

4. [X] No required additional search fees were timely paid by the applicant. Consequently, this international search report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.: 1-41, 43-49 (note however claim 23 has not been searched- see Box II).

Remark on Protest

[ ] The additional search fees were accompanied by the applicant's protest and, where applicable, the payment of a protest fee.

[ ] The additional search fees were accompanied by the applicant's protest but the applicable protest fee was not paid within the time limit specified in the invitation.

[ ] No protest accompanied the payment of additional search fees.

INTERNATIONAL SEARCH REPORT

International application No.
PCT/AU2009/001327

Supplemental Box
(To be used when the space in any of Boxes I to IV is not sufficient)

Continuation of Box No: III

Observations where unity of invention is lacking:

This International Application does not comply with the requirements of unity of invention because it does not relate to one invention or to a group of inventions so linked as to form a single general inventive concept.

In assessing whether there is more than one invention claimed, I have given consideration to those features which can be considered to potentially distinguish the claimed combination of features from the prior art. Where different claims have different distinguishing features they define different inventions.

This International Searching Authority has found that there are different inventions as follows:

Invention 1: Claims 1-41 and 43-49. These claims are directed to a particular Aβ(18-41) crystal structure (Aβ-IgNAR), methods for assessing the interaction of a compound with this structure, methods of selecting or designing compounds that interact with or modulate the Aβ-IgNAR molecule, antibodies raised against the Aβ-IgNAR molecule and methods of detecting the presence of Aβ dimers in a biological sample using the said antibodies. It is considered that the **Aβ-(18-41) crystal structure** as well as associated methods involving the use of this molecule constitutes a first distinguishing feature. (Note: Claim 23 is to excluded subject matter and has not been searched. See Box II).

Invention 2: Claim 42. This claim is directed to a compound for decreasing metal binding by amyloid β-peptide oligomers, wherein the compound interacts with the aligned E22 of the Aβ monomers in the Aβ oligomer (i.e. in claim 42 the Aβ peptide is not fused with an IgNAR molecule (Aβ-IgNAR) nor is it part of a crystal structure). It is considered that compounds which interact with the E22 of the **Aβ peptide** constitutes a second distinguishing feature.

PCT Rule 13.2, first sentence, states that unity of invention is only fulfilled when there is a technical relationship among the claimed inventions involving one or more of the same or corresponding special technical features. PCT Rule 13.2, second sentence, defines a special technical feature as a feature which makes a contribution over the prior art.

The only feature common to all of the claims is the **Aβ protein** itself however this protein is already well known in the art (see for example prior art document: WO 2004/056318 A2 (NEW YORK UNIVERSITY) 08 July 2004 – see sequence 2).

This means that the common feature can not constitute a special technical feature within the meaning of PCT Rule 13.2, second sentence, since it makes no contribution over the prior art.

Because the common feature does not satisfy the requirement for being a special technical feature it follows that it cannot provide the necessary technical relationship between the identified inventions. Therefore the claims do not satisfy the requirement of unity of invention *a posteriori*.

INTERNATIONAL SEARCH REPORT

Information on patent family members

International application No.
PCT/AU2009/001327

This Annex lists the known "A" publication level patent family members relating to the patent documents cited in the above-mentioned international search report. The Australian Patent Office is in no way liable for these particulars which are merely given for the purpose of information.

Patent Document Cited in Search Report		Patent Family Member					
WO	2005/118629	AU	2005250055	AU	2008229687	AU	2009201692
		CA	2567655	EP	1751181	US	2009148438
WO	2004/056318	AU	2003303198	US	2007010435	US	2009175853
WO	2006/066089	AR	052051	CA	2590337	EP	1838348
		US	2006198851	UY	29284		

Due to data integration issues this family listing may not include 10 digit Australian applications filed since May 2001.

END OF ANNEX