Office de la Propriété Intellectuelle du Canada
Un organisme d'Industrie Canada

Canadian Intellectual Property Office
An agency of Industry Canada

CA 2636633 A1 2007/07/19

(21) 2 636 633

(12) DEMANDE DE BREVET CANADIEN
CANADIAN PATENT APPLICATION

(13) A1

(86) Date de dépôt PCT/PCT Filing Date: 2007/01/10
(87) Date publication PCT/PCT Publication Date: 2007/07/19
(85) Entrée phase nationale/National Entry: 2008/07/09
(86) N° demande PCT/PCT Application No.: GB 2007/000064
(87) N° publication PCT/PCT Publication No.: 2007/080400
(30) Priorité/Priority: 2006/01/10 (GB0600406.3)

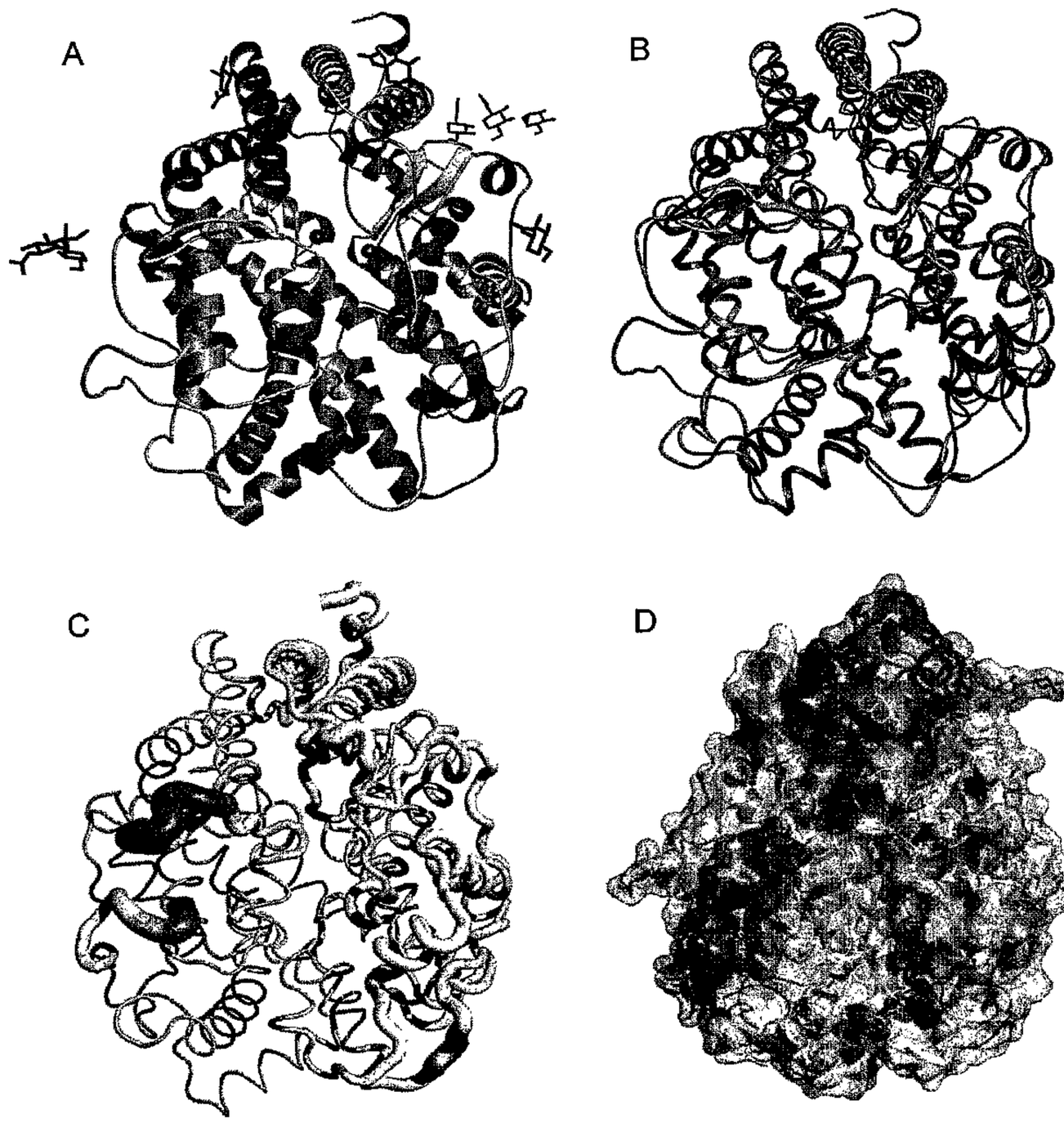
(51) Cl.Int./Int.Cl. *A61K 38/00* (2006.01),
C07K 14/435 (2006.01)

(71) Demandeurs/Applicants:
UNIVERSITY OF CAPE TOWN, ZA;
UNIVERSITY OF BATH, GB

(72) Inventeurs/Inventors:
ACHARYA, RAVI, GB;
STURROCK, EDWARD DAVID, ZA

(74) Agent: SIM & MCBURNEY

(54) Titre : CRISTAL
(54) Title: ACE N-DOMAIN CRYSTAL



(57) Abrégé/Abstract:
The present invention relates to a crystal. In particular the present invention relates to a crystal of the N-domain of ACE protein. The present invention also relates to methods, processes, domain, specific modulators, pharmaceutical compositions and uses of the N-domain crystal and the structure co-ordinates thereof.

(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization
International Bureau

(43) International Publication Date
19 July 2007 (19.07.2007)

PCT

(10) International Publication Number
WO 2007/080400 A3

(51) International Patent Classification:
A61K 38/00 (2006.01) *C07K 14/435* (2006.01)

(21) International Application Number:
PCT/GB2007/000064

(22) International Filing Date: 10 January 2007 (10.01.2007)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
0600406.3 10 January 2006 (10.01.2006) GB

(71) Applicants *(for all designated States except US)*: **UNIVERSITY OF CAPETOWN MEDICAL SCHOOL** [ZA/ZA]; Department of Research and Innovation, Private Bag, Rondebosch 7701 (ZA). **UNIVERSITY OF BATH** [GB/GB]; Claverton Down, Bath BA2 7AY (GB).

(72) Inventors; and

(75) Inventors/Applicants *(for US only)*: **ACHARYA, Ravi** [IN/GB]; Department of Biology and Biochemistry, University of Bath, Claverton Down, Bath BA2 7AY (GB). **STURROCK, Edward, David** [ZA/ZA]; Division of Medical Biochemistry, Institute of Infectious Disease and Molecular Medicine, University of Capetown, Anzio Road, Observatory 7295 (ZA).

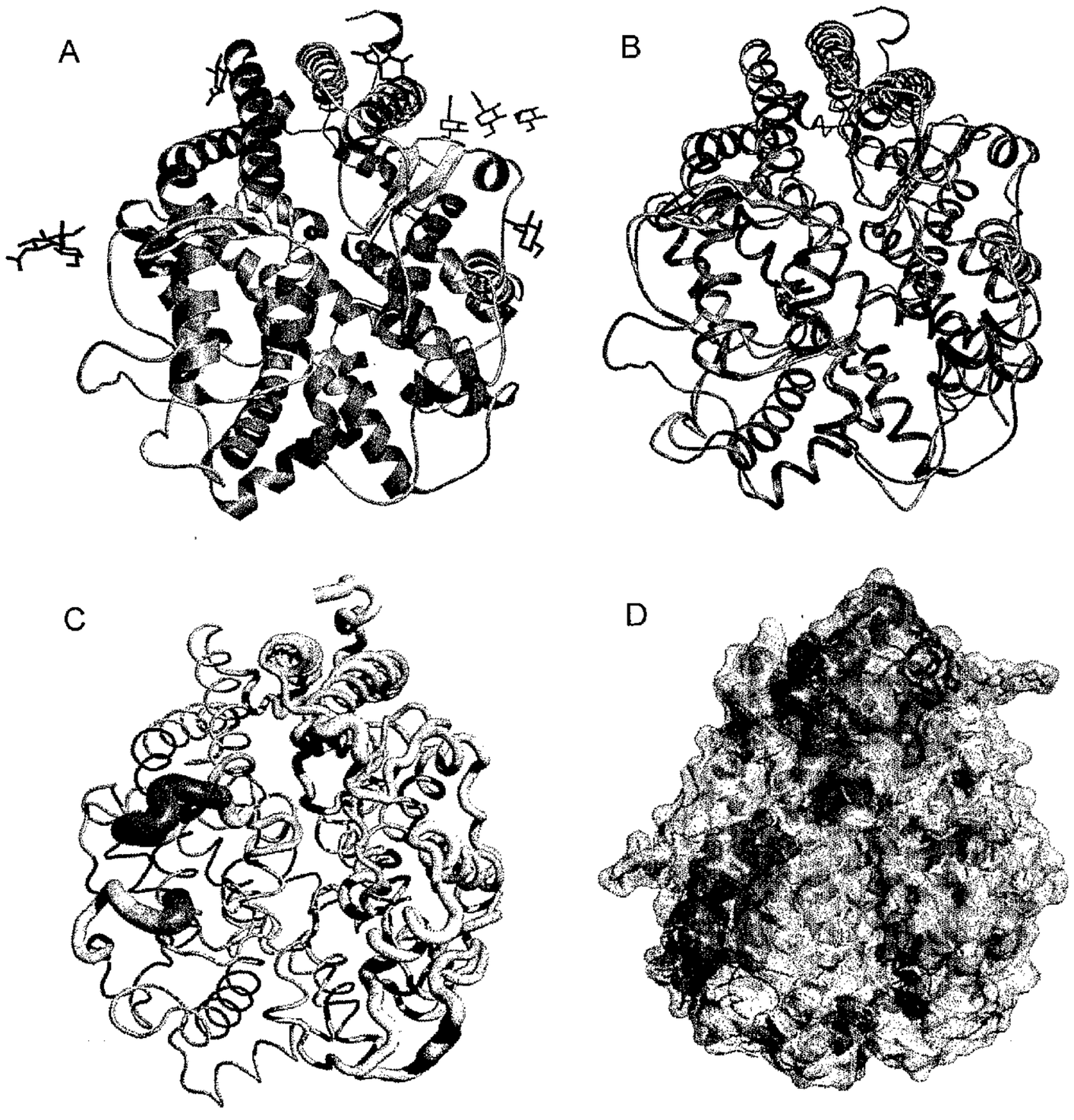
(74) Agents: **MASCHIO, Antonio** et al.; D Young & Co, 120 Holborn, London EC1N 2DY (GB).

(81) Designated States *(unless otherwise indicated, for every kind of national protection available)*: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW.

(84) Designated States *(unless otherwise indicated, for every kind of regional protection available)*: ARIPO (BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM),

[Continued on next page]

(54) Title: ACE N-DOMAIN CRYSTAL



(57) Abstract: The present invention relates to a crystal. In particular the present invention relates to a crystal of the N-domain of ACE protein. The present invention also relates to methods, processes, domain, specific modulators, pharmaceutical compositions and uses of the N-domain crystal and the structure co-ordinates thereof.

WO 2007/080400 A3

WO 2007/080400 A3

European (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

Declaration under Rule 4.17:

— *of inventorship (Rule 4.17(iv))*

Published:

— *with international search report*

— *before the expiration of the time limit for amending the claims and to be republished in the event of receipt of amendments*

(88) Date of publication of the international search report:
8 November 2007

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

DEMANDE OU BREVET VOLUMINEUX

LA PRÉSENTE PARTIE DE CETTE DEMANDE OU CE BREVET COMPREND PLUS D'UN TOME.

CECI EST LE TOME 1 DE 3
CONTENANT LES PAGES 1 À 314

NOTE : Pour les tomes additionels, veuillez contacter le Bureau canadien des brevets

JUMBO APPLICATIONS/PATENTS

THIS SECTION OF THE APPLICATION/PATENT CONTAINS MORE THAN ONE VOLUME

THIS IS VOLUME 1 OF 3
CONTAINING PAGES 1 TO 314

NOTE: For additional volumes, please contact the Canadian Patent Office

NOM DU FICHIER / FILE NAME :

NOTE POUR LE TOME / VOLUME NOTE:

CRYSTAL

FIELD OF INVENTION

The present invention relates to a crystal. In particular the present invention relates to a crystal of the N-domain of ACE protein.

The present invention also relates to methods, processes, domain specific modulators, pharmaceutical compositions and uses of the N-domain crystal and the structure co-ordinates thereof.

BACKGROUND TO THE INVENTION

Angiotensin-converting enzyme (peptidyl dipeptidase A, EC 3.4.15.1, ACE) is a zinc-dependent dipeptidyl carboxypeptidase with diverse physiological functions, including that of blood pressure regulation *via* angiotensin II production and bradykinin inactivation.

Somatic ACE (sACE), a type I transmembrane protein, is composed of two homologous catalytic domains (N- and C- domains) arising from a gene duplication event (Soubrier et al., 1988). The germinal form of ACE (testis ACE, (tACE)) (Ehlers et al., 1989) originates from the same gene as sACE, but has a tissue-specific promoter located within intron 12. Testis-ACE plays a crucial role in reproduction (Hagaman et al., 1998)

Despite sharing ~ 60 % sequence identity with the C-domain, the N-domain has its own distinctive physicochemical and functional properties. It is thermally more stable than the C-domain (Voronov et al., 2002), more resistant to proteolysis under denaturing conditions and is less dependent on chloride activation relative to the C-domain (Wei et al., 1991; Jaspard et al., 1993). The N- and the C-domains are joined by a linker that is susceptible to proteolysis (Sturrock et al., (1997), *Biochem. Biophys. Res.* 236, 16-19). It has also been suggested that the N- and the C-domains have unique physiological roles and that they have negative effect on each other (Woodman et al., 2005).

Substrates such as the hemoregulatory peptide AcSDKP (Rousseau et al., 1995), angiotensin 1-7 (Deddish et al., 1998), and the enkephalin precursor Met^5-Enk-Arg^6-Phe^7 (Deddish et al., 1997) are specific for the N-domain, whereas the physiological substrates bradykinin and angiotensin I are hydrolysed with similar catalytic efficiency as compared with the C-domain.

It has been reported that the N-domain preferentially hydrolyses the A beta peptide of the amyloid precursor protein resulting in inhibition of A beta aggregation and cytotoxicity (Oba et al., 2005). The widely-used ACE inhibitor captopril shows modest selectivity for the N-domain (Wei et al., 1992); however, the phosphinic peptide inhibitor RXP-407 has a dissociation constant three orders of magnitude lower for the N-domain of the enzyme (Dive et al., 1999).

The N-domain has 10 *N*-linked sites of which 7 are unique to the N-domain. The different glycan profile of the N-domain is likely responsible for the carbohydrate-mediated dimerisation of sACE which has been described under certain conditions (Kost et al., 2003). Moreover, the difference in glycosylation could impact on the structural basis for epitope recognition and epitope mapping of the N-domain has revealed a region that might play a role in the relatively inefficient ectodomain shedding of sACE compared to its germinal isoform (Balyasnikova et al., 2005).

Both the N- and the C-domains of ACE protein are heavily glycosylated in nature, a feature that has hampered 3D structural determination of the protein and of each of the domains.

We previously described the 3D structure of the ACE protein (International Patent Application PCT/GB03/03966 (published as WO 04/024765). This 3D structure was that of the underglycosylated C-domain of ACE protein.

This underglycosylated 3D structure, however, provides limited information on the structure of the N-domain of ACE, nor is it ideal for screening or designing domain specific modulators suitable for pharmaceutical use nor indeed for studying the functional interaction between the N- and the C-domains of ACE protein.

Therefore there is a need to obtain a crystal of the N-domain of ACE protein with sufficient quality to allow crystallographic data to be obtained. Further, there is a need for such a crystal to allow the determination of the crystal structure of the N-domain of ACE. Finally there is a need for procedures for studying the interplay between the N- and the C-domains and screening for domain specific modulators using the 3D structural information of the N-domain of ACE protein.

SUMMARY OF THE INVENTION

The present inventors have now for the first time been able to describe the three-dimensional structure of the N-domain of sACE protein.

According to a first aspect of the present invention there is provided a crystal of the N-domain of ACE protein. Preferably the N-domain of ACE protein is minimally glycosylated.

Preferably, the N-domain of ACE protein is minimally glycosylated by incorporating one or more glycosylation sites and/or one or more partially glycosylated sites. More preferably, the minimally glycosylated N-domain of ACE protein is minimally glycosylated at amino acids 25, 45, 117, 289 and 480 of SEQ ID NO: 1.

Preferably the N-domain of ACE protein comprises an inter-domain linker region. This linker region joins the N- and the C-domains and has been reported to be susceptible to proteolysis (Sturrock et al., (1997), *Biochem. Biophys. Res.* 236, 16-19). No one has previously visualised this linker region in a 3D structure. No one has previously analysed the physiological role of this linker region and no one has previously studies the role of the linker in the functional interplay between the N- and the C-domains based on 3D structural data.

Preferably, the crystal of the N-domain of ACE protein comprises atoms arranged in a spatial relationship represented by at least a portion of the structural co-ordinates set forth in Table A or Table B.

Preferably, the crystal belongs to the space group $C222_1$.

Preferably, the crystal has the unit cell dimensions: a=101.12 Å, b=211.32 Å, c=171.27 Å.

Preferably, the crystal is a crystal of the N-domain of human ACE protein.

Preferably, the crystal of the N-domain of ACE protein comprises a ligand bound to the N-domain of ACE protein or a portion thereof. More preferably the ligand modulates the activity of the N-domain of ACE protein. More preferably the ligand is an inhibitor of the N-domain of ACE protein such as lisinopril or a derivative thereof. More preferably the crystal of the N-domain of the ACE protein comprising lisinopril comprises atoms arranged in a spatial relationship represented by at least a portion of the structural co-ordinates set forth in Table B.

Preferably the crystal of the N-domain of the ACE protein comprising the inhibitor lisinopril has the unit cell dimensions of: a=101.32 Å, b=211.90 Å, c=171.03 Å.

In a second aspect, the present invention relates to a method of preparing a crystal of the N-domain of ACE protein comprising the steps of: (a) culturing host cells expressing N-domain of ACE protein; (b) purifying the N-domain of ACE protein; and (c) crystallising the N-domain of ACE protein.

Preferably, the N-domain of ACE protein is crystallised using about 5 mM HEPES and about 0.1 mM PMSF with an equal volume of a reservoir solution containing about 0.2M lithium sulphate, about 15 % PEG 4000, about 100 mM $CH_3COONa.3H_2O$ pH 4.9 and about 10 µM $ZnSO_4.7H_2O$.

Preferably, the crystal that is prepared has a structure defined by at least a portion of the structural co-ordinates set forth in Table A or Table B.

Preferably, the crystal belongs to the space group $C222_1$.

Preferably, the crystal has the unit cell dimensions: a=101.12 Å, b=211.32 Å, c=171.27 Å.

Preferably, the N-domain of ACE protein is the N-domain of human ACE protein.

Preferably, the N-domain of ACE protein is crystallised in the presence of a ligand. More preferably the ligand is a modulator of the N-domain of ACE protein. More preferably the ligand is an inhibitor of the N-domain of ACE protein such as lisinopril or a derivative thereof. More preferably the crystal of the N-domain of the ACE protein comprising lisinopril comprises atoms arranged in a spatial relationship represented by at-least a portion of the structural co-ordinates set forth in Table B.

Preferably the crystal of the N-domain of the ACE protein comprising the inhibitor lisinopril has the unit cell dimensions of: a=101.32 Å, b=211.90 Å, c=171.03 Å.

Preferably the crystal of the N-domain of ACE protein that is prepared in the presence of a ligand is crystallised using about 5 mM HEPES and about 0.1 mM PMSF with an equal volume of a reservoir solution containing about 0.2M lithium sulphate, 18 % PEG 4000, about 100 mM $CH_3COONa.3H_2O$ pH 4.9 and about 10 µM $ZnSO_4.7H_2O$.

In a third aspect, the present invention relates to a method of screening for a modulator of the N-domain of ACE protein wherein the method comprises the use of a crystal according to the present invention. Preferably, the screening method comprises the steps of: (a) providing at least a portion of the structural co-ordinates set forth in Table A or Table B; (b) employing at least a portion of the structural co-ordinates set forth in Table A or Table B to design or select or synthesise a putative modulator of the N-domain of ACE protein; (c) contacting the putative modulator of the N-domain with the N-domain or a mutant, variant, homologue, derivative or fragment thereof in the presence of a substrate; and (d) screening the putative modulator of the N-domain of ACE protein in an assay for the potential to modulate the N-domain.

Comparisons of the 3D structures of the N-domain of ACE protein and C-domain of ACE protein show that the two domains are structurally very similar.

Therefore, according to a fourth aspect, the present invention relates to a method of screening for a modulator of the C-domain of ACE protein wherein the method comprises the use of a crystal according to the present invention. Preferably, the screening method comprises the steps of: (a) providing at least a portion of the structural co-ordinates set forth in Table A or Table B; (b) employing at least a portion of the structural co-ordinates set forth in Table A or Table B to design or select or synthesise a putative modulator of the C-domain of ACE protein; (c) contacting the putative modulator of the C-domain with the C-domain or a mutant, variant, homologue, derivative or fragment thereof; and (d) screening the putative modulator of the C-domain of ACE protein in an assay for the potential to modulate the C-domain.

Preferably, at least a portion of the structural co-ordinates set forth in Table A or Table B and/or the putative modulator of the N-domain of ACE protein or C-domain of ACE protein and/or the substrate are provided on a machine-readable data storage medium comprising a data storage material encoded with machine readable data.

Preferably, the putative N-domain of ACE protein modulator or C-domain of ACE protein modulator is selected from a library of compounds. More preferably, the putative N-domain of ACE protein modulator or C-domain of ACE protein modulator is selected from a database. More preferably, the putative N-domain of ACE protein modulator or C-domain of ACE protein modulator is designed *de novo*. More preferably, the putative N-domain of ACE protein modulator or C-domain of ACE protein modulator is designed from a known ACE modulator. More preferably, the design or selection of the putative N-domain of ACE protein modulator or C-domain of ACE protein modulator is performed in conjunction with computer modelling.

Preferably, the putative N-domain of ACE protein modulator or C-domain of ACE protein modulator is useful in the prevention and/or treatment of ACE related disorder. More preferably, the ACE related disorder is hypertension, myocardial infarction or congestive heart failure.

In a fifth aspect, the present invention relates to a process comprising the steps of: (a) performing the method according to the third aspect and/or the fourth aspect of the present invention; (b) identifying one or more modulators of the N-domain and/or C-domain; and (c) preparing a quantity of those one or more N-domain modulators and/or C-domain modulators.

In a sixth aspect, the present invention relates to a process comprising the steps of: (a) performing the method according to the third aspect and/or the fourth aspect of the present invention; (b) identifying one or more N-domain modulators and/or C-domain modulators; and (c) preparing a pharmaceutical composition comprising those one or more N-domain modulators and/or C-domain modulators.

In a seventh aspect, the present invention relates to a process comprising the steps of: (a) performing the method according to the third aspect and/or the fourth aspect of the present invention; (b) identifying one or more N-domain modulators and/or C-domain modulators; (c) modifying those one or more N-domain modulators and/or C-domain modulators; and (d) optionally preparing a pharmaceutical composition comprising those one or more N-domain modulators and/or C-domain modulators.

In an eighth aspect, the present invention relates to a method of obtaining structural information about a molecule or a molecular complex of unknown structure by using at least a portion of the structure co-ordinates of the N-domain of ACE protein, comprising the steps of: (a) generating X-ray diffraction data from a crystallised molecule or molecular complex; (b) applying at least a portion of the structure co-ordinates of the N-domain of ACE protein to said X-ray diffraction pattern to generate a three dimensional electron density map of at least a portion of the molecule or molecular complex; and (c) using all or a portion of the structure co-ordinates of the N-domain of ACE protein to generate homology models of the N-domain of ACE protein. Preferably the structural information of the structure co-ordinates of ACE protein are used for domain co-operativity studies.

In a ninth aspect, the present invention relates to a modulator of the N-domain of ACE protein and/or the C-domain of ACE protein identified by the method according to the

third aspect and/or the fourth aspect of the present invention. Preferably, the modulator inhibits the N-domain of ACE protein and/or the C-domain of ACE protein.

In a tenth aspect, the present invention relates to a pharmaceutical composition comprising an N-domain of ACE protein modulator and/or a C-domain of ACE protein modulator according to the ninth aspect of the present invention and a pharmaceutically acceptable carrier, diluent, excipient or adjuvant or any combination thereof.

In an eleventh aspect, the present invention relates to a method of preventing and/or treating an ACE related disorder comprising administering a modulator of the N-domain of ACE protein and/or the C-domain of ACE protein according to the ninth aspect of the present invention and/or a pharmaceutical composition according to the tenth aspect of the present invention, wherein said modulator of the N-domain of ACE protein and/or the C-domain of ACE protein and/or said pharmaceutical composition is capable of causing a beneficial preventative and/or therapeutic effect.

In a twelfth aspect, the present invention relates to a computer for producing a three-dimensional representation of the N-domain of ACE protein wherein said computer comprises: (a) a computer-readable data storage medium comprising a data storage material encoded with computer-readable data, wherein said data comprises the structure co-ordinates of the N-domain of ACE protein; (b) a working memory for storing instructions for processing said computer-readable data; (c) a central-processing unit coupled to said working memory and to said computer-readable data storage medium for processing said computer-machine readable data into said three-dimensional representation; and (d) a display coupled to said central-processing unit for displaying said three-dimensional representation.

In a thirteenth aspect, the present invention relates to a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein the data is defined by at least a portion of the structural co-ordinates of the N-domain of ACE protein set forth in Table A or Table B.

In a fourteenth aspect, the present invention relates to the use of an N-domain of ACE protein crystal in the preparation of a medicament to prevent and/or treat an ACE related disorder. Preferably, the ACE related disorder is hypertension, myocardial infarction or congestive heart failure.

In a fifteenth aspect, the present invention relates to the use of at least a portion of the structural co-ordinates set forth in Table A or Table B to screen for modulators of the N-domain of ACE protein and/or C-domain of ACE protein.

In a sixteenth aspect, the present invention relates to the use of at least a portion of the structural co-ordinates set forth in Table A or Table B to solve the structure of the crystalline form of any other domain with significant amino acid sequence homology to any functional domain of the N-domain of ACE protein.

In a seventeenth aspect, the present invention relates to the use of at least a portion of the structural co-ordinates set forth in Table A or Table B in molecular design techniques to design, select and synthesise modulators of the N-domain of ACE protein and/or C-domain of ACE protein.

In an eighteenth aspect, the present invention relates to the use of at least a portion of the structural co-ordinates set forth in Table A or Table B in the development of compounds that can isomerise to reaction intermediates in the chemical reaction of a substrate or other compound that binds to the N-domain of ACE protein and/or the C-domain of ACE protein.

In a nineteenth aspect, the present invention relates to the use of at least a portion of the structural co-ordinates set forth in Table A or Table B to screen small molecule databases for chemical entities or compounds that modulate the N-domain of ACE protein and/or C-domain of ACE protein.

In a twentieth aspect, the present invention relates to the use of at least a portion of the structural co-ordinates set forth in Table A or Table B to solve the structure of the crystalline form of any other domain with significant amino acid sequence homology to any functional domain of the N-domain of ACE protein. Preferably, the structure

of the crystalline form of any other domain with significant amino acid sequence homology to any functional domain of the N-domain of ACE protein is solved using molecular replacement.

In a twenty first aspect, the present invention relates to the use of at least a portion of the structural co-ordinates set forth in Table A or Table B to identify the binding site of any modulator of the N-domain of ACE protein. Preferably the binding site is that of lisinopril or derivatives thereof.

DETAILED DESCRIPTION OF THE INVENTION

N-DOMAIN OF ACE PROTEIN

ACE (EC 3.4.15.1) is a membrane associated peptidyl dipeptidase.

There are two tissues specific isoforms of ACE protein differentially transcribed from the same gene.

Somatic ACE (sACE), a type I transmembrane protein, is composed of two homologous catalytic N- and C- domains, arising from a gene duplication event (Soubrier et al., 1988).

Germinal ACE (testis ACE, (tACE)) has a tissue-specific promoter located within intron 12 (Ehlers et al., 1989).

Despite sharing ~ 60 % sequence identity with the C-domain, the N-domain has its own distinctive physicochemical and functional properties. It has also been reported that the two domains display negative co-operativity effect on each other (Woodman et al., 2005). In the present invention, co-operativity studies between the N- and C-domains of ACE protein is based on studies carried out by Guy et al., 2003 (*Biochemistry*, 42:13185-13192) and Towler et al., 2004 (*The Journal of Biological Chemistry*, 17:17996-18007). In their studies, the authors compare ACE structures with those of the ACE2 homologue that more closely resembles the N-domain of the ACE protein. See Figure 4 below.

As used herein the term "negative co-operativity" refers to the capacity of the two domains of ACE protein to modulate the biochemical activities of each other. By way of example the N-domain may cause steric hindrance of the C-domain by preventing substrate from accessing the active site of the C-domain and vice versa the C-domain may cause steric hindrance of the N-domain by preventing substrate from accessing the active site of the N-domain.

The N- and the C-domains are heavily glycosylated, which has hampered the determination of the 3D structure of the ACE protein.

Previously we described the 3D structure of the C-domain of undeglycosylated ACE protein (see International Patent Application PCT/GB03/03966 (published as WO 04/024765)).

The present inventors have now been able to obtain a minimally glycosylated N-domain of ACE protein.

As used herein the term "minimally glycosylated" means that one or more oligosaccharide chains are linked to one or more amino acid residues in the N-domain of ACE protein. As used herein the term "oligosaccharide" refers to a carbohydrate molecule which comprises less than 10 sugar molecules where the sugar molecules can be any one or more of mono-saccharides, di-, tri-, and/or tetra-saccharides.

As used herein, the term "N-domain of ACE protein" includes all vertebrate and mammalian forms of the N-domain of ACE protein and is intended to cover mutants, variants, homologues, derivatives and fragments thereof. Preferably, the mutants, variants, homologues, derivatives and fragments thereof have the activity of the N-domain of ACE protein. Preferably the N-domain of the ACE protein is minimally glycozylated.

CRYSTAL

In one aspect of the present invention, there is provided a crystal structure of the N-domain of ACE protein in its minimally glycozylated form and its ligand-bound form.

As used herein, the term "crystal" means a structure (such as a three dimensional (3D) solid aggregate) in which the plane faces intersect at definite angles and in which there is a regular structure (such as internal structure) of the constituent chemical species. Thus, the term "crystal" can include any one of: a solid physical crystal form such as an experimentally prepared crystal, a 3D model based on the crystal structure, a representation thereof - such as a schematic representation thereof, a diagramatic representation thereof, or a data set thereof for a computer.

The crystals of the present invention may be prepared by purifying the N-domain of ACE protein and then crystallising the purified protein. The N-domain of ACE protein may also be prepared by expressing a nucleotide sequence encoding the N-domain of ACE protein in a suitable host cell.

In one preferred embodiment, the N-domain of ACE crystal comprises the inter-domain linker region.

The N-domain of ACE protein may be purified using various methods known to a person skilled in the art, for example, from conditioned media by affinity chromatography on a Sepharose-28-lisinopril affinity resin (Yu *et al.* 1997). The protein may be quantified by amino acid analysis and assayed for activity using the substrate hippuryl-L-histidyl-L-leucine, as described previously (Ehlers, MRE, Chen, Y –N, Riordan, JF (1991) *Proc. Natl. Acad. Sci.* USA 88, 1009-1013).

The purified N-domain of ACE proteins may be stored at –20 °C in 5 mM HEPES and 0.1 mM PMSF.

Concentration may be performed with the aid of a filtration system and the protein concentrate may be immediately used for crystallisation purposes. The protein

concentrate may be crystallised using, for example, the vapour diffusion hanging drop method at a temperature of from about 4 °C to about 30 °C, preferably from about 8 °C to about 20 °C, more preferably from about 12 °C to about 18 °C, most preferably at about 16 °C. The crystallisation temperature may be dependent on the additives present in the protein solution.

Typically, the best crystals for the N-domain of ACE proteins are grown at a temperature in the range of from 10 to 20°C, preferably from 12 to 18°C, most preferably at 16 °C by the vapour diffusion hanging drop method by mixing 1 µl of the protein solution at about 4 mg/ml. The solution comprising HEPES in the range of from 1 to 10 mM, preferably in the range of from 2 to 8 mM, more preferably in the range of from 4 to 6 mM, most preferably 5mM HEPES and PMSF in the range of from 0.025 to 0.2%, preferably from 0.05 to 0.15%, more preferably from 0.075 to 0.125, most preferably 0.1% PMSF with an equal volume of a reservoir solution. The reservoir solution comprising lithium sulphate in the range of from 0.025 to 0.4M, preferably in the range of from 0.05 to 0.35M, more preferably from 0.075 to 0.3M, most preferably containing 0.2M lithium sulphate, PEG 4000 in the range of from 5% to 25%, preferably from 10% to 20%, most preferably from 15% to 18% PEG 4000, $CH_3COONa.3H_2O$ in the range of from 50 to 150mM, preferably from 75 to 125 mM, more preferably from 90 to 110 mM, most preferably 100 mM $CH_3COONa.3H_2O$, wherein the $CH_3COONa.3H_2O$ has a pH in the range of from 3.9 to 5.9, preferably a pH from 4.5 to 5.5, more preferably a pH from 4.7 to 5.2, most preferably a pH of 4.9 and $ZnSO_4.7H_2O$ in the range of from 5 to 20µM, preferably from 7.5 to 12.5 µM, most preferably 10 µM $ZnSO_4.7H_2O$.

Crystals usually appear within 1 to 2 weeks and grow to their maximum size after about a month.

The present invention related to a crystal of the N-domain of ACE comprising atoms arranged in a spatial relationship represented by at least a portion of the structural co-ordinates set forth in Table A or Table B.

Preferably, the crystal belongs to the space group $C222_1$ and unit cell dimensions: a=101.12 Å, b=211.32 Å, c=171.27 Å.

Preferably, the N-domain of ACE protein is the N-domain of any vertebrate and mammalian.

Preferably the N-domain of ACE protein is the N-domain of human ACE protein.

Complexes may be obtained by growing the crystals in the presence of a ligand - such as a test compound. In these experiments the protein solution is mixed with the ligand and an equal volume of the reservoir-solution before setting up the crystallisation. Single crystals suitable for diffraction work typically appear after about 1-2 weeks.

Typically, the protein comprising the N-domain of ACE protein is purified to homogeneity for crystallisation. Purity of the N-domain of ACE protein may be measured by typical techniques such as SDS-PAGE, mass spectrometry and hydrophobic HPLC.

The structure of the crystals of the invention may contain a portion – such as at least 25%, at least 50%, at least 75%, or preferably at least 90%, at least 95%, at least 98%, or at least 99% - of the co-ordinates set forth in Table A or Table B. Preferably, the crystal structure of the invention contains all of the co-ordinates set forth in Table A or Table B.

Preferably, the crystals are usable in X-ray crystallography techniques.

Preferably, the crystals used can withstand exposure to X-ray beams used to produce diffraction pattern data necessary to solve the X-ray crystallographic structure.

Preferably, prior to data collection, the crystals are flash-cooled at about 100 K in a cryoprotectant. The cryoprotectant comprising lithium sulphate in the range of from 0.025 to 0.4M, preferably in the range of from 0.05 to 0.35M, more preferably from 0.075 to 0.3M, most preferably containing 0.2M lithium sulphate, PEG 4000 in the range of from 5% to 25%, preferably from 10% to 20%, most preferably from 15% to

18% PEG 4000, $CH_3COONa.3H_2O$ in the range of from 50 to 150mM, preferably from 75 to 125 mM, more preferably from 90 to 110 mM, most preferably 100 mM $CH_3COONa.3H_2O$, wherein the $CH_3COONa.3H_2O$ has a pH in the range of from 3.9 to 5.9, preferably a pH from 4.5 to 5.5, more preferably a pH from 4.7 to 5.2, most preferably a pH of 4.9 and $ZnSO_4.7H_2O$ in the range of from 5 to 20μM, preferably from 7.5 to 12.5 μM, most preferably 10 μM $ZnSO_4.7H_2O$.

The X-ray data may be collected at a Synchrotron Radiation Source. Preferably, the X-ray data are collected at a Synchrotron Radiation Source at 100 °K.

Preferably, the crystal has a resolution determined by X-ray crystallography of about 3.5Å or less, more preferably a resolution of about 3.0 Å or less, more preferably a resolution of about 2.8Å or less, more preferably, a resolution of about 2 Å or less, more preferably, a resolution of about 1.5Å or less, most preferably, 1 Å or less.

GLYCOSYLATION OF THE N-DOMAIN OF ACE PROTEIN

Many proteins in eukaryotic cells are glycoproteins that contain oligosaccharide chains covalently linked to certain amino acids. Glycosylation is known to affect protein folding, interaction between protein domains, localisation and trafficking, protein solubility, antigenicity, biological activity and half-life, as well as cell-cell interactions.

Protein glycosylation can be divided into four main categories mainly depending on the linkage between the amino acid and the sugar molecule. These are *N*-linked glycosylation, O-linked glycosylation, C-mannosylation and GPI anchor attachments. *N*-glycosylation is characterised by the addition of a sugar to the amino group of an asparagine.

For *N*-glycosylation, the sequence motif Asn-Xaa-Ser/Thr (wherein Xaa is any amino acid other than Pro) has been defined as a prerequisite for glycosylation. Although rare, the sequence motif Asn-Xaa-Cys can also be an acceptor site. N-glycans can be subdivided into three distinct groups called 'high mannose type', 'hybrid type', and

'complex type', with the common pentasaccharide core - Manp(alpha1,6)-(Manp(alpha1,3))-Manp(beta1,4)-GlcpNAc(beta1,4) GlcpNAc(beta1,N)-Asn - occurring in all three groups. The relationship between all three types can be ascribed to the fact that they originate from one precursor oligosaccharide which contains the described common pentasaccharide core Man3-GlcNAc2, and some additional sugar residues and the non-reducing end, and is then processed enzymatically to yield these three types. Since the hydroxyl group of Ser/Thr is thought to be involved in hydrogen bonding during the enzymatic attachment of the oligosaccharide precursor molecule to yield a favourable conformation for the action of the oligosaccharyltransferase, it has been suggested for proline that the steric hindrance might be too large (Kornfeld (1985) *Ann. Rev. Biochem.* **54**: 631-64), preventing glycosylation at Pro containing sites. The negative influence of aspartic acid towards glycosylation can be ascribed to the negative charge on the side chain of this residue. In addition some cases have been reported where Ser/Thr is replaced by cysteine. While Ser replacement by Cys generally leads to decreased glycosylation, it has been shown (Kasturi 1995 *J. Biol. Chem.* 270: 14756-61) that substitution by Thr at a given potential glycosylation site can lead to increased glycosylation. This is in accordance with the model of hydrogen bonding being an important factor during the attachment of the precursor molecule to the protein. Although there are usually many potential glycosylation sites in a protein it has been estimated that glycosylation occurs only at one third of them. Mostly at those sites where the surrounding amino acids allow the formation of a beta turn.

Various glycoforms of ACE have been described. By way of example, Sadhukhan & Sen disrupted specific glycosylation sites in rabbit tACE to elucidate the glycosylation requirements for the expression and processing of active testis ACE. There are five potential *N*-linked glycosylation sites in the rabbit tACE sequence, with an additional six in the somatic form. A null mutant, where all five sites had been disrupted, behaved similarly to wild-type tACE expressed in the presence of the glycosylation-inhibitor, tunicamycin. It was degraded intracellularly and failed to be detected in culture medium, confirming previous findings that tACE requires *N*-linked glycosylation to be expressed in an active form. Expression of the remaining mutants showed a preference for *N*-linked glycosylation at the N-terminus and that the presence of sugars at a single N-terminal site was necessary and sufficient to produce enzymatically-active tACE that was solubilised. The presence of glycosylation is not

site-specific, as mutants that have either the first site or second site intact are expressed and active. However, glycosylation at the third site alone is not sufficient to produce active protein in HeLa cells, albeit this mutant was expressed in yeast, indicating that the requirements for glycosylation are cell-specific.

N-linked glycosylation of human tACE expressed in CHO cells at each site has been identified by MALDI-TOF mass spectrometry. There are seven potential *N*-linked sites in human tACE, five of which are complementary to the sites in rabbit tACE (7a). The unique sites lie within the ectodomain (the fourth site) and in the juxtamembrane stalk region, adjacent to the cleavage site (the seventh site). As with the rabbit form, there appears to be a preference for glycosylation at the N-terminus as evidenced by MALDI-TOF mass spectrometry of glycopeptides (Yu et al., 1997) and mutagenesis (Gordon et al., 2003) of glycosylation sites. Inhibition of complex oligosaccharide formation using a glucosidase I inhibitor *N*-butyldeoxynojirimycin (NB-DNJ) led to the production of an active glycoform that was electrophoretically homogeneous.

There are ten putative *N*-glycosylation sites on the human N-domain of ACE protein and Fourier difference density was observed at five of these sites according to the crystal of the present invention.

Suitably, the crystal of the N-domain of ACE protein may comprise minimally glycosylated N-domain of ACE protein or a fragment thereof. For example, the minimally glycosylated N-domain of ACE protein may comprise the sequence presented as SEQ ID No. 1.

To obtain a minimally glycosylated N-domain of ACE protein, various methods known to a person skilled in the art may be used. Both chemical and enzymatic methods may be used. Hydrazinolysis of glycoproteins (Kuraya, N & Hase (1992) J Biochem (Tokyo) 112:122-126), is capable of removing both N- and O-linked sugars, although this results in the complete destruction of the protein component and is therefore not suitable if recovery of the protein is desirable. More delicate chemical methods may be used such as trifluoromethanesulphonic acid (TFMS), however this method may also lead to a partial protein destruction. Alternatively, or in addition,

other methods – such as site directed mutagenesis of glycosylated amino acids may also be employed.

Enzymatic methods which provide for partial sugar removal with no protein degradation may also be used.

Use of the enzyme PNGase F is an effective method of removing most *N*-linked oligosaccharides from glycoproteins (Tarentino & Plummer (1994) *Methods in-Enzymology,* **230**: 44-57). The oligosaccharide is left intact and therefore suitable for further analysis (the asparagine residue from which the sugar is removed is deaminated to aspartic acid, the only modification to the protein).

Other commonly used endoglycosidases include Endoglycosidase H (Kobata (1979) *Anal Biochem* **100**:1-14) and Endoglycosidase F (Trimble & Tarentino (1991) *J. Biochem.* **266**:1646-1651). In a preferred method, the N-domain of ACE protein is digested with Endoglycosidase H (30 mU) in a suitable buffer – such as 100 mM sodium phosphate, 0.1 mM $ZnCl_2$ and 1% BSA, pH 6.0 for 16 h at 37°C. The endo H-treated protein is passed through a lectin affinity column consisting of equal parts of concanavalin A, wheat germ, and lentil lectin, after equilibration with 20 mM Tris-HCl, 0.5 M NaCl at pH 7.4. The minodeglycosylated ACE is collected in the flowthrough. Free oligosaccharides and any other impurities are removed from the flowthrough fraction by a final lisinopril-Sepharose affinity chromatography step. The homogeneity of the ACE protein after deglycosylation is confirmed by SDS-PAGE on a 4-20% acrylamide gel and MALDI-TOF mass spectrometry.

By way of example, a minimally glycosylated N-domain of ACE protein can be obtained by incubating suitable host cells such as CHO cells until confluent and then substituting the growth medium with medium comprising 1% FCS, 0.05% albumax I (Gibco BRL), 20μM MSX and 1.5mM of the glucosidase I inhibitor N-butyldeoxynojirimycin (NB-DNJ) (Toronto Research Chemicals Inc.B691000 Lot 14-EG-91-1 and B691000 12-Cf-146-2).

Preferably, the crystal of the N-domain of ACE protein comprises glycosylated N-domain of ACE protein or a fragment thereof. More preferably, the crystal of the N-domain of ACE protein comprises a minimally glycosylated N-domain of ACE protein or a fragment thereof. More preferably, the crystal of the N-domain of ACE protein comprises *N*-glycosylation of asparagine residues. More, preferably the asparagine residues are *N*-glycosylated with high mannose oligosaccharides.

Preferably, one or more of the asparagine residues of the N-domain of ACE protein can be *N*-glycosylated. More preferably, one or more of the asparagine residue of SEQ ID No: 1 are *N*-glycosylated. More, preferably one or more of the asparagine residues 25, 45, 117, 289 and 480 of SEQ ID No: 1 can be *N*-glycosylated.

PREPARING A CRYSTAL OF THE N-DOMAIN OF ACE PROTEIN

In another aspect, the present invention relates to a method of preparing a crystal of the N-domain of ACE protein, comprising the steps of (a) culturing host cells comprising N-domain of ACE protein; (b) purifying the N-domain of ACE protein; and (c) crystallising the N-domain of ACE protein.

Preferably, the N-domain of ACE protein comprises an inter-domain linker region.

The N-domain of ACE protein may be purified using the methods described herein.

Preferably, the N-domain of ACE protein is crystallised in the presence of a ligand, for example, a modulator of the N-domain of ACE protein.

MODULATORS

The role of ACE protein in the pathogenesis of hypertension has resulted in an intensive search for modulators (eg. inhibitors) of the enzyme that could act as antihypertensive drugs (eg. US 3,891,616, US 3,947,575, US 4,052,511 and US 4,053,651). Therapeutic vasodepressors - such as the compound captopril (D-2-methyl-3-mercaptopropanoyl-L-proline) - have been synthesised as ACE inhibitors. Numerous synthetic peptide derivatives have also been shown to be ACE inhibitors as disclosed in US 3,832,337.

Natural substances that inhibit ACE include snake venom and those derived from foodstuffs – such as ACE inhibiting peptides produced by enzymatic hydrolysis of proteins, such as casein or fish meat protein (by Hiroyuki Ukeda, Nippon Nogei Kagaku Kaishi (*Journal of Japan Society for Bioscience*, Biotechnology, and Agrochemistry, 66(1), 25-29 (1992)).

ACE inhibiting synthetic substances include captopril (D-2-methyl-3-mercaptopropanoyl-L-proline) which has already been put to practical application as an orally administered vasodepressor.

However, many currently used ACE inhibiting substances exhibit side effects in many cases and special attention needs to be exercised.

The present invention offers a novel concept in the field of ACE protein inhibitor design by providing conditions suitable for generating specific inhibitors to more precisely target and regulate the activity of the N- and/or C- domains of ACE protein. Preferably the modulators are N-domain of ACE protein specific and/or C-domain of ACE protein specific. These novel modulators can advantageously have reduced side effects.

The present invention provides the use of molecular design techniques to design, select and synthesise chemical entities and compounds, including ACE modulating compounds, capable of binding to the N-domain of ACE protein, in whole or in part.

Thus, in a further aspect, the present invention relates to a method of screening for a modulator of the N-domain of ACE protein wherein the method comprises the use of a crystal of the N-domain of ACE protein.

Preferably, the method comprises the steps of: (a) providing at least a portion of the structural co-ordinates set forth in Table A or Table B; (b) employing at least a portion of the structural co-ordinates set forth in Table A or Table B to design or select or synthesise a putative modulator of the N-domain of ACE protein; (c) contacting the putative modulator of the N-domain of ACE protein with the N-domain

of ACE protein or a mutant, variant, homologue, derivative or fragment thereof in the presence of a substrate; and (d) screening the putative modulator of the N-domain of ACE protein in an assay for the potential to modulate the N-domain.

By way of example, the structure co-ordinates may be used to design compounds that bind to the N-domain of ACE enzyme and may alter the physical properties of the compounds (e.g. solubility) or the domain or the enzyme itself. This invention may be used to design compounds that act as modulators – such as competitive inhibitors - of the N-domain of ACE protein by binding to all or a portion of the active site of the N-domain of ACE protein. Compounds may also be designed that act as non-competitive inhibitors of the N-domain of ACE protein. These non-competitive inhibitors may bind to all or a portion of the N-domain of ACE protein already bound to its substrate and may be more potent and specific than known N-domain of ACE protein inhibitors that compete only for the N-domain of ACE protein active site. Similarly, non-competitive inhibitors that bind to and inhibit the N-domain of ACE protein whether or not it is bound to another chemical ligand may be designed using the structure co-ordinates of the N-domain of ACE protein as described herein.

By way of example, it may be found that the COOH-binding active site residue differs between the N- and C-domain of ACE protein active sites and/or that it may be amenable to the incorporation of a functionality that can covalently modify this residue to produce an irreversible domain specific inhibitor design.

Due to the significant structural similarity between the N-domain and the C-domain of ACE protein it is envisaged that the structural co-ordinates of the crystal of the N-domain can also be used to design modulators which are specific for the C-domain of ACE protein.

Accordingly, in a further aspect, the present invention relates to a method of screening for a modulator of the C-domain of ACE protein wherein the method comprises the use of a crystal of the N-domain of ACE protein. Preferably, the method comprises the steps of: (a) providing at least a portion of the structural co-ordinates set forth in Table A or Table B; (b) employing at least a portion of the structural co-ordinates set forth in Table A or Table B to design or select or synthesise a putative modulator of

the C-domain of ACE protein; (c) contacting the putative modulator of the C-domain of ACE protein with the C-domain of ACE protein or a mutant, variant, homologue, derivative or fragment thereof in the presence of a substrate; and (d) screening the putative modulator of the C-domain of ACE protein in an assay for the potential to modulate the C-domain.

By way of example, the structure co-ordinates of the N-domain may be used to design compounds that bind to the C-domain of ACE enzyme and may alter the physical properties of the compounds (e.g. solubility) or the domains or the enzyme itself. This invention may be used to design compounds that act as modulators – such as competitive inhibitors - of the C-domain of ACE protein by binding to all or a portion of the active site of the C-domain of ACE protein. Compounds may also be designed that act as non-competitive inhibitors of the C-domain of ACE protein. These non-competitive inhibitors may bind to all or a portion of the C-domain of ACE protein already bound to its substrate and may be more potent and specific than known C-domain of ACE protein inhibitors that compete only for the C-domain of ACE protein active site. Similarly, non-competitive inhibitors that bind to and inhibit the C-domain of ACE protein whether or not it is bound to another chemical ligand may be designed using the structure co-ordinates of the N-domain of ACE protein as described herein. Advantageously, the specific modulators of the C-domain of ACE protein do not adversely affect the enzymatic activity of the N-domain of ACE protein. By way of example, such C-domain specific inhibitors can permit the N-domain to hydrolyse the vasodilator bradykinin and thus alleviate side effects such as persistent cough and angioedema. Accordingly, the C-domain specific modulators identified by the screening methods described herein may have the capacity to overcome certain side effects. By way of a further example, the C-domain specific inhibitors can also permit the hydrolysis of the N-domain specific hemoregulatory peptide AcSDKP.

In a preferred embodiment, at least a portion of the structural co-ordinates set forth in Table A or Table B and/or the putative modulator of the N-domain of ACE protein or C-domain of ACE protein and/or the substrate are provided on a machine-readable data storage medium comprising a data storage material encoded with machine readable data.

A crystal of the N-domain of ACE may be probed with a variety of different chemical entities or test compounds to determine optimal sites for interaction between modulators of the N-domain of ACE protein or the C-domain of ACE protein and the enzyme. For example, X-ray diffraction data collected from crystals grown in the presence of chemical entities or test compounds may allow the elucidation of how the chemical entities or test compounds interact with the N-domain of ACE protein or the C-domain of ACE protein. Molecules that bind to those sites can then be designed and synthesised and tested for their capacity to modulate the activity of the N-domain of ACE protein.

The present invention may also allow the development of compounds that can isomerise to reaction intermediates in the chemical reaction of a substrate or other compound that bind to the N-domain of ACE protein or the C-domain of ACE protein. Thus, the time-dependent analysis of structural changes in the N-domain of ACE protein during its interaction with other molecules may be performed. The reaction intermediates of the N-domain of ACE protein or the C-domain of ACE protein may also be deduced from the reaction product in complex with the N-domain of ACE protein. Such information is especially useful to design improved analogues of known N-domain or C-domain modulators or to design new N-domain or C-domain modulators based on the reaction intermediates and the modulator complex. This may provide a new route for designing N-domain or C-domain of ACE protein modulators with high domain specificity and stability. Preferably, this provides a new route for designing N-domain or C-domain of ACE protein modulators with high domain specificity, high stability and low toxicity.

Small molecule databases or test compounds may be screened for chemical entities or compounds that can bind in whole, or in part, to the N-domain or C-domain of ACE protein. Thus, in a preferred embodiment, the putative N-domain or C-domain modulator is selected from a library of compounds or a database. In this screening, the quality of fit of such entities or compounds to the binding site may be judged by various methods – such as shape complementarity or estimated interaction energy (Meng, E. C. *et al.*, *J. Comp. Chem.*, 13, pp. 505-524 (1992)).

Because the N-domain of ACE protein or a mutant, variant, homologue, derivative or fragment thereof may crystallise in more than one crystal form, the structure co-ordinates of the N-domain of ACE protein, or portions thereof, may be particularly useful to solve the structure of other crystal forms of the N-domain of ACE protein. They may also be used to solve the structure of the N-domain of ACE protein mutants, N-domain of ACE protein variants, N-domain of ACE protein homologues, N-domain of ACE protein derivatives, N-domain of ACE protein fragments and N-domain of ACE protein complexes.

Preferably, the structure co-ordinates of the N-domain of ACE protein are used to solve the structure of the crystalline form of any other protein with significant amino acid sequence homology to any functional domain of the N-domain of ACE protein. By way of example, molecular replacement may be used. In this method, the unknown crystal structure, whether it is another crystal form of the N-domain of ACE protein, N-domain of ACE protein mutant, N-domain of ACE protein variant, N-domain of ACE protein homologue (eg. another protein with significant amino acid sequence homology to any functional domain of the N-domain of ACE protein), N-domain of ACE protein derivative, N-domain of ACE protein fragments or N-domain of ACE protein complex may be determined using the N-domain of ACE protein structure co-ordinates of the present invention. This method will provide a more accurate structural form for the unknown crystal more quickly and efficiently than attempting to determine such information *ab initio*.

Preferably, the structural co-ordinates of the N-domain of ACE protein are used for domain interplay or also referred to as domain co-operativity studies. By way of example, molecular replacement may be used. In this method, unknown domain co-operativity with N-domain of ACE protein, N-domain of ACE protein mutant, N-domain of ACE protein variant, N-domain of ACE protein homologue (e.g. another protein with significant amino acid sequence homology to the N-domain of ACE protein), N-domain of ACE protein derivative, N-domain of ACE protein fragments or N-domain of ACE protein complex may be determined using the N-domain of ACE protein structure co-ordinates of the present invention. This method will provide a more accurate structural form for the unknown crystal more quickly and efficiently than attempting to determine such information *ab initio*.

As used herein the term "domain co-operativity" refers to the capacity of each of the domains of ACE protein to modulate the biochemical activities of each other. As used herein the term "modulate" means to affect, to vary, to adjust, to increase, to decrease or generally to be able to regulate or modify the biochemical activity of the N- or C-domain of ACE ptoein.

Preferably the structural co-ordinates of N-domain of ACE protein are used to study co-operativity between the N-domain of ACE protein and the C-domain of ACE protein.

In a preferred embodiment of the present invention, the crystal of the N-domain of ACE protein further comprises a ligand bound to the ACE protein or a portion thereof. For example, the N-domain of ACE protein may be crystallised in a complex with a ligand that is an inhibitor of the N-domain of ACE protein e.g. lisinopril, captopril or RXP407.

By way of example the inhibitor is bound to the N-domain of ACE protein or a portion thereof by contacting one of more residues of the N-domain of ACE protein selected from: Gln259, Tyr369, Lys489 and Tyr498.

The crystal structures of a series of such complexes may then be solved by molecular replacement or in combination with MAD (Multiwavelength Anomalous Dispersion) and/or MIRAS (Multiple Isomorphous Replacement with Anomalous Scattering) procedures - and compared with that of minimally glycosylated N-domain of ACE protein. Potential sites for modification within the binding sites of the N-domain may thus be identified. This information provides an additional tool for determining the most efficient binding interactions, for example, increased hydrophobic interactions, between the N-domain of ACE protein and a ligand or a compound.

The information will also provide ideal conditions for designing domain specific inhibitors to more precisely regulate the biochemical functions of the N- and C-domains of ACE protein.

The structures and complexes of the N-domain of ACE protein may be refined using computer software - such as X-PLOR (*Meth. Enzymol.*, vol. 114 & 115, H. W. Wyckoff et al., eds., Academic Press (1985)), MLPHARE (Collaborative computational project Number 4. The CCP4 Suite: Programs for Protein Crystallography (1994) *Acta Crystallogr.* D 50, 760-763) and SHARP [De La Fortelle, E. & Bricogne, G. Maximum-likelihood heavy-atom parameters refinement in the MIR and MAD methods (1997) *Methods Enzymol.* 276, 472-494). Preferably, the complexes are refined using the program CNS (Brünger et al., (1998) *Acta Crystallogr.* D 54, 905-921). During the final stages of refinement water molecules, ions and inhibitor molecules may be inserted in the structure. This information may thus be used to optimise known classes of modulators of the N-domain of ACE protein, eg. inhibitors, and more importantly, to design and synthesise novel classes of domain specific modulators.

The overall figure of merit may be improved by iterative solvent flattening, phase combination and phase extension with the program SOLOMON (Abrahams, J. P. & Leslie, A. G. W. Methods used in structure determination of bovine mitochondrial F1 ATPase. (1996) *Acta Crystallogr.* D 52, 110-119).

The structure co-ordinates of the mutants of the N-domain of ACE provided in this invention also facilitate the identification of related domains or enzymes analogous to the N-domain of ACE protein in function, structure or both, thereby further leading to novel therapeutic modes for treating or preventing ACE related diseases.

The design of compounds that bind to or modulate the N-domain of ACE protein or the C-domain of ACE protein according to the present invention generally involves consideration of two factors.

First, the compound must be capable of physically and structurally associating with the N-domain or the C-domain of ACE protein. Non-covalent molecular interactions important in the association of the N-domain of ACE with its substrate may include hydrogen bonding, van der Waals and hydrophobic interactions.

Second, the compound must be able to assume a conformation that allows it to associate with the N-domain or C-domain of ACE protein. Although certain portions of the compound may not directly participate in the association with the N-domain or C-domain of ACE, those portions may still influence the overall conformation of the molecule. This may have a significant impact on potency of the compound. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical ligand or compound in relation to all or a portion of a binding site of the N-domain or C-domain of ACE, or the spacing between functional groups of a compound comprising several chemical entities that directly interact with the N-domain or C-domain of ACE.

The potential modulating or binding effect of a chemical compound on the N-domain or the C-domain of ACE may be analysed prior to its actual synthesis and testing by the use of computer modelling techniques. If the theoretical structure of the given compound suggests insufficient interaction and association with the N-domain or the C-domain of ACE, then synthesis and testing of the compound may be obviated. However, if computer modelling indicates a strong interaction, the molecule may be synthesised and tested for its ability to bind to the N-domain or the C-domain of ACE and modulate (e.g. inhibit) using the fluorescent substrate assay of Thornberry et al., (2000) *Methods Enzymol.* 322, 100–110. In this manner, synthesis of inactive compounds may be avoided.

A modulating or other binding compound of the N-domain or the C-domain of ACE may be computationally evaluated and designed by means of a series of steps in which chemical entities or test compounds are screened and selected for their ability to associate with the N-domain or the C-domain of ACE.

A person skilled in the art may use one of several methods to screen chemical entities or test compounds for their ability to associate with the N-domain or the C-domain of ACE and more particularly with the individual binding sites of the N-domain or the C-domain of ACE. This process may begin by visual inspection of, for example, the active site on the computer screen based on the N-domain or the C-domain of ACE co-ordinates of the present invention. Selected chemical entities or test compounds may then be positioned in a variety of orientations, or docked, with the N-domain or

the C-domain of ACE. Docking may be accomplished using software such as Quanta and Sybyl, followed by energy minimisation and molecular dynamics with standard molecular mechanics force fields - such as CHARMM and AMBER.

Specialised computer programs may also assist in the process of selecting chemical entities or test compounds. These include but are not limited to MCSS (Miranker and Karplus (1991) *Proteins: Structure, Function and Genetics*, 11, 29-34); GRID (Goodford (1985) *J. Med. Chem.*, 28, 849-857) and AUTODOCK (Goodsell and Olsen (1990), *Proteins: Structure. Function, and Genetics*, 8, 195-202).

Once suitable chemical entities or test compounds have been selected, they may be assembled into a single compound capable of modulating the domains of the ACE protein e.g. the N-domain and/or the C-domain of the ACE protein. Assembly may proceed by visual inspection of the relationship of the chemical entities or test compounds in relation to the structure co-ordinates of the N-domain of ACE protein. This may be followed by manual model building using software - such as Quanta, Sybyl or O [Jones, T. A., Zou, J. Y., Cowan, S. W. & Kjeldgaard, M. Improved methods for building protein models in electron density maps and the location of errors in these models (1991) *Acta Crystallogr.* A 47, 110-119].

Refinement of the model may be carried out using the program CNS [Brünger, A. T. et al., Crystallography & NMR System: A new software suite for macromolecular structure determination. (1998) *Acta Crystallogr.* D 54, 905-921].

Various programs may be used by a skilled person to connect the individual chemical entities or test compounds – such as 3D Database systems (Martin (1992) *J. Med. Chem.*, 35, 2145-2154) and CAVEAT (Bartlett et al., (1989) *Royal Chem. Soc.* 78, 182-196).

Rather than build an inhibitor of the N-domain or the C-domain of ACE protein one chemical ligand at a time, modelling of other N-domain or C-domain binding compounds may be designed as a whole or *de novo* using either an empty binding site or optionally including some portion(s) of a known inhibitor(s). Such compounds may be designed using programs that may include but are not limited to LEGEND

(Nishibata and Itai (1991) Tetrahedron, 47, 8985) and LUDI (Bohm (1992) *J. Comp. Aid. Molec. Design*, 6, 61-78).

Other molecular modelling techniques may also be employed in accordance with this invention – such as those described by Cohen et al., *J. Med. Chem.*, 33, 883-894 (1990); Navia and Murcko (1992) *Current Opinions in Structural Biology*, 2, 202-210 (1992).

Once a compound has been designed or selected by the above methods, the efficiency with which that compound may bind to the N-domain or the C-domain of ACE protein may be computationally evaluated. Specific computer software may be used to evaluate the efficiency of binding (eg. to evaluate compound deformation energy and electrostatic interaction) – such as QUANTA/CHARMM (Accelrys Inc., USA) and Insight II/Discover (Biosym Technologies Inc., San Diego, Calif., USA). These programs may be implemented, for instance, using a suitable workstation. Other hardware systems and software packages will be known to those persons skilled in the art.

Once a modulating compound has been selected or designed, as described above, substitutions may be made (eg. in atoms or side groups) to improve or modify the binding properties. The substitutions may be conservative i.e. the replacement group may have approximately the same size, shape, hydrophobicity and charge as the original group. Such substituted chemical compounds may then be analysed for efficiency of binding to the N-domain or C-domain of ACE by the same computer methods described above.

Test compounds and modulators of the N-domain or C-domain of ACE protein which are identified using the crystal and the methods of the present invention may be screened in assays. Screening can be, for example *in vitro*, in cell culture, and/or *in vivo*. Biological screening assays preferably centre on activity-based response models, binding assays (which measure how well a compound binds), and bacterial, yeast and animal cell lines (which measure the biological effect of a compound in a cell). The assays can be automated for high capacity-high throughput screening

(HTS) in which large numbers of compounds can be tested to identify compounds with the desired activity.

Current screening technologies are described in Handbook of Drug Screening, edited by Ramakrishna Seethala, Prabhavathi B. Fernandes. New York, NY, Marcel Dekker, (2001).

DISORDERS

These include, but are not limited to, treatment of high blood pressure; treatment of heart failure; prolonging survival of patients who have had a heart attack; preventing death by heart attack and stroke in patients with vascular disease and in diabetics with other vascular risk factors; prolonging survival of patients with weak heart muscle; helping leaking heart valves; preserving kidney function in diabetics; and the treatment of new indications (e.g. polycythemia). Special groups of patients may also be treated with N-domain or C-domain of ACE inhibitors, including patients with chronic pulmonary disease, patients with schleroderma, patients with atheroschlerosis, and patients with hyperuricemia.

It is also envisaged that the modulators identified by the methods described herein may be used to treat Alzheimer's disease and other degenerative diseases, conditions or disorders of the CNS.

ACE CONSTRUCTS

The N-domain of ACE protein produced by a host recombinant cell may be secreted or may be contained intracellularly depending on the nucleotide sequence and/or the vector used.

The skilled person would understand that expression vectors containing the N-domain of ACE protein encoding nucleotide sequence or a mutant, variant, homologue, derivative or fragment thereof, may be designed with signal sequences which direct secretion of the N-domain of ACE protein coding sequences across a particular prokaryotic or eukaryotic cell membrane.

The N-domain encoding sequence may be fused (e.g. ligated) to nucleotide sequences encoding a polypeptide domain which will facilitate purification of soluble proteins (Kroll DJ et al., (1993) *DNA Cell Biol* 12:441-53). Preferably, the polypeptide domain which facilitates purification of soluble proteins is fused in frame with the N-domain of the ACE protein encoding sequence. Such purification facilitating domains include, but are not limited to, metal chelating peptides – such as histidine-tryptophan modules that allow purification on immobilised metals (Porath J (1992) *Protein Expr Purif* 3, 263-281), protein A domains that allow purification on immobilised immunoglobulin, and the domain utilised in the FLAGS extension/affinity purification system (Immunex Corp, Seattle, WA). The inclusion of a cleavable linker sequence such as Factor XA or enterokinase (Invitrogen, San Diego, CA) between the purification domain and ACE is useful to facilitate purification.

Preferably the N-domain of ACE protein sequence is fused with the glutathione synthetase (GS) signal.

Preferably, the N-domain of ACE protein is secreted in a soluble form host cells and can be harvested from the growth medium.

Preferably, the N-domain of ACE construct is pEE14 N-domain which encodes the N-domain of human tACE. This construct comprises the inter-domain linker region.

HOST CELL

As used herein, the term "host cell" refers to any cell that comprises nucleotide sequences that are of use in the present invention, for example, nucleotide sequences encoding the N-domain of ACE protein.

Host cells may be transformed or transfected with a nucleotide sequence contained in a vector e.g. a cloning vector. Preferably, said nucleotide sequence is carried in a vector for the replication and/or expression of the nucleotide sequence. The cells will be chosen to be compatible with the said vector and may for example be prokaryotic such as bacterial or eukaryotic such as fungal, yeast or plant cells.

The gram-negative bacterium *E. coli* is widely used as a host for cloning nucleotide sequences. This organism is also widely used for heterologous nucleotide sequence expression. However, large amounts of heterologous protein tend to accumulate inside the cell. Subsequent purification of the desired protein from the bulk of *E. coli* intracellular proteins can sometimes be difficult.

In contrast to *E. coli*, bacteria from the genus *Bacillus* are very suitable as heterologous hosts because of their capability to secrete proteins into the culture medium. Other bacteria suitable as hosts are those from the genera *Streptomyces* and *Pseudomonas*.

Depending on the nature of the polynucleotide and/or the desirability for further processing of the expressed protein, eukaryotic hosts including yeast or other fungi may be preferred. In general, yeast cells are preferred over fungal cells because yeast cells are easier to manipulate. However, some proteins are either poorly secreted from the yeast cell, or in some cases are not processed properly (e.g. hyperglycosylation). In these instances, a different fungal host organism should be selected.

Examples of expression hosts are fungi - such as *Aspergillus* species (such as those described in EP-A-0184438 and EP-A-0284603) and *Trichoderma* species; bacteria - such as *Bacillus* species (such as those described in EP-A-0134048 and EP-A-0253455), *Streptomyces* species and *Pseudomonas* species; yeast - such as *Kluyveromyces* species (such as those described in EP-A-0096430 and EP-A-0301670) and *Saccharomyces* species; mammalian cells – such as CHO-K1 cells.

The use of host cells may provide for post-translational modifications (e.g. glycosylation) as may be needed to confer optimal biological activity on recombinant expression products of the present invention.

Aspects of the present invention also relate to host cells comprising the N-domain of ACE protein constructs of the present invention. The N-domain of ACE protein constructs may comprise a nucleotide sequence for replication and expression of the

sequence. The cells will be chosen to be compatible with the vector and may for example be prokaryotic such as bacterial or eukaryotic such as fungal, yeast or plant cells.

In a preferred embodiment, the host cells are mammalian cells – such as CHO-K1 cells. CHO-K1 cells expressing the N-domain of ACE protein may be grown and maintained in accordance with Yu *et al.* (1997).

NUCLEOTIDE SEQUENCES

As used herein, the term "nucleotide sequence" refers to nucleotide sequences, oligonucleotide sequences, polynucleotide sequences and variants, homologues, fragments and derivatives thereof (such as portions thereof) which comprise the nucleotide sequences encoding the N-domain of ACE protein, for example, the N-domain of testis ACE protein or the N-domain of somatic ACE protein.

The nucleotide sequence may be DNA or RNA of genomic or synthetic or recombinant origin, which may be double-stranded or single-stranded whether representing the sense or antisense strand or combinations thereof.

Preferably, the term nucleotide sequence is prepared by use of recombinant DNA techniques (e.g. recombinant DNA). The nucleotide sequences may include within them synthetic or modified nucleotides. A number of different types of modification to oligonucleotides are known in the art. These include methylphosphonate and phosphorothioate backbones addition of acridine or polylysine chains at the 3' and/or 5' ends of the molecule. For the purposes of the present invention, it is to be understood that the nucleotide sequences described herein may be modified by any method available in the art.

It will be understood by a skilled person that numerous different nucleotide sequences can encode the same protein as a result of the degeneracy of the genetic code. In addition, it is to be understood that skilled persons may, using routine techniques, make nucleotide substitutions that do not substantially affect the activity encoded by the

nucleotide sequence of the present invention to reflect the codon usage of any particular host organism in which the target is to be expressed.

The terms "variant", "homologue" or "derivative" in relation to nucleotide sequences include any substitution of, variation of, modification of, replacement of, deletion of or addition of one (or more) nucleic acid from or to the sequence providing the resultant nucleotide sequence encodes a functional protein according to the present invention (or even a modulator of the N-domain of ACE protein according to the present invention if said modulator comprises a nucleotide sequence).

AMINO ACID SEQUENCES

As used herein, the term "amino acid sequence" is synonymous with the term "polypeptide" and/or the term "protein". In some instances, the term "amino acid sequence" is synonymous with the term "peptide".

Aspects of the present invention concern the use of amino acid sequences, which may be available in databases. These amino acid sequences may comprise N-domain of ACE proteins.

The amino acid sequence may be isolated from a suitable source, or it may be made synthetically or it may be prepared by use of recombinant DNA techniques.

The terms "variant", "homologue" or "derivative" in relation to amino acid sequences include any substitution of, variation of, modification of, replacement of, deletion of or addition of one (or more) amino acid from the functional protein according to the present invention (or even a modulator of the N-domain of ACE protein according to the present invention if said modulator comprises an amino acid sequence).

Preferably, the N-domain of ACE protein comprises SEQ ID No. 1 or a mutant, variant, homologue, derivative or a fragment thereof.

PURITY

Preferably the protein solution used for crystallisation is at least 95.5% pure. More preferably the protein solution used for crystallisation is at least 97.5% pure. More preferably, the protein solution used for crystallisation is at least 99.0% pure. Most preferably, the protein solution used for crystallisation is at least 99.5% pure.

MODEL

As used herein, the term "model" refers to a structural model such as a three dimensional (3D) structural model (or representation thereof) comprising the N-domain of ACE protein.

Test compounds can be modelled that bind spatially and preferentially to the N-domain of ACE protein – such as to bind spatially and preferentially to the N-domain of ACE protein – for example, the active site of the N-domain of ACE protein.

Preferably, the crystal model comprising the N-domain of ACE is built from all or a portion of the structural co-ordinates set forth in Table A or Table B.

MUTANT

As used herein, the term "mutant" refers to the N-domain of ACE protein comprising any one or more changes in the wild-type ACE sequence shown as SEQ ID No. 1.

The term "mutant" is not limited to any of the mutations described herein which are reflected in amino acid substitutions of the amino acid residues in the N-domain of ACE protein, but are not limited to, other deletions or insertions of nucleotides which may result in changes in the amino acid residues in the amino acid sequence of the N-domain of ACE protein.

The present invention also enables the solving of the crystal structure of mutants of the N-domain of ACE protein. More particularly, by virtue of the present invention, the location of the active site of the N-domain of ACE protein based on its crystal structure permits the identification of desirable sites for mutation. For example, one or more mutations may be directed to a particular site - such as the active site - or combination of

sites. Similarly, only a location on, at or near the inter-domain linker region may be replaced, resulting in an altered domain co-operativity by changing the charge of one or more charge units, as compared to the wild-type N-domain. Alternatively, an amino acid residue in the inter-domain linker region of the N-domain of ACE may be chosen for replacement based on its hydrophilic or hydrophobic characteristics.

Such mutants may be characterised by any one of several different properties as compared with wild-type N-domain of ACE protein. For example, such mutants may have altered surface charge of one or more charge units, or have an increased stability to subunit dissociation, or an altered substrate specificity in comparison with, or a higher specific activity than, wild-type of the N-domain of ACE protein.

The mutants may be prepared in a number of ways that are known by a person skilled in the art. For example, mutations may be introduced by means of oligonucleotide-directed mutagenesis or other conventional methods. Alternatively, mutants of the N-domain of ACE protein may be generated by site specific replacement of a particular amino acid with an unnaturally occurring amino acid. This may be achieved by growing a host organism capable of expressing either the wild-type or mutant polypeptide on a growth medium depleted of one or more natural amino acids but enriched in one or more corresponding unnaturally occurring amino acids.

The expression, activity (e.g. kinetic constants) and/or the crystallisation properties of the mutants may be determined using the methods described herein.

VARIANTS/HOMOLOGUES/DERIVATIVES/FRAGMENTS

The N-domain of ACE protein described herein is intended to include any polypeptide, which has the activity of the naturally occurring N-domain and includes all vertebrate and mammalian forms. Such terms also include polypeptides that differ from naturally occurring forms of the N-domain by having amino acid deletions, substitutions, and additions, but which retain the activity of the N-domain of ACE protein.

The term "variant" is used to mean a naturally occurring polypeptide or nucleotide sequences which differs from a wild-type or a native sequence.

The term "fragment" indicates that a polypeptide or nucleotide sequence comprises a fraction of a wild-type or a native sequence. It may comprise one or more large contiguous sections of sequence or a plurality of small sections. The sequence may also comprise other elements of sequence, for example, it may be a fusion protein with another protein. Preferably the sequence comprises at least 50%, more preferably at least 65%, more preferably at least 80%, most preferably at least 90% of the wild-type sequence.

The present invention also encompasses the use of variants, homologues and derivatives of nucleotide and amino acid sequences. Here, the term "homologue" means an entity having a certain homology with amino acid sequences or nucleotide sequences. Here, the term "homology" can be equated with "identity".

In the present context, a homologous sequence is taken to include an amino acid sequence which may be at least 75%, 85% or 90% identical, preferably at least 95% or 98% identical to the subject sequence. Although homology can also be considered in terms of similarity (i.e. amino acid residues having similar chemical properties/functions), it is preferred here to express homology in terms of sequence identity.

Homologous sequence is taken to include a nucleotide sequence which may be at least 75%, 85% or 90% identical, preferably at least 95% or 98% identical to the subject sequence.

Homology comparisons can be conducted by eye, or more usually, with the aid of readily available sequence comparison programs. These commercially available computer programs can calculate % homology between two or more sequences.

Homology when based on percentage (%) may be calculated over contiguous sequences, i.e. one sequence is aligned with the other sequence and each amino acid in one sequence is directly compared with the corresponding amino acid in the other

sequence, one residue at a time. This is usually referred to "ungapped" alignment. Typically, such ungapped alignments are performed only over a relatively short number of residues.

Although this is a very simple and consistent method, it fails to take into consideration that, for example, in an otherwise identical pair of sequences, one insertion or deletion will cause the following amino acid residues to be put out of alignment, thus potentially resulting in a large reduction in % homology when a global alignment is performed. Consequently, most sequence comparison methods are designed to produce optimal alignments that take into consideration possible insertions and deletions without penalising unduly the overall homology score. This is achieved by inserting "gaps" in the sequence alignment to try to maximise local homology.

However, these more complex methods assign "gap penalties" to each gap that occurs in the alignment so that, for the same number of identical amino acids, a sequence alignment with as few gaps as possible - reflecting higher relatedness between the two compared sequences - will achieve a higher score than one with many gaps. "Affine gap costs" are typically used that charge a relatively high cost for the existence of a gap and a smaller penalty for each subsequent residue in the gap. This is the most commonly used gap scoring system. High gap penalties will of course produce optimised alignments with fewer gaps. Most alignment programs allow the gap penalties to be modified. However, it is preferred to use the default values when using such software for sequence comparisons. For example when using the GCG Wisconsin Bestfit package the default gap penalty for amino acid sequences is -12 for a gap and -4 for each extension.

Calculation of maximum % homology therefore firstly requires the production of an optimal alignment, taking into consideration gap penalties. A suitable computer program for carrying out such an alignment is the GCG Wisconsin Bestfit package (University of Wisconsin, U.S.A.; Devereux et al., 1984, *Nucleic Acids Research* 12:387). Examples of other software than can perform sequence comparisons include, but are not limited to, the BLAST package (see Ausubel et al., 1999 *ibid* – Chapter 18), FASTA (Atschul et al., 1990, *J. Mol. Biol.,* 403-410) and the

GENEWORKS suite of comparison tools. Both BLAST and FASTA are available for offline and online searching (see Ausubel et al., 1999 *ibid*, pages 7-58 to 7-60). However, for some applications, it is preferred to use the GCG Bestfit program. A new tool, called BLAST 2 Sequences is also available for comparing protein and nucleotide sequence (see *FEMS Microbiol Lett* 1999 174(2): 247-50; *FEMS Microbiol Lett* 1999 177(1): 187-8)

Although the final % homology can be measured in terms of identity, the alignment process itself is typically not based on an all-or-nothing pair comparison. Instead, a scaled similarity score matrix is generally used that assigns scores to each pairwise comparison based on chemical similarity or evolutionary distance. An example of such a matrix commonly used is the BLOSUM62 matrix - the default matrix for the BLAST suite of programs. GCG Wisconsin programs generally use either the public default values or a custom symbol comparison table if supplied (see user manual for further details). For some applications, it is preferred to use the public default values for the GCG package, or in the case of other software, the default matrix, such as BLOSUM62.

Once the software has produced an optimal alignment, it is possible to calculate % homology, preferably % sequence identity. The software typically does this as part of the sequence comparison and generates a numerical result.

By way of example, homologous sequences of the N-domain of ACE protein include, but are not limited to human ACE_S somatic ACE (accession number: J04144), human ACE_T testis ACE (accession number: M26657), human ACEH/ACE2 (accession numbers: AAF78220; BAB40370; AAF99721), chimp ACE_T (accession number: AF193487_2), rabbit ACE_T mature protein (accession number: P22968), rabbit ACE_T full pre-protein (accession number: P22968), mouse ACE_T testis ACE (accession number: P22967), bovine Cdom ACE_S C-domain, rat Cdom ACE_S C-domain (derived from accession number P47820; starting D616), human Ndom ACE_S N-domain (derived from accession number P12821 (J04144)), chimp Ndom ACE_S N-domain (derived from accession number AF193487_1), rabbit Ndom ACE_S N-domain (derived from P12822), bovine Ndom (Bovine {*Bos taurus*} ACE_S N-domain), mouse Ndom ACE_S N-domain (derived from accession number P09470), rat Ndom ACE_S N-

domain (derived from accession number P47820), chick ACE (partial ACE accession number Q10751), dros AnCE (derived from accession number Q10714), dros ACEr (derived from accession number X96913), buffalo fly ACE (derived from accession number Q10715), and silkworm ACE (derived from accession number BAA97657), tick ACE (derived from accession number U62809).

The sequences may also have deletions, insertions or substitutions of amino acid residues, which produce a silent change and result in a functionally equivalent substance. Deliberate amino acid substitutions may be made on the basis of similarity in polarity, charge, solubility, hydrophobicity, hydrophilicity, and/or the amphipathic nature of the residues as long as the secondary binding activity of the substance is retained. For example, negatively charged amino acids include aspartic acid and glutamic acid; positively charged amino acids include lysine and arginine; and amino acids with uncharged polar head groups having similar hydrophilicity values include leucine, isoleucine, valine, glycine, alanine, asparagine, glutamine, serine, threonine, phenylalanine, and tyrosine.

Conservative substitutions may be made, for example according to the Table below. Amino acids in the same block in the second column and preferably in the same line in the third column may be substituted for each other:

ALIPHATIC	Non-polar	G A P
		I L V
	Polar - uncharged	C S T M
		N Q
	Polar - charged	D E
		K R
AROMATIC		H F W Y

Homologous substitution (substitution and replacement are both used herein to mean the interchange of an existing amino acid residue, with an alternative residue) may occur i.e. like-for-like substitution such as basic for basic, acidic for acidic, polar for polar etc.. Non-homologous substitution may also occur i.e. from one class of residue

to another or alternatively involving the inclusion of unnatural amino acids such as ornithine (hereinafter referred to as Z), diaminobutyric acid ornithine (hereinafter referred to as B), norleucine ornithine (hereinafter referred to as O), pyriylalanine, thienylalanine, naphthylalanine and phenylglycine.

Replacements may also be made by unnatural amino acids include; alpha* and alpha-disubstituted* amino acids, N-alkyl amino acids*, lactic acid*, halide derivatives of natural amino acids such as trifluorotyrosine*, p-Cl-phenylalanine*, p-Br-phenylalanine*, p-I-phenylalanine*, L-allyl-glycine*, ß-alanine*, L-α-amino butyric acid*, L-γ-amino butyric acid*, L-α-amino isobutyric acid*, L-ε-amino caproic acid#, 7-amino-heptanoic acid*, L-methionine sulfone#*, L-norleucine*, L-norvaline*, p-nitro-L-phenylalanine*, L-hydroxyproline#, L-thioproline*, methyl derivatives of phenylalanine (Phe) such as 4-methyl-Phe*, pentamethyl-Phe*, L-Phe (4-amino)#, L-Tyr (methyl)*, L-Phe (4-isopropyl)*, L-Tic (1,2,3,4-tetrahydroisoquinoline-3-carboxyl acid)*, L-diaminopropionic acid # and L-Phe (4-benzyl)*. The notation * has been utilised for the purpose of the discussion above (relating to homologous or non-homologous substitution), to indicate the hydrophobic nature of the derivative whereas # has been utilised to indicate the hydrophilic nature of the derivative, #* indicates amphipathic characteristics.

The term "derivative" or "derivatised" as used herein includes chemical modification of a ligand – such as test compound or a modulator of the N-domain of ACE protein. Illustrative of such chemical modifications would be replacement of hydrogen by a halo group, an alkyl group, an acyl group or an amino group.

Variant amino acid sequences may include suitable spacer groups that may be inserted between any two amino acid residues of the sequence including alkyl groups such as methyl, ethyl or propyl groups in addition to amino acid spacers such as glycine or β-alanine residues. A further form of variation, involves the presence of one or more amino acid residues in peptoid form, will be well understood by those skilled in the art. For the avoidance of doubt, "the peptoid form" is used to refer to variant amino acid residues wherein the α-carbon substituent group is on the residue's nitrogen atom rather than the α-carbon. Processes for preparing peptides in the peptoid form are

known in the art, for example Simon RJ et al., *PNAS* (1992) 89(20), 9367-9371 and Horwell DC, *Trends Biotechnol.* (1995) 13(4), 132-134.

TEST COMPOUND

As used herein, the term "test compound" includes, but is not limited to, a compound which may be obtainable from or produced by any suitable source, whether natural or not.

The test compound may be designed or obtained from a small molecule library of compounds, which may comprise peptides, as well as other compounds, such as small organic molecules and particularly new lead compounds. By way of example, the test compound may be a natural substance, a biological macromolecule, or an extract made from biological materials - such as bacteria, fungi, or animal (particularly mammalian) cells or tissues, an organic or an inorganic molecule, a synthetic test compound, a semi-synthetic test compound, a structural or functional mimetic, a peptide, a peptidomimetics, a derivatised test compound, a peptide cleaved from a whole protein, or a peptide synthesised synthetically (such as, by way of example, either using a peptide synthesiser or by recombinant techniques or combinations thereof, a recombinant test compound, a natural or a non-natural test compound, a fusion protein or equivalent thereof and mutants, derivatives or combinations thereof. The test compound may even be a compound that is a modulator of the N-domain or C-domain of ACE protein – such as a known inhibitor of the N-domain or C-domain of ACE protein- that has been modified in some way e.g. by recombinant DNA techniques or chemical synthesis techniques.

Typically, the test compound will be prepared by recombinant DNA techniques and/or chemical synthesis techniques.

Once a test compound capable of interacting with the N-domain or C-domain of ACE protein has been identified, further steps may be carried out to select and/or to modify the test compounds and/or to modify existing compounds, such that they are able to modulate the N-domain or C-domain of ACE protein.

The present invention also relates to a test compound which may be a domain specific compound such as a domain specific inhibitor capable of modulating the activity of the ACE protein in a domain specific manner. That is the compound is capable of modulating the N-domain and/or C-domain of ACE protein.

MODULATING THE ACTIVITY OF ACE

As herein, the term "modulating" refers to preventing, suppressing, inhibiting, alleviating, restoring, elevating, increasing or otherwise affecting the N-domain or C-domain of ACE protein.

The term "modulator of N-domain or C-domain of ACE" may refer to a single ligand or a combination of ligands.

The modulator of the N-domain or C-domain of ACE protein may be an antagonist or an agonist of the N-domain or the C-domain of ACE.

As used herein, the term "agonist" means any ligand, which is capable of interacting (e.g. binding) with N-domain or C-domain of ACE protein and which is capable of increasing a proportion of the N-domain or C-domain of ACE that is in an active form, resulting in an increased biological response.

As used herein, the term "antagonist" means any ligand, which is capable of interacting (e.g. binding) with N-domain or C-domain of ACE protein and which is capable of decreasing (eg. inhibiting) a proportion of the N-domain or C-domain of ACE that is in an active form, resulting in a decreased biological response.

Preferably, the modulators of the N-domain or C-domain of ACE protein of the present invention are antagonists of the N-domain or C-domain of ACE protein.

The modulator may be an organic compound or other chemical. The modulator may be a compound, which is obtainable from or produced by any suitable source, whether natural or artificial. The modulator may be an amino acid molecule, a polypeptide, or

a chemical derivative thereof, or a combination thereof. The modulator may even be a polynucleotide molecule - which may be a sense or an anti-sense molecule. The modulator may even be an antibody.

The modulator of the N-domain or C-domain of ACE protein may be designed or obtained from a small molecule library of compounds, which may comprise peptides, as well as other compounds or small organic molecules.

By way of example, the modulator of the N-domain or C-domain of ACE protein may be a natural substance, a biological macromolecule, or an extract made from biological materials such as bacteria, fungi, or animal (particularly mammalian) cells or tissues, an organic or an inorganic molecule, a synthetic agent, a semi-synthetic agent, a structural or functional mimetic, a peptide, a peptidomimetic, a derivatised agent, a peptide cleaved from a whole protein, or a peptide synthesised synthetically (such as, by way of example, either using a peptide synthesiser or by recombinant techniques or combinations thereof, a recombinant agent, an antibody, a natural or a non-natural agent, a fusion protein or equivalent thereof and mutants, derivatives or combinations thereof).

Typically, the modulator of the N-domain or C-domain of ACE protein will be an organic compound. Typically, the organic compounds will comprise two or more hydrocarbyl groups. Here, the term "hydrocarbyl group" means a group comprising at least C and H and may optionally comprise one or more other suitable substituents. Examples of such substituents may include halo-, alkoxy-, nitro-, an alkyl group, a cyclic group etc. In addition to the possibility of the substituents being a cyclic group, a combination of substituents may form a cyclic group. If the hydrocarbyl group comprises more than one C then those carbons need not necessarily be linked to each other. For example, at least two of the carbons may be linked *via* a suitable element or group. Thus, the hydrocarbyl group may contain hetero atoms. Suitable hetero atoms will be apparent to those skilled in the art and include, for instance, sulphur, nitrogen and oxygen. For some applications, preferably the modulator of the N-domain or C-domain of ACE protein comprises at least one cyclic group. The cyclic group may be a polycyclic group, such as a non-fused polycyclic group. For some applications, the modulator of the N-domain or C-domain of ACE protein comprises

at least the one of said cyclic groups linked to another hydrocarbyl group.

The modulator of the N-domain or C-domain of ACE protein may contain halo groups, for example, fluoro, chloro, bromo or iodo groups.

The modulator of the N-domain or C-domain of ACE protein may contain one or more of alkyl, alkoxy, alkenyl, alkylene and alkenylene groups – which may be unbranched- or branched-chain.

The modulator of the N-domain or C-domain of ACE protein may be in the form of a pharmaceutically acceptable salt – such as an acid addition salt or a base salt – or a solvate thereof, including a hydrate thereof. For a review on suitable salts see Berge et al., (1977) *J. Pharm. Sci.* 66, 1-19.

The modulator of the N-domain or C-domain of ACE protein may be a structurally novel modulator.

The modulators of the N-domain or C-domain of ACE protein may be analogues to other known modulators – such as known inhibitors of the N-domain of ACE protein (for example, snake venom, peptides produced by enzymatic hydrolysis of casein or fish meat protein, or Benazepril, Captopril, Cilazapril, Enalapril, Fosinopril, Lisinopril, Moexipril, Perindopril, Quinapril, Ramipril, Trandolapril and Enalaprilat).

Preferably the inhibitor of the N-domain or C-domain of ACE protein is Lisinopril (N2-[(S)-1-carboxy-3-phenylpropyl]-L-lysyl-L-proline; also known as Prinivil or Zestril).

Preferably, the N-domain or C-domain of ACE protein modulators have improved properties over those previously available, for example, fewer side effects – such as cough (e.g. dry, persistent); fever and chills; hoarseness; swelling of face, mouth, hands, or feet; trouble in swallowing or breathing; itching of skin; yellow eyes or skin; dizziness, light-headedness, or fainting; skin rash, with or without itching; fever, or joint pain; abdominal pain, abdominal distention; nausea, or vomiting; chest pain, confusion; irregular heartbeat; nervousness; numbness or tingling in hands, feet, or lips; weakness

or heaviness of legs; headache, diarrhoea; loss of taste; nausea; unusual tiredness and angioedema.

The modulator of the N-domain or C-domain of ACE protein may be a mimetic.

The modulator of the N-domain or C-domain of ACE protein may also be chemically modified.

The modulator of the N-domain or C-domain of ACE protein may be capable of displaying other therapeutic properties.

The modulator of the N-domain or C-domain of ACE protein may be used in combination with one or more other pharmaceutically active agents.

If combinations of active agents are administered, then these may be administered simultaneously, separately or sequentially.

MIMETIC

As used herein, the term "mimetic" relates to any chemical including, but not limited to, peptide, polypeptide, antibody or other organic chemical with the same qualitative activity or effect as a known compound. That is, the mimetic is a functional equivalent of a known compound.

STEREO AND GEOMETRIC ISOMERS

Modulators of the N-domain or C-domain of ACE protein may exist as stereoisomers and/or geometric isomers – e.g. they may possess one or more asymmetric and/or geometric centres and so may exist in two or more stereoisomeric and/or geometric forms. The present invention contemplates the use of all of the individual stereoisomers and geometric isomers, and mixtures thereof.

PHARMACEUTICAL SALT

Modulators of the N-domain or C-domain of ACE protein may be administered in the form of a pharmaceutically acceptable salt.

Pharmaceutically-acceptable salts are well known to those skilled in the art, and for example include those mentioned by Berge et al., (1977) *J. Pharm. Sci.*, 66, 1-19. Suitable acid addition salts are formed from acids which form non-toxic salts and include the hydrochloride, hydrobromide, hydroiodide, nitrate, sulphate, bisulphate, phosphate, hydrogenphosphate, acetate, trifluoroacetate, gluconate, lactate, salicylate, citrate, tartrate, ascorbate, succinate, maleate, fumarate, gluconate, formate, benzoate, methanesulphonate, ethanesulphonate, benzenesulphonate and p-toluenesulphonate salts.

When one or more acidic moieties are present, suitable pharmaceutically acceptable base addition salts can be formed from bases which form non-toxic salts and include the aluminium, calcium, lithium, magnesium, potassium, sodium, zinc, and pharmaceutically-active amines such as diethanolamine, salts.

A pharmaceutically acceptable salt of a modulator of the N-domain or C-domain of ACE protein may be readily prepared by mixing together solutions of the modulator and the desired acid or base, as appropriate. The salt may precipitate from solution and be collected by filtration or may be recovered by evaporation of the solvent.

The modulator of the N-domain or C-domain of ACE protein may exist in polymorphic form.

The modulator of the N-domain or C-domain of ACE protein may contain one or more asymmetric carbon atoms and therefore exists in two or more stereoisomeric forms. Where a modulator of the N-domain or C-domain of ACE protein contains an alkenyl or alkenylene group, cis (E) and trans (Z) isomerism may also occur. The present invention includes the individual stereoisomers of the modulator of the N-domain or C-domain of ACE protein and, where appropriate, the individual tautomeric forms thereof, together with mixtures thereof.

Separation of diastereoisomers or *cis* and *trans* isomers may be achieved by conventional techniques, e.g. by fractional crystallisation, chromatography or H.P.L.C. of a stereoisomeric mixture of the modulator of the N-domain or C-domain of ACE protein or a suitable salt or derivative thereof. An individual enantiomer of the modulator of the N-domain or C-domain of ACE may also be prepared from a corresponding optically pure intermediate or by resolution, such as by H.P.L.C. of the corresponding racemate using a suitable chiral support or by fractional crystallisation of the diastereoisomeric salts formed by reaction of the corresponding racemate with a suitable optically active acid or base, as appropriate.

The modulator of the N-domain or C-domain of ACE may also include all suitable isotopic variations of the modulator or a pharmaceutically acceptable salt thereof. An isotopic variation of an modulator of the N-domain or C-domain of ACE or a pharmaceutically acceptable salt thereof is defined as one in which at least one atom is replaced by an atom having the same atomic number but an atomic mass different from the atomic mass usually found in nature. Examples of isotopes that can be incorporated into the modulator of ACE and pharmaceutically acceptable salts thereof include isotopes of hydrogen, carbon, nitrogen, oxygen, phosphorus, sulphur, fluorine and chlorine such as ^{2}H, ^{3}H, ^{13}C, ^{14}C, ^{15}N, ^{17}O, ^{18}O, ^{31}P, ^{32}P, ^{35}S, ^{18}F and ^{36}Cl, respectively. Certain isotopic variations of the modulator the N-domain or C-domain of ACE and pharmaceutically acceptable salts thereof, for example, those in which a radioactive isotope such as ^{3}H or ^{14}C is incorporated, are useful in drug and/or substrate tissue distribution studies. Tritiated, i.e., ^{3}H, and carbon-14, i.e., ^{14}C, isotopes are particularly preferred for their ease of preparation and detectability. Further, substitution with isotopes such as deuterium, i.e., ^{2}H, may afford certain therapeutic advantages resulting from greater metabolic stability, for example, increased *in vivo* half-life or reduced dosage requirements and hence may be preferred in some circumstances. Isotopic variations of the modulator of the N-domain or C-domain of ACE and pharmaceutically acceptable salts thereof of this invention can generally be prepared by conventional procedures using appropriate isotopic variations of suitable reagents.

It will be appreciated by those skilled in the art that the agent may be derived from a prodrug. Examples of prodrugs include entities that have certain protected group(s)

and which may not possess pharmacological activity as such, but may, in certain instances, be administered (such as orally or parenterally) and thereafter metabolised in the body to form the modulator of the N-domain or C-domain of ACE which is pharmacologically active.

It will be further appreciated that certain moieties known as "pro-moieties", for example as described in "Design of Prodrugs" by H. Bundgaard, Elsevier, 1985 (the disclosured of which is hereby incorporated by reference), may be placed on appropriate functionalities of the modulator of the N-domain or C-domain of ACE protein. Such prodrugs are also contemplated within the scope of the invention.

PHARMACEUTICALLY ACTIVE SALT

The modulator of the N-domain or C-domain of ACE protein may be administered as a pharmaceutically acceptable salt. Typically, a pharmaceutically acceptable salt may be readily prepared by using a desired acid or base, as appropriate. The salt may precipitate from solution and be collected by filtration or may be recovered by evaporation of the solvent.

CHEMICAL SYNTHESIS METHODS

The modulator of the N-domain or C-domain of ACE protein of the present invention may be prepared by chemical synthesis techniques.

It will be apparent to those skilled in the art that sensitive functional groups may need to be protected and deprotected during synthesis of a compound of the invention. This may be achieved by conventional techniques, for example as described in "Protective Groups in Organic Synthesis" by T W Greene and P G M Wuts, John Wiley and Sons Inc. (1991), and by P.J.Kocienski, in "Protecting Groups", Georg Thieme Verlag (1994).

It is possible during some of the reactions that any stereocentres present could, under certain conditions, be racemised, for example if a base is used in a reaction with a substrate having an having an optical centre comprising a base-sensitive group. This is possible during e.g. a guanylation step. It should be possible to circumvent potential

problems such as this by choice of reaction sequence, conditions, reagents, protection/deprotection regimes, etc. as is well-known in the art.

The compounds and salts may be separated and purified by conventional methods.

Separation of diastereomers may be achieved by conventional techniques, e.g. by fractional crystallisation, chromatography or H.P.L.C. of a stereoisomeric mixture of a compound of formula (I) or a suitable salt or derivative thereof. An individual enantiomer of a compound of formula (I) may also be prepared from a corresponding optically pure intermediate or by resolution, such as by H.P.L.C. of the corresponding racemate using a suitable chiral support or by fractional crystallisation of the diastereomeric salts formed by reaction of the corresponding racemate with a suitably optically active acid or base.

The N-domain or C-domain of ACE protein, modulators of the N-domain or C-domain of ACE protein or variants, homologues, derivatives, fragments or mimetics thereof may be produced using chemical methods to synthesise the N-domain or C-domain of ACE protein or the modulator of the N-domain or C-domain of ACE protein in whole or in part. For example, the N-domain or C-domain peptide or a modulator of the N-domain or C-domain of ACE protein that is a peptide can be synthesised by solid phase techniques, cleaved from the resin, and purified by preparative high performance liquid chromatography (e.g., Creighton (1983) Proteins Structures And Molecular Principles, WH Freeman and Co, New York NY). The composition of the synthetic peptides may be confirmed by amino acid analysis or sequencing (e.g., the Edman degradation procedure; Creighton, *supra*).

Synthesis of peptides (or variants, homologues, derivatives, fragments or mimetics thereof) may be performed using various solid-phase techniques (Roberge JY *et al* (1995) Science 269: 202-204) and automated synthesis may be achieved, for example, using the ABI 43 1 A Peptide Synthesizer (Perkin Elmer) in accordance with the instructions provided by the manufacturer. Additionally, the amino acid sequences comprising the modulator of the N-domain or C-domain of ACE protein, may be altered during direct synthesis and/or combined using chemical methods with a

sequence from other subunits, or any part thereof, to produce a variant modulator of the N-domain or C-domain of ACE protein.

CHEMICAL MODIFICATION

The modulator of the N-domain or C-domain of ACE protein may be a chemically modified modulator.

The chemical modification of a modulator of the N-domain or C-domain of ACE protein may either enhance or reduce interactions between the modulator of the N-domain or C-domain of ACE protein and the target – such as hydrogen bonding interactions, charge interactions, hydrophobic interactions, van der Waals interactions or dipole interactions.

In one aspect, the modulator of the N-domain or C-domain of ACE protein may act as a model (for example, a template) for the development of other compounds.

PHARMACEUTICAL COMPOSITIONS

The components may be administered alone but will generally be administered as a pharmaceutical composition – e.g. when the components are in a mixture with a suitable pharmaceutical excipient, diluent or carrier selected with regard to the intended route of administration and standard pharmaceutical practice.

For example, the components can be administered in the form of tablets, capsules, ovules, elixirs, solutions or suspensions, which may contain flavouring or colouring agents, for immediate-, delayed-, modified-, sustained-, pulsed- or controlled-release applications.

If the pharmaceutical is a tablet, then the tablet may contain excipients such as microcrystalline cellulose, lactose, sodium citrate, calcium carbonate, dibasic calcium phosphate and glycine, disintegrants such as starch (preferably corn, potato or tapioca starch), sodium starch glycollate, croscarmellose sodium and certain complex silicates, and granulation binders - such as polyvinylpyrrolidone,

hydroxypropylmethylcellulose (HPMC), hydroxypropylcellulose (HPC), sucrose, gelatin and acacia. Additionally, lubricating agents - such as magnesium stearate, stearic acid, glyceryl behenate and talc may be included.

Solid compositions of a similar type may also be employed as fillers in gelatin capsules. Preferred excipients in this regard include lactose, starch, a cellulose, milk sugar or high molecular weight polyethylene glycols. For aqueous suspensions and/or elixirs, the modulator of the N-domain or C-domain of ACE protein may be combined with various sweetening or flavouring agents, colouring matter or dyes, with emulsifying and/or suspending agents and with diluents such as water, ethanol, propylene glycol and glycerin, and combinations thereof.

The routes for administration (delivery) may include, but are not limited to, one or more of oral (e.g. as a tablet, capsule, or as an ingestable solution), topical, mucosal (e.g. as a nasal spray or aerosol for inhalation), nasal, parenteral (e.g. by an injectable form), gastrointestinal, intraspinal, intraperitoneal, intramuscular, intravenous, intraventricular, intrauterine, intraocular, intradermal, intracranial, intratracheal, intravaginal, intracerebroventricular, intracerebral, subcutaneous, ophthalmic (including intravitreal or intracameral), transdermal, rectal, buccal, vaginal, epidural, sublingual.

Pharmaceutical compositions of the present invention may comprise a therapeutically effective amount of the N-domain of ACE protein, one or more modulators of the N-domain of ACE protein, one or more modulators of the C-domain of ACE protein or combinations thereof.

The pharmaceutical compositions may be for human or animal usage in human and veterinary medicine and will typically comprise any one or more of a pharmaceutically acceptable diluent, carrier, or excipient. Acceptable carriers or diluents for therapeutic use are well known in the pharmaceutical art, and are described, for example, in Remington's Pharmaceutical Sciences, Mack Publishing Co. (A. R. Gennaro edit. 1985). The choice of pharmaceutical carrier, excipient or diluent can be selected with regard to the intended route of administration and standard pharmaceutical practice. The pharmaceutical compositions may comprise as

- or in addition to - the carrier, excipient or diluent any suitable binder(s), lubricant(s), suspending agent(s), coating agent(s), solubilising agent(s).

Preservatives, stabilisers, dyes and even flavouring agents may be provided in the pharmaceutical composition. Examples of preservatives include sodium benzoate, sorbic acid and esters of p-hydroxybenzoic acid. Antioxidants and suspending agents may be also used.

There may be different composition/formulation requirements dependent on the different delivery systems. By way of example, the pharmaceutical composition of the present invention may be formulated to be administered using a mini-pump or by a mucosal route, for example, as a nasal spray or aerosol for inhalation or ingestable solution, or parenterally in which the composition is formulated by an injectable form, for delivery, by, for example, an intravenous, intramuscular or subcutaneous route. Alternatively, the formulation may be designed to be administered by a number of routes.

If the modulator of the N-domain or C-domain of ACE protein is to be administered mucosally through the gastrointestinal mucosa, it should be able to remain stable during transit though the gastrointestinal tract; for example, it should be resistant to proteolytic degradation, stable at acid pH and resistant to the detergent effects of bile.

Where appropriate, the pharmaceutical compositions may be administered by inhalation, in the form of a suppository or pessary, topically in the form of a lotion, solution, cream, ointment or dusting powder, by use of a skin patch, orally in the form of tablets containing excipients such as starch or lactose, or in capsules or ovules either alone or in admixture with excipients, or in the form of elixirs, solutions or suspensions containing flavouring or colouring agents, or the pharmaceutical compositions can be injected parenterally, for example intravenously, intramuscularly or subcutaneously. For parenteral administration, the compositions may be best used in the form of a sterile aqueous solution which may contain other substances, for example enough salts or monosaccharides to make the solution isotonic with blood. For buccal or sublingual administration the compositions may be administered in the form of tablets or lozenges which can be formulated in a conventional manner.

The modulators of the N-domain or C-domain of ACE protein may be used in combination with a cyclodextrin. Cyclodextrin molecules are known to form inclusion and non-inclusion complexes with drug molecules. Formation of a drug-cyclodextrin complex may modify the solubility, dissolution rate, bioavailability and/or stability property of a drug molecule. Drug-cyclodextrin complexes are generally useful for most dosage forms and administration routes. As an alternative to direct complexation with the drug the cyclodextrin may be used as an auxiliary additive, e.g. as a carrier, diluent or solubiliser. Alpha-, beta- and gamma-cyclodextrins are most commonly used and suitable examples are described in WO-A-91/11172, WO-A-94/02518 and WO-A-98/55148.

If the modulator of the N-domain or C-domain of ACE is a protein, then said protein modulator may be prepared *in situ* in the subject being treated. In this respect, nucleotide sequences encoding said protein may be delivered by use of non-viral techniques (e.g. by use of liposomes) and/or viral techniques (e.g. by use of retroviral vectors) such that the said protein is expressed from said nucleotide sequence.

DOSE LEVELS

Typically, a physician will determine the actual dosage which will be most suitable for an individual subject. The specific dose level and frequency of dosage for any particular patient may be varied and will depend upon a variety of factors including the activity of the specific compound employed, the metabolic stability and length of action of that compound, the age, body weight, general health, sex, diet, mode and time of administration, rate of excretion, drug combination, the severity of the particular condition, and the individual undergoing therapy.

The modulators of the N-domain of ACE protein or the C-domain of ACE protein may be administered separately, concomitantly or sequentially.

FORMULATION

The component(s) may be formulated into a pharmaceutical composition, such as by mixing with one or more of a suitable carrier, diluent or excipient, by using techniques that are known in the art.

VECTOR

Aspects of the present invention relate to a vector comprising a nucleotide sequence – such as a nucleotide sequence encoding the N-domain or the C-domain of ACE protein or a modulator of the N-domain or the C-domain of ACE protein - administered to a subject.

Preferably, the N-domain or the C-domain of ACE and/or the modulator are prepared and/or delivered using a genetic vector.

It is well known in the art, that a vector is a tool that allows or facilitates the transfer of information from one environment to another. In accordance with the present invention, and by way of example, some vectors used in recombinant DNA techniques allow entities, such as a segment of DNA (such as a heterologous DNA segment, such as a heterologous cDNA segment), to be transferred into a host and/or a target cell for the purpose of replicating the vectors comprising nucleotide sequences and/or expressing the proteins encoded by the nucleotide sequences. Examples of vectors used in recombinant DNA techniques include, but are not limited to, plasmids, chromosomes, artificial chromosomes or viruses.

The term "vector" includes expression vectors such as transfection vectors, transduction vectors or transformation vectors.

The term "expression vector" means a construct capable of *in vivo* or *in vitro/ex vivo* expression.

The terms “transfection vectors”, “transduction vectors” or “transformation vectors” describe different constructs capable of being transferred from one organism to another of from one species to another.

REGULATORY SEQUENCES

In some applications, nucleotide sequences are operably linked to a regulatory sequence which is capable of providing for the expression of the nucleotide sequence, such as by a chosen host cell. By way of example, a vector comprising the N-domain or the C-domain of ACE nucleotide sequence is operably linked to such a regulatory sequence i.e. the vector is an expression vector.

The term "operably linked" refers to a juxtaposition wherein the components described are in a relationship permitting them to function in their intended manner. A regulatory sequence "operably linked" to a coding sequence is ligated in such a way that expression of the coding sequence is achieved under conditions compatible with the control sequences.

The term “regulatory sequences” includes promoters and enhancers and other expression regulation signals.

The term "promoter" is used in the normal sense of the art, e.g. an RNA polymerase binding site.

Enhanced expression of a nucleotide sequence, for example, a nucleotide sequence encoding the N-domain or the C-domain of ACE protein - may also be achieved by the selection of heterologous regulatory regions, e.g. promoter, secretion leader and terminator regions, which serve to increase expression and, if desired, secretion levels of the protein of interest from the chosen expression host and/or to provide for the inducible control of the expression of the N-domain or the C-domain of ACE protein. In eukaryotes, polyadenylation sequences may be operably connected to the C-terminus of the nucleotide sequence of the N-domain or the C-domain of ACE protein.

Preferably, the N-domain or the C-domain of ACE protein nucleotide sequence is operably linked to at least a promoter.

Aside from the promoter native to the nucleotide sequence described herein, other promoters may be used to direct its expression. The promoter may be selected for its efficiency in directing the expression of the N-domain or the C-domain of ACE nucleotide sequence in the desired expression host.

In another embodiment, a constitutive promoter may be selected to direct the expression of the N-domain or the C-domain of ACE nucleotide sequence of the present invention. Such an expression construct may provide additional advantages since it circumvents the need to culture the expression hosts on a medium containing an inducing substrate.

Hybrid promoters may also be used to improve inducible regulation of the expression construct.

The promoter can additionally include features to ensure or to increase expression in a suitable host. For example, the features can be conserved regions such as a Pribnow-Box or a TATA box. The promoter may even contain other sequences to affect (such as to maintain, enhance, decrease) the levels of expression of the N-domain or C-domain of ACE nucleotide sequence. For example, suitable other sequences include the Sh1-intron or an ADH intron. Other sequences include inducible elements - such as temperature, chemical, light or stress inducible elements. Also, suitable elements to enhance transcription or translation may be present.

EXPRESSION VECTOR

Preferably, nucleotide sequences – such as nucleotide sequences encoding the N-domain or C-domain of ACE or modulators of the N-domain or C-domain of ACE - are inserted into a vector that is operably linked to a control sequence that is capable of providing for the expression of the coding sequence by the host cell.

Nucleotide sequences produced by a host recombinant cell may be secreted or may be contained intracellularly depending on the sequence and/or the vector used. As will be understood by those of skill in the art, expression vectors can be designed with

signal sequences, which direct secretion of the nucleotide sequence through a particular prokaryotic or eukaryotic cell membrane.

The expression vector may be pEE14 N-domain which encodes the N domain of human ACE and is truncated in the interdomain linker region.

Preferably, the expression vectors are stably expressed in CHO-K1 cells as described previously (Ehlers et al., (1996) *Biochemistry 35*, 9549-9559).

FUSION PROTEINS

The N-domain or C-domain of ACE protein or a modulator of the N-domain or C-domain of ACE protein may be expressed as a fusion protein to aid extraction and purification and/or delivery of the modulator of the N-domain or C-domain of ACE or the N-domain or C-domain of ACE protein to an individual and/or to facilitate the development of a screen for modulators of the N-domain or C-domain of ACE protein.

Examples of fusion protein partners include glutathione-S-transferase (GST), 6xHis, GAL4 (DNA binding and/or transcriptional activation domains) and β-galactosidase.

It may also be convenient to include a proteolytic cleavage site between the fusion protein partner and the protein sequence of interest to allow removal of fusion protein sequences. Preferably, the fusion protein will not hinder the activity of the protein of interest.

The fusion protein may comprise an antigen or an antigenic determinant fused to the substance of the present invention. In this embodiment, the fusion protein may be a non-naturally occurring fusion protein comprising a substance, which may act as an adjuvant in the sense of providing a generalised stimulation of the immune system. The antigen or antigenic determinant may be attached to either the amino or carboxy terminus of the substance.

ORGANISM

The term "organism" in relation to the present invention includes any organism that could comprise the N-domain or C-domain of ACE protein and/or modulators of the N-domain or C-domain of ACE protein. Examples of organisms may include mammals, fungi, yeast, plants or bacteria.

Preferably, the organism is as vertebrate or a mammal. More preferably, the organism is a human.

TRANSFORMATION

As indicated earlier, the host organism can be a prokaryotic or a eukaryotic organism. Examples of suitable prokaryotic hosts include *E. coli* and *Bacillus subtilis*. Teachings on the transformation of prokaryotic hosts are well documented in the art, for example see Sambrook et al., (Molecular Cloning: A Laboratory Manual, 2nd edition, 1989, Cold Spring Harbor Laboratory Press) and Ausubel *et al.*, Current Protocols in Molecular Biology (1995), John Wiley & Sons, Inc. Examples of suitable eukaryotic hosts include mammalian cells.

If a prokaryotic host is used then the nucleotide sequence – such as the N-domain of ACE nucleotide sequence - may need to be suitably modified before transformation - such as by removal of introns.

Thus, the present invention also relates to the transformation of a host cell with a nucleotide sequence – such as those coding for the N-domain or C-domain of ACE protein or a modulator of the N-domain or C-domain of ACE protein. Host cells transformed with the nucleotide sequence may be cultured under conditions suitable for the expression and recovery of the encoded protein from cell culture. The protein produced by a recombinant cell may be secreted or may be contained intracellularly depending on the sequence and/or the vector used. As will be understood by those of skill in the art, expression vectors containing coding sequences can be designed with signal sequences which direct secretion of the coding sequences through a particular prokaryotic or eukaryotic cell membrane. Other recombinant constructions may join

the coding sequence to nucleotide sequence encoding a polypeptide domain, which will facilitate purification of soluble proteins (Kroll DJ et al., (1993) *DNA Cell Biol* 12:441-53) e.g. 6-His or Glutathione-*S*-transferase.

TRANSFECTION

Vectors comprising for example, the nucleotide sequence coding for the N-domain or C-domain of ACE protein, may be introduced into host cells, for example, mammalian cells, using a variety of methods.

Typical transfection methods include electroporation, DNA biolistics, lipid-mediated transfection, compacted DNA-mediated transfection, liposomes, immunoliposomes, lipofectin, cationic agent-mediated, cationic facial amphiphiles (CFAs) (*Nature Biotech.* (1996) 14, 556), multivalent cations such as spermine, cationic lipids or polylysine, 1, 2,-bis (oleoyloxy)-3-(trimethylammonio) propane (DOTAP)-cholesterol complexes (Wolff and Trubetskoy (1998) *Nature Biotech.* 16, 421) and combinations thereof.

Uptake of nucleic acid constructs by mammalian cells is enhanced by several known transfection techniques for example those including the use of transfection agents. Example of these agents include cationic agents (for example calcium phosphate and DEAE-dextran) and lipofectants (for example lipofectam™ and transfectam™). Typically, nucleic acid constructs are mixed with the transfection agent to produce a composition.

Such methods are described in many standard laboratory manuals - such as Sambrook et al., Molecular Cloning: A Laboratory Manual, 2d ed. (1989) Cold Spring Harbor Laboratory Press, Cold Spring Harbor, N.Y.

GENERAL RECOMBINANT DNA METHODOLOGY TECHNIQUES

The present invention employs, unless otherwise indicated, conventional techniques of chemistry, molecular biology, microbiology, recombinant DNA and immunology, which are within the capabilities of a person of ordinary skill in the art. Such techniques are

explained in the literature. See, for example, J. Sambrook, E. F. Fritsch, and T. Maniatis, 1989, *Molecular Cloning: A Laboratory Manual*, Second Edition, Books 1-3, Cold Spring Harbor Laboratory Press; Ausubel, F. M. et al., (1995 and periodic supplements; *Current Protocols in Molecular Biology*, ch. 9, 13, and 16, John Wiley & Sons, New York, N.Y.); B. Roe, J. Crabtree, and A. Kahn, 1996, *DNA Isolation and Sequencing: Essential Techniques*, John Wiley & Sons; J. M. Polak and James O'D. McGee, 1990, *In Situ Hybridization: Principles and Practice*; Oxford University Press; M. J. Gait (Editor), 1984, *Oligonucleotide Synthesis: A Practical Approach*, Irl Press; and, D. M. J. Lilley and J. E. Dahlberg, 1992, *Methods of Enzymology: DNA Structure Part A: Synthesis and Physical Analysis of DNA* Methods in Enzymology, Academic Press. Each of these general texts is herein incorporated by reference.

DESCRIPTION OF THE DRAWINGS

Figure 1. (A) Overall structure of the N-domain with the zinc ion in green, the chloride ion in red and the oligosaccharides in pink. (B) Superposition of the N domain (turquoise) and tACE (pink) with the zinc ion in green. (C) Backbone coloured according to thermal vibration (B factor) with blue for the lowest B factors and red for the highest. (D) Surface diagram showing the lid (dark blue), *N*-linked glycans (green) and the protruding surface patch (pink) comprising the linker and the flexible loop.

Figure 2. (A) Model of the possible domain orientation of ACE. The N-terminus and C-terminal linker of two N-domains (grey) were overlapped and tACE (pink) superimposed. Sugars moieties visible in the N-domain and tACE structures are shown in green, and N-glycosylation sequons where no sugar was observed have been marked by a hypothetical sugar in yellow. The zinc ion in each domain is in green. (B) Close up of the N domain linker and flexible loop (grey). (C) Pink domain lid showing the residues that might be involved in the inter-domain interaction. Charged residues on the C-terminal lid are shown in red (negative) and blue (positive) with the sugar linked asparagine shown in green. Charged and sugar linked residues are marked by the same colours on the N-domain ACE, but their side chains are not visible in the structure.

Figures 3. (A) Close up of the active site of the N-domain ACE (blue with white residues) and tACE (pink with purple residues) with the zinc ion in green and the conserved chloride ion in red. Lisinopril is shown in white/purple and the differing residues between the N- and C-domains shown in ball and stick at the top of the picture. (B) Close up of the minimally glycosylated N-domain active site (blue) with a model of RXP407 (yellow) overlapping the water molecule (grey) adjacent to Tyr 369. Residues differing between the N- and C-domains in the S_2 subsite are also shown in ball and stick along with the conserved residues of the S_1 subsite that interact with lisinopril. Residues conserved between the N- and C- domains are shown in white, N-domain residues shown in blue and C-domain residues shown in pink. The zinc ion is shown in green.

Figure 4. Sequence alignment of the sACE N domain with tACE and ACE2. Helices are highlighted in yellow and strands in blue. The linker region is shown in pink. Helices are numbered sequentially whether α or 3_{10}, and 3_{10} helices are shown with red letters. Chloride I coordinating residues are boxed in dark blue, chloride II in black, and the zinc binding motif in red.

Table 1. Crystallographic Data

Table 2. Active site residues that differ between the N and C domains (C domain numbering is as for tACE).

Table A. Structure co-ordinates of N-domain of ACE protein.

Table B. Structure co-ordinates of N-domain of ACE protein complexed with lisinopril.

The invention will now be further described by way of Examples, which are meant to serve to assist one of ordinary skill in the art in carrying out the invention and are not intended in any way to limit the scope of the invention.

EXAMPLES

Example 1

Materials & Methods

Construction of Expression Vectors

An N-domain construct Leu 1-Asp 629 (D629) cloned into the vector pECE (a kind gift from Sergei Danilov) and encoding the first 629 residues of somatic ACE, was subcloned into pBlueScript using the restriction endonucleases *XbaI* and *EcoRI*. The fragment was then sequenced to verify that the correct fragment was cloned. D629 was then again subcloned into pcDNA3.1(+) using the same restriction enzymes. This N-domain construct was then introduced into the CHO cell glutamine synthetase (GS) expression vector pEE14 using the restriction endonucleases *HindIII* and *XbaI*. The identity of the construct and its correct orientation was confirmed via restriction enzyme digests and further sequencing. The new expression vector was termed pEE N-domain.

Cell Culture and Transfections

CHO-K1 cells were co-transfected with pEE14-N-domain and pSV2neo (10:1). Geneticin (G418) (Sigma) resistant clones expressing soluble N-domain were further selected for resistance to methionine sulfoximine (MSX) (Yu et al., 1997). Cells stably expressing the N-domain were grown in Glasgow Minimum Essential Medium (GMEM) supplemented with 10% dialysed foetal calf serum (Gibco BRL) and 20µM MSX. When confluent growth medium was changed to 1% dialysed FCS, 0.05% albumax I (Gibco BRL), 20µM MSX and 1.5mM N-butyldeoxynojirimycin (NB-DNJ) (Toronto Research Chemicals Inc.B691000 Lot 14-EG-91-1 and B691000 12-Cf-146-2).

Construct purification

Medium containing recombinantly expressed soluble N-domain (N-domain of ACE protein) was harvested and purified in tandem over a protein-G Agarose (Sigma) column followed by an N-domain specific monoclonal antibody (5C5) protein G Agarose column. N-domain was eluted with 50mM ethanolamine pH 11.5. The eluted solution was then dialysed against 5mM HEPES pH 7.5, 0.1mM PMSF and

concentrated in a 30kDa Amicon concentrator at 1000-2000 *g* and 4°C to a concentration of 10mg/ml, and stored at 4°C.

Western Blot Analysis

The N-domain of ACE protein was detected and its purity assessed by Western Blot analysis using 10% SDS-PAGE and transferred on nitrocellulose membrane (Hybond-C, Amersham). The membrane is probed with N-domain specific monoclonal antibody (5C5) and developed with using the ECP chemiluminescent kit (Amersham) and visualised on autoradiographic film according to the manufacturer's instructions.

Crystallisation and X-ray diffraction data collection

1µl of the purified N-domain of ACE protein at 4mg/ml was mixed with 1µl reservoir solution (0.2M lithium sulphate, 0.1M sodium acetate; pH 4.9, 10µM zinc sulphate, 15% polyethylene glycol 4000) and suspended above the reservoir as a hanging drop at 16°C. Crystals grew within 1-2 weeks.

A single crystal was cryocooled (100 K) using reservoir solution plus 25% glycerol as a cryoprotectant. Diffraction data to 3.0 Å were collected on station PX14.1 of the synchrotron radiation source (Daresbury, U.K.) using a Quantum 4 charge-coupled-device detector (Area Detection Systems, Poway, CA). The data were processed and scaled by using the HKL2000 software package (HKL Research, Charlottesville, VA) (Otwinowski, W. Oscillation data reduction program. in *Proceedings of the CCP4 weekend* 56-62 (Daresbury Laboratory, Warrington, UK, 1993). The symmetry and systematic absences were consistent with the $C222_1$ space group (unit cell dimensions, a = 101.12 Å; b = 211.32 Å; and c = 171.27 Å) with two proteins per asymmetric unit. The crystals contained ~54% solvent. Data reduction was carried out by using the CCP4 program TRUNCATE (CCP4. The CCP4 suite: Programs for protein crystallography. *Acta Crystallogr.* **D50**, 760-763 (1994)).

The structure of the N-domain was solved with the program MOLREP (Vagin, A. & Teplyakov, A. An approach to multi-copy search in molecular replacement. *Acta Crystallogr.* **D56**, 1622-1624 (2000)) using a homology model of the N-domain based on the tACE structure (protein data bank entry 1O8A) as a search model. Initial

refinement was performed using REFMAC Murshudov, G.N. Refinement of macromolecular structures by the maximum-likelihood method. *Acta Crystallogr.* **D53**, 240-255 (1997) through the CCP4i interface (CCP4. The CCP4 suite: Programs for protein crystallography. *Acta Crystallogr.* **D50**, 760-763 (1994)). 4% of reflections was kept aside for *R*free calculation (Brünger, A.T. Free *R* value: a novel statistical quantity for assessing the accuracy of crystal structures. *Nature* **355**, 472-475 (1992)). A large part of the C terminal region not present in the tACE structure could be built after the first round of refinement using the program Coot (Emsley, P. & Cowtan, K. Coot: Model building tools for molecular graphics. *Acta Crystallogr.* **60**, 2126-2132 (2004)). Further rounds of refinement and model building allowed the building of the N terminus and the addition of water, carbohydrate and glycerol molecules plus an acetate ion. Final refinement was done using the CNS suite (Brünger, A.T. *et al.* Crystallography & NMR system: A new software suite for macromolecular structure determination. *Acta Crystallogr.* **D54**, 905-921 (1998)).

Sequence alignment of the sACE N domain with tACE and ACE2 is shown in Figure 4.

The N-domain/lisinopril inhibitor complex - 4mg/ml of purified N-domain was incubated with 5mM lisinopril for 5 hours at 4°C. 1µl N-domain with lisinopril was mixed with 1µl reservoir solution (0.2M lithium sulphate, 0.1M sodium acetate, pH 4.9, 10µM zinc sulphate, 18% polyethylene glycol 4000) and suspended above the reservoir as a hanging drop at 16°C. Crystals grew within 1-2 weeks in the same form as the minimally glycosylated N-domain of ACE protein. Single crystal consistent with the $C222_1$ space group (unit cell dimensions, a = 101.32 Å; b = 211.90 Å; and c = 171.03 Å). Diffraction data to 2.8 Å were collected as for the minimally glycosylated N-domain data set. The data were processed with MOSFLM (Leslie, A.G.W. Recent changes to the MOSFLM package for processing film and image plate data. *Joint CCP4+ESF-EAMCB Newsletter on Protein Crystallography* **26**(1992)), scaled with SCALA (CCP4. The CCP4 suite: Programs for protein crystallography. *Acta Crystallogr.* **D50**, 760-763 (1994)) and data reduction carried out by TRUNCATE (CCP4. The CCP4 suite: Programs for protein crystallography. *Acta Crystallogr.* **D50**, 760-763 (1994)).

Refinement (with 2.3% of the reflection kept for the *R*free calculation) of the minimally glycosylated N-domain structure with the CNS suite (Brünger, A.T. *et al.* Crystallography & NMR system: A new software suite for macromolecular structure determination. *Acta Crystallogr.* **D54**, 905-921 (1998)) showed clear difference density for the lisinopril, which was modelled with the program Coot (Emsley, P. & Cowtan, K. Coot: Model building tools for molecular graphics. *Acta Crystallogr.* **60**, 2126-2132 (2004)), along with a few water, carbohydrate, glycerol molecules and an acetate ion.

The atomic coordinates have been deposited with the Protein Data Bank, www.rcsb.org, and the accession codes are 2C6F and 2C6N for the minimally glycosylated and lisinopril complexes for sACE N-domain respectively..

All crystals are isomorphous.

Example 2

Overall structure of the N-domain

The N-domain was crystallised with two molecules per asymmetric unit. The overall fold consists of a mainly helical secondary structure, with the same topology as tACE. The N-domain has the ellipsoid shape with a central groove dividing it into two subdomains, one containing the N-terminal lid that covers the central binding cavity. There are 27 helices, of which 18 of them are α helices, 5 are short 3 helices and 4 are mixed (Woodman, Z.L. et al., The N domain of somatic angiotensin-converting enzyme negatively regulates ectodomain shedding and catalytic activity. *Biochem J.* **389**, 739-744 (2005)). There are also 6 short β-strands. The structures of both molecules in the asymmetric are very similar with a root mean square deviation for the Cα atoms of 0.50Å. Analysis of the Ramachandran plot using the program PROCHECK shows that 94% of the residues lie in the most favoured region, with none in the disallowed region (Laskowski, R.A., MacArthur, M.W., Moss, D.S. & Thronton, J.M. PROCHECK -A program to check the stereochemical quality of protein structures. *J. Appl. Crystallogr.* **26**, 283-291 (1993)). Both termini are well

ordered with all the residues (1-612) being modelled for molecule A and only the N-terminal residue missing in molecule B.

The catalytic zinc ion was observed at the active site and one chloride, equivalent to chloride 2 of tACE, adjacent to Arg500. There are ten putative N-glycosylation sites on the human N-domain protein and Fourier difference density was observed at five of these sites in our structure (Figure 1(A)). Seven N-acetyl glucosamine residues were modelled on molecule A at asparagines 25, 45, 117, 289 and 480, and six on molecule B at residues 25, 45, 117 and 480. A mannose residue was also modelled on both molecules at the end of the disaccharide at Asn25. Although the B-factors for these sugars are high, they are modelled on the basis of clear difference density, at least for the ring portions. Twentyfive water molecules were modelled by visual inspection and a glycerol molecule was modelled on the surface of each molecule adjacent to Glu219. Three acetate molecules were also modelled, one on the surface next to the symmetry axis and one in each of the active sites adjacent to Lys489, where a carboxyalanine was modelled in the tACE structure (Natesh, R., Schwager, S.L.U., Sturrock, E.D. & Acharya, K.R. Crystal structure of the human angiotensin-converting enzyme-lisinopril complex. *Nature* **421**, 551-554 (2003)). We attempted to model N-carboxyalanine at this position however the density was smaller in the N domain structure.

The N-domain protein was also crystallised in the presence of 5mM lisinopril, for which clear difference density was observed upon refinement with the minimally glycosylated N-domain structure. The overall structure is as the minimally glycosylated N-domain, although the lack of completeness in the data results in poorly defined density for the first 30 residues of the N-terminus. The lisinopril is bound at the active site in the same position and conformation as observed for tACE (Natesh, R., Schwager, S.L.U., Sturrock, E.D. & Acharya, K.R. Crystal structure of the human angiotensin-converting enzyme-lisinopril complex. *Nature* **421**, 551-554 (2003)). Four N-acetyl glucosamine residues each were modelled on both molecules at asparagines 25, 117, and 480. Nineteen water molecules, two glycerols and one acetate ion were modelled. The acetate ion was modelled near the symmetry axis and the two the glycerols at equivalent surface positions on the two molecules, similar to as observed in the minimally glycosylated structure.

Comparison of the N and C domains

The N- and C- domains of somatic ACE have ~60% sequence identity and hence share the same overall topology as well as the highly conserved zinc binding motif at the active site (see figure x which will be a sequence alignment). The most easily observable difference between the N- and C- domains (based on tACE) when superimposed (Figure 1(B)) is the extra length of the N- domain at the N- terminus and the C terminus, which includes the inter-domain linker. The N-terminus of the N domain protein, whilst having higher than average B factors, is well defined and packs against helix 3. Also, the loop between helices 19 and 20 (residues 409-417) that was not visible in the tACE structure, is well defined. Three other flexible loops, between helices 3 and 4, strands 1 and 2 and strand 6 and helix 23, show small differences between the domains.

The N-domain has been observed to be activated at lower chloride concentrations and to a lesser extent than the C-domain (Wei, L., Clauser, E., Alhenc-Gelas, F. & Corvol, P. The two homologous domains of human angiotensin I-converting enzyme interact differently with competitive inhibitors. *J. Biol. Chem.* **267**, 13389-13405 (1992)). Consistent with this is the observation of only one chloride bound to the N domain, rather than the two observed for tACE. The chloride ion is observed at the identical site as chloride II in tACE, bound between Tyr 202 and Arg 500. At the equivalent position to the tACE chloride I site, a crucial arginine is substituted by a histidine in the N-domain. Interestingly, ACE2, which was also only observed to bind one chloride ion in the crystal structure, binds chloride in the equivalent position to chloride I in tACE.

The domain arrangement of sACE

The complex kinetics of the somatic ACE catalysis is partly due to the presence of an active site in both the N and C domains and also the potential for interaction between them. The N-and C-domains of sACE are joined by a linker that is susceptible to proteolysis and is assumed to be partly flexible (Sturrock, E.D., Danilov, S.M. & Riordan, J.F. Limited proteolysis of human kidney angiotensin-converting enzyme and generation of catalytically active N- and C-terminal domains. *Biochem. Biophys. Res. Com.* **236**, 16-19 (1997)). The inclusion of the linker in the N-domain construct

allowed us to visualise this region for the first time. The majority of the linker (residues 602-612) was well defined in the electron density map after the first couple of rounds of refinement and was built into the model without ambiguity. The first part of the linker appears to be rigid in our model and is held in place by a hydrogen bond between Tyr607 and Glu161. The last four residues are more flexible as they have high B factors and their side chains are not visible (Fig 1(C)). They form a prominent surface patch, away from the core of the N domain, with a very flexible loop that is anchored by the disulphide bond between Cys128 and Cys136 (Fig 1(C)-(D)). Although this flexible loop is on the symmetry axis, neither its nor the linker's conformation appear to be involved in any crystal packing interactions. Hence it is most likely that the N-terminus of the C-domain would interact with this patch, and that it could adapt its conformation to one or more arrangements.

There is some evidence that only one domain of sACE is capable of catalysis at one time and that the N-domain may be a negative regulator of the C domain Andújar-Sánchez, M., Cámara-Artigas, A. & Jara-Pérez, V. A calorimetric study of the binding of lisinopril, enalaprilat and captopril to angiotensin-converting enzyme. *Biophys. Chem.* **111**, 183-189 (2004); Binevski, P.V., Sizova, E.A., Pozdnev, V.F. & Kost, O.A. Evidence for the negative cooperativity of the two active sites within bovine somatic angiotensin-converting enzyme. *FEBS Lett.* **550**, 84-88 (2003); Woodman, Z.L. et al., The N domain of somatic angiotensin-converting enzyme negatively regulates ectodomain shedding and catalytic activity. *Biochem J.* **389**, 739-744 (2005)). As the flexible region of the linker appears to be short, then it suggests that the N- domain would interact with the N-terminal lid region of the C- domain. The lid region comprise the three (largest) N terminal α-helices in both the N- and C-domains that partly covers the substrate channel (Natesh, R., Schwager, S.L.U., Sturrock, E.D. & Acharya, K.R. Crystal structure of the human angiotensin-converting enzyme-lisinopril complex. *Nature* **421**, 551-554 (2003)). It is thought that a change in conformation of the lid may be necessary for entry of the substrate and might also contribute to the substrate specificity of the domains. The interaction of the N-domain with the C-domain lid might reduce the flexibility of this region to regulate the entry of substrate to the C-domain active site or even to form a surface that partially blocked the cavity opening. By contrast, the position of the linker ensures

that the C-domain is unlikely to interact with the lid region of the N-domain, although it could block the product channel.

The specific interactions between the domains are not obvious, however, particularly as the terminal three residues of the linker are not available in our structure. Furthermore, several side chains on the linker and the flexible loop, which one might assume to play a part in the interaction, are disordered and not visible. We know from the sequence, however, that the flexible loop contains a positively charged lysine, and the linker, three negatively charged residues. These may interact with some of the charged residues protruding from the C-domain lid. The N- and C-domain lids have a different shape, size (due to the extra N-terminal residues) and charge distribution. These differences have been suggested to have a link to the substrate specificity of the two domains, but it seems likely that the shape and charge of the C-domain lid will also influence its interaction with the N-domain linker.

Based on this analysis, and the conformation of the linker, we propose a tentative domain arrangement for sACE. We suggest that the inter-domain linker could pack against the lid of the C-domain, in a similar manner to how the extra N terminal residues of the N domain, pack against the N domain lid. To visualise this, two N domains were overlapped with the N-terminus of one overlaying the linker of the other (allowing for the missing 3 residues), and then the C-domain (using tACE) was superimposed (Fig 2(A)). The initial arrangement caused the C-domain to overlap the flexible loop, suggesting that this loop might mould to the C-domain. Allowing free rotation around the linker produced a model from which it was easier to observe the residues that could be involved in the interaction. Figure 2(B) shows the charged residues on the N- and C-domains which may help form interactions between them. To complicate matters further, though, there is an N-glycosylation sequon on the flexible loop of the N-domain and the top part of the C-domain lid (Fig 2(A)), suggesting that inter-domain interactions and movements may be mediated or aided by sugars.

Binding of Lisinopril and specificity

The lisinopril bound to the active site was clearly defined, despite the poor electron density map in some other regions of the structure. The binding followed the same

orientation as observed for tACE with the central carboxylate coordinating the zinc ion and the phenyl group pointing up towards the lid. The active site residues and the lisinopril molecules for the two structures superimpose well (r.m.s. deviation for Cα atoms, 0.31Å) with nearly all the lisinopril binding residues conserved in the N-domain. tACE Glu 162, which interacts electrostatically with the amine on the lysyl side chain, is replaced by Asp 140 in the N-domain away from the P1' group (Fig 3(A)). Asp 377 of tACE, which forms water mediated interactions with the lysyl group, is also not conserved in the N domain and is replaced by Gln355. Gln355 could potentially form a hydrogen bond with the lysyl group of lisinopril, although this does not appear to be the case in our structure as it is about 4Å away. However, it might form water mediated interactions, but water molecules were not visible due to limited resolution of our structure

A burgeoning area in the field of ACE inhibitor design is the generation of domain specific inhibitors to more precisely regulate the actions of the N- and C-domains of sACE. The structures of two new inhibitors have been published, RXP407 and RXPA380, which are highly specific for the N and C domains, respectively. The structural determinants of RXP470 are known to be the N-terminal aspartate and N-acetyl groups in the P_2 position and the C-terminal amide.

The difference in phosphinic peptides at the P_2 position utilises the differences in the N- and C-domain active site at the S_2 subsite (Table 2). RXPA380 has a large hydrophobic phenyl group at this position, whereas the N-domain specific RXP407 has a charged aspartate residue and an N-terminus acetyl group. This corresponds to the exchange of a phenylalanine residue in the C-domain to Tyr 369 in the N domain. It is probable that the RXPA380 phenyl residue would form a stacking interaction with the Phe391 of tACE, whereas the aspartate or carbonyl (if the aspartate group forms electrostatic interactions with Arg500) of RXP407 would interact with the hydroxyl group of Tyr369 in the N-domain. Interestingly, in both the minimally glycosylated and lisinopril-bound N-domain structure, a patch of difference density was observed adjacent to Tyr369. This was modelled as a water molecule in the minimally glycosylated structure and a cluster of 2-3 water molecules in the lisinopril-bound structure as it was not possible to tell if it was a larger ligand, e.g. from the

crystallisation solution, at this resolution. It is possible that these water molecules in some way mimic the interactions the N-domain would have with extended inhibitors such as RXP407. Indeed, RXP407 can be modelled to make a similar interaction with Tyr369 (Fig 3(B)).

In our structure of the N-domain protein, the triad of residues (Gln259, Lys489, Tyr498), which interact with the carboxyl group of lisinopril, are best placed to interact with the C terminal amide. However, this triad in conserved in the C-domain and the residues that differ between the N- and C-domains are all located further down the cavity. These include Ser357 and Thr358 (both valine in the C-domain) and a patch of acidic residues (Fig 3b). Although the C-domain also has a patch of 2, rather than 3 acidic residues, they are either different in length or position (Table 2). These residues adopt random conformations in our structure, which lack partner/s in the S_2 subsite for them to interact with, but could possibly extend towards the active site and interact in the presence of RXP407. Although the resolution of our structure hinders a more detailed analysis of the active site, the structural details presented here will aid future rational design of domain-specific ACE inhibitors.

In a further aspect, the present invention relates to a composition comprising the N-domain of ACE protein in a crystalline form.

In a further aspect, the present invention relates to a scalable 3D model of the N-domain of ACE protein having at least a portion of the structural co-ordinates set forth in Table A or Table B.

All publications mentioned in the above specification are herein incorporated by reference. Various modifications and variations of the described methods and system of the invention will be apparent to those skilled in the art without departing from the scope and spirit of the invention. Although the invention has been described in connection with specific preferred embodiments, it should be understood that the invention as claimed should not be unduly limited to such specific embodiments. Indeed, various modifications of the described modes for carrying out the invention which are obvious to those skilled in molecular biology or related fields are intended to be within the scope of the following claims.

REFERENCES 1

1. Beldent, V., Michaud, A., Wei, L., Chauvet, M.T., and Corvol, P. (1993) J. Biol. Chem. 268, 26428-26434.

2. Schwager, S.L.U., Chubb, A.J., Scholle, R.R., Brandt, W.F., Riordan, J.F., Mentele, R., Sturrock, E.D and Ehlers, M.R.W. (1999) *Biochemistry 38*, 10388-10397.

3. Schwager, S.L.U., Chubb, A.J., Woodman, Z.L., Yan, L., Mentele, R., Ehlers, M.R.W., and Sturrock, E.D. (2001) *Biochemistry 40*, 15624-15630.

4. Yu, X. C., Sturrock, E. D., Wu, Z., Biemann, K., Ehlers, M. R. W., and Riordan, J. F. (1997) *J. Biol. Chem. 272*, 3511-3519.

5. Sturrock, E. D., Yu, X. C., Wu, Z., Biemann, K., and Riordan, J. F. (1996) *Biochemistry 35*, 9560-9566.

REFERENCES 2

1a. Junot, C., Gonzales, M. F., Ezan, E., Cotton, J., Vazeux, G., Michaud, A., Azizi, M., Vassiliou, S., Yiotakis, A., Corvol, P., and Dive, V. (2001) *J. Pharmacol. Exp. Ther. 297*, 606-611.

2a. Esther, C. R., Marino, E. M., Howard, T. E., Machaud, A., Corvol, P., Capecchi, M. R., and Bernstein, K. E. (1997) *J. Clin. Invest 99*, 2375-2385.

3a. Sadhukhan, R. and Sen, I. (1996) *J. Biol. Chem. 271*, 6429-6434.

4a. Kumar, R. S., Kusari, J., Roy, S. N., Soffer, R. L., and Sen, G. C. (1989) *J. Biol. Chem. 264*, 16754-16758.

5a. Kasturi, S., Jabbar, M. A., Sen, G. C., and Sen, I. (1994) *Biochemistry 33*, 6228-6234.

6a. Ehlers, M. R., Chen, Y. N., and Riordan, J. F. (1992) *Biochem. Biophys. Res. Commun. 183*, 199-205.

7a. Yu, X. C., Sturrock, E. D., Wu, Z., Biemann, K., Ehlers, M. R., and Riordan, J. F. (1997) *J. Biol. Chem. 272*, 3511-3519.

8a. Ehlers, M. R., Schwager, S. L., Scholle, R. R., Manji, G. A., Brandt, W. F., and Riordan, J. F. (1996) *Biochemistry 35*, 9549-9559.

9a. Schwager, S. L., Chubb, A. J., Scholle, R. R., Brandt, W. F., Eckerskorn, C., Sturrock, E. D., and Ehlers, M. R. (1998) *Biochemistry 37*, 15449-15456.

10a. Wei, L., Alhenc-Gelas, F., Corvol, P., and Clauser, E. (1991) *J. Biol. Chem. 266*, 9002-9008.

11a. Nachon, F., Nicolet, Y., Viguie, N., Masson, P., Fontecilla-Camps, J. C., and Lockridge, O. (2002) *Eur. J. Biochem. 269*, 630-637.

12a. Couvineau, A., Fabre, C., Gaudin, P., Maoret, J. J., and Laburthe, M. (1996) *Biochemistry 35*, 1745-1752.

13a. Zhou, A. T., Assil, I., and Abou-Samra, A. B. (2000) *Biochemistry 39*, 6514-6520.

14a. Schwager, S. L., Chubb, A. J., Scholle, R. R., Brandt, W. F., Mentele, R., Riordan, J. F., Sturrock, E. D., and Ehlers, M. R. (1999) *Biochemistry 38*, 10388-10397.

15a. Davis, S. J., Davies, E. A., Barclay, A. N., Daenke, S., Bodian, D. L., Jones, E. Y., Stuart, D. I., Butters, T. D., Dwek, R. A., and van der Merwe, P. A. (1995) *J. Biol. Chem. 270*, 369-375.

16a. Wheeler, S. F., Rudd, P. M., Davis, S. J., Dwek, R. A., and Harvey, D. J. (2002) *Glycobiology 12*, 261-271.

REFERENCES 3

Abrahams, J. P. & Leslie, A. G. W. Methods used in structure determination of bovine mitochondrial F1 ATPase. *Acta Crystallogr. D* **52**, 110-119 (1996).

Brünger, A. T. Free R value: a novel statistical quantity for assessing the accuracy of crystal structure. *Nature* 355, 472-475 (1992).

Brünger, A. T. et al. Crystallography & NMR System: A new software suite for macromolecular structure determination. *Acta Crystallogr. D* 54, 905-921 (1998).

Chubb A. J. Schwager S.L.U., Woodman Z.L., Ehlers, M.R.E., and Sturrock E.D. Defining the ectodomain of angiotensin-converting enzyme. *Biochem. Biophys. Res. Comm.*(2002) in press.

Collaborative computational project Number 4. The CCP4 Suite: Programs for Protein Crystallography. *Acta Crystallogr. D* 50, 760-763 (1994).

Corval, P., Williams, T. A. & Soubrier, F. Peptidyl dipeptidase.A: angiotensin I-converting enzyme. *Methods Enzymol.* **248**, 283-305 (1995).

Cushman, D. W., Cheung, H. S., Sabo, E. F. & Ondetti, M. A. Design of potent competitive inhibitors of angiotensin-converting enzyme. Carboxyalkanoyl and mercaptoalkanoyl amino-acids. *Biochemistry*, 16, 5484-5491 (1977).

De La Fortelle, E. & Bricogne, G. Maximum-likelihood heavy-atom parameters refinement in the MIR and MAD methods. *Methods Enzymol.* 276, 472-494 (1997).

Holm, L. & Sander, C. Protein folds and families: sequence and structure alignments. *Nucleic Acid Res.* 27, 244-247 (1999).

Hooper, N. M. Families of zinc metalloproteases. *FEBS Lett.* 354, 1-6 (1994).

Jones, T. A., Zou, J. Y., Cowan, S. W. & Kjeldgaard, M. Improved methods for building protein models in electron density maps and the location of errors in these models. *Acta Crystallogr. A* 47, 110-119 (1991).

Kraulis, P. MOLSCRIPT: a program to produce both detailed and schematic plots of protein structures. *J. Appl. Crystallogr.* 24, 946-950 (1991).

Liu, X., Fernandez, M., Wouters, M. A., Heyberger, S. & Husain, A. Arg-1098 is critical for the chloride dependence of human angiotensin-1 converting enzyme C-domain catalytic activity. *J. Biol. Chem.* 276, 33518-33525 (2001).

Merritt, E. A. & Bacon, D. J. Raster 3D:photorealistic molecular graphics. *Methods Enzymol.* 277, 505-524 (1997).

Otwinowski, M. & Minor, W. Processing of X-ray diffraction data collected in oscillation mode. *Methods Enzymol* 276, 307-326 (1997).

Rawlings, N. D. & Barrett, A. J. Evolutionary families of metallopeptidases. *Methods Enzymol.* 248, 182-228 (1995).

Waller, C. L. & Marshall, G. R. Three-dimensional quantitative structure-activity relationship of angiotesin-converting enzyme and thermolysin inhibitors. II. A comparison of CoMFA models incorporating molecular orbital fields and desolvation free energies based on active-analog and complementary-receptor-field alignment rules. *J. Med. Chem.* 36, 2390-2403 (1993).

Wei, L., Alhenc-Gelas, F., Corvol, P. & Clauser, E. The two homologous domains of human angiotensin-1 converting enzyme are both catalytically active. *J. Biol. Chem.* 266, 9002-9008 (1991).

Williams, T. A., Corvol, O. & Soubrier, F. Identification of two active site residues in human angiotensin I- converting enzyme. *J. Biol. Chem.* 269, 29430-29434 (1994).

REFERENCES 4

Natesh, R., Schwager, S.L.U., Sturrock, E.D. & Acharya, K.R. Crystal structure of the human angiotensin-converting enzyme-lisinopril complex. *Nature* **421**, 551-554 (2003).

Ehlers, M.R.W. & Riordan, J.F. Angiotensin-converting enzyme: Zinc- and inhibitor-binding stoichiometries of the somatic and testis enzymes. *Biochemistry* **30**, 7118-7125 (1991).

Fuchs, S. et al. Role of the N-terminal catalytic domain of ACE investigated by targeted inactivation in mice. *J. Biol. Chem.* **279**, 15946-15953 (2004).

Azizi, M. et al. Acute angiotensin-converting enzyme inhibition increases the plasma level of the natural stem cell regulator N-acetyl-serly-aspartyl-lysyl-proline. *J. Clin. Invest.* **97**, 839-844 (1996).

Rousseau, A., Michaud, A., Chauvet, M.T., Lenfant, M. & Corvol, P. The hemoregulatory peptide N-acetyl-Ser-Asp-Lys-Pro is a natural and specific substrate of the N-terminal active site of human angiotensin-converting enzyme. *J. Biol. Chem.* **270**, 3656-3661 (1995).

Wei, L., Clauser, E., Alhenc-Gelas, F. & Corvol, P. The two homologous domains of human angiotensin I-converting enzyme interact differently with competitive inhibitors. *J. Biol. Chem.* **267**, 13389-13405 (1992).

Jaspard, E., Wei, L. & Alhenc-Gelas, F. Differences in the properties and enzymatic specificities of the two active sites of the two active sites of angiotensin I-converting enzyme (kininase II). studies with bradykinin and other natural peptides. *J. Biol. Chem.* **268**, 9496-9503 (1993).

Andújar-Sánchez, M., Cámara-Artigas, A. & Jara-Pérez, V. A calorimetric study of the binding of lisinopril, enalaprilat and captopril to angiotensin-converting enzyme. *Biophys. Chem.* **111**, 183-189 (2004).

Binevski, P.V., Sizova, E.A., Pozdnev, V.F. & Kost, O.A. Evidence for the negative cooperativity of the two active sites within bovine somatic angiotensin-converting enzyme. *FEBS Lett.* **550**, 84-88 (2003).

Woodman, Z.L. et al. The N domain of somatic angiotensin-converting enzyme negatively regulates ectodomain shedding and catalytic activity. *Biochem J.* **389**, 739-744 (2005).

Pang, S. et al. Roles of the juxtamembrane and extracellular domains of angiotensin-converting enzyme in ectodomain shedding. *Biochem J.* **358**, 185-192 (2001).

Sturrock, E.D., Danilov, S.M. & Riordan, J.F. Limited proteolysis of human kidney angiotensin-converting enzyme and generation of catalytically active N- and C-terminal domains. *Biochem. Biophys. Res. Com.* **236**, 16-19 (1997).

Voronov, S., Zueva, N., Orlov, V., Arutyunyan, A. & Kost, O. Temperature-induces selective death of the C-domain within angiotensin-converting enzyme molecule. *FEBS Lett.* **522**, 77-82 (2002).

Hagaman, J.R. *et al.* Angiotensin-converting enzyme and male fertility. *Proc. Natl. Acad. Sci. U.S.A.* **95**, 2552-2557 (1998).

Kondoh, G. *et al.* Angiotensin-converting enzyme is a GPI-anchored protein releasing factor crucial for fertilisation. *Nat. Med.* **11**, 160-166 (2005).

Natesh, R., Schwager, S.L.U., Evans, H.R., Sturrock, E.D. & Acharya, K.R. Structural details on the binding of antihypertensive drugs captopril and enalaprilat to human testicular angiotensin I-converting enzyme. *Biochemistry* **43**, 8718-8724 (2004).

Kim, H.M., Shin, D.R., Yoo, O.J., Lee, H. & Lee, J.O. Crystal structure of Drosophila angiotensin I-converting enzyme bound to captopril and lisinopril. *FEBS Lett.* **538**, 65-70 (2003).

Towler, P. *et al.* ACE2 structures reveal a large hinge-bending motion important for inhibitor binding and catalysis. *J. Biol. Chem.* **279**, 17996-18007 (2004).

Otwinowski, W. Oscillation data reduction program. in *Proceedings of the CCP4 weekend* 56-62 (Daresbury Laboratory, Warrington, UK, 1993).

CCP4. The CCP4 suite : Programs for protein crystallography. *Acta Crystallogr.* **D50**, 760-763 (1994).

Vagin, A. & Teplyakov, A. An approach to multi-copy search in molecular replacement. *Acta Crystallogr.* **D56**, 1622-1624 (2000).

Murshudov, G.N. Refinement of macromolecular structures by the maximum-likelihood method. *Acta Crystallogr.* **D53**, 240-255 (1997).

Brünger, A.T. Free *R* value: a novel statistical quantity for assessing the accuracy of crystal structures. *Nature* **355**, 472-475 (1992).

Emsley, P. & Cowtan, K. Coot: Model building tools for molecular graphics. *Acta Crystallogr.* **60**, 2126-2132 (2004).

Brünger, A.T. *et al.* Crystallography & NMR system: A new software suite for macromolecular structure determination. *Acta Crystallogr.* **D54**, 905-921 (1998).

Leslie, A.G.W. Recent changes to the MOSFLM package for processing film and image plate data. *Joint CCP4+ESF-EAMCB Newsletter on Protein Crystallography* **26**(1992).

Laskowski, R.A., MacArthur, M.W., Moss, D.S. & Thronton, J.M. PROCHECK -A program to check the stereochemical quality of protein structures. *J. Appl. Crystallogr.* **26**, 283-291 (1993).

Kost, O.A. *et al.* Epitope-dependent blocking of the angiotensin-converting enzyme dimerization by monoclonal antibodies to the N-terminal domain of ACE: possible

link of ACE dimerization and shedding from the cell surface. *Biochemistry* **42**, 6965-6976 (2003).

Balyasnikova, I.V. *et al.* Localization of an N-domain region of angiotensin-converting enzyme involved in the regulation of ectodomain shedding using monoclonal antibodies. *J. Proteome. Res.* **4**, 258-267 (2005).

Danilov, S.M. *et al.* Structure-function analysis of angiotensin I-converting enzyme using monoclonal antibodies. *J. Biol. Chem.* **269**, 26806-26814 (1994).

TABLE 1.

Crystallographic Data

	Native	Lisinopril complex
Resolution range, Å	48.5-3.0	50-2.8
No. of reflections measured	70398	160032
No. of unique reflections	36858	40318
I/□(*I*) (outer shell*)	9.0 (2.2)	9.2 (1.3)
Completeness (outer shell*), %	99.8 (99.7)	89.0 (57.3)
*R*symm (outer shell*), %	14.1 (59.5)	12.6 (52.8)
*R*cryst, %	22.5	*29.8*
*R*free, %	27.4	31.4
Average temperature factor Å^2		
Protein (mol A / mol B)	35.4 / 38.5	39.3 / 40.2
Carbohydrate (mol A / mol B)	71.8 / 74.6	71.8 / 69.8
Ligand		48.8 / 43.2
Solvent [no. of water molecules]	24.5 [25]	18.3 [16]
Zn^{2+} ion / Cl^{2-} ion	31.6 / 40.1	39.3/35.3
RMSD from ideal values		
Bond lengths, Å	0.02	0.017
Bond angles, °	1.7	2.4

RMSD, root-mean-square deviation.

Outer shell, 3.11-3.00 Å and 2.95-2.8 Å for the native data and lisinopril complex respectively.

*R*free calculation used 4% and 2.3% of the reflections for the native data and lisinopril complex respectively.

TABLE 2.

Active site residues that differ between the N and C domains (C domain numbering is as for tACE).

S_1	**tACE/Cdomain**	V518							
	N domain	T496							
S_2	**tACE/C domain**	N70	E143	S516	A63	Y62	F391	V81	Y69
	N domain	D43	S119	N494	V36	S35	Y369	N54	H42
S_1'	**tACE/C domain**	E162	N374	E376	D377	V380	N277	S284	
	N domain	D140	T352	D354	N355	T358	D255	E262	
S_2'	**tACE/C domain**	D453	S284	V380	V379	E376			
	N domain	E431	D262	T358	S357	D354			

Table A.

REMARK coordinates from restrained individual B-factor refinement
REMARK refinement resolution: 500.0 - 3 A
REMARK starting r= 0.2256 free_r= 0.2748
REMARK final r= 0.2249 free_r= 0.2737
REMARK B rmsd for bonded mainchain atoms= 1.061 target= 1.5
REMARK B rmsd for bonded sidechain atoms= 1.449 target= 2.0
REMARK B rmsd for angle mainchain atoms= 1.846 target= 2.0
REMARK B rmsd for angle sidechain atoms= 2.327 target= 2.5
REMARK rweight= 0.1000 (with wa= 4.39844)
REMARK target= mlf steps= 30
REMARK sg= C222(1) a= 101.12 b= 211.32 c= 171.27 alpha= 90 beta= 90 gamma= 90
REMARK parameter file 1 : CNS_TOPPAR:protein_rep.param
REMARK parameter file 2 : CNS_TOPPAR:ion.param
REMARK parameter file 3 : ../../../nlis/cns/both.par
REMARK parameter file 4 : CNS_TOPPAR:water_rep.param
REMARK parameter file 5 : ../carb.par
REMARK molecular structure file: gen.mtf
REMARK input coordinates: rig.pdb
REMARK reflection file= ../sftools_rf.cv
REMARK ncs= none
REMARK B-correction resolution: 6.0 - 3
REMARK B-factor correction applied to coordinate array B: -0.004
REMARK bulk solvent: density level= 0.337337 e/A^3, B-factor= 25.5172 A^2
REMARK reflections with |Fobs|/sigma_F < 0.0 rejected
REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
REMARK theoretical total number of refl. in resol. range: 37102 (100.0 %)
REMARK number of unobserved reflections (no entry or |F|=0): 1459 (3.9 %)
REMARK number of reflections rejected: 0 (0.0 %)
REMARK total number of reflections used: 35643 (96.1 %)
REMARK number of reflections in working set: 34202 (92.2 %)
REMARK number of reflections in test set: 1441 (3.9 %)

```
CRYST1  101.120  211.320  171.270  90.00  90.00  90.00 C 2 2 21
REMARK FILENAME="rbind.pdb"
REMARK DATE:01-Sep-2005  10:51:14      created by user: hazel
REMARK VERSION:1.1
ATOM    1  CB  ALA A  1    -23.864 -35.275  -7.565  1.00 59.70      A
ATOM    2  C   ALA A  1    -24.294 -37.717  -7.148  1.00 60.38      A
ATOM    3  O   ALA A  1    -23.961 -38.780  -6.618  1.00 59.62      A
ATOM    4  N   ALA A  1    -22.652 -37.006  -8.857  1.00 60.75      A
ATOM    5  CA  ALA A  1    -23.242 -36.679  -7.533  1.00 60.39      A
ATOM    6  N   ASP A  2    -25.560 -37.406  -7.422  1.00 60.30      A
ATOM    7  CA  ASP A  2    -26.661 -38.306  -7.091  1.00 60.51      A
ATOM    8  CB  ASP A  2    -27.942 -37.862  -7.809  1.00 61.34      A
ATOM    9  CG  ASP A  2    -29.144 -38.732  -7.456  1.00 62.14      A
ATOM    10 OD1 ASP A  2    -29.480 -38.824  -6.256  1.00 62.49      A
ATOM    11 OD2 ASP A  2    -29.752 -39.323  -8.377  1.00 62.26      A
ATOM    12 C   ASP A  2    -26.318 -39.742  -7.476  1.00 59.93      A
ATOM    13 O   ASP A  2    -25.833 -40.000  -8.576  1.00 61.20      A
ATOM    14 N   PRO A  3    -26.562 -40.699  -6.568  1.00 58.59      A
ATOM    15 CD  PRO A  3    -27.098 -40.534  -5.206  1.00 58.27      A
ATOM    16 CA  PRO A  3    -26.266 -42.110  -6.842  1.00 57.14      A
ATOM    17 CB  PRO A  3    -26.435 -42.763  -5.473  1.00 57.38      A
ATOM    18 CG  PRO A  3    -27.521 -41.944  -4.857  1.00 57.46      A
ATOM    19 C   PRO A  3    -27.165 -42.740  -7.914  1.00 55.49      A
ATOM    20 O   PRO A  3    -26.738 -43.633  -8.651  1.00 54.12      A
ATOM    21 N   GLY A  4    -28.404 -42.266  -7.993  1.00 54.53      A
ATOM    22 CA  GLY A  4    -29.338 -42.792  -8.972  1.00 53.91      A
ATOM    23 C   GLY A  4    -28.945 -42.517 -10.413  1.00 53.28      A
ATOM    24 O   GLY A  4    -29.479 -43.141 -11.327  1.00 53.35      A
ATOM    25 N   LEU A  5    -28.014 -41.586 -10.617  1.00 52.87      A
ATOM    26 CA  LEU A  5    -27.549 -41.228 -11.955  1.00 51.15      A
ATOM    27 CB  LEU A  5    -27.476 -39.706 -12.108  1.00 48.94      A
ATOM    28 CG  LEU A  5    -28.805 -38.944 -12.068  1.00 47.11      A
ATOM    29 CD1 LEU A  5    -28.548 -37.466 -11.943  1.00 44.60      A
ATOM    30 CD2 LEU A  5    -29.602 -39.232 -13.317  1.00 45.99      A
```

ATOM	31	C	LEU	A	5	-26.188	-41.837	-12.250	1.00 51.49	A
ATOM	32	O	LEU	A	5	-25.695	-41.731	-13.367	1.00 51.18	A
ATOM	33	N	GLN	A	6	-25.640	-42.563	-11.327	1.00 52.94	A
ATOM	34	CA	GLN	A	6	-24.384	-43.191	-11.556	1.00 55.39	A
ATOM	35	CB	GLN	A	6	-23.816	-43.588	-10.244	1.00 55.97	A
ATOM	36	CG	GLN	A	6	-22.367	-43.717	-10.213	1.00 58.03	A
ATOM	37	CD	GLN	A	6	-21.757	-42.560	-9.541	1.00 60.50	A
ATOM	38	OE1	GLN	A	6	-20.540	-42.472	-9.411	1.00 61.49	A
ATOM	39	NE2	GLN	A	6	-22.588	-41.634	-9.128	1.00 61.55	A
ATOM	40	C	GLN	A	6	-24.552	-44.384	-12.408	1.00 56.59	A
ATOM	41	O	GLN	A	6	-25.617	-44.840	-12.561	1.00 57.06	A
ATOM	42	N	PRO	A	7	-23.486	-44.903	-12.966	1.00 57.69	A
ATOM	43	CD	PRO	A	7	-22.106	-44.441	-12.730	1.00 59.02	A
ATOM	44	CA	PRO	A	7	-23.568	-45.839	-14.090	1.00 58.62	A
ATOM	45	CB	PRO	A	7	-22.112	-46.258	-14.295	1.00 58.58	A
ATOM	46	CG	PRO	A	7	-21.323	-45.076	-13.848	1.00 58.80	A
ATOM	47	C	PRO	A	7	-24.422	-47.058	-13.755	1.00 59.55	A
ATOM	48	O	PRO	A	7	-25.532	-47.191	-14.271	1.00 61.74	A
ATOM	49	N	GLY	A	8	-23.904	-47.933	-12.900	1.00 58.50	A
ATOM	50	CA	GLY	A	8	-24.431	-49.279	-12.775	1.00 58.31	A
ATOM	51	C	GLY	A	8	-23.347	-50.336	-12.851	1.00 58.41	A
ATOM	52	O	GLY	A	8	-22.330	-50.246	-12.164	1.00 60.78	A
ATOM	53	N	ASN	A	9	-23.566	-51.343	-13.691	1.00 56.71	A
ATOM	54	CA	ASN	A	9	-22.550	-52.354	-13.957	1.00 54.49	A
ATOM	55	CB	ASN	A	9	-22.144	-53.058	-12.661	1.00 56.78	A
ATOM	56	CG	ASN	A	9	-20.641	-53.085	-12.459	1.00 59.68	A
ATOM	57	OD1	ASN	A	9	-19.884	-53.385	-13.383	1.00 60.14	A
ATOM	58	ND2	ASN	A	9	-20.202	-52.770	-11.246	1.00 60.77	A
ATOM	59	C	ASN	A	9	-23.011	-53.379	-14.988	1.00 52.08	A
ATOM	60	O	ASN	A	9	-24.188	-53.735	-15.040	1.00 51.49	A
ATOM	61	N	PHE	A	10	-22.075	-53.848	-15.808	1.00 48.84	A
ATOM	62	CA	PHE	A	10	-22.390	-54.279	-17.163	1.00 46.09	A
ATOM	63	CB	PHE	A	10	-22.552	-53.069	-18.086	1.00 40.73	A
ATOM	64	CG	PHE	A	10	-23.805	-52.278	-17.837	1.00 36.00	A

ATOM 65 CD1 PHE A 10 -23.749 -51.046 -17.208 1.00 34.11 A
ATOM 66 CD2 PHE A 10 -25.039 -52.766 -18.233 1.00 34.82 A
ATOM 67 CE1 PHE A 10 -24.899 -50.314 -16.978 1.00 33.62 A
ATOM 68 CE2 PHE A 10 -26.193 -52.040 -18.005 1.00 33.24 A
ATOM 69 CZ PHE A 10 -26.123 -50.813 -17.377 1.00 32.41 A
ATOM 70 C PHE A 10 -21.299 -55.200 -17.700 1.00 47.33 A
ATOM 71 O PHE A 10 -20.140 -55.102 -17.298 1.00 47.54 A
ATOM 72 N SER A 11 -21.694 -55.981 -18.685 1.00 49.09 A
ATOM 73 CA SER A 11 -20.944 -57.050 -19.260 1.00 51.16 A
ATOM 74 CB SER A 11 -21.914 -57.969 -19.948 1.00 52.18 A
ATOM 75 OG SER A 11 -23.230 -57.711 -19.528 1.00 55.83 A
ATOM 76 C SER A 11 -20.010 -56.527 -20.270 1.00 51.37 A
ATOM 77 O SER A 11 -20.347 -55.675 -20.997 1.00 51.24 A
ATOM 78 N ALA A 12 -18.805 -57.001 -20.317 1.00 52.26 A
ATOM 79 CA ALA A 12 -17.885 -56.442 -21.234 1.00 53.18 A
ATOM 80 CB ALA A 12 -16.590 -56.722 -20.875 1.00 51.57 A
ATOM 81 C ALA A 12 -18.135 -56.963 -22.575 1.00 54.43 A
ATOM 82 O ALA A 12 -17.211 -57.231 -23.312 1.00 54.12 A
ATOM 83 N ASP A 13 -19.420 -57.091 -22.875 1.00 55.79 A
ATOM 84 CA ASP A 13 -19.948 -57.734 -24.060 1.00 56.36 A
ATOM 85 CB ASP A 13 -21.115 -58.589 -23.693 1.00 59.30 A
ATOM 86 CG ASP A 13 -20.718 -59.905 -23.260 1.00 62.75 A
ATOM 87 OD1 ASP A 13 -19.530 -60.209 -23.368 1.00 63.30 A
ATOM 88 OD2 ASP A 13 -21.523 -60.720 -22.798 1.00 65.19 A
ATOM 89 C ASP A 13 -20.579 -56.691 -24.885 1.00 55.46 A
ATOM 90 O ASP A 13 -20.817 -55.628 -24.438 1.00 55.52 A
ATOM 91 N GLU A 14 -20.926 -57.029 -26.093 1.00 54.03 A
ATOM 92 CA GLU A 14 -21.653 -56.087 -26.934 1.00 51.76 A
ATOM 93 CB GLU A 14 -21.555 -56.497 -28.407 1.00 52.19 A
ATOM 94 CG GLU A 14 -22.396 -55.627 -29.349 1.00 51.31 A
ATOM 95 CD GLU A 14 -22.124 -55.902 -30.814 1.00 49.65 A
ATOM 96 OE1 GLU A 14 -22.807 -55.278 -31.657 1.00 47.71 A
ATOM 97 OE2 GLU A 14 -21.228 -56.730 -31.110 1.00 48.97 A
ATOM 98 C GLU A 14 -23.114 -56.059 -26.496 1.00 50.39 A

ATOM 99 O GLU A 14 -23.824 -55.074 -26.723 1.00 48.36 A
ATOM 100 N ALA A 15 -23.557 -57.152 -25.875 1.00 49.54 A
ATOM 101 CA ALA A 15 -24.931 -57.249 -25.392 1.00 48.17 A
ATOM 102 CB ALA A 15 -25.307 -58.697 -25.151 1.00 48.26 A
ATOM 103 C ALA A 15 -24.995 -56.456 -24.099 1.00 47.03 A
ATOM 104 O ALA A 15 -26.058 -55.989 -23.694 1.00 46.94 A
ATOM 105 N GLY A 16 -23.839 -56.312 -23.458 1.00 45.43 A
ATOM 106 CA GLY A 16 -23.769 -55.537 -22.240 1.00 44.21 A
ATOM 107 C GLY A 16 -23.904 -54.083 -22.638 1.00 44.56 A
ATOM 108 O GLY A 16 -24.717 -53.343 -22.087 1.00 44.15 A
ATOM 109 N ALA A 17 -23.113 -53.686 -23.630 1.00 44.88 A
ATOM 110 CA ALA A 17 -23.111 -52.321 -24.144 1.00 43.99 A
ATOM 111 CB ALA A 17 -22.103 -52.205 -25.277 1.00 42.98 A
ATOM 112 C ALA A 17 -24.490 -51.863 -24.613 1.00 43.79 A
ATOM 113 O ALA A 17 -24.898 -50.734 -24.351 1.00 43.30 A
ATOM 114 N GLN A 18 -25.206 -52.729 -25.319 1.00 44.14 A
ATOM 115 CA GLN A 18 -26.542 -52.377 -25.787 1.00 44.90 A
ATOM 116 CB GLN A 18 -27.218 -53.578 -26.452 1.00 45.72 A
ATOM 117 CG GLN A 18 -27.143 -53.613 -27.976 1.00 47.20 A
ATOM 118 CD GLN A 18 -27.934 -52.490 -28.639 1.00 47.56 A
ATOM 119 OE1 GLN A 18 -28.877 -51.943 -28.056 1.00 46.17 A
ATOM 120 NE2 GLN A 18 -27.563 -52.156 -29.872 1.00 47.95 A
ATOM 121 C GLN A 18 -27.352 -51.948 -24.574 1.00 45.56 A
ATOM 122 O GLN A 18 -28.210 -51.067 -24.658 1.00 46.30 A
ATOM 123 N LEU A 19 -27.073 -52.588 -23.442 1.00 45.38 A
ATOM 124 CA LEU A 19 -27.764 -52.284 -22.189 1.00 44.17 A
ATOM 125 CB LEU A 19 -27.632 -53.475 -21.232 1.00 42.95 A
ATOM 126 CG LEU A 19 -28.423 -54.697 -21.695 1.00 41.27 A
ATOM 127 CD1 LEU A 19 -28.083 -55.910 -20.851 1.00 40.33 A
ATOM 128 CD2 LEU A 19 -29.908 -54.373 -21.616 1.00 41.16 A
ATOM 129 C LEU A 19 -27.190 -51.009 -21.562 1.00 43.72 A
ATOM 130 O LEU A 19 -27.941 -50.121 -21.143 1.00 43.82 A
ATOM 131 N PHE A 20 -25.859 -50.935 -21.517 1.00 42.38 A
ATOM 132 CA PHE A 20 -25.142 -49.783 -20.980 1.00 41.22 A

ATOM 133 CB PHE A 20 -23.656 -49.891 -21.328 1.00 41.22 A
ATOM 134 CG PHE A 20 -22.865 -48.666 -20.991 1.00 42.77 A
ATOM 135 CD1 PHE A 20 -22.194 -48.565 -19.778 1.00 44.56 A
ATOM 136 CD2 PHE A 20 -22.816 -47.592 -21.872 1.00 43.78 A
ATOM 137 CE1 PHE A 20 -21.480 -47.407 -19.437 1.00 44.75 A
ATOM 138 CE2 PHE A 20 -22.109 -46.428 -21.547 1.00 45.36 A
ATOM 139 CZ PHE A 20 -21.438 -46.336 -20.323 1.00 45.39 A
ATOM 140 C PHE A 20 -25.712 -48.507 -21.593 1.00 41.34 A
ATOM 141 O PHE A 20 -26.030 -47.551 -20.884 1.00 41.48 A
ATOM 142 N ALA A 21 -25.839 -48.506 -22.918 1.00 40.47 A
ATOM 143 CA ALA A 21 -26.358 -47.360 -23.644 1.00 39.24 A
ATOM 144 CB ALA A 21 -26.173 -47.572 -25.126 1.00 38.89 A
ATOM 145 C ALA A 21 -27.821 -47.098 -23.337 1.00 39.35 A
ATOM 146 O ALA A 21 -28.235 -45.950 -23.207 1.00 39.42 A
ATOM 147 N ALA A 22 -28.603 -48.164 -23.226 1.00 39.34 A
ATOM 148 CA ALA A 22 -30.025 -48.031 -22.943 1.00 40.16 A
ATOM 149 CB ALA A 22 -30.678 -49.416 -22.866 1.00 39.74 A
ATOM 150 C ALA A 22 -30.212 -47.280 -21.631 1.00 41.24 A
ATOM 151 O ALA A 22 -31.111 -46.444 -21.499 1.00 40.59 A
ATOM 152 N SER A 23 -29.338 -47.575 -20.670 1.00 43.22 A
ATOM 153 CA SER A 23 -29.375 -46.962 -19.342 1.00 45.22 A
ATOM 154 CB SER A 23 -28.454 -47.745 -18.395 1.00 45.73 A
ATOM 155 OG SER A 23 -28.820 -47.579 -17.036 1.00 46.34 A
ATOM 156 C SER A 23 -28.949 -45.489 -19.405 1.00 45.96 A
ATOM 157 O SER A 23 -29.725 -44.587 -19.057 1.00 45.92 A
ATOM 158 N TYR A 24 -27.712 -45.268 -19.851 1.00 45.86 A
ATOM 159 CA TYR A 24 -27.130 -43.933 -20.005 1.00 45.14 A
ATOM 160 CB TYR A 24 -25.937 -44.005 -20.960 1.00 46.13 A
ATOM 161 CG TYR A 24 -25.428 -42.656 -21.418 1.00 48.06 A
ATOM 162 CD1 TYR A 24 -24.937 -41.724 -20.502 1.00 48.24 A
ATOM 163 CE1 TYR A 24 -24.447 -40.487 -20.924 1.00 48.03 A
ATOM 164 CD2 TYR A 24 -25.418 -42.312 -22.773 1.00 48.40 A
ATOM 165 CE2 TYR A 24 -24.926 -41.075 -23.203 1.00 47.52 A
ATOM 166 CZ TYR A 24 -24.441 -40.171 -22.272 1.00 47.46 A

ATOM 167 OH TYR A 24 -23.926 -38.965 -22.681 1.00 46.28 A
ATOM 168 C TYR A 24 -28.135 -42.932 -20.556 1.00 43.62 A
ATOM 169 O TYR A 24 -28.262 -41.813 -20.073 1.00 43.13 A
ATOM 170 N ASN A 25 -28.929 -43.346 -21.524 1.00 42.36 A
ATOM 171 CA ASN A 25 -29.938 -42.520 -22.209 1.00 41.72 A
ATOM 172 CB ASN A 25 -30.661 -43.333 -23.317 1.00 40.46 A
ATOM 173 CG ASN A 25 -31.894 -42.671 -23.871 1.00 40.43 A
ATOM 174 OD1 ASN A 25 -31.786 -41.746 -24.557 1.00 40.06 A
ATOM 175 ND2 ASN A 25 -33.046 -43.226 -23.662 1.00 41.17 A
ATOM 176 C ASN A 25 -30.945 -42.002 -21.299 1.00 42.17 A
ATOM 177 O ASN A 25 -31.347 -40.879 -21.364 1.00 41.04 A
ATOM 178 N ALA A 26 -31.448 -42.883 -20.485 1.00 42.92 A
ATOM 179 CA ALA A 26 -32.520 -42.491 -19.574 1.00 43.29 A
ATOM 180 CB ALA A 26 -33.096 -43.719 -18.906 1.00 43.39 A
ATOM 181 C ALA A 26 -32.033 -41.505 -18.519 1.00 43.47 A
ATOM 182 O ALA A 26 -32.735 -40.546 -18.170 1.00 42.67 A
ATOM 183 N SER A 27 -30.828 -41.756 -18.015 1.00 42.93 A
ATOM 184 CA SER A 27 -30.213 -40.914 -17.000 1.00 42.95 A
ATOM 185 CB SER A 27 -29.057 -41.665 -16.349 1.00 42.26 A
ATOM 186 OG SER A 27 -29.430 -42.996 -16.056 1.00 43.10 A
ATOM 187 C SER A 27 -29.696 -39.602 -17.601 1.00 43.34 A
ATOM 188 O SER A 27 -29.921 -38.519 -17.054 1.00 44.12 A
ATOM 189 N ALA A 28 -28.994 -39.709 -18.725 1.00 43.11 A
ATOM 190 CA ALA A 28 -28.439 -38.551 -19.406 1.00 41.81 A
ATOM 191 CB ALA A 28 -27.744 -38.990 -20.684 1.00 41.60 A
ATOM 192 C ALA A 28 -29.509 -37.522 -19.716 1.00 41.28 A
ATOM 193 O ALA A 28 -29.259 -36.333 -19.638 1.00 40.80 A
ATOM 194 N GLU A 29 -30.705 -37.973 -20.065 1.00 42.45 A
ATOM 195 CA GLU A 29 -31.787 -37.047 -20.383 1.00 44.68 A
ATOM 196 CB GLU A 29 -33.071 -37.805 -20.716 1.00 46.96 A
ATOM 197 CG GLU A 29 -33.234 -38.182 -22.169 1.00 50.48 A
ATOM 198 CD GLU A 29 -34.695 -38.358 -22.535 1.00 53.39 A
ATOM 199 OE1 GLU A 29 -34.996 -38.538 -23.732 1.00 55.17 A
ATOM 200 OE2 GLU A 29 -35.546 -38.313 -21.618 1.00 54.90 A

ATOM 201 C GLU A 29 -32.074 -36.099 -19.235 1.00 44.97 A
ATOM 202 O GLU A 29 -32.508 -34.967 -19.438 1.00 43.63 A
ATOM 203 N GLN A 30 -31.835 -36.582 -18.022 1.00 47.08 A
ATOM 204 CA GLN A 30 -32.075 -35.800 -16.814 1.00 47.50 A
ATOM 205 CB GLN A 30 -32.197 -36.734 -15.603 1.00 48.02 A
ATOM 206 CG GLN A 30 -33.439 -37.630 -15.659 1.00 50.84 A
ATOM 207 CD GLN A 30 -33.578 -38.549 -14.453 1.00 52.87 A
ATOM 208 OE1 GLN A 30 -33.549 -38.090 -13.306 1.00 53.65 A
ATOM 209 NE2 GLN A 30 -33.738 -39.854 -14.704 1.00 52.00 A
ATOM 210 C GLN A 30 -30.961 -34.789 -16.605 1.00 46.87 A
ATOM 211 O GLN A 30 -31.215 -33.586 -16.540 1.00 46.42 A
ATOM 212 N VAL A 31 -29.767 -35.290 -16.426 1.00 45.83 A
ATOM 213 CA VAL A 31 -28.581 -34.501 -16.438 1.00 45.79 A
ATOM 214 CB VAL A 31 -27.435 -35.328 -16.380 1.00 44.91 A
ATOM 215 CG1 VAL A 31 -26.531 -34.815 -17.217 1.00 45.05 A
ATOM 216 CG2 VAL A 31 -26.928 -35.265 -15.128 1.00 44.72 A
ATOM 217 C VAL A 31 -28.393 -33.447 -17.506 1.00 45.62 A
ATOM 218 O VAL A 31 -27.843 -32.406 -17.291 1.00 45.78 A
ATOM 219 N LEU A 32 -28.879 -33.719 -18.668 1.00 44.73 A
ATOM 220 CA LEU A 32 -28.826 -32.778 -19.770 1.00 44.36 A
ATOM 221 CB LEU A 32 -28.927 -33.505 -21.116 1.00 42.88 A
ATOM 222 CG LEU A 32 -27.618 -34.185 -21.522 1.00 40.77 A
ATOM 223 CD1 LEU A 32 -27.789 -34.967 -22.795 1.00 41.40 A
ATOM 224 CD2 LEU A 32 -26.552 -33.126 -21.693 1.00 41.02 A
ATOM 225 C LEU A 32 -29.932 -31.752 -19.628 1.00 44.37 A
ATOM 226 O LEU A 32 -29.697 -30.559 -19.803 1.00 44.83 A
ATOM 227 N PHE A 33 -31.136 -32.206 -19.300 1.00 44.42 A
ATOM 228 CA PHE A 33 -32.247 -31.274 -19.129 1.00 45.58 A
ATOM 229 CB PHE A 33 -33.503 -31.977 -18.615 1.00 41.98 A
ATOM 230 CG PHE A 33 -34.632 -31.034 -18.314 1.00 37.18 A
ATOM 231 CD1 PHE A 33 -35.524 -30.658 -19.304 1.00 36.69 A
ATOM 232 CD2 PHE A 33 -34.776 -30.491 -17.049 1.00 34.63 A
ATOM 233 CE1 PHE A 33 -36.547 -29.752 -19.032 1.00 35.20 A
ATOM 234 CE2 PHE A 33 -35.792 -29.586 -16.771 1.00 33.33 A

ATOM 235 CZ PHE A 33 -36.677 -29.216 -17.761 1.00 33.23 A
ATOM 236 C PHE A 33 -31.884 -30.182 -18.129 1.00 48.29 A
ATOM 237 O PHE A 33 -32.073 -28.994 -18.399 1.00 49.21 A
ATOM 238 N GLN A 34 -31.366 -30.590 -16.972 1.00 50.83 A
ATOM 239 CA GLN A 34 -31.003 -29.637 -15.933 1.00 52.45 A
ATOM 240 CB GLN A 34 -30.497 -30.372 -14.684 1.00 53.44 A
ATOM 241 CG GLN A 34 -29.232 -31.184 -14.853 1.00 56.33 A
ATOM 242 CD GLN A 34 -28.044 -30.587 -14.095 1.00 59.76 A
ATOM 243 OE1 GLN A 34 -28.219 -29.928 -13.058 1.00 60.10 A
ATOM 244 NE2 GLN A 34 -26.827 -30.832 -14.600 1.00 61.38 A
ATOM 245 C GLN A 34 -29.987 -28.598 -16.397 1.00 52.59 A
ATOM 246 O GLN A 34 -30.253 -27.396 -16.298 1.00 53.04 A
ATOM 247 N SER A 35 -28.876 -29.058 -16.928 1.00 51.15 A
ATOM 248 CA SER A 35 -27.868 -28.192 -17.423 1.00 49.99 A
ATOM 249 CB SER A 35 -26.757 -28.984 -17.960 1.00 49.90 A
ATOM 250 OG SER A 35 -26.782 -28.826 -19.334 1.00 53.34 A
ATOM 251 C SER A 35 -28.293 -27.267 -18.482 1.00 48.72 A
ATOM 252 O SER A 35 -27.766 -26.195 -18.545 1.00 48.49 A
ATOM 253 N VAL A 36 -29.193 -27.697 -19.348 1.00 46.52 A
ATOM 254 CA VAL A 36 -29.766 -26.919 -20.440 1.00 44.76 A
ATOM 255 CB VAL A 36 -30.485 -27.832 -21.462 1.00 44.34 A
ATOM 256 CG1 VAL A 36 -31.303 -26.995 -22.437 1.00 41.86 A
ATOM 257 CG2 VAL A 36 -29.460 -28.670 -22.212 1.00 43.46 A
ATOM 258 C VAL A 36 -30.762 -25.888 -19.925 1.00 44.06 A
ATOM 259 O VAL A 36 -30.761 -24.740 -20.372 1.00 43.33 A
ATOM 260 N ALA A 37 -31.610 -26.302 -18.986 1.00 43.05 A
ATOM 261 CA ALA A 37 -32.617 -25.409 -18.420 1.00 42.33 A
ATOM 262 CB ALA A 37 -33.578 -26.191 -17.560 1.00 41.35 A
ATOM 263 C ALA A 37 -31.948 -24.312 -17.602 1.00 41.62 A
ATOM 264 O ALA A 37 -32.443 -23.187 -17.524 1.00 39.76 A
ATOM 265 N ALA A 38 -30.811 -24.658 -17.003 1.00 41.33 A
ATOM 266 CA ALA A 38 -30.037 -23.727 -16.190 1.00 41.12 A
ATOM 267 CB ALA A 38 -28.853 -24.454 -15.540 1.00 40.21 A
ATOM 268 C ALA A 38 -29.532 -22.600 -17.081 1.00 41.12 A

ATOM 269 O ALA A 38 -29.656 -21.416 -16.758 1.00 41.30 A
ATOM 270 N SER A 39 -28.946 -22.985 -18.205 1.00 40.59 A
ATOM 271 CA SER A 39 -28.434 -22.022 -19.148 1.00 38.72 A
ATOM 272 CB SER A 39 -27.790 -22.745 -20.320 1.00 36.81 A
ATOM 273 OG SER A 39 -26.773 -23.617 -19.864 1.00 35.22 A
ATOM 274 C SER A 39 -29.594 -21.169 -19.631 1.00 39.25 A
ATOM 275 O SER A 39 -29.499 -19.944 -19.647 1.00 39.58 A
ATOM 276 N TRP A 40 -30.700 -21.809 -20.005 1.00 39.54 A
ATOM 277 CA TRP A 40 -31.856 -21.064 -20.498 1.00 39.85 A
ATOM 278 CB TRP A 40 -33.053 -21.989 -20.756 1.00 38.38 A
ATOM 279 CG TRP A 40 -34.290 -21.235 -21.204 1.00 37.06 A
ATOM 280 CD2 TRP A 40 -34.594 -20.783 -22.532 1.00 37.49 A
ATOM 281 CE2 TRP A 40 -35.814 -20.076 -22.464 1.00 36.99 A
ATOM 282 CE3 TRP A 40 -33.955 -20.906 -23.771 1.00 37.44 A
ATOM 283 CD1 TRP A 40 -35.311 -20.794 -20.415 1.00 37.37 A
ATOM 284 NE1 TRP A 40 -36.230 -20.098 -21.161 1.00 36.56 A
ATOM 285 CZ2 TRP A 40 -36.406 -19.495 -23.583 1.00 36.70 A
ATOM 286 CZ3 TRP A 40 -34.547 -20.328 -24.882 1.00 37.03 A
ATOM 287 CH2 TRP A 40 -35.761 -19.632 -24.778 1.00 37.26 A
ATOM 288 C TRP A 40 -32.278 -19.940 -19.568 1.00 40.95 A
ATOM 289 O TRP A 40 -32.894 -18.976 -20.017 1.00 41.96 A
ATOM 290 N ALA A 41 -31.955 -20.059 -18.281 1.00 42.31 A
ATOM 291 CA ALA A 41 -32.305 -19.022 -17.304 1.00 42.16 A
ATOM 292 CB ALA A 41 -32.400 -19.623 -15.906 1.00 40.87 A
ATOM 293 C ALA A 41 -31.259 -17.909 -17.331 1.00 42.14 A
ATOM 294 O ALA A 41 -31.583 -16.734 -17.170 1.00 42.22 A
ATOM 295 N HIS A 42 -30.006 -18.296 -17.552 1.00 42.74 A
ATOM 296 CA HIS A 42 -28.895 -17.359 -17.610 1.00 44.17 A
ATOM 297 CB HIS A 42 -27.576 -18.132 -17.510 1.00 47.34 A
ATOM 298 CG HIS A 42 -26.350 -17.288 -17.699 1.00 50.69 A
ATOM 299 CD2 HIS A 42 -25.534 -16.686 -16.801 1.00 51.45 A
ATOM 300 ND1 HIS A 42 -25.828 -16.997 -18.943 1.00 52.32 A
ATOM 301 CE1 HIS A 42 -24.744 -16.255 -18.801 1.00 52.42 A
ATOM 302 NE2 HIS A 42 -24.543 -16.052 -17.511 1.00 52.35 A

ATOM 303 C HIS A 42 -28.904 -16.500 -18.874 1.00 44.50 A
ATOM 304 O HIS A 42 -28.657 -15.297 -18.816 1.00 45.04 A
ATOM 305 N ASP A 43 -29.190 -17.127 -20.010 1.00 44.95 A
ATOM 306 CA ASP A 43 -29.220 -16.424 -21.287 1.00 44.34 A
ATOM 307 CB ASP A 43 -29.186 -17.420 -22.448 1.00 46.25 A
ATOM 308 CG ASP A 43 -27.848 -18.121 -22.575 1.00 48.09 A
ATOM 309 OD1 ASP A 43 -27.624 -18.794 -23.603 1.00 50.16 A
ATOM 310 OD2 ASP A 43 -26.961 -18.057 -21.699 1.00 47.76 A
ATOM 311 C ASP A 43 -30.453 -15.533 -21.397 1.00 43.59 A
ATOM 312 O ASP A 43 -30.359 -14.375 -21.805 1.00 43.18 A
ATOM 313 N THR A 44 -31.608 -16.083 -21.037 1.00 43.46 A
ATOM 314 CA THR A 44 -32.847 -15.315 -21.014 1.00 43.63 A
ATOM 315 CB THR A 44 -34.065 -16.258 -20.972 1.00 43.18 A
ATOM 316 OG1 THR A 44 -34.084 -16.963 -19.724 1.00 44.45 A
ATOM 317 CG2 THR A 44 -33.914 -17.369 -22.000 1.00 42.99 A
ATOM 318 C THR A 44 -32.876 -14.368 -19.821 1.00 43.83 A
ATOM 319 O THR A 44 -33.845 -13.637 -19.618 1.00 42.40 A
ATOM 320 N ASN A 45 -31.805 -14.387 -19.034 1.00 45.28 A
ATOM 321 CA ASN A 45 -31.644 -13.445 -17.934 1.00 45.80 A
ATOM 322 CB ASN A 45 -32.710 -13.684 -16.864 1.00 46.99 A
ATOM 323 CG ASN A 45 -32.704 -12.617 -15.787 1.00 47.94 A
ATOM 324 OD1 ASN A 45 -32.045 -11.586 -15.922 1.00 50.43 A
ATOM 325 ND2 ASN A 45 -33.441 -12.860 -14.709 1.00 47.52 A
ATOM 326 C ASN A 45 -30.214 -13.564 -17.417 1.00 45.21 A
ATOM 327 O ASN A 45 -29.796 -14.627 -16.959 1.00 47.02 A
ATOM 328 N ILE A 46 -29.469 -12.466 -17.496 1.00 42.84 A
ATOM 329 CA ILE A 46 -28.080 -12.457 -17.051 1.00 40.74 A
ATOM 330 CB ILE A 46 -27.199 -11.682 -18.048 1.00 40.63 A
ATOM 331 CG2 ILE A 46 -25.731 -12.016 -17.832 1.00 38.48 A
ATOM 332 CG1 ILE A 46 -27.619 -11.995 -19.486 1.00 40.60 A
ATOM 333 CD1 ILE A 46 -26.617 -11.546 -20.526 1.00 41.08 A
ATOM 334 C ILE A 46 -27.951 -11.852 -15.657 1.00 39.88 A
ATOM 335 O ILE A 46 -27.851 -10.634 -15.506 1.00 40.28 A
ATOM 336 N THR A 47 -27.956 -12.709 -14.642 1.00 39.44 A

ATOM 337 CA THR A 47 -27.669 -12.283 -13.278 1.00 38.92 A
ATOM 338 CB THR A 47 -28.941 -12.349 -12.413 1.00 39.07 A
ATOM 339 OG1 THR A 47 -29.273 -13.718 -12.150 1.00 38.85 A
ATOM 340 CG2 THR A 47 -30.143 -11.840 -13.192 1.00 39.31 A
ATOM 341 C THR A 47 -26.566 -13.131 -12.654 1.00 38.66 A
ATOM 342 O THR A 47 -26.272 -14.230 -13.124 1.00 38.32 A
ATOM 343 N ALA A 48 -25.958 -12.613 -11.592 1.00 38.05 A
ATOM 344 CA ALA A 48 -24.918 -13.336 -10.875 1.00 38.04 A
ATOM 345 CB ALA A 48 -24.364 -12.473 -9.764 1.00 37.51 A
ATOM 346 C ALA A 48 -25.461 -14.651 -10.312 1.00 38.98 A
ATOM 347 O ALA A 48 -24.764 -15.670 -10.306 1.00 37.62 A
ATOM 348 N GLU A 49 -26.709 -14.620 -9.847 1.00 40.23 A
ATOM 349 CA GLU A 49 -27.357 -15.805 -9.290 1.00 41.74 A
ATOM 350 CB GLU A 49 -28.744 -15.457 -8.743 1.00 43.66 A
ATOM 351 CG GLU A 49 -29.516 -16.653 -8.179 1.00 46.92 A
ATOM 352 CD GLU A 49 -28.783 -17.357 -7.036 1.00 49.42 A
ATOM 353 OE1 GLU A 49 -28.329 -16.665 -6.097 1.00 51.14 A
ATOM 354 OE2 GLU A 49 -28.669 -18.604 -7.062 1.00 49.82 A
ATOM 355 C GLU A 49 -27.497 -16.912 -10.332 1.00 41.77 A
ATOM 356 O GLU A 49 -27.112 -18.055 -10.071 1.00 42.26 A
ATOM 357 N ASN A 50 -28.043 -16.575 -11.505 1.00 40.90 A
ATOM 358 CA ASN A 50 -28.234 -17.540 -12.593 1.00 39.66 A
ATOM 359 CB ASN A 50 -29.016 -16.893 -13.744 1.00 40.03 A
ATOM 360 CG ASN A 50 -30.395 -16.405 -13.325 1.00 40.57 A
ATOM 361 OD1 ASN A 50 -31.167 -17.137 -12.716 1.00 39.95 A
ATOM 362 ND2 ASN A 50 -30.713 -15.169 -13.670 1.00 41.49 A
ATOM 363 C ASN A 50 -26.904 -18.102 -13.118 1.00 39.05 A
ATOM 364 O ASN A 50 -26.799 -19.285 -13.453 1.00 38.23 A
ATOM 365 N ALA A 51 -25.891 -17.246 -13.185 1.00 38.53 A
ATOM 366 CA ALA A 51 -24.579 -17.652 -13.653 1.00 38.51 A
ATOM 367 CB ALA A 51 -23.676 -16.454 -13.731 1.00 39.07 A
ATOM 368 C ALA A 51 -24.006 -18.663 -12.694 1.00 38.93 A
ATOM 369 O ALA A 51 -23.490 -19.694 -13.101 1.00 37.64 A
ATOM 370 N ARG A 52 -23.969 -18.359 -11.443 1.00 41.76 A

ATOM 371 CA ARG A 52 -23.634 -19.321 -10.415 1.00 44.00 A
ATOM 372 CB ARG A 52 -24.103 -18.752 -9.118 1.00 45.30 A
ATOM 373 CG ARG A 52 -23.052 -18.588 -8.061 1.00 47.98 A
ATOM 374 CD ARG A 52 -23.670 -18.595 -6.709 1.00 50.52 A
ATOM 375 NE ARG A 52 -24.739 -19.556 -6.775 1.00 52.84 A
ATOM 376 CZ ARG A 52 -25.529 -19.877 -5.820 1.00 53.09 A
ATOM 377 NH1 ARG A 52 -25.406 -19.327 -4.653 1.00 54.58 A
ATOM 378 NH2 ARG A 52 -26.441 -20.773 -6.037 1.00 52.84 A
ATOM 379 C ARG A 52 -24.319 -20.601 -10.557 1.00 44.20 A
ATOM 380 O ARG A 52 -23.738 -21.633 -10.513 1.00 43.62 A
ATOM 381 N ARG A 53 -25.601 -20.519 -10.680 1.00 44.03 A
ATOM 382 CA ARG A 53 -26.411 -21.719 -10.855 1.00 44.62 A
ATOM 383 CB ARG A 53 -27.860 -21.345 -11.130 1.00 45.23 A
ATOM 384 CG ARG A 53 -28.606 -20.787 -9.948 1.00 46.11 A
ATOM 385 CD ARG A 53 -29.942 -20.238 -10.399 1.00 47.87 A
ATOM 386 NE ARG A 53 -30.649 -19.622 -9.288 1.00 48.96 A
ATOM 387 CZ ARG A 53 -31.289 -20.302 -8.346 1.00 49.51 A
ATOM 388 NH1 ARG A 53 -31.317 -21.629 -8.387 1.00 48.90 A
ATOM 389 NH2 ARG A 53 -31.891 -19.648 -7.358 1.00 50.12 A
ATOM 390 C ARG A 53 -25.895 -22.535 -12.026 1.00 44.63 A
ATOM 391 O ARG A 53 -25.558 -23.712 -11.874 1.00 45.30 A
ATOM 392 N GLN A 54 -25.869 -21.901 -13.197 1.00 43.53 A
ATOM 393 CA GLN A 54 -25.387 -22.534 -14.416 1.00 42.03 A
ATOM 394 CB GLN A 54 -25.198 -21.462 -15.497 1.00 42.88 A
ATOM 395 CG GLN A 54 -23.949 -21.610 -16.371 1.00 43.26 A
ATOM 396 CD GLN A 54 -24.194 -22.444 -17.609 1.00 43.52 A
ATOM 397 OE1 GLN A 54 -25.045 -22.099 -18.440 1.00 45.48 A
ATOM 398 NE2 GLN A 54 -23.450 -23.542 -17.747 1.00 41.34 A
ATOM 399 C GLN A 54 -24.066 -23.226 -14.118 1.00 41.21 A
ATOM 400 O GLN A 54 -23.930 -24.432 -14.296 1.00 40.40 A
ATOM 401 N GLU A 55 -23.100 -22.452 -13.644 1.00 40.67 A
ATOM 402 CA GLU A 55 -21.785 -22.985 -13.338 1.00 40.13 A
ATOM 403 CB GLU A 55 -20.938 -21.918 -12.646 1.00 40.90 A
ATOM 404 CG GLU A 55 -20.719 -20.676 -13.496 1.00 41.83 A

ATOM 405 CD GLU A 55 -19.552 -19.827 -13.015 1.00 44.05 A
ATOM 406 OE1 GLU A 55 -18.456 -20.385 -12.787 1.00 44.78 A
ATOM 407 OE2 GLU A 55 -19.719 -18.598 -12.873 1.00 45.51 A
ATOM 408 C GLU A 55 -21.876 -24.232 -12.477 1.00 39.53 A
ATOM 409 O GLU A 55 -20.993 -25.088 -12.511 1.00 39.05 A
ATOM 410 N ALA A 56 -22.953 -24.337 -11.708 1.00 39.28 A
ATOM 411 CA ALA A 56 -23.158 -25.496 -10.845 1.00 38.19 A
ATOM 412 CB ALA A 56 -24.161 -25.159 -9.749 1.00 37.41 A
ATOM 413 C ALA A 56 -23.658 -26.671 -11.682 1.00 36.65 A
ATOM 414 O ALA A 56 -23.057 -27.748 -11.691 1.00 35.00 A
ATOM 415 N ALA A 57 -24.756 -26.441 -12.393 1.00 35.68 A
ATOM 416 CA ALA A 57 -25.364 -27.446 -13.257 1.00 35.13 A
ATOM 417 CB ALA A 57 -26.478 -26.805 -14.064 1.00 35.01 A
ATOM 418 C ALA A 57 -24.332 -28.082 -14.193 1.00 35.36 A
ATOM 419 O ALA A 57 -24.415 -29.272 -14.514 1.00 34.72 A
ATOM 420 N ALA A 58 -23.370 -27.272 -14.631 1.00 35.10 A
ATOM 421 CA ALA A 58 -22.299 -27.717 -15.517 1.00 34.51 A
ATOM 422 CB ALA A 58 -21.453 -26.525 -15.927 1.00 33.24 A
ATOM 423 C ALA A 58 -21.433 -28.747 -14.794 1.00 35.27 A
ATOM 424 O ALA A 58 -21.034 -29.763 -15.366 1.00 35.05 A
ATOM 425 N LEU A 59 -21.155 -28.467 -13.524 1.00 35.58 A
ATOM 426 CA LEU A 59 -20.342 -29.337 -12.683 1.00 34.70 A
ATOM 427 CB LEU A 59 -20.160 -28.694 -11.314 1.00 33.09 A
ATOM 428 CG LEU A 59 -18.727 -28.279 -11.031 1.00 31.07 A
ATOM 429 CD1 LEU A 59 -18.688 -27.478 -9.756 1.00 28.84 A
ATOM 430 CD2 LEU A 59 -17.849 -29.523 -10.958 1.00 29.60 A
ATOM 431 C LEU A 59 -20.954 -30.724 -12.531 1.00 34.78 A
ATOM 432 O LEU A 59 -20.235 -31.723 -12.423 1.00 34.04 A
ATOM 433 N LEU A 60 -22.282 -30.778 -12.510 1.00 34.41 A
ATOM 434 CA LEU A 60 -22.969 -32.053 -12.408 1.00 35.26 A
ATOM 435 CB LEU A 60 -24.475 -31.859 -12.187 1.00 37.35 A
ATOM 436 CG LEU A 60 -24.900 -31.464 -10.766 1.00 39.66 A
ATOM 437 CD1 LEU A 60 -26.401 -31.236 -10.727 1.00 39.89 A
ATOM 438 CD2 LEU A 60 -24.482 -32.551 -9.772 1.00 39.75 A

ATOM 439 C LEU A 60 -22.732 -32.800 -13.708 1.00 34.24 A
ATOM 440 O LEU A 60 -22.224 -33.920 -13.707 1.00 33.75 A
ATOM 441 N SER A 61 -23.093 -32.170 -14.820 1.00 32.82 A
ATOM 442 CA SER A 61 -22.909 -32.780 -16.128 1.00 30.82 A
ATOM 443 CB SER A 61 -23.237 -31.771 -17.221 1.00 30.79 A
ATOM 444 OG SER A 61 -24.610 -31.414 -17.168 1.00 33.24 A
ATOM 445 C SER A 61 -21.484 -33.276 -16.267 1.00 28.63 A
ATOM 446 O SER A 61 -21.248 -34.423 -16.614 1.00 27.43 A
ATOM 447 N GLN A 62 -20.523 -32.416 -15.985 1.00 28.28 A
ATOM 448 CA GLN A 62 -19.138 -32.834 -16.079 1.00 30.22 A
ATOM 449 CB GLN A 62 -18.216 -31.693 -15.640 1.00 29.71 A
ATOM 450 CG GLN A 62 -18.228 -30.511 -16.590 1.00 28.80 A
ATOM 451 CD GLN A 62 -17.735 -29.236 -15.946 1.00 31.00 A
ATOM 452 OE1 GLN A 62 -18.280 -28.794 -14.935 1.00 32.00 A
ATOM 453 NE2 GLN A 62 -16.705 -28.631 -16.528 1.00 31.71 A
ATOM 454 C GLN A 62 -18.958 -34.063 -15.191 1.00 31.66 A
ATOM 455 O GLN A 62 -18.220 -34.985 -15.530 1.00 31.56 A
ATOM 456 N GLU A 63 -19.655 -34.064 -14.057 1.00 33.93 A
ATOM 457 CA GLU A 63 -19.617 -35.176 -13.104 1.00 35.67 A
ATOM 458 CB GLU A 63 -20.452 -34.816 -11.877 1.00 37.75 A
ATOM 459 CG GLU A 63 -19.712 -34.849 -10.559 1.00 43.26 A
ATOM 460 CD GLU A 63 -20.454 -34.079 -9.478 1.00 46.89 A
ATOM 461 OE1 GLU A 63 -21.647 -34.377 -9.253 1.00 47.77 A
ATOM 462 OE2 GLU A 63 -19.846 -33.174 -8.860 1.00 49.33 A
ATOM 463 C GLU A 63 -20.195 -36.429 -13.778 1.00 35.57 A
ATOM 464 O GLU A 63 -19.549 -37.480 -13.840 1.00 35.34 A
ATOM 465 N PHE A 64 -21.418 -36.289 -14.285 1.00 35.16 A
ATOM 466 CA PHE A 64 -22.135 -37.349 -14.985 1.00 35.53 A
ATOM 467 CB PHE A 64 -23.429 -36.774 -15.560 1.00 35.15 A
ATOM 468 CG PHE A 64 -24.342 -37.800 -16.153 1.00 36.52 A
ATOM 469 CD1 PHE A 64 -25.563 -38.084 -15.556 1.00 37.98 A
ATOM 470 CD2 PHE A 64 -24.001 -38.475 -17.314 1.00 37.90 A
ATOM 471 CE1 PHE A 64 -26.437 -39.029 -16.112 1.00 39.80 A
ATOM 472 CE2 PHE A 64 -24.867 -39.419 -17.875 1.00 39.47 A

ATOM 473 CZ PHE A 64 -26.085 -39.695 -17.272 1.00 39.94 A
ATOM 474 C PHE A 64 -21.286 -37.906 -16.125 1.00 36.53 A
ATOM 475 O PHE A 64 -21.051 -39.110 -16.226 1.00 35.88 A
ATOM 476 N ALA A 65 -20.838 -36.999 -16.985 1.00 37.75 A
ATOM 477 CA ALA A 65 -20.032 -37.330 -18.147 1.00 38.12 A
ATOM 478 CB ALA A 65 -19.673 -36.058 -18.887 1.00 38.07 A
ATOM 479 C ALA A 65 -18.769 -38.088 -17.793 1.00 38.81 A
ATOM 480 O ALA A 65 -18.317 -38.955 -18.539 1.00 38.19 A
ATOM 481 N GLU A 66 -18.225 -37.876 -16.643 1.00 40.33 A
ATOM 482 CA GLU A 66 -17.034 -38.578 -16.365 1.00 42.55 A
ATOM 483 CB GLU A 66 -16.340 -38.029 -15.226 1.00 44.34 A
ATOM 484 CG GLU A 66 -15.550 -39.157 -14.711 1.00 48.57 A
ATOM 485 CD GLU A 66 -14.563 -38.725 -13.741 1.00 51.41 A
ATOM 486 OE1 GLU A 66 -14.973 -38.086 -12.771 1.00 53.26 A
ATOM 487 OE2 GLU A 66 -13.393 -39.019 -13.977 1.00 53.13 A
ATOM 488 C GLU A 66 -17.340 -39.915 -15.921 1.00 42.56 A
ATOM 489 O GLU A 66 -16.620 -40.820 -16.190 1.00 42.91 A
ATOM 490 N ALA A 67 -18.383 -40.046 -15.152 1.00 41.53 A
ATOM 491 CA ALA A 67 -18.726 -41.375 -14.651 1.00 41.26 A
ATOM 492 CB ALA A 67 -19.953 -41.297 -13.773 1.00 40.81 A
ATOM 493 C ALA A 67 -18.950 -42.396 -15.759 1.00 41.67 A
ATOM 494 O ALA A 67 -18.253 -43.412 -15.827 1.00 41.02 A
ATOM 495 N TRP A 68 -19.933 -42.137 -16.615 1.00 42.00 A
ATOM 496 CA TRP A 68 -20.219 -43.050 -17.707 1.00 42.69 A
ATOM 497 CB TRP A 68 -21.500 -42.655 -18.428 1.00 43.26 A
ATOM 498 CG TRP A 68 -22.696 -42.663 -17.557 1.00 44.43 A
ATOM 499 CD2 TRP A 68 -23.699 -43.686 -17.485 1.00 44.08 A
ATOM 500 CE2 TRP A 68 -24.651 -43.270 -16.527 1.00 44.43 A
ATOM 501 CE3 TRP A 68 -23.887 -44.914 -18.138 1.00 42.52 A
ATOM 502 CD1 TRP A 68 -23.064 -41.700 -16.667 1.00 45.09 A
ATOM 503 NE1 TRP A 68 -24.239 -42.056 -16.044 1.00 44.76 A
ATOM 504 CZ2 TRP A 68 -25.780 -44.043 -16.206 1.00 44.22 A
ATOM 505 CZ3 TRP A 68 -25.010 -45.679 -17.816 1.00 41.97 A
ATOM 506 CH2 TRP A 68 -25.939 -45.238 -16.860 1.00 42.62 A

ATOM 507 C TRP A 68 -19.069 -43.012 -18.684 1.00 43.00 A
ATOM 508 O TRP A 68 -18.815 -43.979 -19.395 1.00 43.88 A
ATOM 509 N GLY A 69 -18.375 -41.882 -18.718 1.00 42.52 A
ATOM 510 CA GLY A 69 -17.258 -41.754 -19.623 1.00 42.00 A
ATOM 511 C GLY A 69 -16.209 -42.806 -19.339 1.00 42.08 A
ATOM 512 O GLY A 69 -15.985 -43.709 -20.147 1.00 40.81 A
ATOM 513 N ALA A 70 -15.596 -42.719 -18.172 1.00 42.69 A
ATOM 514 CA ALA A 70 -14.524 -43.631 -17.789 1.00 42.80 A
ATOM 515 CB ALA A 70 -13.849 -43.150 -16.514 1.00 41.47 A
ATOM 516 C ALA A 70 -15.047 -45.052 -17.612 1.00 42.51 A
ATOM 517 O ALA A 70 -14.230 -45.992 -17.585 1.00 41.80 A
ATOM 518 N LYS A 71 -16.333 -45.213 -17.470 1.00 43.36 A
ATOM 519 CA LYS A 71 -16.913 -46.542 -17.320 1.00 44.93 A
ATOM 520 CB LYS A 71 -18.306 -46.461 -16.691 1.00 44.65 A
ATOM 521 CG LYS A 71 -19.104 -47.771 -16.748 1.00 44.40 A
ATOM 522 CD LYS A 71 -18.435 -48.919 -15.990 1.00 45.18 A
ATOM 523 CE LYS A 71 -18.565 -48.788 -14.474 1.00 44.52 A
ATOM 524 NZ LYS A 71 -17.937 -49.942 -13.759 1.00 42.88 A
ATOM 525 C LYS A 71 -17.008 -47.162 -18.706 1.00 46.60 A
ATOM 526 O LYS A 71 -16.451 -48.234 -18.953 1.00 48.14 A
ATOM 527 N ALA A 72 -17.703 -46.468 -19.607 1.00 47.30 A
ATOM 528 CA ALA A 72 -17.875 -46.921 -20.983 1.00 46.89 A
ATOM 529 CB ALA A 72 -18.421 -45.792 -21.829 1.00 45.99 A
ATOM 530 C ALA A 72 -16.545 -47.406 -21.549 1.00 47.34 A
ATOM 531 O ALA A 72 -16.506 -48.326 -22.364 1.00 45.93 A
ATOM 532 N LYS A 73 -15.454 -46.787 -21.111 1.00 48.09 A
ATOM 533 CA LYS A 73 -14.137 -47.187 -21.576 1.00 49.46 A
ATOM 534 CB LYS A 73 -13.289 -45.950 -21.927 1.00 50.52 A
ATOM 535 CG LYS A 73 -13.115 -44.913 -20.832 1.00 50.70 A
ATOM 536 CD LYS A 73 -12.898 -43.507 -21.418 1.00 50.52 A
ATOM 537 CE LYS A 73 -11.442 -43.215 -21.738 1.00 49.77 A
ATOM 538 NZ LYS A 73 -11.271 -41.787 -22.118 1.00 50.08 A
ATOM 539 C LYS A 73 -13.413 -48.084 -20.576 1.00 50.62 A
ATOM 540 O LYS A 73 -12.423 -48.731 -20.927 1.00 51.65 A

ATOM 541 N ALA A 74 -13.907 -48.120 -19.343 1.00 51.63 A
ATOM 542 CA ALA A 74 -13.513 -49.149 -18.388 1.00 52.89 A
ATOM 543 CB ALA A 74 -14.553 -49.277 -17.287 1.00 52.93 A
ATOM 544 C ALA A 74 -13.296 -50.491 -19.078 1.00 53.75 A
ATOM 545 O ALA A 74 -12.309 -51.181 -18.817 1.00 54.95 A
ATOM 546 N LEU A 75 -14.222 -50.857 -19.958 1.00 54.15 A
ATOM 547 CA LEU A 75 -14.418 -52.253 -20.326 1.00 54.82 A
ATOM 548 CB LEU A 75 -15.417 -52.923 -19.381 1.00 54.44 A
ATOM 549 CG LEU A 75 -16.848 -52.385 -19.414 1.00 52.75 A
ATOM 550 CD1 LEU A 75 -17.819 -53.405 -18.840 1.00 52.44 A
ATOM 551 CD2 LEU A 75 -16.944 -51.066 -18.662 1.00 50.85 A
ATOM 552 C LEU A 75 -14.891 -52.387 -21.770 1.00 55.25 A
ATOM 553 O LEU A 75 -15.002 -53.494 -22.297 1.00 55.96 A
ATOM 554 N TYR A 76 -15.153 -51.254 -22.413 1.00 55.39 A
ATOM 555 CA TYR A 76 -15.791 -51.251 -23.725 1.00 55.20 A
ATOM 556 CB TYR A 76 -17.093 -50.448 -23.686 1.00 52.59 A
ATOM 557 CG TYR A 76 -18.267 -51.215 -23.122 1.00 49.91 A
ATOM 558 CD1 TYR A 76 -19.457 -50.571 -22.812 1.00 49.81 A
ATOM 559 CE1 TYR A 76 -20.533 -51.268 -22.296 1.00 49.70 A
ATOM 560 CD2 TYR A 76 -18.185 -52.583 -22.899 1.00 48.38 A
ATOM 561 CE2 TYR A 76 -19.256 -53.288 -22.383 1.00 49.58 A
ATOM 562 CZ TYR A 76 -20.427 -52.626 -22.083 1.00 50.30 A
ATOM 563 OH TYR A 76 -21.496 -53.323 -21.570 1.00 50.04 A
ATOM 564 C TYR A 76 -14.868 -50.705 -24.812 1.00 56.57 A
ATOM 565 O TYR A 76 -15.324 -50.335 -25.894 1.00 57.04 A
ATOM 566 N GLU A 77 -13.572 -50.656 -24.521 1.00 57.80 A
ATOM 567 CA GLU A 77 -12.680 -49.703 -25.172 1.00 59.73 A
ATOM 568 CB GLU A 77 -12.097 -48.725 -24.149 1.00 59.93 A
ATOM 569 CG GLU A 77 -12.093 -47.276 -24.610 1.00 61.42 A
ATOM 570 CD GLU A 77 -10.766 -46.858 -25.210 1.00 62.11 A
ATOM 571 OE1 GLU A 77 -10.164 -45.886 -24.708 1.00 63.00 A
ATOM 572 OE2 GLU A 77 -10.323 -47.502 -26.185 1.00 62.74 A
ATOM 573 C GLU A 77 -11.556 -50.398 -25.935 1.00 60.64 A
ATOM 574 O GLU A 77 -10.852 -49.772 -26.726 1.00 61.52 A

ATOM 575 N PRO A 78 -11.393 -51.695 -25.695 1.00 61.01 A
ATOM 576 CD PRO A 78 -11.494 -52.204 -24.316 1.00 61.12 A
ATOM 577 CA PRO A 78 -10.520 -52.528 -26.528 1.00 60.53 A
ATOM 578 CB PRO A 78 -9.875 -53.475 -25.514 1.00 59.65 A
ATOM 579 CG PRO A 78 -10.862 -53.563 -24.407 1.00 60.73 A
ATOM 580 C PRO A 78 -11.312 -53.325 -27.560 1.00 59.82 A
ATOM 581 O PRO A 78 -10.735 -54.110 -28.313 1.00 60.64 A
ATOM 582 N ILE A 79 -12.624 -53.118 -27.587 1.00 57.90 A
ATOM 583 CA ILE A 79 -13.522 -53.929 -28.417 1.00 55.78 A
ATOM 584 CB ILE A 79 -14.293 -54.952 -27.534 1.00 54.00 A
ATOM 585 CG2 ILE A 79 -13.297 -55.791 -26.734 1.00 52.40 A
ATOM 586 CG1 ILE A 79 -15.250 -54.213 -26.583 1.00 53.15 A
ATOM 587 CD1 ILE A 79 -16.078 -55.128 -25.688 1.00 52.14 A
ATOM 588 C ILE A 79 -14.538 -53.172 -29.267 1.00 55.56 A
ATOM 589 O ILE A 79 -14.854 -53.606 -30.380 1.00 56.00 A
ATOM 590 N TRP A 80 -15.071 -52.063 -28.748 1.00 55.26 A
ATOM 591 CA TRP A 80 -16.033 -51.285 -29.528 1.00 55.10 A
ATOM 592 CB TRP A 80 -16.476 -50.014 -28.769 1.00 53.44 A
ATOM 593 CG TRP A 80 -15.518 -48.878 -28.890 1.00 52.46 A
ATOM 594 CD2 TRP A 80 -15.667 -47.715 -29.722 1.00 52.02 A
ATOM 595 CE2 TRP A 80 -14.492 -46.925 -29.567 1.00 51.92 A
ATOM 596 CE3 TRP A 80 -16.676 -47.262 -30.587 1.00 50.25 A
ATOM 597 CD1 TRP A 80 -14.298 -48.756 -28.276 1.00 52.46 A
ATOM 598 NE1 TRP A 80 -13.669 -47.581 -28.682 1.00 52.56 A
ATOM 599 CZ2 TRP A 80 -14.302 -45.709 -30.244 1.00 51.11 A
ATOM 600 CZ3 TRP A 80 -16.485 -46.048 -31.262 1.00 49.92 A
ATOM 601 CH2 TRP A 80 -15.306 -45.287 -31.083 1.00 49.97 A
ATOM 602 C TRP A 80 -15.229 -50.939 -30.789 1.00 56.29 A
ATOM 603 O TRP A 80 -13.996 -51.086 -30.799 1.00 57.19 A
ATOM 604 N GLN A 81 -15.910 -50.478 -31.838 1.00 56.41 A
ATOM 605 CA GLN A 81 -15.247 -50.173 -33.120 1.00 56.79 A
ATOM 606 CB GLN A 81 -13.815 -49.648 -32.952 1.00 56.42 A
ATOM 607 CG GLN A 81 -13.674 -48.181 -32.610 1.00 57.42 A
ATOM 608 CD GLN A 81 -12.196 -47.785 -32.424 1.00 58.57 A

ATOM 609 OE1 GLN A 81 -11.810 -46.612 -32.663 1.00 60.36 A
ATOM 610 NE2 GLN A 81 -11.362 -48.755 -31.999 1.00 57.53 A
ATOM 611 C GLN A 81 -15.159 -51.506 -33.848 1.00 57.17 A
ATOM 612 O GLN A 81 -14.639 -51.588 -34.964 1.00 58.27 A
ATOM 613 N ASN A 82 -15.646 -52.552 -33.196 1.00 56.91 A
ATOM 614 CA ASN A 82 -15.749 -53.890 -33.774 1.00 55.27 A
ATOM 615 CB ASN A 82 -14.704 -54.815 -33.217 1.00 55.80 A
ATOM 616 CG ASN A 82 -13.791 -55.376 -34.269 1.00 57.41 A
ATOM 617 OD1 ASN A 82 -14.046 -56.424 -34.824 1.00 58.53 A
ATOM 618 ND2 ASN A 82 -12.739 -54.665 -34.570 1.00 57.16 A
ATOM 619 C ASN A 82 -17.072 -54.449 -33.470 1.00 54.15 A
ATOM 620 O ASN A 82 -17.333 -55.573 -33.678 1.00 54.13 A
ATOM 621 N PHE A 83 -17.914 -53.615 -32.966 1.00 53.32 A
ATOM 622 CA PHE A 83 -19.298 -53.993 -32.682 1.00 52.75 A
ATOM 623 CB PHE A 83 -19.961 -52.974 -31.744 1.00 52.99 A
ATOM 624 CG PHE A 83 -19.451 -53.012 -30.320 1.00 53.49 A
ATOM 625 CD1 PHE A 83 -18.467 -53.921 -29.926 1.00 53.30 A
ATOM 626 CD2 PHE A 83 -19.966 -52.126 -29.365 1.00 53.02 A
ATOM 627 CE1 PHE A 83 -18.005 -53.947 -28.602 1.00 52.91 A
ATOM 628 CE2 PHE A 83 -19.513 -52.141 -28.041 1.00 51.24 A
ATOM 629 CZ PHE A 83 -18.531 -53.051 -27.659 1.00 52.10 A
ATOM 630 C PHE A 83 -20.079 -54.046 -33.995 1.00 51.90 A
ATOM 631 O PHE A 83 -19.843 -53.241 -34.897 1.00 52.34 A
ATOM 632 N THR A 84 -21.009 -54.990 -34.093 1.00 50.65 A
ATOM 633 CA THR A 84 -21.821 -55.154 -35.294 1.00 49.65 A
ATOM 634 CB THR A 84 -22.723 -56.391 -35.196 1.00 50.02 A
ATOM 635 OG1 THR A 84 -21.929 -57.544 -34.897 1.00 50.23 A
ATOM 636 CG2 THR A 84 -23.459 -56.604 -36.508 1.00 50.80 A
ATOM 637 C THR A 84 -22.725 -53.957 -35.556 1.00 48.61 A
ATOM 638 O THR A 84 -22.694 -53.376 -36.638 1.00 47.86 A
ATOM 639 N ASP A 85 -23.529 -53.605 -34.557 1.00 48.44 A
ATOM 640 CA ASP A 85 -24.467 -52.493 -34.659 1.00 48.10 A
ATOM 641 CB ASP A 85 -25.390 -52.482 -33.444 1.00 47.03 A
ATOM 642 CG ASP A 85 -26.481 -51.455 -33.566 1.00 48.01 A

ATOM 643 OD1 ASP A 85 -27.418 -51.465 -32.736 1.00 48.68 A
ATOM 644 OD2 ASP A 85 -26.399 -50.630 -34.496 1.00 48.69 A
ATOM 645 C ASP A 85 -23.752 -51.153 -34.773 1.00 48.42 A
ATOM 646 O ASP A 85 -23.115 -50.702 -33.829 1.00 48.21 A
ATOM 647 N PRO A 86 -23.856 -50.493 -35.936 1.00 49.03 A
ATOM 648 CD PRO A 86 -24.578 -50.853 -37.167 1.00 49.00 A
ATOM 649 CA PRO A 86 -23.184 -49.203 -36.093 1.00 49.13 A
ATOM 650 CB PRO A 86 -23.457 -48.841 -37.553 1.00 48.95 A
ATOM 651 CG PRO A 86 -23.747 -50.169 -38.207 1.00 48.99 A
ATOM 652 C PRO A 86 -23.770 -48.187 -35.124 1.00 49.61 A
ATOM 653 O PRO A 86 -23.040 -47.430 -34.491 1.00 49.97 A
ATOM 654 N GLN A 87 -25.045 -48.125 -34.995 1.00 50.12 A
ATOM 655 CA GLN A 87 -25.498 -47.134 -34.133 1.00 51.27 A
ATOM 656 CB GLN A 87 -26.977 -47.077 -34.155 1.00 51.50 A
ATOM 657 CG GLN A 87 -27.490 -46.342 -35.342 1.00 54.67 A
ATOM 658 CD GLN A 87 -28.250 -47.170 -36.303 1.00 57.26 A
ATOM 659 OE1 GLN A 87 -29.052 -47.962 -35.905 1.00 60.25 A
ATOM 660 NE2 GLN A 87 -28.015 -46.992 -37.574 1.00 57.43 A
ATOM 661 C GLN A 87 -24.872 -47.349 -32.794 1.00 52.10 A
ATOM 662 O GLN A 87 -24.246 -46.491 -32.313 1.00 53.35 A
ATOM 663 N LEU A 88 -24.924 -48.523 -32.196 1.00 51.21 A
ATOM 664 CA LEU A 88 -24.330 -48.714 -30.874 1.00 49.23 A
ATOM 665 CB LEU A 88 -24.393 -50.193 -30.471 1.00 49.24 A
ATOM 666 CG LEU A 88 -23.777 -50.669 -29.141 1.00 49.77 A
ATOM 667 CD1 LEU A 88 -24.507 -50.073 -27.951 1.00 48.62 A
ATOM 668 CD2 LEU A 88 -23.847 -52.195 -29.081 1.00 50.00 A
ATOM 669 C LEU A 88 -22.896 -48.209 -30.749 1.00 48.48 A
ATOM 670 O LEU A 88 -22.607 -47.400 -29.870 1.00 49.03 A
ATOM 671 N ARG A 89 -21.994 -48.665 -31.616 1.00 47.79 A
ATOM 672 CA ARG A 89 -20.612 -48.215 -31.500 1.00 47.24 A
ATOM 673 CB ARG A 89 -19.652 -49.076 -32.349 1.00 47.26 A
ATOM 674 CG ARG A 89 -19.785 -49.008 -33.844 1.00 48.24 A
ATOM 675 CD ARG A 89 -18.722 -49.918 -34.476 1.00 50.14 A
ATOM 676 NE ARG A 89 -18.695 -49.851 -35.941 1.00 51.64 A

ATOM 677 CZ ARG A 89 -19.684 -50.255 -36.741 1.00 51.94 A
ATOM 678 NH1 ARG A 89 -20.800 -50.766 -36.231 1.00 52.24 A
ATOM 679 NH2 ARG A 89 -19.559 -50.143 -38.058 1.00 51.57 A
ATOM 680 C ARG A 89 -20.412 -46.727 -31.769 1.00 45.67 A
ATOM 681 O ARG A 89 -19.369 -46.173 -31.426 1.00 45.43 A
ATOM 682 N ARG A 90 -21.408 -46.071 -32.361 1.00 44.45 A
ATOM 683 CA ARG A 90 -21.299 -44.631 -32.595 1.00 44.51 A
ATOM 684 CB ARG A 90 -22.147 -44.196 -33.814 1.00 46.30 A
ATOM 685 CG ARG A 90 -21.398 -44.291 -35.177 1.00 49.20 A
ATOM 686 CD ARG A 90 -22.317 -44.118 -36.414 1.00 49.75 A
ATOM 687 NE ARG A 90 -22.788 -42.744 -36.631 1.00 50.61 A
ATOM 688 CZ ARG A 90 -22.255 -41.885 -37.502 1.00 49.63 A
ATOM 689 NH1 ARG A 90 -21.223 -42.246 -38.253 1.00 49.15 A
ATOM 690 NH2 ARG A 90 -22.759 -40.661 -37.627 1.00 48.54 A
ATOM 691 C ARG A 90 -21.738 -43.898 -31.317 1.00 42.92 A
ATOM 692 O ARG A 90 -21.363 -42.750 -31.083 1.00 42.67 A
ATOM 693 N ILE A 91 -22.524 -44.588 -30.489 1.00 41.52 A
ATOM 694 CA ILE A 91 -23.009 -44.047 -29.222 1.00 38.47 A
ATOM 695 CB ILE A 91 -24.278 -44.777 -28.714 1.00 35.72 A
ATOM 696 CG2 ILE A 91 -24.553 -44.395 -27.281 1.00 34.23 A
ATOM 697 CG1 ILE A 91 -25.479 -44.405 -29.572 1.00 34.21 A
ATOM 698 CD1 ILE A 91 -26.770 -44.960 -29.067 1.00 32.27 A
ATOM 699 C ILE A 91 -21.921 -44.234 -28.184 1.00 38.12 A
ATOM 700 O ILE A 91 -21.547 -43.295 -27.491 1.00 38.43 A
ATOM 701 N ILE A 92 -21.445 -45.486 -28.059 1.00 37.74 A
ATOM 702 CA ILE A 92 -20.373 -45.747 -27.107 1.00 38.22 A
ATOM 703 CB ILE A 92 -19.958 -47.230 -27.155 1.00 36.72 A
ATOM 704 CG2 ILE A 92 -18.625 -47.433 -26.451 1.00 35.58 A
ATOM 705 CG1 ILE A 92 -21.041 -48.108 -26.525 1.00 35.09 A
ATOM 706 CD1 ILE A 92 -20.615 -49.542 -26.308 0.00 35.60 A
ATOM 707 C ILE A 92 -19.164 -44.857 -27.377 1.00 38.61 A
ATOM 708 O ILE A 92 -18.522 -44.341 -26.498 1.00 38.70 A
ATOM 709 N GLY A 93 -18.944 -44.609 -28.696 1.00 38.89 A
ATOM 710 CA GLY A 93 -17.838 -43.758 -29.095 1.00 40.10 A

ATOM 711 C GLY A 93 -18.049 -42.301 -28.726 1.00 40.28 A
ATOM 712 O GLY A 93 -17.098 -41.529 -28.633 1.00 39.96 A
ATOM 713 N ALA A 94 -19.304 -41.920 -28.521 1.00 40.47 A
ATOM 714 CA ALA A 94 -19.642 -40.553 -28.149 1.00 40.27 A
ATOM 715 CB ALA A 94 -21.064 -40.230 -28.583 1.00 40.56 A
ATOM 716 C ALA A 94 -19.520 -40.418 -26.643 1.00 40.83 A
ATOM 717 O ALA A 94 -19.254 -39.340 -26.110 1.00 41.36 A
ATOM 718 N VAL A 95 -19.720 -41.530 -25.954 1.00 41.07 A
ATOM 719 CA VAL A 95 -19.639 -41.534 -24.512 1.00 41.37 A
ATOM 720 CB VAL A 95 -20.485 -42.688 -23.934 1.00 42.10 A
ATOM 721 CG1 VAL A 95 -20.365 -42.728 -22.409 1.00 42.19 A
ATOM 722 CG2 VAL A 95 -21.949 -42.497 -24.346 1.00 41.38 A
ATOM 723 C VAL A 95 -18.194 -41.630 -24.036 1.00 41.51 A
ATOM 724 O VAL A 95 -17.828 -41.007 -23.041 1.00 40.85 A
ATOM 725 N ARG A 96 -17.362 -42.381 -24.751 1.00 41.72 A
ATOM 726 CA ARG A 96 -15.973 -42.510 -24.335 1.00 42.44 A
ATOM 727 CB ARG A 96 -15.273 -43.630 -25.124 1.00 43.77 A
ATOM 728 CG ARG A 96 -14.501 -43.215 -26.360 1.00 47.25 A
ATOM 729 CD ARG A 96 -13.413 -44.257 -26.653 1.00 50.07 A
ATOM 730 NE ARG A 96 -12.300 -43.739 -27.451 1.00 52.85 A
ATOM 731 CZ ARG A 96 -11.661 -42.591 -27.214 1.00 54.59 A
ATOM 732 NH1 ARG A 96 -10.657 -42.216 -27.998 1.00 55.63 A
ATOM 733 NH2 ARG A 96 -12.028 -41.800 -26.211 1.00 55.31 A
ATOM 734 C ARG A 96 -15.204 -41.180 -24.431 1.00 42.07 A
ATOM 735 O ARG A 96 -14.075 -41.060 -23.943 1.00 42.27 A
ATOM 736 N THR A 97 -15.822 -40.175 -25.043 1.00 41.50 A
ATOM 737 CA THR A 97 -15.187 -38.867 -25.152 1.00 41.17 A
ATOM 738 CB THR A 97 -15.441 -38.200 -26.516 1.00 41.06 A
ATOM 739 OG1 THR A 97 -14.725 -38.910 -27.531 1.00 41.49 A
ATOM 740 CG2 THR A 97 -14.965 -36.749 -26.500 1.00 40.26 A
ATOM 741 C THR A 97 -15.735 -37.972 -24.055 1.00 40.87 A
ATOM 742 O THR A 97 -16.857 -37.461 -24.148 1.00 39.84 A
ATOM 743 N LEU A 98 -14.913 -37.798 -23.022 1.00 40.81 A
ATOM 744 CA LEU A 98 -15.240 -37.000 -21.845 1.00 40.71 A

ATOM 745 CB LEU A 98 -14.229 -37.300 -20.736 1.00 40.95 A
ATOM 746 CG LEU A 98 -14.339 -38.715 -20.157 1.00 41.19 A
ATOM 747 CD1 LEU A 98 -13.132 -39.035 -19.263 1.00 40.57 A
ATOM 748 CD2 LEU A 98 -15.642 -38.821 -19.379 1.00 40.31 A
ATOM 749 C LEU A 98 -15.307 -35.496 -22.065 1.00 40.30 A
ATOM 750 O LEU A 98 -16.164 -34.812 -21.495 1.00 40.27 A
ATOM 751 N GLY A 99 -14.406 -34.974 -22.882 1.00 39.82 A
ATOM 752 CA GLY A 99 -14.417 -33.548 -23.117 1.00 40.31 A
ATOM 753 C GLY A 99 -13.775 -32.844 -21.943 1.00 41.13 A
ATOM 754 O GLY A 99 -12.667 -33.200 -21.537 1.00 40.81 A
ATOM 755 N SER A 100 -14.474 -31.874 -21.395 1.00 41.93 A
ATOM 756 CA SER A 100 -14.090 -31.107 -20.208 1.00 42.37 A
ATOM 757 CB SER A 100 -15.121 -30.066 -19.965 1.00 41.64 A
ATOM 758 OG SER A 100 -16.066 -30.166 -20.977 1.00 43.45 A
ATOM 759 C SER A 100 -14.045 -31.892 -18.968 1.00 42.69 A
ATOM 760 O SER A 100 -13.487 -31.483 -18.009 1.00 43.42 A
ATOM 761 N ALA A 101 -14.687 -33.015 -18.978 1.00 41.83 A
ATOM 762 CA ALA A 101 -14.911 -33.774 -17.761 1.00 40.33 A
ATOM 763 CB ALA A 101 -16.007 -34.786 -17.974 1.00 41.06 A
ATOM 764 C ALA A 101 -13.663 -34.462 -17.229 1.00 39.60 A
ATOM 765 O ALA A 101 -13.655 -34.903 -16.077 1.00 39.24 A
ATOM 766 N ASN A 102 -12.606 -34.381 -18.025 1.00 38.65 A
ATOM 767 CA ASN A 102 -11.359 -35.035 -17.744 1.00 38.23 A
ATOM 768 CB ASN A 102 -10.537 -35.245 -18.958 1.00 39.91 A
ATOM 769 CG ASN A 102 -11.015 -36.205 -19.819 1.00 40.76 A
ATOM 770 OD1 ASN A 102 -10.811 -37.351 -19.651 1.00 42.53 A
ATOM 771 ND2 ASN A 102 -11.504 -35.749 -20.872 1.00 40.72 A
ATOM 772 C ASN A 102 -10.442 -34.164 -17.024 1.00 36.74 A
ATOM 773 O ASN A 102 -9.287 -34.442 -16.937 1.00 36.79 A
ATOM 774 N LEU A 103 -10.939 -33.058 -16.583 1.00 34.65 A
ATOM 775 CA LEU A 103 -10.129 -31.997 -16.005 1.00 32.93 A
ATOM 776 CB LEU A 103 -10.595 -30.632 -16.509 1.00 34.08 A
ATOM 777 CG LEU A 103 -10.469 -30.233 -17.978 1.00 35.00 A
ATOM 778 CD1 LEU A 103 -11.447 -29.100 -18.270 1.00 36.49 A

ATOM 779 CD2 LEU A 103 -9.043 -29.800 -18.287 1.00 34.67 A
ATOM 780 C LEU A 103 -10.361 -32.049 -14.502 1.00 31.83 A
ATOM 781 O LEU A 103 -11.482 -32.272 -14.053 1.00 32.44 A
ATOM 782 N PRO A 104 -9.310 -31.861 -13.699 1.00 30.30 A
ATOM 783 CD PRO A 104 -7.882 -31.725 -14.023 1.00 30.09 A
ATOM 784 CA PRO A 104 -9.527 -31.895 -12.249 1.00 28.80 A
ATOM 785 CB PRO A 104 -8.133 -31.632 -11.685 1.00 29.17 A
ATOM 786 CG PRO A 104 -7.381 -30.985 -12.831 1.00 30.47 A
ATOM 787 C PRO A 104 -10.570 -30.848 -11.824 1.00 28.11 A
ATOM 788 O PRO A 104 -10.755 -29.839 -12.509 1.00 26.88 A
ATOM 789 N LEU A 105 -11.248 -31.095 -10.702 1.00 28.53 A
ATOM 790 CA LEU A 105 -12.303 -30.205 -10.196 1.00 29.32 A
ATOM 791 CB LEU A 105 -12.632 -30.530 -8.741 1.00 29.17 A
ATOM 792 CG LEU A 105 -14.035 -30.194 -8.208 1.00 28.47 A
ATOM 793 CD1 LEU A 105 -13.925 -30.027 -6.708 1.00 29.08 A
ATOM 794 CD2 LEU A 105 -14.601 -28.939 -8.811 1.00 26.46 A
ATOM 795 C LEU A 105 -12.005 -28.713 -10.285 1.00 29.64 A
ATOM 796 O LEU A 105 -12.817 -27.950 -10.807 1.00 28.80 A
ATOM 797 N ALA A 106 -10.862 -28.291 -9.748 1.00 29.79 A
ATOM 798 CA ALA A 106 -10.490 -26.876 -9.779 1.00 28.52 A
ATOM 799 CB ALA A 106 -9.076 -26.691 -9.245 1.00 27.87 A
ATOM 800 C ALA A 106 -10.578 -26.340 -11.201 1.00 28.31 A
ATOM 801 O ALA A 106 -11.208 -25.309 -11.450 1.00 27.60 A
ATOM 802 N LYS A 107 -9.945 -27.062 -12.124 1.00 27.85 A
ATOM 803 CA LYS A 107 -9.911 -26.698 -13.534 1.00 25.63 A
ATOM 804 CB LYS A 107 -8.931 -27.609 -14.261 1.00 23.73 A
ATOM 805 CG LYS A 107 -7.494 -27.150 -14.105 1.00 20.29 A
ATOM 806 CD LYS A 107 -6.514 -28.187 -14.598 1.00 18.99 A
ATOM 807 CE LYS A 107 -5.150 -27.580 -14.745 1.00 17.99 A
ATOM 808 NZ LYS A 107 -4.152 -28.574 -15.176 1.00 19.62 A
ATOM 809 C LYS A 107 -11.266 -26.688 -14.237 1.00 26.12 A
ATOM 810 O LYS A 107 -11.481 -25.884 -15.139 1.00 26.42 A
ATOM 811 N ARG A 108 -12.180 -27.569 -13.848 1.00 26.37 A
ATOM 812 CA ARG A 108 -13.497 -27.555 -14.470 1.00 27.13 A

ATOM 813 CB ARG A 108 -14.385 -28.674 -13.945 1.00 27.68 A
ATOM 814 CG ARG A 108 -13.895 -30.063 -14.241 1.00 30.61 A
ATOM 815 CD ARG A 108 -14.904 -31.058 -13.729 1.00 33.36 A
ATOM 816 NE ARG A 108 -14.448 -32.434 -13.829 1.00 34.98 A
ATOM 817 CZ ARG A 108 -15.071 -33.447 -13.243 1.00 37.21 A
ATOM 818 NH1 ARG A 108 -16.168 -33.215 -12.522 1.00 37.85 A
ATOM 819 NH2 ARG A 108 -14.608 -34.687 -13.371 1.00 37.76 A
ATOM 820 C ARG A 108 -14.144 -26.247 -14.094 1.00 26.77 A
ATOM 821 O ARG A 108 -14.752 -25.573 -14.920 1.00 25.96 A
ATOM 822 N GLN A 109 -14.003 -25.899 -12.822 1.00 28.19 A
ATOM 823 CA GLN A 109 -14.586 -24.683 -12.285 1.00 30.11 A
ATOM 824 CB GLN A 109 -14.324 -24.599 -10.781 1.00 31.86 A
ATOM 825 CG GLN A 109 -15.095 -25.639 -9.991 1.00 34.48 A
ATOM 826 CD GLN A 109 -14.697 -25.698 -8.523 1.00 37.17 A
ATOM 827 OE1 GLN A 109 -13.516 -25.824 -8.181 1.00 37.80 A
ATOM 828 NE2 GLN A 109 -15.689 -25.627 -7.645 1.00 38.86 A
ATOM 829 C GLN A 109 -14.055 -23.460 -12.993 1.00 29.95 A
ATOM 830 O GLN A 109 -14.819 -22.557 -13.327 1.00 30.00 A
ATOM 831 N GLN A 110 -12.747 -23.428 -13.218 1.00 29.25 A
ATOM 832 CA GLN A 110 -12.140 -22.304 -13.925 1.00 28.38 A
ATOM 833 CB GLN A 110 -10.632 -22.501 -14.066 1.00 27.82 A
ATOM 834 CG GLN A 110 -9.895 -22.419 -12.755 1.00 28.73 A
ATOM 835 CD GLN A 110 -8.477 -22.899 -12.872 1.00 29.68 A
ATOM 836 OE1 GLN A 110 -7.863 -22.803 -13.939 1.00 30.04 A
ATOM 837 NE2 GLN A 110 -7.931 -23.406 -11.769 1.00 29.66 A
ATOM 838 C GLN A 110 -12.785 -22.295 -15.293 1.00 28.27 A
ATOM 839 O GLN A 110 -13.296 -21.276 -15.750 1.00 28.29 A
ATOM 840 N TYR A 111 -12.773 -23.454 -15.933 1.00 28.45 A
ATOM 841 CA TYR A 111 -13.370 -23.597 -17.242 1.00 29.11 A
ATOM 842 CB TYR A 111 -13.489 -25.078 -17.601 1.00 29.47 A
ATOM 843 CG TYR A 111 -13.825 -25.354 -19.049 1.00 31.04 A
ATOM 844 CD1 TYR A 111 -12.908 -25.086 -20.069 1.00 31.34 A
ATOM 845 CE1 TYR A 111 -13.218 -25.355 -21.407 1.00 31.78 A
ATOM 846 CD2 TYR A 111 -15.061 -25.893 -19.401 1.00 32.35 A

ATOM 847 CE2 TYR A 111 -15.381 -26.158 -20.727 1.00 32.85 A
ATOM 848 CZ TYR A 111 -14.461 -25.889 -21.727 1.00 32.48 A
ATOM 849 OH TYR A 111 -14.807 -26.147 -23.038 1.00 32.34 A
ATOM 850 C TYR A 111 -14.751 -22.940 -17.217 1.00 29.25 A
ATOM 851 O TYR A 111 -14.931 -21.846 -17.757 1.00 30.77 A
ATOM 852 N ASN A 112 -15.715 -23.581 -16.565 1.00 27.39 A
ATOM 853 CA ASN A 112 -17.072 -23.046 -16.512 1.00 25.95 A
ATOM 854 CB ASN A 112 -17.905 -23.848 -15.520 1.00 27.89 A
ATOM 855 CG ASN A 112 -17.699 -25.340 -15.666 1.00 29.65 A
ATOM 856 OD1 ASN A 112 -17.919 -25.911 -16.733 1.00 31.17 A
ATOM 857 ND2 ASN A 112 -17.270 -25.982 -14.590 1.00 31.16 A
ATOM 858 C ASN A 112 -17.166 -21.552 -16.183 1.00 25.27 A
ATOM 859 O ASN A 112 -18.080 -20.871 -16.646 1.00 23.98 A
ATOM 860 N ALA A 113 -16.234 -21.035 -15.386 1.00 24.99 A
ATOM 861 CA ALA A 113 -16.255 -19.613 -15.032 1.00 24.81 A
ATOM 862 CB ALA A 113 -15.208 -19.319 -13.987 1.00 23.79 A
ATOM 863 C ALA A 113 -15.979 -18.790 -16.290 1.00 25.80 A
ATOM 864 O ALA A 113 -16.733 -17.870 -16.641 1.00 24.90 A
ATOM 865 N LEU A 114 -14.885 -19.130 -16.966 1.00 25.59 A
ATOM 866 CA LEU A 114 -14.504 -18.451 -18.190 1.00 24.87 A
ATOM 867 CB LEU A 114 -13.347 -19.199 -18.844 1.00 20.71 A
ATOM 868 CG LEU A 114 -12.061 -19.135 -18.019 1.00 19.30 A
ATOM 869 CD1 LEU A 114 -11.064 -20.134 -18.530 1.00 19.65 A
ATOM 870 CD2 LEU A 114 -11.475 -17.739 -18.080 1.00 19.14 A
ATOM 871 C LEU A 114 -15.717 -18.393 -19.123 1.00 26.88 A
ATOM 872 O LEU A 114 -16.132 -17.315 -19.553 1.00 27.99 A
ATOM 873 N LEU A 115 -16.307 -19.548 -19.412 1.00 27.38 A
ATOM 874 CA LEU A 115 -17.456 -19.584 -20.288 1.00 27.82 A
ATOM 875 CB LEU A 115 -17.996 -21.012 -20.371 1.00 27.65 A
ATOM 876 CG LEU A 115 -17.137 -21.958 -21.228 1.00 27.67 A
ATOM 877 CD1 LEU A 115 -17.620 -23.379 -21.104 1.00 27.70 A
ATOM 878 CD2 LEU A 115 -17.198 -21.517 -22.675 1.00 28.16 A
ATOM 879 C LEU A 115 -18.567 -18.595 -19.930 1.00 29.10 A
ATOM 880 O LEU A 115 -18.958 -17.787 -20.769 1.00 30.86 A

ATOM 881 N SER A 116 -19.077 -18.617 -18.703 1.00 29.96 A
ATOM 882 CA SER A 116 -20.155 -17.676 -18.380 1.00 30.94 A
ATOM 883 CB SER A 116 -20.885 -18.051 -17.073 1.00 30.73 A
ATOM 884 OG SER A 116 -19.988 -18.277 -16.015 1.00 32.17 A
ATOM 885 C SER A 116 -19.672 -16.238 -18.332 1.00 31.08 A
ATOM 886 O SER A 116 -20.460 -15.317 -18.512 1.00 31.95 A
ATOM 887 N ASN A 117 -18.428 -16.043 -18.085 1.00 31.34 A
ATOM 888 CA ASN A 117 -17.908 -14.730 -18.078 1.00 33.07 A
ATOM 889 CB ASN A 117 -16.606 -14.739 -17.336 1.00 34.95 A
ATOM 890 CG ASN A 117 -16.774 -14.639 -15.883 1.00 36.53 A
ATOM 891 OD1 ASN A 117 -17.845 -14.748 -15.375 1.00 38.73 A
ATOM 892 ND2 ASN A 117 -15.716 -14.374 -15.203 1.00 38.26 A
ATOM 893 C ASN A 117 -17.782 -14.126 -19.460 1.00 32.72 A
ATOM 894 O ASN A 117 -18.392 -13.142 -19.725 1.00 33.47 A
ATOM 895 N MET A 118 -17.063 -14.767 -20.380 1.00 30.95 A
ATOM 896 CA MET A 118 -16.898 -14.336 -21.757 1.00 27.90 A
ATOM 897 CB MET A 118 -16.178 -15.411 -22.561 1.00 25.75 A
ATOM 898 CG MET A 118 -14.756 -15.652 -22.116 1.00 25.90 A
ATOM 899 SD MET A 118 -13.750 -16.503 -23.346 1.00 26.59 A
ATOM 900 CE MET A 118 -14.410 -18.166 -23.235 1.00 26.36 A
ATOM 901 C MET A 118 -18.244 -14.021 -22.389 1.00 27.71 A
ATOM 902 O MET A 118 -18.427 -12.963 -22.978 1.00 27.53 A
ATOM 903 N SER A 119 -19.197 -14.930 -22.255 1.00 28.05 A
ATOM 904 CA SER A 119 -20.510 -14.690 -22.835 1.00 29.94 A
ATOM 905 CB SER A 119 -21.421 -15.900 -22.628 1.00 30.86 A
ATOM 906 OG SER A 119 -21.835 -15.985 -21.276 1.00 32.58 A
ATOM 907 C SER A 119 -21.154 -13.468 -22.192 1.00 29.70 A
ATOM 908 O SER A 119 -21.998 -12.810 -22.801 1.00 31.63 A
ATOM 909 N ARG A 120 -20.752 -13.177 -20.959 1.00 28.16 A
ATOM 910 CA ARG A 120 -21.290 -12.042 -20.222 1.00 26.54 A
ATOM 911 CB ARG A 120 -21.063 -12.224 -18.716 1.00 25.66 A
ATOM 912 CG ARG A 120 -21.868 -11.263 -17.834 1.00 25.14 A
ATOM 913 CD ARG A 120 -20.965 -10.299 -17.103 1.00 24.89 A
ATOM 914 NE ARG A 120 -19.960 -11.029 -16.347 1.00 26.61 A

ATOM 915 CZ ARG A 120 -18.762 -10.545 -16.051 1.00 27.77 A
ATOM 916 NH1 ARG A 120 -18.438 -9.325 -16.452 1.00 27.49 A
ATOM 917 NH2 ARG A 120 -17.886 -11.286 -15.377 1.00 28.41 A
ATOM 918 C ARG A 120 -20.614 -10.774 -20.697 1.00 26.24 A
ATOM 919 O ARG A 120 -21.269 -9.767 -20.967 1.00 26.86 A
ATOM 920 N ILE A 121 -19.294 -10.822 -20.799 1.00 25.93 A
ATOM 921 CA ILE A 121 -18.548 -9.670 -21.256 1.00 26.42 A
ATOM 922 CB ILE A 121 -17.045 -9.957 -21.270 1.00 24.74 A
ATOM 923 CG2 ILE A 121 -16.309 -8.848 -22.000 1.00 23.96 A
ATOM 924 CG1 ILE A 121 -16.546 -10.110 -19.834 1.00 23.30 A
ATOM 925 CD1 ILE A 121 -15.076 -10.422 -19.721 1.00 23.70 A
ATOM 926 C ILE A 121 -19.010 -9.356 -22.662 1.00 28.33 A
ATOM 927 O ILE A 121 -19.175 -8.195 -23.031 1.00 28.63 A
ATOM 928 N TYR A 122 -19.249 -10.403 -23.439 1.00 30.14 A
ATOM 929 CA TYR A 122 -19.674 -10.215 -24.807 1.00 32.14 A
ATOM 930 CB TYR A 122 -19.659 -11.536 -25.571 1.00 32.05 A
ATOM 931 CG TYR A 122 -20.037 -11.324 -27.012 1.00 32.77 A
ATOM 932 CD1 TYR A 122 -19.105 -10.862 -27.936 1.00 32.36 A
ATOM 933 CE1 TYR A 122 -19.489 -10.514 -29.228 1.00 32.09 A
ATOM 934 CD2 TYR A 122 -21.361 -11.446 -27.423 1.00 33.54 A
ATOM 935 CE2 TYR A 122 -21.750 -11.098 -28.714 1.00 33.15 A
ATOM 936 CZ TYR A 122 -20.814 -10.630 -29.602 1.00 31.88 A
ATOM 937 OH TYR A 122 -21.223 -10.244 -30.846 1.00 31.70 A
ATOM 938 C TYR A 122 -21.053 -9.589 -24.955 1.00 33.94 A
ATOM 939 O TYR A 122 -21.253 -8.721 -25.806 1.00 33.72 A
ATOM 940 N SER A 123 -22.004 -10.020 -24.134 1.00 35.50 A
ATOM 941 CA SER A 123 -23.361 -9.501 -24.237 1.00 37.50 A
ATOM 942 CB SER A 123 -24.360 -10.644 -24.036 1.00 38.28 A
ATOM 943 OG SER A 123 -24.221 -11.631 -25.054 1.00 41.46 A
ATOM 944 C SER A 123 -23.716 -8.324 -23.326 1.00 38.31 A
ATOM 945 O SER A 123 -24.865 -7.880 -23.289 1.00 39.61 A
ATOM 946 N THR A 124 -22.736 -7.804 -22.602 1.00 38.42 A
ATOM 947 CA THR A 124 -22.983 -6.677 -21.720 1.00 38.79 A
ATOM 948 CB THR A 124 -22.378 -6.907 -20.330 1.00 39.60 A

ATOM 949 OG1 THR A 124 -22.860 -8.140 -19.801 1.00 39.76 A
ATOM 950 CG2 THR A 124 -22.765 -5.778 -19.382 1.00 41.57 A
ATOM 951 C THR A 124 -22.320 -5.452 -22.312 1.00 39.15 A
ATOM 952 O THR A 124 -22.689 -4.327 -22.000 1.00 40.07 A
ATOM 953 N ALA A 125 -21.332 -5.685 -23.167 1.00 39.32 A
ATOM 954 CA ALA A 125 -20.577 -4.606 -23.803 1.00 39.33 A
ATOM 955 CB ALA A 125 -19.678 -5.177 -24.893 1.00 40.00 A
ATOM 956 C ALA A 125 -21.448 -3.500 -24.382 1.00 38.70 A
ATOM 957 O ALA A 125 -22.508 -3.761 -24.953 1.00 38.85 A
ATOM 958 N LYS A 126 -20.989 -2.272 -24.234 1.00 37.41 A
ATOM 959 CA LYS A 126 -21.712 -1.113 -24.743 1.00 37.86 A
ATOM 960 CB LYS A 126 -22.572 -0.492 -23.641 1.00 35.30 A
ATOM 961 CG LYS A 126 -23.724 -1.372 -23.182 1.00 34.52 A
ATOM 962 CD LYS A 126 -24.544 -0.689 -22.100 0.00 34.72 A
ATOM 963 CE LYS A 126 -25.686 -1.574 -21.631 0.00 34.81 A
ATOM 964 NZ LYS A 126 -26.490 -0.922 -20.560 0.00 34.68 A
ATOM 965 C LYS A 126 -20.753 -0.071 -25.309 1.00 39.65 A
ATOM 966 O LYS A 126 -19.561 -0.101 -24.992 1.00 39.71 A
ATOM 967 N VAL A 127 -21.274 0.811 -26.136 1.00 41.52 A
ATOM 968 CA VAL A 127 -20.477 1.874 -26.731 1.00 44.12 A
ATOM 969 CB VAL A 127 -20.497 1.806 -28.280 1.00 42.32 A
ATOM 970 CG1 VAL A 127 -19.818 3.030 -28.861 1.00 41.94 A
ATOM 971 CG2 VAL A 127 -19.787 0.556 -28.755 1.00 41.10 A
ATOM 972 C VAL A 127 -21.052 3.213 -26.275 1.00 47.43 A
ATOM 973 O VAL A 127 -22.235 3.494 -26.480 1.00 48.37 A
ATOM 974 N CYS A 128 -20.210 4.035 -25.657 1.00 51.05 A
ATOM 975 CA CYS A 128 -20.649 5.314 -25.111 1.00 55.34 A
ATOM 976 C CYS A 128 -20.054 6.481 -25.891 1.00 58.26 A
ATOM 977 O CYS A 128 -18.947 6.386 -26.420 1.00 58.85 A
ATOM 978 CB CYS A 128 -20.272 5.423 -23.632 1.00 56.55 A
ATOM 979 SG CYS A 128 -20.762 4.000 -22.630 1.00 60.34 A
ATOM 980 N LEU A 129 -20.796 7.581 -25.957 1.00 61.34 A
ATOM 981 CA LEU A 129 -20.387 8.735 -26.749 1.00 65.49 A
ATOM 982 CB LEU A 129 -21.611 9.471 -27.298 1.00 66.04 A

ATOM 983 CG LEU A 129 -22.545 8.657 -28.195 1.00 67.33 A
ATOM 984 CD1 LEU A 129 -23.193 7.525 -27.412 1.00 67.31 A
ATOM 985 CD2 LEU A 129 -23.602 9.552 -28.825 1.00 67.76 A
ATOM 986 C LEU A 129 -19.526 9.689 -25.930 1.00 68.48 A
ATOM 987 O LEU A 129 -19.660 9.768 -24.708 1.00 69.09 A
ATOM 988 N PRO A 130 -18.642 10.413 -26.609 1.00 71.24 A
ATOM 989 CD PRO A 130 -18.625 10.614 -28.069 1.00 71.65 A
ATOM 990 CA PRO A 130 -17.480 11.022 -25.955 1.00 73.58 A
ATOM 991 CB PRO A 130 -16.869 11.879 -27.065 1.00 73.09 A
ATOM 992 CG PRO A 130 -17.261 11.189 -28.323 1.00 72.62 A
ATOM 993 C PRO A 130 -17.888 11.902 -24.778 1.00 75.45 A
ATOM 994 O PRO A 130 -17.423 11.689 -23.658 1.00 76.25 A
ATOM 995 N ALA A 131 -18.750 12.880 -25.035 1.00 76.95 A
ATOM 996 CA ALA A 131 -18.915 14.014 -24.133 1.00 78.20 A
ATOM 997 CB ALA A 131 -18.756 15.323 -24.892 1.00 78.57 A
ATOM 998 C ALA A 131 -20.266 13.966 -23.428 1.00 78.97 A
ATOM 999 O ALA A 131 -20.350 14.155 -22.214 1.00 79.61 A
ATOM 1000 N ALA A 132 -21.320 13.711 -24.196 1.00 79.44 A
ATOM 1001 CA ALA A 132 -22.523 13.084 -23.662 1.00 79.92 A
ATOM 1002 CB ALA A 132 -23.549 12.881 -24.766 1.00 79.50 A
ATOM 1003 C ALA A 132 -22.047 11.805 -22.979 1.00 80.51 A
ATOM 1004 O ALA A 132 -21.729 10.817 -23.642 1.00 81.45 A
ATOM 1005 N ALA A 133 -22.000 11.831 -21.652 1.00 80.60 A
ATOM 1006 CA ALA A 133 -21.816 10.616 -20.867 1.00 80.71 A
ATOM 1007 CB ALA A 133 -21.190 10.939 -19.519 1.00 80.73 A
ATOM 1008 C ALA A 133 -23.192 9.987 -20.679 1.00 80.64 A
ATOM 1009 O ALA A 133 -23.499 9.446 -19.616 1.00 81.87 A
ATOM 1010 N ALA A 134 -24.018 10.061 -21.718 1.00 79.37 A
ATOM 1011 CA ALA A 134 -25.338 9.442 -21.692 1.00 77.64 A
ATOM 1012 CB ALA A 134 -26.260 10.199 -20.748 1.00 77.18 A
ATOM 1013 C ALA A 134 -25.943 9.376 -23.091 1.00 76.11 A
ATOM 1014 O ALA A 134 -25.924 10.358 -23.833 1.00 75.64 A
ATOM 1015 N ALA A 135 -26.479 8.213 -23.443 1.00 73.99 A
ATOM 1016 CA ALA A 135 -26.035 6.955 -22.855 1.00 71.71 A

ATOM 1017 CB ALA A 135 -26.716 6.725 -21.515 1.00 71.45 A
ATOM 1018 C ALA A 135 -26.298 5.783 -23.796 1.00 69.72 A
ATOM 1019 O ALA A 135 -26.801 5.965 -24.904 1.00 69.55 A
ATOM 1020 N CYS A 136 -25.954 4.581 -23.347 1.00 66.91 A
ATOM 1021 CA CYS A 136 -25.192 3.661 -24.152 1.00 63.04 A
ATOM 1022 C CYS A 136 -25.757 3.166 -25.465 1.00 60.52 A
ATOM 1023 O CYS A 136 -26.933 2.952 -25.496 1.00 61.18 A
ATOM 1024 CB CYS A 136 -23.777 4.038 -24.137 1.00 63.64 A
ATOM 1025 SG CYS A 136 -23.037 3.962 -22.504 1.00 63.19 A
ATOM 1026 N TRP A 137 -24.998 2.925 -26.540 1.00 56.74 A
ATOM 1027 CA TRP A 137 -25.496 2.011 -27.562 1.00 53.00 A
ATOM 1028 CB TRP A 137 -24.915 2.372 -28.930 1.00 53.22 A
ATOM 1029 CG TRP A 137 -25.453 3.652 -29.491 1.00 52.74 A
ATOM 1030 CD2 TRP A 137 -24.817 4.505 -30.450 1.00 53.34 A
ATOM 1031 CE2 TRP A 137 -25.681 5.593 -30.685 1.00 53.26 A
ATOM 1032 CE3 TRP A 137 -23.598 4.460 -31.137 1.00 53.76 A
ATOM 1033 CD1 TRP A 137 -26.647 4.242 -29.190 1.00 52.29 A
ATOM 1034 NE1 TRP A 137 -26.792 5.408 -29.903 1.00 52.49 A
ATOM 1035 CZ2 TRP A 137 -25.368 6.620 -31.573 1.00 54.51 A
ATOM 1036 CZ3 TRP A 137 -23.290 5.481 -32.017 1.00 54.60 A
ATOM 1037 CH2 TRP A 137 -24.171 6.546 -32.228 1.00 55.17 A
ATOM 1038 C TRP A 137 -25.159 0.564 -27.215 1.00 50.69 A
ATOM 1039 O TRP A 137 -24.154 0.291 -26.559 1.00 50.68 A
ATOM 1040 N SER A 138 -26.005 -0.359 -27.661 1.00 48.30 A
ATOM 1041 CA SER A 138 -25.738 -1.781 -27.496 1.00 47.22 A
ATOM 1042 CB SER A 138 -26.810 -2.427 -26.629 1.00 47.36 A
ATOM 1043 OG SER A 138 -28.039 -2.497 -27.338 1.00 49.91 A
ATOM 1044 C SER A 138 -25.736 -2.476 -28.855 1.00 46.23 A
ATOM 1045 O SER A 138 -26.389 -2.026 -29.802 1.00 46.74 A
ATOM 1046 N LEU A 139 -25.000 -3.579 -28.948 1.00 44.33 A
ATOM 1047 CA LEU A 139 -25.027 -4.415 -30.142 1.00 43.44 A
ATOM 1048 CB LEU A 139 -24.104 -5.623 -29.974 1.00 42.26 A
ATOM 1049 CG LEU A 139 -23.668 -6.320 -31.265 1.00 41.48 A
ATOM 1050 CD1 LEU A 139 -22.912 -5.357 -32.168 1.00 40.20 A

ATOM 1051 CD2 LEU A 139 -22.823 -7.546 -30.956 1.00 41.40 A
ATOM 1052 C LEU A 139 -26.445 -4.877 -30.461 1.00 44.09 A
ATOM 1053 O LEU A 139 -26.767 -5.175 -31.610 1.00 44.26 A
ATOM 1054 N ALA A 140 -27.288 -4.934 -29.434 1.00 44.75 A
ATOM 1055 CA ALA A 140 -28.554 -5.652 -29.522 1.00 44.45 A
ATOM 1056 CB ALA A 140 -29.328 -5.523 -28.218 1.00 45.62 A
ATOM 1057 C ALA A 140 -29.392 -5.152 -30.692 1.00 44.51 A
ATOM 1058 O ALA A 140 -29.687 -5.903 -31.622 1.00 46.05 A
ATOM 1059 N PRO A 141 -29.774 -3.880 -30.640 1.00 43.55 A
ATOM 1060 CD PRO A 141 -30.362 -3.576 -29.324 1.00 42.16 A
ATOM 1061 CA PRO A 141 -30.522 -3.255 -31.736 1.00 42.50 A
ATOM 1062 CB PRO A 141 -31.819 -2.813 -31.058 1.00 40.78 A
ATOM 1063 CG PRO A 141 -31.431 -2.567 -29.642 1.00 41.73 A
ATOM 1064 C PRO A 141 -29.788 -2.044 -32.301 1.00 42.45 A
ATOM 1065 O PRO A 141 -29.740 -1.863 -33.517 1.00 42.34 A
ATOM 1066 N ASP A 142 -29.223 -1.225 -31.419 1.00 42.51 A
ATOM 1067 CA ASP A 142 -28.560 0.015 -31.832 1.00 41.53 A
ATOM 1068 CB ASP A 142 -28.075 0.769 -30.589 1.00 43.54 A
ATOM 1069 CG ASP A 142 -29.108 0.776 -29.469 1.00 45.42 A
ATOM 1070 OD1 ASP A 142 -30.251 1.219 -29.728 1.00 46.75 A
ATOM 1071 OD2 ASP A 142 -28.774 0.338 -28.337 1.00 46.53 A
ATOM 1072 C ASP A 142 -27.403 -0.089 -32.829 1.00 40.21 A
ATOM 1073 O ASP A 142 -27.522 0.357 -33.974 1.00 40.40 A
ATOM 1074 N LEU A 143 -26.278 -0.649 -32.389 1.00 37.85 A
ATOM 1075 CA LEU A 143 -25.116 -0.779 -33.255 1.00 33.85 A
ATOM 1076 CB LEU A 143 -23.990 -1.524 -32.535 1.00 32.00 A
ATOM 1077 CG LEU A 143 -23.373 -0.899 -31.282 1.00 29.79 A
ATOM 1078 CD1 LEU A 143 -22.148 -1.706 -30.893 1.00 29.29 A
ATOM 1079 CD2 LEU A 143 -22.981 0.540 -31.534 1.00 28.65 A
ATOM 1080 C LEU A 143 -25.457 -1.493 -34.561 1.00 32.65 A
ATOM 1081 O LEU A 143 -25.023 -1.069 -35.627 1.00 31.77 A
ATOM 1082 N THR A 144 -26.238 -2.565 -34.489 1.00 31.41 A
ATOM 1083 CA THR A 144 -26.595 -3.289 -35.706 1.00 30.58 A
ATOM 1084 CB THR A 144 -27.569 -4.463 -35.448 1.00 29.30 A

ATOM 1085 OG1 THR A 144 -26.921 -5.482 -34.683 1.00 26.22 A
ATOM 1086 CG2 THR A 144 -28.013 -5.060 -36.766 1.00 29.15 A
ATOM 1087 C THR A 144 -27.256 -2.378 -36.724 1.00 31.46 A
ATOM 1088 O THR A 144 -26.841 -2.330 -37.882 1.00 33.05 A
ATOM 1089 N ASN A 145 -28.289 -1.662 -36.294 1.00 31.21 A
ATOM 1090 CA ASN A 145 -29.002 -0.773 -37.195 1.00 30.28 A
ATOM 1091 CB ASN A 145 -30.184 -0.109 -36.479 1.00 30.00 A
ATOM 1092 CG ASN A 145 -31.226 -1.127 -36.007 1.00 31.64 A
ATOM 1093 OD1 ASN A 145 -31.334 -2.224 -36.569 1.00 30.95 A
ATOM 1094 ND2 ASN A 145 -32.002 -0.765 -34.977 1.00 30.66 A
ATOM 1095 C ASN A 145 -28.084 0.277 -37.794 1.00 29.79 A
ATOM 1096 O ASN A 145 -28.160 0.561 -38.989 1.00 30.68 A
ATOM 1097 N ILE A 146 -27.203 0.845 -36.978 1.00 28.91 A
ATOM 1098 CA ILE A 146 -26.282 1.863 -37.476 1.00 27.87 A
ATOM 1099 CB ILE A 146 -25.392 2.424 -36.341 1.00 26.57 A
ATOM 1100 CG2 ILE A 146 -24.606 3.626 -36.847 1.00 25.00 A
ATOM 1101 CG1 ILE A 146 -26.262 2.854 -35.158 1.00 25.04 A
ATOM 1102 CD1 ILE A 146 -25.485 3.403 -33.998 1.00 22.52 A
ATOM 1103 C ILE A 146 -25.394 1.304 -38.589 1.00 27.70 A
ATOM 1104 O ILE A 146 -25.043 2.017 -39.522 1.00 28.17 A
ATOM 1105 N LEU A 147 -25.030 0.032 -38.498 1.00 26.79 A
ATOM 1106 CA LEU A 147 -24.206 -0.565 -39.534 1.00 26.74 A
ATOM 1107 CB LEU A 147 -23.448 -1.780 -39.010 1.00 25.85 A
ATOM 1108 CG LEU A 147 -22.169 -1.367 -38.299 1.00 26.60 A
ATOM 1109 CD1 LEU A 147 -22.387 -1.440 -36.800 1.00 27.70 A
ATOM 1110 CD2 LEU A 147 -21.026 -2.264 -38.726 1.00 25.46 A
ATOM 1111 C LEU A 147 -25.071 -0.982 -40.694 1.00 27.42 A
ATOM 1112 O LEU A 147 -24.642 -0.957 -41.838 1.00 28.47 A
ATOM 1113 N ALA A 148 -26.303 -1.356 -40.391 1.00 28.57 A
ATOM 1114 CA ALA A 148 -27.230 -1.797 -41.419 1.00 28.61 A
ATOM 1115 CB ALA A 148 -28.420 -2.515 -40.779 1.00 27.26 A
ATOM 1116 C ALA A 148 -27.738 -0.679 -42.315 1.00 28.77 A
ATOM 1117 O ALA A 148 -27.989 -0.916 -43.490 1.00 30.51 A
ATOM 1118 N SER A 149 -27.877 0.538 -41.794 1.00 28.61 A

ATOM 1119 CA SER A 149 -28.427 1.598 -42.625 1.00 29.83 A
ATOM 1120 CB SER A 149 -29.940 1.638 -42.433 1.00 32.08 A
ATOM 1121 OG SER A 149 -30.264 1.661 -41.054 1.00 35.97 A
ATOM 1122 C SER A 149 -27.890 3.014 -42.527 1.00 30.09 A
ATOM 1123 O SER A 149 -28.455 3.928 -43.134 1.00 30.41 A
ATOM 1124 N SER A 150 -26.816 3.213 -41.776 1.00 30.03 A
ATOM 1125 CA SER A 150 -26.235 4.544 -41.664 1.00 29.89 A
ATOM 1126 CB SER A 150 -25.566 4.738 -40.309 1.00 28.85 A
ATOM 1127 OG SER A 150 -24.658 5.826 -40.363 1.00 29.04 A
ATOM 1128 C SER A 150 -25.190 4.700 -42.745 1.00 30.56 A
ATOM 1129 O SER A 150 -24.345 3.820 -42.895 1.00 32.30 A
ATOM 1130 N ARG A 151 -25.238 5.808 -43.487 1.00 30.10 A
ATOM 1131 CA ARG A 151 -24.265 6.062 -44.556 1.00 29.48 A
ATOM 1132 CB ARG A 151 -24.973 6.433 -45.857 1.00 29.10 A
ATOM 1133 CG ARG A 151 -25.201 5.261 -46.784 1.00 27.67 A
ATOM 1134 CD ARG A 151 -25.751 4.058 -46.057 1.00 26.00 A
ATOM 1135 NE ARG A 151 -26.422 3.157 -46.984 1.00 27.68 A
ATOM 1136 CZ ARG A 151 -26.752 1.901 -46.702 1.00 29.23 A
ATOM 1137 NH1 ARG A 151 -27.368 1.159 -47.613 1.00 29.67 A
ATOM 1138 NH2 ARG A 151 -26.450 1.384 -45.520 1.00 29.14 A
ATOM 1139 C ARG A 151 -23.234 7.127 -44.233 1.00 29.24 A
ATOM 1140 O ARG A 151 -22.654 7.735 -45.133 1.00 28.27 A
ATOM 1141 N SER A 152 -23.011 7.340 -42.943 1.00 29.98 A
ATOM 1142 CA SER A 152 -22.030 8.314 -42.479 1.00 31.53 A
ATOM 1143 CB SER A 152 -22.532 9.029 -41.235 1.00 31.24 A
ATOM 1144 OG SER A 152 -21.428 9.450 -40.454 1.00 32.43 A
ATOM 1145 C SER A 152 -20.754 7.575 -42.125 1.00 31.98 A
ATOM 1146 O SER A 152 -20.731 6.812 -41.161 1.00 33.79 A
ATOM 1147 N TYR A 153 -19.693 7.812 -42.886 1.00 32.16 A
ATOM 1148 CA TYR A 153 -18.427 7.125 -42.638 1.00 32.05 A
ATOM 1149 CB TYR A 153 -17.330 7.661 -43.567 1.00 30.78 A
ATOM 1150 CG TYR A 153 -16.021 6.906 -43.493 1.00 30.24 A
ATOM 1151 CD1 TYR A 153 -15.767 5.809 -44.319 1.00 28.08 A
ATOM 1152 CE1 TYR A 153 -14.540 5.136 -44.261 1.00 28.12 A

ATOM 1153 CD2 TYR A 153 -15.020 7.305 -42.604 1.00 30.77 A
ATOM 1154 CE2 TYR A 153 -13.796 6.637 -42.541 1.00 29.39 A
ATOM 1155 CZ TYR A 153 -13.564 5.565 -43.369 1.00 28.84 A
ATOM 1156 OH TYR A 153 -12.340 4.956 -43.306 1.00 30.48 A
ATOM 1157 C TYR A 153 -17.989 7.256 -41.182 1.00 32.22 A
ATOM 1158 O TYR A 153 -17.770 6.250 -40.502 1.00 31.46 A
ATOM 1159 N ALA A 154 -17.877 8.487 -40.697 1.00 32.75 A
ATOM 1160 CA ALA A 154 -17.461 8.704 -39.319 1.00 33.09 A
ATOM 1161 CB ALA A 154 -17.472 10.183 -38.984 1.00 33.13 A
ATOM 1162 C ALA A 154 -18.357 7.949 -38.347 1.00 33.88 A
ATOM 1163 O ALA A 154 -17.863 7.276 -37.436 1.00 34.69 A
ATOM 1164 N MET A 155 -19.670 8.044 -38.537 1.00 34.13 A
ATOM 1165 CA MET A 155 -20.580 7.366 -37.629 1.00 34.65 A
ATOM 1166 CB MET A 155 -22.023 7.650 -38.001 1.00 36.37 A
ATOM 1167 CG MET A 155 -22.961 7.246 -36.896 1.00 39.93 A
ATOM 1168 SD MET A 155 -24.408 8.288 -36.875 1.00 46.60 A
ATOM 1169 CE MET A 155 -25.720 7.070 -37.147 1.00 45.28 A
ATOM 1170 C MET A 155 -20.338 5.863 -37.597 1.00 34.24 A
ATOM 1171 O MET A 155 -20.213 5.261 -36.521 1.00 35.09 A
ATOM 1172 N LEU A 156 -20.272 5.249 -38.773 1.00 32.59 A
ATOM 1173 CA LEU A 156 -20.018 3.818 -38.842 1.00 31.17 A
ATOM 1174 CB LEU A 156 -19.966 3.371 -40.305 1.00 30.51 A
ATOM 1175 CG LEU A 156 -21.242 3.682 -41.094 1.00 30.45 A
ATOM 1176 CD1 LEU A 156 -20.962 3.623 -42.579 1.00 30.10 A
ATOM 1177 CD2 LEU A 156 -22.341 2.711 -40.704 1.00 30.97 A
ATOM 1178 C LEU A 156 -18.679 3.545 -38.143 1.00 30.43 A
ATOM 1179 O LEU A 156 -18.551 2.595 -37.372 1.00 30.53 A
ATOM 1180 N LEU A 157 -17.691 4.399 -38.394 1.00 28.38 A
ATOM 1181 CA LEU A 157 -16.375 4.226 -37.791 1.00 25.45 A
ATOM 1182 CB LEU A 157 -15.427 5.322 -38.273 1.00 22.41 A
ATOM 1183 CG LEU A 157 -14.046 5.256 -37.625 1.00 21.22 A
ATOM 1184 CD1 LEU A 157 -13.459 3.881 -37.885 1.00 19.32 A
ATOM 1185 CD2 LEU A 157 -13.143 6.368 -38.162 1.00 17.85 A
ATOM 1186 C LEU A 157 -16.430 4.235 -36.267 1.00 25.60 A

ATOM 1187 O LEU A 157 -15.715 3.483 -35.602 1.00 24.45 A
ATOM 1188 N PHE A 158 -17.281 5.088 -35.710 1.00 25.96 A
ATOM 1189 CA PHE A 158 -17.394 5.175 -34.265 1.00 26.41 A
ATOM 1190 CB PHE A 158 -18.243 6.381 -33.863 1.00 26.80 A
ATOM 1191 CG PHE A 158 -18.208 6.669 -32.390 1.00 28.55 A
ATOM 1192 CD1 PHE A 158 -17.053 7.170 -31.794 1.00 28.95 A
ATOM 1193 CD2 PHE A 158 -19.310 6.391 -31.582 1.00 29.43 A
ATOM 1194 CE1 PHE A 158 -16.995 7.383 -30.418 1.00 29.17 A
ATOM 1195 CE2 PHE A 158 -19.261 6.605 -30.197 1.00 29.54 A
ATOM 1196 CZ PHE A 158 -18.100 7.099 -29.618 1.00 29.43 A
ATOM 1197 C PHE A 158 -17.980 3.895 -33.671 1.00 25.38 A
ATOM 1198 O PHE A 158 -17.543 3.424 -32.623 1.00 25.67 A
ATOM 1199 N ALA A 159 -18.964 3.326 -34.346 1.00 22.91 A
ATOM 1200 CA ALA A 159 -19.569 2.108 -33.857 1.00 21.66 A
ATOM 1201 CB ALA A 159 -20.922 1.924 -34.491 1.00 20.98 A
ATOM 1202 C ALA A 159 -18.689 0.896 -34.138 1.00 22.12 A
ATOM 1203 O ALA A 159 -18.649 -0.039 -33.349 1.00 23.01 A
ATOM 1204 N TRP A 160 -17.987 0.894 -35.267 1.00 21.57 A
ATOM 1205 CA TRP A 160 -17.134 -0.236 -35.602 1.00 19.02 A
ATOM 1206 CB TRP A 160 -16.546 -0.084 -37.008 1.00 16.65 A
ATOM 1207 CG TRP A 160 -15.862 -1.334 -37.464 1.00 14.59 A
ATOM 1208 CD2 TRP A 160 -14.509 -1.717 -37.193 1.00 12.86 A
ATOM 1209 CE2 TRP A 160 -14.330 -3.011 -37.713 1.00 12.44 A
ATOM 1210 CE3 TRP A 160 -13.430 -1.091 -36.556 1.00 12.60 A
ATOM 1211 CD1 TRP A 160 -16.430 -2.378 -38.120 1.00 14.53 A
ATOM 1212 NE1 TRP A 160 -15.520 -3.393 -38.273 1.00 13.78 A
ATOM 1213 CZ2 TRP A 160 -13.117 -3.696 -37.621 1.00 11.68 A
ATOM 1214 CZ3 TRP A 160 -12.222 -1.773 -36.462 1.00 13.49 A
ATOM 1215 CH2 TRP A 160 -12.078 -3.063 -36.996 1.00 13.10 A
ATOM 1216 C TRP A 160 -16.001 -0.330 -34.588 1.00 18.73 A
ATOM 1217 O TRP A 160 -15.690 -1.407 -34.080 1.00 17.22 A
ATOM 1218 N GLU A 161 -15.391 0.818 -34.311 1.00 18.89 A
ATOM 1219 CA GLU A 161 -14.293 0.917 -33.350 1.00 20.59 A
ATOM 1220 CB GLU A 161 -13.631 2.285 -33.466 1.00 20.57 A

ATOM 1221 CG GLU A 161 -12.363 2.478 -32.679 1.00 19.67 A
ATOM 1222 CD GLU A 161 -11.864 3.906 -32.811 1.00 23.41 A
ATOM 1223 OE1 GLU A 161 -10.711 4.192 -32.432 1.00 24.99 A
ATOM 1224 OE2 GLU A 161 -12.632 4.764 -33.297 1.00 25.21 A
ATOM 1225 C GLU A 161 -14.838 0.735 -31.933 1.00 20.85 A
ATOM 1226 O GLU A 161 -14.281 -0.016 -31.128 1.00 21.38 A
ATOM 1227 N GLY A 162 -15.928 1.431 -31.635 1.00 19.77 A
ATOM 1228 CA GLY A 162 -16.525 1.299 -30.329 1.00 19.18 A
ATOM 1229 C GLY A 162 -16.738 -0.154 -29.950 1.00 18.38 A
ATOM 1230 O GLY A 162 -16.212 -0.625 -28.941 1.00 18.23 A
ATOM 1231 N TRP A 163 -17.499 -0.871 -30.768 1.00 17.70 A
ATOM 1232 CA TRP A 163 -17.788 -2.275 -30.513 1.00 18.49 A
ATOM 1233 CB TRP A 163 -18.734 -2.830 -31.578 1.00 18.18 A
ATOM 1234 CG TRP A 163 -18.950 -4.281 -31.392 1.00 18.34 A
ATOM 1235 CD2 TRP A 163 -19.613 -4.909 -30.290 1.00 20.41 A
ATOM 1236 CE2 TRP A 163 -19.505 -6.311 -30.479 1.00 20.44 A
ATOM 1237 CE3 TRP A 163 -20.288 -4.425 -29.158 1.00 19.02 A
ATOM 1238 CD1 TRP A 163 -18.484 -5.287 -32.181 1.00 19.93 A
ATOM 1239 NE1 TRP A 163 -18.811 -6.516 -31.641 1.00 20.04 A
ATOM 1240 CZ2 TRP A 163 -20.044 -7.227 -29.583 1.00 20.00 A
ATOM 1241 CZ3 TRP A 163 -20.820 -5.335 -28.274 1.00 20.37 A
ATOM 1242 CH2 TRP A 163 -20.697 -6.725 -28.490 1.00 21.38 A
ATOM 1243 C TRP A 163 -16.578 -3.199 -30.418 1.00 17.96 A
ATOM 1244 O TRP A 163 -16.540 -4.087 -29.581 1.00 17.36 A
ATOM 1245 N HIS A 164 -15.598 -2.994 -31.284 1.00 18.34 A
ATOM 1246 CA HIS A 164 -14.413 -3.839 -31.295 1.00 17.82 A
ATOM 1247 CB HIS A 164 -13.650 -3.660 -32.604 1.00 16.85 A
ATOM 1248 CG HIS A 164 -14.261 -4.400 -33.744 1.00 16.73 A
ATOM 1249 CD2 HIS A 164 -13.885 -5.541 -34.365 1.00 17.16 A
ATOM 1250 ND1 HIS A 164 -15.445 -4.012 -34.334 1.00 17.12 A
ATOM 1251 CE1 HIS A 164 -15.771 -4.883 -35.271 1.00 17.19 A
ATOM 1252 NE2 HIS A 164 -14.840 -5.821 -35.308 1.00 18.43 A
ATOM 1253 C HIS A 164 -13.475 -3.659 -30.124 1.00 18.06 A
ATOM 1254 O HIS A 164 -12.782 -4.602 -29.739 1.00 19.00 A

ATOM 1255 N ASN A 165 -13.417 -2.453 -29.575 1.00 17.86 A
ATOM 1256 CA ASN A 165 -12.571 -2.230 -28.421 1.00 18.54 A
ATOM 1257 CB ASN A 165 -12.261 -0.743 -28.243 1.00 19.00 A
ATOM 1258 CG ASN A 165 -11.290 -0.213 -29.280 1.00 19.84 A
ATOM 1259 OD1 ASN A 165 -10.396 -0.928 -29.748 1.00 20.57 A
ATOM 1260 ND2 ASN A 165 -11.438 1.061 -29.622 1.00 18.82 A
ATOM 1261 C ASN A 165 -13.377 -2.740 -27.232 1.00 18.66 A
ATOM 1262 O ASN A 165 -12.934 -3.595 -26.470 1.00 18.73 A
ATOM 1263 N ALA A 166 -14.590 -2.229 -27.113 1.00 18.96 A
ATOM 1264 CA ALA A 166 -15.482 -2.596 -26.032 1.00 19.93 A
ATOM 1265 CB ALA A 166 -16.831 -1.950 -26.266 1.00 20.24 A
ATOM 1266 C ALA A 166 -15.664 -4.100 -25.792 1.00 21.43 A
ATOM 1267 O ALA A 166 -15.717 -4.541 -24.648 1.00 22.01 A
ATOM 1268 N ALA A 167 -15.752 -4.893 -26.855 1.00 22.58 A
ATOM 1269 CA ALA A 167 -15.977 -6.329 -26.700 1.00 22.94 A
ATOM 1270 CB ALA A 167 -16.909 -6.844 -27.822 1.00 21.51 A
ATOM 1271 C ALA A 167 -14.708 -7.152 -26.684 1.00 22.80 A
ATOM 1272 O ALA A 167 -14.594 -8.140 -25.948 1.00 23.45 A
ATOM 1273 N GLY A 168 -13.746 -6.738 -27.492 1.00 22.08 A
ATOM 1274 CA GLY A 168 -12.523 -7.501 -27.598 1.00 21.25 A
ATOM 1275 C GLY A 168 -11.498 -7.414 -26.495 1.00 20.15 A
ATOM 1276 O GLY A 168 -11.168 -8.419 -25.867 1.00 19.24 A
ATOM 1277 N ILE A 169 -10.985 -6.211 -26.274 1.00 18.66 A
ATOM 1278 CA ILE A 169 -9.949 -5.993 -25.287 1.00 16.77 A
ATOM 1279 CB ILE A 169 -9.762 -4.490 -25.046 1.00 14.93 A
ATOM 1280 CG2 ILE A 169 -8.839 -4.271 -23.867 1.00 16.10 A
ATOM 1281 CG1 ILE A 169 -9.199 -3.837 -26.313 1.00 12.45 A
ATOM 1282 CD1 ILE A 169 -9.185 -2.328 -26.308 1.00 8.11 A
ATOM 1283 C ILE A 169 -10.120 -6.735 -23.954 1.00 17.46 A
ATOM 1284 O ILE A 169 -9.190 -7.415 -23.493 1.00 16.93 A
ATOM 1285 N PRO A 170 -11.304 -6.638 -23.322 1.00 17.31 A
ATOM 1286 CD PRO A 170 -12.531 -5.922 -23.709 1.00 17.07 A
ATOM 1287 CA PRO A 170 -11.490 -7.336 -22.043 1.00 17.22 A
ATOM 1288 CB PRO A 170 -12.798 -6.761 -21.527 1.00 15.27 A

ATOM 1289 CG PRO A 170 -13.555 -6.538 -22.772 1.00 17.40 A
ATOM 1290 C PRO A 170 -11.539 -8.853 -22.167 1.00 17.28 A
ATOM 1291 O PRO A 170 -11.133 -9.580 -21.263 1.00 20.22 A
ATOM 1292 N LEU A 171 -12.028 -9.323 -23.302 1.00 16.32 A
ATOM 1293 CA LEU A 171 -12.170 -10.744 -23.555 1.00 15.46 A
ATOM 1294 CB LEU A 171 -13.045 -10.900 -24.799 1.00 16.04 A
ATOM 1295 CG LEU A 171 -14.142 -11.951 -24.892 1.00 17.35 A
ATOM 1296 CD1 LEU A 171 -14.453 -12.499 -23.513 1.00 18.46 A
ATOM 1297 CD2 LEU A 171 -15.372 -11.311 -25.540 1.00 16.09 A
ATOM 1298 C LEU A 171 -10.851 -11.513 -23.726 1.00 14.92 A
ATOM 1299 O LEU A 171 -10.716 -12.638 -23.283 1.00 14.35 A
ATOM 1300 N LYS A 172 -9.871 -10.887 -24.352 1.00 15.48 A
ATOM 1301 CA LYS A 172 -8.589 -11.527 -24.638 1.00 15.25 A
ATOM 1302 CB LYS A 172 -7.578 -10.479 -25.114 1.00 15.19 A
ATOM 1303 CG LYS A 172 -6.358 -11.052 -25.799 1.00 13.13 A
ATOM 1304 CD LYS A 172 -5.506 -9.950 -26.373 1.00 13.80 A
ATOM 1305 CE LYS A 172 -4.215 -10.505 -26.932 1.00 17.48 A
ATOM 1306 NZ LYS A 172 -3.317 -9.409 -27.409 1.00 22.33 A
ATOM 1307 C LYS A 172 -7.941 -12.403 -23.576 1.00 16.09 A
ATOM 1308 O LYS A 172 -7.716 -13.585 -23.815 1.00 16.40 A
ATOM 1309 N PRO A 173 -7.606 -11.842 -22.397 1.00 17.54 A
ATOM 1310 CD PRO A 173 -7.938 -10.515 -21.852 1.00 17.58 A
ATOM 1311 CA PRO A 173 -6.977 -12.676 -21.361 1.00 16.61 A
ATOM 1312 CB PRO A 173 -6.850 -11.713 -20.182 1.00 14.04 A
ATOM 1313 CG PRO A 173 -7.994 -10.802 -20.374 1.00 14.81 A
ATOM 1314 C PRO A 173 -7.782 -13.946 -21.027 1.00 16.99 A
ATOM 1315 O PRO A 173 -7.212 -15.030 -20.866 1.00 15.72 A
ATOM 1316 N LEU A 174 -9.103 -13.814 -20.940 1.00 16.94 A
ATOM 1317 CA LEU A 174 -9.934 -14.968 -20.653 1.00 18.28 A
ATOM 1318 CB LEU A 174 -11.390 -14.568 -20.436 1.00 17.54 A
ATOM 1319 CG LEU A 174 -11.760 -13.499 -19.422 1.00 16.03 A
ATOM 1320 CD1 LEU A 174 -13.263 -13.575 -19.190 1.00 14.81 A
ATOM 1321 CD2 LEU A 174 -11.007 -13.725 -18.133 1.00 19.24 A
ATOM 1322 C LEU A 174 -9.885 -15.981 -21.797 1.00 20.50 A

ATOM 1323 O LEU A 174 -9.888 -17.193 -21.543 1.00 22.07 A
ATOM 1324 N TYR A 175 -9.835 -15.505 -23.049 1.00 20.40 A
ATOM 1325 CA TYR A 175 -9.811 -16.430 -24.172 1.00 19.86 A
ATOM 1326 CB TYR A 175 -9.903 -15.716 -25.526 1.00 19.84 A
ATOM 1327 CG TYR A 175 -10.312 -16.689 -26.626 1.00 22.29 A
ATOM 1328 CD1 TYR A 175 -11.632 -17.146 -26.718 1.00 21.79 A
ATOM 1329 CE1 TYR A 175 -11.999 -18.124 -27.639 1.00 20.79 A
ATOM 1330 CD2 TYR A 175 -9.366 -17.245 -27.504 1.00 21.75 A
ATOM 1331 CE2 TYR A 175 -9.733 -18.232 -28.433 1.00 21.02 A
ATOM 1332 CZ TYR A 175 -11.053 -18.663 -28.489 1.00 20.85 A
ATOM 1333 OH TYR A 175 -11.449 -19.625 -29.391 1.00 20.12 A
ATOM 1334 C TYR A 175 -8.563 -17.298 -24.144 1.00 19.71 A
ATOM 1335 O TYR A 175 -8.637 -18.514 -24.330 1.00 18.68 A
ATOM 1336 N GLU A 176 -7.421 -16.673 -23.899 1.00 20.37 A
ATOM 1337 CA GLU A 176 -6.157 -17.397 -23.847 1.00 22.98 A
ATOM 1338 CB GLU A 176 -5.021 -16.446 -23.492 1.00 21.56 A
ATOM 1339 CG GLU A 176 -4.980 -15.194 -24.331 1.00 24.69 A
ATOM 1340 CD GLU A 176 -3.896 -14.264 -23.857 1.00 27.39 A
ATOM 1341 OE1 GLU A 176 -3.195 -14.658 -22.895 1.00 27.62 A
ATOM 1342 OE2 GLU A 176 -3.739 -13.159 -24.430 1.00 29.89 A
ATOM 1343 C GLU A 176 -6.206 -18.517 -22.807 1.00 24.35 A
ATOM 1344 O GLU A 176 -5.634 -19.603 -23.016 1.00 23.59 A
ATOM 1345 N ASP A 177 -6.877 -18.242 -21.684 1.00 25.65 A
ATOM 1346 CA ASP A 177 -6.994 -19.214 -20.604 1.00 26.37 A
ATOM 1347 CB ASP A 177 -7.384 -18.523 -19.300 1.00 27.89 A
ATOM 1348 CG ASP A 177 -6.198 -17.844 -18.621 1.00 29.60 A
ATOM 1349 OD1 ASP A 177 -5.039 -18.151 -18.992 1.00 30.03 A
ATOM 1350 OD2 ASP A 177 -6.428 -17.018 -17.707 1.00 29.64 A
ATOM 1351 C ASP A 177 -7.989 -20.311 -20.934 1.00 26.19 A
ATOM 1352 O ASP A 177 -7.763 -21.480 -20.591 1.00 26.80 A
ATOM 1353 N PHE A 178 -9.085 -19.942 -21.594 1.00 25.24 A
ATOM 1354 CA PHE A 178 -10.088 -20.923 -21.990 1.00 24.34 A
ATOM 1355 CB PHE A 178 -11.247 -20.260 -22.734 1.00 23.81 A
ATOM 1356 CG PHE A 178 -12.017 -21.214 -23.602 1.00 24.94 A

ATOM 1357 CD1 PHE A 178 -12.892 -22.135 -23.037 1.00 25.82 A
ATOM 1358 CD2 PHE A 178 -11.811 -21.240 -24.987 1.00 26.05 A
ATOM 1359 CE1 PHE A 178 -13.548 -23.073 -23.829 1.00 26.52 A
ATOM 1360 CE2 PHE A 178 -12.458 -22.173 -25.796 1.00 25.55 A
ATOM 1361 CZ PHE A 178 -13.328 -23.094 -25.215 1.00 27.71 A
ATOM 1362 C PHE A 178 -9.428 -21.928 -22.924 1.00 23.93 A
ATOM 1363 O PHE A 178 -9.625 -23.133 -22.807 1.00 24.07 A
ATOM 1364 N THR A 179 -8.644 -21.408 -23.859 1.00 23.29 A
ATOM 1365 CA THR A 179 -7.967 -22.234 -24.831 1.00 21.77 A
ATOM 1366 CB THR A 179 -7.227 -21.358 -25.843 1.00 22.07 A
ATOM 1367 OG1 THR A 179 -8.190 -20.655 -26.634 1.00 23.35 A
ATOM 1368 CG2 THR A 179 -6.350 -22.195 -26.743 1.00 22.80 A
ATOM 1369 C THR A 179 -7.013 -23.224 -24.186 1.00 21.05 A
ATOM 1370 O THR A 179 -7.020 -24.400 -24.523 1.00 21.08 A
ATOM 1371 N ALA A 180 -6.200 -22.771 -23.245 1.00 20.85 A
ATOM 1372 CA ALA A 180 -5.267 -23.683 -22.609 1.00 20.51 A
ATOM 1373 CB ALA A 180 -4.475 -22.965 -21.549 1.00 19.20 A
ATOM 1374 C ALA A 180 -6.041 -24.837 -21.994 1.00 21.84 A
ATOM 1375 O ALA A 180 -5.694 -26.003 -22.185 1.00 22.70 A
ATOM 1376 N LEU A 181 -7.102 -24.513 -21.263 1.00 22.15 A
ATOM 1377 CA LEU A 181 -7.896 -25.552 -20.625 1.00 23.71 A
ATOM 1378 CB LEU A 181 -8.925 -24.927 -19.677 1.00 22.43 A
ATOM 1379 CG LEU A 181 -8.309 -24.446 -18.355 1.00 23.09 A
ATOM 1380 CD1 LEU A 181 -9.353 -23.716 -17.510 1.00 24.25 A
ATOM 1381 CD2 LEU A 181 -7.733 -25.644 -17.602 1.00 19.40 A
ATOM 1382 C LEU A 181 -8.578 -26.484 -21.623 1.00 24.68 A
ATOM 1383 O LEU A 181 -8.405 -27.708 -21.559 1.00 24.19 A
ATOM 1384 N SER A 182 -9.340 -25.905 -22.550 1.00 26.24 A
ATOM 1385 CA SER A 182 -10.046 -26.692 -23.562 1.00 27.19 A
ATOM 1386 CB SER A 182 -10.627 -25.785 -24.653 1.00 26.85 A
ATOM 1387 OG SER A 182 -11.620 -26.471 -25.399 1.00 25.48 A
ATOM 1388 C SER A 182 -9.120 -27.723 -24.188 1.00 27.63 A
ATOM 1389 O SER A 182 -9.501 -28.880 -24.351 1.00 28.48 A
ATOM 1390 N ASN A 183 -7.905 -27.308 -24.535 1.00 27.62 A

ATOM 1391 CA ASN A 183 -6.951 -28.239 -25.122 1.00 28.51 A
ATOM 1392 CB ASN A 183 -5.653 -27.538 -25.519 1.00 27.48 A
ATOM 1393 CG ASN A 183 -5.714 -26.947 -26.903 1.00 26.22 A
ATOM 1394 OD1 ASN A 183 -6.687 -27.147 -27.626 1.00 26.51 A
ATOM 1395 ND2 ASN A 183 -4.670 -26.220 -27.286 1.00 25.36 A
ATOM 1396 C ASN A 183 -6.629 -29.326 -24.125 1.00 29.14 A
ATOM 1397 O ASN A 183 -6.794 -30.510 -24.408 1.00 31.09 A
ATOM 1398 N GLU A 184 -6.179 -28.919 -22.946 1.00 29.46 A
ATOM 1399 CA GLU A 184 -5.824 -29.880 -21.918 1.00 29.59 A
ATOM 1400 CB GLU A 184 -5.642 -29.191 -20.574 1.00 28.57 A
ATOM 1401 CG GLU A 184 -5.186 -30.160 -19.518 1.00 30.32 A
ATOM 1402 CD GLU A 184 -5.170 -29.544 -18.151 1.00 32.53 A
ATOM 1403 OE1 GLU A 184 -6.159 -28.862 -17.825 1.00 36.27 A
ATOM 1404 OE2 GLU A 184 -4.186 -29.744 -17.405 1.00 33.30 A
ATOM 1405 C GLU A 184 -6.866 -30.972 -21.778 1.00 29.07 A
ATOM 1406 O GLU A 184 -6.530 -32.145 -21.623 1.00 29.26 A
ATOM 1407 N ALA A 185 -8.133 -30.586 -21.842 1.00 27.98 A
ATOM 1408 CA ALA A 185 -9.205 -31.553 -21.702 1.00 28.32 A
ATOM 1409 CB ALA A 185 -10.555 -30.836 -21.660 1.00 27.02 A
ATOM 1410 C ALA A 185 -9.195 -32.607 -22.809 1.00 28.74 A
ATOM 1411 O ALA A 185 -9.037 -33.802 -22.539 1.00 28.55 A
ATOM 1412 N TYR A 186 -9.344 -32.162 -24.054 1.00 28.92 A
ATOM 1413 CA TYR A 186 -9.388 -33.076 -25.199 1.00 28.19 A
ATOM 1414 CB TYR A 186 -9.866 -32.343 -26.443 1.00 23.52 A
ATOM 1415 CG TYR A 186 -11.304 -31.941 -26.342 1.00 21.10 A
ATOM 1416 CD1 TYR A 186 -11.671 -30.613 -26.173 1.00 20.03 A
ATOM 1417 CE1 TYR A 186 -12.994 -30.252 -26.059 1.00 20.85 A
ATOM 1418 CD2 TYR A 186 -12.301 -32.897 -26.390 1.00 21.19 A
ATOM 1419 CE2 TYR A 186 -13.623 -32.549 -26.271 1.00 21.88 A
ATOM 1420 CZ TYR A 186 -13.968 -31.229 -26.108 1.00 21.84 A
ATOM 1421 OH TYR A 186 -15.299 -30.904 -26.001 1.00 25.30 A
ATOM 1422 C TYR A 186 -8.083 -33.767 -25.494 1.00 29.57 A
ATOM 1423 O TYR A 186 -8.042 -34.749 -26.241 1.00 29.52 A
ATOM 1424 N LYS A 187 -7.016 -33.248 -24.908 1.00 30.88 A

ATOM 1425 CA LYS A 187 -5.712 -33.831 -25.107 1.00 32.68 A
ATOM 1426 CB LYS A 187 -4.672 -33.018 -24.357 1.00 31.40 A
ATOM 1427 CG LYS A 187 -3.481 -32.631 -25.194 1.00 31.79 A
ATOM 1428 CD LYS A 187 -2.576 -33.815 -25.416 1.00 33.70 A
ATOM 1429 CE LYS A 187 -1.212 -33.363 -25.913 1.00 36.69 A
ATOM 1430 NZ LYS A 187 -0.573 -32.366 -25.003 1.00 36.36 A
ATOM 1431 C LYS A 187 -5.813 -35.239 -24.547 1.00 33.95 A
ATOM 1432 O LYS A 187 -5.274 -36.186 -25.128 1.00 35.18 A
ATOM 1433 N ALA A 188 -6.564 -35.373 -23.453 1.00 34.52 A
ATOM 1434 CA ALA A 188 -6.755 -36.641 -22.759 1.00 35.58 A
ATOM 1435 CB ALA A 188 -7.217 -36.399 -21.330 1.00 35.35 A
ATOM 1436 C ALA A 188 -7.750 -37.530 -23.498 1.00 35.94 A
ATOM 1437 O ALA A 188 -7.810 -38.735 -23.201 1.00 36.53 A
ATOM 1438 N ASP A 189 -8.521 -36.969 -24.384 1.00 35.63 A
ATOM 1439 CA ASP A 189 -9.460 -37.773 -25.145 1.00 34.84 A
ATOM 1440 CB ASP A 189 -10.725 -36.977 -25.456 1.00 35.18 A
ATOM 1441 CG ASP A 189 -11.688 -36.959 -24.291 1.00 37.17 A
ATOM 1442 OD1 ASP A 189 -12.012 -38.062 -23.794 1.00 39.05 A
ATOM 1443 OD2 ASP A 189 -12.120 -35.860 -23.868 1.00 37.85 A
ATOM 1444 C ASP A 189 -8.779 -38.246 -26.428 1.00 34.33 A
ATOM 1445 O ASP A 189 -9.419 -38.830 -27.307 1.00 34.30 A
ATOM 1446 N GLY A 190 -7.476 -37.986 -26.529 1.00 33.17 A
ATOM 1447 CA GLY A 190 -6.729 -38.425 -27.691 1.00 33.93 A
ATOM 1448 C GLY A 190 -6.499 -37.466 -28.852 1.00 34.38 A
ATOM 1449 O GLY A 190 -5.748 -37.798 -29.768 1.00 35.03 A
ATOM 1450 N PHE A 191 -7.127 -36.297 -28.857 1.00 33.48 A
ATOM 1451 CA PHE A 191 -6.895 -35.372 -29.956 1.00 33.46 A
ATOM 1452 CB PHE A 191 -8.163 -34.587 -30.251 1.00 34.42 A
ATOM 1453 CG PHE A 191 -9.387 -35.452 -30.467 1.00 36.71 A
ATOM 1454 CD1 PHE A 191 -10.078 -35.996 -29.382 1.00 37.61 A
ATOM 1455 CD2 PHE A 191 -9.887 -35.673 -31.751 1.00 36.64 A
ATOM 1456 CE1 PHE A 191 -11.251 -36.737 -29.570 1.00 36.78 A
ATOM 1457 CE2 PHE A 191 -11.058 -36.413 -31.949 1.00 36.92 A
ATOM 1458 CZ PHE A 191 -11.741 -36.944 -30.852 1.00 37.59 A

ATOM 1459 C PHE A 191 -5.745 -34.434 -29.577 1.00 33.90 A
ATOM 1460 O PHE A 191 -5.426 -34.301 -28.401 1.00 34.85 A
ATOM 1461 N THR A 192 -5.111 -33.790 -30.553 1.00 33.56 A
ATOM 1462 CA THR A 192 -3.982 -32.906 -30.250 1.00 32.85 A
ATOM 1463 CB THR A 192 -3.248 -32.468 -31.526 1.00 33.17 A
ATOM 1464 OG1 THR A 192 -2.710 -33.616 -32.179 1.00 32.51 A
ATOM 1465 CG2 THR A 192 -2.107 -31.499 -31.193 1.00 34.09 A
ATOM 1466 C THR A 192 -4.406 -31.639 -29.534 1.00 32.64 A
ATOM 1467 O THR A 192 -3.763 -31.193 -28.574 1.00 33.35 A
ATOM 1468 N ASP A 193 -5.486 -31.055 -30.034 1.00 31.01 A
ATOM 1469 CA ASP A 193 -6.028 -29.822 -29.497 1.00 29.62 A
ATOM 1470 CB ASP A 193 -5.354 -28.622 -30.169 1.00 31.85 A
ATOM 1471 CG ASP A 193 -5.295 -28.750 -31.683 1.00 34.55 A
ATOM 1472 OD1 ASP A 193 -6.364 -28.647 -32.336 1.00 36.69 A
ATOM 1473 OD2 ASP A 193 -4.174 -28.959 -32.217 1.00 33.64 A
ATOM 1474 C ASP A 193 -7.507 -29.849 -29.810 1.00 28.55 A
ATOM 1475 O ASP A 193 -7.971 -30.759 -30.492 1.00 28.38 A
ATOM 1476 N THR A 194 -8.254 -28.873 -29.312 1.00 26.56 A
ATOM 1477 CA THR A 194 -9.680 -28.856 -29.564 1.00 25.02 A
ATOM 1478 CB THR A 194 -10.355 -27.722 -28.804 1.00 22.89 A
ATOM 1479 OG1 THR A 194 -9.754 -27.607 -27.515 1.00 21.60 A
ATOM 1480 CG2 THR A 194 -11.834 -28.010 -28.625 1.00 22.30 A
ATOM 1481 C THR A 194 -9.947 -28.707 -31.056 1.00 25.03 A
ATOM 1482 O THR A 194 -11.006 -29.081 -31.542 1.00 25.44 A
ATOM 1483 N GLY A 195 -8.977 -28.173 -31.784 1.00 24.71 A
ATOM 1484 CA GLY A 195 -9.154 -27.995 -33.213 1.00 24.87 A
ATOM 1485 C GLY A 195 -9.409 -29.326 -33.882 1.00 24.39 A
ATOM 1486 O GLY A 195 -10.394 -29.503 -34.612 1.00 23.80 A
ATOM 1487 N ALA A 196 -8.514 -30.272 -33.623 1.00 23.14 A
ATOM 1488 CA ALA A 196 -8.631 -31.604 -34.195 1.00 22.46 A
ATOM 1489 CB ALA A 196 -7.446 -32.451 -33.783 1.00 21.22 A
ATOM 1490 C ALA A 196 -9.928 -32.275 -33.766 1.00 23.07 A
ATOM 1491 O ALA A 196 -10.559 -32.968 -34.557 1.00 23.22 A
ATOM 1492 N TYR A 197 -10.321 -32.074 -32.512 1.00 23.57 A

ATOM 1493 CA TYR A 197 -11.548 -32.667 -32.007 1.00 23.71 A
ATOM 1494 CB TYR A 197 -11.723 -32.374 -30.506 1.00 21.55 A
ATOM 1495 CG TYR A 197 -13.102 -32.745 -29.987 1.00 19.57 A
ATOM 1496 CD1 TYR A 197 -13.552 -34.064 -30.037 1.00 17.58 A
ATOM 1497 CE1 TYR A 197 -14.841 -34.395 -29.663 1.00 17.81 A
ATOM 1498 CD2 TYR A 197 -13.988 -31.764 -29.533 1.00 17.97 A
ATOM 1499 CE2 TYR A 197 -15.287 -32.088 -29.156 1.00 17.52 A
ATOM 1500 CZ TYR A 197 -15.702 -33.406 -29.226 1.00 19.36 A
ATOM 1501 OH TYR A 197 -16.979 -33.745 -28.860 1.00 21.39 A
ATOM 1502 C TYR A 197 -12.738 -32.111 -32.783 1.00 25.29 A
ATOM 1503 O TYR A 197 -13.667 -32.839 -33.131 1.00 26.51 A
ATOM 1504 N TRP A 198 -12.704 -30.812 -33.046 1.00 26.31 A
ATOM 1505 CA TRP A 198 -13.768 -30.143 -33.777 1.00 28.39 A
ATOM 1506 CB TRP A 198 -13.504 -28.643 -33.798 1.00 29.93 A
ATOM 1507 CG TRP A 198 -13.851 -27.944 -32.541 1.00 29.91 A
ATOM 1508 CD2 TRP A 198 -13.854 -26.531 -32.331 1.00 30.12 A
ATOM 1509 CE2 TRP A 198 -14.257 -26.308 -30.996 1.00 29.70 A
ATOM 1510 CE3 TRP A 198 -13.556 -25.429 -33.142 1.00 29.59 A
ATOM 1511 CD1 TRP A 198 -14.238 -28.511 -31.364 1.00 29.26 A
ATOM 1512 NE1 TRP A 198 -14.485 -27.533 -30.428 1.00 29.22 A
ATOM 1513 CZ2 TRP A 198 -14.371 -25.026 -30.454 1.00 29.64 A
ATOM 1514 CZ3 TRP A 198 -13.669 -24.156 -32.603 1.00 28.69 A
ATOM 1515 CH2 TRP A 198 -14.073 -23.965 -31.272 1.00 29.30 A
ATOM 1516 C TRP A 198 -13.917 -30.643 -35.221 1.00 29.07 A
ATOM 1517 O TRP A 198 -15.039 -30.779 -35.728 1.00 29.99 A
ATOM 1518 N ARG A 199 -12.790 -30.899 -35.882 1.00 27.49 A
ATOM 1519 CA ARG A 199 -12.819 -31.380 -37.260 1.00 27.87 A
ATOM 1520 CB ARG A 199 -11.476 -31.086 -37.945 1.00 27.08 A
ATOM 1521 CG ARG A 199 -11.105 -29.607 -37.977 1.00 26.10 A
ATOM 1522 CD ARG A 199 -9.832 -29.354 -38.760 1.00 24.86 A
ATOM 1523 NE ARG A 199 -8.694 -30.096 -38.231 1.00 24.73 A
ATOM 1524 CZ ARG A 199 -7.889 -29.663 -37.268 1.00 25.61 A
ATOM 1525 NH1 ARG A 199 -6.878 -30.424 -36.865 1.00 24.88 A
ATOM 1526 NH2 ARG A 199 -8.083 -28.467 -36.717 1.00 27.52 A

ATOM 1527 C ARG A 199 -13.149 -32.882 -37.375 1.00 28.57 A
ATOM 1528 O ARG A 199 -13.650 -33.348 -38.412 1.00 28.45 A
ATOM 1529 N SER A 200 -12.883 -33.640 -36.313 1.00 28.56 A
ATOM 1530 CA SER A 200 -13.150 -35.071 -36.334 1.00 28.62 A
ATOM 1531 CB SER A 200 -12.630 -35.758 -35.049 1.00 27.96 A
ATOM 1532 OG SER A 200 -13.445 -35.526 -33.909 1.00 25.96 A
ATOM 1533 C SER A 200 -14.634 -35.351 -36.520 1.00 29.44 A
ATOM 1534 O SER A 200 -15.020 -36.480 -36.825 1.00 30.91 A
ATOM 1535 N TRP A 201 -15.463 -34.325 -36.362 1.00 29.47 A
ATOM 1536 CA TRP A 201 -16.902 -34.497 -36.502 1.00 31.15 A
ATOM 1537 CB TRP A 201 -17.655 -33.293 -35.969 1.00 32.45 A
ATOM 1538 CG TRP A 201 -17.537 -33.076 -34.515 1.00 34.41 A
ATOM 1539 CD2 TRP A 201 -17.717 -31.835 -33.832 1.00 36.18 A
ATOM 1540 CE2 TRP A 201 -17.598 -32.097 -32.452 1.00 36.64 A
ATOM 1541 CE3 TRP A 201 -17.969 -30.521 -34.255 1.00 37.31 A
ATOM 1542 CD1 TRP A 201 -17.320 -34.018 -33.555 1.00 35.12 A
ATOM 1543 NE1 TRP A 201 -17.357 -33.439 -32.308 1.00 35.59 A
ATOM 1544 CZ2 TRP A 201 -17.726 -31.096 -31.490 1.00 38.14 A
ATOM 1545 CZ3 TRP A 201 -18.097 -29.525 -33.300 1.00 38.49 A
ATOM 1546 CH2 TRP A 201 -17.974 -29.819 -31.932 1.00 39.40 A
ATOM 1547 C TRP A 201 -17.377 -34.731 -37.918 1.00 32.29 A
ATOM 1548 O TRP A 201 -18.514 -35.131 -38.122 1.00 33.48 A
ATOM 1549 N TYR A 202 -16.531 -34.464 -38.902 1.00 34.08 A
ATOM 1550 CA TYR A 202 -16.945 -34.671 -40.285 1.00 35.38 A
ATOM 1551 CB TYR A 202 -16.472 -33.503 -41.152 1.00 33.78 A
ATOM 1552 CG TYR A 202 -17.084 -32.188 -40.717 1.00 32.32 A
ATOM 1553 CD1 TYR A 202 -16.549 -31.466 -39.647 1.00 29.78 A
ATOM 1554 CE1 TYR A 202 -17.145 -30.287 -39.201 1.00 28.18 A
ATOM 1555 CD2 TYR A 202 -18.238 -31.697 -41.335 1.00 32.06 A
ATOM 1556 CE2 TYR A 202 -18.846 -30.519 -40.893 1.00 30.70 A
ATOM 1557 CZ TYR A 202 -18.290 -29.823 -39.829 1.00 29.44 A
ATOM 1558 OH TYR A 202 -18.876 -28.656 -39.404 1.00 29.12 A
ATOM 1559 C TYR A 202 -16.463 -36.009 -40.827 1.00 36.33 A
ATOM 1560 O TYR A 202 -16.789 -36.396 -41.945 1.00 36.92 A

ATOM 1561 N ASN A 203 -15.635 -36.685 -40.113 1.00 37.74 A
ATOM 1562 CA ASN A 203 -15.179 -37.941 -40.552 1.00 39.33 A
ATOM 1563 CB ASN A 203 -16.231 -38.969 -40.431 1.00 43.18 A
ATOM 1564 CG ASN A 203 -15.786 -40.134 -39.658 1.00 45.83 A
ATOM 1565 OD1 ASN A 203 -14.873--40.835 -40.015 1.00 47.58 A
ATOM 1566 ND2 ASN A 203 -16.408 -40.331 -38.566 1.00 47.49 A
ATOM 1567 C ASN A 203 -14.805 -37.915 -41.902 1.00 38.72 A
ATOM 1568 O ASN A 203 -15.382 -38.509 -42.717 1.00 38.77 A
ATOM 1569 N SER A 204 -13.722 -37.285 -42.132 1.00 37.19 A
ATOM 1570 CA SER A 204 -13.150 -37.261 -43.466 1.00 35.18 A
ATOM 1571 CB SER A 204 -13.762 -36.129 -44.303 1.00 36.26 A
ATOM 1572 OG SER A 204 -13.164 -36.048 -45.593 1.00 37.84 A
ATOM 1573 C SER A 204 -11.675 -37.012 -43.269 1.00 33.37 A
ATOM 1574 O SER A 204 -11.274 -35.949 -42.815 1.00 32.63 A
ATOM 1575 N PRO A 205 -10.840 -37.996 -43.590 1.00 32.65 A
ATOM 1576 CD PRO A 205 -11.074 -39.290 -44.248 1.00 32.73 A
ATOM 1577 CA PRO A 205 -9.412 -37.751 -43.397 1.00 32.64 A
ATOM 1578 CB PRO A 205 -8.782 -39.088 -43.767 1.00 32.64 A
ATOM 1579 CG PRO A 205 -9.711 -39.588 -44.831 1.00 33.78 A
ATOM 1580 C PRO A 205 -8.948 -36.626 -44.301 1.00 32.05 A
ATOM 1581 O PRO A 205 -7.885 -36.040 -44.104 1.00 32.56 A
ATOM 1582 N THR A 206 -9.731 -36.243 -45.280 1.00 31.92 A
ATOM 1583 CA THR A 206 -9.378 -35.135 -46.187 1.00 32.25 A
ATOM 1584 CB THR A 206 -9.539 -35.537 -47.596 1.00 33.66 A
ATOM 1585 OG1 THR A 206 -8.686 -36.634 -47.879 1.00 37.55 A
ATOM 1586 CG2 THR A 206 -10.841 -36.058 -47.836 1.00 31.82 A
ATOM 1587 C THR A 206 -10.167 -33.869 -46.025 1.00 30.64 A
ATOM 1588 O THR A 206 -10.056 -32.996 -46.758 1.00 30.14 A
ATOM 1589 N PHE A 207 -10.986 -33.797 -45.050 1.00 29.01 A
ATOM 1590 CA PHE A 207 -11.760 -32.580 -44.738 1.00 27.83 A
ATOM 1591 CB PHE A 207 -12.092 -32.559 -43.231 1.00 23.61 A
ATOM 1592 CG PHE A 207 -13.055 -31.469 -42.814 1.00 20.03 A
ATOM 1593 CD1 PHE A 207 -14.247 -31.263 -43.502 1.00 19.48 A
ATOM 1594 CD2 PHE A 207 -12.788 -30.676 -41.707 1.00 19.62 A

ATOM 1595 CE1 PHE A 207 -15.157 -30.286 -43.095 1.00 19.21 A
ATOM 1596 CE2 PHE A 207 -13.701 -29.692 -41.294 1.00 20.24 A
ATOM 1597 CZ PHE A 207 -14.884 -29.503 -41.993 1.00 19.86 A
ATOM 1598 C PHE A 207 -11.152 -31.220 -45.134 1.00 29.12 A
ATOM 1599 O PHE A 207 -11.700 -30.509 -45.975 1.00 29.17 A
ATOM 1600 N GLU A 208 -10.035 -30.851 -44.513 1.00 30.63 A
ATOM 1601 CA GLU A 208 -9.385 -29.570 -44.791 1.00 31.48 A
ATOM 1602 CB GLU A 208 -8.122 -29.412 -43.932 1.00 32.82 A
ATOM 1603 CG GLU A 208 -8.389 -29.079 -42.469 1.00 34.96 A
ATOM 1604 CD GLU A 208 -7.112 -28.814 -41.685 1.00 37.11 A
ATOM 1605 OE1 GLU A 208 -6.452 -27.781 -41.936 1.00 39.09 A
ATOM 1606 OE2 GLU A 208 -6.764 -29.644 -40.817 1.00 37.55 A
ATOM 1607 C GLU A 208 -9.029 -29.344 -46.254 1.00 31.27 A
ATOM 1608 O GLU A 208 -9.201 -28.242 -46.772 1.00 30.68 A
ATOM 1609 N ASP A 209 -8.518 -30.377 -46.912 1.00 31.49 A
ATOM 1610 CA ASP A 209 -8.151 -30.267 -48.319 1.00 31.77 A
ATOM 1611 CB ASP A 209 -7.342 -31.494 -48.761 1.00 33.73 A
ATOM 1612 CG ASP A 209 -6.050 -31.660 -47.965 1.00 35.68 A
ATOM 1613 OD1 ASP A 209 -5.141 -30.811 -48.114 1.00 35.82 A
ATOM 1614 OD2 ASP A 209 -5.953 -32.637 -47.180 1.00 37.43 A
ATOM 1615 C ASP A 209 -9.414 -30.134 -49.166 1.00 31.09 A
ATOM 1616 O ASP A 209 -9.453 -29.348 -50.120 1.00 30.79 A
ATOM 1617 N ASP A 210 -10.446 -30.897 -48.817 1.00 30.27 A
ATOM 1618 CA ASP A 210 -11.709 -30.821 -49.537 1.00 30.96 A
ATOM 1619 CB ASP A 210 -12.710 -31.822 -48.977 1.00 32.23 A
ATOM 1620 CG ASP A 210 -12.234 -33.251 -49.106 1.00 36.73 A
ATOM 1621 OD1 ASP A 210 -11.490 -33.545 -50.069 1.00 38.00 A
ATOM 1622 OD2 ASP A 210 -12.618 -34.085 -48.251 1.00 39.18 A
ATOM 1623 C ASP A 210 -12.295 -29.410 -49.433 1.00 31.77 A
ATOM 1624 O ASP A 210 -12.963 -28.937 -50.353 1.00 32.47 A
ATOM 1625 N LEU A 211 -12.038 -28.739 -48.312 1.00 31.59 A
ATOM 1626 CA LEU A 211 -12.532 -27.389 -48.088 1.00 29.86 A
ATOM 1627 CB LEU A 211 -12.525 -27.059 -46.598 1.00 30.57 A
ATOM 1628 CG LEU A 211 -13.491 -27.794 -45.666 1.00 30.22 A

ATOM 1629 CD1 LEU A 211 -13.291 -27.280 -44.237 1.00 30.65 A
ATOM 1630 CD2 LEU A 211 -14.925 -27.563 -46.115 1.00 30.10 A
ATOM 1631 C LEU A 211 -11.688 -26.375 -48.819 1.00 29.78 A
ATOM 1632 O LEU A 211 -12.210 -25.413 -49.357 1.00 29.06 A
ATOM 1633 N GLU A 212 -10.378 -26.581 -48.828 1.00 30.65 A
ATOM 1634 CA GLU A 212 -9.494 -25.651 -49.514 1.00 32.04 A
ATOM 1635 CB GLU A 212 -8.021 -25.971 -49.250 1.00 31.48 A
ATOM 1636 CG GLU A 212 -7.097 -24.862 -49.738 1.00 34.76 A
ATOM 1637 CD GLU A 212 -5.613 -25.156 -49.524 1.00 37.96 A
ATOM 1638 OE1 GLU A 212 -4.779 -24.226 -49.665 1.00 38.12 A
ATOM 1639 OE2 GLU A 212 -5.273 -26.319 -49.225 1.00 40.56 A
ATOM 1640 C GLU A 212 -9.773 -25.716 -51.011 1.00 32.66 A
ATOM 1641 O GLU A 212 -9.800 -24.691 -51.700 1.00 31.82 A
ATOM 1642 N HIS A 213 -9.980 -26.933 -51.508 1.00 34.42 A
ATOM 1643 CA HIS A 213 -10.286 -27.140 -52.918 1.00 35.64 A
ATOM 1644 CB HIS A 213 -10.339 -28.643 -53.235 1.00 38.66 A
ATOM 1645 CG HIS A 213 -10.629 -28.953 -54.677 1.00 44.15 A
ATOM 1646 CD2 HIS A 213 -11.760 -29.395 -55.286 1.00 45.39 A
ATOM 1647 ND1 HIS A 213 -9.684 -28.825 -55.677 1.00 46.46 A
ATOM 1648 CE1 HIS A 213 -10.218 -29.179 -56.836 1.00 45.63 A
ATOM 1649 NE2 HIS A 213 -11.476 -29.528 -56.625 1.00 45.48 A
ATOM 1650 C HIS A 213 -11.651 -26.497 -53.183 1.00 34.67 A
ATOM 1651 O HIS A 213 -11.813 -25.721 -54.112 1.00 35.37 A
ATOM 1652 N LEU A 214 -12.629 -26.811 -52.347 1.00 33.40 A
ATOM 1653 CA LEU A 214 -13.966 -26.265 -52.504 1.00 32.39 A
ATOM 1654 CB LEU A 214 -14.865 -26.777 -51.378 1.00 33.01 A
ATOM 1655 CG LEU A 214 -16.033 -27.684 -51.763 1.00 33.48 A
ATOM 1656 CD1 LEU A 214 -16.700 -28.245 -50.512 1.00 33.80 A
ATOM 1657 CD2 LEU A 214 -17.019 -26.884 -52.584 1.00 33.84 A
ATOM 1658 C LEU A 214 -13.994 -24.743 -52.522 1.00 32.41 A
ATOM 1659 O LEU A 214 -14.870 -24.152 -53.148 1.00 32.47 A
ATOM 1660 N TYR A 215 -13.047 -24.103 -51.836 1.00 31.93 A
ATOM 1661 CA TYR A 215 -13.018 -22.639 -51.802 1.00 31.13 A
ATOM 1662 CB TYR A 215 -12.162 -22.117 -50.639 1.00 29.43 A

ATOM 1663 CG TYR A 215 -12.300 -20.625 -50.445 1.00 26.75 A
ATOM 1664 CD1 TYR A 215 -13.501 -20.070 -50.010 1.00 26.25 A
ATOM 1665 CE1 TYR A 215 -13.674 -18.693 -49.936 1.00 25.59 A
ATOM 1666 CD2 TYR A 215 -11.269 -19.763 -50.791 1.00 26.05 A
ATOM 1667 CE2 TYR A 215 -11.430 -18.387 -50.723 1.00 24.66 A
ATOM 1668 CZ TYR A 215 -12.635 -17.856 -50.299 1.00 24.65 A
ATOM 1669 OH TYR A 215 -12.814 -16.489 -50.267 1.00 22.67 A
ATOM 1670 C TYR A 215 -12.509 -22.028 -53.108 1.00 32.06 A
ATOM 1671 O TYR A 215 -13.078 -21.037 -53.581 1.00 33.33 A
ATOM 1672 N GLN A 216 -11.442 -22.603 -53.678 1.00 31.48 A
ATOM 1673 CA GLN A 216 -10.875 -22.123 -54.946 1.00 30.38 A
ATOM 1674 CB GLN A 216 -9.804 -23.069 -55.466 1.00 32.17 A
ATOM 1675 CG GLN A 216 -8.593 -23.241 -54.590 1.00 36.67 A
ATOM 1676 CD GLN A 216 -7.585 -24.185 -55.227 1.00 39.16 A
ATOM 1677 OE1 GLN A 216 -7.008 -23.871 -56.273 1.00 42.34 A
ATOM 1678 NE2 GLN A 216 -7.373 -25.350 -54.608 1.00 39.00 A
ATOM 1679 C GLN A 216 -11.957 -22.030 -56.013 1.00 28.68 A
ATOM 1680 O GLN A 216 -12.018 -21.062 -56.770 1.00 28.67 A
ATOM 1681 N GLN A 217 -12.790 -23.060 -56.089 1.00 26.10 A
ATOM 1682 CA GLN A 217 -13.877 -23.092 -57.048 1.00 24.85 A
ATOM 1683 CB GLN A 217 -14.706 -24.354 -56.852 1.00 26.43 A
ATOM 1684 CG GLN A 217 -14.118 -25.587 -57.496 1.00 30.91 A
ATOM 1685 CD GLN A 217 -14.968 -26.834 -57.274 1.00 34.33 A
ATOM 1686 OE1 GLN A 217 -16.190 -26.814 -57.447 1.00 34.46 A
ATOM 1687 NE2 GLN A 217 -14.314 -27.935 -56.897 1.00 37.13 A
ATOM 1688 C GLN A 217 -14.788 -21.890 -56.909 1.00 23.15 A
ATOM 1689 O GLN A 217 -15.319 -21.393 -57.894 1.00 23.64 A
ATOM 1690 N LEU A 218 -14.968 -21.427 -55.678 1.00 21.40 A
ATOM 1691 CA LEU A 218 -15.850 -20.299 -55.406 1.00 19.68 A
ATOM 1692 CB LEU A 218 -16.653 -20.571 -54.126 1.00 19.60 A
ATOM 1693 CG LEU A 218 -17.485 -21.860 -54.007 1.00 19.16 A
ATOM 1694 CD1 LEU A 218 -17.764 -22.162 -52.554 1.00 20.40 A
ATOM 1695 CD2 LEU A 218 -18.781 -21.717 -54.749 1.00 19.39 A
ATOM 1696 C LEU A 218 -15.160 -18.941 -55.290 1.00 19.45 A

ATOM 1697 O LEU A 218 -15.796 -17.915 -55.516 1.00 20.36 A
ATOM 1698 N GLU A 219 -13.872 -18.912 -54.959 1.00 17.63 A
ATOM 1699 CA GLU A 219 -13.195 -17.624 -54.810 1.00 17.26 A
ATOM 1700 CB GLU A 219 -11.667 -17.769 -54.692 1.00 18.09 A
ATOM 1701 CG GLU A 219 -10.997 -16.407 -54.393 1.00 20.56 A
ATOM 1702 CD GLU A 219 -9.559 -16.501 -53.863 1.00 24.38 A
ATOM 1703 OE1 GLU A 219 -9.140 -15.580 -53.111 1.00 25.10 A
ATOM 1704 OE2 GLU A 219 -8.844 -17.474 -54.204 1.00 26.01 A
ATOM 1705 C GLU A 219 -13.498 -16.609 -55.902 1.00 16.81 A
ATOM 1706 O GLU A 219 -13.770 -15.450 -55.603 1.00 15.63 A
ATOM 1707 N PRO A 220 -13.456 -17.026 -57.183 1.00 17.05 A
ATOM 1708 CD PRO A 220 -13.126 -18.365 -57.701 1.00 16.40 A
ATOM 1709 CA PRO A 220 -13.730 -16.114 -58.298 1.00 15.17 A
ATOM 1710 CB PRO A 220 -13.701 -17.032 -59.506 1.00 14.61 A
ATOM 1711 CG PRO A 220 -12.723 -18.053 -59.109 1.00 15.77 A
ATOM 1712 C PRO A 220 -15.077 -15.443 -58.128 1.00 14.32 A
ATOM 1713 O PRO A 220 -15.251 -14.274 -58.475 1.00 12.98 A
ATOM 1714 N LEU A 221 -16.025 -16.196 -57.582 1.00 12.90 A
ATOM 1715 CA LEU A 221 -17.362 -15.678 -57.363 1.00 13.21 A
ATOM 1716 CB LEU A 221 -18.258 -16.755 -56.756 1.00 12.43 A
ATOM 1717 CG LEU A 221 -19.442 -17.271 -57.568 1.00 10.59 A
ATOM 1718 CD1 LEU A 221 -18.936 -18.069 -58.742 1.00 11.21 A
ATOM 1719 CD2 LEU A 221 -20.320 -18.133 -56.695 1.00 10.88 A
ATOM 1720 C LEU A 221 -17.300 -14.486 -56.435 1.00 14.12 A
ATOM 1721 O LEU A 221 -17.850 -13.429 -56.746 1.00 15.39 A
ATOM 1722 N TYR A 222 -16.623 -14.656 -55.299 1.00 14.17 A
ATOM 1723 CA TYR A 222 -16.493 -13.587 -54.312 1.00 14.92 A
ATOM 1724 CB TYR A 222 -15.769 -14.077 -53.049 1.00 14.94 A
ATOM 1725 CG TYR A 222 -15.613 -12.997 -51.996 1.00 15.02 A
ATOM 1726 CD1 TYR A 222 -16.726 -12.406 -51.420 1.00 14.51 A
ATOM 1727 CE1 TYR A 222 -16.595 -11.392 -50.497 1.00 14.97 A
ATOM 1728 CD2 TYR A 222 -14.357 -12.540 -51.612 1.00 14.88 A
ATOM 1729 CE2 TYR A 222 -14.214 -11.519 -50.681 1.00 13.42 A
ATOM 1730 CZ TYR A 222 -15.338 -10.952 -50.128 1.00 14.66 A

ATOM 1731 OH TYR A 222 -15.222 -9.957 -49.185 1.00 14.60 A
ATOM 1732 C TYR A 222 -15.742 -12.397 -54.877 1.00 15.63 A
ATOM 1733 O TYR A 222 -16.262 -11.291 -54.884 1.00 15.35 A
ATOM 1734 N LEU A 223 -14.516 -12.631 -55.336 1.00 16.33 A
ATOM 1735 CA LEU A 223 -13.681 -11.582 -55.911 1.00 17.18 A
ATOM 1736 CB LEU A 223 -12.520 -12.199 -56.681 1.00 17.93 A
ATOM 1737 CG LEU A 223 -11.505 -12.977 -55.853 1.00 19.84 A
ATOM 1738 CD1 LEU A 223 -10.408 -13.506 -56.780 1.00 21.41 A
ATOM 1739 CD2 LEU A 223 -10.909 -12.079 -54.776 1.00 20.01 A
ATOM 1740 C LEU A 223 -14.452 -10.647 -56.841 1.00 17.64 A
ATOM 1741 O LEU A 223 -14.187 -9.440 -56.872 1.00 16.48 A
ATOM 1742 N ASN A 224 -15.397 -11.198 -57.600 1.00 18.65 A
ATOM 1743 CA ASN A 224 -16.176 -10.374 -58.503 1.00 20.39 A
ATOM 1744 CB ASN A 224 -16.752 -11.199 -59.648 1.00 21.74 A
ATOM 1745 CG ASN A 224 -15.840 -11.199 -60.864 1.00 24.90 A
ATOM 1746 OD1 ASN A 224 -15.636 -10.161 -61.521 1.00 25.95 A
ATOM 1747 ND2 ASN A 224 -15.264 -12.358 -61.160 1.00 26.25 A
ATOM 1748 C ASN A 224 -17.268 -9.613 -57.791 1.00 20.79 A
ATOM 1749 O ASN A 224 -17.481 -8.429 -58.081 1.00 22.75 A
ATOM 1750 N LEU A 225 -17.967 -10.261 -56.863 1.00 19.82 A
ATOM 1751 CA LEU A 225 -18.994 -9.537 -56.118 1.00 18.61 A
ATOM 1752 CB LEU A 225 -19.674 -10.452 -55.098 1.00 16.99 A
ATOM 1753 CG LEU A 225 -20.771 -9.750 -54.293 1.00 17.82 A
ATOM 1754 CD1 LEU A 225 -21.827 -9.178 -55.243 1.00 15.88 A
ATOM 1755 CD2 LEU A 225 -21.385 -10.727 -53.300 1.00 17.09 A
ATOM 1756 C LEU A 225 -18.277 -8.385 -55.390 1.00 17.52 A
ATOM 1757 O LEU A 225 -18.796 -7.282 -55.253 1.00 16.16 A
ATOM 1758 N HIS A 226 -17.061 -8.679 -54.950 1.00 17.71 A
ATOM 1759 CA HIS A 226 -16.215 -7.747 -54.236 1.00 18.86 A
ATOM 1760 CB HIS A 226 -14.933 -8.466 -53.801 1.00 19.59 A
ATOM 1761 CG HIS A 226 -13.997 -7.618 -52.999 1.00 20.50 A
ATOM 1762 CD2 HIS A 226 -13.465 -7.801 -51.770 1.00 20.55 A
ATOM 1763 ND1 HIS A 226 -13.449 -6.449 -53.481 1.00 21.68 A
ATOM 1764 CE1 HIS A 226 -12.617 -5.952 -52.585 1.00 21.11 A

ATOM 1765 NE2 HIS A 226 -12.608 -6.753 -51.538 1.00 20.14 A
ATOM 1766 C HIS A 226 -15.885 -6.503 -55.058 1.00 19.34 A
ATOM 1767 O HIS A 226 -16.320 -5.410 -54.705 1.00 20.11 A
ATOM 1768 N ALA A 227 -15.122 -6.649 -56.143 1.00 19.62 A
ATOM 1769 CA ALA A 227 -14.765 -5.490 -56.974 1.00 19.73 A
ATOM 1770 CB ALA A 227 -13.999 -5.950 -58.203 1.00 17.75 A
ATOM 1771 C ALA A 227 -15.980 -4.635 -57.391 1.00 19.72 A
ATOM 1772 O ALA A 227 -15.884 -3.405 -57.465 1.00 18.83 A
ATOM 1773 N PHE A 228 -17.114 -5.295 -57.639 1.00 18.98 A
ATOM 1774 CA PHE A 228 -18.360 -4.641 -58.049 1.00 19.35 A
ATOM 1775 CB PHE A 228 -19.403 -5.707 -58.409 1.00 20.24 A
ATOM 1776 CG PHE A 228 -20.707 -5.148 -58.931 1.00 22.58 A
ATOM 1777 CD1 PHE A 228 -20.804 -4.640 -60.224 1.00 22.95 A
ATOM 1778 CD2 PHE A 228 -21.853 -5.159 -58.137 1.00 23.62 A
ATOM 1779 CE1 PHE A 228 -22.029 -4.155 -60.721 1.00 22.86 A
ATOM 1780 CE2 PHE A 228 -23.074 -4.680 -58.622 1.00 23.72 A
ATOM 1781 CZ PHE A 228 -23.161 -4.178 -59.917 1.00 23.32 A
ATOM 1782 C PHE A 228 -18.914 -3.740 -56.957 1.00 19.51 A
ATOM 1783 O PHE A 228 -19.348 -2.624 -57.218 1.00 20.82 A
ATOM 1784 N VAL A 229 -18.914 -4.244 -55.729 1.00 18.14 A
ATOM 1785 CA VAL A 229 -19.407 -3.489 -54.592 1.00 16.73 A
ATOM 1786 CB VAL A 229 -19.636 -4.403 -53.377 1.00 17.01 A
ATOM 1787 CG1 VAL A 229 -19.956 -3.567 -52.146 1.00 16.68 A
ATOM 1788 CG2 VAL A 229 -20.773 -5.373 -53.675 1.00 15.78 A
ATOM 1789 C VAL A 229 -18.393 -2.427 -54.229 1.00 16.22 A
ATOM 1790 O VAL A 229 -18.746 -1.301 -53.924 1.00 15.22 A
ATOM 1791 N ARG A 230 -17.124 -2.795 -54.267 1.00 16.84 A
ATOM 1792 CA ARG A 230 -16.073 -1.850 -53.948 1.00 18.28 A
ATOM 1793 CB ARG A 230 -14.692 -2.486 -54.117 1.00 16.72 A
ATOM 1794 CG ARG A 230 -13.549 -1.565 -53.704 1.00 17.78 A
ATOM 1795 CD ARG A 230 -12.196 -2.240 -53.844 1.00 20.55 A
ATOM 1796 NE ARG A 230 -11.911 -2.616 -55.224 1.00 22.59 A
ATOM 1797 CZ ARG A 230 -10.983 -3.499 -55.572 1.00 22.87 A
ATOM 1798 NH1 ARG A 230 -10.253 -4.099 -54.649 1.00 22.74 A

ATOM 1799 NH2 ARG A 230 -10.791 -3.791 -56.845 1.00 26.21 A
ATOM 1800 C ARG A 230 -16.206 -0.652 -54.878 1.00 19.38 A
ATOM 1801 O ARG A 230 -15.901 0.480 -54.496 1.00 20.34 A
ATOM 1802 N ARG A 231 -16.658 -0.897 -56.104 1.00 19.18 A
ATOM 1803 CA ARG A 231 -16.833 0.196 -57.048 1.00 19.52 A
ATOM 1804 CB ARG A 231 -17.038 -0.341 -58.473 1.00 22.02 A
ATOM 1805 CG ARG A 231 -17.794 0.599 -59.424 1.00 23.90 A
ATOM 1806 CD ARG A 231 -16.992 1.814 -59.835 1.00 24.71 A
ATOM 1807 NE ARG A 231 -16.221 1.551 -61.040 1.00 28.82 A
ATOM 1808 CZ ARG A 231 -15.664 2.489 -61.802 1.00 30.31 A
ATOM 1809 NH1 ARG A 231 -14.979 2.142 -62.886 1.00 30.51 A
ATOM 1810 NH2 ARG A 231 -15.798 3.772 -61.484 1.00 30.50 A
ATOM 1811 C ARG A 231 -18.043 1.000 -56.594 1.00 18.41 A
ATOM 1812 O ARG A 231 -17.957 2.207 -56.414 1.00 16.85 A
ATOM 1813 N ALA A 232 -19.169 0.327 -56.395 1.00 18.30 A
ATOM 1814 CA ALA A 232 -20.367 1.016 -55.950 1.00 19.22 A
ATOM 1815 CB ALA A 232 -21.460 0.021 -55.647 1.00 18.29 A
ATOM 1816 C ALA A 232 -20.071 1.854 -54.707 1.00 20.02 A
ATOM 1817 O ALA A 232 -20.560 2.974 -54.581 1.00 20.83 A
ATOM 1818 N LEU A 233 -19.273 1.318 -53.785 1.00 20.27 A
ATOM 1819 CA LEU A 233 -18.948 2.055 -52.568 1.00 20.99 A
ATOM 1820 CB LEU A 233 -18.268 1.148 -51.530 1.00 21.27 A
ATOM 1821 CG LEU A 233 -19.198 0.240 -50.709 1.00 21.28 A
ATOM 1822 CD1 LEU A 233 -18.391 -0.572 -49.722 1.00 21.97 A
ATOM 1823 CD2 LEU A 233 -20.232 1.074 -49.972 1.00 20.87 A
ATOM 1824 C LEU A 233 -18.084 3.272 -52.853 1.00 21.85 A
ATOM 1825 O LEU A 233 -18.303 4.338 -52.280 1.00 22.22 A
ATOM 1826 N HIS A 234 -17.104 3.120 -53.734 1.00 23.04 A
ATOM 1827 CA HIS A 234 -16.240 4.242 -54.094 1.00 24.21 A
ATOM 1828 CB HIS A 234 -15.310 3.831 -55.241 1.00 23.12 A
ATOM 1829 CG HIS A 234 -14.398 4.919 -55.715 1.00 24.28 A
ATOM 1830 CD2 HIS A 234 -13.137 5.253 -55.345 1.00 25.28 A
ATOM 1831 ND1 HIS A 234 -14.749 5.807 -56.708 1.00 25.58 A
ATOM 1832 CE1 HIS A 234 -13.745 6.639 -56.931 1.00 25.62 A

ATOM 1833 NE2 HIS A 234 -12.754 6.324 -56.118 1.00 24.61 A
ATOM 1834 C HIS A 234 -17.145 5.394 -54.525 1.00 26.31 A
ATOM 1835 O HIS A 234 -17.010 6.536 -54.066 1.00 26.73 A
ATOM 1836 N ARG A 235 -18.095 5.061 -55.391 1.00 28.34 A
ATOM 1837 CA ARG A 235 -19.063 6.010 -55.925 1.00 29.79 A
ATOM 1838 CB ARG A 235 -20.129 5.247 -56.710 1.00 30.15 A
ATOM 1839 CG ARG A 235 -20.588 5.924 -57.981 1.00 35.12 A
ATOM 1840 CD ARG A 235 -20.542 4.948 -59.173 1.00 38.02 A
ATOM 1841 NE ARG A 235 -21.241 3.693 -58.880 1.00 42.20 A
ATOM 1842 CZ ARG A 235 -21.171 2.592 -59.632 1.00 43.47 A
ATOM 1843 NH1 ARG A 235 -20.430 2.580 -60.742 1.00 42.94 A
ATOM 1844 NH2 ARG A 235 -21.827 1.491 -59.258 1.00 44.85 A
ATOM 1845 C ARG A 235 -19.738 6.869 -54.858 1.00 30.19 A
ATOM 1846 O ARG A 235 -20.067 8.023 -55.115 1.00 31.22 A
ATOM 1847 N ARG A 236 -19.933 6.313 -53.662 1.00 30.20 A
ATOM 1848 CA ARG A 236 -20.617 7.031 -52.582 1.00 29.55 A
ATOM 1849 CB ARG A 236 -21.591 6.076 -51.879 1.00 28.72 A
ATOM 1850 CG ARG A 236 -21.603 6.173 -50.363 1.00 29.76 A
ATOM 1851 CD ARG A 236 -22.687 7.107 -49.824 1.00 30.73 A
ATOM 1852 NE ARG A 236 -24.047 6.662 -50.144 1.00 30.46 A
ATOM 1853 CZ ARG A 236 -25.147 7.105 -49.533 1.00 29.88 A
ATOM 1854 NH1 ARG A 236 -25.057 8.006 -48.559 1.00 29.80 A
ATOM 1855 NH2 ARG A 236 -26.338 6.657 -49.902 1.00 28.85 A
ATOM 1856 C ARG A 236 -19.747 7.738 -51.545 1.00 28.16 A
ATOM 1857 O ARG A 236 -20.078 8.834 -51.112 1.00 27.16 A
ATOM 1858 N TYR A 237 -18.645 7.118 -51.144 1.00 27.62 A
ATOM 1859 CA TYR A 237 -17.778 7.727 -50.140 1.00 27.49 A
ATOM 1860 CB TYR A 237 -17.281 6.681 -49.146 1.00 25.75 A
ATOM 1861 CG TYR A 237 -18.401 5.983 -48.419 1.00 24.79 A
ATOM 1862 CD1 TYR A 237 -18.678 4.641 -48.667 1.00 24.20 A
ATOM 1863 CE1 TYR A 237 -19.705 3.993 -48.023 1.00 23.82 A
ATOM 1864 CD2 TYR A 237 -19.195 6.665 -47.497 1.00 23.05 A
ATOM 1865 CE2 TYR A 237 -20.236 6.022 -46.845 1.00 23.34 A
ATOM 1866 CZ TYR A 237 -20.482 4.679 -47.114 1.00 24.38 A

ATOM 1867 OH TYR A 237 -21.485 3.994 -46.465 1.00 25.67 A
ATOM 1868 C TYR A 237 -16.597 8.445 -50.745 1.00 27.96 A
ATOM 1869 O TYR A 237 -15.905 9.201 -50.067 1.00 27.80 A
ATOM 1870 N GLY A 238 -16.347 8.194 -52.022 1.00 28.93 A
ATOM 1871 CA GLY A 238 -15.254 8.884 -52.670 1.00 30.62 A
ATOM 1872 C GLY A 238 -13.929 8.180 -52.823 1.00 31.40 A
ATOM 1873 O GLY A 238 -13.807 6.981 -52.630 1.00 31.57 A
ATOM 1874 N ASP A 239 -12.920 8.972 -53.157 1.00 32.87 A
ATOM 1875 CA ASP A 239 -11.583 8.472 -53.407 1.00 34.23 A
ATOM 1876 CB ASP A 239 -10.965 9.289 -54.533 1.00 35.99 A
ATOM 1877 CG ASP A 239 -9.996 8.482 -55.350 1.00 39.51 A
ATOM 1878 OD1 ASP A 239 -10.449 7.482 -55.970 1.00 40.93 A
ATOM 1879 OD2 ASP A 239 -8.790 8.842 -55.358 1.00 41.81 A
ATOM 1880 C ASP A 239 -10.639 8.456 -52.210 1.00 34.21 A
ATOM 1881 O ASP A 239 -9.596 7.795 -52.249 1.00 33.86 A
ATOM 1882 N ALA A 240 -10.997 9.187 -51.157 1.00 34.02 A
ATOM 1883 CA ALA A 240 -10.175 9.238 -49.954 1.00 32.33 A
ATOM 1884 CB ALA A 240 -10.491 10.490 -49.146 1.00 32.59 A
ATOM 1885 C ALA A 240 -10.410 8.003 -49.095 1.00 31.67 A
ATOM 1886 O ALA A 240 -9.465 7.442 -48.547 1.00 31.77 A
ATOM 1887 N TYR A 241 -11.664 7.568 -49.000 1.00 30.56 A
ATOM 1888 CA TYR A 241 -11.996 6.430 -48.167 1.00 30.16 A
ATOM 1889 CB TYR A 241 -13.308 6.700 -47.447 1.00 33.72 A
ATOM 1890 CG TYR A 241 -13.199 7.863 -46.493 1.00 38.47 A
ATOM 1891 CD1 TYR A 241 -14.240 8.778 -46.348 1.00 39.86 A
ATOM 1892 CE1 TYR A 241 -14.105 9.906 -45.534 1.00 42.05 A
ATOM 1893 CD2 TYR A 241 -12.014 8.097 -45.788 1.00 40.76 A
ATOM 1894 CE2 TYR A 241 -11.867 9.224 -44.976 1.00 42.77 A
ATOM 1895 CZ TYR A 241 -12.913 10.127 -44.855 1.00 43.05 A
ATOM 1896 OH TYR A 241 -12.755 11.264 -44.084 1.00 44.78 A
ATOM 1897 C TYR A 241 -12.036 5.075 -48.833 1.00 29.36 A
ATOM 1898 O TYR A 241 -11.894 4.060 -48.151 1.00 29.97 A
ATOM 1899 N ILE A 242 -12.243 5.023 -50.145 1.00 27.23 A
ATOM 1900 CA ILE A 242 -12.247 3.728 -50.822 1.00 24.93 A

ATOM 1901 CB ILE A 242 -13.614 3.416 -51.468 1.00 23.59 A
ATOM 1902 CG2 ILE A 242 -13.531 2.112 -52.246 1.00 22.19 A
ATOM 1903 CG1 ILE A 242 -14.701 3.283 -50.395 1.00 23.82 A
ATOM 1904 CD1 ILE A 242 -14.634 1.996 -49.572 1.00 23.69 A
ATOM 1905 C ILE A 242 -11.158 3.664 -51.890 1.00 24.88 A
ATOM 1906 O ILE A 242 -11.046 4.554 -52.726 1.00 25.34 A
ATOM 1907 N ASN A 243 -10.343 2.614 -51.839 1.00 25.53 A
ATOM 1908 CA ASN A 243 -9.262 2.420 -52.800 1.00 24.99 A
ATOM 1909 CB ASN A 243 -7.993 1.968 -52.093 1.00 23.45 A
ATOM 1910 CG ASN A 243 -6.866 1.702 -53.048 1.00 22.10 A
ATOM 1911 OD1 ASN A 243 -7.079 1.242 -54.164 1.00 24.32 A
ATOM 1912 ND2 ASN A 243 -5.650 1.972 -52.613 1.00 20.21 A
ATOM 1913 C ASN A 243 -9.690 1.345 -53.789 1.00 25.06 A
ATOM 1914 O ASN A 243 -9.888 0.184 -53.408 1.00 24.68 A
ATOM 1915 N LEU A 244 -9.819 1.744 -55.054 1.00 23.94 A
ATOM 1916 CA LEU A 244 -10.248 0.848 -56.125 1.00 24.23 A
ATOM 1917 CB LEU A 244 -10.497 1.669 -57.394 1.00 24.31 A
ATOM 1918 CG LEU A 244 -11.687 2.621 -57.325 1.00 23.51 A
ATOM 1919 CD1 LEU A 244 -11.731 3.523 -58.545 1.00 23.41 A
ATOM 1920 CD2 LEU A 244 -12.962 1.805 -57.209 1.00 23.41 A
ATOM 1921 C LEU A 244 -9.281 -0.305 -56.420 1.00 24.46 A
ATOM 1922 O LEU A 244 -9.556 -1.169 -57.255 1.00 25.01 A
ATOM 1923 N ARG A 245 -8.158 -0.308 -55.756 1.00 24.99 A
ATOM 1924 CA ARG A 245 -7.172 -1.326 -55.891 1.00 26.08 A
ATOM 1925 CB ARG A 245 -5.990 -0.689 -56.467 1.00 29.72 A
ATOM 1926 CG ARG A 245 -5.726 -0.908 -57.869 1.00 33.61 A
ATOM 1927 CD ARG A 245 -5.639 0.310 -58.543 1.00 37.88 A
ATOM 1928 NE ARG A 245 -4.312 0.632 -58.987 1.00 41.48 A
ATOM 1929 CZ ARG A 245 -3.651 1.666 -58.567 1.00 43.64 A
ATOM 1930 NH1 ARG A 245 -4.188 2.451 -57.661 1.00 45.14 A
ATOM 1931 NH2 ARG A 245 -2.462 1.921 -59.032 1.00 42.67 A
ATOM 1932 C ARG A 245 -6.697 -1.827 -54.575 1.00 25.61 A
ATOM 1933 O ARG A 245 -5.640 -2.313 -54.516 1.00 25.99 A
ATOM 1934 N GLY A 246 -7.462 -1.622 -53.508 1.00 23.55 A

ATOM 1935 CA GLY A 246 -7.100 -2.060 -52.176 1.00 21.78 A
ATOM 1936 C GLY A 246 -8.263 -2.749 -51.506 1.00 20.67 A
ATOM 1937 O GLY A 246 -9.354 -2.775 -52.073 1.00 22.09 A
ATOM 1938 N PRO A 247 -8.077 -3.305 -50.296 1.00 18.33 A
ATOM 1939 CD PRO A 247 -6.892 -3.206 -49.426 1.00 16.92 A
ATOM 1940 CA PRO A 247 -9.162 -3.989 -49.602 1.00 17.28 A
ATOM 1941 CB PRO A 247 -8.452 -4.638 -48.436 1.00 15.74 A
ATOM 1942 CG PRO A 247 -7.435 -3.639 -48.094 1.00 16.89 A
ATOM 1943 C PRO A 247 -10.170 -2.961 -49.167 1.00 18.49 A
ATOM 1944 O PRO A 247 -9.819 -1.797 -48.985 1.00 19.02 A
ATOM 1945 N ILE A 248 -11.424 -3.377 -49.021 1.00 19.95 A
ATOM 1946 CA ILE A 248 -12.486 -2.462 -48.597 1.00 20.23 A
ATOM 1947 CB ILE A 248 -13.865 -3.024 -48.934 1.00 17.37 A
ATOM 1948 CG2 ILE A 248 -14.922 -2.037 -48.542 1.00 16.91 A
ATOM 1949 CG1 ILE A 248 -13.936 -3.378 -50.414 1.00 16.65 A
ATOM 1950 CD1 ILE A 248 -15.157 -4.196 -50.794 1.00 15.12 A
ATOM 1951 C ILE A 248 -12.429 -2.288 -47.085 1.00 21.54 A
ATOM 1952 O ILE A 248 -12.104 -3.230 -46.369 1.00 23.11 A
ATOM 1953 N PRO A 249 -12.727 -1.081 -46.580 1.00 22.23 A
ATOM 1954 CD PRO A 249 -12.834 0.173 -47.347 1.00 22.95 A
ATOM 1955 CA PRO A 249 -12.713 -0.808 -45.134 1.00 22.55 A
ATOM 1956 CB PRO A 249 -12.881 0.710 -45.069 1.00 24.10 A
ATOM 1957 CG PRO A 249 -12.273 1.179 -46.377 1.00 23.02 A
ATOM 1958 C PRO A 249 -13.871 -1.562 -44.451 1.00 21.70 A
ATOM 1959 O PRO A 249 -15.035 -1.330 -44.755 1.00 21.66 A
ATOM 1960 N ALA A 250 -13.525 -2.442 -43.517 1.00 21.79 A
ATOM 1961 CA ALA A 250 -14.469 -3.315 -42.803 1.00 22.32 A
ATOM 1962 CB ALA A 250 -13.716 -4.054 -41.708 1.00 21.30 A
ATOM 1963 C ALA A 250 -15.801 -2.807 -42.234 1.00 22.16 A
ATOM 1964 O ALA A 250 -16.661 -3.622 -41.882 1.00 22.88 A
ATOM 1965 N HIS A 251 -16.002 -1.496 -42.149 1.00 21.29 A
ATOM 1966 CA HIS A 251 -17.241 -0.976 -41.582 1.00 20.38 A
ATOM 1967 CB HIS A 251 -16.922 0.130 -40.588 1.00 17.81 A
ATOM 1968 CG HIS A 251 -16.249 1.320 -41.199 1.00 15.99 A

ATOM 1969 CD2 HIS A 251 -16.609 2.625 -41.239 1.00 14.54 A
ATOM 1970 ND1 HIS A 251 -15.032 1.238 -41.842 1.00 15.78 A
ATOM 1971 CE1 HIS A 251 -14.672 2.441 -42.249 1.00 15.30 A
ATOM 1972 NE2 HIS A 251 -15.610 3.300 -41.895 1.00 14.34 A
ATOM 1973 C HIS A 251 -18.265 -0.444 -42.573 1.00 22.18 A
ATOM 1974 O HIS A 251 -19.306 0.084 -42.167 1.00 23.18 A
ATOM 1975 N LEU A 252 -17.991 -0.587 -43.867 1.00 23.49 A
ATOM 1976 CA LEU A 252 -18.893 -0.066 -44.890 1.00 24.01 A
ATOM 1977 CB LEU A 252 -18.080 0.665 -45.944 1.00 23.45 A
ATOM 1978 CG LEU A 252 -17.175 1.707 -45.295 1.00 24.28 A
ATOM 1979 CD1 LEU A 252 -16.230 2.280 -46.328 1.00 25.33 A
ATOM 1980 CD2 LEU A 252 -18.019 2.796 -44.658 1.00 23.14 A
ATOM 1981 C LEU A 252 -19.800 -1.083 -45.566 1.00 23.89 A
ATOM 1982 O LEU A 252 -20.723 -0.694 -46.283 1.00 23.72 A
ATOM 1983 N LEU A 253 -19.551 -2.373 -45.340 1.00 23.56 A
ATOM 1984 CA LEU A 253 -20.369 -3.413 -45.967 1.00 23.63 A
ATOM 1985 CB LEU A 253 -19.592 -4.736 -46.036 1.00 22.61 A
ATOM 1986 CG LEU A 253 -18.524 -4.854 -47.136 1.00 21.86 A
ATOM 1987 CD1 LEU A 253 -19.040 -4.201 -48.397 1.00 19.44 A
ATOM 1988 CD2 LEU A 253 -17.244 -4.190 -46.726 1.00 22.98 A
ATOM 1989 C LEU A 253 -21.744 -3.634 -45.328 1.00 24.62 A
ATOM 1990 O LEU A 253 -22.450 -4.594 -45.655 1.00 23.77 A
ATOM 1991 N GLY A 254 -22.111 -2.737 -44.412 1.00 25.84 A
ATOM 1992 CA GLY A 254 -23.413 -2.806 -43.757 1.00 26.23 A
ATOM 1993 C GLY A 254 -23.642 -3.820 -42.649 1.00 26.43 A
ATOM 1994 O GLY A 254 -24.792 -4.077 -42.278 1.00 26.24 A
ATOM 1995 N ASP A 255 -22.562 -4.387 -42.118 1.00 25.95 A
ATOM 1996 CA ASP A 255 -22.645 -5.378 -41.053 1.00 25.40 A
ATOM 1997 CB ASP A 255 -22.907 -6.753 -41.661 1.00 25.91 A
ATOM 1998 CG ASP A 255 -22.713 -7.864 -40.667 1.00 27.96 A
ATOM 1999 OD1 ASP A 255 -21.542 -8.137 -40.322 1.00 27.24 A
ATOM 2000 OD2 ASP A 255 -23.723 -8.457 -40.224 1.00 30.03 A
ATOM 2001 C ASP A 255 -21.344 -5.369 -40.248 1.00 25.58 A
ATOM 2002 O ASP A 255 -20.259 -5.402 -40.816 1.00 26.44 A

```
ATOM  2003  N   MET A 256     -21.466  -5.320 -38.925  1.00 25.26      A
ATOM  2004  CA  MET A 256     -20.324  -5.256 -38.011  1.00 24.59      A
ATOM  2005  CB  MET A 256     -20.807  -5.577 -36.582  1.00 24.40      A
ATOM  2006  CG  MET A 256     -19.795  -5.338 -35.466  1.00 24.15      A
ATOM  2007  SD  MET A 256     -19.032  -3.673 -35.411  1.00 28.25      A
ATOM  2008  CE  MET A 256     -20.276  -2.681 -34.581  1.00 26.00      A
ATOM  2009  C   MET A 256     -19.088  -6.100 -38.363  1.00 24.12      A
ATOM  2010  O   MET A 256     -17.957  -5.700 -38.088  1.00 22.54      A
ATOM  2011  N   TRP A 257     -19.288  -7.250 -38.992  1.00 24.84      A
ATOM  2012  CA  TRP A 257     -18.160  -8.110 -39.332  1.00 25.64      A
ATOM  2013  CB  TRP A 257     -18.387  -9.506 -38.748  1.00 26.31      A
ATOM  2014  CG  TRP A 257     -18.674  -9.427 -37.286  1.00 27.74      A
ATOM  2015  CD2 TRP A 257     -19.966  -9.393 -36.665  1.00 27.64      A
ATOM  2016  CE2 TRP A 257     -19.766  -9.124 -35.294  1.00 28.34      A
ATOM  2017  CE3 TRP A 257     -21.276  -9.555 -37.138  1.00 26.67      A
ATOM  2018  CD1 TRP A 257     -17.765  -9.197 -36.287  1.00 28.15      A
ATOM  2019  NE1 TRP A 257     -18.415  -9.009 -35.091  1.00 28.29      A
ATOM  2020  CZ2 TRP A 257     -20.828  -9.011 -34.391  1.00 27.86      A
ATOM  2021  CZ3 TRP A 257     -22.324  -9.442 -36.243  1.00 26.13      A
ATOM  2022  CH2 TRP A 257     -22.096  -9.172 -34.884  1.00 27.49      A
ATOM  2023  C   TRP A 257     -17.935  -8.194 -40.822  1.00 25.79      A
ATOM  2024  O   TRP A 257     -16.976  -8.812 -41.269  1.00 26.17      A
ATOM  2025  N   ALA A 258     -18.826  -7.561 -41.577  1.00 26.43      A
ATOM  2026  CA  ALA A 258     -18.757  -7.544 -43.033  1.00 27.30      A
ATOM  2027  CB  ALA A 258     -17.386  -7.044 -43.491  1.00 26.85      A
ATOM  2028  C   ALA A 258     -19.000  -8.944 -43.568  1.00 28.20      A
ATOM  2029  O   ALA A 258     -18.509  -9.297 -44.636  1.00 29.54      A
ATOM  2030  N   GLN A 259     -19.765  -9.740 -42.830  1.00 28.07      A
ATOM  2031  CA  GLN A 259     -20.029 -11.109 -43.235  1.00 28.16      A
ATOM  2032  CB  GLN A 259     -20.311 -11.981 -42.003  1.00 29.12      A
ATOM  2033  CG  GLN A 259     -21.475 -11.527 -41.126  1.00 29.26      A
ATOM  2034  CD  GLN A 259     -21.774 -12.515 -40.018  1.00 29.00      A
ATOM  2035  OE1 GLN A 259     -20.900 -12.839 -39.221  1.00 30.26      A
ATOM  2036  NE2 GLN A 259     -23.010 -13.004 -39.965  1.00 29.36      A
```

ATOM 2037 C GLN A 259 -21.152 -11.264 -44.257 1.00 28.46 A
ATOM 2038 O GLN A 259 -21.252 -12.305 -44.908 1.00 28.34 A
ATOM 2039 N SER A 260 -22.007 -10.255 -44.387 1.00 27.96 A
ATOM 2040 CA SER A 260 -23.087 -10.296 -45.373 1.00 28.23 A
ATOM 2041 CB SER A 260 -24.305 -11.049 -44.834 1.00 27.92 A
ATOM 2042 OG SER A 260 -24.716 -10.530 -43.589 1.00 30.62 A
ATOM 2043 C SER A 260 -23.438 -8.856 -45.741 1.00 27.80 A
ATOM 2044 O SER A 260 -23.689 -8.023 -44.864 1.00 29.05 A
ATOM 2045 N TRP A 261 -23.457 -8.570 -47.041 1.00 26.57 A
ATOM 2046 CA TRP A 261 -23.698 -7.220 -47.525 1.00 25.94 A
ATOM 2047 CB TRP A 261 -22.712 -6.927 -48.665 1.00 26.22 A
ATOM 2048 CG TRP A 261 -21.312 -7.449 -48.398 1.00 25.14 A
ATOM 2049 CD2 TRP A 261 -20.223 -7.512 -49.325 1.00 24.03 A
ATOM 2050 CE2 TRP A 261 -19.115 -8.053 -48.632 1.00 24.07 A
ATOM 2051 CE3 TRP A 261 -20.072 -7.163 -50.673 1.00 23.98 A
ATOM 2052 CD1 TRP A 261 -20.829 -7.940 -47.216 1.00 25.00 A
ATOM 2053 NE1 TRP A 261 -19.518 -8.304 -47.347 1.00 23.79 A
ATOM 2054 CZ2 TRP A 261 -17.868 -8.254 -49.242 1.00 23.28 A
ATOM 2055 CZ3 TRP A 261 -18.834 -7.363 -51.280 1.00 24.44 A
ATOM 2056 CH2 TRP A 261 -17.747 -7.905 -50.561 1.00 23.12 A
ATOM 2057 C TRP A 261 -25.117 -6.871 -47.959 1.00 25.26 A
ATOM 2058 O TRP A 261 -25.355 -5.766 -48.433 1.00 25.24 A
ATOM 2059 N GLU A 262 -26.057 -7.795 -47.782 1.00 25.04 A
ATOM 2060 CA GLU A 262 -27.453 -7.567 -48.169 1.00 24.87 A
ATOM 2061 CB GLU A 262 -28.317 -8.775 -47.777 1.00 26.29 A
ATOM 2062 CG GLU A 262 -27.844 -9.486 -46.538 1.00 31.88 A
ATOM 2063 CD GLU A 262 -28.950 -9.659 -45.519 1.00 36.83 A
ATOM 2064 OE1 GLU A 262 -29.555 -8.630 -45.120 1.00 39.12 A
ATOM 2065 OE2 GLU A 262 -29.215 -10.819 -45.110 1.00 39.09 A
ATOM 2066 C GLU A 262 -28.093 -6.292 -47.630 1.00 23.59 A
ATOM 2067 O GLU A 262 -29.167 -5.907 -48.080 1.00 22.95 A
ATOM 2068 N ASN A 263 -27.447 -5.637 -46.670 1.00 23.44 A
ATOM 2069 CA ASN A 263 -27.990 -4.402 -46.113 1.00 23.32 A
ATOM 2070 CB ASN A 263 -27.619 -4.245 -44.630 1.00 24.10 A

ATOM 2071 CG ASN A 263 -28.667 -4.823 -43.695 1.00 25.41 A
ATOM 2072 OD1 ASN A 263 -29.834 -4.441 -43.741 1.00 25.12 A
ATOM 2073 ND2 ASN A 263 -28.254 -5.745 -42.840 1.00 26.98 A
ATOM 2074 C ASN A 263 -27.528 -3.173 -46.885 1.00 23.36 A
ATOM 2075 O ASN A 263 -27.873 -2.061 -46.527 1.00 23.63 A
ATOM 2076 N ILE A 264 -26.729 -3.355 -47.927 1.00 23.51 A
ATOM 2077 CA ILE A 264 -26.312 -2.208 -48.717 1.00 23.66 A
ATOM 2078 CB ILE A 264 -24.767 -2.033 -48.722 1.00 21.36 A
ATOM 2079 CG2 ILE A 264 -24.289 -1.678 -47.347 1.00 19.65 A
ATOM 2080 CG1 ILE A 264 -24.073 -3.304 -49.180 1.00 21.03 A
ATOM 2081 CD1 ILE A 264 -22.579 -3.131 -49.319 1.00 22.40 A
ATOM 2082 C ILE A 264 -26.855 -2.346 -50.151 1.00 25.45 A
ATOM 2083 O ILE A 264 -26.478 -1.599 -51.052 1.00 25.94 A
ATOM 2084 N TYR A 265 -27.767 -3.301 -50.327 1.00 26.29 A
ATOM 2085 CA TYR A 265 -28.405 -3.594 -51.607 1.00 27.39 A
ATOM 2086 CB TYR A 265 -29.619 -4.492 -51.372 1.00 26.33 A
ATOM 2087 CG TYR A 265 -30.450 -4.781 -52.602 1.00 25.96 A
ATOM 2088 CD1 TYR A 265 -29.920 -5.498 -53.684 1.00 26.77 A
ATOM 2089 CE1 TYR A 265 -30.699 -5.778 -54.821 1.00 25.68 A
ATOM 2090 CD2 TYR A 265 -31.771 -4.352 -52.685 1.00 25.38 A
ATOM 2091 CE2 TYR A 265 -32.553 -4.625 -53.812 1.00 24.95 A
ATOM 2092 CZ TYR A 265 -32.011 -5.336 -54.869 1.00 24.52 A
ATOM 2093 OH TYR A 265 -32.784 -5.603 -55.960 1.00 21.97 A
ATOM 2094 C TYR A 265 -28.845 -2.341 -52.356 1.00 29.31 A
ATOM 2095 O TYR A 265 -28.706 -2.243 -53.580 1.00 29.95 A
ATOM 2096 N ASP A 266 -29.382 -1.381 -51.615 1.00 31.14 A
ATOM 2097 CA ASP A 266 -29.858 -0.140 -52.210 1.00 32.38 A
ATOM 2098 CB ASP A 266 -30.668 0.669 -51.182 1.00 34.67 A
ATOM 2099 CG ASP A 266 -29.895 0.918 -49.891 1.00 37.51 A
ATOM 2100 OD1 ASP A 266 -29.605 -0.070 -49.182 1.00 39.06 A
ATOM 2101 OD2 ASP A 266 -29.570 2.092 -49.584 1.00 38.58 A
ATOM 2102 C ASP A 266 -28.730 0.717 -52.772 1.00 31.88 A
ATOM 2103 O ASP A 266 -28.990 1.704 -53.442 1.00 32.84 A
ATOM 2104 N MET A 267 -27.483 0.344 -52.507 1.00 31.37 A

```
ATOM  2105  CA  MET A 267     -26.336   1.102  -53.004  1.00 31.65      A
ATOM  2106  CB  MET A 267     -25.321   1.338  -51.887  1.00 32.28      A
ATOM  2107  CG  MET A 267     -25.722   2.326  -50.806  1.00 33.91      A
ATOM  2108  SD  MET A 267     -24.417   2.386  -49.544  1.00 37.42      A
ATOM  2109  CE  MET A 267     -23.479   3.731  -50.089  1.00 34.59      A
ATOM  2110  C   MET A 267     -25.618   0.390  -54.143  1.00 31.66      A
ATOM  2111  O   MET A 267     -24.748   0.967  -54.792  1.00 31.58      A
ATOM  2112  N   VAL A 268     -25.957  -0.872  -54.370  1.00 32.25      A
ATOM  2113  CA  VAL A 268     -25.314  -1.633  -55.428  1.00 34.03      A
ATOM  2114  CB  VAL A 268     -24.474  -2.803  -54.879  1.00 33.65      A
ATOM  2115  CG1 VAL A 268     -23.445  -2.289  -53.889  1.00 34.73      A
ATOM  2116  CG2 VAL A 268     -25.380  -3.830  -54.241  1.00 33.63      A
ATOM  2117  C   VAL A 268     -26.334  -2.209  -56.384  1.00 34.93      A
ATOM  2118  O   VAL A 268     -25.977  -2.654  -57.479  1.00 35.38      A
ATOM  2119  N   VAL A 269     -27.601  -2.211  -55.968  1.00 35.41      A
ATOM  2120  CA  VAL A 269     -28.664  -2.746  -56.813  1.00 34.96      A
ATOM  2121  CB  VAL A 269     -30.061  -2.215  -56.379  1.00 34.56      A
ATOM  2122  CG1 VAL A 269     -30.236  -0.780  -56.791  1.00 34.65      A
ATOM  2123  CG2 VAL A 269     -31.148  -3.064  -56.983  1.00 34.54      A
ATOM  2124  C   VAL A 269     -28.340  -2.302  -58.234  1.00 34.42      A
ATOM  2125  O   VAL A 269     -28.244  -1.111  -58.517  1.00 32.82      A
ATOM  2126  N   PRO A 270     -28.113  -3.266  -59.138  1.00 35.25      A
ATOM  2127  CD  PRO A 270     -28.156  -4.725  -58.945  1.00 35.71      A
ATOM  2128  CA  PRO A 270     -27.791  -2.934  -60.530  1.00 36.32      A
ATOM  2129  CB  PRO A 270     -27.493  -4.302  -61.152  1.00 35.28      A
ATOM  2130  CG  PRO A 270     -28.349  -5.228  -60.354  1.00 35.54      A
ATOM  2131  C   PRO A 270     -28.909  -2.171  -61.241  1.00 36.97      A
ATOM  2132  O   PRO A 270     -28.724  -1.021  -61.639  1.00 36.77      A
ATOM  2133  N   PHE A 271     -30.070  -2.798  -61.392  1.00 37.97      A
ATOM  2134  CA  PHE A 271     -31.173  -2.117  -62.056  1.00 38.41      A
ATOM  2135  CB  PHE A 271     -31.855  -3.056  -63.051  1.00 35.40      A
ATOM  2136  CG  PHE A 271     -30.891  -3.766  -63.940  1.00 33.92      A
ATOM  2137  CD1 PHE A 271     -30.571  -5.104  -63.713  1.00 33.83      A
ATOM  2138  CD2 PHE A 271     -30.232  -3.081  -64.955  1.00 31.74      A
```

ATOM 2139 CE1 PHE A 271 -29.605 -5.747 -64.481 1.00 32.50 A
ATOM 2140 CE2 PHE A 271 -29.265 -3.711 -65.724 1.00 30.97 A
ATOM 2141 CZ PHE A 271 -28.949 -5.045 -65.489 1.00 31.01 A
ATOM 2142 C PHE A 271 -32.163 -1.611 -61.032 1.00 39.65 A
ATOM 2143 O PHE A 271 -33.078 -2.323 -60.625 1.00 39.71 A
ATOM 2144 N PRO A 272 -31.969 -0.364 -60.577 1.00 41.11 A
ATOM 2145 CD PRO A 272 -30.902 0.580 -60.946 1.00 40.91 A
ATOM 2146 CA PRO A 272 -32.871 0.228 -59.588 1.00 42.37 A
ATOM 2147 CB PRO A 272 -32.069 1.413 -59.070 1.00 40.22 A
ATOM 2148 CG PRO A 272 -31.361 1.871 -60.290 1.00 40.26 A
ATOM 2149 C PRO A 272 -34.123 0.651 -60.330 1.00 44.54 A
ATOM 2150 O PRO A 272 -34.342 0.231 -61.467 1.00 46.26 A
ATOM 2151 N ALA A 273 -34.949 1.472 -59.700 1.00 45.82 A
ATOM 2152 CA ALA A 273 -36.165 1.943 -60.351 1.00 47.58 A
ATOM 2153 CB ALA A 273 -35.809 2.746 -61.607 1.00 46.24 A
ATOM 2154 C ALA A 273 -37.120 0.811 -60.711 1.00 48.33 A
ATOM 2155 O ALA A 273 -38.050 1.002 -61.491 1.00 48.66 A
ATOM 2156 N LYS A 274 -36.879 -0.370 -60.155 1.00 49.18 A
ATOM 2157 CA LYS A 274 -37.754 -1.519 -60.399 1.00 50.03 A
ATOM 2158 CB LYS A 274 -36.971 -2.665 -61.059 1.00 47.73 A
ATOM 2159 CG LYS A 274 -36.763 -2.459 -62.545 1.00 46.69 A
ATOM 2160 CD LYS A 274 -36.933 -3.775 -63.307 1.00 46.49 A
ATOM 2161 CE LYS A 274 -36.994 -3.576 -64.843 0.00 46.63 A
ATOM 2162 NZ LYS A 274 -37.527 -4.793 -65.572 0.00 46.61 A
ATOM 2163 C LYS A 274 -38.326 -1.964 -59.050 1.00 51.79 A
ATOM 2164 O LYS A 274 -37.891 -1.475 -58.007 1.00 53.02 A
ATOM 2165 N PRO A 275 -39.319 -2.874 -59.053 1.00 53.15 A
ATOM 2166 CD PRO A 275 -39.766 -3.777 -60.126 1.00 54.47 A
ATOM 2167 CA PRO A 275 -39.861 -3.298 -57.759 1.00 54.20 A
ATOM 2168 CB PRO A 275 -40.773 -4.466 -58.131 1.00 54.12 A
ATOM 2169 CG PRO A 275 -40.124 -5.026 -59.359 1.00 53.83 A
ATOM 2170 C PRO A 275 -38.697 -3.702 -56.860 1.00 55.38 A
ATOM 2171 O PRO A 275 -37.789 -4.424 -57.281 1.00 55.50 A
ATOM 2172 N ASN A 276 -38.836 -3.423 -55.555 1.00 56.34 A

ATOM 2173 CA ASN A 276 -37.812 -3.576 -54.509 1.00 56.65 A
ATOM 2174 CB ASN A 276 -38.078 -2.614 -53.331 1.00 56.86 A
ATOM 2175 CG ASN A 276 -37.089 -2.793 -52.113 1.00 57.47 A
ATOM 2176 OD1 ASN A 276 -35.894 -2.721 -52.255 1.00 57.85 A
ATOM 2177 ND2 ASN A 276 -37.627 -2.961 -50.934 1.00 56.05 A
ATOM 2178 C ASN A 276 -37.907 -4.897 -53.931 1.00 57.14 A
ATOM 2179 O ASN A 276 -38.925 -5.231 -53.411 1.00 56.94 A
ATOM 2180 N LEU A 277 -36.832 -5.675 -54.010 1.00 58.10 A
ATOM 2181 CA LEU A 277 -36.814 -7.016 -53.439 1.00 59.18 A
ATOM 2182 CB LEU A 277 -35.778 -7.888 -54.151 1.00 58.57 A
ATOM 2183 CG LEU A 277 -36.166 -8.408 -55.537 1.00 58.13 A
ATOM 2184 CD1 LEU A 277 -35.064 -9.284 -56.110 1.00 57.72 A
ATOM 2185 CD2 LEU A 277 -37.483 -9.167 -55.476 1.00 57.80 A
ATOM 2186 C LEU A 277 -36.525 -6.978 -51.941 1.00 60.04 A
ATOM 2187 O LEU A 277 -35.678 -7.720 -51.444 1.00 60.90 A
ATOM 2188 N ALA A 278 -37.234 -6.109 -51.228 1.00 61.14 A
ATOM 2189 CA ALA A 278 -36.741 -5.573 -49.964 1.00 61.66 A
ATOM 2190 CB ALA A 278 -35.525 -6.357 -49.495 1.00 61.93 A
ATOM 2191 C ALA A 278 -37.828 -5.583 -48.894 1.00 61.84 A
ATOM 2192 O ALA A 278 -37.998 -4.610 -48.160 1.00 62.55 A
ATOM 2193 N VAL A 279 -38.561 -6.688 -48.812 1.00 61.25 A
ATOM 2194 CA VAL A 279 -39.821 -6.720 -48.078 1.00 59.93 A
ATOM 2195 CB VAL A 279 -40.267 -8.164 -47.783 1.00 60.99 A
ATOM 2196 CG1 VAL A 279 -41.600 -8.172 -47.052 1.00 63.71 A
ATOM 2197 CG2 VAL A 279 -40.353 -8.968 -49.072 1.00 61.48 A
ATOM 2198 C VAL A 279 -39.716 -5.953 -46.764 1.00 58.97 A
ATOM 2199 O VAL A 279 -40.717 -5.472 -46.232 1.00 58.01 A
ATOM 2200 N THR A 280 -38.497 -5.842 -46.245 1.00 57.82 A
ATOM 2201 CA THR A 280 -38.271 -5.230 -44.947 1.00 56.13 A
ATOM 2202 CB THR A 280 -36.755 -4.933 -44.775 1.00 56.62 A
ATOM 2203 OG1 THR A 280 -36.509 -4.381 -43.477 1.00 56.46 A
ATOM 2204 CG2 THR A 280 -36.271 -3.968 -45.857 1.00 58.61 A
ATOM 2205 C THR A 280 -39.106 -3.967 -44.663 1.00 54.28 A
ATOM 2206 O THR A 280 -39.262 -3.579 -43.508 1.00 53.27 A

ATOM 2207 N SER A 281 -39.658 -3.343 -45.701 1.00 53.32 A
ATOM 2208 CA SER A 281 -40.468 -2.133 -45.513 1.00 52.73 A
ATOM 2209 CB SER A 281 -40.044 -1.042 -46.503 1.00 52.38 A
ATOM 2210 OG SER A 281 -40.067 -1.520 -47.835 1.00 53.37 A
ATOM 2211 C SER A 281 -41.974 -2.372 -45.633 1.00 51.84 A
ATOM 2212 O SER A 281 -42.777 -1.546 -45.201 1.00 51.21 A
ATOM 2213 N THR A 282 -42.352 -3.500 -46.225 1.00 51.37 A
ATOM 2214 CA THR A 282 -43.762 -3.848 -46.385 1.00 49.74 A
ATOM 2215 CB THR A 282 -43.979 -4.756 -47.617 1.00 49.52 A
ATOM 2216 OG1 THR A 282 -43.150 -4.305 -48.690 1.00 49.62 A
ATOM 2217 CG2 THR A 282 -45.429 -4.712 -48.068 1.00 48.30 A
ATOM 2218 C THR A 282 -44.191 -4.605 -45.124 1.00 49.01 A
ATOM 2219 O THR A 282 -45.371 -4.639 -44.761 1.00 47.11 A
ATOM 2220 N MET A 283 -43.209 -5.217 -44.469 1.00 48.67 A
ATOM 2221 CA MET A 283 -43.453 -5.962 -43.248 1.00 48.47 A
ATOM 2222 CB MET A 283 -42.161 -6.654 -42.782 1.00 48.13 A
ATOM 2223 CG MET A 283 -41.786 -7.900 -43.595 1.00 46.77 A
ATOM 2224 SD MET A 283 -40.176 -8.623 -43.179 1.00 46.24 A
ATOM 2225 CE MET A 283 -40.646 -10.050 -42.250 1.00 46.37 A
ATOM 2226 C MET A 283 -43.952 -4.973 -42.198 1.00 48.36 A
ATOM 2227 O MET A 283 -44.939 -5.228 -41.508 1.00 48.36 A
ATOM 2228 N LEU A 284 -43.270 -3.836 -42.097 1.00 48.06 A
ATOM 2229 CA LEU A 284 -43.648 -2.798 -41.149 1.00 47.85 A
ATOM 2230 CB LEU A 284 -42.602 -1.679 -41.150 1.00 45.38 A
ATOM 2231 CG LEU A 284 -41.172 -2.099 -40.797 1.00 44.66 A
ATOM 2232 CD1 LEU A 284 -40.202 -0.987 -41.109 1.00 43.61 A
ATOM 2233 CD2 LEU A 284 -41.098 -2.475 -39.339 1.00 44.96 A
ATOM 2234 C LEU A 284 -45.007 -2.237 -41.552 1.00 49.52 A
ATOM 2235 O LEU A 284 -45.898 -2.065 -40.721 1.00 49.98 A
ATOM 2236 N GLN A 285 -45.163 -1.961 -42.841 1.00 51.60 A
ATOM 2237 CA GLN A 285 -46.408 -1.414 -43.369 1.00 52.65 A
ATOM 2238 CB GLN A 285 -46.380 -1.443 -44.894 1.00 53.91 A
ATOM 2239 CG GLN A 285 -47.373 -0.517 -45.563 1.00 55.92 A
ATOM 2240 CD GLN A 285 -46.799 0.869 -45.757 1.00 57.90 A

ATOM 2241 OE1 GLN A 285 -45.664 1.015 -46.221 1.00 58.70 A
ATOM 2242 NE2 GLN A 285 -47.578 1.898 -45.419 1.00 58.62 A
ATOM 2243 C GLN A 285 -47.611 -2.208 -42.888 1.00 52.55 A
ATOM 2244 O GLN A 285 -48.619 -1.636 -42.489 1.00 52.52 A
ATOM 2245 N GLN A 286 -47.493 -3.505 -42.823 1.00 53.29 A
ATOM 2246 CA GLN A 286 -48.636 -4.322 -42.471 1.00 53.87 A
ATOM 2247 CB GLN A 286 -48.564 -5.695 -43.104 1.00 54.49 A
ATOM 2248 CG GLN A 286 -48.784 -5.715 -44.580 1.00 56.17 A
ATOM 2249 CD GLN A 286 -48.751 -7.073 -45.174 1.00 57.63 A
ATOM 2250 OE1 GLN A 286 -47.792 -7.411 -45.818 1.00 57.51 A
ATOM 2251 NE2 GLN A 286 -49.816 -7.860 -44.983 1.00 57.60 A
ATOM 2252 C GLN A 286 -48.747 -4.482 -41.006 1.00 53.42 A
ATOM 2253 O GLN A 286 -49.698 -5.016 -40.551 1.00 54.29 A
ATOM 2254 N GLY A 287 -47.768 -4.012 -40.261 1.00 51.73 A
ATOM 2255 CA GLY A 287 -47.767 -4.186 -38.816 1.00 49.64 A
ATOM 2256 C GLY A 287 -47.339 -5.567 -38.343 1.00 47.95 A
ATOM 2257 O GLY A 287 -47.920 -6.129 -37.422 1.00 46.72 A
ATOM 2258 N TRP A 288 -46.306 -6.113 -38.964 1.00 47.50 A
ATOM 2259 CA TRP A 288 -45.824 -7.433 -38.593 1.00 47.59 A
ATOM 2260 CB TRP A 288 -44.801 -7.912 -39.639 1.00 48.03 A
ATOM 2261 CG TRP A 288 -45.440 -8.535 -40.870 1.00 48.77 A
ATOM 2262 CD2 TRP A 288 -45.045 -9.749 -41.528 1.00 48.54 A
ATOM 2263 CE2 TRP A 288 -45.943 -9.959 -42.596 1.00 48.23 A
ATOM 2264 CE3 TRP A 288 -44.019 -10.680 -41.317 1.00 47.80 A
ATOM 2265 CD1 TRP A 288 -46.530 -8.068 -41.558 1.00 48.71 A
ATOM 2266 NE1 TRP A 288 -46.837 -8.921 -42.593 1.00 48.14 A
ATOM 2267 CZ2 TRP A 288 -45.847 -11.058 -43.447 1.00 47.68 A
ATOM 2268 CZ3 TRP A 288 -43.926 -11.772 -42.167 1.00 46.79 A
ATOM 2269 CH2 TRP A 288 -44.835 -11.951 -43.216 1.00 46.87 A
ATOM 2270 C TRP A 288 -45.259 -7.585 -37.162 1.00 47.03 A
ATOM 2271 O TRP A 288 -44.282 -6.950 -36.767 1.00 45.80 A
ATOM 2272 N ASN A 289 -45.913 -8.455 -36.405 1.00 47.78 A
ATOM 2273 CA ASN A 289 -45.565 -8.797 -35.028 1.00 47.54 A
ATOM 2274 CB ASN A 289 -46.684 -9.689 -34.469 1.00 47.90 A

ATOM 2275 CG ASN A 289 -47.121 -9.303 -33.080 1.00 49.23 A
ATOM 2276 OD1 ASN A 289 -47.347 -8.129 -32.786 1.00 49.13 A
ATOM 2277 ND2 ASN A 289 -47.276 -10.304 -32.214 1.00 51.71 A
ATOM 2278 C ASN A 289 -44.264 -9.600 -35.091 1.00 47.29 A
ATOM 2279 O ASN A 289 -43.860 -10.047 -36.161 1.00 47.17 A
ATOM 2280 N ALA A 290 -43.601 -9.787 -33.959 1.00 47.24 A
ATOM 2281 CA ALA A 290 -42.393 -10.594 -33.977 1.00 47.47 A
ATOM 2282 CB ALA A 290 -41.562 -10.334 -32.732 1.00 47.04 A
ATOM 2283 C ALA A 290 -42.892 -12.038 -34.004 1.00 47.73 A
ATOM 2284 O ALA A 290 -42.207 -12.949 -34.454 1.00 47.18 A
ATOM 2285 N THR A 291 -44.111 -12.230 -33.517 1.00 49.29 A
ATOM 2286 CA THR A 291 -44.720 -13.554 -33.485 1.00 50.78 A
ATOM 2287 CB THR A 291 -45.945 -13.594 -32.535 1.00 50.18 A
ATOM 2288 OG1 THR A 291 -45.535 -13.266 -31.205 1.00 48.53 A
ATOM 2289 CG2 THR A 291 -46.568 -14.975 -32.524 1.00 49.17 A
ATOM 2290 C THR A 291 -45.188 -13.882 -34.895 1.00 51.55 A
ATOM 2291 O THR A 291 -44.998 -14.997 -35.387 1.00 50.92 A
ATOM 2292 N HIS A 292 -45.802 -12.895 -35.538 1.00 52.39 A
ATOM 2293 CA HIS A 292 -46.295 -13.049 -36.899 1.00 53.14 A
ATOM 2294 CB HIS A 292 -46.678 -11.675 -37.467 1.00 56.29 A
ATOM 2295 CG HIS A 292 -47.468 -11.737 -38.741 1.00 60.35 A
ATOM 2296 CD2 HIS A 292 -48.221 -10.803 -39.375 1.00 61.48 A
ATOM 2297 ND1 HIS A 292 -47.542 -12.878 -39.515 1.00 62.05 A
ATOM 2298 CE1 HIS A 292 -48.303 -12.645 -40.571 1.00 62.15 A
ATOM 2299 NE2 HIS A 292 -48.728 -11.393 -40.509 1.00 62.89 A
ATOM 2300 C HIS A 292 -45.202 -13.696 -37.753 1.00 52.03 A
ATOM 2301 O HIS A 292 -45.479 -14.502 -38.640 1.00 52.05 A
ATOM 2302 N MET A 293 -43.955 -13.342 -37.470 1.00 50.45 A
ATOM 2303 CA MET A 293 -42.829 -13.889 -38.208 1.00 48.16 A
ATOM 2304 CB MET A 293 -41.552 -13.108 -37.884 1.00 48.42 A
ATOM 2305 CG MET A 293 -41.447 -11.790 -38.646 1.00 48.32 A
ATOM 2306 SD MET A 293 -40.158 -10.699 -38.034 1.00 48.72 A
ATOM 2307 CE MET A 293 -38.711 -11.698 -38.354 1.00 48.96 A
ATOM 2308 C MET A 293 -42.635 -15.366 -37.929 1.00 46.73 A

ATOM 2309 O MET A 293 -42.374 -16.136 -38.845 1.00 47.63 A
ATOM 2310 N PHE A 294 -42.773 -15.777 -36.676 1.00 45.17 A
ATOM 2311 CA PHE A 294 -42.603 -17.189 -36.351 1.00 43.68 A
ATOM 2312 CB PHE A 294 -42.352 -17.374 -34.852 1.00 40.35 A
ATOM 2313 CG PHE A 294 -40.981 -16.956 -34.417 1.00 36.79 A
ATOM 2314 CD1 PHE A 294 -40.661 -15.615 -34.274 1.00 35.06 A
ATOM 2315 CD2 PHE A 294 -39.997 -17.908 -34.185 1.00 35.75 A
ATOM 2316 CE1 PHE A 294 -39.387 -15.231 -33.907 1.00 33.22 A
ATOM 2317 CE2 PHE A 294 -38.721 -17.533 -33.820 1.00 34.26 A
ATOM 2318 CZ PHE A 294 -38.416 -16.192 -33.680 1.00 33.79 A
ATOM 2319 C PHE A 294 -43.786 -18.046 -36.801 1.00 44.38 A
ATOM 2320 O PHE A 294 -43.745 -19.272 -36.712 1.00 44.86 A
ATOM 2321 N ARG A 295 -44.760 -17.442 -37.422 1.00 45.00 A
ATOM 2322 CA ARG A 295 -45.944 -18.153 -37.833 1.00 46.23 A
ATOM 2323 CB ARG A 295 -47.163 -17.338 -37.499 1.00 48.19 A
ATOM 2324 CG ARG A 295 -47.787 -17.628 -36.218 1.00 50.42 A
ATOM 2325 CD ARG A 295 -49.122 -17.065 -36.126 1.00 52.42 A
ATOM 2326 NE ARG A 295 -49.561 -16.478 -37.371 1.00 54.53 A
ATOM 2327 CZ ARG A 295 -50.660 -16.813 -38.006 1.00 55.99 A
ATOM 2328 NH1 ARG A 295 -51.439 -17.739 -37.537 1.00 55.63 A
ATOM 2329 NH2 ARG A 295 -50.985 -16.231 -39.126 1.00 56.81 A
ATOM 2330 C ARG A 295 -45.995 -18.387 -39.287 1.00 45.96 A
ATOM 2331 O ARG A 295 -46.498 -19.376 -39.733 1.00 45.98 A
ATOM 2332 N VAL A 296 -45.529 -17.408 -40.034 1.00 45.29 A
ATOM 2333 CA VAL A 296 -45.275 -17.532 -41.459 1.00 44.03 A
ATOM 2334 CB VAL A 296 -44.818 -16.182 -42.044 1.00 43.10 A
ATOM 2335 CG1 VAL A 296 -44.973 -16.179 -43.556 1.00 42.43 A
ATOM 2336 CG2 VAL A 296 -45.626 -15.061 -41.429 1.00 42.76 A
ATOM 2337 C VAL A 296 -44.190 -18.576 -41.695 1.00 43.78 A
ATOM 2338 O VAL A 296 -44.310 -19.430 -42.570 1.00 44.52 A
ATOM 2339 N ALA A 297 -43.126 -18.504 -40.908 1.00 42.69 A
ATOM 2340 CA ALA A 297 -42.042 -19.457 -41.040 1.00 43.01 A
ATOM 2341 CB ALA A 297 -40.955 -19.147 -40.047 1.00 41.85 A
ATOM 2342 C ALA A 297 -42.578 -20.853 -40.797 1.00 44.05 A

ATOM 2343 O ALA A 297 -42.228 -21.791 -41.507 1.00 44.98 A
ATOM 2344 N GLU A 298 -43.430 -20.988 -39.787 1.00 44.72 A
ATOM 2345 CA GLU A 298 -44.012 -22.281 -39.453 1.00 44.68 A
ATOM 2346 CB GLU A 298 -44.837 -22.177 -38.163 1.00 45.17 A
ATOM 2347 CG GLU A 298 -45.570 -23.459 -37.768 1.00 45.21 A
ATOM 2348 CD GLU A 298 -46.475 -23.277 -36.548 1.00 45.68 A
ATOM 2349 OE1 GLU A 298 -47.214 -22.273 -36.505 1.00 46.03 A
ATOM 2350 OE2 GLU A 298 -46.460 -24.141 -35.641 1.00 45.61 A
ATOM 2351 C GLU A 298 -44.896 -22.745 -40.598 1.00 44.42 A
ATOM 2352 O GLU A 298 -44.772 -23.870 -41.071 1.00 42.67 A
ATOM 2353 N GLU A 299 -45.844 -21.951 -40.994 1.00 45.21 A
ATOM 2354 CA GLU A 299 -46.650 -22.294 -42.117 1.00 47.08 A
ATOM 2355 CB GLU A 299 -47.336 -21.086 -42.612 1.00 47.94 A
ATOM 2356 CG GLU A 299 -48.581 -21.413 -43.325 1.00 51.36 A
ATOM 2357 CD GLU A 299 -48.657 -20.698 -44.593 1.00 53.85 A
ATOM 2358 OE1 GLU A 299 -49.464 -21.114 -45.407 1.00 55.01 A
ATOM 2359 OE2 GLU A 299 -47.894 -19.746 -44.767 1.00 55.05 A
ATOM 2360 C GLU A 299 -45.950 -22.950 -43.274 1.00 47.09 A
ATOM 2361 O GLU A 299 -46.414 -23.897 -43.814 1.00 47.43 A
ATOM 2362 N PHE A 300 -44.830 -22.446 -43.683 1.00 45.66 A
ATOM 2363 CA PHE A 300 -44.119 -23.088 -44.786 1.00 43.98 A
ATOM 2364 CB PHE A 300 -42.782 -22.379 -45.063 1.00 43.64 A
ATOM 2365 CG PHE A 300 -42.061 -22.879 -46.303 1.00 43.14 A
ATOM 2366 CD1 PHE A 300 -42.093 -22.148 -47.490 1.00 42.21 A
ATOM 2367 CD2 PHE A 300 -41.355 -24.083 -46.285 1.00 43.25 A
ATOM 2368 CE1 PHE A 300 -41.438 -22.608 -48.629 1.00 41.02 A
ATOM 2369 CE2 PHE A 300 -40.696 -24.549 -47.427 1.00 41.50 A
ATOM 2370 CZ PHE A 300 -40.739 -23.813 -48.594 1.00 41.03 A
ATOM 2371 C PHE A 300 -43.850 -24.524 -44.336 1.00 43.56 A
ATOM 2372 O PHE A 300 -44.262 -25.476 -44.989 1.00 44.47 A
ATOM 2373 N PHE A 301 -43.172 -24.660 -43.199 1.00 42.19 A
ATOM 2374 CA PHE A 301 -42.825 -25.965 -42.645 1.00 40.18 A
ATOM 2375 CB PHE A 301 -42.283 -25.814 -41.219 1.00 37.78 A
ATOM 2376 CG PHE A 301 -40.811 -25.523 -41.146 1.00 34.84 A

ATOM 2377 CD1 PHE A 301 -40.337 -24.223 -41.246 1.00 34.08 A
ATOM 2378 CD2 PHE A 301 -39.895 -26.558 -40.971 1.00 33.67 A
ATOM 2379 CE1 PHE A 301 -38.971 -23.959 -41.171 1.00 33.29 A
ATOM 2380 CE2 PHE A 301 -38.527 -26.301 -40.897 1.00 32.70 A
ATOM 2381 CZ PHE A 301 -38.068 -25.000 -40.996 1.00 32.07 A
ATOM 2382 C PHE A 301 -43.961 -26.982 -42.622 1.00 39.60 A
ATOM 2383 O PHE A 301 -43.761 -28.160 -42.925 1.00 38.51 A
ATOM 2384 N THR A 302 -45.152 -26.539 -42.244 1.00 39.59 A
ATOM 2385 CA THR A 302 -46.274 -27.459 -42.172 1.00 41.02 A
ATOM 2386 CB THR A 302 -47.509 -26.800 -41.479 1.00 39.84 A
ATOM 2387 OG1 THR A 302 -47.864 -25.589 -42.155 1.00 39.60 A
ATOM 2388 CG2 THR A 302 -47.203 -26.483 -40.028 1.00 39.29 A
ATOM 2389 C THR A 302 -46.663 -27.988 -43.563 1.00 42.86 A
ATOM 2390 O THR A 302 -46.840 -29.203 -43.760 1.00 42.70 A
ATOM 2391 N SER A 303 -46.768 -27.081 -44.531 1.00 43.58 A
ATOM 2392 CA SER A 303 -47.149 -27.452 -45.890 1.00 44.01 A
ATOM 2393 CB SER A 303 -47.096 -26.225 -46.809 1.00 44.17 A
ATOM 2394 OG SER A 303 -45.763 -25.830 -47.079 1.00 44.37 A
ATOM 2395 C SER A 303 -46.296 -28.574 -46.484 1.00 44.52 A
ATOM 2396 O SER A 303 -46.769 -29.326 -47.339 1.00 45.65 A
ATOM 2397 N LEU A 304 -45.050 -28.696 -46.038 1.00 44.20 A
ATOM 2398 CA LEU A 304 -44.174 -29.736 -46.558 1.00 43.61 A
ATOM 2399 CB LEU A 304 -42.709 -29.325 -46.441 1.00 44.13 A
ATOM 2400 CG LEU A 304 -42.283 -27.946 -46.931 1.00 44.53 A
ATOM 2401 CD1 LEU A 304 -40.756 -27.892 -46.955 1.00 45.82 A
ATOM 2402 CD2 LEU A 304 -42.858 -27.674 -48.309 1.00 44.97 A
ATOM 2403 C LEU A 304 -44.386 -31.021 -45.791 1.00 43.16 A
ATOM 2404 O LEU A 304 -43.546 -31.911 -45.833 1.00 43.58 A
ATOM 2405 N ALA A 305 -45.509 -31.108 -45.086 1.00 43.29 A
ATOM 2406 CA ALA A 305 -45.846 -32.293 -44.297 1.00 44.68 A
ATOM 2407 CB ALA A 305 -46.010 -33.526 -45.218 1.00 45.41 A
ATOM 2408 C ALA A 305 -44.826 -32.580 -43.184 1.00 44.56 A
ATOM 2409 O ALA A 305 -44.503 -33.741 -42.892 1.00 43.53 A
ATOM 2410 N LEU A 306 -44.317 -31.505 -42.584 1.00 45.06 A

ATOM 2411 CA LEU A 306 -43.373 -31.581 -41.470 1.00 45.51 A
ATOM 2412 CB LEU A 306 -42.164 -30.679 -41.729 1.00 45.35 A
ATOM 2413 CG LEU A 306 -41.140 -31.202 -42.737 1.00 44.52 A
ATOM 2414 CD1 LEU A 306 -40.056 -30.165 -42.937 1.00 44.63 A
ATOM 2415 CD2 LEU A 306 -40.535 -32.504 -42.241 1.00 43.49 A
ATOM 2416 C LEU A 306 -44.152 -31.106 -40.229 1.00 46.15 A
ATOM 2417 O LEU A 306 -45.150 -30.389 -40.366 1.00 46.08 A
ATOM 2418 N SER A 307 -43.716 -31.496 -39.031 1.00 46.01 A
ATOM 2419 CA SER A 307 -44.443 -31.108 -37.814 1.00 45.51 A
ATOM 2420 CB SER A 307 -43.982 -31.942 -36.614 1.00 43.93 A
ATOM 2421 OG SER A 307 -42.579 -31.999 -36.543 1.00 44.26 A
ATOM 2422 C SER A 307 -44.357 -29.628 -37.487 1.00 45.68 A
ATOM 2423 O SER A 307 -43.357 -28.983 -37.797 1.00 46.29 A
ATOM 2424 N PRO A 308 -45.426 -29.066 -36.873 1.00 45.91 A
ATOM 2425 CD PRO A 308 -46.707 -29.743 -36.585 1.00 45.44 A
ATOM 2426 CA PRO A 308 -45.503 -27.650 -36.490 1.00 45.32 A
ATOM 2427 CB PRO A 308 -47.003 -27.387 -36.458 1.00 44.65 A
ATOM 2428 CG PRO A 308 -47.519 -28.655 -35.878 1.00 45.01 A
ATOM 2429 C PRO A 308 -44.860 -27.439 -35.129 1.00 45.03 A
ATOM 2430 O PRO A 308 -44.426 -28.396 -34.485 1.00 44.68 A
ATOM 2431 N MET A 309 -44.796 -26.194 -34.687 1.00 45.07 A
ATOM 2432 CA MET A 309 -44.188 -25.917 -33.399 1.00 46.33 A
ATOM 2433 CB MET A 309 -43.944 -24.416 -33.245 1.00 47.46 A
ATOM 2434 CG MET A 309 -42.849 -23.876 -34.154 1.00 48.16 A
ATOM 2435 SD MET A 309 -41.287 -24.765 -33.963 1.00 49.70 A
ATOM 2436 CE MET A 309 -41.229 -25.740 -35.483 1.00 48.35 A
ATOM 2437 C MET A 309 -45.083 -26.428 -32.278 1.00 46.90 A
ATOM 2438 O MET A 309 -46.283 -26.129 -32.249 1.00 47.22 A
ATOM 2439 N PRO A 310 -44.513 -27.214 -31.343 1.00 46.78 A
ATOM 2440 CD PRO A 310 -43.105 -27.626 -31.258 1.00 46.29 A
ATOM 2441 CA PRO A 310 -45.269 -27.767 -30.216 1.00 46.85 A
ATOM 2442 CB PRO A 310 -44.238 -28.619 -29.482 1.00 45.99 A
ATOM 2443 CG PRO A 310 -43.226 -28.923 -30.512 1.00 46.44 A
ATOM 2444 C PRO A 310 -45.778 -26.631 -29.336 1.00 47.87 A

ATOM 2445 O PRO A 310 -45.324 -25.487 -29.455 1.00 48.50 A
ATOM 2446 N PRO A 311 -46.749 -26.917 -28.460 1.00 47.98 A
ATOM 2447 CD PRO A 311 -47.712 -28.033 -28.482 1.00 47.84 A
ATOM 2448 CA PRO A 311 -47.229 -25.825 -27.608 1.00 47.56 A
ATOM 2449 CB PRO A 311 -48.452 -26.433 -26.933 1.00 47.83 A
ATOM 2450 CG PRO A 311 -48.984 -27.361 -28.001 1.00 47.61 A
ATOM 2451 C PRO A 311 -46.140 -25.380 -26.612 1.00 47.35 A
ATOM 2452 O PRO A 311 -46.028 -24.191 -26.298 1.00 47.68 A
ATOM 2453 N GLU A 312 -45.332 -26.327 -26.130 1.00 45.60 A
ATOM 2454 CA GLU A 312 -44.255 -26.006 -25.192 1.00 45.03 A
ATOM 2455 CB GLU A 312 -43.391 -27.237 -24.889 1.00 46.14 A
ATOM 2456 CG GLU A 312 -44.110 -28.378 -24.184 1.00 48.91 A
ATOM 2457 CD GLU A 312 -44.872 -29.279 -25.144 1.00 51.53 A
ATOM 2458 OE1 GLU A 312 -45.686 -28.761 -25.943 1.00 52.09 A
ATOM 2459 OE2 GLU A 312 -44.659 -30.511 -25.098 1.00 52.72 A
ATOM 2460 C GLU A 312 -43.368 -24.915 -25.778 1.00 44.55 A
ATOM 2461 O GLU A 312 -42.958 -23.995 -25.071 1.00 43.54 A
ATOM 2462 N PHE A 313 -43.076 -25.034 -27.074 1.00 44.47 A
ATOM 2463 CA PHE A 313 -42.236 -24.074 -27.794 1.00 43.27 A
ATOM 2464 CB PHE A 313 -42.063 -24.498 -29.261 1.00 41.88 A
ATOM 2465 CG PHE A 313 -41.521 -23.404 -30.160 1.00 40.31 A
ATOM 2466 CD1 PHE A 313 -40.156 -23.192 -30.284 1.00 38.59 A
ATOM 2467 CD2 PHE A 313 -42.388 -22.581 -30.879 1.00 39.97 A
ATOM 2468 CE1 PHE A 313 -39.664 -22.179 -31.109 1.00 37.54 A
ATOM 2469 CE2 PHE A 313 -41.903 -21.565 -31.704 1.00 38.36 A
ATOM 2470 CZ PHE A 313 -40.540 -21.366 -31.819 1.00 37.59 A
ATOM 2471 C PHE A 313 -42.850 -22.688 -27.755 1.00 43.49 A
ATOM 2472 O PHE A 313 -42.147 -21.693 -27.589 1.00 43.91 A
ATOM 2473 N TRP A 314 -44.162 -22.617 -27.916 1.00 43.61 A
ATOM 2474 CA TRP A 314 -44.814 -21.327 -27.910 1.00 45.36 A
ATOM 2475 CB TRP A 314 -46.198 -21.427 -28.541 1.00 47.01 A
ATOM 2476 CG TRP A 314 -46.154 -21.566 -30.023 1.00 48.38 A
ATOM 2477 CD2 TRP A 314 -45.872 -20.531 -30.967 1.00 49.14 A
ATOM 2478 CE2 TRP A 314 -45.959 -21.104 -32.255 1.00 49.83 A

ATOM 2479 CE3 TRP A 314 -45.556 -19.172 -30.851 1.00 49.92 A
ATOM 2480 CD1 TRP A 314 -46.386 -22.695 -30.749 1.00 49.75 A
ATOM 2481 NE1 TRP A 314 -46.273 -22.427 -32.093 1.00 50.05 A
ATOM 2482 CZ2 TRP A 314 -45.742 -20.368 -33.421 1.00 50.47 A
ATOM 2483 CZ3 TRP A 314 -45.340 -18.439 -32.010 1.00 50.46 A
ATOM 2484 CH2 TRP A 314 -45.436 -19.043 -33.281 1.00 50.94 A
ATOM 2485 C TRP A 314 -44.919 -20.723 -26.529 1.00 45.57 A
ATOM 2486 O TRP A 314 -44.947 -19.511 -26.392 1.00 45.84 A
ATOM 2487 N ALA A 315 -44.971 -21.558 -25.501 1.00 46.64 A
ATOM 2488 CA ALA A 315 -45.078 -21.046 -24.142 1.00 46.92 A
ATOM 2489 CB ALA A 315 -45.768 -22.072 -23.241 1.00 46.47 A
ATOM 2490 C ALA A 315 -43.700 -20.713 -23.592 1.00 47.83 A
ATOM 2491 O ALA A 315 -43.514 -19.684 -22.934 1.00 48.24 A
ATOM 2492 N GLY A 316 -42.730 -21.573 -23.887 1.00 48.69 A
ATOM 2493 CA GLY A 316 -41.386 -21.372 -23.374 1.00 50.26 A
ATOM 2494 C GLY A 316 -40.348 -20.620 -24.192 1.00 50.83 A
ATOM 2495 O GLY A 316 -39.219 -20.452 -23.729 1.00 52.01 A
ATOM 2496 N SER A 317 -40.695 -20.153 -25.386 1.00 50.48 A
ATOM 2497 CA SER A 317 -39.712 -19.440 -26.203 1.00 50.05 A
ATOM 2498 CB SER A 317 -39.959 -19.687 -27.696 1.00 49.41 A
ATOM 2499 OG SER A 317 -39.559 -20.992 -28.081 1.00 50.33 A
ATOM 2500 C SER A 317 -39.701 -17.950 -25.954 1.00 49.75 A
ATOM 2501 O SER A 317 -40.701 -17.378 -25.526 1.00 51.07 A
ATOM 2502 N MET A 318 -38.558 -17.329 -26.219 1.00 48.28 A
ATOM 2503 CA MET A 318 -38.413 -15.889 -26.067 1.00 46.77 A
ATOM 2504 CB MET A 318 -37.232 -15.553 -25.166 1.00 47.20 A
ATOM 2505 CG MET A 318 -37.151 -14.083 -24.820 1.00 48.61 A
ATOM 2506 SD MET A 318 -35.537 -13.650 -24.189 1.00 51.05 A
ATOM 2507 CE MET A 318 -34.589 -13.681 -25.702 1.00 50.70 A
ATOM 2508 C MET A 318 -38.159 -15.369 -27.470 1.00 45.29 A
ATOM 2509 O MET A 318 -37.072 -15.536 -28.013 1.00 45.05 A
ATOM 2510 N LEU A 319 -39.160 -14.736 -28.058 1.00 43.87 A
ATOM 2511 CA LEU A 319 -39.020 -14.260 -29.416 1.00 43.93 A
ATOM 2512 CB LEU A 319 -40.201 -14.768 -30.239 1.00 42.93 A

ATOM 2513 CG LEU A 319 -40.633 -16.205 -29.939 1.00 41.40 A
ATOM 2514 CD1 LEU A 319 -41.803 -16.570 -30.825 1.00 41.02 A
ATOM 2515 CD2 LEU A 319 -39.476 -17.158 -30.155 1.00 41.65 A
ATOM 2516 C LEU A 319 -38.920 -12.748 -29.534 1.00 45.15 A
ATOM 2517 O LEU A 319 -39.087 -12.192 -30.623 1.00 46.47 A
ATOM 2518 N GLU A 320 -38.651 -12.082 -28.418 1.00 45.25 A
ATOM 2519 CA GLU A 320 -38.527 -10.629 -28.402 1.00 45.68 A
ATOM 2520 CB GLU A 320 -39.890 -9.973 -28.188 1.00 45.43 A
ATOM 2521 CG GLU A 320 -40.809 -10.022 -29.399 1.00 48.16 A
ATOM 2522 CD GLU A 320 -42.225 -9.535 -29.096 1.00 49.53 A
ATOM 2523 OE1 GLU A 320 -42.903 -10.185 -28.274 1.00 50.45 A
ATOM 2524 OE2 GLU A 320 -42.665 -8.511 -29.673 1.00 49.57 A
ATOM 2525 C GLU A 320 -37.607 -10.229 -27.274 1.00 46.46 A
ATOM 2526 O GLU A 320 -37.471 -10.955 -26.299 1.00 47.25 A
ATOM 2527 N LYS A 321 -36.963 -9.079 -27.408 1.00 47.42 A
ATOM 2528 CA LYS A 321 -36.079 -8.603 -26.360 1.00 48.46 A
ATOM 2529 CB LYS A 321 -35.230 -7.439 -26.868 1.00 47.61 A
ATOM 2530 CG LYS A 321 -34.024 -7.124 -26.004 1.00 47.19 A
ATOM 2531 CD LYS A 321 -33.313 -5.870 -26.474 1.00 46.34 A
ATOM 2532 CE LYS A 321 -32.160 -5.518 -25.553 1.00 46.22 A
ATOM 2533 NZ LYS A 321 -31.593 -4.177 -25.879 1.00 46.44 A
ATOM 2534 C LYS A 321 -37.027 -8.128 -25.268 1.00 49.93 A
ATOM 2535 O LYS A 321 -37.778 -7.176 -25.465 1.00 50.39 A
ATOM 2536 N PRO A 322 -36.986 -8.795 -24.119 1.00 51.31 A
ATOM 2537 CD PRO A 322 -36.159 -9.984 -23.846 1.00 52.43 A
ATOM 2538 CA PRO A 322 -37.932 -8.519 -23.033 1.00 52.25 A
ATOM 2539 CB PRO A 322 -37.472 -9.466 -21.925 1.00 53.08 A
ATOM 2540 CG PRO A 322 -36.824 -10.594 -22.646 1.00 52.83 A
ATOM 2541 C PRO A 322 -37.839 -7.072 -22.557 1.00 53.49 A
ATOM 2542 O PRO A 322 -37.014 -6.310 -23.059 1.00 53.08 A
ATOM 2543 N ALA A 323 -38.682 -6.705 -21.596 1.00 55.17 A
ATOM 2544 CA ALA A 323 -38.864 -5.306 -21.231 1.00 56.32 A
ATOM 2545 CB ALA A 323 -40.206 -4.797 -21.739 1.00 55.48 A
ATOM 2546 C ALA A 323 -38.756 -5.111 -19.722 1.00 57.50 A

ATOM 2547 O ALA A 323 -38.791 -3.984 -19.229 1.00 58.43 A
ATOM 2548 N ALA A 324 -38.624 -6.216 -18.995 1.00 58.32 A
ATOM 2549 CA ALA A 324 -38.367 -6.163 -17.561 1.00 58.25 A
ATOM 2550 CB ALA A 324 -38.533 -7.542 -16.942 1.00 57.56 A
ATOM 2551 C ALA A 324 -36.975 -5.612 -17.271 1.00 58.53 A
ATOM 2552 O ALA A 324 -36.475 -5.720 -16.151 1.00 58.53 A
ATOM 2553 N GLY A 325 -36.354 -5.020 -18.286 1.00 58.98 A
ATOM 2554 CA GLY A 325 -34.995 -4.527 -18.166 1.00 58.88 A
ATOM 2555 C GLY A 325 -33.974 -5.646 -18.119 1.00 58.25 A
ATOM 2556 O GLY A 325 -32.772 -5.409 -18.240 1.00 58.50 A
ATOM 2557 N ARG A 326 -34.455 -6.873 -17.943 1.00 56.31 A
ATOM 2558 CA ARG A 326 -33.588 -8.045 -17.954 1.00 55.26 A
ATOM 2559 CB ARG A 326 -34.412 -9.320 -18.144 1.00 55.27 A
ATOM 2560 CG ARG A 326 -35.821 -9.238 -17.580 1.00 55.77 A
ATOM 2561 CD ARG A 326 -36.344 -10.552 -17.023 1.00 55.61 A
ATOM 2562 NE ARG A 326 -35.988 -11.686 -17.870 1.00 54.23 A
ATOM 2563 CZ ARG A 326 -36.667 -12.053 -18.949 1.00 54.37 A
ATOM 2564 NH1 ARG A 326 -37.745 -11.376 -19.318 1.00 54.32 A
ATOM 2565 NH2 ARG A 326 -36.269 -13.099 -19.661 1.00 53.97 A
ATOM 2566 C ARG A 326 -32.528 -7.938 -19.046 1.00 55.56 A
ATOM 2567 O ARG A 326 -32.819 -7.519 -20.166 1.00 56.77 A
ATOM 2568 N GLU A 327 -31.325 -8.354 -18.746 1.00 54.37 A
ATOM 2569 CA GLU A 327 -30.265 -8.346 -19.692 1.00 52.58 A
ATOM 2570 CB GLU A 327 -29.016 -7.959 -18.950 1.00 53.30 A
ATOM 2571 CG GLU A 327 -27.884 -7.486 -19.804 1.00 55.73 A
ATOM 2572 CD GLU A 327 -27.298 -6.217 -19.300 1.00 56.88 A
ATOM 2573 OE1 GLU A 327 -27.147 -6.091 -18.088 1.00 57.95 A
ATOM 2574 OE2 GLU A 327 -27.000 -5.359 -20.113 1.00 57.03 A
ATOM 2575 C GLU A 327 -30.103 -9.706 -20.280 1.00 50.91 A
ATOM 2576 O GLU A 327 -29.875 -10.634 -19.573 1.00 49.89 A
ATOM 2577 N VAL A 328 -30.197 -9.814 -21.602 1.00 48.95 A
ATOM 2578 CA VAL A 328 -30.160 -11.111 -22.282 1.00 46.42 A
ATOM 2579 CB VAL A 328 -31.546 -11.467 -22.851 1.00 44.97 A
ATOM 2580 CG1 VAL A 328 -32.573 -11.469 -21.747 1.00 45.10 A

ATOM 2581 CG2 VAL A 328 -31.941 -10.471 -23.928 1.00 44.05 A
ATOM 2582 C VAL A 328 -29.172 -11.267 -23.432 1.00 45.65 A
ATOM 2583 O VAL A 328 -28.794 -10.301 -24.087 1.00 46.39 A
ATOM 2584 N VAL A 329 -28.768 -12.512 -23.667 1.00 44.93 A
ATOM 2585 CA VAL A 329 -27.862 -12.842 -24.758 1.00 43.67 A
ATOM 2586 CB VAL A 329 -27.294 -14.261 -24.611 1.00 42.47 A
ATOM 2587 CG1 VAL A 329 -26.215 -14.493 -25.643 1.00 41.51 A
ATOM 2588 CG2 VAL A 329 -26.752 -14.462 -23.214 1.00 41.53 A
ATOM 2589 C VAL A 329 -28.766 -12.801 -25.982 1.00 43.98 A
ATOM 2590 O VAL A 329 -29.410 -13.792 -26.325 1.00 42.84 A
ATOM 2591 N CYS A 330 -28.822 -11.641 -26.628 1.00 44.30 A
ATOM 2592 CA CYS A 330 -29.678 -11.444 -27.784 1.00 44.94 A
ATOM 2593 C CYS A 330 -29.435 -12.296 -29.022 1.00 44.95 A
ATOM 2594 O CYS A 330 -30.324 -12.421 -29.871 1.00 45.34 A
ATOM 2595 CB CYS A 330 -29.668 -9.974 -28.186 1.00 45.77 A
ATOM 2596 SG CYS A 330 -30.970 -8.984 -27.379 1.00 51.29 A
ATOM 2597 N HIS A 331 -28.252 -12.886 -29.142 1.00 44.35 A
ATOM 2598 CA HIS A 331 -27.970 -13.703 -30.315 1.00 43.52 A
ATOM 2599 CB HIS A 331 -26.609 -14.368 -30.180 1.00 44.40 A
ATOM 2600 CG HIS A 331 -25.948 -14.665 -31.491 1.00 46.22 A
ATOM 2601 CD2 HIS A 331 -25.537 -15.833 -32.040 1.00 47.00 A
ATOM 2602 ND1 HIS A 331 -25.603 -13.676 -32.389 1.00 47.55 A
ATOM 2603 CE1 HIS A 331 -25.004 -14.220 -33.431 1.00 48.36 A
ATOM 2604 NE2 HIS A 331 -24.952 -15.528 -33.246 1.00 48.19 A
ATOM 2605 C HIS A 331 -29.042 -14.768 -30.473 1.00 42.85 A
ATOM 2606 O HIS A 331 -29.392 -15.449 -29.514 1.00 43.53 A
ATOM 2607 N ALA A 332 -29.569 -14.904 -31.681 1.00 41.47 A
ATOM 2608 CA ALA A 332 -30.593 -15.898 -31.955 1.00 39.57 A
ATOM 2609 CB ALA A 332 -31.170 -15.678 -33.339 1.00 39.70 A
ATOM 2610 C ALA A 332 -29.989 -17.295 -31.860 1.00 38.69 A
ATOM 2611 O ALA A 332 -28.869 -17.522 -32.316 1.00 37.97 A
ATOM 2612 N SER A 333 -30.733 -18.223 -31.259 1.00 38.48 A
ATOM 2613 CA SER A 333 -30.287 -19.608 -31.111 1.00 38.16 A
ATOM 2614 CB SER A 333 -29.315 -19.729 -29.943 1.00 38.29 A

ATOM 2615 OG SER A 333 -29.890 -19.203 -28.765 1.00 39.09 A
ATOM 2616 C SER A 333 -31.479 -20.537 -30.890 1.00 37.81 A
ATOM 2617 O SER A 333 -32.588 -20.079 -30.600 1.00 36.94 A
ATOM 2618 N ALA A 334 -31.245 -21.840 -31.039 1.00 37.25 A
ATOM 2619 CA ALA A 334 -32.293 -22.843 -30.857 1.00 37.13 A
ATOM 2620 CB ALA A 334 -32.559 -23.552 -32.165 1.00 37.00 A
ATOM 2621 C ALA A 334 -31.895 -23.846 -29.771 1.00 37.29 A
ATOM 2622 O ALA A 334 -30.770 -24.339 -29.742 1.00 37.22 A
ATOM 2623 N TRP A 335 -32.839 -24.159 -28.892 1.00 37.54 A
ATOM 2624 CA TRP A 335 -32.578 -25.048 -27.768 1.00 37.20 A
ATOM 2625 CB TRP A 335 -32.927 -24.312 -26.474 1.00 36.46 A
ATOM 2626 CG TRP A 335 -32.198 -23.011 -26.337 1.00 36.46 A
ATOM 2627 CD2 TRP A 335 -31.272 -22.654 -25.309 1.00 36.03 A
ATOM 2628 CE2 TRP A 335 -30.803 -21.351 -25.601 1.00 36.00 A
ATOM 2629 CE3 TRP A 335 -30.791 -23.308 -24.169 1.00 35.11 A
ATOM 2630 CD1 TRP A 335 -32.256 -21.937 -27.189 1.00 36.40 A
ATOM 2631 NE1 TRP A 335 -31.419 -20.940 -26.754 1.00 35.90 A
ATOM 2632 CZ2 TRP A 335 -29.876 -20.693 -24.795 1.00 35.28 A
ATOM 2633 CZ3 TRP A 335 -29.873 -22.655 -23.371 1.00 35.70 A
ATOM 2634 CH2 TRP A 335 -29.423 -21.357 -23.686 1.00 35.28 A
ATOM 2635 C TRP A 335 -33.249 -26.413 -27.765 1.00 36.99 A
ATOM 2636 O TRP A 335 -34.454 -26.535 -27.975 1.00 36.86 A
ATOM 2637 N ASP A 336 -32.444 -27.435 -27.502 1.00 37.04 A
ATOM 2638 CA ASP A 336 -32.916 -28.808 -27.428 1.00 37.26 A
ATOM 2639 CB ASP A 336 -32.114 -29.685 -28.395 1.00 37.58 A
ATOM 2640 CG ASP A 336 -32.640 -31.109 -28.484 1.00 36.98 A
ATOM 2641 OD1 ASP A 336 -33.836 -31.323 -28.194 1.00 36.61 A
ATOM 2642 OD2 ASP A 336 -31.855 -32.007 -28.869 1.00 35.00 A
ATOM 2643 C ASP A 336 -32.677 -29.239 -25.984 1.00 37.95 A
ATOM 2644 O ASP A 336 -31.526 -29.379 -25.558 1.00 38.41 A
ATOM 2645 N PHE A 337 -33.764 -29.427 -25.233 1.00 38.07 A
ATOM 2646 CA PHE A 337 -33.681 -29.815 -23.825 1.00 38.41 A
ATOM 2647 CB PHE A 337 -34.916 -29.327 -23.055 1.00 38.35 A
ATOM 2648 CG PHE A 337 -34.926 -27.845 -22.770 1.00 38.46 A

ATOM 2649 CD1 PHE A 337 -35.230 -26.925 -23.774 1.00 37.31 A
ATOM 2650 CD2 PHE A 337 -34.663 -27.371 -21.481 1.00 38.07 A
ATOM 2651 CE1 PHE A 337 -35.278 -25.544 -23.499 1.00 35.95 A
ATOM 2652 CE2 PHE A 337 -34.706 -26.001 -21.194 1.00 38.33 A
ATOM 2653 CZ PHE A 337 -35.017 -25.082 -22.208 1.00 36.81 A
ATOM 2654 C PHE A 337 -33.503 -31.312 -23.569 1.00 38.17 A
ATOM 2655 O PHE A 337 -33.529 -31.749 -22.424 1.00 38.13 A
ATOM 2656 N TYR A 338 -33.332 -32.091 -24.628 1.00 38.35 A
ATOM 2657 CA TYR A 338 -33.137 -33.535 -24.502 1.00 39.02 A
ATOM 2658 CB TYR A 338 -31.731 -33.821 -23.973 1.00 39.49 A
ATOM 2659 CG TYR A 338 -30.654 -33.403 -24.942 1.00 41.28 A
ATOM 2660 CD1 TYR A 338 -30.351 -32.058 -25.147 1.00 41.85 A
ATOM 2661 CE1 TYR A 338 -29.403 -31.671 -26.086 1.00 43.04 A
ATOM 2662 CD2 TYR A 338 -29.978 -34.349 -25.699 1.00 41.89 A
ATOM 2663 CE2 TYR A 338 -29.031 -33.980 -26.639 1.00 43.62 A
ATOM 2664 CZ TYR A 338 -28.747 -32.641 -26.834 1.00 44.33 A
ATOM 2665 OH TYR A 338 -27.833 -32.287 -27.809 1.00 46.76 A
ATOM 2666 C TYR A 338 -34.170 -34.280 -23.659 1.00 39.09 A
ATOM 2667 O TYR A 338 -33.858 -35.273 -23.003 1.00 38.65 A
ATOM 2668 N ASN A 339 -35.409 -33.812 -23.704 1.00 39.78 A
ATOM 2669 CA ASN A 339 -36.487 -34.434 -22.957 1.00 40.08 A
ATOM 2670 CB ASN A 339 -36.898 -33.515 -21.801 1.00 39.81 A
ATOM 2671 CG ASN A 339 -37.743 -32.346 -22.260 1.00 40.39 A
ATOM 2672 OD1 ASN A 339 -37.720 -31.969 -23.437 1.00 41.41 A
ATOM 2673 ND2 ASN A 339 -38.491 -31.757 -21.332 1.00 39.35 A
ATOM 2674 C ASN A 339 -37.683 -34.702 -23.884 1.00 40.40 A
ATOM 2675 O ASN A 339 -38.804 -34.911 -23.427 1.00 40.77 A
ATOM 2676 N ARG A 340 -37.436 -34.677 -25.191 1.00 40.46 A
ATOM 2677 CA ARG A 340 -38.478 -34.929 -26.191 1.00 40.15 A
ATOM 2678 CB ARG A 340 -38.864 -36.409 -26.173 1.00 38.95 A
ATOM 2679 CG ARG A 340 -37.783 -37.327 -26.691 1.00 39.69 A
ATOM 2680 CD ARG A 340 -37.887 -38.712 -26.087 1.00 40.72 A
ATOM 2681 NE ARG A 340 -37.636 -38.675 -24.647 1.00 42.72 A
ATOM 2682 CZ ARG A 340 -38.581 -38.667 -23.711 1.00 42.69 A

ATOM 2683 NH1 ARG A 340 -39.865 -38.701 -24.045 1.00 42.55 A
ATOM 2684 NH2 ARG A 340 -38.239 -38.611 -22.433 1.00 43.16 A
ATOM 2685 C ARG A 340 -39.741 -34.094 -26.034 1.00 39.90 A
ATOM 2686 O ARG A 340 -40.710 -34.307 -26.758 1.00 40.12 A
ATOM 2687 N LYS A 341 -39.739 -33.113 -25.162 1.00 40.32 A
ATOM 2688 CA LYS A 341 -40.911 -32.307 -24.855 1.00 41.89 A
ATOM 2689 CB LYS A 341 -41.266 -32.528 -23.414 1.00 42.25 A
ATOM 2690 CG LYS A 341 -42.689 -32.503 -23.030 1.00 42.88 A
ATOM 2691 CD LYS A 341 -42.863 -31.927 -21.641 1.00 43.46 A
ATOM 2692 CE LYS A 341 -43.858 -30.810 -21.581 1.00 43.41 A
ATOM 2693 NZ LYS A 341 -44.044 -30.295 -20.231 1.00 41.57 A
ATOM 2694 C LYS A 341 -40.638 -30.848 -25.047 1.00 42.97 A
ATOM 2695 O LYS A 341 -41.375 -30.195 -25.710 1.00 42.21 A
ATOM 2696 N ASP A 342 -39.553 -30.351 -24.468 1.00 44.11 A
ATOM 2697 CA ASP A 342 -39.157 -28.944 -24.489 1.00 44.52 A
ATOM 2698 CB ASP A 342 -38.560 -28.558 -23.131 1.00 46.94 A
ATOM 2699 CG ASP A 342 -39.573 -27.912 -22.201 1.00 48.86 A
ATOM 2700 OD1 ASP A 342 -40.685 -28.459 -22.038 1.00 49.85 A
ATOM 2701 OD2 ASP A 342 -39.246 -26.854 -21.619 1.00 51.55 A
ATOM 2702 C ASP A 342 -38.164 -28.571 -25.571 1.00 43.48 A
ATOM 2703 O ASP A 342 -37.020 -29.029 -25.562 1.00 43.17 A
ATOM 2704 N PHE A 343 -38.616 -27.722 -26.491 1.00 42.53 A
ATOM 2705 CA PHE A 343 -37.799 -27.230 -27.603 1.00 40.78 A
ATOM 2706 CB PHE A 343 -38.145 -27.946 -28.920 1.00 37.68 A
ATOM 2707 CG PHE A 343 -38.231 -29.450 -28.810 1.00 36.00 A
ATOM 2708 CD1 PHE A 343 -39.457 -30.075 -28.582 1.00 34.52 A
ATOM 2709 CD2 PHE A 343 -37.092 -30.242 -28.951 1.00 35.25 A
ATOM 2710 CE1 PHE A 343 -39.548 -31.462 -28.498 1.00 34.50 A
ATOM 2711 CE2 PHE A 343 -37.173 -31.629 -28.870 1.00 35.37 A
ATOM 2712 CZ PHE A 343 -38.406 -32.239 -28.642 1.00 35.35 A
ATOM 2713 C PHE A 343 -38.148 -25.750 -27.740 1.00 41.36 A
ATOM 2714 O PHE A 343 -39.308 -25.405 -27.986 1.00 41.25 A
ATOM 2715 N ARG A 344 -37.164 -24.870 -27.581 1.00 42.08 A
ATOM 2716 CA ARG A 344 -37.452 -23.438 -27.676 1.00 42.64 A

ATOM 2717 CB ARG A 344 -37.593 -22.829 -26.278 1.00 44.23 A
ATOM 2718 CG ARG A 344 -38.053 -23.793 -25.203 1.00 47.79 A
ATOM 2719 CD ARG A 344 -38.267 -23.054 -23.901 1.00 49.33 A
ATOM 2720 NE ARG A 344 -38.104 -23.920 -22.738 1.00 51.50 A
ATOM 2721 CZ ARG A 344 -38.145 -23.485 -21.482 1.00 51.72 A
ATOM 2722 NH1 ARG A 344 -38.349 -22.193 -21.245 1.00 52.80 A
ATOM 2723 NH2 ARG A 344 -37.966 -24.333 -20.470 1.00 51.44 A
ATOM 2724 C ARG A 344 -36.421 -22.623 -28.446 1.00 41.75 A
ATOM 2725 O ARG A 344 -35.312 -23.078 -28.714 1.00 41.86 A
ATOM 2726 N ILE A 345 -36.803 -21.398 -28.780 1.00 40.33 A
ATOM 2727 CA ILE A 345 -35.930 -20.493 -29.502 1.00 40.05 A
ATOM 2728 CB ILE A 345 -36.515 -20.171 -30.898 1.00 39.92 A
ATOM 2729 CG2 ILE A 345 -35.901 -18.892 -31.448 1.00 39.29 A
ATOM 2730 CG1 ILE A 345 -36.296 -21.369 -31.834 1.00 39.58 A
ATOM 2731 CD1 ILE A 345 -36.752 -21.150 -33.262 1.00 36.26 A
ATOM 2732 C ILE A 345 -35.745 -19.198 -28.718 1.00 40.50 A
ATOM 2733 O ILE A 345 -36.705 -18.660 -28.162 1.00 41.70 A
ATOM 2734 N LYS A 346 -34.541 -18.660 -28.674 1.00 39.94 A
ATOM 2735 CA LYS A 346 -34.199 -17.422 -27.983 1.00 38.69 A
ATOM 2736 CB LYS A 346 -33.112 -17.723 -26.989 1.00 37.09 A
ATOM 2737 CG LYS A 346 -32.590 -16.622 -26.110 1.00 34.23 A
ATOM 2738 CD LYS A 346 -31.181 -16.892 -25.693 1.00 32.44 A
ATOM 2739 CE LYS A 346 -30.163 -16.352 -26.684 1.00 32.66 A
ATOM 2740 NZ LYS A 346 -29.155 -17.270 -27.313 1.00 31.32 A
ATOM 2741 C LYS A 346 -33.653 -16.423 -28.943 1.00 38.97 A
ATOM 2742 O LYS A 346 -32.616 -16.595 -29.446 1.00 39.50 A
ATOM 2743 N GLN A 347 -34.373 -15.370 -29.216 1.00 38.55 A
ATOM 2744 CA GLN A 347 -33.947 -14.398 -30.213 1.00 39.05 A
ATOM 2745 CB GLN A 347 -34.221 -14.950 -31.604 1.00 38.68 A
ATOM 2746 CG GLN A 347 -33.932 -13.975 -32.710 1.00 39.12 A
ATOM 2747 CD GLN A 347 -34.500 -14.435 -34.019 1.00 39.67 A
ATOM 2748 OE1 GLN A 347 -34.371 -15.601 -34.383 1.00 40.23 A
ATOM 2749 NE2 GLN A 347 -35.133 -13.521 -34.743 1.00 40.20 A
ATOM 2750 C GLN A 347 -34.642 -13.054 -30.073 1.00 39.55 A

ATOM 2751 O GLN A 347 -35.872 -12.979 -30.131 1.00 39.14 A
ATOM 2752 N CYS A 348 -33.853 -11.995 -29.909 1.00 40.47 A
ATOM 2753 CA CYS A 348 -34.403 -10.650 -29.765 1.00 42.70 A
ATOM 2754 C CYS A 348 -34.872 -10.164 -31.140 1.00 42.61 A
ATOM 2755 O CYS A 348 -34.354 -9.190 -31.691 1.00 43.38 A
ATOM 2756 CB CYS A 348 -33.350 -9.688 -29.182 1.00 44.58 A
ATOM 2757 SG CYS A 348 -32.665 -10.127 -27.537 1.00 46.39 A
ATOM 2758 N THR A 349 -35.867 -10.860 -31.676 1.00 41.20 A
ATOM 2759 CA THR A 349 -36.421 -10.566 -32.989 1.00 39.39 A
ATOM 2760 CB THR A 349 -37.674 -11.426 -33.261 1.00 39.50 A
ATOM 2761 OG1 THR A 349 -37.364 -12.808 -33.050 1.00 39.71 A
ATOM 2762 CG2 THR A 349 -38.150 -11.241 -34.687 1.00 38.77 A
ATOM 2763 C THR A 349 -36.796 -9.112 -33.226 1.00 38.24 A
ATOM 2764 O THR A 349 -37.486 -8.496 -32.425 1.00 37.73 A
ATOM 2765 N ALA A 350 -36.321 -8.586 -34.348 1.00 37.86 A
ATOM 2766 CA ALA A 350 -36.606 -7.228 -34.790 1.00 37.83 A
ATOM 2767 CB ALA A 350 -35.311 -6.439 -34.943 1.00 37.69 A
ATOM 2768 C ALA A 350 -37.278 -7.440 -36.152 1.00 38.23 A
ATOM 2769 O ALA A 350 -36.843 -8.275 -36.938 1.00 38.55 A
ATOM 2770 N VAL A 351 -38.349 -6.711 -36.429 1.00 38.82 A
ATOM 2771 CA VAL A 351 -39.062 -6.872 -37.695 1.00 39.43 A
ATOM 2772 CB VAL A 351 -40.398 -6.111 -37.644 1.00 39.64 A
ATOM 2773 CG1 VAL A 351 -40.981 -5.969 -39.035 1.00 40.50 A
ATOM 2774 CG2 VAL A 351 -41.369 -6.862 -36.734 1.00 37.94 A
ATOM 2775 C VAL A 351 -38.240 -6.430 -38.907 1.00 40.64 A
ATOM 2776 O VAL A 351 -38.272 -5.265 -39.313 1.00 40.10 A
ATOM 2777 N THR A 352 -37.516 -7.388 -39.486 1.00 41.79 A
ATOM 2778 CA THR A 352 -36.646 -7.146 -40.633 1.00 41.94 A
ATOM 2779 CB THR A 352 -35.244 -6.784 -40.145 1.00 41.83 A
ATOM 2780 OG1 THR A 352 -35.304 -5.521 -39.484 1.00 42.07 A
ATOM 2781 CG2 THR A 352 -34.266 -6.695 -41.295 1.00 43.79 A
ATOM 2782 C THR A 352 -36.557 -8.372 -41.537 1.00 42.51 A
ATOM 2783 O THR A 352 -36.625 -9.500 -41.061 1.00 42.27 A
ATOM 2784 N MET A 353 -36.394 -8.153 -42.839 1.00 43.29 A

ATOM 2785 CA MET A 353 -36.309 -9.272 -43.758 1.00 44.08 A
ATOM 2786 CB MET A 353 -36.152 -8.795 -45.205 1.00 47.53 A
ATOM 2787 CG MET A 353 -36.519 -9.861 -46.251 1.00 50.24 A
ATOM 2788 SD MET A 353 -36.263 -9.368 -47.997 1.00 54.12 A
ATOM 2789 CE MET A 353 -34.603 -10.060 -48.297 1.00 53.08 A
ATOM 2790 C MET A 353 -35.145 -10.159 -43.375 1.00 43.41 A
ATOM 2791 O MET A 353 -35.321 -11.358 -43.215 1.00 42.34 A
ATOM 2792 N ASP A 354 -33.954 -9.587 -43.217 1.00 44.64 A
ATOM 2793 CA ASP A 354 -32.806 -10.411 -42.839 1.00 46.57 A
ATOM 2794 CB ASP A 354 -31.499 -9.594 -42.702 1.00 48.00 A
ATOM 2795 CG ASP A 354 -31.717 -8.077 -42.745 1.00 51.83 A
ATOM 2796 OD1 ASP A 354 -32.396 -7.580 -43.675 1.00 52.68 A
ATOM 2797 OD2 ASP A 354 -31.186 -7.371 -41.850 1.00 54.11 A
ATOM 2798 C ASP A 354 -33.111 -11.141 -41.532 1.00 47.53 A
ATOM 2799 O ASP A 354 -32.511 -12.174 -41.231 1.00 47.38 A
ATOM 2800 N GLN A 355 -34.132 -10.704 -40.838 1.00 48.81 A
ATOM 2801 CA GLN A 355 -34.475 -11.300 -39.587 1.00 48.08 A
ATOM 2802 CB GLN A 355 -34.843 -10.270 -38.556 1.00 47.13 A
ATOM 2803 CG GLN A 355 -33.683 -9.789 -37.770 1.00 48.31 A
ATOM 2804 CD GLN A 355 -33.594 -10.305 -36.388 1.00 48.09 A
ATOM 2805 OE1 GLN A 355 -34.148 -9.774 -35.507 1.00 48.37 A
ATOM 2806 NE2 GLN A 355 -32.982 -11.406 -36.235 1.00 47.82 A
ATOM 2807 C GLN A 355 -35.550 -12.284 -39.749 1.00 47.78 A
ATOM 2808 O GLN A 355 -35.702 -13.129 -38.954 1.00 48.60 A
ATOM 2809 N LEU A 356 -36.295 -12.169 -40.807 1.00 46.44 A
ATOM 2810 CA LEU A 356 -37.297 -13.164 -41.176 1.00 43.62 A
ATOM 2811 CB LEU A 356 -38.203 -12.637 -42.291 1.00 42.36 A
ATOM 2812 CG LEU A 356 -39.241 -13.630 -42.828 1.00 41.19 A
ATOM 2813 CD1 LEU A 356 -40.126 -14.149 -41.704 1.00 40.62 A
ATOM 2814 CD2 LEU A 356 -40.081 -12.947 -43.877 1.00 39.57 A
ATOM 2815 C LEU A 356 -36.676 -14.480 -41.609 1.00 42.99 A
ATOM 2816 O LEU A 356 -37.253 -15.538 -41.376 1.00 43.36 A
ATOM 2817 N SER A 357 -35.505 -14.423 -42.239 1.00 42.07 A
ATOM 2818 CA SER A 357 -34.851 -15.652 -42.675 1.00 41.18 A

ATOM 2819 CB SER A 357 -33.919 -15.393 -43.865 1.00 39.62 A
ATOM 2820 OG SER A 357 -32.977 -14.394 -43.576 1.00 38.03 A
ATOM 2821 C SER A 357 -34.095 -16.289 -41.522 1.00 40.65 A
ATOM 2822 O SER A 357 -33.914 -17.505 -41.494 1.00 40.23 A
ATOM 2823 N THR A 358 -33.659 -15.471 -40.566 1.00 40.85 A
ATOM 2824 CA THR A 358 -32.958 -15.993 -39.396 1.00 40.86 A
ATOM 2825 CB THR A 358 -32.406 -14.875 -38.492 1.00 40.84 A
ATOM 2826 OG1 THR A 358 -31.246 -14.285 -39.097 1.00 39.27 A
ATOM 2827 CG2 THR A 358 -32.036 -15.443 -37.122 1.00 40.75 A
ATOM 2828 C THR A 358 -33.981 -16.786 -38.595 1.00 40.77 A
ATOM 2829 O THR A 358 -33.651 -17.766 -37.922 1.00 39.94 A
ATOM 2830 N VAL A 359 -35.231 -16.350 -38.668 1.00 40.24 A
ATOM 2831 CA VAL A 359 -36.290 -17.050 -37.971 1.00 39.58 A
ATOM 2832 CB VAL A 359 -37.620 -16.279 -38.043 1.00 39.32 A
ATOM 2833 CG1 VAL A 359 -38.758 -17.153 -37.539 1.00 39.04 A
ATOM 2834 CG2 VAL A 359 -37.520 -15.010 -37.199 1.00 38.97 A
ATOM 2835 C VAL A 359 -36.442 -18.418 -38.618 1.00 39.18 A
ATOM 2836 O VAL A 359 -36.568 -19.422 -37.915 1.00 39.87 A
ATOM 2837 N HIS A 360 -36.417 -18.462 -39.951 1.00 37.66 A
ATOM 2838 CA HIS A 360 -36.525 -19.738 -40.657 1.00 36.81 A
ATOM 2839 CB HIS A 360 -36.575 -19.536 -42.171 1.00 35.97 A
ATOM 2840 CG HIS A 360 -37.878 -18.994 -42.666 1.00 37.14 A
ATOM 2841 CD2 HIS A 360 -38.898 -19.589 -43.329 1.00 37.42 A
ATOM 2842 ND1 HIS A 360 -38.253 -17.679 -42.490 1.00 38.78 A
ATOM 2843 CE1 HIS A 360 -39.446 -17.486 -43.024 1.00 39.34 A
ATOM 2844 NE2 HIS A 360 -39.862 -18.629 -43.540 1.00 39.00 A
ATOM 2845 C HIS A 360 -35.321 -20.602 -40.301 1.00 35.68 A
ATOM 2846 O HIS A 360 -35.455 -21.795 -40.007 1.00 34.73 A
ATOM 2847 N HIS A 361 -34.147 -19.980 -40.321 1.00 34.03 A
ATOM 2848 CA HIS A 361 -32.903 -20.659 -39.988 1.00 33.65 A
ATOM 2849 CB HIS A 361 -31.768 -19.650 -39.882 1.00 33.34 A
ATOM 2850 CG HIS A 361 -30.513 -20.221 -39.302 1.00 31.80 A
ATOM 2851 CD2 HIS A 361 -29.993 -20.140 -38.058 1.00 31.41 A
ATOM 2852 ND1 HIS A 361 -29.648 -21.007 -40.027 1.00 31.30 A

ATOM 2853 CE1 HIS A 361 -28.647 -21.386 -39.254 1.00 30.91 A
ATOM 2854 NE2 HIS A 361 -28.832 -20.874 -38.053 1.00 31.01 A
ATOM 2855 C HIS A 361 -33.016 -21.388 -38.659 1.00 33.70 A
ATOM 2856 O HIS A 361 -32.649 -22.561 -38.543 1.00 32.65 A
ATOM 2857 N GLU A 362 -33.513 -20.669 -37.655 1.00 34.07 A
ATOM 2858 CA GLU A 362 -33.680 -21.218 -36.319 1.00 33.62 A
ATOM 2859 CB GLU A 362 -34.036 -20.100 -35.333 1.00 33.93 A
ATOM 2860 CG GLU A 362 -32.940 -19.044 -35.137 1.00 34.15 A
ATOM 2861 CD GLU A 362 -31.596 -19.639 -34.754 1.00 35.22 A
ATOM 2862 OE1 GLU A 362 -31.574 -20.670 -34.070 1.00 36.91 A
ATOM 2863 OE2 GLU A 362 -30.551 -19.071 -35.116 1.00 35.16 A
ATOM 2864 C GLU A 362 -34.738 -22.325 -36.297 1.00 33.91 A
ATOM 2865 O GLU A 362 -34.499 -23.392 -35.720 1.00 33.70 A
ATOM 2866 N MET A 363 -35.893 -22.085 -36.924 1.00 33.63 A
ATOM 2867 CA MET A 363 -36.945 -23.102 -36.981 1.00 34.31 A
ATOM 2868 CB MET A 363 -38.100 -22.649 -37.863 1.00 35.71 A
ATOM 2869 CG MET A 363 -39.049 -21.692 -37.206 1.00 38.96 A
ATOM 2870 SD MET A 363 -40.759 -22.252 -37.392 1.00 41.06 A
ATOM 2871 CE MET A 363 -41.588 -21.035 -36.330 1.00 39.57 A
ATOM 2872 C MET A 363 -36.373 -24.383 -37.571 1.00 34.10 A
ATOM 2873 O MET A 363 -36.830 -25.481 -37.275 1.00 33.78 A
ATOM 2874 N GLY A 364 -35.375 -24.225 -38.428 1.00 33.86 A
ATOM 2875 CA GLY A 364 -34.756 -25.375 -39.043 1.00 33.52 A
ATOM 2876 C GLY A 364 -34.107 -26.247 -38.004 1.00 33.69 A
ATOM 2877 O GLY A 364 -34.082 -27.460 -38.158 1.00 34.93 A
ATOM 2878 N HIS A 365 -33.567 -25.635 -36.953 1.00 34.17 A
ATOM 2879 CA HIS A 365 -32.927 -26.383 -35.867 1.00 34.86 A
ATOM 2880 CB HIS A 365 -32.141 -25.436 -34.958 1.00 33.95 A
ATOM 2881 CG HIS A 365 -30.864 -24.947 -35.561 1.00 34.55 A
ATOM 2882 CD2 HIS A 365 -30.405 -23.692 -35.790 1.00 34.78 A
ATOM 2883 ND1 HIS A 365 -29.876 -25.803 -36.000 1.00 33.79 A
ATOM 2884 CE1 HIS A 365 -28.863 -25.096 -36.472 1.00 34.38 A
ATOM 2885 NE2 HIS A 365 -29.159 -23.813 -36.357 1.00 33.95 A
ATOM 2886 C HIS A 365 -33.997 -27.105 -35.047 1.00 35.07 A

ATOM 2887 O HIS A 365 -33.877 -28.299 -34.752 1.00 33.51 A
ATOM 2888 N ILE A 366 -35.042 -26.360 -34.696 1.00 34.86 A
ATOM 2889 CA ILE A 366 -36.163 -26.888 -33.936 1.00 35.34 A
ATOM 2890 CB ILE A 366 -37.239 -25.799 -33.741 1.00 35.51 A
ATOM 2891 CG2 ILE A 366 -38.415 -26.349 -32.965 1.00 35.57 A
ATOM 2892 CG1 ILE A 366 -36.623 -24.593 -33.033 1.00 35.55 A
ATOM 2893 CD1 ILE A 366 -35.759 -24.958 -31.845 1.00 36.59 A
ATOM 2894 C ILE A 366 -36.788 -28.087 -34.652 1.00 35.58 A
ATOM 2895 O ILE A 366 -37.058 -29.118 -34.032 1.00 35.58 A
ATOM 2896 N GLN A 367 -37.006 -27.943 -35.959 1.00 35.53 A
ATOM 2897 CA GLN A 367 -37.600 -29.005 -36.768 1.00 35.60 A
ATOM 2898 CB GLN A 367 -37.871 -28.527 -38.195 1.00 34.08 A
ATOM 2899 CG GLN A 367 -38.606 -29.563 -39.040 1.00 33.86 A
ATOM 2900 CD GLN A 367 -40.074 -29.697 -38.668 1.00 34.01 A
ATOM 2901 OE1 GLN A 367 -40.688 -30.742 -38.875 1.00 35.15 A
ATOM 2902 NE2 GLN A 367 -40.646 -28.630 -38.132 1.00 33.31 A
ATOM 2903 C GLN A 367 -36.702 -30.229 -36.828 1.00 36.04 A
ATOM 2904 O GLN A 367 -37.186 -31.349 -36.988 1.00 36.40 A
ATOM 2905 N TYR A 368 -35.396 -30.017 -36.707 1.00 35.45 A
ATOM 2906 CA TYR A 368 -34.462 -31.120 -36.744 1.00 35.55 A
ATOM 2907 CB TYR A 368 -33.039 -30.600 -36.923 1.00 35.74 A
ATOM 2908 CG TYR A 368 -32.116 -31.545 -37.670 1.00 37.21 A
ATOM 2909 CD1 TYR A 368 -30.992 -31.065 -38.348 1.00 37.93 A
ATOM 2910 CE1 TYR A 368 -30.121 -31.929 -39.022 1.00 38.53 A
ATOM 2911 CD2 TYR A 368 -32.348 -32.916 -37.689 1.00 38.05 A
ATOM 2912 CE2 TYR A 368 -31.485 -33.789 -38.362 1.00 39.18 A
ATOM 2913 CZ TYR A 368 -30.371 -33.291 -39.025 1.00 39.10 A
ATOM 2914 OH TYR A 368 -29.500 -34.155 -39.666 1.00 37.48 A
ATOM 2915 C TYR A 368 -34.609 -31.848 -35.420 1.00 36.64 A
ATOM 2916 O TYR A 368 -34.580 -33.075 -35.374 1.00 36.91 A
ATOM 2917 N TYR A 369 -34.791 -31.082 -34.344 1.00 37.50 A
ATOM 2918 CA TYR A 369 -34.959 -31.646 -33.003 1.00 37.48 A
ATOM 2919 CB TYR A 369 -35.098 -30.536 -31.961 1.00 35.62 A
ATOM 2920 CG TYR A 369 -33.899 -29.635 -31.850 1.00 33.19 A

ATOM 2921 CD1 TYR A 369 -34.057 -28.275 -31.618 1.00 32.92 A
ATOM 2922 CE1 TYR A 369 -32.964 -27.434 -31.531 1.00 34.36 A
ATOM 2923 CD2 TYR A 369 -32.612 -30.139 -31.986 1.00 32.70 A
ATOM 2924 CE2 TYR A 369 -31.506 -29.309 -31.900 1.00 34.01 A
ATOM 2925 CZ TYR A 369 -31.689 -27.953 -31.675 1.00 35.30 A
ATOM 2926 OH TYR A 369 -30.598 -27.112 -31.616 1.00 36.23 A
ATOM 2927 C TYR A 369 -36.213 -32.493 -32.971 1.00 38.49 A
ATOM 2928 O TYR A 369 -36.166 -33.680 -32.650 1.00 39.60 A
ATOM 2929 N LEU A 370 -37.334 -31.862 -33.307 1.00 38.26 A
ATOM 2930 CA LEU A 370 -38.627 -32.528 -33.326 1.00 37.47 A
ATOM 2931 CB LEU A 370 -39.681 -31.615 -33.958 1.00 34.09 A
ATOM 2932 CG LEU A 370 -39.867 -30.226 -33.358 1.00 32.59 A
ATOM 2933 CD1 LEU A 370 -40.775 -29.406 -34.245 1.00 32.73 A
ATOM 2934 CD2 LEU A 370 -40.441 -30.349 -31.973 1.00 32.20 A
ATOM 2935 C LEU A 370 -38.567 -33.832 -34.111 1.00 38.97 A
ATOM 2936 O LEU A 370 -39.213 -34.807 -33.748 1.00 40.37 A
ATOM 2937 N GLN A 371 -37.783 -33.856 -35.180 1.00 40.33 A
ATOM 2938 CA GLN A 371 -37.699 -35.050 -36.014 1.00 41.82 A
ATOM 2939 CB GLN A 371 -37.193 -34.693 -37.420 1.00 42.99 A
ATOM 2940 CG GLN A 371 -38.129 -33.803 -38.249 1.00 41.62 A
ATOM 2941 CD GLN A 371 -39.520 -34.384 -38.410 1.00 40.46 A
ATOM 2942 OE1 GLN A 371 -39.696 -35.601 -38.488 1.00 39.12 A
ATOM 2943 NE2 GLN A 371 -40.516 -33.513 -38.477 1.00 39.61 A
ATOM 2944 C GLN A 371 -36.870 -36.206 -35.467 1.00 42.33 A
ATOM 2945 O GLN A 371 -37.235 -37.364 -35.670 1.00 43.17 A
ATOM 2946 N TYR A 372 -35.765 -35.927 -34.785 1.00 42.69 A
ATOM 2947 CA TYR A 372 -34.965 -37.035 -34.282 1.00 44.21 A
ATOM 2948 CB TYR A 372 -33.479 -36.872 -34.671 1.00 45.88 A
ATOM 2949 CG TYR A 372 -32.744 -35.624 -34.189 1.00 47.12 A
ATOM 2950 CD1 TYR A 372 -33.264 -34.794 -33.193 1.00 47.39 A
ATOM 2951 CE1 TYR A 372 -32.540 -33.688 -32.719 1.00 47.90 A
ATOM 2952 CD2 TYR A 372 -31.486 -35.313 -34.705 1.00 48.58 A
ATOM 2953 CE2 TYR A 372 -30.758 -34.212 -34.241 1.00 49.61 A
ATOM 2954 CZ TYR A 372 -31.285 -33.406 -33.250 1.00 48.82 A

```
ATOM  2955 OH  TYR A 372     -30.542 -32.338 -32.795  1.00 47.60      A
ATOM  2956 C   TYR A 372     -35.087 -37.315 -32.790  1.00 44.50      A
ATOM  2957 O   TYR A 372     -34.360 -38.164 -32.251  1.00 44.28      A
ATOM  2958 N   LYS A 373     -36.024 -36.634 -32.129  1.00 44.11      A
ATOM  2959 CA  LYS A 373     -36.220 -36.815 -30.690  1.00 43.18      A
ATOM  2960 CB  LYS A 373     -37.437 -36.017 -30.204  1.00 42.04      A
ATOM  2961 CG  LYS A 373     -38.785 -36.531 -30.674  1.00 41.69      A
ATOM  2962 CD  LYS A 373     -39.900 -35.630 -30.150  1.00 42.07      A
ATOM  2963 CE  LYS A 373     -41.268 -35.981 -30.733  1.00 41.86      A
ATOM  2964 NZ  LYS A 373     -41.712 -37.361 -30.388  1.00 41.51      A
ATOM  2965 C   LYS A 373     -36.380 -38.280 -30.288  1.00 43.21      A
ATOM  2966 O   LYS A 373     -36.198 -38.624 -29.124  1.00 43.14      A
ATOM  2967 N   ASP A 374     -36.696 -39.145 -31.246  1.00 43.39      A
ATOM  2968 CA  ASP A 374     -36.881 -40.554 -30.947  1.00 43.26      A
ATOM  2969 CB  ASP A 374     -38.095 -41.076 -31.696  1.00 46.24      A
ATOM  2970 CG  ASP A 374     -39.382 -40.458 -31.191  1.00 50.04      A
ATOM  2971 OD1 ASP A 374     -39.625 -40.531 -29.960  1.00 51.44      A
ATOM  2972 OD2 ASP A 374     -40.143 -39.897 -32.013  1.00 51.92      A
ATOM  2973 C   ASP A 374     -35.681 -41.442 -31.209  1.00 42.09      A
ATOM  2974 O   ASP A 374     -35.816 -42.527 -31.757  1.00 42.02      A
ATOM  2975 N   LEU A 375     -34.510 -40.980 -30.788  1.00 41.94      A
ATOM  2976 CA  LEU A 375     -33.269 -41.728 -30.957  1.00 41.84      A
ATOM  2977 CB  LEU A 375     -32.433 -41.123 -32.091  1.00 43.30      A
ATOM  2978 CG  LEU A 375     -33.024 -41.038 -33.499  1.00 43.82      A
ATOM  2979 CD1 LEU A 375     -32.274 -39.990 -34.306  1.00 44.15      A
ATOM  2980 CD2 LEU A 375     -32.952 -42.402 -34.161  1.00 43.55      A
ATOM  2981 C   LEU A 375     -32.454 -41.640 -29.674  1.00 40.70      A
ATOM  2982 O   LEU A 375     -32.677 -40.752 -28.852  1.00 39.20      A
ATOM  2983 N   PRO A 376     -31.508 -42.573 -29.478  1.00 40.63      A
ATOM  2984 CD  PRO A 376     -31.149 -43.761 -30.274  1.00 40.97      A
ATOM  2985 CA  PRO A 376     -30.701 -42.500 -28.264  1.00 40.75      A
ATOM  2986 CB  PRO A 376     -29.571 -43.479 -28.558  1.00 40.90      A
ATOM  2987 CG  PRO A 376     -30.277 -44.551 -29.311  1.00 40.74      A
ATOM  2988 C   PRO A 376     -30.210 -41.059 -28.165  1.00 40.76      A
```

ATOM 2989 O PRO A 376 -29.806 -40.468 -29.165 1.00 42.46 A
ATOM 2990 N VAL A 377 -30.277 -40.488 -26.971 1.00 39.66 A
ATOM 2991 CA VAL A 377 -29.844 -39.114 -26.745 1.00 37.92 A
ATOM 2992 CB VAL A 377 -29.704 -38.836 -25.220 1.00 36.49 A
ATOM 2993 CG1 VAL A 377 -28.517 -39.608 -24.647 1.00 37.67 A
ATOM 2994 CG2 VAL A 377 -29.556 -37.367 -24.966 1.00 34.14 A
ATOM 2995 C VAL A 377 -28.521 -38.769 -27.453 1.00 37.64 A
ATOM 2996 O VAL A 377 -28.445 -37.779 -28.180 1.00 37.60 A
ATOM 2997 N SER A 378 -27.491 -39.588 -27.259 1.00 36.49 A
ATOM 2998 CA SER A 378 -26.192 -39.317 -27.860 1.00 36.63 A
ATOM 2999 CB SER A 378 -25.167 -40.336 -27.362 1.00 36.94 A
ATOM 3000 OG SER A 378 -25.657 -41.653 -27.517 1.00 39.91 A
ATOM 3001 C SER A 378 -26.165 -39.253 -29.389 1.00 35.84 A
ATOM 3002 O SER A 378 -25.116 -39.014 -29.979 1.00 34.67 A
ATOM 3003 N LEU A 379 -27.311 -39.459 -30.028 1.00 36.12 A
ATOM 3004 CA LEU A 379 -27.392 -39.398 -31.485 1.00 36.83 A
ATOM 3005 CB LEU A 379 -27.896 -40.723 -32.066 1.00 36.62 A
ATOM 3006 CG LEU A 379 -27.108 -42.020 -31.849 1.00 36.80 A
ATOM 3007 CD1 LEU A 379 -27.862 -43.168 -32.495 1.00 35.69 A
ATOM 3008 CD2 LEU A 379 -25.728 -41.917 -32.444 1.00 36.45 A
ATOM 3009 C LEU A 379 -28.320 -38.270 -31.954 1.00 37.73 A
ATOM 3010 O LEU A 379 -28.655 -38.195 -33.136 1.00 37.11 A
ATOM 3011 N ARG A 380 -28.733 -37.400 -31.032 1.00 39.25 A
ATOM 3012 CA ARG A 380 -29.623 -36.283 -31.367 1.00 40.66 A
ATOM 3013 CB ARG A 380 -30.497 -35.904 -30.159 1.00 42.63 A
ATOM 3014 CG ARG A 380 -31.322 -37.066 -29.630 1.00 43.18 A
ATOM 3015 CD ARG A 380 -32.250 -36.697 -28.482 1.00 43.72 A
ATOM 3016 NE ARG A 380 -32.791 -37.919 -27.878 1.00 45.88 A
ATOM 3017 CZ ARG A 380 -33.611 -37.958 -26.829 1.00 45.83 A
ATOM 3018 NH1 ARG A 380 -34.011 -36.835 -26.238 1.00 44.45 A
ATOM 3019 NH2 ARG A 380 -34.030 -39.129 -26.366 1.00 46.80 A
ATOM 3020 C ARG A 380 -28.820 -35.072 -31.832 1.00 40.70 A
ATOM 3021 O ARG A 380 -28.738 -34.039 -31.148 1.00 40.70 A
ATOM 3022 N ARG A 381 -28.204 -35.234 -32.989 1.00 40.89 A

```
ATOM  3023  CA  ARG A 381     -27.228 -34.356 -33.590  1.00 40.63      A
ATOM  3024  CB  ARG A 381     -25.912 -35.107 -33.457  1.00 42.06      A
ATOM  3025  CG  ARG A 381     -25.121 -34.798 -32.290  1.00 42.26      A
ATOM  3026  CD  ARG A 381     -25.766 -33.841 -31.430  1.00 45.08      A
ATOM  3027  NE  ARG A 381     -24.839 -32.818 -30.976  1.00 48.47      A
ATOM  3028  CZ  ARG A 381     -25.127 -31.572 -30.662  1.00 49.05      A
ATOM  3029  NH1 ARG A 381     -26.333 -31.086 -30.742  1.00 48.20      A
ATOM  3030  NH2 ARG A 381     -24.147 -30.804 -30.287  1.00 49.59      A
ATOM  3031  C   ARG A 381     -27.657 -34.270 -35.089  1.00 39.16      A
ATOM  3032  O   ARG A 381     -28.411 -35.066 -35.456  1.00 39.48      A
ATOM  3033  N   GLY A 382     -27.192 -33.349 -35.938  1.00 37.16      A
ATOM  3034  CA  GLY A 382     -27.314 -33.456 -37.386  1.00 35.25      A
ATOM  3035  C   GLY A 382     -26.297 -34.434 -37.946  1.00 33.42      A
ATOM  3036  O   GLY A 382     -25.360 -34.800 -37.241  1.00 33.53      A
ATOM  3037  N   ALA A 383     -26.478 -34.871 -39.191  1.00 32.75      A
ATOM  3038  CA  ALA A 383     -25.535 -35.809 -39.815  1.00 31.91      A
ATOM  3039  CB  ALA A 383     -25.734 -35.837 -41.323  1.00 33.76      A
ATOM  3040  C   ALA A 383     -24.144 -35.308 -39.472  1.00 30.27      A
ATOM  3041  O   ALA A 383     -23.248 -36.083 -39.136  1.00 29.89      A
ATOM  3042  N   ASN A 384     -23.989 -33.995 -39.603  1.00 28.03      A
ATOM  3043  CA  ASN A 384     -22.785 -33.278 -39.227  1.00 28.64      A
ATOM  3044  CB  ASN A 384     -21.659 -33.331 -40.295  1.00 30.24      A
ATOM  3045  CG  ASN A 384     -21.994 -32.605 -41.602  1.00 31.98      A
ATOM  3046  OD1 ASN A 384     -22.546 -31.503 -41.610  1.00 33.11      A
ATOM  3047  ND2 ASN A 384     -21.611 -33.219 -42.718  1.00 29.17      A
ATOM  3048  C   ASN A 384     -23.300 -31.865 -38.958  1.00 28.56      A
ATOM  3049  O   ASN A 384     -24.369 -31.488 -39.451  1.00 27.53      A
ATOM  3050  N   PRO A 385     -22.575 -31.081 -38.145  1.00 28.51      A
ATOM  3051  CD  PRO A 385     -21.184 -31.334 -37.731  1.00 27.49      A
ATOM  3052  CA  PRO A 385     -22.974 -29.712 -37.801  1.00 28.96      A
ATOM  3053  CB  PRO A 385     -21.703 -29.117 -37.211  1.00 28.26      A
ATOM  3054  CG  PRO A 385     -21.002 -30.312 -36.658  1.00 27.98      A
ATOM  3055  C   PRO A 385     -23.471 -28.922 -39.003  1.00 30.29      A
ATOM  3056  O   PRO A 385     -24.345 -28.059 -38.875  1.00 32.12      A
```

ATOM 3057 N GLY A 386 -22.902 -29.223 -40.168 1.00 29.85 A
ATOM 3058 CA GLY A 386 -23.285 -28.541 -41.386 1.00 28.62 A
ATOM 3059 C GLY A 386 -24.734 -28.769 -41.747 1.00 29.23 A
ATOM 3060 O GLY A 386 -25.450 -27.812 -42.022 1.00 29.20 A
ATOM 3061 N PHE A 387 -25.173 -30.026 -41.752 1.00 29.65 A
ATOM 3062 CA PHE A 387 -26.563 -30.326 -42.082 1.00 30.14 A
ATOM 3063 CB PHE A 387 -26.869 -31.817 -41.885 1.00 30.04 A
ATOM 3064 CG PHE A 387 -26.269 -32.719 -42.939 1.00 30.84 A
ATOM 3065 CD1 PHE A 387 -24.892 -32.735 -43.176 1.00 31.00 A
ATOM 3066 CD2 PHE A 387 -27.080 -33.585 -43.673 1.00 29.77 A
ATOM 3067 CE1 PHE A 387 -24.334 -33.606 -44.131 1.00 30.68 A
ATOM 3068 CE2 PHE A 387 -26.531 -34.457 -44.627 1.00 30.22 A
ATOM 3069 CZ PHE A 387 -25.158 -34.468 -44.855 1.00 29.38 A
ATOM 3070 C PHE A 387 -27.496 -29.504 -41.198 1.00 30.14 A
ATOM 3071 O PHE A 387 -28.506 -28.980 -41.666 1.00 29.35 A
ATOM 3072 N HIS A 388 -27.142 -29.379 -39.921 1.00 29.68 A
ATOM 3073 CA HIS A 388 -27.974 -28.635 -38.990 1.00 29.23 A
ATOM 3074 CB HIS A 388 -27.406 -28.699 -37.562 1.00 29.87 A
ATOM 3075 CG HIS A 388 -28.407 -29.145 -36.526 1.00 30.57 A
ATOM 3076 CD2 HIS A 388 -28.415 -30.213 -35.695 1.00 30.18 A
ATOM 3077 ND1 HIS A 388 -29.587 -28.465 -36.283 1.00 30.81 A
ATOM 3078 CE1 HIS A 388 -30.276 -29.099 -35.352 1.00 30.16 A
ATOM 3079 NE2 HIS A 388 -29.590 -30.162 -34.976 1.00 30.14 A
ATOM 3080 C HIS A 388 -28.149 -27.193 -39.413 1.00 28.54 A
ATOM 3081 O HIS A 388 -29.274 -26.709 -39.502 1.00 29.28 A
ATOM 3082 N GLU A 389 -27.051 -26.500 -39.689 1.00 28.07 A
ATOM 3083 CA GLU A 389 -27.149 -25.098 -40.089 1.00 28.29 A
ATOM 3084 CB GLU A 389 -25.761 -24.452 -40.120 1.00 28.13 A
ATOM 3085 CG GLU A 389 -24.948 -24.544 -38.820 1.00 29.84 A
ATOM 3086 CD GLU A 389 -25.696 -24.021 -37.600 1.00 30.64 A
ATOM 3087 OE1 GLU A 389 -26.468 -23.051 -37.732 1.00 30.20 A
ATOM 3088 OE2 GLU A 389 -25.500 -24.574 -36.499 1.00 30.65 A
ATOM 3089 C GLU A 389 -27.825 -24.915 -41.453 1.00 28.36 A
ATOM 3090 O GLU A 389 -28.266 -23.815 -41.795 1.00 29.82 A

ATOM 3091 N ALA A 390 -27.901 -25.997 -42.221 1.00 26.14 A
ATOM 3092 CA ALA A 390 -28.527 -25.959 -43.537 1.00 23.23 A
ATOM 3093 CB ALA A 390 -28.124 -27.179 -44.352 1.00 23.61 A
ATOM 3094 C ALA A 390 -30.046 -25.872 -43.424 1.00 23.38 A
ATOM 3095 O ALA A 390 -30.685 -25.081 -44.117 1.00 22.78 A
ATOM 3096 N ILE A 391 -30.616 -26.690 -42.546 1.00 23.42 A
ATOM 3097 CA ILE A 391 -31.985 -27.162 -42.716 1.00 22.36 A
ATOM 3098 CB ILE A 391 -32.419 -28.008 -41.504 1.00 20.22 A
ATOM 3099 CG2 ILE A 391 -33.909 -28.305 -41.567 1.00 16.75 A
ATOM 3100 CG1 ILE A 391 -31.611 -29.305 -41.442 1.00 20.32 A
ATOM 3101 CD1 ILE A 391 -31.501 -30.019 -42.771 1.00 19.50 A
ATOM 3102 C ILE A 391 -32.950 -25.998 -42.914 1.00 23.56 A
ATOM 3103 O ILE A 391 -33.849 -26.059 -43.753 1.00 24.41 A
ATOM 3104 N GLY A 392 -32.758 -24.938 -42.136 1.00 24.03 A
ATOM 3105 CA GLY A 392 -33.619 -23.772 -42.209 1.00 25.24 A
ATOM 3106 C GLY A 392 -33.303 -22.893 -43.403 1.00 26.93 A
ATOM 3107 O GLY A 392 -34.193 -22.264 -43.975 1.00 27.39 A
ATOM 3108 N ASP A 393 -32.030 -22.851 -43.782 1.00 29.78 A
ATOM 3109 CA ASP A 393 -31.590 -22.029 -44.902 1.00 30.91 A
ATOM 3110 CB ASP A 393 -30.062 -22.004 -44.982 1.00 33.01 A
ATOM 3111 CG ASP A 393 -29.451 -20.924 -44.110 1.00 35.37 A
ATOM 3112 OD1 ASP A 393 -29.786 -20.868 -42.908 1.00 34.06 A
ATOM 3113 OD2 ASP A 393 -28.628 -20.089 -44.538 1.00 37.74 A
ATOM 3114 C ASP A 393 -32.176 -22.532 -46.218 1.00 30.46 A
ATOM 3115 O ASP A 393 -32.612 -21.742 -47.055 1.00 30.15 A
ATOM 3116 N VAL A 394 -32.182 -23.849 -46.393 1.00 30.06 A
ATOM 3117 CA VAL A 394 -32.780 -24.464 -47.578 1.00 29.38 A
ATOM 3118 CB VAL A 394 -32.974 -25.976 -47.399 1.00 27.50 A
ATOM 3119 CG1 VAL A 394 -33.667 -26.543 -48.606 1.00 25.21 A
ATOM 3120 CG2 VAL A 394 -31.639 -26.660 -47.188 1.00 27.06 A
ATOM 3121 C VAL A 394 -34.159 -23.841 -47.813 1.00 30.78 A
ATOM 3122 O VAL A 394 -34.371 -23.117 -48.788 1.00 31.67 A
ATOM 3123 N LEU A 395 -35.094 -24.123 -46.908 1.00 31.02 A
ATOM 3124 CA LEU A 395 -36.447 -23.587 -47.007 1.00 30.35 A

ATOM 3125 CB LEU A 395 -37.275 -23.938 -45.766 1.00 29.21 A
ATOM 3126 CG LEU A 395 -37.739 -25.380 -45.585 1.00 29.04 A
ATOM 3127 CD1 LEU A 395 -36.565 -26.295 -45.245 1.00 28.67 A
ATOM 3128 CD2 LEU A 395 -38.771 -25.404 -44.484 1.00 28.50 A
ATOM 3129 C LEU A 395 -36.428 -22.079 -47.174 1.00 30.38 A
ATOM 3130 O LEU A 395 -37.343 -21.505 -47.753 1.00 31.31 A
ATOM 3131 N ALA A 396 -35.395 -21.432 -46.658 1.00 29.84 A
ATOM 3132 CA ALA A 396 -35.303 -19.987 -46.788 1.00 30.81 A
ATOM 3133 CB ALA A 396 -34.127 -19.467 -45.993 1.00 32.14 A
ATOM 3134 C ALA A 396 -35.148 -19.605 -48.262 1.00 31.43 A
ATOM 3135 O ALA A 396 -35.729 -18.608 -48.714 1.00 31.32 A
ATOM 3136 N LEU A 397 -34.371 -20.402 -49.006 1.00 31.49 A
ATOM 3137 CA LEU A 397 -34.132 -20.152 -50.434 1.00 30.57 A
ATOM 3138 CB LEU A 397 -33.337 -21.294 -51.075 1.00 28.20 A
ATOM 3139 CG LEU A 397 -31.837 -21.312 -50.763 1.00 27.50 A
ATOM 3140 CD1 LEU A 397 -31.204 -22.558 -51.340 1.00 26.24 A
ATOM 3141 CD2 LEU A 397 -31.171 -20.072 -51.325 1.00 25.83 A
ATOM 3142 C LEU A 397 -35.446 -19.985 -51.161 1.00 31.24 A
ATOM 3143 O LEU A 397 -35.624 -19.020 -51.912 1.00 32.54 A
ATOM 3144 N SER A 398 -36.369 -20.914 -50.920 1.00 31.26 A
ATOM 3145 CA SER A 398 -37.679 -20.875 -51.553 1.00 30.66 A
ATOM 3146 CB SER A 398 -38.452 -22.170 -51.264 1.00 29.37 A
ATOM 3147 OG SER A 398 -37.731 -23.325 -51.672 1.00 27.56 A
ATOM 3148 C SER A 398 -38.488 -19.667 -51.075 1.00 31.33 A
ATOM 3149 O SER A 398 -39.273 -19.102 -51.825 1.00 32.06 A
ATOM 3150 N VAL A 399 -38.296 -19.251 -49.833 1.00 31.71 A
ATOM 3151 CA VAL A 399 -39.061 -18.123 -49.331 1.00 32.24 A
ATOM 3152 CB VAL A 399 -38.953 -18.011 -47.788 1.00 32.17 A
ATOM 3153 CG1 VAL A 399 -39.932 -16.965 -47.259 1.00 29.97 A
ATOM 3154 CG2 VAL A 399 -39.223 -19.359 -47.154 1.00 31.41 A
ATOM 3155 C VAL A 399 -38.593 -16.819 -49.958 1.00 33.12 A
ATOM 3156 O VAL A 399 -39.402 -15.971 -50.308 1.00 33.08 A
ATOM 3157 N SER A 400 -37.286 -16.665 -50.112 1.00 33.88 A
ATOM 3158 CA SER A 400 -36.727 -15.440 -50.682 1.00 35.80 A

ATOM 3159 CB SER A 400 -35.207 -15.497 -50.625 1.00 36.18 A
ATOM 3160 OG SER A 400 -34.781 -15.742 -49.303 1.00 38.27 A
ATOM 3161 C SER A 400 -37.150 -15.107 -52.118 1.00 36.52 A
ATOM 3162 O SER A 400 -37.155 -13.933 -52.505 1.00 34.84 A
ATOM 3163 N THR A 401 -37.493 -16.133 -52.900 1.00 37.13 A
ATOM 3164 CA THR A 401 -37.888 -15.932 -54.295 1.00 37.30 A
ATOM 3165 CB THR A 401 -38.338 -17.252 -54.967 1.00 37.10 A
ATOM 3166 OG1 THR A 401 -39.593 -17.668 -54.421 1.00 36.11 A
ATOM 3167 CG2 THR A 401 -37.304 -18.347 -54.759 1.00 36.99 A
ATOM 3168 C THR A 401 -39.017 -14.917 -54.450 1.00 38.52 A
ATOM 3169 O THR A 401 -40.007 -14.961 -53.723 1.00 37.77 A
ATOM 3170 N PRO A 402 -38.886 -13.994 -55.420 1.00 39.99 A
ATOM 3171 CD PRO A 402 -37.767 -13.852 -56.369 1.00 39.57 A
ATOM 3172 CA PRO A 402 -39.904 -12.966 -55.669 1.00 40.77 A
ATOM 3173 CB PRO A 402 -39.359 -12.229 -56.889 1.00 40.32 A
ATOM 3174 CG PRO A 402 -37.883 -12.409 -56.762 1.00 39.62 A
ATOM 3175 C PRO A 402 -41.291 -13.574 -55.928 1.00 42.35 A
ATOM 3176 O PRO A 402 -42.317 -12.973 -55.610 1.00 42.08 A
ATOM 3177 N ALA A 403 -41.313 -14.768 -56.514 1.00 44.09 A
ATOM 3178 CA ALA A 403 -42.571 -15.438 -56.801 1.00 45.34 A
ATOM 3179 CB ALA A 403 -42.336 -16.653 -57.689 1.00 46.00 A
ATOM 3180 C ALA A 403 -43.227 -15.865 -55.500 1.00 46.02 A
ATOM 3181 O ALA A 403 -44.440 -15.744 -55.346 1.00 46.35 A
ATOM 3182 N HIS A 404 -42.428 -16.359 -54.561 1.00 47.34 A
ATOM 3183 CA HIS A 404 -42.956 -16.798 -53.273 1.00 48.51 A
ATOM 3184 CB HIS A 404 -41.917 -17.622 -52.510 1.00 47.98 A
ATOM 3185 CG HIS A 404 -42.453 -18.268 -51.270 1.00 47.58 A
ATOM 3186 CD2 HIS A 404 -42.403 -17.885 -49.972 1.00 48.35 A
ATOM 3187 ND1 HIS A 404 -43.142 -19.461 -51.291 1.00 47.43 A
ATOM 3188 CE1 HIS A 404 -43.494 -19.786 -50.060 1.00 47.17 A
ATOM 3189 NE2 HIS A 404 -43.057 -18.846 -49.241 1.00 48.26 A
ATOM 3190 C HIS A 404 -43.421 -15.620 -52.423 1.00 49.15 A
ATOM 3191 O HIS A 404 -44.490 -15.666 -51.815 1.00 49.82 A
ATOM 3192 N LEU A 405 -42.612 -14.567 -52.384 1.00 49.09 A

ATOM 3193 CA LEU A 405 -42.931 -13.386 -51.590 1.00 48.81 A
ATOM 3194 CB LEU A 405 -41.879 -12.295 -51.803 1.00 47.87 A
ATOM 3195 CG LEU A 405 -40.477 -12.590 -51.267 1.00 46.76 A
ATOM 3196 CD1 LEU A 405 -39.578 -11.372 -51.418 1.00 45.74 A
ATOM 3197 CD2 LEU A 405 -40.538 -13.039 -49.815 1.00 44.69 A
ATOM 3198 C LEU A 405 -44.317 -12.851 -51.933 1.00 49.57 A
ATOM 3199 O LEU A 405 -45.057 -12.408 -51.055 1.00 49.79 A
ATOM 3200 N HIS A 406 -44.661 -12.895 -53.216 1.00 49.82 A
ATOM 3201 CA HIS A 406 -45.953 -12.406 -53.681 1.00 48.66 A
ATOM 3202 CB HIS A 406 -45.971 -12.312 -55.208 1.00 48.91 A
ATOM 3203 CG HIS A 406 -47.241 -11.748 -55.765 1.00 50.76 A
ATOM 3204 CD2 HIS A 406 -47.471 -10.652 -56.527 1.00 50.86 A
ATOM 3205 ND1 HIS A 406 -48.471 -12.333 -55.553 1.00 52.42 A
ATOM 3206 CE1 HIS A 406 -49.404 -11.621 -56.159 1.00 52.24 A
ATOM 3207 NE2 HIS A 406 -48.824 -10.596 -56.758 1.00 51.03 A
ATOM 3208 C HIS A 406 -47.088 -13.303 -53.198 1.00 48.17 A
ATOM 3209 O HIS A 406 -48.176 -12.825 -52.876 1.00 48.24 A
ATOM 3210 N ALA A 407 -46.803 -14.570 -53.155 1.00 47.55 A
ATOM 3211 CA ALA A 407 -47.778 -15.544 -52.849 1.00 47.09 A
ATOM 3212 CB ALA A 407 -47.175 -16.843 -52.913 1.00 45.58 A
ATOM 3213 C ALA A 407 -48.231 -15.287 -51.492 1.00 47.12 A
ATOM 3214 O ALA A 407 -49.247 -15.777 -51.088 1.00 48.12 A
ATOM 3215 N ILE A 408 -47.472 -14.502 -50.769 1.00 45.69 A
ATOM 3216 CA ILE A 408 -47.679 -14.381 -49.356 1.00 44.43 A
ATOM 3217 CB ILE A 408 -46.788 -15.239 -48.621 1.00 43.09 A
ATOM 3218 CG2 ILE A 408 -45.856 -15.842 -49.486 1.00 42.85 A
ATOM 3219 CG1 ILE A 408 -45.985 -14.416 -47.723 1.00 41.20 A
ATOM 3220 CD1 ILE A 408 -44.720 -14.866 -47.743 1.00 39.90 A
ATOM 3221 C ILE A 408 -47.529 -13.065 -48.762 1.00 43.91 A
ATOM 3222 O ILE A 408 -47.701 -12.895 -47.612 1.00 44.14 A
ATOM 3223 N GLY A 409 -47.238 -12.100 -49.551 1.00 43.79 A
ATOM 3224 CA GLY A 409 -47.990 -10.922 -49.425 1.00 44.50 A
ATOM 3225 C GLY A 409 -47.088 -9.774 -49.438 1.00 45.74 A
ATOM 3226 O GLY A 409 -47.515 -8.698 -49.288 1.00 45.92 A

ATOM 3227 N LEU A 410 -45.827 -9.951 -49.621 1.00 46.73 A
ATOM 3228 CA LEU A 410 -45.112 -8.763 -49.518 1.00 48.68 A
ATOM 3229 CB LEU A 410 -44.218 -8.769 -48.346 1.00 48.91 A
ATOM 3230 CG LEU A 410 -43.682 -10.023 -47.758 1.00 48.12 A
ATOM 3231 CD1 LEU A 410 -42.242 -9.906 -47.755 1.00 48.34 A
ATOM 3232 CD2 LEU A 410 -44.092 -9.912 -46.445 1.00 47.14 A
ATOM 3233 C LEU A 410 -44.429 -8.247 -50.695 1.00 50.39 A
ATOM 3234 O LEU A 410 -43.682 -7.330 -50.599 1.00 50.07 A
ATOM 3235 N LEU A 411 -44.689 -8.826 -51.836 1.00 52.00 A
ATOM 3236 CA LEU A 411 -44.150 -8.292 -53.033 1.00 53.63 A
ATOM 3237 CB LEU A 411 -43.240 -9.257 -53.669 1.00 53.77 A
ATOM 3238 CG LEU A 411 -41.880 -8.727 -53.950 1.00 54.20 A
ATOM 3239 CD1 LEU A 411 -41.193 -9.481 -54.990 1.00 54.49 A
ATOM 3240 CD2 LEU A 411 -42.082 -7.444 -54.409 1.00 54.08 A
ATOM 3241 C LEU A 411 -45.253 -8.047 -53.932 1.00 55.43 A
ATOM 3242 O LEU A 411 -45.773 -8.911 -54.522 1.00 56.12 A
ATOM 3243 N ALA A 412 -45.617 -6.810 -53.994 1.00 57.46 A
ATOM 3244 CA ALA A 412 -46.861 -6.343 -54.595 1.00 59.06 A
ATOM 3245 CB ALA A 412 -47.020 -4.845 -54.386 1.00 57.79 A
ATOM 3246 C ALA A 412 -46.919 -6.685 -56.080 1.00 60.36 A
ATOM 3247 O ALA A 412 -47.943 -6.483 -56.733 1.00 60.73 A
ATOM 3248 N ALA A 413 -45.815 -7.204 -56.606 1.00 63.14 A
ATOM 3249 CA ALA A 413 -45.596 -7.238 -58.047 1.00 65.57 A
ATOM 3250 CB ALA A 413 -44.249 -6.623 -58.393 1.00 64.50 A
ATOM 3251 C ALA A 413 -45.687 -8.663 -58.584 1.00 67.19 A
ATOM 3252 O ALA A 413 -45.907 -9.608 -57.827 1.00 68.89 A
ATOM 3253 N ALA A 414 -45.514 -8.808 -59.893 1.00 68.04 A
ATOM 3254 CA ALA A 414 -44.461 -9.656 -60.438 1.00 68.43 A
ATOM 3255 CB ALA A 414 -44.977 -11.070 -60.655 1.00 67.74 A
ATOM 3256 C ALA A 414 -43.909 -9.083 -61.739 1.00 68.56 A
ATOM 3257 O ALA A 414 -44.663 -8.770 -62.660 1.00 70.23 A
ATOM 3258 N ALA A 415 -42.589 -8.947 -61.807 1.00 67.29 A
ATOM 3259 CA ALA A 415 -41.924 -8.521 -63.033 1.00 65.61 A
ATOM 3260 CB ALA A 415 -41.123 -7.252 -62.789 1.00 65.25 A

ATOM 3261 C ALA A 415 -41.025 -9.623 -63.584 1.00 64.49 A
ATOM 3262 O ALA A 415 -39.840 -9.692 -63.256 1.00 66.13 A
ATOM 3263 N ALA A 416 -41.596 -10.483 -64.421 1.00 61.83 A
ATOM 3264 CA ALA A 416 -40.875 -11.638 -64.942 1.00 59.70 A
ATOM 3265 CB ALA A 416 -41.850 -12.729 -65.355 1.00 59.64 A
ATOM 3266 C ALA A 416 -39.982 -11.248 -66.115 1.00 58.20 A
ATOM 3267 O ALA A 416 -40.388 -11.338 -67.274 1.00 58.88 A
ATOM 3268 N ASP A 417 -38.764 -10.814 -65.807 1.00 55.91 A
ATOM 3269 CA ASP A 417 -37.804 -10.423 -66.838 1.00 53.90 A
ATOM 3270 CB ASP A 417 -37.966 -8.952 -67.139 1.00 53.38 A
ATOM 3271 CG ASP A 417 -37.997 -8.135 -65.886 1.00 53.91 A
ATOM 3272 OD1 ASP A 417 -39.050 -8.150 -65.195 1.00 54.73 A
ATOM 3273 OD2 ASP A 417 -36.960 -7.507 -65.580 1.00 54.90 A
ATOM 3274 C ASP A 417 -36.387 -10.659 -66.321 1.00 53.34 A
ATOM 3275 O ASP A 417 -36.203 -11.159 -65.207 1.00 54.14 A
ATOM 3276 N THR A 418 -35.390 -10.292 -67.126 1.00 51.46 A
ATOM 3277 CA THR A 418 -33.998 -10.480 -66.732 1.00 49.15 A
ATOM 3278 CB THR A 418 -33.029 -10.367 -67.938 1.00 47.43 A
ATOM 3279 OG1 THR A 418 -33.309 -9.166 -68.664 1.00 48.09 A
ATOM 3280 CG2 THR A 418 -33.170 -11.559 -68.861 1.00 47.09 A
ATOM 3281 C THR A 418 -33.588 -9.465 -65.678 1.00 48.82 A
ATOM 3282 O THR A 418 -33.194 -9.840 -64.575 1.00 48.64 A
ATOM 3283 N GLU A 419 -33.689 -8.183 -66.014 1.00 48.45 A
ATOM 3284 CA GLU A 419 -33.306 -7.126 -65.087 1.00 47.51 A
ATOM 3285 CB GLU A 419 -33.871 -5.777 -65.549 1.00 48.99 A
ATOM 3286 CG GLU A 419 -33.042 -5.123 -66.650 1.00 51.51 A
ATOM 3287 CD GLU A 419 -33.451 -3.684 -66.926 1.00 54.24 A
ATOM 3288 OE1 GLU A 419 -34.131 -3.079 -66.064 1.00 55.87 A
ATOM 3289 OE2 GLU A 419 -33.080 -3.152 -67.997 1.00 55.58 A
ATOM 3290 C GLU A 419 -33.725 -7.426 -63.649 1.00 45.73 A
ATOM 3291 O GLU A 419 -32.907 -7.382 -62.736 1.00 44.88 A
ATOM 3292 N SER A 420 -34.995 -7.739 -63.440 1.00 44.44 A
ATOM 3293 CA SER A 420 -35.446 -8.051 -62.097 1.00 43.27 A
ATOM 3294 CB SER A 420 -36.963 -8.244 -62.078 1.00 43.75 A

```
ATOM  3295  OG  SER A 420     -37.629  -7.024 -62.360  1.00 43.55      A
ATOM  3296  C   SER A 420     -34.736  -9.325 -61.643  1.00 42.24      A
ATOM  3297  O   SER A 420     -34.327  -9.441 -60.493  1.00 42.70      A
ATOM  3298  N   ASP A 421     -34.577 -10.267 -62.566  1.00 41.02      A
ATOM  3299  CA  ASP A 421     -33.921 -11.532 -62.277  1.00 40.29      A
ATOM  3300  CB  ASP A 421     -33.928 -12.412 -63.537  1.00 43.85      A
ATOM  3301  CG  ASP A 421     -33.562 -13.867 -63.249  1.00 47.18      A
ATOM  3302  OD1 ASP A 421     -34.019 -14.402 -62.210  1.00 49.21      A
ATOM  3303  OD2 ASP A 421     -32.830 -14.482 -64.069  1.00 48.36      A
ATOM  3304  C   ASP A 421     -32.496 -11.286 -61.778  1.00 38.50      A
ATOM  3305  O   ASP A 421     -32.072 -11.886 -60.791  1.00 38.87      A
ATOM  3306  N   ILE A 422     -31.759 -10.408 -62.456  1.00 35.45      A
ATOM  3307  CA  ILE A 422     -30.389 -10.066 -62.050  1.00 32.47      A
ATOM  3308  CB  ILE A 422     -29.726  -9.052 -63.065  1.00 31.16      A
ATOM  3309  CG2 ILE A 422     -28.496  -8.388 -62.457  1.00 29.04      A
ATOM  3310  CG1 ILE A 422     -29.326  -9.772 -64.352  1.00 27.41      A
ATOM  3311  CD1 ILE A 422     -28.151 -10.677 -64.201  1.00 26.09      A
ATOM  3312  C   ILE A 422     -30.412  -9.449 -60.640  1.00 31.94      A
ATOM  3313  O   ILE A 422     -29.665  -9.884 -59.768  1.00 32.22      A
ATOM  3314  N   ASN A 423     -31.268  -8.445 -60.422  1.00 30.22      A
ATOM  3315  CA  ASN A 423     -31.395  -7.796 -59.113  1.00 27.60      A
ATOM  3316  CB  ASN A 423     -32.623  -6.882 -59.056  1.00 26.15      A
ATOM  3317  CG  ASN A 423     -32.411  -5.552 -59.762  1.00 24.67      A
ATOM  3318  OD1 ASN A 423     -31.528  -4.775 -59.414  1.00 24.01      A
ATOM  3319  ND2 ASN A 423     -33.235  -5.285 -60.755  1.00 26.39      A
ATOM  3320  C   ASN A 423     -31.537  -8.845 -58.026  1.00 27.25      A
ATOM  3321  O   ASN A 423     -30.765  -8.860 -57.076  1.00 27.16      A
ATOM  3322  N   TYR A 424     -32.537  -9.712 -58.164  1.00 27.02      A
ATOM  3323  CA  TYR A 424     -32.759 -10.772 -57.191  1.00 29.02      A
ATOM  3324  CB  TYR A 424     -33.839 -11.753 -57.667  1.00 29.19      A
ATOM  3325  CG  TYR A 424     -33.965 -12.996 -56.796  1.00 29.82      A
ATOM  3326  CD1 TYR A 424     -34.273 -12.900 -55.431  1.00 30.39      A
ATOM  3327  CE1 TYR A 424     -34.339 -14.045 -54.614  1.00 30.56      A
ATOM  3328  CD2 TYR A 424     -33.732 -14.266 -57.324  1.00 30.81      A
```

ATOM 3329 CE2 TYR A 424 -33.795 -15.411 -56.521 1.00 31.64 A
ATOM 3330 CZ TYR A 424 -34.097 -15.296 -55.169 1.00 31.87 A
ATOM 3331 OH TYR A 424 -34.146 -16.434 -54.383 1.00 30.68 A
ATOM 3332 C TYR A 424 -31.469 -11.541 -56.929 1.00 30.18 A
ATOM 3333 O TYR A 424 -31.005 -11.627 -55.785 1.00 31.16 A
ATOM 3334 N LEU A 425 -30.892 -12.103 -57.986 1.00 29.73 A
ATOM 3335 CA LEU A 425 -29.661 -12.867 -57.852 1.00 28.67 A
ATOM 3336 CB LEU A 425 -29.203 -13.396 -59.216 1.00 28.70 A
ATOM 3337 CG LEU A 425 -29.818 -14.711 -59.683 1.00 26.91 A
ATOM 3338 CD1 LEU A 425 -29.093 -15.196 -60.929 1.00 28.16 A
ATOM 3339 CD2 LEU A 425 -29.693 -15.739 -58.577 1.00 27.02 A
ATOM 3340 C LEU A 425 -28.530 -12.081 -57.192 1.00 28.01 A
ATOM 3341 O LEU A 425 -27.731 -12.654 -56.449 1.00 27.72 A
ATOM 3342 N LEU A 426 -28.443 -10.780 -57.462 1.00 26.90 A
ATOM 3343 CA LEU A 426 -27.392 -9.995 -56.834 1.00 26.80 A
ATOM 3344 CB LEU A 426 -27.280 -8.594 -57.434 1.00 23.93 A
ATOM 3345 CG LEU A 426 -26.255 -7.783 -56.634 1.00 22.44 A
ATOM 3346 CD1 LEU A 426 -24.859 -8.146 -57.067 1.00 21.13 A
ATOM 3347 CD2 LEU A 426 -26.486 -6.317 -56.822 1.00 22.57 A
ATOM 3348 C LEU A 426 -27.698 -9.880 -55.343 1.00 27.65 A
ATOM 3349 O LEU A 426 -26.813 -10.047 -54.508 1.00 27.73 A
ATOM 3350 N LYS A 427 -28.953 -9.605 -55.003 1.00 29.51 A
ATOM 3351 CA LYS A 427 -29.315 -9.495 -53.595 1.00 30.79 A
ATOM 3352 CB LYS A 427 -30.822 -9.299 -53.407 1.00 31.88 A
ATOM 3353 CG LYS A 427 -31.125 -8.564 -52.111 1.00 33.97 A
ATOM 3354 CD LYS A 427 -32.565 -8.674 -51.676 1.00 36.42 A
ATOM 3355 CE LYS A 427 -32.721 -8.095 -50.272 1.00 38.43 A
ATOM 3356 NZ LYS A 427 -31.879 -8.808 -49.261 1.00 38.08 A
ATOM 3357 C LYS A 427 -28.874 -10.764 -52.873 1.00 30.16 A
ATOM 3358 O LYS A 427 -28.168 -10.689 -51.863 1.00 29.92 A
ATOM 3359 N MET A 428 -29.284 -11.923 -53.393 1.00 29.18 A
ATOM 3360 CA MET A 428 -28.899 -13.206 -52.807 1.00 29.18 A
ATOM 3361 CB MET A 428 -29.530 -14.361 -53.584 1.00 28.83 A
ATOM 3362 CG MET A 428 -31.039 -14.459 -53.461 1.00 30.84 A

ATOM 3363 SD MET A 428 -31.605 -14.982 -51.840 1.00 30.63 A
ATOM 3364 CE MET A 428 -31.200 -16.689 -51.913 1.00 31.50 A
ATOM 3365 C MET A 428 -27.376 -13.388 -52.797 1.00 29.60 A
ATOM 3366 O MET A 428 -26.837 -14.088 -51.947 1.00 29.55 A
ATOM 3367 N ALA A 429 -26.687 -12.762 -53.748 1.00 29.39 A
ATOM 3368 CA ALA A 429 -25.235 -12.861 -53.835 1.00 27.95 A
ATOM 3369 CB ALA A 429 -24.757 -12.285 -55.158 1.00 26.44 A
ATOM 3370 C ALA A 429 -24.603 -12.102 -52.674 1.00 28.08 A
ATOM 3371 O ALA A 429 -23.583 -12.520 -52.117 1.00 27.22 A
ATOM 3372 N LEU A 430 -25.217 -10.979 -52.318 1.00 27.70 A
ATOM 3373 CA LEU A 430 -24.734 -10.154 -51.227 1.00 27.41 A
ATOM 3374 CB LEU A 430 -25.547 -8.864 -51.139 1.00 25.13 A
ATOM 3375 CG LEU A 430 -25.372 -7.807 -52.223 1.00 22.90 A
ATOM 3376 CD1 LEU A 430 -26.216 -6.595 -51.873 1.00 21.30 A
ATOM 3377 CD2 LEU A 430 -23.914 -7.416 -52.330 1.00 22.15 A
ATOM 3378 C LEU A 430 -24.842 -10.906 -49.909 1.00 28.84 A
ATOM 3379 O LEU A 430 -24.035 -10.695 -49.006 1.00 28.53 A
ATOM 3380 N GLU A 431 -25.843 -11.780 -49.809 1.00 30.41 A
ATOM 3381 CA GLU A 431 -26.075 -12.575 -48.600 1.00 32.53 A
ATOM 3382 CB GLU A 431 -27.557 -12.948 -48.464 1.00 34.07 A
ATOM 3383 CG GLU A 431 -27.849 -13.840 -47.250 1.00 38.11 A
ATOM 3384 CD GLU A 431 -29.347 -14.056 -46.997 1.00 40.47 A
ATOM 3385 OE1 GLU A 431 -30.135 -13.105 -47.244 1.00 40.48 A
ATOM 3386 OE2 GLU A 431 -29.731 -15.166 -46.534 1.00 41.87 A
ATOM 3387 C GLU A 431 -25.256 -13.860 -48.512 1.00 32.79 A
ATOM 3388 O GLU A 431 -24.610 -14.115 -47.500 1.00 34.98 A
ATOM 3389 N LYS A 432 -25.281 -14.668 -49.565 1.00 32.40 A
ATOM 3390 CA LYS A 432 -24.564 -15.939 -49.562 1.00 30.94 A
ATOM 3391 CB LYS A 432 -25.350 -16.984 -50.372 1.00 31.16 A
ATOM 3392 CG LYS A 432 -26.856 -17.105 -50.041 1.00 32.62 A
ATOM 3393 CD LYS A 432 -27.144 -17.685 -48.660 1.00 34.17 A
ATOM 3394 CE LYS A 432 -28.650 -17.888 -48.447 1.00 35.49 A
ATOM 3395 NZ LYS A 432 -29.009 -18.228 -47.027 1.00 35.42 A
ATOM 3396 C LYS A 432 -23.122 -15.907 -50.066 1.00 29.30 A

ATOM 3397 O LYS A 432 -22.249 -16.523 -49.477 1.00 30.16 A
ATOM 3398 N ILE A 433 -22.860 -15.200 -51.152 1.00 28.39 A
ATOM 3399 CA ILE A 433 -21.507 -15.170 -51.696 1.00 27.71 A
ATOM 3400 CB ILE A 433 -21.472 -14.510 -53.098 1.00 27.80 A
ATOM 3401 CG2 ILE A 433 -20.043 -14.525 -53.650 1.00 27.34 A
ATOM 3402 CG1 ILE A 433 -22.422 -15.236 -54.049 1.00 26.64 A
ATOM 3403 CD1 ILE A 433 -22.099 -16.684 -54.250 1.00 24.29 A
ATOM 3404 C ILE A 433 -20.539 -14.412 -50.803 1.00 27.67 A
ATOM 3405 O ILE A 433 -19.449 -14.892 -50.498 1.00 28.26 A
ATOM 3406 N ALA A 434 -20.946 -13.214 -50.401 1.00 27.14 A
ATOM 3407 CA ALA A 434 -20.117 -12.351 -49.565 1.00 25.55 A
ATOM 3408 CB ALA A 434 -20.862 -11.034 -49.269 1.00 24.31 A
ATOM 3409 C ALA A 434 -19.694 -13.007 -48.263 1.00 24.09 A
ATOM 3410 O ALA A 434 -18.704 -12.604 -47.657 1.00 25.45 A
ATOM 3411 N PHE A 435 -20.440 -14.020 -47.842 1.00 22.38 A
ATOM 3412 CA PHE A 435 -20.175 -14.711 -46.593 1.00 21.70 A
ATOM 3413 CB PHE A 435 -21.469 -15.354 -46.085 1.00 22.37 A
ATOM 3414 CG PHE A 435 -21.334 -16.029 -44.752 1.00 24.26 A
ATOM 3415 CD1 PHE A 435 -21.473 -15.304 -43.570 1.00 26.04 A
ATOM 3416 CD2 PHE A 435 -21.036 -17.394 -44.675 1.00 24.68 A
ATOM 3417 CE1 PHE A 435 -21.314 -15.930 -42.316 1.00 27.05 A
ATOM 3418 CE2 PHE A 435 -20.875 -18.032 -43.443 1.00 25.53 A
ATOM 3419 CZ PHE A 435 -21.014 -17.295 -42.252 1.00 27.01 A
ATOM 3420 C PHE A 435 -19.089 -15.770 -46.710 1.00 20.54 A
ATOM 3421 O PHE A 435 -18.278 -15.945 -45.803 1.00 21.12 A
ATOM 3422 N LEU A 436 -19.071 -16.474 -47.832 1.00 20.28 A
ATOM 3423 CA LEU A 436 -18.108 -17.544 -48.057 1.00 19.96 A
ATOM 3424 CB LEU A 436 -18.047 -17.871 -49.545 1.00 21.67 A
ATOM 3425 CG LEU A 436 -19.382 -18.370 -50.068 1.00 22.94 A
ATOM 3426 CD1 LEU A 436 -19.192 -18.883 -51.484 1.00 25.86 A
ATOM 3427 CD2 LEU A 436 -19.908 -19.471 -49.166 1.00 21.18 A
ATOM 3428 C LEU A 436 -16.701 -17.291 -47.527 1.00 18.76 A
ATOM 3429 O LEU A 436 -16.159 -18.103 -46.764 1.00 16.27 A
ATOM 3430 N PRO A 437 -16.079 -16.172 -47.932 1.00 17.95 A

ATOM 3431 CD PRO A 437 -16.517 -14.990 -48.698 1.00 15.22 A
ATOM 3432 CA PRO A 437 -14.735 -15.984 -47.390 1.00 18.02 A
ATOM 3433 CB PRO A 437 -14.329 -14.609 -47.948 1.00 16.08 A
ATOM 3434 CG PRO A 437 -15.638 -13.907 -48.135 1.00 14.85 A
ATOM 3435 C PRO A 437 -14.736 -16.070 -45.846 1.00 18.39 A
ATOM 3436 O PRO A 437 -14.114 -16.964 -45.279 1.00 17.93 A
ATOM 3437 N PHE A 438 -15.462 -15.167 -45.187 1.00 18.36 A
ATOM 3438 CA PHE A 438 -15.548 -15.133 -43.729 1.00 20.27 A
ATOM 3439 CB PHE A 438 -16.668 -14.185 -43.297 1.00 20.49 A
ATOM 3440 CG PHE A 438 -16.686 -13.902 -41.818 1.00 22.05 A
ATOM 3441 CD1 PHE A 438 -15.652 -13.188 -41.221 1.00 22.96 A
ATOM 3442 CD2 PHE A 438 -17.739 -14.349 -41.023 1.00 22.81 A
ATOM 3443 CE1 PHE A 438 -15.667 -12.920 -39.857 1.00 25.14 A
ATOM 3444 CE2 PHE A 438 -17.767 -14.086 -39.650 1.00 24.16 A
ATOM 3445 CZ PHE A 438 -16.728 -13.369 -39.066 1.00 24.81 A
ATOM 3446 C PHE A 438 -15.785 -16.510 -43.099 1.00 20.79 A
ATOM 3447 O PHE A 438 -15.004 -16.964 -42.261 1.00 20.02 A
ATOM 3448 N GLY A 439 -16.872 -17.165 -43.490 1.00 21.12 A
ATOM 3449 CA GLY A 439 -17.163 -18.478 -42.949 1.00 21.27 A
ATOM 3450 C GLY A 439 -15.950 -19.398 -42.967 1.00 23.22 A
ATOM 3451 O GLY A 439 -15.722 -20.169 -42.033 1.00 26.53 A
ATOM 3452 N TYR A 440 -15.164 -19.325 -44.033 1.00 22.35 A
ATOM 3453 CA TYR A 440 -13.974 -20.155 -44.175 1.00 21.52 A
ATOM 3454 CB TYR A 440 -13.423 -19.998 -45.594 1.00 20.29 A
ATOM 3455 CG TYR A 440 -12.311 -20.952 -45.925 1.00 17.52 A
ATOM 3456 CD1 TYR A 440 -12.555 -22.316 -46.017 1.00 17.12 A
ATOM 3457 CE1 TYR A 440 -11.534 -23.211 -46.316 1.00 16.95 A
ATOM 3458 CD2 TYR A 440 -11.015 -20.494 -46.137 1.00 16.21 A
ATOM 3459 CE2 TYR A 440 -9.983 -21.378 -46.434 1.00 16.47 A
ATOM 3460 CZ TYR A 440 -10.250 -22.739 -46.523 1.00 16.21 A
ATOM 3461 OH TYR A 440 -9.249 -23.639 -46.811 1.00 12.39 A
ATOM 3462 C TYR A 440 -12.914 -19.721 -43.163 1.00 22.02 A
ATOM 3463 O TYR A 440 -12.441 -20.503 -42.341 1.00 22.67 A
ATOM 3464 N LEU A 441 -12.564 -18.447 -43.256 1.00 21.90 A

ATOM 3465 CA LEU A 441 -11.565 -17.775 -42.435 1.00 21.58 A
ATOM 3466 CB LEU A 441 -11.641 -16.284 -42.767 1.00 22.89 A
ATOM 3467 CG LEU A 441 -11.317 -15.166 -41.769 1.00 24.57 A
ATOM 3468 CD1 LEU A 441 -11.375 -13.869 -42.552 1.00 27.81 A
ATOM 3469 CD2 LEU A 441 -12.301 -15.091 -40.618 1.00 23.70 A
ATOM 3470 C LEU A 441 -11.577 -17.962 -40.906 1.00 21.14 A
ATOM 3471 O LEU A 441 -10.539 -18.244 -40.301 1.00 20.90 A
ATOM 3472 N VAL A 442 -12.740 -17.795 -40.283 1.00 19.63 A
ATOM 3473 CA VAL A 442 -12.846 -17.887 -38.833 1.00 18.48 A
ATOM 3474 CB VAL A 442 -14.314 -17.749 -38.385 1.00 16.57 A
ATOM 3475 CG1 VAL A 442 -14.452 -18.127 -36.923 1.00 15.46 A
ATOM 3476 CG2 VAL A 442 -14.780 -16.307 -38.599 1.00 14.72 A
ATOM 3477 C VAL A 442 -12.213 -19.117 -38.188 1.00 19.80 A
ATOM 3478 O VAL A 442 -11.294 -18.988 -37.368 1.00 19.92 A
ATOM 3479 N ASP A 443 -12.687 -20.305 -38.537 1.00 20.90 A
ATOM 3480 CA ASP A 443 -12.110 -21.494 -37.944 1.00 21.62 A
ATOM 3481 CB ASP A 443 -13.021 -22.689 -38.159 1.00 22.30 A
ATOM 3482 CG ASP A 443 -13.945 -22.930 -36.980 1.00 22.13 A
ATOM 3483 OD1 ASP A 443 -14.328 -21.951 -36.298 1.00 18.75 A
ATOM 3484 OD2 ASP A 443 -14.287 -24.110 -36.747 1.00 23.90 A
ATOM 3485 C ASP A 443 -10.727 -21.746 -38.505 1.00 22.11 A
ATOM 3486 O ASP A 443 -9.995 -22.603 -38.019 1.00 22.37 A
ATOM 3487 N GLN A 444 -10.375 -20.996 -39.542 1.00 23.37 A
ATOM 3488 CA GLN A 444 -9.042 -21.089 -40.118 1.00 24.45 A
ATOM 3489 CB GLN A 444 -8.935 -20.215 -41.374 1.00 27.22 A
ATOM 3490 CG GLN A 444 -9.581 -20.796 -42.616 1.00 31.23 A
ATOM 3491 CD GLN A 444 -8.948 -22.120 -42.998 1.00 34.10 A
ATOM 3492 OE1 GLN A 444 -7.725 -22.203 -43.199 1.00 36.11 A
ATOM 3493 NE2 GLN A 444 -9.772 -23.168 -43.092 1.00 33.25 A
ATOM 3494 C GLN A 444 -8.146 -20.504 -39.027 1.00 23.80 A
ATOM 3495 O GLN A 444 -7.129 -21.084 -38.636 1.00 22.44 A
ATOM 3496 N TRP A 445 -8.557 -19.336 -38.540 1.00 23.38 A
ATOM 3497 CA TRP A 445 -7.850 -18.623 -37.493 1.00 23.09 A
ATOM 3498 CB TRP A 445 -8.567 -17.307 -37.185 1.00 22.16 A

```
ATOM  3499  CG  TRP A 445     -7.989 -16.574 -36.004  1.00 22.85      A
ATOM  3500  CD2 TRP A 445     -8.513 -16.544 -34.658  1.00 23.14      A
ATOM  3501  CE2 TRP A 445     -7.630 -15.762 -33.884  1.00 22.08      A
ATOM  3502  CE3 TRP A 445     -9.640 -17.104 -34.036  1.00 22.69      A
ATOM  3503  CD1 TRP A 445     -6.848 -15.831 -35.984  1.00 22.23      A
ATOM  3504  NE1 TRP A 445     -6.626 -15.340 -34.714  1.00 22.96      A
ATOM  3505  CZ2 TRP A 445     -7.836 -15.522 -32.521  1.00 20.49      A
ATOM  3506  CZ3 TRP A 445     -9.846 -16.866 -32.679  1.00 21.70      A
ATOM  3507  CH2 TRP A 445     -8.948 -16.082 -31.937  1.00 20.61      A
ATOM  3508  C   TRP A 445     -7.788 -19.463 -36.223  1.00 23.41      A
ATOM  3509  O   TRP A 445     -6.710 -19.633 -35.634  1.00 24.33      A
ATOM  3510  N   ARG A 446     -8.943 -19.987 -35.813  1.00 21.70      A
ATOM  3511  CA  ARG A 446     -9.036 -20.779 -34.592  1.00 20.79      A
ATOM  3512  CB  ARG A 446    -10.490 -21.064 -34.230  1.00 21.22      A
ATOM  3513  CG  ARG A 446    -10.929 -20.327 -33.005  1.00 21.94      A
ATOM  3514  CD  ARG A 446    -12.220 -20.853 -32.456  1.00 23.12      A
ATOM  3515  NE  ARG A 446    -13.324 -20.718 -33.396  1.00 25.87      A
ATOM  3516  CZ  ARG A 446    -14.598 -20.602 -33.025  1.00 28.25      A
ATOM  3517  NH1 ARG A 446    -14.923 -20.602 -31.731  1.00 31.49      A
ATOM  3518  NH2 ARG A 446    -15.550 -20.489 -33.936  1.00 28.83      A
ATOM  3519  C   ARG A 446     -8.276 -22.083 -34.546  1.00 21.40      A
ATOM  3520  O   ARG A 446     -7.632 -22.357 -33.547  1.00 21.39      A
ATOM  3521  N   TRP A 447     -8.350 -22.898 -35.595  1.00 21.41      A
ATOM  3522  CA  TRP A 447     -7.629 -24.167 -35.561  1.00 21.71      A
ATOM  3523  CB  TRP A 447     -7.742 -24.934 -36.891  1.00 24.23      A
ATOM  3524  CG  TRP A 447     -9.111 -25.409 -37.242  1.00 25.09      A
ATOM  3525  CD2 TRP A 447     -9.606 -25.669 -38.554  1.00 26.47      A
ATOM  3526  CE2 TRP A 447    -10.948 -26.090 -38.421  1.00 27.09      A
ATOM  3527  CE3 TRP A 447     -9.046 -25.586 -39.836  1.00 26.63      A
ATOM  3528  CD1 TRP A 447    -10.135 -25.679 -36.386  1.00 26.21      A
ATOM  3529  NE1 TRP A 447    -11.250 -26.088 -37.085  1.00 27.08      A
ATOM  3530  CZ2 TRP A 447    -11.740 -26.422 -39.520  1.00 27.29      A
ATOM  3531  CZ3 TRP A 447     -9.833 -25.915 -40.929  1.00 26.72      A
ATOM  3532  CH2 TRP A 447    -11.168 -26.327 -40.763  1.00 27.26      A
```

ATOM 3533 C TRP A 447 -6.167 -23.899 -35.276 1.00 20.17 A
ATOM 3534 O TRP A 447 -5.471 -24.736 -34.703 1.00 19.06 A
ATOM 3535 N GLY A 448 -5.719 -22.720 -35.688 1.00 19.58 A
ATOM 3536 CA GLY A 448 -4.340 -22.318 -35.494 1.00 20.58 A
ATOM 3537 C GLY A 448 -4.038 -21.785 -34.104 1.00 21.48 A
ATOM 3538 O GLY A 448 -2.888 -21.836 -33.655 1.00 21.72 A
ATOM 3539 N VAL A 449 -5.054 -21.248 -33.430 1.00 21.03 A
ATOM 3540 CA VAL A 449 -4.874 -20.754 -32.075 1.00 20.32 A
ATOM 3541 CB VAL A 449 -6.068 -19.902 -31.609 1.00 21.00 A
ATOM 3542 CG1 VAL A 449 -5.955 -19.631 -30.115 1.00 21.02 A
ATOM 3543 CG2 VAL A 449 -6.110 -18.595 -32.376 1.00 19.62 A
ATOM 3544 C VAL A 449 -4.787 -21.974 -31.177 1.00 19.42 A
ATOM 3545 O VAL A 449 -3.926 -22.061 -30.314 1.00 19.23 A
ATOM 3546 N PHE A 450 -5.701 -22.908 -31.403 1.00 19.35 A
ATOM 3547 CA PHE A 450 -5.779 -24.154 -30.648 1.00 20.25 A
ATOM 3548 CB PHE A 450 -6.993 -24.984 -31.090 1.00 20.48 A
ATOM 3549 CG PHE A 450 -8.288 -24.573 -30.457 1.00 20.63 A
ATOM 3550 CD1 PHE A 450 -9.445 -24.500 -31.212 1.00 21.06 A
ATOM 3551 CD2 PHE A 450 -8.365 -24.301 -29.098 1.00 21.32 A
ATOM 3552 CE1 PHE A 450 -10.660 -24.164 -30.618 1.00 21.58 A
ATOM 3553 CE2 PHE A 450 -9.580 -23.964 -28.503 1.00 20.59 A
ATOM 3554 CZ PHE A 450 -10.721 -23.898 -29.262 1.00 19.68 A
ATOM 3555 C PHE A 450 -4.546 -25.007 -30.847 1.00 21.17 A
ATOM 3556 O PHE A 450 -4.212 -25.823 -29.989 1.00 21.95 A
ATOM 3557 N SER A 451 -3.875 -24.841 -31.982 1.00 21.31 A
ATOM 3558 CA SER A 451 -2.689 -25.646 -32.259 1.00 22.22 A
ATOM 3559 CB SER A 451 -2.649 -26.060 -33.730 1.00 22.35 A
ATOM 3560 OG SER A 451 -2.021 -25.074 -34.536 1.00 25.87 A
ATOM 3561 C SER A 451 -1.388 -24.947 -31.902 1.00 22.43 A
ATOM 3562 O SER A 451 -0.333 -25.574 -31.894 1.00 23.31 A
ATOM 3563 N GLY A 452 -1.456 -23.652 -31.623 1.00 22.54 A
ATOM 3564 CA GLY A 452 -0.251 -22.929 -31.266 1.00 24.09 A
ATOM 3565 C GLY A 452 0.463 -22.228 -32.402 1.00 26.41 A
ATOM 3566 O GLY A 452 1.543 -21.686 -32.201 1.00 27.59 A

ATOM 3567 N ARG A 453 -0.182 -22.037 -33.498 1.00 28.87 A
ATOM 3568 CA ARG A 453 0.506 -21.502 -34.599 1.00 31.83 A
ATOM 3569 CB ARG A 453 0.004 -22.197 -35.842 1.00 34.80 A
ATOM 3570 CG ARG A 453 -0.023 -21.387 -37.106 1.00 39.04 A
ATOM 3571 CD ARG A 453 -1.380 -21.323 -37.750 1.00 42.67 A
ATOM 3572 NE ARG A 453 -1.460 -21.864 -39.073 1.00 47.08 A
ATOM 3573 CZ ARG A 453 -2.539 -22.362 -39.625 1.00 47.43 A
ATOM 3574 NH1 ARG A 453 -3.674 -22.416 -38.977 1.00 46.12 A
ATOM 3575 NH2 ARG A 453 -2.465 -22.771 -40.877 1.00 47.15 A
ATOM 3576 C ARG A 453 0.163 -20.088 -34.590 1.00 31.42 A
ATOM 3577 O ARG A 453 0.751 -19.262 -35.226 1.00 31.97 A
ATOM 3578 N THR A 454 -0.817 -19.817 -33.793 1.00 30.21 A
ATOM 3579 CA THR A 454 -1.213 -18.453 -33.499 1.00 30.22 A
ATOM 3580 CB THR A 454 -2.576 -18.101 -34.141 1.00 31.51 A
ATOM 3581 OG1 THR A 454 -2.502 -18.244 -35.569 1.00 32.11 A
ATOM 3582 CG2 THR A 454 -2.959 -16.658 -33.792 1.00 31.46 A
ATOM 3583 C THR A 454 -1.309 -18.234 -31.985 1.00 28.81 A
ATOM 3584 O THR A 454 -2.381 -18.394 -31.393 1.00 30.11 A
ATOM 3585 N PRO A 455 -0.179 -17.891 -31.334 1.00 26.25 A
ATOM 3586 CD PRO A 455 1.185 -17.833 -31.892 1.00 24.90 A
ATOM 3587 CA PRO A 455 -0.157 -17.648 -29.889 1.00 24.44 A
ATOM 3588 CB PRO A 455 1.329 -17.645 -29.571 1.00 25.03 A
ATOM 3589 CG PRO A 455 1.936 -17.101 -30.822 1.00 23.84 A
ATOM 3590 C PRO A 455 -0.812 -16.300 -29.608 1.00 22.90 A
ATOM 3591 O PRO A 455 -1.032 -15.515 -30.520 1.00 22.71 A
ATOM 3592 N PRO A 456 -1.131 -16.006 -28.344 1.00 22.53 A
ATOM 3593 CD PRO A 456 -1.051 -16.811 -27.118 1.00 21.88 A
ATOM 3594 CA PRO A 456 -1.763 -14.711 -28.073 1.00 22.90 A
ATOM 3595 CB PRO A 456 -1.946 -14.743 -26.562 1.00 21.95 A
ATOM 3596 CG PRO A 456 -2.126 -16.194 -26.284 1.00 20.73 A
ATOM 3597 C PRO A 456 -0.915 -13.527 -28.550 1.00 23.24 A
ATOM 3598 O PRO A 456 -1.393 -12.396 -28.678 1.00 22.92 A
ATOM 3599 N SER A 457 0.352 -13.806 -28.822 1.00 22.64 A
ATOM 3600 CA SER A 457 1.263 -12.780 -29.275 1.00 22.95 A

ATOM 3601 CB SER A 457 2.713 -13.262 -29.150 1.00 23.24 A
ATOM 3602 OG SER A 457 3.032 -14.239 -30.125 1.00 26.16 A
ATOM 3603 C SER A 457 0.963 -12.382 -30.713 1.00 22.84 A
ATOM 3604 O SER A 457 1.475 -11.366 -31.186 1.00 23.98 A
ATOM 3605 N ARG A 458 0.140 -13.184 -31.398 1.00 22.74 A
ATOM 3606 CA ARG A 458 -0.256 -12.919 -32.801 1.00 22.56 A
ATOM 3607 CB ARG A 458 0.465 -13.857 -33.779 1.00 21.47 A
ATOM 3608 CG ARG A 458 1.976 -13.767 -33.757 1.00 20.43 A
ATOM 3609 CD ARG A 458 2.589 -14.587 -34.873 1.00 19.60 A
ATOM 3610 NE ARG A 458 3.838 -15.191 -34.445 1.00 17.93 A
ATOM 3611 CZ ARG A 458 4.002 -16.489 -34.229 1.00 18.97 A
ATOM 3612 NH1 ARG A 458 2.994 -17.332 -34.404 1.00 19.09 A
ATOM 3613 NH2 ARG A 458 5.177 -16.945 -33.834 1.00 20.45 A
ATOM 3614 C ARG A 458 -1.758 -13.062 -33.047 1.00 21.81 A
ATOM 3615 O ARG A 458 -2.187 -13.262 -34.175 1.00 20.92 A
ATOM 3616 N TYR A 459 -2.551 -12.955 -31.991 1.00 22.24 A
ATOM 3617 CA TYR A 459 -3.993 -13.083 -32.121 1.00 22.70 A
ATOM 3618 CB TYR A 459 -4.681 -12.850 -30.765 1.00 24.47 A
ATOM 3619 CG TYR A 459 -4.814 -14.075 -29.874 1.00 24.77 A
ATOM 3620 CD1 TYR A 459 -5.664 -14.062 -28.768 1.00 24.45 A
ATOM 3621 CE1 TYR A 459 -5.790 -15.168 -27.937 1.00 24.34 A
ATOM 3622 CD2 TYR A 459 -4.091 -15.238 -30.125 1.00 26.41 A
ATOM 3623 CE2 TYR A 459 -4.213 -16.348 -29.298 1.00 26.68 A
ATOM 3624 CZ TYR A 459 -5.064 -16.305 -28.204 1.00 25.83 A
ATOM 3625 OH TYR A 459 -5.172 -17.404 -27.375 1.00 29.52 A
ATOM 3626 C TYR A 459 -4.578 -12.113 -33.143 1.00 22.65 A
ATOM 3627 O TYR A 459 -5.332 -12.521 -34.028 1.00 22.41 A
ATOM 3628 N ASN A 460 -4.248 -10.828 -33.024 1.00 21.50 A
ATOM 3629 CA ASN A 460 -4.804 -9.852 -33.950 1.00 20.16 A
ATOM 3630 CB ASN A 460 -4.844 -8.464 -33.318 1.00 19.14 A
ATOM 3631 CG ASN A 460 -6.166 -7.756 -33.570 1.00 19.69 A
ATOM 3632 OD1 ASN A 460 -7.239 -8.321 -33.326 1.00 18.65 A
ATOM 3633 ND2 ASN A 460 -6.100 -6.520 -34.059 1.00 19.97 A
ATOM 3634 C ASN A 460 -4.058 -9.798 -35.266 1.00 19.78 A

ATOM 3635 O ASN A 460 -4.660 -9.607 -36.323 1.00 21.02 A
ATOM 3636 N PHE A 461 -2.749 -9.981 -35.210 1.00 17.97 A
ATOM 3637 CA PHE A 461 -1.955 -9.954 -36.408 1.00 15.62 A
ATOM 3638 CB PHE A 461 -0.495 -9.957 -36.032 1.00 16.13 A
ATOM 3639 CG PHE A 461 0.425 -10.351 -37.133 1.00 16.86 A
ATOM 3640 CD1 PHE A 461 0.837 -11.673 -37.266 1.00 17.09 A
ATOM 3641 CD2 PHE A 461 0.964 -9.397 -37.978 1.00 18.04 A
ATOM 3642 CE1 PHE A 461 1.776 -12.038 -38.210 1.00 17.01 A
ATOM 3643 CE2 PHE A 461 1.912 -9.755 -38.934 1.00 18.08 A
ATOM 3644 CZ PHE A 461 2.321 -11.074 -39.049 1.00 17.61 A
ATOM 3645 C PHE A 461 -2.296 -11.117 -37.306 1.00 16.41 A
ATOM 3646 O PHE A 461 -2.204 -10.979 -38.512 1.00 19.34 A
ATOM 3647 N ASP A 462 -2.698 -12.262 -36.755 1.00 16.99 A
ATOM 3648 CA ASP A 462 -3.056 -13.395 -37.624 1.00 18.19 A
ATOM 3649 CB ASP A 462 -2.724 -14.753 -36.977 1.00 19.47 A
ATOM 3650 CG ASP A 462 -1.301 -15.203 -37.265 1.00 20.73 A
ATOM 3651 OD1 ASP A 462 -0.629 -14.525 -38.064 1.00 22.71 A
ATOM 3652 OD2 ASP A 462 -0.849 -16.229 -36.706 1.00 21.37 A
ATOM 3653 C ASP A 462 -4.529 -13.355 -38.035 1.00 18.57 A
ATOM 3654 O ASP A 462 -4.939 -14.029 -38.987 1.00 18.85 A
ATOM 3655 N TRP A 463 -5.321 -12.562 -37.319 1.00 17.77 A
ATOM 3656 CA TRP A 463 -6.734 -12.408 -37.640 1.00 16.92 A
ATOM 3657 CB TRP A 463 -7.486 -11.829 -36.432 1.00 14.22 A
ATOM 3658 CG TRP A 463 -8.936 -11.401 -36.665 1.00 10.02 A
ATOM 3659 CD2 TRP A 463 -10.092 -12.253 -36.711 1.00 9.24 A
ATOM 3660 CE2 TRP A 463 -11.224 -11.414 -36.833 1.00 8.76 A
ATOM 3661 CE3 TRP A 463 -10.281 -13.645 -36.657 1.00 9.71 A
ATOM 3662 CD1 TRP A 463 -9.406 -10.122 -36.770 1.00 9.37 A
ATOM 3663 NE1 TRP A 463 -10.773 -10.121 -36.865 1.00 9.69 A
ATOM 3664 CZ2 TRP A 463 -12.526 -11.914 -36.896 1.00 8.90 A
ATOM 3665 CZ3 TRP A 463 -11.577 -14.145 -36.722 1.00 10.56 A
ATOM 3666 CH2 TRP A 463 -12.684 -13.277 -36.839 1.00 11.27 A
ATOM 3667 C TRP A 463 -6.858 -11.490 -38.855 1.00 17.54 A
ATOM 3668 O TRP A 463 -7.564 -11.799 -39.796 1.00 18.14 A

```
ATOM   3669  N   TRP A 464     -6.165 -10.360 -38.849  1.00 19.35      A
ATOM   3670  CA  TRP A 464     -6.255  -9.464 -39.998  1.00 21.50      A
ATOM   3671  CB  TRP A 464     -5.818  -8.050 -39.620  1.00 22.37      A
ATOM   3672  CG  TRP A 464     -6.867  -7.391 -38.799  1.00 25.27      A
ATOM   3673  CD2 TRP A 464     -8.082  -6.818 -39.287  1.00 27.31      A
ATOM   3674  CE2 TRP A 464     -8.855  -6.457 -38.161  1.00 27.82      A
ATOM   3675  CE3 TRP A 464     -8.595  -6.577 -40.571  1.00 28.49      A
ATOM   3676  CD1 TRP A 464     -6.944  -7.346 -37.433  1.00 25.51      A
ATOM   3677  NE1 TRP A 464     -8.136  -6.790 -37.043  1.00 26.13      A
ATOM   3678  CZ2 TRP A 464    -10.118  -5.867 -38.278  1.00 29.60      A
ATOM   3679  CZ3 TRP A 464     -9.851  -5.988 -40.691  1.00 29.45      A
ATOM   3680  CH2 TRP A 464    -10.598  -5.640 -39.548  1.00 30.76      A
ATOM   3681  C   TRP A 464     -5.470  -9.988 -41.199  1.00 22.46      A
ATOM   3682  O   TRP A 464     -5.627  -9.504 -42.328  1.00 22.21      A
ATOM   3683  N   TYR A 465     -4.613 -10.977 -40.968  1.00 21.92      A
ATOM   3684  CA  TYR A 465     -3.908 -11.565 -42.089  1.00 20.47      A
ATOM   3685  CB  TYR A 465     -2.855 -12.574 -41.628  1.00 21.55      A
ATOM   3686  CG  TYR A 465     -2.345 -13.418 -42.773  1.00 23.60      A
ATOM   3687  CD1 TYR A 465     -1.445 -12.904 -43.707  1.00 23.50      A
ATOM   3688  CE1 TYR A 465     -1.045 -13.653 -44.819  1.00 25.30      A
ATOM   3689  CD2 TYR A 465     -2.832 -14.708 -42.979  1.00 25.25      A
ATOM   3690  CE2 TYR A 465     -2.448 -15.458 -44.089  1.00 27.28      A
ATOM   3691  CZ  TYR A 465     -1.555 -14.927 -45.006  1.00 26.75      A
ATOM   3692  OH  TYR A 465     -1.198 -15.671 -46.112  1.00 27.23      A
ATOM   3693  C   TYR A 465     -5.025 -12.300 -42.839  1.00 19.15      A
ATOM   3694  O   TYR A 465     -5.264 -12.078 -44.024  1.00 19.77      A
ATOM   3695  N   LEU A 466     -5.736 -13.153 -42.114  1.00 16.19      A
ATOM   3696  CA  LEU A 466     -6.807 -13.934 -42.706  1.00 14.96      A
ATOM   3697  CB  LEU A 466     -7.356 -14.937 -41.683  1.00 12.13      A
ATOM   3698  CG  LEU A 466     -6.351 -15.981 -41.208  1.00 10.49      A
ATOM   3699  CD1 LEU A 466     -7.035 -16.923 -40.276  1.00 11.32      A
ATOM   3700  CD2 LEU A 466     -5.790 -16.751 -42.382  1.00  9.40      A
ATOM   3701  C   LEU A 466     -7.941 -13.117 -43.292  1.00 15.16      A
ATOM   3702  O   LEU A 466     -8.439 -13.451 -44.353  1.00 16.26      A
```

```
ATOM  3703  N   ARG A 467     -8.344 -12.053 -42.604  1.00 16.10      A
ATOM  3704  CA  ARG A 467     -9.444 -11.194 -43.058  1.00 16.29      A
ATOM  3705  CB  ARG A 467     -9.795 -10.167 -41.980  1.00 16.59      A
ATOM  3706  CG  ARG A 467    -10.258 -10.788 -40.674  1.00 16.94      A
ATOM  3707  CD  ARG A 467    -11.777 -10.847 -40.567  1.00 19.18      A
ATOM  3708  NE  ARG A 467    -12.389  -9.513 -40.595  1.00 20.42      A
ATOM  3709  CZ  ARG A 467    -13.687  -9.268 -40.433  1.00 19.37      A
ATOM  3710  NH1 ARG A 467    -14.127  -8.025 -40.482  1.00 19.86      A
ATOM  3711  NH2 ARG A 467    -14.544 -10.258 -40.211  1.00 18.20      A
ATOM  3712  C   ARG A 467     -9.076 -10.486 -44.353  1.00 17.10      A
ATOM  3713  O   ARG A 467     -9.831 -10.534 -45.327  1.00 18.11      A
ATOM  3714  N   THR A 468     -7.918  -9.832 -44.374  1.00 17.19      A
ATOM  3715  CA  THR A 468     -7.486  -9.159 -45.590  1.00 17.27      A
ATOM  3716  CB  THR A 468     -6.098  -8.478 -45.438  1.00 16.69      A
ATOM  3717  OG1 THR A 468     -6.202  -7.317 -44.594  1.00 15.44      A
ATOM  3718  CG2 THR A 468     -5.565  -8.058 -46.806  1.00 14.50      A
ATOM  3719  C   THR A 468     -7.392 -10.233 -46.667  1.00 18.27      A
ATOM  3720  O   THR A 468     -8.063 -10.142 -47.699  1.00 20.61      A
ATOM  3721  N   LYS A 469     -6.585 -11.262 -46.403  1.00 17.40      A
ATOM  3722  CA  LYS A 469     -6.392 -12.354 -47.347  1.00 15.93      A
ATOM  3723  CB  LYS A 469     -5.616 -13.505 -46.705  1.00 14.24      A
ATOM  3724  CG  LYS A 469     -5.509 -14.715 -47.625  1.00 12.48      A
ATOM  3725  CD  LYS A 469     -4.649 -15.828 -47.059  1.00 11.60      A
ATOM  3726  CE  LYS A 469     -4.944 -17.116 -47.805  1.00 12.05      A
ATOM  3727  NZ  LYS A 469     -3.917 -18.181 -47.635  1.00 13.38      A
ATOM  3728  C   LYS A 469     -7.647 -12.923 -47.975  1.00 16.31      A
ATOM  3729  O   LYS A 469     -7.688 -13.124 -49.170  1.00 18.59      A
ATOM  3730  N   TYR A 470     -8.676 -13.196 -47.192  1.00 17.11      A
ATOM  3731  CA  TYR A 470     -9.874 -13.780 -47.783  1.00 18.71      A
ATOM  3732  CB  TYR A 470    -10.441 -14.897 -46.894  1.00 17.17      A
ATOM  3733  CG  TYR A 470     -9.572 -16.132 -46.842  1.00 17.88      A
ATOM  3734  CD1 TYR A 470     -8.549 -16.250 -45.905  1.00 17.58      A
ATOM  3735  CE1 TYR A 470     -7.721 -17.365 -45.892  1.00 18.02      A
ATOM  3736  CD2 TYR A 470     -9.744 -17.170 -47.765  1.00 16.98      A
```

ATOM 3737 CE2 TYR A 470 -8.923 -18.289 -47.757 1.00 14.63 A
ATOM 3738 CZ TYR A 470 -7.916 -18.381 -46.821 1.00 16.45 A
ATOM 3739 OH TYR A 470 -7.099 -19.489 -46.794 1.00 18.19 A
ATOM 3740 C TYR A 470 -10.986 -12.803 -48.132 1.00 20.06 A
ATOM 3741 O TYR A 470 -11.574 -12.907 -49.208 1.00 22.88 A
ATOM 3742 N GLN A 471 -11.281 -11.857 -47.249 1.00 18.91 A
ATOM 3743 CA GLN A 471 -12.348 -10.917 -47.545 1.00 18.37 A
ATOM 3744 CB GLN A 471 -13.053 -10.512 -46.254 1.00 19.72 A
ATOM 3745 CG GLN A 471 -14.005 -11.593 -45.753 1.00 23.55 A
ATOM 3746 CD GLN A 471 -14.758 -11.204 -44.495 1.00 25.32 A
ATOM 3747 OE1 GLN A 471 -14.180 -11.125 -43.409 1.00 23.98 A
ATOM 3748 NE2 GLN A 471 -16.056 -10.953 -44.638 1.00 26.86 A
ATOM 3749 C GLN A 471 -11.900 -9.678 -48.319 1.00 17.38 A
ATOM 3750 O GLN A 471 -12.706 -9.039 -49.003 1.00 15.73 A
ATOM 3751 N GLY A 472 -10.615 -9.353 -48.241 1.00 15.54 A
ATOM 3752 CA GLY A 472 -10.143 -8.175 -48.930 1.00 16.10 A
ATOM 3753 C GLY A 472 -10.736 -6.939 -48.284 1.00 16.73 A
ATOM 3754 O GLY A 472 -11.252 -6.019 -48.935 1.00 14.53 A
ATOM 3755 N ILE A 473 -10.681 -6.947 -46.961 1.00 18.68 A
ATOM 3756 CA ILE A 473 -11.172 -5.842 -46.169 1.00 18.10 A
ATOM 3757 CB ILE A 473 -12.436 -6.216 -45.398 1.00 17.35 A
ATOM 3758 CG2 ILE A 473 -13.540 -6.551 -46.370 1.00 17.73 A
ATOM 3759 CG1 ILE A 473 -12.158 -7.402 -44.478 1.00 17.91 A
ATOM 3760 CD1 ILE A 473 -13.266 -7.654 -43.427 1.00 17.89 A
ATOM 3761 C ILE A 473 -10.078 -5.498 -45.186 1.00 18.37 A
ATOM 3762 O ILE A 473 -9.259 -6.344 -44.815 1.00 18.23 A
ATOM 3763 N CYS A 474 -10.049 -4.245 -44.775 1.00 17.91 A
ATOM 3764 CA CYS A 474 -9.052 -3.817 -43.830 1.00 17.96 A
ATOM 3765 CB CYS A 474 -7.982 -3.010 -44.549 1.00 18.69 A
ATOM 3766 SG CYS A 474 -8.596 -1.500 -45.248 1.00 22.40 A
ATOM 3767 C CYS A 474 -9.732 -2.987 -42.741 1.00 17.38 A
ATOM 3768 O CYS A 474 -10.836 -2.473 -42.941 1.00 15.98 A
ATOM 3769 N PRO A 475 -9.091 -2.880 -41.560 1.00 17.21 A
ATOM 3770 CD PRO A 475 -7.790 -3.513 -41.265 1.00 16.36 A

ATOM 3771 CA PRO A 475 -9.567 -2.135 -40.391 1.00 16.16 A
ATOM 3772 CB PRO A 475 -8.580 -2.553 -39.307 1.00 16.23 A
ATOM 3773 CG PRO A 475 -7.321 -2.741 -40.078 1.00 15.68 A
ATOM 3774 C PRO A 475 -9.548 -0.637 -40.648 1.00 15.46 A
ATOM 3775 O PRO A 475 -8.561 -0.106 -41.140 1.00 15.04 A
ATOM 3776 N PRO A 476 -10.642 0.060 -40.324 1.00 15.80 A
ATOM 3777 CD PRO A 476 -11.945 -0.501 -39.940 1.00 16.17 A
ATOM 3778 CA PRO A 476 -10.741 1.510 -40.529 1.00 16.16 A
ATOM 3779 CB PRO A 476 -12.229 1.789 -40.312 1.00 15.24 A
ATOM 3780 CG PRO A 476 -12.652 0.704 -39.399 1.00 17.52 A
ATOM 3781 C PRO A 476 -9.831 2.384 -39.663 1.00 16.09 A
ATOM 3782 O PRO A 476 -9.530 3.520 -40.025 1.00 17.93 A
ATOM 3783 N VAL A 477 -9.409 1.853 -38.520 1.00 15.57 A
ATOM 3784 CA VAL A 477 -8.506 2.546 -37.607 1.00 15.66 A
ATOM 3785 CB VAL A 477 -9.182 2.885 -36.273 1.00 12.96 A
ATOM 3786 CG1 VAL A 477 -10.222 3.957 -36.473 1.00 11.95 A
ATOM 3787 CG2 VAL A 477 -9.814 1.645 -35.695 1.00 13.14 A
ATOM 3788 C VAL A 477 -7.376 1.561 -37.346 1.00 18.07 A
ATOM 3789 O VAL A 477 -7.545 0.361 -37.579 1.00 18.65 A
ATOM 3790 N THR A 478 -6.233 2.044 -36.867 1.00 20.51 A
ATOM 3791 CA THR A 478 -5.091 1.165 -36.615 1.00 22.21 A
ATOM 3792 CB THR A 478 -3.849 1.970 -36.248 1.00 22.13 A
ATOM 3793 OG1 THR A 478 -3.673 3.027 -37.202 1.00 23.83 A
ATOM 3794 CG2 THR A 478 -2.617 1.073 -36.269 1.00 22.49 A
ATOM 3795 C THR A 478 -5.369 0.167 -35.500 1.00 23.29 A
ATOM 3796 O THR A 478 -6.208 -0.432 -34.641 1.00 25.09 A
ATOM 3797 N ARG A 479 -4.682 -0.980 -35.526 1.00 23.91 A
ATOM 3798 CA ARG A 479 -4.856 -2.026 -34.506 1.00 25.43 A
ATOM 3799 CB ARG A 479 -5.751 -3.166 -35.021 1.00 26.26 A
ATOM 3800 CG ARG A 479 -6.837 -2.784 -36.036 1.00 25.49 A
ATOM 3801 CD ARG A 479 -7.930 -1.981 -35.383 1.00 25.49 A
ATOM 3802 NE ARG A 479 -8.647 -2.732 -34.351 1.00 24.68 A
ATOM 3803 CZ ARG A 479 -9.124 -2.188 -33.234 1.00 23.89 A
ATOM 3804 NH1 ARG A 479 -8.953 -0.891 -32.986 1.00 23.48 A

ATOM 3805 NH2 ARG A 479 -9.804 -2.929 -32.386 1.00 23.53 A
ATOM 3806 C ARG A 479 -3.499 -2.626 -34.111 1.00 26.31 A
ATOM 3807 O ARG A 479 -2.512 -2.491 -34.838 1.00 25.83 A
ATOM 3808 N ASN A 480 -3.477 -3.145 -32.891 1.00 27.66 A
ATOM 3809 CA ASN A 480 -2.369 -3.838 -32.282 1.00 29.08 A
ATOM 3810 CB ASN A 480 -1.521 -2.922 -31.467 1.00 30.24 A
ATOM 3811 CG ASN A 480 -2.241 -1.804 -30.920 1.00 32.70 A
ATOM 3812 OD1 ASN A 480 -3.160 -1.968 -30.239 1.00 34.75 A
ATOM 3813 ND2 ASN A 480 -1.783 -0.631 -31.175 1.00 34.84 A
ATOM 3814 C ASN A 480 -2.597 -5.099 -31.512 1.00 30.15 A
ATOM 3815 O ASN A 480 -3.677 -5.407 -31.267 1.00 30.54 A
ATOM 3816 N GLU A 481 -1.593 -5.786 -31.105 1.00 30.84 A
ATOM 3817 CA GLU A 481 -1.869 -6.885 -30.273 1.00 31.75 A
ATOM 3818 CB GLU A 481 -0.639 -7.692 -30.101 1.00 30.91 A
ATOM 3819 CG GLU A 481 -0.277 -8.612 -31.210 1.00 32.71 A
ATOM 3820 CD GLU A 481 -1.396 -9.356 -31.756 1.00 34.29 A
ATOM 3821 OE1 GLU A 481 -1.246 -9.789 -32.845 1.00 34.23 A
ATOM 3822 OE2 GLU A 481 -2.401 -9.534 -31.151 1.00 34.75 A
ATOM 3823 C GLU A 481 -2.315 -6.420 -28.935 1.00 32.11 A
ATOM 3824 O GLU A 481 -1.839 -6.896 -27.996 1.00 34.79 A
ATOM 3825 N THR A 482 -3.218 -5.498 -28.818 1.00 31.25 A
ATOM 3826 CA THR A 482 -3.813 -5.277 -27.560 1.00 30.63 A
ATOM 3827 CB THR A 482 -3.519 -3.972 -27.024 1.00 31.03 A
ATOM 3828 OG1 THR A 482 -4.696 -3.347 -26.610 1.00 32.48 A
ATOM 3829 CG2 THR A 482 -3.155 -3.167 -27.958 1.00 31.00 A
ATOM 3830 C THR A 482 -5.217 -5.424 -27.781 1.00 29.91 A
ATOM 3831 O THR A 482 -6.012 -5.193 -26.968 1.00 31.06 A
ATOM 3832 N HIS A 483 -5.519 -5.904 -28.934 1.00 28.71 A
ATOM 3833 CA HIS A 483 -6.789 -5.728 -29.433 1.00 26.10 A
ATOM 3834 CB HIS A 483 -6.620 -5.049 -30.695 1.00 26.58 A
ATOM 3835 CG HIS A 483 -6.584 -3.578 -30.618 1.00 28.00 A
ATOM 3836 CD2 HIS A 483 -7.405 -2.701 -30.033 1.00 27.05 A
ATOM 3837 ND1 HIS A 483 -5.507 -2.866 -31.010 1.00 30.09 A
ATOM 3838 CE1 HIS A 483 -5.702 -1.600 -30.771 1.00 28.75 A

```
ATOM  3839  NE2 HIS A 483     -6.855  -1.470 -30.185  1.00 27.98      A
ATOM  3840  C   HIS A 483     -7.138  -7.116 -29.686  1.00 24.65      A
ATOM  3841  O   HIS A 483     -6.304  -7.918 -29.713  1.00 23.77      A
ATOM  3842  N   PHE A 484     -8.380  -7.432 -29.859  1.00 23.61      A
ATOM  3843  CA  PHE A 484     -8.741  -8.822 -30.040  1.00 23.94      A
ATOM  3844  CB  PHE A 484     -8.922  -9.491 -28.683  1.00 23.00      A
ATOM  3845  CG  PHE A 484     -9.232 -10.947 -28.773  1.00 24.55      A
ATOM  3846  CD1 PHE A 484     -8.502 -11.772 -29.629  1.00 25.25      A
ATOM  3847  CD2 PHE A 484    -10.252 -11.500 -28.009  1.00 25.69      A
ATOM  3848  CE1 PHE A 484     -8.786 -13.126 -29.730  1.00 25.29      A
ATOM  3849  CE2 PHE A 484    -10.547 -12.853 -28.098  1.00 25.95      A
ATOM  3850  CZ  PHE A 484     -9.813 -13.668 -28.964  1.00 26.91      A
ATOM  3851  C   PHE A 484    -10.040  -8.816 -30.823  1.00 24.58      A
ATOM  3852  O   PHE A 484    -11.103  -9.196 -30.327  1.00 25.89      A
ATOM  3853  N   ASP A 485     -9.928  -8.372 -32.066  1.00 23.54      A
ATOM  3854  CA  ASP A 485    -11.064  -8.247 -32.944  1.00 22.07      A
ATOM  3855  CB  ASP A 485    -10.601  -7.500 -34.199  1.00 22.77      A
ATOM  3856  CG  ASP A 485     -9.993  -6.132 -33.859  1.00 22.94      A
ATOM  3857  OD1 ASP A 485    -10.671  -5.329 -33.188  1.00 22.56      A
ATOM  3858  OD2 ASP A 485     -8.840  -5.852 -34.250  1.00 23.07      A
ATOM  3859  C   ASP A 485    -11.784  -9.558 -33.254  1.00 21.18      A
ATOM  3860  O   ASP A 485    -12.961  -9.553 -33.605  1.00 20.14      A
ATOM  3861  N   ALA A 486    -11.097 -10.683 -33.101  1.00 20.66      A
ATOM  3862  CA  ALA A 486    -11.738 -11.961 -33.356  1.00 21.29      A
ATOM  3863  CB  ALA A 486    -10.719 -13.073 -33.348  1.00 20.40      A
ATOM  3864  C   ALA A 486    -12.748 -12.170 -32.244  1.00 22.27      A
ATOM  3865  O   ALA A 486    -13.785 -12.807 -32.426  1.00 23.34      A
ATOM  3866  N   GLY A 487    -12.437 -11.608 -31.084  1.00 22.55      A
ATOM  3867  CA  GLY A 487    -13.311 -11.744 -29.936  1.00 23.10      A
ATOM  3868  C   GLY A 487    -14.593 -10.936 -29.985  1.00 23.85      A
ATOM  3869  O   GLY A 487    -15.486 -11.154 -29.163  1.00 25.35      A
ATOM  3870  N   ALA A 488    -14.702 -10.006 -30.929  1.00 23.27      A
ATOM  3871  CA  ALA A 488    -15.903  -9.185 -31.035  1.00 23.25      A
ATOM  3872  CB  ALA A 488    -15.572  -7.849 -31.661  1.00 22.67      A
```

ATOM 3873 C ALA A 488 -16.974 -9.893 -31.854 1.00 24.16 A
ATOM 3874 O ALA A 488 -18.035 -9.328 -32.124 1.00 25.32 A
ATOM 3875 N LYS A 489 -16.693 -11.131 -32.246 1.00 23.93 A
ATOM 3876 CA LYS A 489 -17.651 -11.929 -33.004 1.00 24.18 A
ATOM 3877 CB LYS A 489 -16.961 -12.622 -34.180 1.00 23.27 A
ATOM 3878 CG LYS A 489 -17.865 -13.560 -34.964 1.00 20.31 A
ATOM 3879 CD LYS A 489 -19.061 -12.819 -35.542 1.00 21.67 A
ATOM 3880 CE LYS A 489 -20.101 -13.788 -36.081 1.00 21.97 A
ATOM 3881 NZ LYS A 489 -21.392 -13.109 -36.379 1.00 25.09 A
ATOM 3882 C LYS A 489 -18.337 -12.962 -32.115 1.00 24.77 A
ATOM 3883 O LYS A 489 -17.683 -13.835 -31.543 1.00 25.27 A
ATOM 3884 N PHE A 490 -19.638 -12.892 -32.001 1.00 23.86 A
ATOM 3885 CA PHE A 490 -20.316 -13.692 -31.056 1.00 24.54 A
ATOM 3886 CB PHE A 490 -21.715 -13.813 -31.360 1.00 24.42 A
ATOM 3887 CG PHE A 490 -22.435 -14.790 -30.527 1.00 25.79 A
ATOM 3888 CD1 PHE A 490 -23.287 -14.428 -29.587 1.00 25.24 A
ATOM 3889 CD2 PHE A 490 -22.348 -16.066 -30.771 1.00 25.91 A
ATOM 3890 CE1 PHE A 490 -23.926 -15.318 -28.939 1.00 24.39 A
ATOM 3891 CE2 PHE A 490 -23.040 -16.933 -30.128 1.00 25.39 A
ATOM 3892 CZ PHE A 490 -23.781 -16.561 -29.210 1.00 24.73 A
ATOM 3893 C PHE A 490 -19.786 -15.001 -30.818 1.00 25.27 A
ATOM 3894 O PHE A 490 -19.787 -15.476 -29.758 1.00 25.38 A
ATOM 3895 N HIS A 491 -19.288 -15.640 -31.816 1.00 25.15 A
ATOM 3896 CA HIS A 491 -19.061 -17.081 -31.807 1.00 24.46 A
ATOM 3897 CB HIS A 491 -19.072 -17.632 -33.234 1.00 23.77 A
ATOM 3898 CG HIS A 491 -20.429 -17.647 -33.866 1.00 24.58 A
ATOM 3899 CD2 HIS A 491 -21.081 -16.716 -34.603 1.00 25.02 A
ATOM 3900 ND1 HIS A 491 -21.284 -18.725 -33.769 1.00 25.73 A
ATOM 3901 CE1 HIS A 491 -22.401 -18.457 -34.419 1.00 26.06 A
ATOM 3902 NE2 HIS A 491 -22.304 -17.245 -34.934 1.00 26.09 A
ATOM 3903 C HIS A 491 -17.743 -17.426 -31.121 1.00 24.46 A
ATOM 3904 O HIS A 491 -17.552 -18.549 -30.655 1.00 23.14 A
ATOM 3905 N VAL A 492 -16.846 -16.434 -31.078 1.00 24.78 A
ATOM 3906 CA VAL A 492 -15.512 -16.655 -30.508 1.00 26.46 A

```
ATOM  3907  CB  VAL A 492     -14.467 -15.594 -30.959  1.00 27.00      A
ATOM  3908  CG1 VAL A 492     -13.158 -15.801 -30.182  1.00 26.88      A
ATOM  3909  CG2 VAL A 492     -14.188 -15.729 -32.454  1.00 25.03      A
ATOM  3910  C   VAL A 492     -15.578 -16.697 -28.985  1.00 26.30      A
ATOM  3911  O   VAL A 492     -15.014 -17.599 -28.370  1.00 27.38      A
ATOM  3912  N   PRO A 493     -16.260 -15.724 -28.389  1.00 25.57      A
ATOM  3913  CD  PRO A 493     -16.768 -14.503 -29.035  1.00 25.53      A
ATOM  3914  CA  PRO A 493     -16.461 -15.705 -26.936  1.00 24.27      A
ATOM  3915  CB  PRO A 493     -17.189 -14.378 -26.700  1.00 23.63      A
ATOM  3916  CG  PRO A 493     -17.756 -14.007 -28.027  1.00 25.03      A
ATOM  3917  C   PRO A 493     -17.324 -16.871 -26.466  1.00 23.96      A
ATOM  3918  O   PRO A 493     -16.996 -17.517 -25.471  1.00 26.34      A
ATOM  3919  N   ASN A 494     -18.415 -17.132 -27.179  1.00 22.69      A
ATOM  3920  CA  ASN A 494     -19.312 -18.229 -26.833  1.00 22.06      A
ATOM  3921  CB  ASN A 494     -20.752 -17.886 -27.219  1.00 23.76      A
ATOM  3922  CG  ASN A 494     -21.264 -16.645 -26.513  1.00 27.02      A
ATOM  3923  OD1 ASN A 494     -22.279 -16.687 -25.818  1.00 30.57      A
ATOM  3924  ND2 ASN A 494     -20.563 -15.533 -26.689  1.00 28.71      A
ATOM  3925  C   ASN A 494     -18.893 -19.544 -27.484  1.00 21.16      A
ATOM  3926  O   ASN A 494     -19.722 -20.425 -27.713  1.00 20.92      A
ATOM  3927  N   VAL A 495     -17.604 -19.668 -27.779  1.00 20.40      A
ATOM  3928  CA  VAL A 495     -17.025 -20.951 -28.162  1.00 20.97      A
ATOM  3929  CB  VAL A 495     -16.618 -21.778 -26.928  1.00 19.61      A
ATOM  3930  CG1 VAL A 495     -15.980 -23.092 -27.354  1.00 18.76      A
ATOM  3931  CG2 VAL A 495     -15.674 -20.982 -26.040  1.00 19.94      A
ATOM  3932  C   VAL A 495     -17.999 -21.764 -29.010  1.00 21.79      A
ATOM  3933  O   VAL A 495     -18.423 -22.849 -28.615  1.00 20.46      A
ATOM  3934  N   THR A 496     -18.346 -21.231 -30.177  1.00 22.69      A
ATOM  3935  CA  THR A 496     -18.966 -22.028 -31.229  1.00 23.52      A
ATOM  3936  CB  THR A 496     -20.254 -21.349 -31.731  1.00 24.42      A
ATOM  3937  OG1 THR A 496     -21.364 -21.773 -30.930  1.00 23.96      A
ATOM  3938  CG2 THR A 496     -20.614 -21.852 -33.121  1.00 25.36      A
ATOM  3939  C   THR A 496     -18.003 -22.251 -32.391  1.00 23.29      A
ATOM  3940  O   THR A 496     -17.408 -21.305 -32.906  1.00 24.04      A
```

```
ATOM   3941  N   PRO A 497     -17.856 -23.508 -32.799  1.00 23.40      A
ATOM   3942  CD  PRO A 497     -18.380 -24.706 -32.123  1.00 22.06      A
ATOM   3943  CA  PRO A 497     -17.173 -23.835 -34.055  1.00 23.92      A
ATOM   3944  CB  PRO A 497     -17.335 -25.355 -34.154  1.00 24.09      A
ATOM   3945  CG  PRO A 497     -17.584 -25.804 -32.757  1.00 23.68      A
ATOM   3946  C   PRO A 497     -17.842 -23.161 -35.249  1.00 23.61      A
ATOM   3947  O   PRO A 497     -19.067 -23.053 -35.285  1.00 22.86      A
ATOM   3948  N   TYR A 498     -17.042 -22.713 -36.211  1.00 23.19      A
ATOM   3949  CA  TYR A 498     -17.561 -21.932 -37.326  1.00 23.11      A
ATOM   3950  CB  TYR A 498     -16.848 -20.572 -37.382  1.00 22.02      A
ATOM   3951  CG  TYR A 498     -17.719 -19.401 -37.825  1.00 20.52      A
ATOM   3952  CD1 TYR A 498     -18.567 -18.754 -36.928  1.00 19.83      A
ATOM   3953  CE1 TYR A 498     -19.373 -17.672 -37.336  1.00 19.95      A
ATOM   3954  CD2 TYR A 498     -17.693 -18.940 -39.148  1.00 20.70      A
ATOM   3955  CE2 TYR A 498     -18.495 -17.862 -39.567  1.00 20.22      A
ATOM   3956  CZ  TYR A 498     -19.331 -17.233 -38.659  1.00 20.07      A
ATOM   3957  OH  TYR A 498     -20.125 -16.184 -39.075  1.00 20.11      A
ATOM   3958  C   TYR A 498     -17.502 -22.603 -38.701  1.00 24.48      A
ATOM   3959  O   TYR A 498     -18.372 -22.348 -39.546  1.00 24.64      A
ATOM   3960  N   ILE A 499     -16.515 -23.472 -38.934  1.00 24.67      A
ATOM   3961  CA  ILE A 499     -16.388 -24.114 -40.256  1.00 25.17      A
ATOM   3962  CB  ILE A 499     -15.229 -25.144 -40.318  1.00 24.77      A
ATOM   3963  CG2 ILE A 499     -15.610 -26.429 -39.585  1.00 24.34      A
ATOM   3964  CG1 ILE A 499     -14.936 -25.511 -41.777  1.00 24.35      A
ATOM   3965  CD1 ILE A 499     -14.635 -24.337 -42.673  1.00 22.78      A
ATOM   3966  C   ILE A 499     -17.639 -24.819 -40.714  1.00 25.28      A
ATOM   3967  O   ILE A 499     -17.694 -25.316 -41.825  1.00 26.23      A
ATOM   3968  N   ARG A 500     -18.639 -24.870 -39.849  1.00 26.48      A
ATOM   3969  CA  ARG A 500     -19.900 -25.524 -40.162  1.00 27.79      A
ATOM   3970  CB  ARG A 500     -20.647 -25.834 -38.872  1.00 29.54      A
ATOM   3971  CG  ARG A 500     -19.860 -25.377 -37.649  1.00 33.75      A
ATOM   3972  CD  ARG A 500     -20.715 -25.292 -36.415  1.00 34.51      A
ATOM   3973  NE  ARG A 500     -20.356 -26.323 -35.448  1.00 35.82      A
ATOM   3974  CZ  ARG A 500     -21.046 -26.557 -34.341  1.00 36.29      A
```

ATOM 3975 NH1 ARG A 500 -22.124 -25.819 -34.071 1.00 33.84 A
ATOM 3976 NH2 ARG A 500 -20.659 -27.534 -33.525 1.00 39.33 A
ATOM 3977 C ARG A 500 -20.761 -24.607 -41.030 1.00 27.43 A
ATOM 3978 O ARG A 500 -21.547 -25.087 -41.841 1.00 27.93 A
ATOM 3979 N TYR A 501 -20.623 -23.292 -40.854 1.00 27.12 A
ATOM 3980 CA TYR A 501 -21.412 -22.344 -41.636 1.00 27.51 A
ATOM 3981 CB TYR A 501 -21.349 -20.950 -41.018 1.00 29.59 A
ATOM 3982 CG TYR A 501 -22.002 -20.893 -39.663 1.00 31.64 A
ATOM 3983 CD1 TYR A 501 -21.249 -20.667 -38.513 1.00 33.80 A
ATOM 3984 CE1 TYR A 501 -21.844 -20.671 -37.251 1.00 33.88 A
ATOM 3985 CD2 TYR A 501 -23.372 -21.116 -39.521 1.00 30.84 A
ATOM 3986 CE2 TYR A 501 -23.976 -21.123 -38.275 1.00 31.43 A
ATOM 3987 CZ TYR A 501 -23.206 -20.903 -37.138 1.00 33.23 A
ATOM 3988 OH TYR A 501 -23.788 -20.939 -35.891 1.00 33.38 A
ATOM 3989 C TYR A 501 -20.982 -22.289 -43.090 1.00 26.81 A
ATOM 3990 O TYR A 501 -21.765 -21.909 -43.959 1.00 26.18 A
ATOM 3991 N PHE A 502 -19.731 -22.664 -43.342 1.00 26.48 A
ATOM 3992 CA PHE A 502 -19.177 -22.704 -44.692 1.00 23.75 A
ATOM 3993 CB PHE A 502 -17.662 -22.898 -44.636 1.00 23.92 A
ATOM 3994 CG PHE A 502 -16.991 -22.826 -45.972 1.00 24.93 A
ATOM 3995 CD1 PHE A 502 -16.830 -21.602 -46.626 1.00 25.73 A
ATOM 3996 CD2 PHE A 502 -16.506 -23.973 -46.579 1.00 24.29 A
ATOM 3997 CE1 PHE A 502 -16.192 -21.530 -47.865 1.00 24.82 A
ATOM 3998 CE2 PHE A 502 -15.871 -23.904 -47.815 1.00 24.05 A
ATOM 3999 CZ PHE A 502 -15.714 -22.682 -48.455 1.00 25.14 A
ATOM 4000 C PHE A 502 -19.819 -23.915 -45.346 1.00 22.84 A
ATOM 4001 O PHE A 502 -20.491 -23.801 -46.376 1.00 22.64 A
ATOM 4002 N VAL A 503 -19.612 -25.070 -44.718 1.00 21.04 A
ATOM 4003 CA VAL A 503 -20.161 -26.329 -45.195 1.00 20.36 A
ATOM 4004 CB VAL A 503 -20.016 -27.418 -44.114 1.00 19.43 A
ATOM 4005 CG1 VAL A 503 -20.684 -28.700 -44.561 1.00 18.92 A
ATOM 4006 CG2 VAL A 503 -18.547 -27.660 -43.819 1.00 17.50 A
ATOM 4007 C VAL A 503 -21.632 -26.107 -45.504 1.00 20.09 A
ATOM 4008 O VAL A 503 -22.140 -26.490 -46.559 1.00 20.21 A

```
ATOM  4009  N   SER A 504     -22.290 -25.448 -44.566  1.00 19.89      A
ATOM  4010  CA  SER A 504     -23.696 -25.126 -44.659  1.00 21.30      A
ATOM  4011  CB  SER A 504     -24.096 -24.338 -43.416  1.00 20.48      A
ATOM  4012  OG  SER A 504     -25.436 -23.918 -43.485  1.00 19.72      A
ATOM  4013  C   SER A 504     -24.034 -24.324 -45.919  1.00 23.58      A
ATOM  4014  O   SER A 504     -24.906 -24.702 -46.703  1.00 24.73      A
ATOM  4015  N   PHE A 505     -23.336 -23.215 -46.122  1.00 24.99      A
ATOM  4016  CA  PHE A 505     -23.610 -22.388 -47.278  1.00 25.81      A
ATOM  4017  CB  PHE A 505     -22.820 -21.083 -47.172  1.00 26.60      A
ATOM  4018  CG  PHE A 505     -23.547 -20.007 -46.400  1.00 28.93      A
ATOM  4019  CD1 PHE A 505     -24.062 -20.273 -45.136  1.00 30.23      A
ATOM  4020  CD2 PHE A 505     -23.739 -18.738 -46.946  1.00 28.87      A
ATOM  4021  CE1 PHE A 505     -24.756 -19.300 -44.429  1.00 31.44      A
ATOM  4022  CE2 PHE A 505     -24.434 -17.746 -46.246  1.00 29.34      A
ATOM  4023  CZ  PHE A 505     -24.944 -18.029 -44.985  1.00 31.07      A
ATOM  4024  C   PHE A 505     -23.364 -23.095 -48.606  1.00 25.85      A
ATOM  4025  O   PHE A 505     -23.994 -22.784 -49.620  1.00 25.28      A
ATOM  4026  N   VAL A 506     -22.464 -24.065 -48.612  1.00 26.29      A
ATOM  4027  CA  VAL A 506     -22.219 -24.783 -49.848  1.00 25.96      A
ATOM  4028  CB  VAL A 506     -20.777 -25.356 -49.923  1.00 25.44      A
ATOM  4029  CG1 VAL A 506     -20.719 -26.528 -50.908  1.00 22.82      A
ATOM  4030  CG2 VAL A 506     -19.799 -24.241 -50.358  1.00 23.64      A
ATOM  4031  C   VAL A 506     -23.228 -25.904 -50.036  1.00 26.77      A
ATOM  4032  O   VAL A 506     -23.761 -26.052 -51.136  1.00 29.18      A
ATOM  4033  N   LEU A 507     -23.526 -26.683 -48.993  1.00 25.74      A
ATOM  4034  CA  LEU A 507     -24.483 -27.770 -49.194  1.00 25.50      A
ATOM  4035  CB  LEU A 507     -24.096 -29.029 -48.400  1.00 25.94      A
ATOM  4036  CG  LEU A 507     -24.809 -29.424 -47.108  1.00 25.15      A
ATOM  4037  CD1 LEU A 507     -24.733 -30.918 -46.903  1.00 24.78      A
ATOM  4038  CD2 LEU A 507     -24.168 -28.694 -45.961  1.00 25.90      A
ATOM  4039  C   LEU A 507     -25.941 -27.438 -48.947  1.00 25.50      A
ATOM  4040  O   LEU A 507     -26.769 -28.336 -48.862  1.00 26.83      A
ATOM  4041  N   GLN A 508     -26.273 -26.158 -48.842  1.00 26.02      A
ATOM  4042  CA  GLN A 508     -27.670 -25.793 -48.639  1.00 26.02      A
```

ATOM 4043 CB GLN A 508 -27.801 -24.419 -47.964 1.00 25.89 A
ATOM 4044 CG GLN A 508 -27.631 -23.180 -48.838 1.00 27.95 A
ATOM 4045 CD GLN A 508 -27.623 -21.886 -48.004 1.00 30.56 A
ATOM 4046 OE1 GLN A 508 -28.133 -20.839 -48.434 1.00 30.96 A
ATOM 4047 NE2 GLN A 508 -27.030 -21.958 -46.807 1.00 30.26 A
ATOM 4048 C GLN A 508 -28.310 -25.796 -50.010 1.00 26.18 A
ATOM 4049 O GLN A 508 -29.500 -26.049 -50.149 1.00 26.89 A
ATOM 4050 N PHE A 509 -27.500 -25.533 -51.030 1.00 26.98 A
ATOM 4051 CA PHE A 509 -27.988 -25.531 -52.403 1.00 27.26 A
ATOM 4052 CB PHE A 509 -27.099 -24.657 -53.294 1.00 27.15 A
ATOM 4053 CG PHE A 509 -27.132 -23.193 -52.943 1.00 27.97 A
ATOM 4054 CD1 PHE A 509 -26.263 -22.669 -51.992 1.00 28.60 A
ATOM 4055 CD2 PHE A 509 -28.028 -22.336 -53.562 1.00 26.97 A
ATOM 4056 CE1 PHE A 509 -26.285 -21.316 -51.670 1.00 27.01 A
ATOM 4057 CE2 PHE A 509 -28.054 -20.984 -53.241 1.00 27.79 A
ATOM 4058 CZ PHE A 509 -27.183 -20.477 -52.296 1.00 26.34 A
ATOM 4059 C PHE A 509 -28.057 -26.963 -52.967 1.00 27.40 A
ATOM 4060 O PHE A 509 -28.881 -27.247 -53.839 1.00 27.00 A
ATOM 4061 N GLN A 510 -27.192 -27.860 -52.482 1.00 27.28 A
ATOM 4062 CA GLN A 510 -27.233 -29.245 -52.956 1.00 26.52 A
ATOM 4063 CB GLN A 510 -26.187 -30.127 -52.270 1.00 23.00 A
ATOM 4064 CG GLN A 510 -24.748 -29.757 -52.518 1.00 19.85 A
ATOM 4065 CD GLN A 510 -23.831 -30.950 -52.393 1.00 19.65 A
ATOM 4066 OE1 GLN A 510 -22.654 -30.817 -52.088 1.00 19.40 A
ATOM 4067 NE2 GLN A 510 -24.369 -32.128 -52.642 1.00 20.64 A
ATOM 4068 C GLN A 510 -28.616 -29.751 -52.573 1.00 27.40 A
ATOM 4069 O GLN A 510 -29.264 -30.483 -53.331 1.00 28.47 A
ATOM 4070 N PHE A 511 -29.048 -29.336 -51.383 1.00 26.68 A
ATOM 4071 CA PHE A 511 -30.351 -29.695 -50.837 1.00 26.98 A
ATOM 4072 CB PHE A 511 -30.497 -29.202 -49.383 1.00 29.08 A
ATOM 4073 CG PHE A 511 -29.799 -30.047 -48.343 1.00 28.82 A
ATOM 4074 CD1 PHE A 511 -28.818 -30.968 -48.684 1.00 29.51 A
ATOM 4075 CD2 PHE A 511 -30.097 -29.857 -46.998 1.00 29.18 A
ATOM 4076 CE1 PHE A 511 -28.140 -31.686 -47.693 1.00 29.62 A

ATOM 4077 CE2 PHE A 511 -29.427 -30.562 -46.008 1.00 29.58 A
ATOM 4078 CZ PHE A 511 -28.444 -31.481 -46.358 1.00 29.77 A
ATOM 4079 C PHE A 511 -31.436 -29.024 -51.672 1.00 25.88 A
ATOM 4080 O PHE A 511 -32.415 -29.655 -52.045 1.00 25.35 A
ATOM 4081 N HIS A 512 -31.256 -27.735 -51.943 1.00 26.06 A
ATOM 4082 CA HIS A 512 -32.226 -26.968 -52.714 1.00 26.84 A
ATOM 4083 CB HIS A 512 -31.762 -25.518 -52.862 1.00 26.99 A
ATOM 4084 CG HIS A 512 -32.778 -24.616 -53.493 1.00 27.39 A
ATOM 4085 CD2 HIS A 512 -32.653 -23.652 -54.434 1.00 28.09 A
ATOM 4086 ND1 HIS A 512 -34.107 -24.620 -53.126 1.00 29.00 A
ATOM 4087 CE1 HIS A 512 -34.757 -23.698 -53.816 1.00 30.09 A
ATOM 4088 NE2 HIS A 512 -33.897 -23.096 -54.616 1.00 29.35 A
ATOM 4089 C HIS A 512 -32.451 -27.571 -54.087 1.00 27.69 A
ATOM 4090 O HIS A 512 -33.562 -27.553 -54.603 1.00 28.48 A
ATOM 4091 N GLU A 513 -31.394 -28.104 -54.683 1.00 27.80 A
ATOM 4092 CA GLU A 513 -31.514 -28.712 -55.996 1.00 27.64 A
ATOM 4093 CB GLU A 513 -30.125 -28.999 -56.576 1.00 27.10 A
ATOM 4094 CG GLU A 513 -30.122 -29.406 -58.039 1.00 27.91 A
ATOM 4095 CD GLU A 513 -28.728 -29.715 -58.564 1.00 28.74 A
ATOM 4096 OE1 GLU A 513 -28.028 -30.533 -57.940 1.00 29.15 A
ATOM 4097 OE2 GLU A 513 -28.327 -29.150 -59.602 1.00 29.07 A
ATOM 4098 C GLU A 513 -32.277 -30.008 -55.786 1.00 28.18 A
ATOM 4099 O GLU A 513 -33.372 -30.190 -56.307 1.00 27.93 A
ATOM 4100 N ALA A 514 -31.693 -30.891 -54.987 1.00 28.71 A
ATOM 4101 CA ALA A 514 -32.287 -32.187 -54.691 1.00 29.81 A
ATOM 4102 CB ALA A 514 -31.496 -32.880 -53.573 1.00 29.28 A
ATOM 4103 C ALA A 514 -33.771 -32.119 -54.320 1.00 31.13 A
ATOM 4104 O ALA A 514 -34.557 -32.976 -54.736 1.00 31.89 A
ATOM 4105 N LEU A 515 -34.162 -31.117 -53.539 1.00 31.68 A
ATOM 4106 CA LEU A 515 -35.560 -31.006 -53.146 1.00 33.55 A
ATOM 4107 CB LEU A 515 -35.712 -30.095 -51.919 1.00 33.56 A
ATOM 4108 CG LEU A 515 -35.091 -30.687 -50.636 1.00 33.78 A
ATOM 4109 CD1 LEU A 515 -35.297 -29.733 -49.462 1.00 32.18 A
ATOM 4110 CD2 LEU A 515 -35.710 -32.059 -50.334 1.00 32.77 A

ATOM 4111 C LEU A 515 -36.422 -30.516 -54.295 1.00 34.69 A
ATOM 4112 O LEU A 515 -37.514 -31.034 -54.525 1.00 35.01 A
ATOM 4113 N CYS A 516 -35.929 -29.532 -55.033 1.00 35.86 A
ATOM 4114 CA CYS A 516 -36.682 -29.012 -56.160 1.00 36.89 A
ATOM 4115 C CYS A 516 -36.934 -30.094 -57.198 1.00 38.08 A
ATOM 4116 O CYS A 516 -37.950 -30.074 -57.890 1.00 37.74 A
ATOM 4117 CB CYS A 516 -35.941 -27.844 -56.791 1.00 36.33 A
ATOM 4118 SG CYS A 516 -35.898 -26.398 -55.700 1.00 37.29 A
ATOM 4119 N LYS A 517 -36.009 -31.042 -57.307 1.00 39.90 A
ATOM 4120 CA LYS A 517 -36.181 -32.121 -58.267 1.00 41.39 A
ATOM 4121 CB LYS A 517 -34.907 -32.960 -58.397 1.00 40.02 A
ATOM 4122 CG LYS A 517 -34.962 -33.956 -59.545 1.00 39.66 A
ATOM 4123 CD LYS A 517 -33.669 -34.730 -59.677 1.00 41.10 A
ATOM 4124 CE LYS A 517 -33.794 -35.860 -60.699 1.00 42.94 A
ATOM 4125 NZ LYS A 517 -34.016 -35.375 -62.096 1.00 44.20 A
ATOM 4126 C LYS A 517 -37.348 -33.001 -57.832 1.00 43.56 A
ATOM 4127 O LYS A 517 -38.252 -33.264 -58.629 1.00 45.90 A
ATOM 4128 N GLU A 518 -37.439 -33.408 -56.591 1.00 44.27 A
ATOM 4129 CA GLU A 518 -38.564 -34.244 -56.219 1.00 44.14 A
ATOM 4130 CB GLU A 518 -38.345 -34.915 -54.937 1.00 44.65 A
ATOM 4131 CG GLU A 518 -37.595 -36.179 -55.118 1.00 46.27 A
ATOM 4132 CD GLU A 518 -38.448 -37.300 -54.855 1.00 47.80 A
ATOM 4133 OE1 GLU A 518 -38.079 -38.241 -54.197 1.00 48.96 A
ATOM 4134 OE2 GLU A 518 -39.532 -37.229 -55.321 1.00 49.99 A
ATOM 4135 C GLU A 518 -39.812 -33.534 -56.105 1.00 43.66 A
ATOM 4136 O GLU A 518 -40.832 -34.091 -56.204 1.00 43.02 A
ATOM 4137 N ALA A 519 -39.748 -32.277 -55.852 1.00 43.95 A
ATOM 4138 CA ALA A 519 -40.985 -31.513 -55.873 1.00 44.83 A
ATOM 4139 CB ALA A 519 -40.709 -30.050 -55.540 1.00 44.04 A
ATOM 4140 C ALA A 519 -41.579 -31.630 -57.270 1.00 45.48 A
ATOM 4141 O ALA A 519 -42.798 -31.608 -57.448 1.00 46.33 A
ATOM 4142 N GLY A 520 -40.704 -31.768 -58.260 1.00 45.57 A
ATOM 4143 CA GLY A 520 -41.150 -31.871 -59.632 1.00 45.67 A
ATOM 4144 C GLY A 520 -41.102 -30.508 -60.288 1.00 46.39 A

ATOM 4145 O GLY A 520 -41.801 -30.238 -61.265 1.00 46.26 A
ATOM 4146 N TYR A 521 -40.263 -29.633 -59.744 1.00 47.25 A
ATOM 4147 CA TYR A 521 -40.041 -28.319 -60.336 1.00 47.13 A
ATOM 4148 CB TYR A 521 -39.465 -27.351 -59.300 1.00 46.85 A
ATOM 4149 CG TYR A 521 -39.260 -25.948 -59.823 1.00 47.30 A
ATOM 4150 CD1 TYR A 521 -40.257 -24.988 -59.704 1.00 47.81 A
ATOM 4151 CE1 TYR A 521 -40.074 -23.704 -60.181 1.00 46.74 A
ATOM 4152 CD2 TYR A 521 -38.070 -25.582 -60.439 1.00 46.23 A
ATOM 4153 CE2 TYR A 521 -37.878 -24.301 -60.919 1.00 45.27 A
ATOM 4154 CZ TYR A 521 -38.883 -23.366 -60.788 1.00 46.11 A
ATOM 4155 OH TYR A 521 -38.698 -22.089 -61.265 1.00 47.40 A
ATOM 4156 C TYR A 521 -39.115 -28.405 -61.544 1.00 47.94 A
ATOM 4157 O TYR A 521 -38.236 -29.264 -61.605 1.00 47.33 A
ATOM 4158 N GLU A 522 -39.426 -27.639 -62.553 1.00 49.45 A
ATOM 4159 CA GLU A 522 -38.468 -27.386 -63.567 1.00 50.87 A
ATOM 4160 CB GLU A 522 -38.577 -28.379 -64.670 1.00 51.32 A
ATOM 4161 CG GLU A 522 -37.546 -29.445 -64.618 1.00 53.71 A
ATOM 4162 CD GLU A 522 -38.129 -30.732 -65.034 1.00 55.56 A
ATOM 4163 OE1 GLU A 522 -39.214 -30.679 -65.622 1.00 56.26 A
ATOM 4164 OE2 GLU A 522 -37.515 -31.767 -64.760 1.00 56.12 A
ATOM 4165 C GLU A 522 -38.686 -26.043 -64.114 1.00 50.80 A
ATOM 4166 O GLU A 522 -39.743 -25.488 -63.989 1.00 52.29 A
ATOM 4167 N GLY A 523 -37.664 -25.521 -64.732 1.00 49.28 A
ATOM 4168 CA GLY A 523 -37.346 -24.156 -64.560 1.00 47.02 A
ATOM 4169 C GLY A 523 -36.123 -24.125 -63.740 1.00 45.60 A
ATOM 4170 O GLY A 523 -35.501 -25.131 -63.594 1.00 46.37 A
ATOM 4171 N PRO A 524 -35.806 -22.963 -63.199 1.00 43.67 A
ATOM 4172 CD PRO A 524 -36.442 -21.859 -63.887 1.00 42.87 A
ATOM 4173 CA PRO A 524 -34.474 -22.577 -62.960 1.00 42.11 A
ATOM 4174 CB PRO A 524 -34.503 -21.187 -63.455 1.00 41.55 A
ATOM 4175 CG PRO A 524 -35.290 -21.243 -64.400 1.00 41.14 A
ATOM 4176 C PRO A 524 -34.144 -22.554 -61.546 1.00 41.51 A
ATOM 4177 O PRO A 524 -34.832 -22.077 -60.705 1.00 41.91 A
ATOM 4178 N LEU A 525 -33.005 -23.081 -61.249 1.00 39.56 A

ATOM 4179 CA LEU A 525 -32.867 -23.540 -59.873 1.00 37.93 A
ATOM 4180 CB LEU A 525 -31.477 -24.136 -59.643 1.00 35.41 A
ATOM 4181 CG LEU A 525 -31.190 -24.660 -58.235 1.00 33.34 A
ATOM 4182 CD1 LEU A 525 -32.248 -25.667 -57.809 1.00 31.38 A
ATOM 4183 CD2 LEU A 525 -29.800 -25.274 -58.162 1.00 31.54 A
ATOM 4184 C LEU A 525 -33.121 -22.406 -58.885 1.00 38.05 A
ATOM 4185 O LEU A 525 -33.595 -22.633 -57.772 1.00 38.87 A
ATOM 4186 N HIS A 526 -32.803 -21.184 -59.300 1.00 36.81 A
ATOM 4187 CA HIS A 526 -32.948 -20.026 -58.440 1.00 35.30 A
ATOM 4188 CB HIS A 526 -31.924 -18.948 -58.813 1.00 34.19 A
ATOM 4189 CG HIS A 526 -32.271 -18.173 -60.042 1.00 33.72 A
ATOM 4190 CD2 HIS A 526 -32.839 -16.951 -60.191 1.00 33.62 A
ATOM 4191 ND1 HIS A 526 -32.026 -18.638 -61.313 1.00 33.80 A
ATOM 4192 CE1 HIS A 526 -32.424 -17.737 -62.194 1.00 33.94 A
ATOM 4193 NE2 HIS A 526 -32.921 -16.704 -61.537 1.00 32.71 A
ATOM 4194 C HIS A 526 -34.346 -19.428 -58.430 1.00 35.67 A
ATOM 4195 O HIS A 526 -34.572 -18.374 -57.837 1.00 36.50 A
ATOM 4196 N GLN A 527 -35.287 -20.085 -59.090 1.00 35.11 A
ATOM 4197 CA GLN A 527 -36.650 -19.579 -59.099 1.00 35.85 A
ATOM 4198 CB GLN A 527 -37.081 -19.175 -60.512 1.00 37.47 A
ATOM 4199 CG GLN A 527 -36.416 -17.900 -61.012 1.00 39.32 A
ATOM 4200 CD GLN A 527 -36.988 -17.414 -62.331 1.00 39.65 A
ATOM 4201 OE1 GLN A 527 -37.165 -18.196 -63.262 1.00 38.71 A
ATOM 4202 NE2 GLN A 527 -37.273 -16.116 -62.418 1.00 39.83 A
ATOM 4203 C GLN A 527 -37.565 -20.653 -58.550 1.00 35.52 A
ATOM 4204 O GLN A 527 -38.779 -20.486 -58.469 1.00 34.58 A
ATOM 4205 N CYS A 528 -36.961 -21.762 -58.160 1.00 36.50 A
ATOM 4206 CA CYS A 528 -37.717 -22.864 -57.605 1.00 37.51 A
ATOM 4207 C CYS A 528 -38.269 -22.515 -56.235 1.00 38.13 A
ATOM 4208 O CYS A 528 -37.653 -21.759 -55.476 1.00 38.75 A
ATOM 4209 CB CYS A 528 -36.838 -24.107 -57.489 1.00 37.95 A
ATOM 4210 SG CYS A 528 -37.497 -25.289 -56.279 1.00 38.36 A
ATOM 4211 N ASP A 529 -39.432 -23.076 -55.927 1.00 37.97 A
ATOM 4212 CA ASP A 529 -40.086 -22.852 -54.652 1.00 38.25 A

ATOM 4213 CB ASP A 529 -41.087 -21.708 -54.767 1.00 37.84 A
ATOM 4214 CG ASP A 529 -41.956 -21.572 -53.537 1.00 38.24 A
ATOM 4215 OD1 ASP A 529 -41.405 -21.649 -52.419 1.00 37.67 A
ATOM 4216 OD2 ASP A 529 -43.184 -21.378 -53.687 1.00 38.42 A
ATOM 4217 C ASP A 529 -40.798 -24.128 -54.270 1.00 38.73 A
ATOM 4218 O ASP A 529 -41.890 -24.396 -54.749 1.00 37.90 A
ATOM 4219 N ILE A 530 -40.175 -24.917 -53.402 1.00 40.75 A
ATOM 4220 CA ILE A 530 -40.762 -26.188 -52.988 1.00 43.46 A
ATOM 4221 CB ILE A 530 -39.710 -27.097 -52.280 1.00 43.25 A
ATOM 4222 CG2 ILE A 530 -38.561 -27.410 -53.230 1.00 42.14 A
ATOM 4223 CG1 ILE A 530 -39.192 -26.420 -51.010 1.00 43.02 A
ATOM 4224 CD1 ILE A 530 -38.241 -27.276 -50.215 1.00 40.90 A
ATOM 4225 C ILE A 530 -41.993 -26.062 -52.082 1.00 45.79 A
ATOM 4226 O ILE A 530 -42.406 -27.042 -51.451 1.00 45.86 A
ATOM 4227 N TYR A 531 -42.581 -24.868 -52.027 1.00 47.88 A
ATOM 4228 CA TYR A 531 -43.764 -24.630 -51.202 1.00 50.06 A
ATOM 4229 CB TYR A 531 -44.304 -23.222 -51.459 1.00 52.41 A
ATOM 4230 CG TYR A 531 -45.457 -22.800 -50.561 1.00 55.58 A
ATOM 4231 CD1 TYR A 531 -45.318 -22.766 -49.169 1.00 55.79 A
ATOM 4232 CE1 TYR A 531 -46.365 -22.329 -48.343 1.00 56.94 A
ATOM 4233 CD2 TYR A 531 -46.675 -22.389 -51.108 1.00 57.15 A
ATOM 4234 CE2 TYR A 531 -47.726 -21.949 -50.296 1.00 58.69 A
ATOM 4235 CZ TYR A 531 -47.566 -21.919 -48.915 1.00 58.51 A
ATOM 4236 OH TYR A 531 -48.606 -21.469 -48.124 1.00 58.41 A
ATOM 4237 C TYR A 531 -44.868 -25.668 -51.460 1.00 50.33 A
ATOM 4238 O TYR A 531 -45.072 -26.115 -52.593 1.00 50.83 A
ATOM 4239 N ARG A 532 -45.566 -26.044 -50.387 1.00 49.47 A
ATOM 4240 CA ARG A 532 -46.652 -27.026 -50.416 1.00 47.50 A
ATOM 4241 CB ARG A 532 -47.924 -26.409 -51.028 1.00 47.42 A
ATOM 4242 CG ARG A 532 -48.614 -25.369 -50.132 1.00 49.55 A
ATOM 4243 CD ARG A 532 -50.088 -25.138 -50.509 1.00 51.61 A
ATOM 4244 NE ARG A 532 -50.816 -24.354 -49.506 1.00 53.81 A
ATOM 4245 CZ ARG A 532 -51.041 -24.753 -48.252 1.00 55.83 A
ATOM 4246 NH1 ARG A 532 -50.600 -25.932 -47.832 1.00 55.39 A

ATOM 4247 NH2 ARG A 532 -51.694 -23.964 -47.402 1.00 57.46 A
ATOM 4248 C ARG A 532 -46.336 -28.365 -51.095 1.00 45.89 A
ATOM 4249 O ARG A 532 -47.247 -29.119 -51.435 1.00 46.40 A
ATOM 4250 N SER A 533 -45.054 -28.675 -51.278 1.00 43.49 A
ATOM 4251 CA SER A 533 -44.673 -29.942 -51.905 1.00 41.83 A
ATOM 4252 CB SER A 533 -43.392 -29.794 -52.722 1.00 40.57 A
ATOM 4253 OG SER A 533 -42.873 -31.077 -53.034 1.00 38.66 A
ATOM 4254 C SER A 533 -44.458 -31.041 -50.880 1.00 41.32 A
ATOM 4255 O SER A 533 -43.346 -31.223 -50.385 1.00 41.93 A
ATOM 4256 N THR A 534 -45.515 -31.782 -50.571 1.00 40.96 A
ATOM 4257 CA THR A 534 -45.414 -32.865 -49.599 1.00 40.54 A
ATOM 4258 CB THR A 534 -46.768 -33.566 -49.391 1.00 40.76 A
ATOM 4259 OG1 THR A 534 -47.106 -34.302 -50.568 1.00 39.34 A
ATOM 4260 CG2 THR A 534 -47.863 -32.546 -49.119 1.00 41.67 A
ATOM 4261 C THR A 534 -44.400 -33.908 -50.053 1.00 39.66 A
ATOM 4262 O THR A 534 -43.838 -34.638 -49.237 1.00 38.39 A
ATOM 4263 N ALA A 535 -44.167 -33.972 -51.361 1.00 39.88 A
ATOM 4264 CA ALA A 535 -43.214 -34.931 -51.907 1.00 40.44 A
ATOM 4265 CB ALA A 535 -43.433 -35.103 -53.403 1.00 39.16 A
ATOM 4266 C ALA A 535 -41.778 -34.504 -51.624 1.00 40.59 A
ATOM 4267 O ALA A 535 -40.913 -35.327 -51.307 1.00 39.93 A
ATOM 4268 N ALA A 536 -41.512 -33.199 -51.734 1.00 40.33 A
ATOM 4269 CA ALA A 536 -40.184 -32.671 -51.443 1.00 39.48 A
ATOM 4270 CB ALA A 536 -40.116 -31.208 -51.829 1.00 38.83 A
ATOM 4271 C ALA A 536 -39.897 -32.833 -49.941 1.00 39.46 A
ATOM 4272 O ALA A 536 -38.883 -33.417 -49.547 1.00 39.07 A
ATOM 4273 N GLY A 537 -40.808 -32.315 -49.117 1.00 38.56 A
ATOM 4274 CA GLY A 537 -40.661 -32.392 -47.676 1.00 37.77 A
ATOM 4275 C GLY A 537 -40.377 -33.772 -47.104 1.00 38.59 A
ATOM 4276 O GLY A 537 -39.642 -33.898 -46.122 1.00 38.61 A
ATOM 4277 N ALA A 538 -40.956 -34.807 -47.703 1.00 38.64 A
ATOM 4278 CA ALA A 538 -40.757 -36.172 -47.230 1.00 38.07 A
ATOM 4279 CB ALA A 538 -41.687 -37.096 -47.959 1.00 37.50 A
ATOM 4280 C ALA A 538 -39.316 -36.621 -47.436 1.00 38.33 A

```
ATOM  4281  O   ALA A 538     -38.796 -37.451 -46.691  1.00 37.98      A
ATOM  4282  N   LYS A 539     -38.625 -36.017 -48.361  1.00 38.99      A
ATOM  4283  CA  LYS A 539     -37.288 -36.383 -48.695  1.00 38.67      A
ATOM  4284  CB  LYS A 539     -37.003 -35.788 -50.035  1.00 37.54      A
ATOM  4285  CG  LYS A 539     -35.942 -36.423 -50.882  1.00 35.92      A
ATOM  4286  CD  LYS A 539     -35.301 -35.464 -51.742  1.00 33.76      A
ATOM  4287  CE  LYS A 539     -34.236 -36.111 -52.423  1.00 32.69      A
ATOM  4288  NZ  LYS A 539     -34.501 -37.487 -52.430  1.00 31.05      A
ATOM  4289  C   LYS A 539     -36.373 -35.756 -47.747  1.00 39.63      A
ATOM  4290  O   LYS A 539     -35.362 -36.289 -47.449  1.00 38.85      A
ATOM  4291  N   LEU A 540     -36.716 -34.559 -47.330  1.00 40.03      A
ATOM  4292  CA  LEU A 540     -35.961 -33.819 -46.325  1.00 40.45      A
ATOM  4293  CB  LEU A 540     -36.488 -32.390 -46.216  1.00 38.46      A
ATOM  4294  CG  LEU A 540     -35.563 -31.266 -45.725  1.00 37.54      A
ATOM  4295  CD1 LEU A 540     -36.417 -30.246 -45.003  1.00 36.97      A
ATOM  4296  CD2 LEU A 540     -34.480 -31.776 -44.805  1.00 36.47      A
ATOM  4297  C   LEU A 540     -36.096 -34.491 -44.964  1.00 41.98      A
ATOM  4298  O   LEU A 540     -35.103 -34.732 -44.271  1.00 42.60      A
ATOM  4299  N   ARG A 541     -37.296 -34.866 -44.604  1.00 42.12      A
ATOM  4300  CA  ARG A 541     -37.442 -35.405 -43.320  1.00 43.15      A
ATOM  4301  CB  ARG A 541     -38.847 -35.536 -42.962  1.00 45.48      A
ATOM  4302  CG  ARG A 541     -39.056 -36.861 -42.458  1.00 49.39      A
ATOM  4303  CD  ARG A 541     -40.446 -37.160 -41.901  1.00 52.41      A
ATOM  4304  NE  ARG A 541     -41.481 -36.323 -42.440  1.00 56.57      A
ATOM  4305  CZ  ARG A 541     -42.285 -36.685 -43.406  1.00 58.70      A
ATOM  4306  NH1 ARG A 541     -42.171 -37.860 -43.963  1.00 59.03      A
ATOM  4307  NH2 ARG A 541     -43.204 -35.872 -43.844  1.00 59.11      A
ATOM  4308  C   ARG A 541     -36.828 -36.709 -43.081  1.00 42.29      A
ATOM  4309  O   ARG A 541     -36.591 -37.060 -41.998  1.00 42.33      A
ATOM  4310  N   ALA A 542     -36.587 -37.466 -44.094  1.00 40.90      A
ATOM  4311  CA  ALA A 542     -35.796 -38.685 -43.980  1.00 39.39      A
ATOM  4312  CB  ALA A 542     -35.738 -39.408 -45.318  1.00 39.38      A
ATOM  4313  C   ALA A 542     -34.389 -38.383 -43.475  1.00 38.42      A
ATOM  4314  O   ALA A 542     -33.823 -39.164 -42.698  1.00 37.57      A
```

ATOM 4315 N VAL A 543 -33.806 -37.294 -43.933 1.00 37.79 A
ATOM 4316 CA VAL A 543 -32.458 -36.928 -43.520 1.00 36.54 A
ATOM 4317 CB VAL A 543 -31.866 -35.790 -44.433 1.00 35.43 A
ATOM 4318 CG1 VAL A 543 -32.566 -35.795 -45.774 1.00 34.12 A
ATOM 4319 CG2 VAL A 543 -31.998 -34.431 -43.777 1.00 33.76 A
ATOM 4320 C VAL A 543 -32.539 -36.461 -42.069 1.00 36.60 A
ATOM 4321 O VAL A 543 -31.673 -36.777 -41.243 1.00 36.23 A
ATOM 4322 N LEU A 544 -33.597 -35.715 -41.763 1.00 35.55 A
ATOM 4323 CA LEU A 544 -33.788 -35.212 -40.418 1.00 34.72 A
ATOM 4324 CB LEU A 544 -35.048 -34.345 -40.352 1.00 31.47 A
ATOM 4325 CG LEU A 544 -34.969 -33.064 -41.178 1.00 29.88 A
ATOM 4326 CD1 LEU A 544 -36.157 -32.173 -40.903 1.00 28.15 A
ATOM 4327 CD2 LEU A 544 -33.709 -32.340 -40.818 1.00 30.33 A
ATOM 4328 C LEU A 544 -33.880 -36.372 -39.429 1.00 35.59 A
ATOM 4329 O LEU A 544 -33.066 -36.483 -38.511 1.00 36.79 A
ATOM 4330 N GLN A 545 -34.855 -37.222 -39.610 1.00 34.97 A
ATOM 4331 CA GLN A 545 -34.966 -38.369 -38.804 1.00 34.10 A
ATOM 4332 CB GLN A 545 -36.104 -39.207 -39.247 1.00 36.14 A
ATOM 4333 CG GLN A 545 -37.387 -38.539 -39.387 1.00 39.28 A
ATOM 4334 CD GLN A 545 -38.515 -39.393 -38.928 1.00 41.95 A
ATOM 4335 OE1 GLN A 545 -39.461 -38.930 -38.356 1.00 42.64 A
ATOM 4336 NE2 GLN A 545 -38.402 -40.646 -39.152 1.00 44.00 A
ATOM 4337 C GLN A 545 -33.810 -39.258 -38.642 1.00 32.73 A
ATOM 4338 O GLN A 545 -33.933 -40.249 -38.034 1.00 32.74 A
ATOM 4339 N ALA A 546 -32.687 -38.957 -39.207 1.00 31.78 A
ATOM 4340 CA ALA A 546 -31.499 -39.803 -39.098 1.00 31.70 A
ATOM 4341 CB ALA A 546 -30.780 -39.866 -40.448 1.00 32.23 A
ATOM 4342 C ALA A 546 -30.511 -39.382 -38.001 1.00 32.11 A
ATOM 4343 O ALA A 546 -29.747 -40.215 -37.496 1.00 30.61 A
ATOM 4344 N GLY A 547 -30.513 -38.097 -37.644 1.00 31.92 A
ATOM 4345 CA GLY A 547 -29.604 -37.611 -36.620 1.00 32.99 A
ATOM 4346 C GLY A 547 -28.161 -37.989 -36.902 1.00 34.11 A
ATOM 4347 O GLY A 547 -27.674 -37.748 -37.997 1.00 36.15 A
ATOM 4348 N SER A 548 -27.473 -38.577 -35.925 1.00 34.90 A

```
ATOM   4349  CA  SER A 548     -26.078 -38.985 -36.100  1.00 35.56      A
ATOM   4350  CB  SER A 548     -25.237 -38.553 -34.900  1.00 35.52      A
ATOM   4351  OG  SER A 548     -23.897 -38.961 -35.047  1.00 40.49      A
ATOM   4352  C   SER A 548     -25.992 -40.500 -36.206  1.00 35.33      A
ATOM   4353  O   SER A 548     -24.903 -41.065 -36.091  1.00 35.14      A
ATOM   4354  N   SER A 549     -27.136 -41.154 -36.408  1.00 35.30      A
ATOM   4355  CA  SER A 549     -27.191 -42.614 -36.502  1.00 35.97      A
ATOM   4356  CB  SER A 549     -28.642 -43.068 -36.625  1.00 35.82      A
ATOM   4357  OG  SER A 549     -29.026 -43.161 -37.984  1.00 37.19      A
ATOM   4358  C   SER A 549     -26.373 -43.159 -37.679  1.00 37.05      A
ATOM   4359  O   SER A 549     -25.585 -44.098 -37.517  1.00 37.43      A
ATOM   4360  N   ARG A 550     -26.516 -42.567 -38.851  1.00 36.97      A
ATOM   4361  CA  ARG A 550     -25.850 -42.961 -40.073  1.00 34.91      A
ATOM   4362  CB  ARG A 550     -26.917 -42.895 -41.111  1.00 36.08      A
ATOM   4363  CG  ARG A 550     -27.291 -44.110 -41.791  1.00 37.62      A
ATOM   4364  CD  ARG A 550     -28.712 -44.164 -42.083  1.00 39.72      A
ATOM   4365  NE  ARG A 550     -29.083 -43.597 -43.365  1.00 42.07      A
ATOM   4366  CZ  ARG A 550     -28.629 -43.984 -44.533  1.00 43.03      A
ATOM   4367  NH1 ARG A 550     -27.767 -44.953 -44.632  1.00 41.88      A
ATOM   4368  NH2 ARG A 550     -29.042 -43.387 -45.608  1.00 41.87      A
ATOM   4369  C   ARG A 550     -24.826 -41.910 -40.436  1.00 33.07      A
ATOM   4370  O   ARG A 550     -25.024 -40.800 -40.024  1.00 33.25      A
ATOM   4371  N   PRO A 551     -23.790 -42.238 -41.237  1.00 30.88      A
ATOM   4372  CD  PRO A 551     -23.413 -43.637 -41.512  1.00 29.57      A
ATOM   4373  CA  PRO A 551     -22.728 -41.326 -41.694  1.00 29.44      A
ATOM   4374  CB  PRO A 551     -21.768 -42.255 -42.427  1.00 27.57      A
ATOM   4375  CG  PRO A 551     -21.922 -43.533 -41.705  1.00 28.24      A
ATOM   4376  C   PRO A 551     -23.330 -40.265 -42.638  1.00 30.00      A
ATOM   4377  O   PRO A 551     -24.123 -40.596 -43.525  1.00 29.79      A
ATOM   4378  N   TRP A 552     -22.956 -39.001 -42.464  1.00 30.11      A
ATOM   4379  CA  TRP A 552     -23.517 -37.959 -43.307  1.00 30.55      A
ATOM   4380  CB  TRP A 552     -22.907 -36.590 -42.992  1.00 30.80      A
ATOM   4381  CG  TRP A 552     -21.430 -36.407 -43.277  1.00 31.69      A
ATOM   4382  CD2 TRP A 552     -20.836 -35.948 -44.506  1.00 32.33      A
```

ATOM 4383 CE2 TRP A 552 -19.444 -35.829 -44.280 1.00 30.88 A
ATOM 4384 CE3 TRP A 552 -21.345 -35.625 -45.775 1.00 31.15 A
ATOM 4385 CD1 TRP A 552 -20.399 -36.550 -42.390 1.00 32.16 A
ATOM 4386 NE1 TRP A 552 -19.206 -36.199 -42.982 1.00 31.05 A
ATOM 4387 CZ2 TRP A 552 -18.560 -35.402 -45.272 1.00 29.55 A
ATOM 4388 CZ3 TRP A 552 -20.463 -35.203 -46.757 1.00 28.79 A
ATOM 4389 CH2 TRP A 552 -19.087 -35.096 -46.500 1.00 28.84 A
ATOM 4390 C TRP A 552 -23.282 -38.302 -44.758 1.00 32.02 A
ATOM 4391 O TRP A 552 -24.173 -38.167 -45.604 1.00 32.80 A
ATOM 4392 N GLN A 553 -22.171 -38.913 -45.020 1.00 32.51 A
ATOM 4393 CA GLN A 553 -21.772 -39.118 -46.347 1.00 32.38 A
ATOM 4394 CB GLN A 553 -20.358 -39.527 -46.327 1.00 29.30 A
ATOM 4395 CG GLN A 553 -19.774 -39.316 -45.079 1.00 29.37 A
ATOM 4396 CD GLN A 553 -18.381 -39.023 -45.159 1.00 31.64 A
ATOM 4397 OE1 GLN A 553 -17.970 -38.134 -45.818 1.00 33.64 A
ATOM 4398 NE2 GLN A 553 -17.633 -39.712 -44.440 1.00 32.32 A
ATOM 4399 C GLN A 553 -22.615 -40.121 -47.006 1.00 34.38 A
ATOM 4400 O GLN A 553 -22.602 -40.200 -48.159 1.00 36.53 A
ATOM 4401 N GLU A 554 -23.381 -40.888 -46.250 1.00 35.52 A
ATOM 4402 CA GLU A 554 -24.466 -41.751 -46.739 1.00 35.47 A
ATOM 4403 CB GLU A 554 -24.577 -43.005 -45.876 1.00 35.47 A
ATOM 4404 CG GLU A 554 -23.670 -44.134 -46.307 1.00 37.05 A
ATOM 4405 CD GLU A 554 -23.624 -45.267 -45.293 1.00 38.51 A
ATOM 4406 OE1 GLU A 554 -24.677 -45.565 -44.669 1.00 38.37 A
ATOM 4407 OE2 GLU A 554 -22.533 -45.865 -45.132 1.00 38.33 A
ATOM 4408 C GLU A 554 -25.824 -41.055 -46.775 1.00 34.92 A
ATOM 4409 O GLU A 554 -26.534 -41.106 -47.775 1.00 35.11 A
ATOM 4410 N VAL A 555 -26.187 -40.413 -45.674 1.00 33.96 A
ATOM 4411 CA VAL A 555 -27.456 -39.710 -45.604 1.00 33.42 A
ATOM 4412 CB VAL A 555 -27.607 -39.033 -44.244 1.00 32.99 A
ATOM 4413 CG1 VAL A 555 -29.044 -38.602 -44.031 1.00 33.19 A
ATOM 4414 CG2 VAL A 555 -27.157 -39.989 -43.161 1.00 33.03 A
ATOM 4415 C VAL A 555 -27.513 -38.662 -46.714 1.00 33.13 A
ATOM 4416 O VAL A 555 -28.586 -38.274 -47.172 1.00 31.30 A

ATOM 4417 N LEU A 556 -26.341 -38.208 -47.143 1.00 33.88 A
ATOM 4418 CA LEU A 556 -26.262 -37.223 -48.213 1.00 34.54 A
ATOM 4419 CB LEU A 556 -24.878 -36.556 -48.228 1.00 30.87 A
ATOM 4420 CG LEU A 556 -24.660 -35.441 -49.257 1.00 26.08 A
ATOM 4421 CD1 LEU A 556 -25.774 -34.418 -49.159 1.00 23.27 A
ATOM 4422 CD2 LEU A 556 -23.317 -34.789 -49.015 1.00 25.07 A
ATOM 4423 C LEU A 556 -26.538 -37.914 -49.557 1.00 36.26 A
ATOM 4424 O LEU A 556 -27.387 -37.463 -50.336 1.00 36.12 A
ATOM 4425 N LYS A 557 -25.833 -39.017 -49.818 1.00 37.08 A
ATOM 4426 CA LYS A 557 -26.021 -39.753 -51.060 1.00 37.81 A
ATOM 4427 CB LYS A 557 -25.208 -41.046 -51.051 1.00 38.58 A
ATOM 4428 CG LYS A 557 -25.098 -41.700 -52.427 1.00 40.17 A
ATOM 4429 CD LYS A 557 -23.977 -42.730 -52.466 1.00 40.16 A
ATOM 4430 CE LYS A 557 -23.497 -42.963 -53.883 1.00 40.05 A
ATOM 4431 NZ LYS A 557 -22.163 -43.630 -53.898 1.00 41.51 A
ATOM 4432 C LYS A 557 -27.496 -40.069 -51.285 1.00 38.35 A
ATOM 4433 O LYS A 557 -28.039 -39.751 -52.336 1.00 39.42 A
ATOM 4434 N ASP A 558 -28.149 -40.685 -50.304 1.00 38.40 A
ATOM 4435 CA ASP A 558 -29.567 -41.009 -50.436 1.00 38.70 A
ATOM 4436 CB ASP A 558 -30.138 -41.530 -49.113 1.00 41.45 A
ATOM 4437 CG ASP A 558 -29.797 -42.988 -48.854 1.00 43.30 A
ATOM 4438 OD1 ASP A 558 -28.601 -43.347 -48.909 1.00 43.83 A
ATOM 4439 OD2 ASP A 558 -30.729 -43.781 -48.584 1.00 45.51 A
ATOM 4440 C ASP A 558 -30.378 -39.793 -50.862 1.00 37.89 A
ATOM 4441 O ASP A 558 -31.229 -39.878 -51.739 1.00 39.11 A
ATOM 4442 N MET A 559 -30.101 -38.651 -50.252 1.00 36.74 A
ATOM 4443 CA MET A 559 -30.857 -37.451 -50.563 1.00 36.08 A
ATOM 4444 CB MET A 559 -30.832 -36.498 -49.372 1.00 35.23 A
ATOM 4445 CG MET A 559 -31.526 -35.184 -49.641 1.00 33.32 A
ATOM 4446 SD MET A 559 -30.816 -33.837 -48.703 1.00 34.42 A
ATOM 4447 CE MET A 559 -32.264 -32.714 -48.592 1.00 34.45 A
ATOM 4448 C MET A 559 -30.439 -36.678 -51.799 1.00 36.27 A
ATOM 4449 O MET A 559 -31.290 -36.214 -52.541 1.00 37.04 A
ATOM 4450 N VAL A 560 -29.140 -36.514 -52.015 1.00 36.42 A

ATOM 4451 CA VAL A 560 -28.679 -35.737 -53.157 1.00 36.76 A
ATOM 4452 CB VAL A 560 -27.699 -34.646 -52.693 1.00 37.57 A
ATOM 4453 CG1 VAL A 560 -27.073 -33.930 -53.892 1.00 39.11 A
ATOM 4454 CG2 VAL A 560 -28.444 -33.648 -51.829 1.00 37.61 A
ATOM 4455 C VAL A 560 -28.054 -36.538 -54.294 1.00 37.22 A
ATOM 4456 O VAL A 560 -28.033 -36.085 -55.437 1.00 37.49 A
ATOM 4457 N GLY A 561 -27.558 -37.729 -53.993 1.00 37.69 A
ATOM 4458 CA GLY A 561 -26.957 -38.537 -55.033 1.00 37.89 A
ATOM 4459 C GLY A 561 -25.451 -38.397 -55.033 1.00 39.63 A
ATOM 4460 O GLY A 561 -24.759 -38.963 -55.884 1.00 39.91 A
ATOM 4461 N LEU A 562 -24.929 -37.648 -54.069 1.00 40.38 A
ATOM 4462 CA LEU A 562 -23.490 -37.453 -53.995 1.00 40.49 A
ATOM 4463 CB LEU A 562 -23.141 -35.996 -54.281 1.00 40.15 A
ATOM 4464 CG LEU A 562 -22.278 -35.771 -55.522 1.00 38.21 A
ATOM 4465 CD1 LEU A 562 -22.013 -34.279 -55.672 1.00 38.58 A
ATOM 4466 CD2 LEU A 562 -20.974 -36.530 -55.397 1.00 37.81 A
ATOM 4467 C LEU A 562 -22.847 -37.876 -52.682 1.00 40.88 A
ATOM 4468 O LEU A 562 -23.404 -37.703 -51.604 1.00 41.96 A
ATOM 4469 N ASP A 563 -21.651 -38.430 -52.808 1.00 41.70 A
ATOM 4470 CA ASP A 563 -20.858 -38.897 -51.685 1.00 41.52 A
ATOM 4471 CB ASP A 563 -19.703 -39.747 -52.206 1.00 44.46 A
ATOM 4472 CG ASP A 563 -19.740 -41.162 -51.690 1.00 47.87 A
ATOM 4473 OD1 ASP A 563 -20.654 -41.918 -52.094 1.00 50.42 A
ATOM 4474 OD2 ASP A 563 -18.850 -41.521 -50.882 1.00 50.12 A
ATOM 4475 C ASP A 563 -20.267 -37.745 -50.875 1.00 40.90 A
ATOM 4476 O ASP A 563 -19.759 -37.974 -49.783 1.00 40.76 A
ATOM 4477 N ALA A 564 -20.308 -36.520 -51.404 1.00 40.56 A
ATOM 4478 CA ALA A 564 -19.720 -35.392 -50.684 1.00 40.46 A
ATOM 4479 CB ALA A 564 -18.222 -35.431 -50.848 1.00 40.73 A
ATOM 4480 C ALA A 564 -20.222 -33.998 -51.047 1.00 40.57 A
ATOM 4481 O ALA A 564 -21.196 -33.846 -51.793 1.00 41.16 A
ATOM 4482 N LEU A 565 -19.545 -32.986 -50.493 1.00 39.99 A
ATOM 4483 CA LEU A 565 -19.867 -31.577 -50.746 1.00 39.32 A
ATOM 4484 CB LEU A 565 -19.061 -30.667 -49.824 1.00 39.32 A

ATOM 4485 CG LEU A 565 -19.600 -30.446 -48.417 1.00 38.64 A
ATOM 4486 CD1 LEU A 565 -18.531 -29.822 -47.548 1.00 36.75 A
ATOM 4487 CD2 LEU A 565 -20.821 -29.561 -48.493 1.00 38.36 A
ATOM 4488 C LEU A 565 -19.535 -31.249 -52.193 1.00 39.34 A
ATOM 4489 O LEU A 565 -18.527 -31.709 -52.729 1.00 39.75 A
ATOM 4490 N ASP A 566 -20.383 -30.446 -52.819 1.00 39.00 A
ATOM 4491 CA ASP A 566 -20.205 -30.087 -54.218 1.00 38.57 A
ATOM 4492 CB ASP A 566 -21.020 -31.047 -55.099 1.00 41.07 A
ATOM 4493 CG ASP A 566 -20.621 -30.991 -56.573 1.00 43.49 A
ATOM 4494 OD1 ASP A 566 -19.428 -31.235 -56.875 1.00 45.98 A
ATOM 4495 OD2 ASP A 566 -21.500 -30.719 -57.429 1.00 42.49 A
ATOM 4496 C ASP A 566 -20.684 -28.666 -54.421 1.00 37.25 A
ATOM 4497 O ASP A 566 -21.771 -28.294 -53.971 1.00 36.53 A
ATOM 4498 N ALA A 567 -19.874 -27.865 -55.100 1.00 36.23 A
ATOM 4499 CA ALA A 567 -20.249 -26.478 -55.345 1.00 36.56 A
ATOM 4500 CB ALA A 567 -19.020 -25.586 -55.320 1.00 35.28 A
ATOM 4501 C ALA A 567 -20.980 -26.318 -56.670 1.00 36.76 A
ATOM 4502 O ALA A 567 -21.542 -25.257 -56.946 1.00 37.78 A
ATOM 4503 N GLN A 568 -20.876 -27.308 -57.498 1.00 36.41 A
ATOM 4504 CA GLN A 568 -21.680 -27.373 -58.645 1.00 37.22 A
ATOM 4505 CB GLN A 568 -21.602 -28.736 -59.257 1.00 40.15 A
ATOM 4506 CG GLN A 568 -20.424 -28.904 -60.220 1.00 46.32 A
ATOM 4507 CD GLN A 568 -20.439 -30.185 -61.066 1.00 49.52 A
ATOM 4508 OE1 GLN A 568 -19.679 -30.298 -61.998 1.00 51.19 A
ATOM 4509 NE2 GLN A 568 -21.291 -31.111 -60.752 1.00 49.78 A
ATOM 4510 C GLN A 568 -23.057 -26.835 -58.577 1.00 35.58 A
ATOM 4511 O GLN A 568 -23.371 -25.974 -59.261 1.00 35.56 A
ATOM 4512 N PRO A 569 -23.922 -27.381 -57.796 1.00 33.57 A
ATOM 4513 CD PRO A 569 -23.674 -28.464 -56.833 1.00 32.71 A
ATOM 4514 CA PRO A 569 -25.308 -26.910 -57.699 1.00 31.89 A
ATOM 4515 CB PRO A 569 -25.954 -27.919 -56.748 1.00 30.76 A
ATOM 4516 CG PRO A 569 -24.837 -28.303 -55.878 1.00 32.42 A
ATOM 4517 C PRO A 569 -25.424 -25.472 -57.211 1.00 30.38 A
ATOM 4518 O PRO A 569 -26.486 -24.856 -57.317 1.00 30.62 A

ATOM 4519 N LEU A 570 -24.323 -24.943 -56.685 1.00 28.88 A
ATOM 4520 CA LEU A 570 -24.276 -23.572 -56.184 1.00 27.54 A
ATOM 4521 CB LEU A 570 -23.195 -23.463 -55.094 1.00 28.82 A
ATOM 4522 CG LEU A 570 -22.585 -22.122 -54.677 1.00 28.45 A
ATOM 4523 CD1 LEU A 570 -23.635 -21.047 -54.597 1.00 29.24 A
ATOM 4524 CD2 LEU A 570 -21.910 -22.297 -53.338 1.00 30.17 A
ATOM 4525 C LEU A 570 -23.975 -22.647 -57.351 1.00 25.68 A
ATOM 4526 O LEU A 570 -24.564 -21.580 -57.490 1.00 24.41 A
ATOM 4527 N LEU A 571 -23.055 -23.088 -58.198 1.00 25.15 A
ATOM 4528 CA LEU A 571 -22.647 -22.344 -59.379 1.00 24.44 A
ATOM 4529 CB LEU A 571 -21.480 -23.076 -60.040 1.00 23.38 A
ATOM 4530 CG LEU A 571 -20.314 -23.285 -59.071 1.00 21.69 A
ATOM 4531 CD1 LEU A 571 -19.214 -24.082 -59.734 1.00 22.99 A
ATOM 4532 CD2 LEU A 571 -19.787 -21.936 -58.613 1.00 18.93 A
ATOM 4533 C LEU A 571 -23.835 -22.232 -60.329 1.00 24.74 A
ATOM 4534 O LEU A 571 -24.047 -21.200 -60.966 1.00 23.72 A
ATOM 4535 N LYS A 572 -24.608 -23.309 -60.398 1.00 25.06 A
ATOM 4536 CA LYS A 572 -25.802 -23.381 -61.225 1.00 25.39 A
ATOM 4537 CB LYS A 572 -26.331 -24.820 -61.212 1.00 25.47 A
ATOM 4538 CG LYS A 572 -27.797 -24.985 -61.612 1.00 26.69 A
ATOM 4539 CD LYS A 572 -28.360 -26.323 -61.121 1.00 29.14 A
ATOM 4540 CE LYS A 572 -27.823 -27.513 -61.899 1.00 30.91 A
ATOM 4541 NZ LYS A 572 -28.763 -27.923 -62.986 1.00 31.97 A
ATOM 4542 C LYS A 572 -26.875 -22.417 -60.703 1.00 26.09 A
ATOM 4543 O LYS A 572 -27.677 -21.889 -61.469 1.00 25.40 A
ATOM 4544 N TYR A 573 -26.890 -22.191 -59.394 1.00 26.67 A
ATOM 4545 CA TYR A 573 -27.869 -21.291 -58.804 1.00 27.18 A
ATOM 4546 CB TYR A 573 -27.796 -21.336 -57.272 1.00 26.16 A
ATOM 4547 CG TYR A 573 -28.849 -20.499 -56.560 1.00 24.43 A
ATOM 4548 CD1 TYR A 573 -30.057 -21.064 -56.147 1.00 23.61 A
ATOM 4549 CE1 TYR A 573 -31.050 -20.284 -55.557 1.00 22.31 A
ATOM 4550 CD2 TYR A 573 -28.664 -19.129 -56.356 1.00 23.50 A
ATOM 4551 CE2 TYR A 573 -29.651 -18.343 -55.771 1.00 22.00 A
ATOM 4552 CZ TYR A 573 -30.840 -18.924 -55.376 1.00 22.66 A

ATOM 4553 OH TYR A 573 -31.826 -18.142 -54.814 1.00 21.99 A
ATOM 4554 C TYR A 573 -27.621 -19.860 -59.272 1.00 28.87 A
ATOM 4555 O TYR A 573 -28.519 -19.211 -59.806 1.00 30.92 A
ATOM 4556 N PHE A 574 -26.399 -19.378 -59.072 1.00 29.72 A
ATOM 4557 CA PHE A 574 -26.075 -17.980 -59.334 1.00 31.82 A
ATOM 4558 CB PHE A 574 -24.916 -17.524 -58.446 1.00 30.39 A
ATOM 4559 CG PHE A 574 -25.277 -17.400 -56.993 1.00 29.94 A
ATOM 4560 CD1 PHE A 574 -24.958 -18.408 -56.098 1.00 29.90 A
ATOM 4561 CD2 PHE A 574 -25.937 -16.277 -56.523 1.00 29.44 A
ATOM 4562 CE1 PHE A 574 -25.290 -18.297 -54.761 1.00 29.15 A
ATOM 4563 CE2 PHE A 574 -26.271 -16.161 -55.187 1.00 30.19 A
ATOM 4564 CZ PHE A 574 -25.947 -17.173 -54.305 1.00 30.65 A
ATOM 4565 C PHE A 574 -25.730 -17.755 -60.803 1.00 33.75 A
ATOM 4566 O PHE A 574 -25.151 -16.730 -61.164 1.00 33.71 A
ATOM 4567 N GLN A 575 -25.949 -18.677 -61.676 1.00 35.97 A
ATOM 4568 CA GLN A 575 -25.174 -18.614 -62.886 1.00 37.07 A
ATOM 4569 CB GLN A 575 -25.603 -19.614 -63.877 1.00 37.27 A
ATOM 4570 CG GLN A 575 -24.541 -20.018 -64.743 1.00 38.94 A
ATOM 4571 CD GLN A 575 -24.519 -21.413 -64.873 1.00 41.24 A
ATOM 4572 OE1 GLN A 575 -25.528 -22.000 -65.112 1.00 42.36 A
ATOM 4573 NE2 GLN A 575 -23.396 -21.987 -64.678 1.00 40.35 A
ATOM 4574 C GLN A 575 -25.295 -17.359 -63.584 1.00 37.79 A
ATOM 4575 O GLN A 575 -24.361 -16.904 -64.126 1.00 37.54 A
ATOM 4576 N PRO A 576 -26.482 -16.819 -63.658 1.00 38.00 A
ATOM 4577 CD PRO A 576 -27.762 -17.460 -63.310 1.00 38.94 A
ATOM 4578 CA PRO A 576 -26.666 -15.667 -64.545 1.00 36.92 A
ATOM 4579 CB PRO A 576 -28.169 -15.397 -64.450 1.00 36.94 A
ATOM 4580 CG PRO A 576 -28.765 -16.729 -64.160 1.00 39.57 A
ATOM 4581 C PRO A 576 -25.883 -14.448 -64.066 1.00 36.37 A
ATOM 4582 O PRO A 576 -25.077 -13.900 -64.819 1.00 37.47 A
ATOM 4583 N VAL A 577 -26.121 -14.034 -62.827 1.00 35.25 A
ATOM 4584 CA VAL A 577 -25.401 -12.909 -62.243 1.00 33.71 A
ATOM 4585 CB VAL A 577 -25.911 -12.587 -60.827 1.00 33.58 A
ATOM 4586 CG1 VAL A 577 -25.383 -13.603 -59.825 1.00 33.24 A

ATOM 4587 CG2 VAL A 577 -25.512 -11.175 -60.425 1.00 33.14 A
ATOM 4588 C VAL A 577 -23.902 -13.187 -62.183 1.00 32.37 A
ATOM 4589 O VAL A 577 -23.089 -12.263 -62.194 1.00 31.50 A
ATOM 4590 N THR A 578 -23.545 -14.465 -62.118 1.00 30.79 A
ATOM 4591 CA THR A 578 -22.137 -14.874 -62.112 1.00 30.70 A
ATOM 4592 CB THR A 578 -21.972 -16.415 -62.088 1.00 32.00 A
ATOM 4593 OG1 THR A 578 -22.225 -16.912 -60.769 1.00 32.60 A
ATOM 4594 CG2 THR A 578 -20.553 -16.811 -62.523 1.00 31.30 A
ATOM 4595 C THR A 578 -21.456 -14.386 -63.377 1.00 29.66 A
ATOM 4596 O THR A 578 -20.321 -13.907 -63.360 1.00 29.88 A
ATOM 4597 N GLN A 579 -22.157 -14.538 -64.485 1.00 28.21 A
ATOM 4598 CA GLN A 579 -21.623 -14.118 -65.755 1.00 27.07 A
ATOM 4599 CB GLN A 579 -22.349 -14.848 -66.881 1.00 28.54 A
ATOM 4600 CG GLN A 579 -21.443 -15.711 -67.754 1.00 30.37 A
ATOM 4601 CD GLN A 579 -20.793 -16.840 -66.989 1.00 31.95 A
ATOM 4602 OE1 GLN A 579 -21.475 -17.666 -66.361 1.00 31.51 A
ATOM 4603 NE2 GLN A 579 -19.465 -16.892 -67.041 1.00 32.32 A
ATOM 4604 C GLN A 579 -21.802 -12.615 -65.893 1.00 26.12 A
ATOM 4605 O GLN A 579 -20.938 -11.931 -66.435 1.00 26.25 A
ATOM 4606 N TRP A 580 -22.920 -12.106 -65.380 1.00 25.28 A
ATOM 4607 CA TRP A 580 -23.231 -10.680 -65.454 1.00 24.40 A
ATOM 4608 CB TRP A 580 -24.592 -10.388 -64.837 1.00 25.33 A
ATOM 4609 CG TRP A 580 -24.967 -8.939 -64.925 1.00 25.88 A
ATOM 4610 CD2 TRP A 580 -24.711 -7.931 -63.947 1.00 27.17 A
ATOM 4611 CE2 TRP A 580 -25.195 -6.708 -64.471 1.00 26.50 A
ATOM 4612 CE3 TRP A 580 -24.117 -7.936 -62.682 1.00 27.87 A
ATOM 4613 CD1 TRP A 580 -25.579 -8.312 -65.970 1.00 25.36 A
ATOM 4614 NE1 TRP A 580 -25.721 -6.971 -65.707 1.00 25.53 A
ATOM 4615 CZ2 TRP A 580 -25.109 -5.511 -63.775 1.00 26.77 A
ATOM 4616 CZ3 TRP A 580 -24.030 -6.747 -61.991 1.00 29.98 A
ATOM 4617 CH2 TRP A 580 -24.523 -5.546 -62.541 1.00 29.15 A
ATOM 4618 C TRP A 580 -22.199 -9.817 -64.759 1.00 24.40 A
ATOM 4619 O TRP A 580 -21.709 -8.846 -65.336 1.00 24.06 A
ATOM 4620 N LEU A 581 -21.890 -10.154 -63.510 1.00 24.30 A

ATOM 4621 CA LEU A 581 -20.906 -9.400 -62.745 1.00 22.28 A
ATOM 4622 CB LEU A 581 -20.770 -9.993 -61.338 1.00 19.79 A
ATOM 4623 CG LEU A 581 -21.872 -9.624 -60.341 1.00 16.53 A
ATOM 4624 CD1 LEU A 581 -21.722 -10.445 -59.071 1.00 11.65 A
ATOM 4625 CD2 LEU A 581 -21.797 -8.121 -60.051 1.00 13.00 A
ATOM 4626 C LEU A 581 -19.566 -9.424 -63.467 1.00 22.52 A
ATOM 4627 O LEU A 581 -18.944 -8.389 -63.694 1.00 21.61 A
ATOM 4628 N GLN A 582 -19.104 -10.577 -63.779 1.00 24.14 A
ATOM 4629 CA GLN A 582 -17.938 -10.790 -64.543 1.00 26.12 A
ATOM 4630 CB GLN A 582 -17.915 -12.253 -64.855 1.00 25.87 A
ATOM 4631 CG GLN A 582 -16.679 -12.958 -64.637 1.00 26.45 A
ATOM 4632 CD GLN A 582 -16.743 -14.290 -65.071 1.00 27.48 A
ATOM 4633 OE1 GLN A 582 -15.847 -14.768 -65.605 1.00 28.08 A
ATOM 4634 NE2 GLN A 582 -17.804 -14.905 -64.853 1.00 27.82 A
ATOM 4635 C GLN A 582 -17.796 -9.973 -65.764 1.00 27.32 A
ATOM 4636 O GLN A 582 -16.756 -9.527 -66.032 1.00 28.70 A
ATOM 4637 N GLU A 583 -18.838 -9.833 -66.550 1.00 28.10 A
ATOM 4638 CA GLU A 583 -18.875 -8.973 -67.729 1.00 28.29 A
ATOM 4639 CB GLU A 583 -20.133 -9.254 -68.567 1.00 29.77 A
ATOM 4640 CG GLU A 583 -20.277 -8.351 -69.800 1.00 32.20 A
ATOM 4641 CD GLU A 583 -19.389 -8.755 -70.982 1.00 33.73 A
ATOM 4642 OE1 GLU A 583 -18.291 -9.329 -70.780 1.00 33.02 A
ATOM 4643 OE2 GLU A 583 -19.795 -8.470 -72.130 1.00 35.04 A
ATOM 4644 C GLU A 583 -18.830 -7.502 -67.361 1.00 27.34 A
ATOM 4645 O GLU A 583 -18.180 -6.721 -68.041 1.00 26.86 A
ATOM 4646 N GLN A 584 -19.518 -7.135 -66.281 1.00 27.16 A
ATOM 4647 CA GLN A 584 -19.570 -5.750 -65.813 1.00 26.73 A
ATOM 4648 CB GLN A 584 -20.544 -5.612 -64.641 1.00 26.26 A
ATOM 4649 CG GLN A 584 -21.998 -5.626 -65.040 1.00 28.23 A
ATOM 4650 CD GLN A 584 -22.372 -4.411 -65.864 1.00 29.96 A
ATOM 4651 OE1 GLN A 584 -22.299 -3.267 -65.387 1.00 29.56 A
ATOM 4652 NE2 GLN A 584 -22.771 -4.645 -67.112 1.00 30.43 A
ATOM 4653 C GLN A 584 -18.228 -5.203 -65.379 1.00 26.45 A
ATOM 4654 O GLN A 584 -17.850 -4.093 -65.761 1.00 26.75 A

ATOM 4655 N ASN A 585 -17.510 -5.980 -64.573 1.00 26.22 A
ATOM 4656 CA ASN A 585 -16.212 -5.539 -64.059 1.00 26.73 A
ATOM 4657 CB ASN A 585 -15.654 -6.538 -63.028 1.00 26.93 A
ATOM 4658 CG ASN A 585 -16.498 -6.614 -61.769 1.00 25.15 A
ATOM 4659 OD1 ASN A 585 -16.959 -5.592 -61.266 1.00 24.88 A
ATOM 4660 ND2 ASN A 585 -16.689 -7.823 -61.249 1.00 23.32 A
ATOM 4661 C ASN A 585 -15.204 -5.340 -65.165 1.00 26.33 A
ATOM 4662 O ASN A 585 -14.513 -4.321 -65.218 1.00 26.21 A
ATOM 4663 N GLN A 586 -15.081 -6.269 -66.051 1.00 26.16 A
ATOM 4664 CA GLN A 586 -14.193 -6.124 -67.170 1.00 26.25 A
ATOM 4665 CB GLN A 586 -14.357 -7.302 -68.067 1.00 26.28 A
ATOM 4666 CG GLN A 586 -13.187 -7.712 -68.837 1.00 28.40 A
ATOM 4667 CD GLN A 586 -13.094 -7.031 -70.183 1.00 31.43 A
ATOM 4668 OE1 GLN A 586 -14.052 -6.867 -70.882 1.00 30.94 A
ATOM 4669 NE2 GLN A 586 -11.934 -6.666 -70.523 1.00 31.92 A
ATOM 4670 C GLN A 586 -14.470 -4.867 -67.875 1.00 25.95 A
ATOM 4671 O GLN A 586 -13.668 -4.015 -67.918 1.00 25.77 A
ATOM 4672 N GLN A 587 -15.631 -4.712 -68.426 1.00 25.45 A
ATOM 4673 CA GLN A 587 -15.850 -3.493 -69.192 1.00 25.83 A
ATOM 4674 CB GLN A 587 -17.312 -3.347 -69.628 1.00 24.59 A
ATOM 4675 CG GLN A 587 -18.125 -4.602 -69.535 1.00 25.62 A
ATOM 4676 CD GLN A 587 -19.299 -4.628 -70.497 1.00 25.90 A
ATOM 4677 OE1 GLN A 587 -19.144 -4.994 -71.656 1.00 28.21 A
ATOM 4678 NE2 GLN A 587 -20.479 -4.239 -70.021 1.00 26.35 A
ATOM 4679 C GLN A 587 -15.428 -2.273 -68.370 1.00 26.63 A
ATOM 4680 O GLN A 587 -14.654 -1.438 -68.844 1.00 27.64 A
ATOM 4681 N ASN A 588 -15.911 -2.116 -67.185 1.00 26.37 A
ATOM 4682 CA ASN A 588 -15.525 -0.994 -66.381 1.00 25.51 A
ATOM 4683 CB ASN A 588 -16.490 -0.874 -65.238 1.00 26.51 A
ATOM 4684 CG ASN A 588 -17.773 -0.287 -65.620 1.00 28.12 A
ATOM 4685 OD1 ASN A 588 -18.003 0.856 -65.470 1.00 29.79 A
ATOM 4686 ND2 ASN A 588 -18.638 -1.082 -66.087 1.00 29.14 A
ATOM 4687 C ASN A 588 -14.129 -1.060 -65.833 1.00 23.78 A
ATOM 4688 O ASN A 588 -13.815 -0.406 -64.943 1.00 24.20 A

ATOM 4689 N GLY A 589 -13.290 -1.883 -66.369 1.00 22.64 A
ATOM 4690 CA GLY A 589 -11.889 -1.967 -65.979 1.00 22.40 A
ATOM 4691 C GLY A 589 -11.493 -2.263 -64.542 1.00 23.13 A
ATOM 4692 O GLY A 589 -10.353 -1.995 -64.150 1.00 22.13 A
ATOM 4693 N GLU A 590 -12.409 -2.818 -63.754 1.00 23.77 A
ATOM 4694 CA GLU A 590 -12.114 -3.159 -62.358 1.00 23.91 A
ATOM 4695 CB GLU A 590 -13.314 -3.869 -61.702 1.00 24.72 A
ATOM 4696 CG GLU A 590 -14.491 -2.967 -61.410 1.00 25.46 A
ATOM 4697 CD GLU A 590 -14.032 -1.618 -60.910 1.00 27.80 A
ATOM 4698 OE1 GLU A 590 -13.125 -1.571 -60.049 1.00 29.68 A
ATOM 4699 OE2 GLU A 590 -14.572 -0.600 -61.377 1.00 29.62 A
ATOM 4700 C GLU A 590 -10.891 -4.063 -62.217 1.00 23.01 A
ATOM 4701 O GLU A 590 -10.376 -4.594 -63.198 1.00 22.59 A
ATOM 4702 N VAL A 591 -10.429 -4.220 -60.984 1.00 22.69 A
ATOM 4703 CA VAL A 591 -9.299 -5.089 -60.693 1.00 22.33 A
ATOM 4704 CB VAL A 591 -8.105 -4.325 -60.057 1.00 21.36 A
ATOM 4705 CG1 VAL A 591 -6.995 -5.309 -59.687 1.00 20.78 A
ATOM 4706 CG2 VAL A 591 -7.563 -3.303 -61.014 1.00 22.39 A
ATOM 4707 C VAL A 591 -9.777 -6.128 -59.682 1.00 22.85 A
ATOM 4708 O VAL A 591 -10.099 -5.785 -58.545 1.00 23.91 A
ATOM 4709 N LEU A 592 -9.850 -7.388 -60.093 1.00 22.75 A
ATOM 4710 CA LEU A 592 -10.273 -8.419 -59.162 1.00 22.24 A
ATOM 4711 CB LEU A 592 -10.523 -9.739 -59.895 1.00 20.48 A
ATOM 4712 CG LEU A 592 -11.584 -9.633 -60.991 1.00 21.02 A
ATOM 4713 CD1 LEU A 592 -11.820 -11.009 -61.620 1.00 18.66 A
ATOM 4714 CD2 LEU A 592 -12.882 -9.060 -60.412 1.00 19.20 A
ATOM 4715 C LEU A 592 -9.154 -8.579 -58.134 1.00 22.73 A
ATOM 4716 O LEU A 592 -8.013 -8.879 -58.486 1.00 22.22 A
ATOM 4717 N GLY A 593 -9.493 -8.376 -56.866 1.00 23.72 A
ATOM 4718 CA GLY A 593 -8.555 -8.599 -55.783 1.00 24.39 A
ATOM 4719 C GLY A 593 -8.060 -7.305 -55.169 1.00 24.68 A
ATOM 4720 O GLY A 593 -8.429 -6.214 -55.606 1.00 24.14 A
ATOM 4721 N TRP A 594 -7.219 -7.430 -54.150 1.00 25.24 A
ATOM 4722 CA TRP A 594 -6.435 -6.307 -53.652 1.00 25.37 A

```
ATOM  4723  CB  TRP A 594     -6.699  -6.108 -52.160  1.00 24.18      A
ATOM  4724  CG  TRP A 594     -7.074  -7.377 -51.462  1.00 22.76      A
ATOM  4725  CD2 TRP A 594     -8.218  -8.195 -51.727  1.00 19.95      A
ATOM  4726  CE2 TRP A 594     -8.168  -9.289 -50.840  1.00 20.25      A
ATOM  4727  CE3 TRP A 594     -9.287  -8.114 -52.625  1.00 17.34      A
ATOM  4728  CD1 TRP A 594     -6.390  -7.993 -50.454  1.00 22.71      A
ATOM  4729  NE1 TRP A 594     -7.042  -9.141 -50.073  1.00 22.24      A
ATOM  4730  CZ2 TRP A 594     -9.140 -10.287 -50.825  1.00 17.38      A
ATOM  4731  CZ3 TRP A 594     -10.250  -9.106 -52.609  1.00 15.88      A
ATOM  4732  CH2 TRP A 594     -10.170 -10.178 -51.716  1.00 15.40      A
ATOM  4733  C   TRP A 594     -4.950  -6.567 -53.882  1.00 26.34      A
ATOM  4734  O   TRP A 594     -4.362  -7.453 -53.257  1.00 29.44      A
ATOM  4735  N   PRO A 595     -4.346  -5.793 -54.777  1.00 25.15      A
ATOM  4736  CD  PRO A 595     -5.038  -5.242 -55.956  1.00 24.93      A
ATOM  4737  CA  PRO A 595     -2.890  -5.814 -54.950  1.00 24.29      A
ATOM  4738  CB  PRO A 595     -2.707  -5.402 -56.413  1.00 23.44      A
ATOM  4739  CG  PRO A 595     -3.922  -4.608 -56.732  1.00 24.15      A
ATOM  4740  C   PRO A 595     -2.198  -4.814 -54.031  1.00 24.14      A
ATOM  4741  O   PRO A 595     -1.061  -5.041 -53.619  1.00 23.50      A
ATOM  4742  N   GLU A 596     -2.883  -3.719 -53.715  1.00 24.08      A
ATOM  4743  CA  GLU A 596     -2.395  -2.770 -52.722  1.00 23.76      A
ATOM  4744  CB  GLU A 596     -2.888  -1.358 -53.043  1.00 23.78      A
ATOM  4745  CG  GLU A 596     -2.254  -0.747 -54.282  1.00 27.03      A
ATOM  4746  CD  GLU A 596     -2.600   0.719 -54.450  1.00 28.65      A
ATOM  4747  OE1 GLU A 596     -3.172   1.309 -53.509  1.00 30.60      A
ATOM  4748  OE2 GLU A 596     -2.301   1.283 -55.524  1.00 28.49      A
ATOM  4749  C   GLU A 596     -2.830  -3.171 -51.316  1.00 24.12      A
ATOM  4750  O   GLU A 596     -3.460  -2.390 -50.603  1.00 23.58      A
ATOM  4751  N   TYR A 597     -2.488  -4.394 -50.923  1.00 24.18      A
ATOM  4752  CA  TYR A 597     -2.719  -4.855 -49.551  1.00 22.41      A
ATOM  4753  CB  TYR A 597     -2.150  -6.267 -49.384  1.00 21.40      A
ATOM  4754  CG  TYR A 597     -0.653  -6.297 -49.472  1.00 20.52      A
ATOM  4755  CD1 TYR A 597      0.120  -5.914 -48.390  1.00 22.43      A
ATOM  4756  CE1 TYR A 597      1.505  -5.852 -48.470  1.00 23.20      A
```

ATOM 4757 CD2 TYR A 597 -0.004 -6.629 -50.651 1.00 21.96 A
ATOM 4758 CE2 TYR A 597 1.389 -6.570 -50.745 1.00 22.63 A
ATOM 4759 CZ TYR A 597 2.135 -6.180 -49.641 1.00 22.77 A
ATOM 4760 OH TYR A 597 3.507 -6.127 -49.665 1.00 21.93 A
ATOM 4761 C TYR A 597 -1.871 -3.844 -48.787 1.00 21.79 A
ATOM 4762 O TYR A 597 -1.057 -3.141 -49.399 1.00 24.79 A
ATOM 4763 N GLN A 598 -2.034 -3.748 -47.477 1.00 20.07 A
ATOM 4764 CA GLN A 598 -1.238 -2.781 -46.715 1.00 19.86 A
ATOM 4765 CB GLN A 598 0.215 -2.733 -47.242 1.00 17.95 A
ATOM 4766 CG GLN A 598 1.138 -1.710 -46.574 1.00 19.57 A
ATOM 4767 CD GLN A 598 2.606 -1.839 -47.013 1.00 22.24 A
ATOM 4768 OE1 GLN A 598 3.470 -1.096 -46.556 1.00 20.34 A
ATOM 4769 NE2 GLN A 598 2.885 -2.791 -47.898 1.00 24.70 A
ATOM 4770 C GLN A 598 -1.838 -1.379 -46.737 1.00 18.63 A
ATOM 4771 O GLN A 598 -1.391 -0.525 -45.989 1.00 20.57 A
ATOM 4772 N TRP A 599 -2.840 -1.138 -47.581 1.00 16.87 A
ATOM 4773 CA TRP A 599 -3.463 0.176 -47.648 1.00 17.34 A
ATOM 4774 CB TRP A 599 -4.126 0.420 -48.998 1.00 14.85 A
ATOM 4775 CG TRP A 599 -4.924 1.715 -49.038 1.00 13.15 A
ATOM 4776 CD2 TRP A 599 -6.340 1.870 -48.819 1.00 12.61 A
ATOM 4777 CE2 TRP A 599 -6.616 3.253 -48.849 1.00 11.73 A
ATOM 4778 CE3 TRP A 599 -7.397 0.975 -48.596 1.00 12.39 A
ATOM 4779 CD1 TRP A 599 -4.429 2.970 -49.193 1.00 13.43 A
ATOM 4780 NE1 TRP A 599 -5.432 3.898 -49.080 1.00 13.08 A
ATOM 4781 CZ2 TRP A 599 -7.904 3.768 -48.664 1.00 10.88 A
ATOM 4782 CZ3 TRP A 599 -8.683 1.490 -48.411 1.00 12.53 A
ATOM 4783 CH2 TRP A 599 -8.920 2.875 -48.446 1.00 11.35 A
ATOM 4784 C TRP A 599 -4.540 0.333 -46.587 1.00 21.33 A
ATOM 4785 O TRP A 599 -5.339 -0.586 -46.376 1.00 22.64 A
ATOM 4786 N HIS A 600 -4.576 1.499 -45.935 1.00 23.11 A
ATOM 4787 CA HIS A 600 -5.589 1.764 -44.933 1.00 23.61 A
ATOM 4788 CB HIS A 600 -5.015 1.642 -43.526 1.00 23.42 A
ATOM 4789 CG HIS A 600 -4.704 0.235 -43.118 1.00 24.52 A
ATOM 4790 CD2 HIS A 600 -5.379 -0.632 -42.325 1.00 25.01 A

ATOM 4791 ND1 HIS A 600 -3.585 -0.441 -43.560 1.00 24.98 A
ATOM 4792 CE1 HIS A 600 -3.582 -1.663 -43.056 1.00 25.67 A
ATOM 4793 NE2 HIS A 600 -4.661 -1.804 -42.304 1.00 27.07 A
ATOM 4794 C HIS A 600 -6.174 3.145 -45.118 1.00 24.86 A
ATOM 4795 O HIS A 600 -5.479 4.086 -45.480 1.00 24.64 A
ATOM 4796 N PRO A 601 -7.480 3.281 -44.867 1.00 26.30 A
ATOM 4797 CD PRO A 601 -8.418 2.255 -44.375 1.00 25.90 A
ATOM 4798 CA PRO A 601 -8.159 4.563 -45.006 1.00 27.16 A
ATOM 4799 CB PRO A 601 -9.626 4.170 -44.923 1.00 26.61 A
ATOM 4800 CG PRO A 601 -9.602 3.080 -43.919 1.00 24.21 A
ATOM 4801 C PRO A 601 -7.763 5.463 -43.861 1.00 28.60 A
ATOM 4802 O PRO A 601 -7.460 4.985 -42.773 1.00 29.64 A
ATOM 4803 N PRO A 602 -7.756 6.780 -44.089 1.00 29.79 A
ATOM 4804 CD PRO A 602 -7.958 7.416 -45.402 1.00 29.35 A
ATOM 4805 CA PRO A 602 -7.406 7.786 -43.079 1.00 30.76 A
ATOM 4806 CB PRO A 602 -7.022 8.985 -43.932 1.00 30.16 A
ATOM 4807 CG PRO A 602 -7.999 8.884 -45.048 1.00 30.18 A
ATOM 4808 C PRO A 602 -8.626 8.078 -42.182 1.00 30.93 A
ATOM 4809 O PRO A 602 -9.755 7.749 -42.544 1.00 30.56 A
ATOM 4810 N LEU A 603 -8.449 8.795 -41.109 1.00 31.81 A
ATOM 4811 CA LEU A 603 -9.572 8.991 -40.277 1.00 33.57 A
ATOM 4812 CB LEU A 603 -9.163 9.391 -38.904 1.00 33.75 A
ATOM 4813 CG LEU A 603 -8.353 8.445 -38.107 1.00 35.18 A
ATOM 4814 CD1 LEU A 603 -7.812 9.165 -37.029 1.00 34.73 A
ATOM 4815 CD2 LEU A 603 -9.256 7.503 -37.588 1.00 36.50 A
ATOM 4816 C LEU A 603 -10.324 10.089 -40.783 1.00 34.61 A
ATOM 4817 O LEU A 603 -9.815 10.867 -41.477 1.00 33.86 A
ATOM 4818 N PRO A 604 -11.601 10.158 -40.421 1.00 36.13 A
ATOM 4819 CD PRO A 604 -12.419 9.046 -39.906 1.00 37.13 A
ATOM 4820 CA PRO A 604 -12.383 11.386 -40.587 1.00 38.71 A
ATOM 4821 CB PRO A 604 -13.660 11.089 -39.800 1.00 37.28 A
ATOM 4822 CG PRO A 604 -13.813 9.611 -39.890 1.00 38.37 A
ATOM 4823 C PRO A 604 -11.670 12.596 -39.992 1.00 42.28 A
ATOM 4824 O PRO A 604 -10.740 12.436 -39.201 1.00 43.26 A

ATOM 4825 N ASP A 605 -12.106 13.792 -40.373 1.00 46.22 A
ATOM 4826 CA ASP A 605 -11.237 14.963 -40.364 1.00 49.85 A
ATOM 4827 CB ASP A 605 -11.967 16.177 -40.941 1.00 52.55 A
ATOM 4828 CG ASP A 605 -11.598 16.447 -42.386 1.00 56.03 A
ATOM 4829 OD1 ASP A 605 -11.342 15.475 -43.127 1.00 58.27 A
ATOM 4830 OD2 ASP A 605 -11.538 17.597 -42.869 1.00 55.38 A
ATOM 4831 C ASP A 605 -10.741 15.270 -38.955 1.00 50.73 A
ATOM 4832 O ASP A 605 -9.658 15.828 -38.776 1.00 52.03 A
ATOM 4833 N ASN A 606 -11.539 14.901 -37.959 1.00 49.99 A
ATOM 4834 CA ASN A 606 -11.482 15.547 -36.653 1.00 49.37 A
ATOM 4835 CB ASN A 606 -12.243 16.874 -36.678 1.00 49.35 A
ATOM 4836 CG ASN A 606 -11.361 18.057 -36.329 1.00 49.40 A
ATOM 4837 OD1 ASN A 606 -10.154 17.911 -36.134 1.00 47.80 A
ATOM 4838 ND2 ASN A 606 -11.961 19.239 -36.250 1.00 50.01 A
ATOM 4839 C ASN A 606 -12.026 14.652 -35.544 1.00 49.33 A
ATOM 4840 O ASN A 606 -13.010 14.990 -34.887 1.00 49.38 A
ATOM 4841 N TYR A 607 -11.378 13.510 -35.341 1.00 48.23 A
ATOM 4842 CA TYR A 607 -12.077 12.288 -34.963 1.00 47.20 A
ATOM 4843 CB TYR A 607 -11.829 11.186 -35.995 1.00 43.84 A
ATOM 4844 CG TYR A 607 -12.574 9.902 -35.712 1.00 40.46 A
ATOM 4845 CD1 TYR A 607 -13.913 9.765 -36.053 1.00 39.31 A
ATOM 4846 CE1 TYR A 607 -14.600 8.594 -35.797 1.00 37.91 A
ATOM 4847 CD2 TYR A 607 -11.940 8.827 -35.105 1.00 39.08 A
ATOM 4848 CE2 TYR A 607 -12.618 7.651 -34.845 1.00 38.02 A
ATOM 4849 CZ TYR A 607 -13.948 7.540 -35.193 1.00 38.36 A
ATOM 4850 OH TYR A 607 -14.628 6.371 -34.937 1.00 38.19 A
ATOM 4851 C TYR A 607 -11.652 11.814 -33.577 1.00 49.21 A
ATOM 4852 O TYR A 607 -10.500 11.434 -33.368 1.00 49.55 A
ATOM 4853 N PRO A 608 -12.589 11.837 -32.636 1.00 50.72 A
ATOM 4854 CD PRO A 608 -12.041 10.852 -31.687 1.00 50.76 A
ATOM 4855 CA PRO A 608 -13.999 11.579 -32.947 1.00 52.91 A
ATOM 4856 CB PRO A 608 -14.239 10.195 -32.340 1.00 51.54 A
ATOM 4857 CG PRO A 608 -13.259 10.105 -31.224 1.00 50.50 A
ATOM 4858 C PRO A 608 -14.920 12.604 -32.295 1.00 55.88 A

ATOM 4859 O PRO A 608 -15.386 12.391 -31.176 1.00 56.24 A
ATOM 4860 N ALA A 609 -15.176 13.705 -32.994 1.00 59.30 A
ATOM 4861 CA ALA A 609 -16.201 14.655 -32.579 1.00 61.97 A
ATOM 4862 CB ALA A 609 -15.570 15.826 -31.840 1.00 59.71 A
ATOM 4863 C ALA A 609 -17.011 15.151 -33.773 1.00 64.52 A
ATOM 4864 O ALA A 609 -16.555 16.007 -34.532 1.00 65.49 A
ATOM 4865 N GLY A 610 -18.213 14.607 -33.934 1.00 66.84 A
ATOM 4866 CA GLY A 610 -18.876 14.591 -35.225 1.00 69.46 A
ATOM 4867 C GLY A 610 -20.381 14.561 -35.038 1.00 71.87 A
ATOM 4868 O GLY A 610 -20.900 15.044 -34.032 1.00 73.10 A
ATOM 4869 N ALA A 611 -21.081 13.991 -36.013 1.00 73.56 A
ATOM 4870 CA ALA A 611 -22.464 13.572 -35.818 1.00 75.56 A
ATOM 4871 CB ALA A 611 -23.315 14.135 -36.946 1.00 75.02 A
ATOM 4872 C ALA A 611 -22.641 12.061 -35.719 1.00 76.97 A
ATOM 4873 O ALA A 611 -22.846 11.383 -36.726 1.00 77.36 A
ATOM 4874 N ALA A 612 -22.559 11.539 -34.499 1.00 77.67 A
ATOM 4875 CA ALA A 612 -21.337 10.910 -34.014 1.00 77.73 A
ATOM 4876 CB ALA A 612 -21.669 9.767 -33.067 1.00 76.94 A
ATOM 4877 C ALA A 612 -20.477 10.412 -35.171 1.00 77.77 A
ATOM 4878 O ALA A 612 -19.412 10.965 -35.448 1.00 77.11 A
ATOM 4879 ZN+2 ZN2 A 701 -27.749 -21.950 -36.694 1.00 31.58 A
ATOM 4880 CL CL A 702 -27.997 -18.440 -91.633 1.00 37.15 A
ATOM 4881 C1 NAG A 691 -2.656 0.205 -29.595 1.00 42.25 A
ATOM 4882 C2 NAG A 691 -1.485 1.001 -29.153 1.00 41.75 A
ATOM 4883 C3 NAG A 691 -2.114 1.986 -28.304 1.00 43.62 A
ATOM 4884 C4 NAG A 691 -2.940 2.962 -28.971 1.00 45.06 A
ATOM 4885 C5 NAG A 691 -4.088 2.162 -29.383 1.00 44.59 A
ATOM 4886 C6 NAG A 691 -4.770 3.098 -30.312 1.00 44.13 A
ATOM 4887 C7 NAG A 691 -0.347 -0.600 -27.831 1.00 41.96 A
ATOM 4888 C8 NAG A 691 -0.334 -1.075 -26.654 1.00 41.29 A
ATOM 4889 N2 NAG A 691 -1.199 0.302 -28.002 1.00 41.51 A
ATOM 4890 O3 NAG A 691 -1.197 2.696 -27.526 1.00 44.90 A
ATOM 4891 O4 NAG A 691 -3.264 3.946 -28.002 1.00 46.21 A
ATOM 4892 O5 NAG A 691 -3.686 1.023 -30.082 1.00 43.99 A

ATOM 4893 O6 NAG A 691 -4.754 4.380 -29.685 1.00 44.45 A
ATOM 4894 O7 NAG A 691 0.377 -0.980 -28.643 1.00 43.03 A
ATOM 4895 C1 NAG A 692 -34.269 -12.671 -13.273 1.00 63.56 A
ATOM 4896 C2 NAG A 692 -34.229 -12.631 -11.772 1.00 64.49 A
ATOM 4897 C3 NAG A 692 -34.947 -13.777 -11.168 1.00 64.22 A
ATOM 4898 C4 NAG A 692 -36.333 -13.672 -11.711 1.00 63.84 A
ATOM 4899 C5 NAG A 692 -36.280 -13.595 -13.216 1.00 62.95 A
ATOM 4900 C6 NAG A 692 -37.605 -13.487 -13.905 1.00 61.07 A
ATOM 4901 C7 NAG A 692 -32.270 -13.676 -10.711 1.00 64.23 A
ATOM 4902 C8 NAG A 692 -32.980 -14.689 -10.404 1.00 63.59 A
ATOM 4903 N2 NAG A 692 -32.852 -12.712 -11.363 1.00 65.15 A
ATOM 4904 O3 NAG A 692 -35.045 -13.606 -9.759 1.00 63.03 A
ATOM 4905 O4 NAG A 692 -36.991 -14.825 -11.227 1.00 64.82 A
ATOM 4906 O5 NAG A 692 -35.617 -12.414 -13.490 1.00 62.81 A
ATOM 4907 O6 NAG A 692 -37.828 -12.112 -14.039 1.00 59.24 A
ATOM 4908 O7 NAG A 692 -31.123 -13.642 -10.443 1.00 63.59 A
ATOM 4909 C1 NAG A 693 -34.477 -42.696 -23.324 1.00 58.53 A
ATOM 4910 C2 NAG A 693 -35.699 -41.795 -23.191 1.00 58.49 A
ATOM 4911 C3 NAG A 693 -36.964 -42.523 -23.630 1.00 57.95 A
ATOM 4912 C4 NAG A 693 -36.768 -43.187 -24.987 1.00 58.71 A
ATOM 4913 C5 NAG A 693 -35.481 -44.004 -25.016 1.00 58.21 A
ATOM 4914 C6 NAG A 693 -35.246 -44.604 -26.397 1.00 57.38 A
ATOM 4915 C7 NAG A 693 -35.806 -42.606 -20.909 1.00 60.85 A
ATOM 4916 C8 NAG A 693 -35.964 -42.315 -19.631 1.00 60.71 A
ATOM 4917 N2 NAG A 693 -35.860 -41.586 -21.760 1.00 58.86 A
ATOM 4918 O3 NAG A 693 -38.049 -41.592 -23.705 1.00 56.80 A
ATOM 4919 O4 NAG A 693 -37.882 -44.043 -25.265 1.00 59.25 A
ATOM 4920 O5 NAG A 693 -34.379 -43.169 -24.666 1.00 58.94 A
ATOM 4921 O6 NAG A 693 -34.034 -45.366 -26.386 1.00 54.16 A
ATOM 4922 O7 NAG A 693 -35.620 -43.758 -21.263 1.00 61.99 A
ATOM 4923 C1 NAG A 694 -39.567 -42.058 -22.933 1.00 68.25 A
ATOM 4924 C2 NAG A 694 -40.705 -41.687 -22.007 1.00 68.16 A
ATOM 4925 C3 NAG A 694 -41.719 -42.766 -21.825 1.00 67.96 A
ATOM 4926 C4 NAG A 694 -42.350 -42.900 -23.140 1.00 68.00 A

ATOM 4927 C5 NAG A 694 -41.230 -43.316 -23.993 1.00 67.98 A
ATOM 4928 C6 NAG A 694 -41.799 -43.349 -25.349 1.00 68.09 A
ATOM 4929 C7 NAG A 694 -39.966 -40.544 -20.061 1.00 65.37 A
ATOM 4930 C8 NAG A 694 -39.269 -40.754 -19.058 1.00 65.62 A
ATOM 4931 N2 NAG A 694 -40.022 -41.610 -20.774 1.00 66.47 A
ATOM 4932 O3 NAG A 694 -42.727 -42.236 -21.005 1.00 67.28 A
ATOM 4933 O4 NAG A 694 -43.327 -43.904 -23.056 1.00 68.33 A
ATOM 4934 O5 NAG A 694 -40.179 -42.368 -24.135 1.00 69.20 A
ATOM 4935 O6 NAG A 694 -40.635 -43.547 -26.130 1.00 68.13 A
ATOM 4936 O7 NAG A 694 -40.424 -39.468 -20.184 1.00 64.59 A
ATOM 4937 C1 NAG A 695 -15.374 -13.838 -13.994 1.00 67.83 A
ATOM 4938 C2 NAG A 695 -14.178 -14.613 -13.421 1.00 67.87 A
ATOM 4939 C3 NAG A 695 -14.382 -15.025 -11.956 1.00 67.82 A
ATOM 4940 C4 NAG A 695 -15.092 -13.946 -11.110 1.00 67.67 A
ATOM 4941 C5 NAG A 695 -16.291 -13.421 -11.872 1.00 67.30 A
ATOM 4942 C6 NAG A 695 -17.075 -12.361 -11.147 1.00 67.41 A
ATOM 4943 C7 NAG A 695 -12.804 -16.128 -14.727 1.00 67.19 A
ATOM 4944 C8 NAG A 695 -12.059 -17.299 -14.106 1.00 66.22 A
ATOM 4945 N2 NAG A 695 -13.989 -15.819 -14.208 1.00 67.85 A
ATOM 4946 O3 NAG A 695 -13.113 -15.308 -11.389 1.00 67.82 A
ATOM 4947 O4 NAG A 695 -15.524 -14.503 -9.876 1.00 67.46 A
ATOM 4948 O5 NAG A 695 -15.843 -12.847 -13.092 1.00 66.86 A
ATOM 4949 O6 NAG A 695 -18.092 -11.833 -11.987 1.00 68.27 A
ATOM 4950 O7 NAG A 695 -12.305 -15.522 -15.673 1.00 67.16 A
ATOM 4951 C1 NAG A 696 -3.891 5.074 -27.035 1.00102.35 A
ATOM 4952 C2 NAG A 696 -3.388 6.568 -27.106 1.00102.66 A
ATOM 4953 C3 NAG A 696 -3.831 7.253 -25.770 1.00102.62 A
ATOM 4954 C4 NAG A 696 -5.375 7.216 -25.734 1.00102.43 A
ATOM 4955 C5 NAG A 696 -5.832 5.693 -25.728 1.00102.39 A
ATOM 4956 C6 NAG A 696 -7.292 5.492 -25.676 1.00102.27 A
ATOM 4957 C7 NAG A 696 -1.211 7.219 -28.116 1.00103.23 A
ATOM 4958 C8 NAG A 696 0.233 7.137 -27.992 1.00102.86 A
ATOM 4959 N2 NAG A 696 -1.925 6.588 -27.139 1.00103.15 A
ATOM 4960 O3 NAG A 696 -3.384 8.619 -25.788 1.00102.27 A

ATOM 4961 O4 NAG A 696 -5.827 7.839 -24.519 1.00102.23 A
ATOM 4962 O5 NAG A 696 -5.319 5.086 -26.994 1.00102.41 A
ATOM 4963 O6 NAG A 696 -7.615 4.171 -25.330 1.00102.70 A
ATOM 4964 O7 NAG A 696 -1.709 7.786 -28.990 1.00103.24 A
ATOM 4965 C1 NAG A 697 -48.304 -10.691 -31.326 1.00114.89 A
ATOM 4966 C2 NAG A 697 -48.808 -10.576 -29.834 1.00115.54 A
ATOM 4967 C3 NAG A 697 -48.914 -12.037 -29.285 1.00115.59 A
ATOM 4968 C4 NAG A 697 -49.968 -12.768 -30.144 1.00115.33 A
ATOM 4969 C5 NAG A 697 -49.445 -12.800 -31.645 1.00114.98 A
ATOM 4970 C6 NAG A 697 -50.343 -13.487 -32.592 1.00115.31 A
ATOM 4971 C7 NAG A 697 -48.076 -8.771 -28.290 1.00116.10 A
ATOM 4972 C8 NAG A 697 -46.954 -8.212 -27.555 1.00115.13 A
ATOM 4973 N2 NAG A 697 -47.800 -9.883 -29.032 1.00115.82 A
ATOM 4974 O3 NAG A 697 -49.364 -11.980 -27.920 1.00115.61 A
ATOM 4975 O4 NAG A 697 -50.100 -14.120 -29.670 1.00114.93 A
ATOM 4976 O5 NAG A 697 -49.302 -11.378 -32.082 1.00114.30 A
ATOM 4977 O6 NAG A 697 -49.686 -13.784 -33.797 1.00115.94 A
ATOM 4978 O7 NAG A 697 -49.126 -8.294 -28.239 1.00116.05 A
ATOM 4979 C1 BMA A 900 -44.667 -44.071 -23.041 1.00105.78 A
ATOM 4980 C2 BMA A 900 -45.437 -42.905 -22.415 1.00105.64 A
ATOM 4981 O2 BMA A 900 -45.349 -41.763 -23.267 1.00105.46 A
ATOM 4982 C3 BMA A 900 -46.904 -43.309 -22.243 1.00105.88 A
ATOM 4983 O3 BMA A 900 -47.663 -42.183 -21.799 1.00105.67 A
ATOM 4984 C4 BMA A 900 -47.439 -43.793 -23.596 1.00106.16 A
ATOM 4985 O4 BMA A 900 -48.760 -44.312 -23.430 1.00107.54 A
ATOM 4986 C5 BMA A 900 -46.519 -44.891 -24.131 1.00105.89 A
ATOM 4987 C6 BMA A 900 -47.065 -45.407 -25.465 1.00104.97 A
ATOM 4988 O6 BMA A 900 -46.210 -46.437 -25.965 1.00104.32 A
ATOM 4989 O5 BMA A 900 -45.207 -44.371 -24.325 1.00105.59 A
ATOM 4990 C ACT A 800 -1.026 -18.401 -40.484 1.00 54.57 A
ATOM 4991 O ACT A 800 -0.975 -17.772 -41.626 1.00 54.77 A
ATOM 4992 OXT ACT A 800 -0.105 -19.110 -39.954 1.00 55.42 A
ATOM 4993 CH3 ACT A 800 -2.356 -18.236 -39.753 1.00 51.84 A
ATOM 4994 C1 GOL A2433 -11.417 -6.356 -73.980 1.00 28.25 A

ATOM 4995 O1 GOL A2433 -10.614 -5.261 -74.222 1.00 26.33 A
ATOM 4996 C2 GOL A2433 -12.311 -6.641 -75.118 1.00 28.99 A
ATOM 4997 O2 GOL A2433 -13.475 -7.164 -74.711 1.00 28.06 A
ATOM 4998 C3 GOL A2433 -12.737 -5.379 -75.637 1.00 30.22 A
ATOM 4999 O3 GOL A2433 -13.346 -5.606 -76.838 1.00 27.87 A
ATOM 5000 C1 GOL A2434 -6.493 -11.083 -54.520 1.00 33.16 A
ATOM 5001 O1 GOL A2434 -5.388 -10.288 -54.300 1.00 35.07 A
ATOM 5002 C2 GOL A2434 -6.772 -11.964 -53.371 1.00 33.47 A
ATOM 5003 O2 GOL A2434 -7.311 -13.127 -53.761 1.00 31.95 A
ATOM 5004 C3 GOL A2434 -5.507 -12.397 -52.864 1.00 34.38 A
ATOM 5005 O3 GOL A2434 -5.724 -12.994 -51.655 1.00 29.91 A
ATOM 5006 C ACT A 801 -23.630 -15.606 -37.570 1.00 39.60 A
ATOM 5007 O ACT A 801 -22.537 -16.066 -38.117 1.00 38.76 A
ATOM 5008 OXT ACT A 801 -23.875 -14.398 -37.239 1.00 40.11 A
ATOM 5009 CH3 ACT A 801 -24.689 -16.678 -37.326 1.00 37.10 A
ATOM 5010 C ACT B 801 -16.292 -23.491 -90.598 1.00 55.71 B
ATOM 5011 O ACT B 801 -15.020 -23.630 -90.853 1.00 56.05 B
ATOM 5012 OXT ACT B 801 -16.906 -22.409 -90.307 1.00 55.98 B
ATOM 5013 CH3 ACT B 801 -17.077 -24.798 -90.672 1.00 54.50 B
ATOM 5014 ZN+2 ZN2 B 701 -22.723 -27.770 -91.593 1.00 29.74 B
ATOM 5015 CL CL B 703 -18.098 -27.730 -36.933 1.00 30.54 B
ATOM 5016 N ALA B 2 -38.012 -26.571 -119.812 1.00 52.55 B
ATOM 5017 CA ALA B 2 -39.222 -26.174 -120.521 1.00 52.71 B
ATOM 5018 CB ALA B 2 -39.770 -24.876 -119.947 1.00 51.48 B
ATOM 5019 C ALA B 2 -40.280 -27.271 -120.466 1.00 53.65 B
ATOM 5020 O ALA B 2 -39.956 -28.452 -120.343 1.00 52.07 B
ATOM 5021 N PRO B 3 -41.544 -26.872 -120.559 1.00 55.09 B
ATOM 5022 CD PRO B 3 -41.623 -25.599 -121.296 1.00 54.55 B
ATOM 5023 CA PRO B 3 -42.618 -27.797 -120.937 1.00 55.17 B
ATOM 5024 CB PRO B 3 -43.441 -26.985 -121.941 1.00 54.73 B
ATOM 5025 CG PRO B 3 -42.498 -25.955 -122.457 1.00 54.66 B
ATOM 5026 C PRO B 3 -43.483 -28.179 -119.740 1.00 54.78 B
ATOM 5027 O PRO B 3 -44.118 -27.313 -119.138 1.00 53.82 B
ATOM 5028 N GLY B 4 -43.503 -29.465 -119.405 1.00 54.86 B

ATOM 5029 CA GLY B 4 -44.281 -29.947-118.279 1.00 55.34 B
ATOM 5030 C GLY B 4 -44.103 -28.934-117.165 1.00 55.83 B
ATOM 5031 O GLY B 4 -44.991 -28.750-116.332 1.00 56.40 B
ATOM 5032 N LEU B 5 -42.950 -28.274-117.150 1.00 55.59 B
ATOM 5033 CA LEU B 5 -42.434 -27.659-115.933 1.00 53.55 B
ATOM 5034 CB LEU B 5 -40.945 -27.474-116.230 1.00 49.69 B
ATOM 5035 CG LEU B 5 -40.081 -28.736-116.177 1.00 48.03 B
ATOM 5036 CD1 LEU B 5 -38.603 -28.378-116.200 1.00 46.32 B
ATOM 5037 CD2 LEU B 5 -40.417 -29.566-114.948 1.00 47.27 B
ATOM 5038 C LEU B 5 -43.043 -26.342-115.466 1.00 53.87 B
ATOM 5039 O LEU B 5 -42.473 -25.646-114.626 1.00 54.92 B
ATOM 5040 N GLN B 6 -44.205 -26.005-116.017 1.00 54.78 B
ATOM 5041 CA GLN B 6 -44.722 -24.688-115.921 1.00 55.58 B
ATOM 5042 CB GLN B 6 -45.062 -24.190-117.280 1.00 55.83 B
ATOM 5043 CG GLN B 6 -43.999 -23.475-117.913 1.00 56.58 B
ATOM 5044 CD GLN B 6 -43.947 -23.741-119.328 1.00 57.43 B
ATOM 5045 OE1 GLN B 6 -44.435 -22.971-120.110 1.00 58.66 B
ATOM 5046 NE2 GLN B 6 -43.352 -24.838-119.696 1.00 57.55 B
ATOM 5047 C GLN B 6 -45.947 -24.761-115.151 1.00 56.30 B
ATOM 5048 O GLN B 6 -46.575 -25.767-115.099 1.00 55.49 B
ATOM 5049 N PRO B 7 -46.298 -23.664-114.544 1.00 57.56 B
ATOM 5050 CD PRO B 7 -45.535 -22.411-114.386 1.00 57.46 B
ATOM 5051 CA PRO B 7 -47.528 -23.624-113.759 1.00 59.00 B
ATOM 5052 CB PRO B 7 -47.292 -22.443-112.825 1.00 58.23 B
ATOM 5053 CG PRO B 7 -46.531 -21.505-113.696 1.00 57.87 B
ATOM 5054 C PRO B 7 -48.813 -23.474-114.564 1.00 60.29 B
ATOM 5055 O PRO B 7 -49.064 -22.428-115.170 1.00 59.73 B
ATOM 5056 N GLY B 8 -49.621 -24.530-114.569 1.00 61.70 B
ATOM 5057 CA GLY B 8 -50.889 -24.469-115.260 1.00 62.99 B
ATOM 5058 C GLY B 8 -51.685 -23.407-114.532 1.00 64.39 B
ATOM 5059 O GLY B 8 -51.243 -22.903-113.500 1.00 65.52 B
ATOM 5060 N ALA B 9 -52.854 -23.068-115.066 1.00 65.21 B
ATOM 5061 CA ALA B 9 -53.715 -22.064-114.452 1.00 65.89 B
ATOM 5062 CB ALA B 9 -54.630 -21.441-115.495 1.00 65.51 B

ATOM 5063 C ALA B 9 -54.533 -22.662-113.312 1.00 66.35 B
ATOM 5064 O ALA B 9 -55.752 -22.797-113.414 1.00 67.27 B
ATOM 5065 N PHE B 10 -53.854 -23.018-112.227 1.00 66.12 B
ATOM 5066 CA PHE B 10 -54.527 -23.493-111.024 1.00 65.35 B
ATOM 5067 CB PHE B 10 -53.503 -23.911-109.966 1.00 61.40 B
ATOM 5068 CG PHE B 10 -52.683 -25.108-110.356 1.00 57.57 B
ATOM 5069 CD1 PHE B 10 -51.410 -24.951-110.879 1.00 55.45 B
ATOM 5070 CD2 PHE B 10 -53.184 -26.389-110.200 1.00 56.75 B
ATOM 5071 CE1 PHE B 10 -50.653 -26.050-111.239 1.00 55.89 B
ATOM 5072 CE2 PHE B 10 -52.432 -27.492-110.558 1.00 56.98 B
ATOM 5073 CZ PHE B 10 -51.165 -27.322-111.078 1.00 56.71 B
ATOM 5074 C PHE B 10 -55.460 -22.429-110.457 1.00 67.11 B
ATOM 5075 O PHE B 10 -55.086 -21.263-110.333 1.00 67.71 B
ATOM 5076 N ALA B 11 -56.678 -22.838-110.115 1.00 68.67 B
ATOM 5077 CA ALA B 11 -57.707 -21.902-109.680 1.00 70.27 B
ATOM 5078 CB ALA B 11 -58.896 -22.652-109.100 1.00 68.57 B
ATOM 5079 C ALA B 11 -57.155 -20.909-108.663 1.00 71.71 B
ATOM 5080 O ALA B 11 -56.225 -21.219-107.918 1.00 72.90 B
ATOM 5081 N ALA B 12 -57.733 -19.712-108.638 1.00 72.92 B
ATOM 5082 CA ALA B 12 -57.859 -18.947-107.403 1.00 74.07 B
ATOM 5083 CB ALA B 12 -58.040 -17.469-107.710 1.00 72.91 B
ATOM 5084 C ALA B 12 -59.011 -19.500-106.570 1.00 75.73 B
ATOM 5085 O ALA B 12 -60.156 -19.071-106.716 1.00 77.85 B
ATOM 5086 N ALA B 13 -58.701 -20.453-105.697 1.00 76.25 B
ATOM 5087 CA ALA B 13 -59.416 -20.599-104.435 1.00 75.92 B
ATOM 5088 CB ALA B 13 -60.097 -21.956-104.349 1.00 75.43 B
ATOM 5089 C ALA B 13 -58.368 -20.453-103.337 1.00 75.80 B
ATOM 5090 O ALA B 13 -57.430 -19.668-103.462 1.00 75.94 B
ATOM 5091 N GLU B 14 -58.537 -21.216-102.261 1.00 74.83 B
ATOM 5092 CA GLU B 14 -57.429 -21.541-101.372 1.00 73.72 B
ATOM 5093 CB GLU B 14 -57.877 -21.346 -99.922 1.00 74.12 B
ATOM 5094 CG GLU B 14 -57.058 -22.129 -98.908 1.00 73.92 B
ATOM 5095 CD GLU B 14 -57.272 -21.644 -97.488 1.00 74.21 B
ATOM 5096 OE1 GLU B 14 -57.842 -20.546 -97.312 1.00 74.20 B

ATOM 5097 OE2 GLU B 14 -56.871 -22.360 -96.547 1.00 74.30 B
ATOM 5098 C GLU B 14 -56.850 -22.940-101.558 1.00 73.11 B
ATOM 5099 O GLU B 14 -55.634 -23.130-101.530 1.00 73.96 B
ATOM 5100 N ALA B 15 -57.731 -23.917-101.749 1.00 72.25 B
ATOM 5101 CA ALA B 15 -57.319 -25.246-102.185 1.00 71.72 B
ATOM 5102 CB ALA B 15 -58.323 -26.291-101.722 1.00 71.15 B
ATOM 5103 C ALA B 15 -57.153 -25.302-103.700 1.00 70.77 B
ATOM 5104 O ALA B 15 -56.965 -26.398-104.252 1.00 70.75 B
ATOM 5105 N GLY B 16 -57.212 -24.163-104.343 1.00 69.58 B
ATOM 5106 CA GLY B 16 -56.501 -23.953-105.591 1.00 68.31 B
ATOM 5107 C GLY B 16 -55.011 -23.765-105.384 1.00 67.70 B
ATOM 5108 O GLY B 16 -54.198 -24.288-106.147 1.00 67.48 B
ATOM 5109 N ALA B 17 -54.652 -23.014-104.348 1.00 67.05 B
ATOM 5110 CA ALA B 17 -53.256 -22.828-103.986 1.00 65.80 B
ATOM 5111 CB ALA B 17 -53.135 -21.823-102.843 1.00 64.98 B
ATOM 5112 C ALA B 17 -52.723 -24.186-103.559 1.00 65.24 B
ATOM 5113 O ALA B 17 -51.549 -24.504-103.757 1.00 65.62 B
ATOM 5114 N GLN B 18 -53.594 -25.019-103.051 1.00 64.06 B
ATOM 5115 CA GLN B 18 -53.152 -26.309-102.623 1.00 63.82 B
ATOM 5116 CB GLN B 18 -54.247 -27.059-101.950 1.00 63.41 B
ATOM 5117 CG GLN B 18 -54.334 -26.761-100.555 1.00 63.99 B
ATOM 5118 CD GLN B 18 -53.178 -27.285 -99.803 1.00 64.56 B
ATOM 5119 OE1 GLN B 18 -53.147 -27.199 -98.601 1.00 64.89 B
ATOM 5120 NE2 GLN B 18 -52.217 -27.825-100.495 1.00 63.79 B
ATOM 5121 C GLN B 18 -52.737 -27.095-103.785 1.00 63.64 B
ATOM 5122 O GLN B 18 -51.691 -27.685-103.795 1.00 64.23 B
ATOM 5123 N ALA B 19 -53.613 -27.168-104.763 1.00 63.04 B
ATOM 5124 CA ALA B 19 -53.338 -27.971-105.952 1.00 61.37 B
ATOM 5125 CB ALA B 19 -54.534 -27.927-106.894 1.00 61.30 B
ATOM 5126 C ALA B 19 -52.103 -27.368-106.615 1.00 60.04 B
ATOM 5127 O ALA B 19 -51.296 -28.065-107.242 1.00 58.73 B
ATOM 5128 N PHE B 20 -51.971 -26.054-106.455 1.00 58.60 B
ATOM 5129 CA PHE B 20 -50.840 -25.314-106.991 1.00 57.84 B
ATOM 5130 CB PHE B 20 -50.975 -23.832-106.645 1.00 57.99 B

```
ATOM  5131  CG  PHE B  20     -49.794 -23.012-107.060  1.00 58.34      B
ATOM  5132  CD1 PHE B  20     -49.730 -22.454-108.330  1.00 59.68      B
ATOM  5133  CD2 PHE B  20     -48.720 -22.840-106.205  1.00 58.61      B
ATOM  5134  CE1 PHE B  20     -48.610 -21.738-108.743  1.00 59.80      B
ATOM  5135  CE2 PHE B  20     -47.597 -22.128-106.609  1.00 59.35      B
ATOM  5136  CZ  PHE B  20     -47.543 -21.577-107.881  1.00 59.69      B
ATOM  5137  C   PHE B  20     -49.549 -25.862-106.374  1.00 57.25      B
ATOM  5138  O   PHE B  20     -48.666 -26.346-107.092  1.00 57.78      B
ATOM  5139  N   ALA B  21     -49.450 -25.777-105.045  1.00 55.66      B
ATOM  5140  CA  ALA B  21     -48.284 -26.253-104.301  1.00 54.60      B
ATOM  5141  CB  ALA B  21     -48.451 -25.943-102.828  1.00 55.05      B
ATOM  5142  C   ALA B  21     -48.065 -27.748-104.493  1.00 54.24      B
ATOM  5143  O   ALA B  21     -46.935 -28.239-104.404  1.00 54.07      B
ATOM  5144  N   ALA B  22     -49.185 -28.473-104.702  1.00 53.94      B
ATOM  5145  CA  ALA B  22     -49.107 -29.905-104.968  1.00 53.41      B
ATOM  5146  CB  ALA B  22     -50.501 -30.487-105.148  1.00 53.91      B
ATOM  5147  C   ALA B  22     -48.248 -30.192-106.194  1.00 52.65      B
ATOM  5148  O   ALA B  22     -47.327 -30.966-106.170  1.00 51.91      B
ATOM  5149  N   ALA B  23     -48.549 -29.407-107.268  1.00 51.94      B
ATOM  5150  CA  ALA B  23     -47.814 -29.485-108.544  1.00 51.68      B
ATOM  5151  CB  ALA B  23     -48.618 -28.774-109.678  1.00 51.03      B
ATOM  5152  C   ALA B  23     -46.401 -28.874-108.446  1.00 51.12      B
ATOM  5153  O   ALA B  23     -45.414 -29.521-108.818  1.00 50.79      B
ATOM  5154  N   TYR B  24     -46.304 -27.639-107.954  1.00 49.86      B
ATOM  5155  CA  TYR B  24     -45.007 -26.982-107.813  1.00 49.14      B
ATOM  5156  CB  TYR B  24     -45.090 -25.832-106.811  1.00 49.68      B
ATOM  5157  CG  TYR B  24     -43.726 -25.288-106.425  1.00 50.26      B
ATOM  5158  CD1 TYR B  24     -43.164 -24.207-107.100  1.00 50.10      B
ATOM  5159  CE1 TYR B  24     -41.875 -23.761-106.797  1.00 49.95      B
ATOM  5160  CD2 TYR B  24     -42.963 -25.907-105.427  1.00 50.66      B
ATOM  5161  CE2 TYR B  24     -41.676 -25.470-105.121  1.00 49.95      B
ATOM  5162  CZ  TYR B  24     -41.138 -24.399-105.809  1.00 49.59      B
ATOM  5163  OH  TYR B  24     -39.864 -23.974-105.514  1.00 48.79      B
ATOM  5164  C   TYR B  24     -43.933 -27.950-107.332  1.00 48.54      B
```

ATOM 5165 O TYR B 24 -42.851 -28.048-107.905 1.00 47.92 B
ATOM 5166 N ASN B 25 -44.291 -28.723-106.331 1.00 47.79 B
ATOM 5167 CA ASN B 25 -43.399 -29.676-105.707 1.00 48.42 B
ATOM 5168 CB ASN B 25 -44.137 -30.483-104.674 1.00 48.76 B
ATOM 5169 CG ASN B 25 -43.354 -31.700-104.180 1.00 50.17 B
ATOM 5170 OD1 ASN B 25 -42.261 -31.583-103.608 1.00 50.11 B
ATOM 5171 ND2 ASN B 25 -43.881 -32.861-104.433 1.00 50.41 B
ATOM 5172 C ASN B 25 -42.840 -30.646-106.644 1.00 49.22 B
ATOM 5173 O ASN B 25 -41.685 -30.978-106.588 1.00 48.88 B
ATOM 5174 N SER B 26 -43.708 -31.174-107.482 1.00 49.87 B
ATOM 5175 CA SER B 26 -43.369 -32.229-108.442 1.00 49.71 B
ATOM 5176 CB SER B 26 -44.643 -32.799-109.052 1.00 50.34 B
ATOM 5177 OG SER B 26 -44.320 -33.802-109.997 1.00 53.39 B
ATOM 5178 C SER B 26 -42.462 -31.732-109.556 1.00 49.13 B
ATOM 5179 O SER B 26 -41.587 -32.458-110.039 1.00 48.44 B
ATOM 5180 N SER B 27 -42.698 -30.493-109.972 1.00 47.88 B
ATOM 5181 CA SER B 27 -41.901 -29.873-111.017 1.00 48.23 B
ATOM 5182 CB SER B 27 -42.605 -28.608-111.523 1.00 48.36 B
ATOM 5183 OG SER B 27 -43.979 -28.846-111.788 1.00 46.35 B
ATOM 5184 C SER B 27 -40.551 -29.507-110.397 1.00 48.69 B
ATOM 5185 O SER B 27 -39.493 -29.762-110.975 1.00 49.04 B
ATOM 5186 N ALA B 28 -40.618 -28.921-109.202 1.00 48.59 B
ATOM 5187 CA ALA B 28 -39.447 -28.496-108.438 1.00 47.29 B
ATOM 5188 CB ALA B 28 -39.895 -27.934-107.098 1.00 47.03 B
ATOM 5189 C ALA B 28 -38.412 -29.603-108.221 1.00 46.49 B
ATOM 5190 O ALA B 28 -37.224 -29.398-108.440 1.00 45.72 B
ATOM 5191 N GLU B 29 -38.801 -30.740-107.812 1.00 46.46 B
ATOM 5192 CA GLU B 29 -37.893 -31.804-107.577 1.00 46.37 B
ATOM 5193 CB GLU B 29 -38.701 -33.009-107.153 1.00 47.98 B
ATOM 5194 CG GLU B 29 -38.290 -33.785-105.911 1.00 50.51 B
ATOM 5195 CD GLU B 29 -39.075 -35.049-105.759 1.00 52.32 B
ATOM 5196 OE1 GLU B 29 -40.250 -34.983-105.472 1.00 53.33 B
ATOM 5197 OE2 GLU B 29 -38.527 -36.109-105.937 1.00 53.21 B
ATOM 5198 C GLU B 29 -37.083 -32.114-108.777 1.00 45.28 B

```
ATOM  5199  O   GLU B  29     -36.033 -32.579-108.645  1.00 44.73      B
ATOM  5200  N   GLN B  30     -37.600 -31.920-109.953  1.00 44.58      B
ATOM  5201  CA  GLN B  30     -36.865 -32.169-111.183  1.00 44.92      B
ATOM  5202  CB  GLN B  30     -37.841 -32.240-112.368  1.00 46.05      B
ATOM  5203  CG  GLN B  30     -38.964 -33.266-112.208  1.00 48.19      B
ATOM  5204  CD  GLN B  30     -39.831 -33.390-113.453  1.00 49.32      B
ATOM  5205  OE1 GLN B  30     -39.345 -33.763-114.519  1.00 50.12      B
ATOM  5206  NE2 GLN B  30     -41.120 -33.078-113.323  1.00 48.99      B
ATOM  5207  C   GLN B  30     -35.812 -31.098-111.444  1.00 44.65      B
ATOM  5208  O   GLN B  30     -34.626 -31.394-111.621  1.00 43.93      B
ATOM  5209  N   VAL B  31     -36.258 -29.849-111.467  1.00 44.19      B
ATOM  5210  CA  VAL B  31     -35.374 -28.722-111.713  1.00 43.44      B
ATOM  5211  CB  VAL B  31     -36.204 -27.417-111.863  1.00 41.66      B
ATOM  5212  CG1 VAL B  31     -36.954 -27.131-110.593  1.00 42.68      B
ATOM  5213  CG2 VAL B  31     -35.304 -26.260-112.234  1.00 43.06      B
ATOM  5214  C   VAL B  31     -34.317 -28.594-110.603  1.00 44.24      B
ATOM  5215  O   VAL B  31     -33.183 -28.164-110.852  1.00 45.27      B
ATOM  5216  N   LEU B  32     -34.679 -28.988-109.385  1.00 44.27      B
ATOM  5217  CA  LEU B  32     -33.749 -28.934-108.263  1.00 43.44      B
ATOM  5218  CB  LEU B  32     -34.513 -29.006-106.939  1.00 43.05      B
ATOM  5219  CG  LEU B  32     -35.272 -27.718-106.597  1.00 42.75      B
ATOM  5220  CD1 LEU B  32     -36.415 -28.039-105.666  1.00 43.93      B
ATOM  5221  CD2 LEU B  32     -34.330 -26.684-105.983  1.00 41.86      B
ATOM  5222  C   LEU B  32     -32.722 -30.063-108.363  1.00 43.54      B
ATOM  5223  O   LEU B  32     -31.522 -29.824-108.228  1.00 44.21      B
ATOM  5224  N   PHE B  33     -33.181 -31.290-108.598  1.00 42.66      B
ATOM  5225  CA  PHE B  33     -32.254 -32.402-108.742  1.00 41.35      B
ATOM  5226  CB  PHE B  33     -32.984 -33.679-109.150  1.00 38.10      B
ATOM  5227  CG  PHE B  33     -32.065 -34.852-109.365  1.00 36.01      B
ATOM  5228  CD1 PHE B  33     -31.623 -35.617-108.295  1.00 34.93      B
ATOM  5229  CD2 PHE B  33     -31.604 -35.168-110.633  1.00 34.86      B
ATOM  5230  CE1 PHE B  33     -30.734 -36.678-108.486  1.00 33.37      B
ATOM  5231  CE2 PHE B  33     -30.716 -36.226-110.830  1.00 33.59      B
ATOM  5232  CZ  PHE B  33     -30.283 -36.980-109.753  1.00 32.83      B
```

ATOM 5233 C PHE B 33 -31.285 -32.016-109.856 1.00 42.35 B
ATOM 5234 O PHE B 33 -30.077 -32.256-109.772 1.00 41.76 B
ATOM 5235 N ALA B 34 -31.835 -31.409-110.902 1.00 42.78 B
ATOM 5236 CA ALA B 34 -31.040 -30.987-112.045 1.00 43.77 B
ATOM 5237 CB ALA B 34 -31.923 -30.267-113.058 1.00 42.82 B
ATOM 5238 C ALA B 34 -29.899 -30.077-111.623 1.00 44.38 B
ATOM 5239 O ALA B 34 -28.732 -30.334-111.938 1.00 44.30 B
ATOM 5240 N SER B 35 -30.248 -29.013-110.906 1.00 44.38 B
ATOM 5241 CA SER B 35 -29.271 -28.034-110.456 1.00 44.59 B
ATOM 5242 CB SER B 35 -30.000 -26.825-109.858 1.00 45.78 B
ATOM 5243 OG SER B 35 -29.184 -25.663-109.880 1.00 47.82 B
ATOM 5244 C SER B 35 -28.250 -28.591-109.458 1.00 43.59 B
ATOM 5245 O SER B 35 -27.059 -28.287-109.562 1.00 44.28 B
ATOM 5246 N VAL B 36 -28.707 -29.404-108.505 1.00 41.95 B
ATOM 5247 CA VAL B 36 -27.821 -29.990-107.494 1.00 40.39 B
ATOM 5248 CB VAL B 36 -28.609 -30.762-106.428 1.00 39.58 B
ATOM 5249 CG1 VAL B 36 -27.642 -31.451-105.468 1.00 36.88 B
ATOM 5250 CG2 VAL B 36 -29.527 -29.814-105.679 1.00 38.79 B
ATOM 5251 C VAL B 36 -26.811 -30.949-108.089 1.00 40.71 B
ATOM 5252 O VAL B 36 -25.675 -31.027-107.633 1.00 39.96 B
ATOM 5253 N ALA B 37 -27.246 -31.693-109.098 1.00 41.39 B
ATOM 5254 CA ALA B 37 -26.385 -32.656-109.775 1.00 40.62 B
ATOM 5255 CB ALA B 37 -27.227 -33.581-110.642 1.00 39.52 B
ATOM 5256 C ALA B 37 -25.380 -31.889-110.628 1.00 40.74 B
ATOM 5257 O ALA B 37 -24.226 -32.297-110.780 1.00 39.89 B
ATOM 5258 N ALA B 38 -25.835 -30.767-111.176 1.00 41.60 B
ATOM 5259 CA ALA B 38 -24.995 -29.918-112.009 1.00 42.68 B
ATOM 5260 CB ALA B 38 -25.827 -28.794-112.621 1.00 42.51 B
ATOM 5261 C ALA B 38 -23.884 -29.345-111.146 1.00 42.95 B
ATOM 5262 O ALA B 38 -22.756 -29.160-111.602 1.00 44.56 B
ATOM 5263 N SER B 39 -24.214 -29.065-109.892 1.00 42.49 B
ATOM 5264 CA SER B 39 -23.240 -28.529-108.958 1.00 42.08 B
ATOM 5265 CB SER B 39 -23.951 -27.859-107.786 1.00 42.41 B
ATOM 5266 OG SER B 39 -24.828 -26.847-108.248 1.00 44.05 B

ATOM 5267 C SER B 39 -22.333 -29.646-108.454 1.00 41.88 B
ATOM 5268 O SER B 39 -21.125 -29.462-108.357 1.00 41.65 B
ATOM 5269 N TRP B 40 -22.908 -30.807-108.137 1.00 42.21 B
ATOM 5270 CA TRP B 40 -22.104 -31.927-107.659 1.00 41.85 B
ATOM 5271 CB TRP B 40 -22.960 -33.176-107.409 1.00 42.00 B
ATOM 5272 CG TRP B 40 -22.120 -34.359-107.007 1.00 42.09 B
ATOM 5273 CD2 TRP B 40 -21.790 -34.766-105.672 1.00 42.28 B
ATOM 5274 CE2 TRP B 40 -20.867 -35.829-105.772 1.00 42.93 B
ATOM 5275 CE3 TRP B 40 -22.180 -34.332-104.399 1.00 41.18 B
ATOM 5276 CD1 TRP B 40 -21.411 -35.176-107.835 1.00 42.40 B
ATOM 5277 NE1 TRP B 40 -20.653 -36.059-107.104 1.00 42.64 B
ATOM 5278 CZ2 TRP B 40 -20.324 -36.462-104.651 1.00 43.20 B
ATOM 5279 CZ3 TRP B 40 -21.640 -34.964-103.284 1.00 41.22 B
ATOM 5280 CH2 TRP B 40 -20.723 -36.017-103.420 1.00 41.92 B
ATOM 5281 C TRP B 40 -21.002 -32.271-108.647 1.00 42.30 B
ATOM 5282 O TRP B 40 -19.906 -32.626-108.242 1.00 40.84 B
ATOM 5283 N ALA B 41 -21.297 -32.173-109.939 1.00 44.15 B
ATOM 5284 CA ALA B 41 -20.311 -32.471-110.976 1.00 45.82 B
ATOM 5285 CB ALA B 41 -20.956 -32.384-112.342 1.00 47.01 B
ATOM 5286 C ALA B 41 -19.127 -31.517-110.906 1.00 47.23 B
ATOM 5287 O ALA B 41 -17.982 -31.939-111.034 1.00 47.49 B
ATOM 5288 N HIS B 42 -19.415 -30.232-110.704 1.00 49.24 B
ATOM 5289 CA HIS B 42 -18.384 -29.189-110.605 1.00 50.67 B
ATOM 5290 CB HIS B 42 -19.047 -27.801-110.536 1.00 52.13 B
ATOM 5291 CG HIS B 42 -18.075 -26.660-110.452 1.00 54.64 B
ATOM 5292 CD2 HIS B 42 -17.029 -26.315-111.243 1.00 55.35 B
ATOM 5293 ND1 HIS B 42 -18.141 -25.697-109.466 1.00 56.25 B
ATOM 5294 CE1 HIS B 42 -17.179 -24.810-109.651 1.00 55.97 B
ATOM 5295 NE2 HIS B 42 -16.491 -25.162-110.723 1.00 56.01 B
ATOM 5296 C HIS B 42 -17.466 -29.370-109.389 1.00 50.68 B
ATOM 5297 O HIS B 42 -16.261 -29.574-109.538 1.00 50.30 B
ATOM 5298 N ASP B 43 -18.048 -29.297-108.196 1.00 50.66 B
ATOM 5299 CA ASP B 43 -17.270 -29.280-106.963 1.00 50.96 B
ATOM 5300 CB ASP B 43 -18.188 -29.097-105.753 1.00 50.64 B

ATOM 5301 CG ASP B 43 -18.951 -27.788-105.793 1.00 51.47 B
ATOM 5302 OD1 ASP B 43 -19.919 -27.637-105.018 1.00 50.88 B
ATOM 5303 OD2 ASP B 43 -18.656 -26.852-106.566 1.00 51.69 B
ATOM 5304 C ASP B 43 -16.445 -30.554-106.809 1.00 51.63 B
ATOM 5305 O ASP B 43 -15.338 -30.525-106.272 1.00 51.56 B
ATOM 5306 N THR B 44 -16.992 -31.670-107.280 1.00 53.02 B
ATOM 5307 CA THR B 44 -16.305 -32.953-107.197 1.00 54.36 B
ATOM 5308 CB THR B 44 -17.308 -34.113-107.335 1.00 54.74 B
ATOM 5309 OG1 THR B 44 -18.272 -34.043-106.278 1.00 57.07 B
ATOM 5310 CG2 THR B 44 -16.617 -35.447-107.091 1.00 56.01 B
ATOM 5311 C THR B 44 -15.221 -33.069-108.263 1.00 54.48 B
ATOM 5312 O THR B 44 -14.387 -33.974-108.218 1.00 54.85 B
ATOM 5313 N ASN B 45 -15.238 -32.148-109.220 1.00 54.87 B
ATOM 5314 CA ASN B 45 -14.275 -32.162-110.315 1.00 54.77 B
ATOM 5315 CB ASN B 45 -14.558 -33.331-111.262 1.00 55.85 B
ATOM 5316 CG ASN B 45 -13.603 -33.371-112.438 1.00 57.81 B
ATOM 5317 OD1 ASN B 45 -12.418 -33.068-112.302 1.00 58.60 B
ATOM 5318 ND2 ASN B 45 -14.116 -33.748-113.604 1.00 58.79 B
ATOM 5319 C ASN B 45 -14.268 -30.850-111.092 1.00 54.31 B
ATOM 5320 O ASN B 45 -14.972 -30.704-112.091 1.00 55.11 B
ATOM 5321 N ILE B 46 -13.467 -29.897-110.625 1.00 53.32 B
ATOM 5322 CA ILE B 46 -13.453 -28.558-111.202 1.00 52.23 B
ATOM 5323 CB ILE B 46 -12.720 -27.576-110.268 1.00 52.28 B
ATOM 5324 CG2 ILE B 46 -12.999 -26.139-110.682 1.00 53.29 B
ATOM 5325 CG1 ILE B 46 -13.137 -27.811-108.815 1.00 52.05 B
ATOM 5326 CD1 ILE B 46 -12.513 -26.840-107.837 1.00 51.23 B
ATOM 5327 C ILE B 46 -12.798 -28.558-112.580 1.00 51.88 B
ATOM 5328 O ILE B 46 -11.579 -28.683-112.698 1.00 51.48 B
ATOM 5329 N THR B 47 -13.616 -28.418-113.618 1.00 51.27 B
ATOM 5330 CA THR B 47 -13.121 -28.051-114.939 1.00 49.36 B
ATOM 5331 CB THR B 47 -13.576 -29.082-115.990 1.00 48.57 B
ATOM 5332 OG1 THR B 47 -15.002 -29.218-115.944 1.00 46.98 B
ATOM 5333 CG2 THR B 47 -13.080 -30.472-115.623 1.00 47.03 B
ATOM 5334 C THR B 47 -13.589 -26.656-115.335 1.00 49.58 B

ATOM 5335 O THR B 47 -13.743 -25.778-114.486 1.00 50.94 B
ATOM 5336 N ALA B 48 -13.815 -26.457-116.630 1.00 48.24 B
ATOM 5337 CA ALA B 48 -14.425 -25.231-117.118 1.00 46.89 B
ATOM 5338 CB ALA B 48 -13.529 -24.570-118.114 1.00 45.80 B
ATOM 5339 C ALA B 48 -15.725 -25.637-117.774 1.00 47.35 B
ATOM 5340 O ALA B 48 -16.640 -24.837-117.944 1.00 46.78 B
ATOM 5341 N GLU B 49 -15.876 -26.895-118.004 1.00 48.84 B
ATOM 5342 CA GLU B 49 -17.075 -27.337-118.623 1.00 48.83 B
ATOM 5343 CB GLU B 49 -16.838 -28.598-119.351 1.00 50.26 B
ATOM 5344 CG GLU B 49 -18.145 -29.149-119.789 1.00 53.34 B
ATOM 5345 CD GLU B 49 -18.281 -29.144-121.254 1.00 54.70 B
ATOM 5346 OE1 GLU B 49 -17.881 -30.131-121.837 1.00 56.93 B
ATOM 5347 OE2 GLU B 49 -18.771 -28.164-121.814 1.00 54.66 B
ATOM 5348 C GLU B 49 -18.100 -27.630-117.656 1.00 46.95 B
ATOM 5349 O GLU B 49 -19.221 -27.304-117.823 1.00 45.53 B
ATOM 5350 N ASN B 50 -17.718 -28.327-116.629 1.00 44.90 B
ATOM 5351 CA ASN B 50 -18.694 -28.578-115.590 1.00 42.44 B
ATOM 5352 CB ASN B 50 -18.067 -29.424-114.488 1.00 40.63 B
ATOM 5353 CG ASN B 50 -17.760 -30.827-114.952 1.00 39.27 B
ATOM 5354 OD1 ASN B 50 -18.610 -31.481-115.545 1.00 40.19 B
ATOM 5355 ND2 ASN B 50 -16.550 -31.300-114.683 1.00 36.86 B
ATOM 5356 C ASN B 50 -19.169 -27.249-115.045 1.00 42.45 B
ATOM 5357 O ASN B 50 -20.295 -27.136-114.565 1.00 42.37 B
ATOM 5358 N ALA B 51 -18.298 -26.244-115.144 1.00 42.60 B
ATOM 5359 CA ALA B 51 -18.597 -24.891-114.672 1.00 42.52 B
ATOM 5360 CB ALA B 51 -17.327 -24.058-114.643 1.00 41.75 B
ATOM 5361 C ALA B 51 -19.636 -24.223-115.565 1.00 42.31 B
ATOM 5362 O ALA B 51 -20.491 -23.471-115.089 1.00 41.82 B
ATOM 5363 N ALA B 52 -19.549 -24.499-116.864 1.00 41.98 B
ATOM 5364 CA ALA B 52 -20.481 -23.945-117.832 1.00 41.01 B
ATOM 5365 CB ALA B 52 -19.937 -24.108-119.233 1.00 40.47 B
ATOM 5366 C ALA B 52 -21.791 -24.691-117.682 1.00 41.28 B
ATOM 5367 O ALA B 52 -22.859 -24.125-117.882 1.00 41.39 B
ATOM 5368 N ALA B 53 -21.700 -25.980-117.328 1.00 42.57 B

ATOM 5369 CA ALA B 53 -22.867 -26.828-117.117 1.00 43.00 B
ATOM 5370 CB ALA B 53 -22.454 -28.290-117.047 1.00 41.61 B
ATOM 5371 C ALA B 53 -23.619 -26.425-115.853 1.00 43.73 B
ATOM 5372 O ALA B 53 -24.847 -26.383-115.810 1.00 43.23 B
ATOM 5373 N GLN B 54 -22.957 -26.216-114.750 1.00 44.28 B
ATOM 5374 CA GLN B 54 -23.683 -25.627-113.678 1.00 44.98 B
ATOM 5375 CB GLN B 54 -22.850 -25.405-112.459 1.00 47.10 B
ATOM 5376 CG GLN B 54 -23.633 -24.635-111.420 1.00 51.27 B
ATOM 5377 CD GLN B 54 -22.892 -23.476-110.929 1.00 53.99 B
ATOM 5378 OE1 GLN B 54 -21.720 -23.390-111.181 1.00 56.99 B
ATOM 5379 NE2 GLN B 54 -23.561 -22.544-110.289 1.00 53.73 B
ATOM 5380 C GLN B 54 -24.254 -24.340-114.041 1.00 43.60 B
ATOM 5381 O GLN B 54 -25.396 -24.099-113.825 1.00 43.14 B
ATOM 5382 N GLU B 55 -23.424 -23.457-114.530 1.00 41.89 B
ATOM 5383 CA GLU B 55 -23.952 -22.140-114.873 1.00 41.00 B
ATOM 5384 CB GLU B 55 -22.883 -21.304-115.586 1.00 41.89 B
ATOM 5385 CG GLU B 55 -21.760 -20.845-114.672 1.00 45.11 B
ATOM 5386 CD GLU B 55 -20.838 -19.824-115.319 1.00 46.58 B
ATOM 5387 OE1 GLU B 55 -21.353 -18.802-115.831 1.00 48.54 B
ATOM 5388 OE2 GLU B 55 -19.602 -20.037-115.305 1.00 46.69 B
ATOM 5389 C GLU B 55 -25.215 -22.207-115.726 1.00 39.95 B
ATOM 5390 O GLU B 55 -26.002 -21.257-115.754 1.00 39.02 B
ATOM 5391 N ALA B 56 -25.389 -23.314-116.460 1.00 38.40 B
ATOM 5392 CA ALA B 56 -26.604 -23.483-117.249 1.00 36.55 B
ATOM 5393 CB ALA B 56 -26.387 -24.517-118.343 1.00 36.66 B
ATOM 5394 C ALA B 56 -27.783 -23.880-116.367 1.00 35.55 B
ATOM 5395 O ALA B 56 -28.797 -23.236-116.347 1.00 35.02 B
ATOM 5396 N ALA B 57 -27.518 -24.924-115.550 1.00 35.05 B
ATOM 5397 CA ALA B 57 -28.517 -25.431-114.611 1.00 34.53 B
ATOM 5398 CB ALA B 57 -27.924 -26.545-113.766 1.00 34.14 B
ATOM 5399 C ALA B 57 -29.000 -24.306-113.722 1.00 33.93 B
ATOM 5400 O ALA B 57 -30.163 -24.269-113.330 1.00 33.13 B
ATOM 5401 N ALA B 58 -28.090 -23.390-113.413 1.00 33.78 B
ATOM 5402 CA ALA B 58 -28.398 -22.234-112.583 1.00 34.55 B

ATOM 5403 CB ALA B 58 -27.121 -21.478-112.274 1.00 34.34 B
ATOM 5404 C ALA B 58 -29.399 -21.315-113.284 1.00 35.08 B
ATOM 5405 O ALA B 58 -30.341 -20.820-112.667 1.00 34.71 B
ATOM 5406 N LEU B 59 -29.177 -21.080-114.574 1.00 35.83 B
ATOM 5407 CA LEU B 59 -30.068 -20.239-115.360 1.00 36.67 B
ATOM 5408 CB LEU B 59 -29.495 -20.007-116.757 1.00 36.51 B
ATOM 5409 CG LEU B 59 -28.641 -18.751-116.931 1.00 36.85 B
ATOM 5410 CD1 LEU B 59 -28.183 -18.618-118.370 1.00 35.53 B
ATOM 5411 CD2 LEU B 59 -29.459 -17.543-116.527 1.00 37.97 B
ATOM 5412 C LEU B 59 -31.406 -20.935-115.474 1.00 36.99 B
ATOM 5413 O LEU B 59 -32.456 -20.298-115.517 1.00 37.58 B
ATOM 5414 N LEU B 60 -31.346 -22.259-115.524 1.00 37.01 B
ATOM 5415 CA LEU B 60 -32.534 -23.096-115.624 1.00 36.41 B
ATOM 5416 CB LEU B 60 -32.109 -24.562-115.720 1.00 36.62 B
ATOM 5417 CG LEU B 60 -32.923 -25.499-116.616 1.00 37.02 B
ATOM 5418 CD1 LEU B 60 -32.148 -26.801-116.830 1.00 36.13 B
ATOM 5419 CD2 LEU B 60 -34.280 -25.761-115.992 1.00 37.37 B
ATOM 5420 C LEU B 60 -33.411 -22.878-114.389 1.00 35.97 B
ATOM 5421 O LEU B 60 -34.581 -22.500-114.497 1.00 34.67 B
ATOM 5422 N SER B 61 -32.827 -23.112-113.215 1.00 35.05 B
ATOM 5423 CA SER B 61 -33.526 -22.943-111.951 1.00 33.47 B
ATOM 5424 CB SER B 61 -32.569 -23.207-110.790 1.00 33.42 B
ATOM 5425 OG SER B 61 -31.968 -24.485-110.885 1.00 32.02 B
ATOM 5426 C SER B 61 -34.084 -21.533-111.837 1.00 33.67 B
ATOM 5427 O SER B 61 -35.223 -21.333-111.422 1.00 33.63 B
ATOM 5428 N GLN B 62 -33.274 -20.555-112.210 1.00 34.66 B
ATOM 5429 CA GLN B 62 -33.687 -19.162-112.136 1.00 37.21 B
ATOM 5430 CB GLN B 62 -32.557 -18.258-112.607 1.00 36.85 B
ATOM 5431 CG GLN B 62 -31.340 -18.318-111.732 1.00 36.38 B
ATOM 5432 CD GLN B 62 -30.381 -17.200-112.030 1.00 37.93 B
ATOM 5433 OE1 GLN B 62 -29.512 -17.318-112.888 1.00 37.21 B
ATOM 5434 NE2 GLN B 62 -30.548 -16.093-111.328 1.00 40.42 B
ATOM 5435 C GLN B 62 -34.939 -18.899-112.952 1.00 39.48 B
ATOM 5436 O GLN B 62 -35.773 -18.075-112.583 1.00 39.62 B

ATOM 5437 N GLU B 63 -35.060 -19.597-114.073 1.00 42.76 B
ATOM 5438 CA GLU B 63 -36.236 -19.458-114.929 1.00 45.86 B
ATOM 5439 CB GLU B 63 -36.043 -20.230-116.231 1.00 47.89 B
ATOM 5440 CG GLU B 63 -35.319 -19.468-117.314 1.00 52.67 B
ATOM 5441 CD GLU B 63 -35.119 -20.314-118.547 1.00 55.44 B
ATOM 5442 OE1 GLU B 63 -34.156 -21.116-118.561 1.00 56.48 B
ATOM 5443 OE2 GLU B 63 -35.931 -20.183-119.494 1.00 57.55 B
ATOM 5444 C GLU B 63 -37.439 -20.030-114.192 1.00 45.69 B
ATOM 5445 O GLU B 63 -38.459 -19.359-114.018 1.00 45.83 B
ATOM 5446 N PHE B 64 -37.293 -21.283-113.768 1.00 45.52 B
ATOM 5447 CA PHE B 64 -38.320 -22.008-113.039 1.00 44.84 B
ATOM 5448 CB PHE B 64 -37.698 -23.230-112.378 1.00 43.76 B
ATOM 5449 CG PHE B 64 -38.689 -24.114-111.699 1.00 44.45 B
ATOM 5450 CD1 PHE B 64 -39.525 -24.938-112.440 1.00 45.22 B
ATOM 5451 CD2 PHE B 64 -38.784 -24.135-110.314 1.00 45.07 B
ATOM 5452 CE1 PHE B 64 -40.442 -25.778-111.813 1.00 46.26 B
ATOM 5453 CE2 PHE B 64 -39.699 -24.968-109.674 1.00 45.80 B
ATOM 5454 CZ PHE B 64 -40.530 -25.792-110.426 1.00 46.14 B
ATOM 5455 C PHE B 64 -38.961 -21.139-111.969 1.00 45.88 B
ATOM 5456 O PHE B 64 -40.144 -20.803-112.040 1.00 46.68 B
ATOM 5457 N ALA B 65 -38.157 -20.778-110.976 1.00 46.35 B
ATOM 5458 CA ALA B 65 -38.622 -19.964-109.868 1.00 47.08 B
ATOM 5459 CB ALA B 65 -37.451 -19.611-108.973 1.00 46.91 B
ATOM 5460 C ALA B 65 -39.344 -18.700-110.316 1.00 47.88 B
ATOM 5461 O ALA B 65 -40.204 -18.191-109.604 1.00 48.37 B
ATOM 5462 N GLU B 66 -39.103 -18.235-111.507 1.00 49.09 B
ATOM 5463 CA GLU B 66 -39.786 -17.050-111.932 1.00 50.96 B
ATOM 5464 CB GLU B 66 -39.024 -16.326-112.964 1.00 52.58 B
ATOM 5465 CG GLU B 66 -39.513 -14.922-113.044 1.00 56.18 B
ATOM 5466 CD GLU B 66 -39.814 -14.476-114.417 1.00 58.98 B
ATOM 5467 OE1 GLU B 66 -38.978 -14.703-115.283 1.00 60.94 B
ATOM 5468 OE2 GLU B 66 -40.875 -13.889-114.605 1.00 60.27 B
ATOM 5469 C GLU B 66 -41.087 -17.308-112.499 1.00 51.26 B
ATOM 5470 O GLU B 66 -41.987 -16.558-112.315 1.00 51.03 B

ATOM 5471 N ALA B 67 -41.178 -18.365-113.254 1.00 52.07 B
ATOM 5472 CA ALA B 67 -42.476 -18.728-113.811 1.00 52.84 B
ATOM 5473 CB ALA B 67 -42.365 -20.012-114.621 1.00 52.70 B
ATOM 5474 C ALA B 67 -43.432 -18.930-112.647 1.00 53.22 B
ATOM 5475 O ALA B 67 -44.400 -18.182-112.476 1.00 52.93 B
ATOM 5476 N TRP B 68 -43.139 -19.948-111.845 1.00 53.86 B
ATOM 5477 CA TRP B 68 -43.946 -20.270-110.679 1.00 54.39 B
ATOM 5478 CB TRP B 68 -43.308 -21.408-109.905 1.00 53.62 B
ATOM 5479 CG TRP B 68 -43.258 -22.646-110.700 1.00 53.60 B
ATOM 5480 CD2 TRP B 68 -44.245 -23.681-110.720 1.00 54.03 B
ATOM 5481 CE2 TRP B 68 -43.830 -24.634-111.675 1.00 54.11 B
ATOM 5482 CE3 TRP B 68 -45.446 -23.893-110.023 1.00 53.39 B
ATOM 5483 CD1 TRP B 68 -42.310 -22.996-111.610 1.00 53.21 B
ATOM 5484 NE1 TRP B 68 -42.646 -24.189-112.203 1.00 53.29 B
ATOM 5485 CZ2 TRP B 68 -44.575 -25.791-111.955 1.00 53.76 B
ATOM 5486 CZ3 TRP B 68 -46.185 -25.041-110.298 1.00 53.38 B
ATOM 5487 CH2 TRP B 68 -45.745 -25.976-111.258 1.00 54.05 B
ATOM 5488 C TRP B 68 -44.100 -19.072-109.770 1.00 54.62 B
ATOM 5489 O TRP B 68 -45.218 -18.674-109.449 1.00 55.22 B
ATOM 5490 N GLY B 69 -42.969 -18.506-109.359 1.00 54.53 B
ATOM 5491 CA GLY B 69 -42.987 -17.350-108.484 1.00 54.46 B
ATOM 5492 C GLY B 69 -43.985 -16.302-108.932 1.00 54.90 B
ATOM 5493 O GLY B 69 -44.798 -15.820-108.140 1.00 54.98 B
ATOM 5494 N ALA B 70 -43.918 -15.942-110.212 1.00 55.33 B
ATOM 5495 CA ALA B 70 -44.846 -14.949-110.737 1.00 55.94 B
ATOM 5496 CB ALA B 70 -44.465 -14.565-112.159 1.00 54.48 B
ATOM 5497 C ALA B 70 -46.283 -15.456-110.689 1.00 56.35 B
ATOM 5498 O ALA B 70 -47.195 -14.723-110.402 1.00 56.93 B
ATOM 5499 N LYS B 71 -46.455 -16.741-110.980 1.00 56.48 B
ATOM 5500 CA LYS B 71 -47.760 -17.384-110.871 1.00 57.25 B
ATOM 5501 CB LYS B 71 -47.676 -18.845-111.314 1.00 57.24 B
ATOM 5502 CG LYS B 71 -49.026 -19.494-111.574 1.00 58.19 B
ATOM 5503 CD LYS B 71 -49.706 -18.887-112.790 1.00 59.03 B
ATOM 5504 CE LYS B 71 -50.937 -19.684-113.189 1.00 60.21 B

ATOM 5505 NZ LYS B 71 -51.728 -18.991-114.243 1.00 61.81 B
ATOM 5506 C LYS B 71 -48.299 -17.298-109.447 1.00 58.14 B
ATOM 5507 O LYS B 71 -49.313 -16.646-109.194 1.00 58.38 B
ATOM 5508 N ALA B 72 -47.615 -17.961-108.520 1.00 58.44 B
ATOM 5509 CA ALA B 72 -47.947 -17.859-107.103 1.00 58.43 B
ATOM 5510 CB ALA B 72 -46.757 -18.269-106.250 1.00 58.00 B
ATOM 5511 C ALA B 72 -48.401 -16.448-106.744 1.00 59.21 B
ATOM 5512 O ALA B 72 -49.500 -16.254-106.220 1.00 59.26 B
ATOM 5513 N LYS B 73 -47.552 -15.468-107.029 1.00 60.84 B
ATOM 5514 CA LYS B 73 -47.935 -14.065-106.920 1.00 63.02 B
ATOM 5515 CB LYS B 73 -46.831 -13.163-107.475 1.00 63.27 B
ATOM 5516 CG LYS B 73 -45.547 -13.183-106.662 1.00 64.91 B
ATOM 5517 CD LYS B 73 -45.072 -11.773-106.347 1.00 65.70 B
ATOM 5518 CE LYS B 73 -43.562 -11.657-106.474 1.00 65.97 B
ATOM 5519 NZ LYS B 73 -43.125 -11.648-107.898 1.00 66.77 B
ATOM 5520 C LYS B 73 -49.248 -13.794-107.645 1.00 63.67 B
ATOM 5521 O LYS B 73 -50.252 -13.444-107.024 1.00 64.03 B
ATOM 5522 N ALA B 74 -49.233 -13.959-108.963 1.00 64.36 B
ATOM 5523 CA ALA B 74 -50.398 -13.659-109.786 1.00 65.23 B
ATOM 5524 CB ALA B 74 -50.208 -14.202-111.194 1.00 65.04 B
ATOM 5525 C ALA B 74 -51.672 -14.220-109.164 1.00 66.04 B
ATOM 5526 O ALA B 74 -52.680 -13.522-109.052 1.00 66.53 B
ATOM 5527 N LEU B 75 -51.620 -15.486-108.763 1.00 66.61 B
ATOM 5528 CA LEU B 75 -52.812 -16.199-108.320 1.00 67.26 B
ATOM 5529 CB LEU B 75 -52.581 -17.710-108.364 1.00 66.75 B
ATOM 5530 CG LEU B 75 -53.155 -18.449-109.574 1.00 66.11 B
ATOM 5531 CD1 LEU B 75 -52.414 -18.057-110.844 1.00 66.73 B
ATOM 5532 CD2 LEU B 75 -53.102 -19.954-109.362 1.00 65.62 B
ATOM 5533 C LEU B 75 -53.222 -15.771-106.914 1.00 68.72 B
ATOM 5534 O LEU B 75 -54.392 -15.487-106.658 1.00 68.73 B
ATOM 5535 N TYR B 76 -52.255 -15.732-106.003 1.00 70.14 B
ATOM 5536 CA TYR B 76 -52.531 -15.372-104.617 1.00 71.22 B
ATOM 5537 CB TYR B 76 -52.842 -16.619-103.786 1.00 69.54 B
ATOM 5538 CG TYR B 76 -53.005 -17.880-104.604 1.00 68.51 B

ATOM 5539 CD1 TYR B 76 -51.897 -18.598-105.033 1.00 67.40 B
ATOM 5540 CE1 TYR B 76 -52.041 -19.753-105.781 1.00 67.84 B
ATOM 5541 CD2 TYR B 76 -54.264 -18.352-104.944 1.00 69.41 B
ATOM 5542 CE2 TYR B 76 -54.418 -19.505-105.690 1.00 68.68 B
ATOM 5543 CZ TYR B 76 -53.303 -20.201-106.106 1.00 68.39 B
ATOM 5544 OH TYR B 76 -53.450 -21.350-106.850 1.00 68.32 B
ATOM 5545 C TYR B 76 -51.369 -14.603-103.996 1.00 72.88 B
ATOM 5546 O TYR B 76 -50.439 -15.198-103.451 1.00 74.95 B
ATOM 5547 N GLU B 77 -51.457 -13.289-104.081 1.00 73.68 B
ATOM 5548 CA GLU B 77 -50.807 -12.427-103.101 1.00 74.63 B
ATOM 5549 CB GLU B 77 -49.519 -11.836-103.678 1.00 72.74 B
ATOM 5550 CG GLU B 77 -49.258 -10.397-103.268 1.00 72.09 B
ATOM 5551 CD GLU B 77 -47.907 -9.892-103.736 0.00 72.26 B
ATOM 5552 OE1 GLU B 77 -47.168 -10.672-104.373 0.00 72.20 B
ATOM 5553 OE2 GLU B 77 -47.584 -8.716-103.467 0.00 72.20 B
ATOM 5554 C GLU B 77 -51.737 -11.309-102.643 1.00 75.85 B
ATOM 5555 O GLU B 77 -51.316 -10.382-101.952 1.00 76.28 B
ATOM 5556 N PRO B 78 -52.977 -11.393-103.032 1.00 76.51 B
ATOM 5557 CD PRO B 78 -53.276 -11.091-104.443 1.00 76.61 B
ATOM 5558 CA PRO B 78 -54.085 -11.029-102.143 1.00 75.80 B
ATOM 5559 CB PRO B 78 -55.243 -10.797-103.115 1.00 75.82 B
ATOM 5560 CG PRO B 78 -54.585 -10.353-104.374 1.00 76.15 B
ATOM 5561 C PRO B 78 -54.430 -12.155-101.175 1.00 74.94 B
ATOM 5562 O PRO B 78 -55.145 -13.087-101.543 1.00 74.00 B
ATOM 5563 N ALA B 79 -53.923 -12.063 -99.950 1.00 74.56 B
ATOM 5564 CA ALA B 79 -54.173 -13.091 -98.932 1.00 74.34 B
ATOM 5565 CB ALA B 79 -55.666 -13.080 -98.520 1.00 74.65 B
ATOM 5566 C ALA B 79 -53.723 -14.543 -99.170 1.00 73.65 B
ATOM 5567 O ALA B 79 -54.534 -15.427 -99.477 1.00 73.27 B
ATOM 5568 N TRP B 80 -52.416 -14.763 -99.027 1.00 72.73 B
ATOM 5569 CA TRP B 80 -51.819 -16.106 -99.099 1.00 70.85 B
ATOM 5570 CB TRP B 80 -50.666 -16.168-100.107 1.00 70.16 B
ATOM 5571 CG TRP B 80 -49.599 -15.166 -99.822 1.00 69.64 B
ATOM 5572 CD2 TRP B 80 -48.476 -15.338 -98.946 1.00 69.59 B

```
ATOM  5573  CE2 TRP B  80     -47.746 -14.116 -98.950  1.00 69.38      B
ATOM  5574  CE3 TRP B  80     -48.009 -16.407 -98.156  1.00 69.30      B
ATOM  5575  CD1 TRP B  80     -49.519 -13.889-100.308  1.00 69.39      B
ATOM  5576  NE1 TRP B  80     -48.404 -13.249 -99.789  1.00 69.33      B
ATOM  5577  CZ2 TRP B  80     -46.573 -13.933 -98.192  1.00 69.58      B
ATOM  5578  CZ3 TRP B  80     -46.840 -16.229 -97.401  1.00 69.01      B
ATOM  5579  CH2 TRP B  80     -46.134 -14.995 -97.429  1.00 69.74      B
ATOM  5580  C   TRP B  80     -51.278 -16.146 -97.669  1.00 69.95      B
ATOM  5581  O   TRP B  80     -50.867 -17.184 -97.146  1.00 70.22      B
ATOM  5582  N   GLN B  81     -51.291 -14.946 -97.077  1.00 68.65      B
ATOM  5583  CA  GLN B  81     -50.878 -14.682 -95.695  1.00 66.69      B
ATOM  5584  CB  GLN B  81     -50.405 -13.224 -95.548  1.00 65.39      B
ATOM  5585  CG  GLN B  81     -49.116 -12.950 -96.320  1.00 64.47      B
ATOM  5586  CD  GLN B  81     -48.756 -11.463 -96.372  1.00 64.63      B
ATOM  5587  OE1 GLN B  81     -49.619 -10.611 -96.665  1.00 64.56      B
ATOM  5588  NE2 GLN B  81     -47.472 -11.142 -96.105  1.00 64.97      B
ATOM  5589  C   GLN B  81     -52.101 -14.925 -94.815  1.00 65.94      B
ATOM  5590  O   GLN B  81     -51.997 -14.961 -93.587  1.00 66.29      B
ATOM  5591  N   ASN B  82     -53.253 -15.078 -95.472  1.00 64.93      B
ATOM  5592  CA  ASN B  82     -54.517 -15.346 -94.788  1.00 64.58      B
ATOM  5593  CB  ASN B  82     -55.507 -14.184 -94.975  1.00 64.45      B
ATOM  5594  CG  ASN B  82     -55.346 -13.110 -93.898  1.00 65.32      B
ATOM  5595  OD1 ASN B  82     -55.301 -13.428 -92.691  1.00 65.52      B
ATOM  5596  ND2 ASN B  82     -55.268 -11.832 -94.318  1.00 65.10      B
ATOM  5597  C   ASN B  82     -55.167 -16.652 -95.237  1.00 64.34      B
ATOM  5598  O   ASN B  82     -56.341 -16.672 -95.596  1.00 64.53      B
ATOM  5599  N   PHE B  83     -54.388 -17.731 -95.236  1.00 64.08      B
ATOM  5600  CA  PHE B  83     -54.896 -19.047 -95.602  1.00 63.81      B
ATOM  5601  CB  PHE B  83     -53.910 -19.802 -96.495  1.00 65.00      B
ATOM  5602  CG  PHE B  83     -53.864 -19.315 -97.916  1.00 66.37      B
ATOM  5603  CD1 PHE B  83     -55.026 -18.926 -98.576  1.00 66.97      B
ATOM  5604  CD2 PHE B  83     -52.662 -19.307 -98.620  1.00 66.72      B
ATOM  5605  CE1 PHE B  83     -54.992 -18.538 -99.924  1.00 66.50      B
ATOM  5606  CE2 PHE B  83     -52.618 -18.924 -99.963  1.00 66.08      B
```

ATOM 5607 CZ PHE B 83 -53.783 -18.538-100.614 1.00 65.97 B
ATOM 5608 C PHE B 83 -55.098 -19.834 -94.312 1.00 63.24 B
ATOM 5609 O PHE B 83 -54.177 -19.943 -93.496 1.00 62.79 B
ATOM 5610 N ALA B 84 -56.302 -20.376 -94.134 1.00 62.37 B
ATOM 5611 CA ALA B 84 -56.634 -21.145 -92.941 1.00 61.04 B
ATOM 5612 CB ALA B 84 -57.897 -21.958 -93.178 1.00 59.69 B
ATOM 5613 C ALA B 84 -55.471 -22.060 -92.597 1.00 60.47 B
ATOM 5614 O ALA B 84 -55.125 -22.224 -91.427 1.00 60.60 B
ATOM 5615 N ASP B 85 -54.856 -22.626 -93.631 1.00 59.57 B
ATOM 5616 CA ASP B 85 -53.725 -23.535 -93.469 1.00 58.77 B
ATOM 5617 CB ASP B 85 -53.647 -24.474 -94.677 1.00 58.50 B
ATOM 5618 CG ASP B 85 -52.538 -25.499 -94.553 1.00 58.22 B
ATOM 5619 OD1 ASP B 85 -52.469 -26.408 -95.406 1.00 58.02 B
ATOM 5620 OD2 ASP B 85 -51.729 -25.399 -93.609 1.00 58.06 B
ATOM 5621 C ASP B 85 -52.383 -22.811 -93.282 1.00 58.05 B
ATOM 5622 O ASP B 85 -51.975 -22.006 -94.119 1.00 58.00 B
ATOM 5623 N PRO B 86 -51.676 -23.103 -92.176 1.00 57.25 B
ATOM 5624 CD PRO B 86 -52.109 -23.982 -91.068 1.00 56.47 B
ATOM 5625 CA PRO B 86 -50.382 -22.487 -91.868 1.00 55.96 B
ATOM 5626 CB PRO B 86 -50.212 -22.790 -90.384 1.00 55.63 B
ATOM 5627 CG PRO B 86 -50.842 -24.147 -90.261 1.00 55.32 B
ATOM 5628 C PRO B 86 -49.204 -22.997 -92.706 1.00 55.16 B
ATOM 5629 O PRO B 86 -48.350 -22.212 -93.124 1.00 55.12 B
ATOM 5630 N GLN B 87 -49.157 -24.307 -92.943 1.00 54.06 B
ATOM 5631 CA GLN B 87 -48.076 -24.913 -93.721 1.00 53.10 B
ATOM 5632 CB GLN B 87 -48.124 -26.434 -93.620 1.00 53.20 B
ATOM 5633 CG GLN B 87 -47.661 -26.948 -92.281 1.00 54.29 B
ATOM 5634 CD GLN B 87 -47.323 -28.413 -92.323 1.00 55.03 B
ATOM 5635 OE1 GLN B 87 -46.966 -28.944 -93.375 1.00 54.19 B
ATOM 5636 NE2 GLN B 87 -47.404 -29.076 -91.174 1.00 56.03 B
ATOM 5637 C GLN B 87 -48.101 -24.520 -95.182 1.00 52.82 B
ATOM 5638 O GLN B 87 -47.055 -24.426 -95.819 1.00 51.91 B
ATOM 5639 N LEU B 88 -49.304 -24.310 -95.707 1.00 52.94 B
ATOM 5640 CA LEU B 88 -49.483 -23.920 -97.097 1.00 52.51 B

ATOM 5641 CB LEU B 88 -50.968 -23.945 -97.463 1.00 52.31 B
ATOM 5642 CG LEU B 88 -51.375 -23.696 -98.916 1.00 51.90 B
ATOM 5643 CD1 LEU B 88 -51.359 -22.205 -99.198 1.00 51.78 B
ATOM 5644 CD2 LEU B 88 -50.448 -24.461 -99.858 1.00 50.60 B
ATOM 5645 C LEU B 88 -48.934 -22.521 -97.224 1.00 52.55 B
ATOM 5646 O LEU B 88 -48.169 -22.227 -98.141 1.00 53.01 B
ATOM 5647 N ARG B 89 -49.324 -21.657 -96.292 1.00 52.50 B
ATOM 5648 CA ARG B 89 -48.838 -20.287 -96.290 1.00 52.36 B
ATOM 5649 CB ARG B 89 -49.257 -19.558 -95.015 1.00 53.45 B
ATOM 5650 CG ARG B 89 -50.694 -19.078 -94.999 1.00 56.38 B
ATOM 5651 CD ARG B 89 -51.015 -18.361 -93.692 1.00 58.61 B
ATOM 5652 NE ARG B 89 -50.727 -19.213 -92.536 1.00 61.93 B
ATOM 5653 CZ ARG B 89 -50.904 -18.858 -91.264 1.00 63.12 B
ATOM 5654 NH1 ARG B 89 -51.375 -17.656 -90.956 1.00 63.76 B
ATOM 5655 NH2 ARG B 89 -50.601 -19.711 -90.296 1.00 63.67 B
ATOM 5656 C ARG B 89 -47.318 -20.319 -96.375 1.00 51.93 B
ATOM 5657 O ARG B 89 -46.722 -19.646 -97.216 1.00 52.75 B
ATOM 5658 N ALA B 90 -46.686 -21.110 -95.510 1.00 51.05 B
ATOM 5659 CA ALA B 90 -45.231 -21.199 -95.521 1.00 50.06 B
ATOM 5660 CB ALA B 90 -44.754 -22.219 -94.498 1.00 49.30 B
ATOM 5661 C ALA B 90 -44.712 -21.554 -96.910 1.00 48.77 B
ATOM 5662 O ALA B 90 -43.669 -21.057 -97.349 1.00 47.78 B
ATOM 5663 N ILE B 91 -45.447 -22.401 -97.639 1.00 47.76 B
ATOM 5664 CA ILE B 91 -45.040 -22.814 -98.976 1.00 46.12 B
ATOM 5665 CB ILE B 91 -45.765 -24.106 -99.400 1.00 44.36 B
ATOM 5666 CG2 ILE B 91 -45.402 -24.468 -100.831 1.00 43.40 B
ATOM 5667 CG1 ILE B 91 -45.356 -25.245 -98.468 1.00 43.64 B
ATOM 5668 CD1 ILE B 91 -46.077 -26.540 -98.728 1.00 42.97 B
ATOM 5669 C ILE B 91 -45.257 -21.736 -100.039 1.00 46.70 B
ATOM 5670 O ILE B 91 -44.457 -21.617 -100.964 1.00 47.53 B
ATOM 5671 N ILE B 92 -46.318 -20.946 -99.914 1.00 46.42 B
ATOM 5672 CA ILE B 92 -46.579 -19.893 -100.897 1.00 46.92 B
ATOM 5673 CB ILE B 92 -47.989 -19.267 -100.713 1.00 46.13 B
ATOM 5674 CG2 ILE B 92 -48.169 -18.071 -101.643 1.00 45.20 B

ATOM 5675 CG1 ILE B 92 -49.057 -20.318-101.008 1.00 45.96 B
ATOM 5676 CD1 ILE B 92 -48.913 -20.979-102.368 1.00 44.82 B
ATOM 5677 C ILE B 92 -45.540 -18.775-100.841 1.00 47.32 B
ATOM 5678 O ILE B 92 -45.041 -18.320-101.872 1.00 47.67 B
ATOM 5679 N GLY B 93 -45.217 -18.334 -99.633 1.00 47.82 B
ATOM 5680 CA GLY B 93 -44.249 -17.264 -99.474 1.00 47.90 B
ATOM 5681 C GLY B 93 -42.856 -17.673 -99.899 1.00 47.72 B
ATOM 5682 O GLY B 93 -42.056 -16.831-100.311 1.00 47.80 B
ATOM 5683 N ALA B 94 -42.562 -18.965 -99.797 1.00 47.39 B
ATOM 5684 CA ALA B 94 -41.247 -19.482-100.156 1.00 47.90 B
ATOM 5685 CB ALA B 94 -41.007 -20.830 -99.492 1.00 47.50 B
ATOM 5686 C ALA B 94 -41.099 -19.598-101.669 1.00 48.08 B
ATOM 5687 O ALA B 94 -39.989 -19.709-102.187 1.00 48.55 B
ATOM 5688 N VAL B 95 -42.227 -19.572-102.372 1.00 47.56 B
ATOM 5689 CA VAL B 95 -42.230 -19.727-103.821 1.00 46.85 B
ATOM 5690 CB VAL B 95 -43.375 -20.646-104.287 1.00 46.92 B
ATOM 5691 CG1 VAL B 95 -43.196 -21.019-105.750 1.00 47.97 B
ATOM 5692 CG2 VAL B 95 -43.446 -21.891-103.416 1.00 46.06 B
ATOM 5693 C VAL B 95 -42.360 -18.376-104.518 1.00 46.10 B
ATOM 5694 O VAL B 95 -41.969 -18.225-105.676 1.00 45.83 B
ATOM 5695 N ARG B 96 -42.810 -17.400-103.769 1.00 45.40 B
ATOM 5696 CA ARG B 96 -42.858 -16.064-104.247 1.00 46.52 B
ATOM 5697 CB ARG B 96 -44.099 -15.340-103.779 1.00 47.87 B
ATOM 5698 CG ARG B 96 -44.292 -15.226-102.355 1.00 50.18 B
ATOM 5699 CD ARG B 96 -45.131 -14.079-101.929 1.00 51.91 B
ATOM 5700 NE ARG B 96 -44.301 -12.945-101.680 1.00 54.40 B
ATOM 5701 CZ ARG B 96 -44.690 -11.709-101.783 1.00 55.18 B
ATOM 5702 NH1 ARG B 96 -43.813 -10.757-101.581 1.00 55.24 B
ATOM 5703 NH2 ARG B 96 -45.943 -11.408-102.088 1.00 54.73 B
ATOM 5704 C ARG B 96 -41.643 -15.296-103.946 1.00 46.01 B
ATOM 5705 O ARG B 96 -41.553 -14.121-104.150 1.00 45.68 B
ATOM 5706 N THR B 97 -40.667 -16.006-103.470 1.00 45.22 B
ATOM 5707 CA THR B 97 -39.344 -15.436-103.249 1.00 43.82 B
ATOM 5708 CB THR B 97 -38.795 -15.865-101.875 1.00 43.46 B

ATOM 5709 OG1 THR B 97 -39.387 -15.060-100.848 1.00 43.97 B
ATOM 5710 CG2 THR B 97 -37.314 -15.536-101.767 1.00 43.77 B
ATOM 5711 C THR B 97 -38.375 -15.847-104.352 1.00 42.65 B
ATOM 5712 O THR B 97 -37.635 -16.820-104.209 1.00 42.62 B
ATOM 5713 N LEU B 98 -38.386 -15.100-105.451 1.00 40.69 B
ATOM 5714 CA LEU B 98 -37.612 -15.465-106.633 1.00 38.65 B
ATOM 5715 CB LEU B 98 -37.943 -14.517-107.788 1.00 39.37 B
ATOM 5716 CG LEU B 98 -39.395 -14.062-107.982 1.00 40.00 B
ATOM 5717 CD1 LEU B 98 -39.507 -13.285-109.281 1.00 39.79 B
ATOM 5718 CD2 LEU B 98 -40.325 -15.256-108.009 1.00 40.11 B
ATOM 5719 C LEU B 98 -36.105 -15.494-106.419 1.00 36.62 B
ATOM 5720 O LEU B 98 -35.401 -16.341-106.972 1.00 35.19 B
ATOM 5721 N GLY B 99 -35.599 -14.567-105.623 1.00 35.46 B
ATOM 5722 CA GLY B 99 -34.171 -14.550-105.386 1.00 35.63 B
ATOM 5723 C GLY B 99 -33.432 -13.971-106.572 1.00 35.30 B
ATOM 5724 O GLY B 99 -33.822 -12.920-107.085 1.00 35.61 B
ATOM 5725 N SER B 100 -32.372 -14.641-107.018 1.00 34.26 B
ATOM 5726 CA SER B 100 -31.606 -14.130-108.148 1.00 34.02 B
ATOM 5727 CB SER B 100 -30.299 -14.913-108.319 1.00 32.58 B
ATOM 5728 OG SER B 100 -30.528 -16.292-108.463 1.00 32.34 B
ATOM 5729 C SER B 100 -32.403 -14.135-109.452 1.00 35.22 B
ATOM 5730 O SER B 100 -31.966 -13.558-110.453 1.00 36.47 B
ATOM 5731 N ALA B 101 -33.579 -14.766-109.433 1.00 35.34 B
ATOM 5732 CA ALA B 101 -34.442 -14.838-110.605 1.00 34.69 B
ATOM 5733 CB ALA B 101 -35.532 -15.851-110.372 1.00 32.59 B
ATOM 5734 C ALA B 101 -35.052 -13.482-110.980 1.00 35.10 B
ATOM 5735 O ALA B 101 -35.535 -13.307-112.091 1.00 34.17 B
ATOM 5736 N ASN B 102 -35.021 -12.531-110.105 1.00 36.09 B
ATOM 5737 CA ASN B 102 -35.556 -11.262-110.413 1.00 38.24 B
ATOM 5738 CB ASN B 102 -35.732 -10.476-109.154 1.00 40.55 B
ATOM 5739 CG ASN B 102 -36.581 -11.121-108.177 1.00 43.37 B
ATOM 5740 OD1 ASN B 102 -37.709 -10.793-108.001 1.00 43.56 B
ATOM 5741 ND2 ASN B 102 -36.016 -11.979-107.465 1.00 44.99 B
ATOM 5742 C ASN B 102 -34.614 -10.481-111.250 1.00 38.50 B

ATOM 5743 O ASN B 102 -34.892 -9.394-111.612 1.00 38.68 B
ATOM 5744 N LEU B 103 -33.452 -11.023-111.477 1.00 38.33 B
ATOM 5745 CA LEU B 103 -32.419 -10.435-112.330 1.00 38.19 B
ATOM 5746 CB LEU B 103 -31.048 -10.922-111.879 1.00 38.90 B
ATOM 5747 CG LEU B 103 -30.458 -10.510-110.540 1.00 38.35 B
ATOM 5748 CD1 LEU B 103 -29.236 -11.377-110.306 1.00 39.52 B
ATOM 5749 CD2 LEU B 103 -30.077 -9.035-110.540 1.00 37.04 B
ATOM 5750 C LEU B 103 -32.559 -10.781-113.804 1.00 38.46 B
ATOM 5751 O LEU B 103 -32.816 -11.926-114.145 1.00 40.19 B
ATOM 5752 N PRO B 104 -32.356 -9.804-114.701 1.00 38.13 B
ATOM 5753 CD PRO B 104 -32.082 -8.389-114.407 1.00 37.73 B
ATOM 5754 CA PRO B 104 -32.454 -10.020-116.154 1.00 37.48 B
ATOM 5755 CB PRO B 104 -32.084 -8.659-116.735 1.00 37.53 B
ATOM 5756 CG PRO B 104 -32.529 -7.722-115.694 1.00 38.10 B
ATOM 5757 C PRO B 104 -31.487 -11.110-116.631 1.00 37.39 B
ATOM 5758 O PRO B 104 -30.482 -11.395-115.979 1.00 38.14 B
ATOM 5759 N LEU B 105 -31.790 -11.701-117.778 1.00 37.39 B
ATOM 5760 CA LEU B 105 -30.965 -12.759-118.352 1.00 37.58 B
ATOM 5761 CB LEU B 105 -31.298 -12.909-119.839 1.00 37.86 B
ATOM 5762 CG LEU B 105 -30.881 -14.144-120.664 1.00 37.80 B
ATOM 5763 CD1 LEU B 105 -30.401 -13.654-122.037 1.00 38.43 B
ATOM 5764 CD2 LEU B 105 -29.790 -14.968-119.972 1.00 36.90 B
ATOM 5765 C LEU B 105 -29.471 -12.472-118.202 1.00 37.40 B
ATOM 5766 O LEU B 105 -28.716 -13.266-117.640 1.00 37.08 B
ATOM 5767 N ALA B 106 -29.054 -11.323-118.713 1.00 37.50 B
ATOM 5768 CA ALA B 106 -27.650 -10.934-118.668 1.00 37.81 B
ATOM 5769 CB ALA B 106 -27.465 -9.603-119.396 1.00 39.21 B
ATOM 5770 C ALA B 106 -27.057 -10.852-117.261 1.00 37.11 B
ATOM 5771 O ALA B 106 -25.964 -11.372-117.015 1.00 35.72 B
ATOM 5772 N LYS B 107 -27.794 -10.344-116.311 1.00 36.02 B
ATOM 5773 CA LYS B 107 -27.252 -10.174-115.003 1.00 34.66 B
ATOM 5774 CB LYS B 107 -28.053 -9.192-114.258 1.00 32.76 B
ATOM 5775 CG LYS B 107 -27.463 -7.847-114.235 1.00 32.04 B
ATOM 5776 CD LYS B 107 -28.495 -6.846-114.113 1.00 32.22 B

ATOM 5777 CE LYS B 107 -27.990 -5.562-113.602 1.00 32.16 B
ATOM 5778 NZ LYS B 107 -29.042 -4.713-113.064 1.00 33.81 B
ATOM 5779 C LYS B 107 -27.237 -11.426-114.283 1.00 34.84 B
ATOM 5780 O LYS B 107 -26.344 -11.699-113.561 1.00 34.84 B
ATOM 5781 N ARG B 108 -28.206 -12.262-114.562 1.00 34.86 B
ATOM 5782 CA ARG B 108 -28.226 -13.599-113.976 1.00 34.64 B
ATOM 5783 CB ARG B 108 -29.373 -14.446-114.532 1.00 35.23 B
ATOM 5784 CG ARG B 108 -30.768 -14.052-114.087 1.00 37.13 B
ATOM 5785 CD ARG B 108 -31.790 -15.043-114.636 1.00 37.58 B
ATOM 5786 NE ARG B 108 -33.166 -14.586-114.469 1.00 38.63 B
ATOM 5787 CZ ARG B 108 -34.224 -15.231-114.947 1.00 40.00 B
ATOM 5788 NH1 ARG B 108 -34.056 -16.366-115.622 1.00 40.70 B
ATOM 5789 NH2 ARG B 108 -35.445 -14.739-114.761 1.00 39.30 B
ATOM 5790 C ARG B 108 -26.933 -14.306-114.311 1.00 33.82 B
ATOM 5791 O ARG B 108 -26.312 -14.905-113.451 1.00 35.13 B
ATOM 5792 N GLN B 109 -26.449 -14.157-115.483 1.00 33.17 B
ATOM 5793 CA GLN B 109 -25.322 -14.882-115.884 1.00 33.27 B
ATOM 5794 CB GLN B 109 -25.172 -14.823-117.384 1.00 35.11 B
ATOM 5795 CG GLN B 109 -26.411 -14.925-118.182 1.00 39.24 B
ATOM 5796 CD GLN B 109 -26.188 -14.747-119.634 1.00 41.81 B
ATOM 5797 OE1 GLN B 109 -26.946 -15.170-120.458 1.00 42.07 B
ATOM 5798 NE2 GLN B 109 -25.137 -14.111-119.945 1.00 44.57 B
ATOM 5799 C GLN B 109 -24.106 -14.343-115.278 1.00 31.70 B
ATOM 5800 O GLN B 109 -23.140 -15.030-115.140 1.00 29.58 B
ATOM 5801 N GLN B 110 -24.121 -13.060-114.989 1.00 30.31 B
ATOM 5802 CA GLN B 110 -23.011 -12.423-114.276 1.00 28.78 B
ATOM 5803 CB GLN B 110 -23.194 -10.906-114.218 1.00 28.75 B
ATOM 5804 CG GLN B 110 -23.096 -10.203-115.562 1.00 29.71 B
ATOM 5805 CD GLN B 110 -23.256 -8.699-115.448 1.00 30.63 B
ATOM 5806 OE1 GLN B 110 -22.498 -8.035-114.749 1.00 32.66 B
ATOM 5807 NE2 GLN B 110 -24.247 -8.155-116.136 1.00 30.94 B
ATOM 5808 C GLN B 110 -23.014 -12.992-112.871 1.00 28.29 B
ATOM 5809 O GLN B 110 -21.981 -13.431-112.353 1.00 27.01 B
ATOM 5810 N TYR B 111 -24.196 -12.987-112.264 I.00 28.31 B

ATOM 5811 CA TYR B 111 -24.377 -13.527-110.930 1.00 28.17 B
ATOM 5812 CB TYR B 111 -25.856 -13.544-110.564 1.00 29.89 B
ATOM 5813 CG TYR B 111 -26.084 -13.901-109.118 1.00 33.73 B
ATOM 5814 CD1 TYR B 111 -25.674 -13.037-108.098 1.00 35.22 B
ATOM 5815 CE1 TYR B 111 -25.836 -13.378-106.758 1.00 35.54 B
ATOM 5816 CD2 TYR B 111 -26.668 -15.118-108.757 1.00 34.56 B
ATOM 5817 CE2 TYR B 111 -26.834 -15.465-107.420 1.00 34.92 B
ATOM 5818 CZ TYR B 111 -26.412 -14.590-106.428 1.00 34.87 B
ATOM 5819 OH TYR B 111 -26.537 -14.930-105.108 1.00 33.82 B
ATOM 5820 C TYR B 111 -23.839 -14.951-110.893 1.00 27.36 B
ATOM 5821 O TYR B 111 -22.829 -15.223-110.246 1.00 25.91 B
ATOM 5822 N ASN B 112 -24.516 -15.850-111.601 1.00 26.45 B
ATOM 5823 CA ASN B 112 -24.120 -17.248-111.659 1.00 26.53 B
ATOM 5824 CB ASN B 112 -24.935 -18.014-112.710 1.00 26.18 B
ATOM 5825 CG ASN B 112 -26.433 -17.886-112.514 1.00 27.14 B
ATOM 5826 OD1 ASN B 112 -26.923 -17.746-111.400 1.00 28.72 B
ATOM 5827 ND2 ASN B 112 -27.170 -17.955-113.606 1.00 25.93 B
ATOM 5828 C ASN B 112 -22.638 -17.420-111.974 1.00 27.84 B
ATOM 5829 O ASN B 112 -22.025 -18.399-111.565 1.00 29.00 B
ATOM 5830 N ALA B 113 -22.056 -16.481-112.707 1.00 28.57 B
ATOM 5831 CA ALA B 113 -20.647 -16.600-113.053 1.00 28.33 B
ATOM 5832 CB ALA B 113 -20.361 -15.859-114.336 1.00 28.02 B
ATOM 5833 C ALA B 113 -19.766 -16.076-111.928 1.00 28.74 B
ATOM 5834 O ALA B 113 -18.699 -16.632-111.650 1.00 29.93 B
ATOM 5835 N LEU B 114 -20.205 -15.003-111.277 1.00 27.27 B
ATOM 5836 CA LEU B 114 -19.436 -14.457-110.171 1.00 23.99 B
ATOM 5837 CB LEU B 114 -20.108 -13.208-109.623 1.00 21.03 B
ATOM 5838 CG LEU B 114 -19.789 -11.931-110.386 1.00 18.99 B
ATOM 5839 CD1 LEU B 114 -20.527 -10.762-109.766 1.00 16.91 B
ATOM 5840 CD2 LEU B 114 -18.292 -11.697-110.355 1.00 18.53 B
ATOM 5841 C LEU B 114 -19.330 -15.516-109.085 1.00 24.15 B
ATOM 5842 O LEU B 114 -18.307 -15.628-108.410 1.00 23.67 B
ATOM 5843 N LEU B 115 -20.381 -16.312-108.930 1.00 23.42 B
ATOM 5844 CA LEU B 115 -20.366 -17.356-107.926 1.00 24.25 B

ATOM 5845 CB LEU B 115 -21.774 -17.933-107.742 1.00 23.35 B
ATOM 5846 CG LEU B 115 -22.804 -16.946-107.168 1.00 24.76 B
ATOM 5847 CD1 LEU B 115 -24.191 -17.539-107.268 1.00 24.18 B
ATOM 5848 CD2 LEU B 115 -22.472 -16.600-105.722 1.00 23.13 B
ATOM 5849 C LEU B 115 -19.355 -18.462-108.236 1.00 25.52 B
ATOM 5850 O LEU B 115 -18.517 -18.779-107.395 1.00 26.64 B
ATOM 5851 N SER B 116 -19.400 -19.035-109.435 1.00 25.75 B
ATOM 5852 CA SER B 116 -18.464 -20.115-109.750 1.00 27.89 B
ATOM 5853 CB SER B 116 -18.887 -20.908-111.007 1.00 29.85 B
ATOM 5854 OG SER B 116 -19.204 -20.089-112.116 1.00 32.83 B
ATOM 5855 C SER B 116 -17.023 -19.685-109.885 1.00 28.57 B
ATOM 5856 O SER B 116 -16.118 -20.495-109.665 1.00 29.06 B
ATOM 5857 N ASN B 117 -16.789 -18.424-110.241 1.00 28.87 B
ATOM 5858 CA ASN B 117 -15.413 -17.950-110.369 1.00 29.76 B
ATOM 5859 CB ASN B 117 -15.355 -16.651-111.165 1.00 32.05 B
ATOM 5860 CG ASN B 117 -15.284 -16.885-112.657 1.00 35.00 B
ATOM 5861 OD1 ASN B 117 -14.346 -17.513-113.163 1.00 36.45 B
ATOM 5862 ND2 ASN B 117 -16.279 -16.375-113.375 1.00 38.76 B
ATOM 5863 C ASN B 117 -14.772 -17.740-108.999 1.00 29.89 B
ATOM 5864 O ASN B 117 -13.598 -18.068-108.810 1.00 30.05 B
ATOM 5865 N MET B 118 -15.543 -17.199-108.049 1.00 28.94 B
ATOM 5866 CA MET B 118 -15.042 -16.961-106.697 1.00 27.77 B
ATOM 5867 CB MET B 118 -16.100 -16.267-105.828 1.00 27.42 B
ATOM 5868 CG MET B 118 -16.344 -14.803-106.136 1.00 25.18 B
ATOM 5869 SD MET B 118 -17.236 -13.945-104.812 1.00 25.98 B
ATOM 5870 CE MET B 118 -18.861 -14.689-104.875 1.00 21.78 B
ATOM 5871 C MET B 118 -14.696 -18.304-106.080 1.00 27.16 B
ATOM 5872 O MET B 118 -13.610 -18.495-105.537 1.00 25.49 B
ATOM 5873 N SER B 119 -15.644 -19.228-106.175 1.00 27.22 B
ATOM 5874 CA SER B 119 -15.475 -20.573-105.650 1.00 28.14 B
ATOM 5875 CB SER B 119 -16.713 -21.403-105.972 1.00 28.24 B
ATOM 5876 OG SER B 119 -16.556 -22.739-105.551 1.00 28.89 B
ATOM 5877 C SER B 119 -14.239 -21.214-106.266 1.00 28.98 B
ATOM 5878 O SER B 119 -13.468 -21.880-105.577 1.00 29.88 B

ATOM 5879 N ARG B 120 -14.055 -20.996-107.566 1.00 29.36 B
ATOM 5880 CA ARG B 120 -12.914 -21.531-108.294 1.00 29.46 B
ATOM 5881 CB ARG B 120 -13.060 -21.211-109.788 1.00 31.11 B
ATOM 5882 CG ARG B 120 -12.111 -21.983-110.714 1.00 33.43 B
ATOM 5883 CD ARG B 120 -10.970 -21.117-111.236 1.00 32.95 B
ATOM 5884 NE ARG B 120 -11.475 -19.949-111.950 1.00 34.34 B
ATOM 5885 CZ ARG B 120 -10.718 -18.908-112.281 1.00 37.43 B
ATOM 5886 NH1 ARG B 120 -9.425 -18.906-111.964 1.00 38.82 B
ATOM 5887 NH2 ARG B 120 -11.253 -17.854-112.895 1.00 37.48 B
ATOM 5888 C ARG B 120 -11.619 -20.933-107.746 1.00 28.97 B
ATOM 5889 O ARG B 120 -10.688 -21.653-107.400 1.00 28.04 B
ATOM 5890 N ILE B 121 -11.573 -19.610-107.662 1.00 29.72 B
ATOM 5891 CA ILE B 121 -10.399 -18.907-107.166 1.00 31.47 B
ATOM 5892 CB ILE B 121 -10.676 -17.401-107.103 1.00 30.68 B
ATOM 5893 CG2 ILE B 121 -9.508 -16.673-106.461 1.00 29.67 B
ATOM 5894 CG1 ILE B 121 -10.930 -16.875-108.515 1.00 29.18 B
ATOM 5895 CD1 ILE B 121 -11.517 -15.481-108.556 1.00 29.36 B
ATOM 5896 C ILE B 121 -9.963 -19.392-105.782 1.00 33.55 B
ATOM 5897 O ILE B 121 -8.773 -19.632-105.537 1.00 32.52 B
ATOM 5898 N TYR B 122 -10.936 -19.539-104.884 1.00 35.43 B
ATOM 5899 CA TYR B 122 -10.682 -19.978-103.515 1.00 36.24 B
ATOM 5900 CB TYR B 122 -11.979 -19.933-102.703 1.00 36.82 B
ATOM 5901 CG TYR B 122 -11.792 -20.310-101.246 1.00 39.78 B
ATOM 5902 CD1 TYR B 122 -11.296 -19.391-100.312 1.00 39.28 B
ATOM 5903 CE1 TYR B 122 -11.078 -19.763 -98.983 1.00 39.78 B
ATOM 5904 CD2 TYR B 122 -12.071 -21.605-100.806 1.00 40.82 B
ATOM 5905 CE2 TYR B 122 -11.858 -21.981 -99.483 1.00 40.96 B
ATOM 5906 CZ TYR B 122 -11.360 -21.066 -98.578 1.00 40.89 B
ATOM 5907 OH TYR B 122 -11.115 -21.483 -97.286 1.00 41.76 B
ATOM 5908 C TYR B 122 -10.070 -21.372-103.405 1.00 37.05 B
ATOM 5909 O TYR B 122 -9.058 -21.546-102.728 1.00 38.31 B
ATOM 5910 N SER B 123 -10.684 -22.360-104.062 1.00 37.62 B
ATOM 5911 CA SER B 123 -10.203 -23.747-104.024 1.00 37.93 B
ATOM 5912 CB SER B 123 -11.345 -24.715-104.345 1.00 38.45 B

ATOM 5913 OG SER B 123 -12.397 -24.608-103.399 1.00 41.52 B
ATOM 5914 C SER B 123 -9.046 -24.017-104.978 1.00 37.83 B
ATOM 5915 O SER B 123 -8.708 -25.170-105.234 1.00 39.02 B
ATOM 5916 N THR B 124 -8.435 -22.954-105.488 1.00 37.34 B
ATOM 5917 CA THR B 124 -7.327 -23.073-106.423 1.00 36.97 B
ATOM 5918 CB THR B 124 -7.713 -22.463-107.788 1.00 37.35 B
ATOM 5919 OG1 THR B 124 -8.637 -23.334-108.439 1.00 36.59 B
ATOM 5920 CG2 THR B 124 -6.488 -22.248-108.677 1.00 37.71 B
ATOM 5921 C THR B 124 -6.076 -22.374-105.911 1.00 37.32 B
ATOM 5922 O THR B 124 -4.965 -22.749-106.269 1.00 37.40 B
ATOM 5923 N ALA B 125 -6.265 -21.352-105.083 1.00 37.57 B
ATOM 5924 CA ALA B 125 -5.149 -20.586-104.538 1.00 37.41 B
ATOM 5925 CB ALA B 125 -5.650 -19.606-103.505 1.00 38.08 B
ATOM 5926 C ALA B 125 -4.103 -21.500-103.924 1.00 37.32 B
ATOM 5927 O ALA B 125 -4.435 -22.442-103.205 1.00 37.16 B
ATOM 5928 N LYS B 126 -2.862 -21.110-103.942 1.00 37.43 B
ATOM 5929 CA LYS B 126 -1.809 -21.991-103.613 1.00 38.28 B
ATOM 5930 CB LYS B 126 -1.254 -22.480-104.905 1.00 38.47 B
ATOM 5931 CG LYS B 126 -1.642 -23.827-105.250 1.00 37.76 B
ATOM 5932 CD LYS B 126 -1.822 -23.997-106.684 0.00 39.24 B
ATOM 5933 CE LYS B 126 -3.159 -24.689-107.003 0.00 40.00 B
ATOM 5934 NZ LYS B 126 -3.310 -25.229-108.400 1.00 41.87 B
ATOM 5935 C LYS B 126 -0.780 -21.121-103.019 1.00 39.38 B
ATOM 5936 O LYS B 126 -0.830 -19.981-103.274 1.00 39.61 B
ATOM 5937 N VAL B 127 0.186 -21.641-102.274 1.00 40.25 B
ATOM 5938 CA VAL B 127 1.262 -20.850-101.688 1.00 41.29 B
ATOM 5939 CB VAL B 127 1.231 -20.852-100.131 1.00 38.75 B
ATOM 5940 CG1 VAL B 127 2.331 -19.956 -99.595 1.00 34.32 B
ATOM 5941 CG2 VAL B 127 -0.115 -20.381 -99.622 1.00 37.27 B
ATOM 5942 C VAL B 127 2.590 -21.439-102.128 1.00 44.41 B
ATOM 5943 O VAL B 127 2.855 -22.605-101.874 1.00 44.51 B
ATOM 5944 N CYS B 128 3.417 -20.634-102.787 1.00 49.53 B
ATOM 5945 CA CYS B 128 4.728 -21.094-103.243 1.00 55.69 B
ATOM 5946 C CYS B 128 5.814 -20.453-102.401 1.00 59.00 B

ATOM 5947 O CYS B 128 5.624 -19.357-101.859 1.00 59.77 B
ATOM 5948 CB CYS B 128 4.961 -20.726-104.705 1.00 58.13 B
ATOM 5949 SG CYS B 128 3.552 -21.099-105.793 1.00 64.19 B
ATOM 5950 N LEU B 129 6.956 -21.132-102.304 1.00 62.86 B
ATOM 5951 CA LEU B 129 8.084 -20.640-101.514 1.00 66.84 B
ATOM 5952 CB LEU B 129 8.643 -21.776-100.654 1.00 65.97 B
ATOM 5953 CG LEU B 129 7.608 -22.564 -99.833 1.00 65.39 B
ATOM 5954 CD1 LEU B 129 6.840 -23.550-100.716 1.00 63.89 B
ATOM 5955 CD2 LEU B 129 8.326 -23.318 -98.736 1.00 66.31 B
ATOM 5956 C LEU B 129 9.177 -20.088-102.429 1.00 70.03 B
ATOM 5957 O LEU B 129 9.255 -20.475-103.597 1.00 71.38 B
ATOM 5958 N PRO B 130 10.009 -19.197-101.898 1.00 72.61 B
ATOM 5959 CD PRO B 130 9.934 -18.670-100.524 1.00 73.19 B
ATOM 5960 CA PRO B 130 10.985 -18.470-102.716 1.00 74.33 B
ATOM 5961 CB PRO B 130 11.720 -17.606-101.690 1.00 73.98 B
ATOM 5962 CG PRO B 130 10.729 -17.398-100.602 1.00 73.61 B
ATOM 5963 C PRO B 130 11.964 -19.417-103.401 1.00 76.13 B
ATOM 5964 O PRO B 130 12.729 -18.991-104.267 1.00 76.31 B
ATOM 5965 N ASN B 131 11.932 -20.690-103.020 1.00 78.25 B
ATOM 5966 CA ASN B 131 11.843 -21.775-103.990 1.00 80.47 B
ATOM 5967 CB ASN B 131 11.625 -23.113-103.281 1.00 80.79 B
ATOM 5968 CG ASN B 131 12.572 -24.192-103.768 1.00 81.80 B
ATOM 5969 OD1 ASN B 131 12.423 -24.711-104.874 1.00 82.36 B
ATOM 5970 ND2 ASN B 131 13.553 -24.535-102.942 1.00 82.32 B
ATOM 5971 C ASN B 131 10.742 -21.540-105.019 1.00 82.02 B
ATOM 5972 O ASN B 131 9.557 -21.534-104.684 1.00 83.75 B
ATOM 5973 N ALA B 132 11.141 -21.347-106.272 1.00 82.27 B
ATOM 5974 CA ALA B 132 10.229 -21.502-107.399 1.00 82.57 B
ATOM 5975 CB ALA B 132 8.823 -21.806-106.905 1.00 81.85 B
ATOM 5976 C ALA B 132 10.709 -22.593-108.350 1.00 83.10 B
ATOM 5977 O ALA B 132 10.441 -22.545-109.551 1.00 83.95 B
ATOM 5978 N ALA B 133 11.419 -23.575-107.806 1.00 83.24 B
ATOM 5979 CA ALA B 133 11.193 -24.971-108.160 1.00 82.83 B
ATOM 5980 CB ALA B 133 12.309 -25.846-107.610 1.00 82.51 B

ATOM 5981 C ALA B 133 9.837 -25.349-107.572 1.00 82.52 B
ATOM 5982 O ALA B 133 9.748 -25.789-106.426 1.00 82.68 B
ATOM 5983 N ALA B 134 8.785 -25.175-108.364 1.00 81.72 B
ATOM 5984 CA ALA B 134 7.421 -25.228-107.850 1.00 80.22 B
ATOM 5985 CB ALA B 134 6.423 -25.264-108.997 1.00 79.70 B
ATOM 5986 C ALA B 134 7.292 -26.480-106.990 1.00 79.10 B
ATOM 5987 O ALA B 134 7.320 -27.600-107.499 1.00 80.44 B
ATOM 5988 N ALA B 135 7.152 -26.282-105.683 1.00 75.95 B
ATOM 5989 CA ALA B 135 6.269 -27.113-104.873 1.00 72.56 B
ATOM 5990 CB ALA B 135 7.075 -28.142-104.096 1.00 72.03 B
ATOM 5991 C ALA B 135 5.430 -26.263-103.924 1.00 70.69 B
ATOM 5992 O ALA B 135 5.774 -26.102-102.753 1.00 72.07 B
ATOM 5993 N CYS B 136 4.330 -25.722-104.437 1.00 66.42 B
ATOM 5994 CA CYS B 136 3.487 -24.819-103.663 1.00 61.77 B
ATOM 5995 C CYS B 136 2.474 -25.593-102.825 1.00 57.93 B
ATOM 5996 O CYS B 136 2.082 -26.705-103.179 1.00 56.21 B
ATOM 5997 CB CYS B 136 2.765 -23.836-104.586 1.00 62.97 B
ATOM 5998 SG CYS B 136 3.772 -23.223-105.957 1.00 65.22 B
ATOM 5999 N TRP B 137 2.054 -24.997-101.714 1.00 54.83 B
ATOM 6000 CA TRP B 137 1.148 -25.664-100.780 1.00 51.24 B
ATOM 6001 CB TRP B 137 1.509 -25.329-99.335 1.00 50.75 B
ATOM 6002 CG TRP B 137 2.909 -25.621 -98.955 1.00 49.82 B
ATOM 6003 CD2 TRP B 137 3.713 -24.876 -98.040 1.00 50.08 B
ATOM 6004 CE2 TRP B 137 4.959 -25.533 -97.950 1.00 50.41 B
ATOM 6005 CE3 TRP B 137 3.502 -23.716 -97.283 1.00 50.57 B
ATOM 6006 CD1 TRP B 137 3.670 -26.666 -99.372 1.00 50.20 B
ATOM 6007 NE1 TRP B 137 4.905 -26.624 -98.775 1.00 50.22 B
ATOM 6008 CZ2 TRP B 137 5.999 -25.066 -97.132 1.00 51.03 B
ATOM 6009 CZ3 TRP B 137 4.537 -23.248 -96.464 1.00 50.81 B
ATOM 6010 CH2 TRP B 137 5.769 -23.924 -96.398 1.00 51.17 B
ATOM 6011 C TRP B 137 -0.306 -25.274-100.993 1.00 49.56 B
ATOM 6012 O TRP B 137 -0.607 -24.134-101.342 1.00 48.92 B
ATOM 6013 N SER B 138 -1.204 -26.227-100.771 1.00 47.87 B
ATOM 6014 CA SER B 138 -2.638 -25.997-100.910 1.00 47.70 B

ATOM 6015 CB SER B 138 -3.320 -27.248-101.451 1.00 49.86 B
ATOM 6016 OG SER B 138 -3.276 -28.303-100.498 1.00 51.82 B
ATOM 6017 C SER B 138 -3.179 -25.707 -99.518 1.00 46.54 B
ATOM 6018 O SER B 138 -2.448 -25.814 -98.542 1.00 46.69 B
ATOM 6019 N LEU B 139 -4.453 -25.353 -99.410 1.00 45.24 B
ATOM 6020 CA LEU B 139 -5.006 -25.077 -98.092 1.00 44.11 B
ATOM 6021 CB LEU B 139 -6.338 -24.327 -98.193 1.00 42.44 B
ATOM 6022 CG LEU B 139 -6.878 -23.775 -96.869 1.00 40.14 B
ATOM 6023 CD1 LEU B 139 -5.857 -22.843 -96.235 1.00 38.80 B
ATOM 6024 CD2 LEU B 139 -8.185 -23.038 -97.111 1.00 40.13 B
ATOM 6025 C LEU B 139 -5.186 -26.377 -97.306 1.00 43.65 B
ATOM 6026 O LEU B 139 -4.782 -26.467 -96.150 1.00 45.06 B
ATOM 6027 N ALA B 140 -5.820 -27.339 -97.917 1.00 43.12 B
ATOM 6028 CA ALA B 140 -5.973 -28.605 -97.308 1.00 43.98 B
ATOM 6029 CB ALA B 140 -7.346 -28.933 -97.215 1.00 43.65 B
ATOM 6030 C ALA B 140 -5.277 -29.648 -98.084 1.00 44.72 B
ATOM 6031 O ALA B 140 -5.759 -30.082 -99.069 1.00 43.99 B
ATOM 6032 N PRO B 141 -4.105 -30.049 -97.632 1.00 45.40 B
ATOM 6033 CD PRO B 141 -3.626 -31.230 -98.320 1.00 45.17 B
ATOM 6034 CA PRO B 141 -3.791 -30.166 -96.240 1.00 44.46 B
ATOM 6035 CB PRO B 141 -3.424 -31.569 -96.170 1.00 43.90 B
ATOM 6036 CG PRO B 141 -2.766 -31.716 -97.259 1.00 43.51 B
ATOM 6037 C PRO B 141 -2.557 -29.465 -95.988 1.00 43.98 B
ATOM 6038 O PRO B 141 -2.198 -29.186 -94.931 1.00 42.90 B
ATOM 6039 N ASP B 142 -1.811 -29.224 -96.996 1.00 44.16 B
ATOM 6040 CA ASP B 142 -0.531 -28.702 -96.718 1.00 44.45 B
ATOM 6041 CB ASP B 142 0.124 -28.227 -97.954 1.00 45.88 B
ATOM 6042 CG ASP B 142 0.337 -29.291 -98.883 1.00 47.41 B
ATOM 6043 OD1 ASP B 142 1.095 -30.166 -98.562 1.00 48.71 B
ATOM 6044 OD2 ASP B 142 -0.211 -29.368 -99.952 1.00 48.31 B
ATOM 6045 C ASP B 142 -0.510 -27.713 -95.648 1.00 43.39 B
ATOM 6046 O ASP B 142 0.312 -27.799 -94.814 1.00 43.73 B
ATOM 6047 N LEU B 143 -1.395 -26.739 -95.675 1.00 41.46 B
ATOM 6048 CA LEU B 143 -1.206 -25.487 -94.945 1.00 37.84 B

ATOM 6049 CB LEU B 143 -1.798 -24.323 -95.692 1.00 35.27 B
ATOM 6050 CG LEU B 143 -1.169 -23.669 -96.873 1.00 32.82 B
ATOM 6051 CD1 LEU B 143 -1.878 -22.500 -97.122 1.00 31.32 B
ATOM 6052 CD2 LEU B 143 0.172 -23.405 -96.665 1.00 32.19 B
ATOM 6053 C LEU B 143 -1.946 -25.624 -93.695 1.00 36.02 B
ATOM 6054 O LEU B 143 -1.502 -25.315 -92.660 1.00 34.20 B
ATOM 6055 N THR B 144 -3.080 -26.224 -93.825 1.00 34.66 B
ATOM 6056 CA THR B 144 -3.879 -26.628 -92.677 1.00 35.14 B
ATOM 6057 CB THR B 144 -5.020 -27.565 -93.108 1.00 33.95 B
ATOM 6058 OG1 THR B 144 -6.114 -26.790 -93.597 1.00 34.56 B
ATOM 6059 CG2 THR B 144 -5.489 -28.405 -91.956 1.00 34.68 B
ATOM 6060 C THR B 144 -3.014 -27.348 -91.627 1.00 36.48 B
ATOM 6061 O THR B 144 -3.182 -27.134 -90.423 1.00 37.23 B
ATOM 6062 N ASN B 145 -2.090 -28.190 -92.092 1.00 36.61 B
ATOM 6063 CA ASN B 145 -1.193 -28.938 -91.210 1.00 36.30 B
ATOM 6064 CB ASN B 145 -0.537 -30.106 -91.959 1.00 37.66 B
ATOM 6065 CG ASN B 145 -1.550 -31.107 -92.498 1.00 39.36 B
ATOM 6066 OD1 ASN B 145 -2.687 -31.202 -92.014 1.00 40.56 B
ATOM 6067 ND2 ASN B 145 -1.131 -31.878 -93.493 1.00 40.33 B
ATOM 6068 C ASN B 145 -0.091 -28.073 -90.623 1.00 35.25 B
ATOM 6069 O ASN B 145 0.338 -28.277 -89.490 1.00 35.88 B
ATOM 6070 N ILE B 146 0.385 -27.112 -91.401 1.00 33.91 B
ATOM 6071 CA ILE B 146 1.444 -26.238 -90.926 1.00 32.64 B
ATOM 6072 CB ILE B 146 1.985 -25.343 -92.054 1.00 31.27 B
ATOM 6073 CG2 ILE B 146 3.176 -24.548 -91.552 1.00 31.11 B
ATOM 6074 CG1 ILE B 146 2.404 -26.210 -93.244 1.00 30.05 B
ATOM 6075 CD1 ILE B 146 3.039 -25.442 -94.382 1.00 27.91 B
ATOM 6076 C ILE B 146 0.909 -25.365 -89.800 1.00 32.26 B
ATOM 6077 O ILE B 146 1.615 -25.069 -88.837 1.00 31.55 B
ATOM 6078 N LEU B 147 -0.352 -24.972 -89.925 1.00 31.71 B
ATOM 6079 CA LEU B 147 -0.975 -24.140 -88.919 1.00 30.28 B
ATOM 6080 CB LEU B 147 -2.044 -23.248 -89.544 1.00 28.79 B
ATOM 6081 CG LEU B 147 -1.532 -21.827 -89.736 1.00 27.68 B
ATOM 6082 CD1 LEU B 147 -1.121 -21.638 -91.177 1.00 28.13 B

ATOM 6083 CD2 LEU B 147 -2.611 -20.842 -89.326 1.00 27.77 B
ATOM 6084 C LEU B 147 -1.592 -24.944 -87.807 1.00 29.94 B
ATOM 6085 O LEU B 147 -2.200 -24.388 -86.908 1.00 30.96 B
ATOM 6086 N ALA B 148 -1.440 -26.255 -87.861 1.00 29.46 B
ATOM 6087 CA ALA B 148 -2.016 -27.092 -86.829 1.00 29.71 B
ATOM 6088 CB ALA B 148 -2.817 -28.215 -87.440 1.00 29.09 B
ATOM 6089 C ALA B 148 -0.939 -27.664 -85.944 1.00 31.02 B
ATOM 6090 O ALA B 148 -1.172 -27.877 -84.756 1.00 34.09 B
ATOM 6091 N SER B 149 0.249 -27.896 -86.502 1.00 30.60 B
ATOM 6092 CA SER B 149 1.334 -28.488 -85.721 1.00 29.80 B
ATOM 6093 CB SER B 149 1.465 -29.958 -86.092 1.00 31.93 B
ATOM 6094 OG SER B 149 1.449 -30.088 -87.502 1.00 35.83 B
ATOM 6095 C SER B 149 2.702 -27.832 -85.800 1.00 27.68 B
ATOM 6096 O SER B 149 3.622 -28.235 -85.093 1.00 26.70 B
ATOM 6097 N SER B 150 2.859 -26.846 -86.666 1.00 26.48 B
ATOM 6098 CA SER B 150 4.139 -26.174 -86.751 1.00 25.72 B
ATOM 6099 CB SER B 150 4.268 -25.415 -88.062 1.00 25.19 B
ATOM 6100 OG SER B 150 5.468 -24.661 -88.073 1.00 25.83 B
ATOM 6101 C SER B 150 4.245 -25.194 -85.590 1.00 26.29 B
ATOM 6102 O SER B 150 3.256 -24.548 -85.212 1.00 27.01 B
ATOM 6103 N ARG B 151 5.443 -25.085 -85.021 1.00 25.75 B
ATOM 6104 CA ARG B 151 5.673 -24.179 -83.902 1.00 24.93 B
ATOM 6105 CB ARG B 151 6.048 -24.966 -82.652 1.00 23.31 B
ATOM 6106 CG ARG B 151 4.907 -25.187 -81.689 1.00 20.68 B
ATOM 6107 CD ARG B 151 3.705 -25.788 -82.350 1.00 17.57 B
ATOM 6108 NE ARG B 151 2.773 -26.295 -81.355 1.00 18.49 B
ATOM 6109 CZ ARG B 151 1.506 -26.607 -81.600 1.00 20.11 B
ATOM 6110 NH1 ARG B 151 0.741 -27.066 -80.620 1.00 19.83 B
ATOM 6111 NH2 ARG B 151 1.000 -26.446 -82.823 1.00 19.20 B
ATOM 6112 C ARG B 151 6.759 -23.167 -84.219 1.00 25.26 B
ATOM 6113 O ARG B 151 7.386 -22.605 -83.315 1.00 25.50 B
ATOM 6114 N SER B 152 6.976 -22.942 -85.511 1.00 25.18 B
ATOM 6115 CA SER B 152 7.970 -21.979 -85.974 1.00 25.84 B
ATOM 6116 CB SER B 152 8.627 -22.487 -87.246 1.00 25.77 B

ATOM 6117 OG SER B 152 9.677 -21.633 -87.630 1.00 29.32 B
ATOM 6118 C SER B 152 7.200 -20.693 -86.259 1.00 25.83 B
ATOM 6119 O SER B 152 6.311 -20.677 -87.107 1.00 26.18 B
ATOM 6120 N TYR B 153 7.520 -19.618 -85.550 1.00 25.42 B
ATOM 6121 CA TYR B 153 6.772 -18.388 -85.754 1.00 26.24 B
ATOM 6122 CB TYR B 153 7.286 -17.261 -84.850 1.00 25.10 B
ATOM 6123 CG TYR B 153 6.469 -15.983 -84.934 1.00 23.31 B
ATOM 6124 CD1 TYR B 153 5.386 -15.761 -84.082 1.00 22.93 B
ATOM 6125 CE1 TYR B 153 4.636 -14.587 -84.163 1.00 21.05 B
ATOM 6126 CD2 TYR B 153 6.774 -14.999 -85.877 1.00 22.03 B
ATOM 6127 CE2 TYR B 153 6.027 -13.831 -85.969 1.00 20.86 B
ATOM 6128 CZ TYR B 153 4.967 -13.632 -85.109 1.00 20.89 B
ATOM 6129 OH TYR B 153 4.252 -12.469 -85.201 1.00 21.99 B
ATOM 6130 C TYR B 153 6.871 -17.970 -87.208 1.00 27.73 B
ATOM 6131 O TYR B 153 5.866 -17.583 -87.819 1.00 28.80 B
ATOM 6132 N ALA B 154 8.077 -18.061 -87.765 1.00 27.76 B
ATOM 6133 CA ALA B 154 8.302 -17.691 -89.161 1.00 26.90 B
ATOM 6134 CB ALA B 154 9.771 -17.818 -89.501 1.00 24.70 B
ATOM 6135 C ALA B 154 7.467 -18.530 -90.138 1.00 27.11 B
ATOM 6136 O ALA B 154 6.706 -17.982 -90.940 1.00 27.43 B
ATOM 6137 N MET B 155 7.598 -19.852 -90.071 1.00 27.29 B
ATOM 6138 CA MET B 155 6.852 -20.713 -90.981 1.00 29.02 B
ATOM 6139 CB MET B 155 7.225 -22.170 -90.741 1.00 31.49 B
ATOM 6140 CG MET B 155 6.692 -23.129 -91.795 1.00 35.56 B
ATOM 6141 SD MET B 155 7.652 -24.678 -91.814 1.00 42.16 B
ATOM 6142 CE MET B 155 7.269 -25.399 -90.175 1.00 38.82 B
ATOM 6143 C MET B 155 5.340 -20.518 -90.855 1.00 28.34 B
ATOM 6144 O MET B 155 4.612 -20.551 -91.852 1.00 28.97 B
ATOM 6145 N LEU B 156 4.867 -20.311 -89.630 1.00 27.74 B
ATOM 6146 CA LEU B 156 3.445 -20.086 -89.399 1.00 26.72 B
ATOM 6147 CB LEU B 156 3.152 -20.074 -87.892 1.00 26.42 B
ATOM 6148 CG LEU B 156 3.191 -21.449 -87.193 1.00 26.17 B
ATOM 6149 CD1 LEU B 156 3.188 -21.285 -85.691 1.00 26.48 B
ATOM 6150 CD2 LEU B 156 1.981 -22.275 -87.618 1.00 26.59 B

ATOM 6151 C LEU B 156 3.028 -18.763 -90.057 1.00 26.46 B
ATOM 6152 O LEU B 156 1.985 -18.684 -90.699 1.00 27.74 B
ATOM 6153 N LEU B 157 3.858 -17.733 -89.914 1.00 25.37 B
ATOM 6154 CA LEU B 157 3.577 -16.426 -90.507 1.00 24.75 B
ATOM 6155 CB LEU B 157 4.636 -15.411 -90.057 1.00 23.32 B
ATOM 6156 CG LEU B 157 4.623 -13.992 -90.644 1.00 21.40 B
ATOM 6157 CD1 LEU B 157 3.377 -13.258 -90.188 1.00 20.32 B
ATOM 6158 CD2 LEU B 157 5.883 -13.241 -90.215 1.00 18.46 B
ATOM 6159 C LEU B 157 3.576 -16.518 -92.031 1.00 25.81 B
ATOM 6160 O LEU B 157 2.756 -15.892 -92.707 1.00 26.08 B
ATOM 6161 N PHE B 158 4.502 -17.306 -92.570 1.00 27.08 B
ATOM 6162 CA PHE B 158 4.614 -17.468 -94.017 1.00 27.48 B
ATOM 6163 CB PHE B 158 5.850 -18.297 -94.363 1.00 29.80 B
ATOM 6164 CG PHE B 158 6.301 -18.147 -95.790 1.00 32.74 B
ATOM 6165 CD1 PHE B 158 7.000 -17.009 -96.192 1.00 33.67 B
ATOM 6166 CD2 PHE B 158 6.001 -19.125 -96.739 1.00 33.80 B
ATOM 6167 CE1 PHE B 158 7.393 -16.838 -97.515 1.00 34.00 B
ATOM 6168 CE2 PHE B 158 6.392 -18.968 -98.073 1.00 34.45 B
ATOM 6169 CZ PHE B 158 7.088 -17.821 -98.460 1.00 34.54 B
ATOM 6170 C PHE B 158 3.370 -18.117 -94.626 1.00 25.89 B
ATOM 6171 O PHE B 158 2.882 -17.674 -95.661 1.00 26.78 B
ATOM 6172 N ALA B 159 2.862 -19.162 -93.978 1.00 23.43 B
ATOM 6173 CA ALA B 159 1.672 -19.847 -94.457 1.00 22.10 B
ATOM 6174 CB ALA B 159 1.529 -21.175 -93.746 1.00 20.41 B
ATOM 6175 C ALA B 159 0.418 -18.999 -94.241 1.00 22.11 B
ATOM 6176 O ALA B 159 -0.493 -19.016 -95.070 1.00 22.05 B
ATOM 6177 N TRP B 160 0.371 -18.265 -93.129 1.00 21.46 B
ATOM 6178 CA TRP B 160 -0.781 -17.419 -92.822 1.00 20.90 B
ATOM 6179 CB TRP B 160 -0.690 -16.818 -91.412 1.00 20.05 B
ATOM 6180 CG TRP B 160 -1.927 -16.015 -91.035 1.00 19.37 B
ATOM 6181 CD2 TRP B 160 -2.161 -14.622 -91.279 1.00 17.74 B
ATOM 6182 CE2 TRP B 160 -3.465 -14.330 -90.823 1.00 17.70 B
ATOM 6183 CE3 TRP B 160 -1.397 -13.591 -91.840 1.00 17.57 B
ATOM 6184 CD1 TRP B 160 -3.067 -16.491 -90.456 1.00 19.51 B

ATOM 6185 NE1 TRP B 160 -3.995 -15.489 -90.324 1.00 17.96 B
ATOM 6186 CZ2 TRP B 160 -4.022 -13.056 -90.908 1.00 17.76 B
ATOM 6187 CZ3 TRP B 160 -1.951 -12.319 -91.924 1.00 17.92 B
ATOM 6188 CH2 TRP B 160 -3.252 -12.064 -91.459 1.00 17.97 B
ATOM 6189 C TRP B 160 -0.860 -16.279 -93.821 1.00 20.47 B
ATOM 6190 O TRP B 160 -1.884 -16.075 -94.465 1.00 19.77 B
ATOM 6191 N GLU B 161 0.223 -15.523 -93.926 1.00 20.40 B
ATOM 6192 CA GLU B 161 0.272 -14.405 -94.860 1.00 21.66 B
ATOM 6193 CB GLU B 161 1.640 -13.730 -94.792 1.00 21.38 B
ATOM 6194 CG GLU B 161 1.765 -12.498 -95.661 1.00 21.93 B
ATOM 6195 CD GLU B 161 3.189 -11.970 -95.726 1.00 23.97 B
ATOM 6196 OE1 GLU B 161 3.354 -10.792 -96.099 1.00 24.83 B
ATOM 6197 OE2 GLU B 161 4.139 -12.727 -95.420 1.00 24.15 B
ATOM 6198 C GLU B 161 0.028 -14.933 -96.275 1.00 22.07 B
ATOM 6199 O GLU B 161 -0.868 -14.465 -96.981 1.00 22.73 B
ATOM 6200 N GLY B 162 0.834 -15.920 -96.669 1.00 20.98 B
ATOM 6201 CA GLY B 162 0.727 -16.524 -97.980 1.00 20.61 B
ATOM 6202 C GLY B 162 -0.681 -16.900 -98.384 1.00 21.17 B
ATOM 6203 O GLY B 162 -1.123 -16.563 -99.481 1.00 20.65 B
ATOM 6204 N TRP B 163 -1.399 -17.598 -97.516 1.00 21.90 B
ATOM 6205 CA TRP B 163 -2.761 -17.982 -97.855 1.00 22.40 B
ATOM 6206 CB TRP B 163 -3.347 -18.933 -96.791 1.00 21.14 B
ATOM 6207 CG TRP B 163 -4.831 -19.118 -96.949 1.00 21.06 B
ATOM 6208 CD2 TRP B 163 -5.508 -19.798 -98.018 1.00 20.23 B
ATOM 6209 CE2 TRP B 163 -6.902 -19.612 -97.820 1.00 19.98 B
ATOM 6210 CE3 TRP B 163 -5.076 -20.541 -99.127 1.00 18.38 B
ATOM 6211 CD1 TRP B 163 -5.812 -18.573 -96.168 1.00 21.95 B
ATOM 6212 NE1 TRP B 163 -7.058 -18.863 -96.684 1.00 21.61 B
ATOM 6213 CZ2 TRP B 163 -7.864 -20.143 -98.692 1.00 18.48 B
ATOM 6214 CZ3 TRP B 163 -6.037 -21.065 -99.991 1.00 18.64 B
ATOM 6215 CH2 TRP B 163 -7.414 -20.861 -99.766 1.00 19.27 B
ATOM 6216 C TRP B 163 -3.658 -16.751 -98.029 1.00 22.99 B
ATOM 6217 O TRP B 163 -4.404 -16.653 -98.999 1.00 24.04 B
ATOM 6218 N HIS B 164 -3.537 -15.776 -97.187 1.00 23.15 B

ATOM 6219 CA HIS B 164 -4.349 -14.597 -97.202 1.00 23.12 B
ATOM 6220 CB HIS B 164 -4.145 -13.864 -95.884 1.00 20.50 B
ATOM 6221 CG HIS B 164 -4.945 -14.411 -94.773 1.00 20.07 B
ATOM 6222 CD2 HIS B 164 -6.091 -13.993 -94.249 1.00 18.68 B
ATOM 6223 ND1 HIS B 164 -4.635 -15.560 -94.128 1.00 21.35 B
ATOM 6224 CE1 HIS B 164 -5.544 -15.792 -93.217 1.00 19.71 B
ATOM 6225 NE2 HIS B 164 -6.443 -14.856 -93.274 1.00 17.81 B
ATOM 6226 C HIS B 164 -4.101 -13.664 -98.322 1.00 23.62 B
ATOM 6227 O HIS B 164 -4.974 -12.997 -98.779 1.00 24.09 B
ATOM 6228 N ASN B 165 -2.882 -13.534 -98.737 1.00 22.79 B
ATOM 6229 CA ASN B 165 -2.616 -12.723 -99.896 1.00 22.21 B
ATOM 6230 CB ASN B 165 -1.128 -12.417 -99.989 1.00 21.27 B
ATOM 6231 CG ASN B 165 -0.684 -11.421 -98.955 1.00 21.74 B
ATOM 6232 OD1 ASN B 165 -1.447 -10.537 -98.559 1.00 21.90 B
ATOM 6233 ND2 ASN B 165 0.564 -11.539 -98.518 1.00 24.17 B
ATOM 6234 C ASN B 165 -3.099 -13.453-101.156 1.00 23.12 B
ATOM 6235 O ASN B 165 -3.767 -12.873-102.014 1.00 23.53 B
ATOM 6236 N ALA B 166 -2.784 -14.739-101.240 1.00 22.60 B
ATOM 6237 CA ALA B 166 -3.147 -15.547-102.384 1.00 22.62 B
ATOM 6238 CB ALA B 166 -2.501 -16.892-102.258 1.00 21.38 B
ATOM 6239 C ALA B 166 -4.641 -15.721-102.605 1.00 23.93 B
ATOM 6240 O ALA B 166 -5.102 -15.771-103.741 1.00 24.10 B
ATOM 6241 N ALA B 167 -5.407 -15.796-101.526 1.00 25.58 B
ATOM 6242 CA ALA B 167 -6.848 -16.026-101.641 1.00 26.26 B
ATOM 6243 CB ALA B 167 -7.300 -16.944-100.501 1.00 24.91 B
ATOM 6244 C ALA B 167 -7.787 -14.812-101.719 1.00 26.74 B
ATOM 6245 O ALA B 167 -8.716 -14.784-102.541 1.00 26.76 B
ATOM 6246 N GLY B 168 -7.559 -13.814-100.874 1.00 26.24 B
ATOM 6247 CA GLY B 168 -8.452 -12.671-100.864 1.00 26.08 B
ATOM 6248 C GLY B 168 -8.210 -11.533-101.844 1.00 26.01 B
ATOM 6249 O GLY B 168 -9.159 -10.874-102.280 1.00 26.61 B
ATOM 6250 N ILE B 169 -6.953 -11.280-102.186 1.00 24.10 B
ATOM 6251 CA ILE B 169 -6.652 -10.187-103.094 1.00 21.99 B
ATOM 6252 CB ILE B 169 -5.116 -10.073-103.306 1.00 20.82 B

ATOM 6253 CG2 ILE B 169 -4.799 -9.121-104.457 1.00 20.39 B
ATOM 6254 CG1 ILE B 169 -4.466 -9.588-102.005 1.00 18.16 B
ATOM 6255 CD1 ILE B 169 -2.976 -9.386-102.087 1.00 16.47 B
ATOM 6256 C ILE B 169 -7.390 -10.305-104.436 1.00 22.26 B
ATOM 6257 O ILE B 169 -8.159 -9.417-104.817 1.00 22.63 B
ATOM 6258 N PRO B 170 -7.202 -11.421-105.146 1.00 21.78 B
ATOM 6259 CD PRO B 170 -6.507 -12.653-104.734 1.00 21.83 B
ATOM 6260 CA PRO B 170 -7.859 -11.611-106.440 1.00 22.05 B
ATOM 6261 CB PRO B 170 -7.226 -12.895-106.943 1.00 21.58 B
ATOM 6262 CG PRO B 170 -7.085 -13.678-105.683 1.00 20.96 B
ATOM 6263 C PRO B 170 -9.371 -11.734-106.354 1.00 23.00 B
ATOM 6264 O PRO B 170 -10.080 -11.543-107.339 1.00 25.16 B
ATOM 6265 N LEU B 171 -9.857 -12.042-105.164 1.00 22.86 B
ATOM 6266 CA LEU B 171 -11.273 -12.257-104.940 1.00 22.27 B
ATOM 6267 CB LEU B 171 -11.400 -13.250-103.782 1.00 23.41 B
ATOM 6268 CG LEU B 171 -12.583 -14.200-103.599 1.00 25.26 B
ATOM 6269 CD1 LEU B 171 -13.098 -14.707-104.957 1.00 25.82 B
ATOM 6270 CD2 LEU B 171 -12.123 -15.348-102.689 1.00 22.07 B
ATOM 6271 C LEU B 171 -12.066 -10.988-104.656 1.00 21.04 B
ATOM 6272 O LEU B 171 -13.266 -10.946-104.884 1.00 19.44 B
ATOM 6273 N LYS B 172 -11.416 -9.919-104.431 1.00 21.74 B
ATOM 6274 CA LYS B 172 -12.089 -8.783-103.962 1.00 22.67 B
ATOM 6275 CB LYS B 172 -11.080 -7.831-103.431 1.00 24.19 B
ATOM 6276 CG LYS B 172 -11.627 -6.647-102.764 1.00 24.87 B
ATOM 6277 CD LYS B 172 -10.595 -5.918-102.143 1.00 28.85 B
ATOM 6278 CE LYS B 172 -11.144 -4.753-101.628 1.00 31.11 B
ATOM 6279 NZ LYS B 172 -10.321 -4.242-100.530 1.00 33.52 B
ATOM 6280 C LYS B 172 -12.865 -8.103-104.966 1.00 22.23 B
ATOM 6281 O LYS B 172 -13.959 -7.787-104.738 1.00 20.81 B
ATOM 6282 N PRO B 173 -12.288 -7.811-106.102 1.00 21.45 B
ATOM 6283 CD PRO B 173 -10.959 -8.201-106.600 1.00 20.21 B
ATOM 6284 CA PRO B 173 -13.072 -7.175-107.166 1.00 20.49 B
ATOM 6285 CB PRO B 173 -12.108 -7.175-108.349 1.00 19.32 B
ATOM 6286 CG PRO B 173 -11.219 -8.343-108.063 1.00 18.88 B

ATOM 6287 C PRO B 173 -14.386 -7.916-107.444 1.00 20.61 B
ATOM 6288 O PRO B 173 -15.427 -7.292-107.680 1.00 19.71 B
ATOM 6289 N LEU B 174 -14.336 -9.243-107.377 1.00 20.23 B
ATOM 6290 CA LEU B 174 -15.522 -10.048-107.618 1.00 21.74 B
ATOM 6291 CB LEU B 174 -15.132 -11.513-107.824 1.00 20.66 B
ATOM 6292 CG LEU B 174 -14.030 -11.848-108.825 1.00 19.15 B
ATOM 6293 CD1 LEU B 174 -14.028 -13.343-109.045 1.00 19.68 B
ATOM 6294 CD2 LEU B 174 -14.272 -11.157-110.141 1.00 23.72 B
ATOM 6295 C LEU B 174 -16.581 -9.946-106.496 1.00 23.56 B
ATOM 6296 O LEU B 174 -17.787 -9.838-106.788 1.00 22.95 B
ATOM 6297 N TYR B 175 -16.151 -9.971-105.226 1.00 24.30 B
ATOM 6298 CA TYR B 175 -17.102 -9.898-104.113 1.00 23.75 B
ATOM 6299 CB TYR B 175 -16.387 -9.979-102.756 1.00 23.38 B
ATOM 6300 CG TYR B 175 -17.317 -10.363-101.616 1.00 23.97 B
ATOM 6301 CD1 TYR B 175 -17.823 -11.661-101.515 1.00 25.47 B
ATOM 6302 CE1 TYR B 175 -18.712 -12.016-100.509 1.00 24.83 B
ATOM 6303 CD2 TYR B 175 -17.725 -9.428-100.668 1.00 23.22 B
ATOM 6304 CE2 TYR B 175 -18.615 -9.773 -99.654 1.00 24.06 B
ATOM 6305 CZ TYR B 175 -19.104 -11.069 -99.587 1.00 25.23 B
ATOM 6306 OH TYR B 175 -20.007 -11.429 -98.619 1.00 26.03 B
ATOM 6307 C TYR B 175 -17.936 -8.620-104.169 1.00 23.95 B
ATOM 6308 O TYR B 175 -19.080 -8.618-103.742 1.00 23.28 B
ATOM 6309 N GLU B 176 -17.365 -7.542-104.700 1.00 24.82 B
ATOM 6310 CA GLU B 176 -18.067 -6.268-104.798 1.00 25.91 B
ATOM 6311 CB GLU B 176 -17.089 -5.157-105.164 1.00 25.46 B
ATOM 6312 CG GLU B 176 -15.842 -5.149-104.314 1.00 26.82 B
ATOM 6313 CD GLU B 176 -14.773 -4.231-104.863 1.00 27.26 B
ATOM 6314 OE1 GLU B 176 -15.136 -3.151-105.368 1.00 26.04 B
ATOM 6315 OE2 GLU B 176 -13.576 -4.584-104.780 1.00 28.08 B
ATOM 6316 C GLU B 176 -19.171 -6.328-105.840 1.00 27.43 B
ATOM 6317 O GLU B 176 -20.258 -5.801-105.616 1.00 27.23 B
ATOM 6318 N ASP B 177 -18.895 -6.953-106.986 1.00 29.55 B
ATOM 6319 CA ASP B 177 -19.901 -7.067-108.042 1.00 31.28 B
ATOM 6320 CB ASP B 177 -19.288 -7.587-109.346 1.00 34.46 B

ATOM 6321 CG ASP B 177 -18.276 -6.631-109.945 1.00 36.90 B
ATOM 6322 OD1 ASP B 177 -18.446 -5.398-109.773 1.00 40.15 B
ATOM 6323 OD2 ASP B 177 -17.322 -7.113-110.602 1.00 36.84 B
ATOM 6324 C ASP B 177 -21.005 -8.019-107.606 1.00 31.25 B
ATOM 6325 O ASP B 177 -22.193 -7.751-107.846 1.00 31.48 B
ATOM 6326 N PHE B 178 -20.604 -9.133-106.982 1.00 29.44 B
ATOM 6327 CA PHE B 178 -21.547 -10.136-106.481 1.00 27.60 B
ATOM 6328 CB PHE B 178 -20.812 -11.285-105.781 1.00 28.75 B
ATOM 6329 CG PHE B 178 -21.680 -12.045-104.809 1.00 30.90 B
ATOM 6330 CD1 PHE B 178 -22.544 -13.045-105.257 1.00 32.62 B
ATOM 6331 CD2 PHE B 178 -21.708 -11.690-103.454 1.00 30.92 B
ATOM 6332 CE1 PHE B 178 -23.425 -13.671-104.371 1.00 33.94 B
ATOM 6333 CE2 PHE B 178 -22.585 -12.307-102.562 1.00 31.13 B
ATOM 6334 CZ PHE B 178 -23.445 -13.295-103.017 1.00 32.44 B
ATOM 6335 C PHE B 178 -22.488 -9.498-105.469 1.00 26.24 B
ATOM 6336 O PHE B 178 -23.692 -9.750-105.474 1.00 26.05 B
ATOM 6337 N THR B 179 -21.911 -8.687-104.589 1.00 24.87 B
ATOM 6338 CA THR B 179 -22.656 -8.015-103.544 1.00 24.19 B
ATOM 6339 CB THR B 179 -21.695 -7.238-102.588 1.00 25.28 B
ATOM 6340 OG1 THR B 179 -20.697 -8.131-102.081 1.00 27.02 B
ATOM 6341 CG2 THR B 179 -22.445 -6.665-101.407 1.00 24.11 B
ATOM 6342 C THR B 179 -23.707 -7.071-104.122 1.00 23.34 B
ATOM 6343 O THR B 179 -24.850 -7.095-103.692 1.00 23.51 B
ATOM 6344 N ALA B 180 -23.342 -6.255-105.105 1.00 22.63 B
ATOM 6345 CA ALA B 180 -24.305 -5.325-105.688 1.00 22.75 B
ATOM 6346 CB ALA B 180 -23.630 -4.435-106.703 1.00 22.36 B
ATOM 6347 C ALA B 180 -25.464 -6.050-106.347 1.00 23.53 B
ATOM 6348 O ALA B 180 -26.618 -5.641-106.215 1.00 23.46 B
ATOM 6349 N LEU B 181 -25.154 -7.128-107.059 1.00 23.65 B
ATOM 6350 CA LEU B 181 -26.176 -7.884-107.757 1.00 25.45 B
ATOM 6351 CB LEU B 181 -25.529 -8.862-108.743 1.00 25.20 B
ATOM 6352 CG LEU B 181 -25.015 -8.251-110.043 1.00 25.19 B
ATOM 6353 CD1 LEU B 181 -24.421 -9.332-110.933 1.00 27.40 B
ATOM 6354 CD2 LEU B 181 -26.167 -7.553-110.747 1.00 25.23 B

ATOM 6355 C LEU B 181 -27.096 -8.631-106.816 1.00 27.21 B
ATOM 6356 O LEU B 181 -28.319 -8.647-107.002 1.00 27.42 B
ATOM 6357 N SER B 182 -26.499 -9.255-105.805 1.00 29.06 B
ATOM 6358 CA SER B 182 -27.249 -10.026-104.821 1.00 29.37 B
ATOM 6359 CB SER B 182 -26.286 -10.661-103.818 1.00 29.10 B
ATOM 6360 OG SER B 182 -26.978 -11.548-102.961 1.00 30.68 B
ATOM 6361 C SER B 182 -28.246 -9.125-104.108 1.00 29.03 B
ATOM 6362 O SER B 182 -29.281 -9.577-103.622 1.00 29.67 B
ATOM 6363 N ASN B 183 -27.926 -7.841-104.061 1.00 28.04 B
ATOM 6364 CA ASN B 183 -28.786 -6.871-103.422 1.00 28.99 B
ATOM 6365 CB ASN B 183 -27.983 -5.649-102.991 1.00 29.74 B
ATOM 6366 CG ASN B 183 -27.490 -5.747-101.567 1.00 28.04 B
ATOM 6367 OD1 ASN B 183 -26.610 -6.531-101.250 1.00 27.45 B
ATOM 6368 ND2 ASN B 183 -28.070 -4.948-100.700 1.00 30.48 B
ATOM 6369 C ASN B 183 -29.908 -6.436-104.341 1.00 30.37 B
ATOM 6370 O ASN B 183 -31.069 -6.413-103.938 1.00 30.99 B
ATOM 6371 N GLU B 184 -29.626 -6.008-105.536 1.00 31.98 B
ATOM 6372 CA GLU B 184 -30.646 -5.772-106.520 1.00 32.35 B
ATOM 6373 CB GLU B 184 -30.008 -5.927-107.842 1.00 34.05 B
ATOM 6374 CG GLU B 184 -29.957 -4.701-108.688 1.00 39.02 B
ATOM 6375 CD GLU B 184 -30.137 -4.981-110.129 1.00 42.29 B
ATOM 6376 OE1 GLU B 184 -29.260 -4.659-110.921 1.00 44.06 B
ATOM 6377 OE2 GLU B 184 -31.184 -5.514-110.462 1.00 43.81 B
ATOM 6378 C GLU B 184 -31.593 -6.833-106.520 1.00 31.06 B
ATOM 6379 O GLU B 184 -32.732 -6.656-106.559 1.00 29.94 B
ATOM 6380 N ALA B 185 -31.070 -7.993-106.621 1.00 29.58 B
ATOM 6381 CA ALA B 185 -31.899 -9.175-106.693 1.00 30.05 B
ATOM 6382 CB ALA B 185 -31.033 -10.413-106.553 1.00 27.67 B
ATOM 6383 C ALA B 185 -32.960 -9.152-105.605 1.00 31.55 B
ATOM 6384 O ALA B 185 -34.140 -8.931-105.875 1.00 32.15 B
ATOM 6385 N TYR B 186 -32.521 -9.365-104.367 1.00 33.02 B
ATOM 6386 CA TYR B 186 -33.411 -9.403-103.212 1.00 33.17 B
ATOM 6387 CB TYR B 186 -32.644 -9.943-102.005 1.00 31.22 B
ATOM 6388 CG TYR B 186 -32.403 -11.432-102.089 1.00 30.76 B

ATOM 6389 CD1 TYR B 186 -31.128 -11.944-102.310 1.00 28.96 B
ATOM 6390 CE1 TYR B 186 -30.920 -13.318-102.429 1.00 29.24 B
ATOM 6391 CD2 TYR B 186 -33.469 -12.334-101.987 1.00 31.10 B
ATOM 6392 CE2 TYR B 186 -33.270 -13.707-102.112 1.00 29.79 B
ATOM 6393 CZ TYR B 186 -31.998 -14.189-102.333 1.00 29.11 B
ATOM 6394 OH TYR B 186 -31.813 -15.538-102.480 1.00 29.59 B
ATOM 6395 C TYR B 186 -34.167 -8.122-102.838 1.00 34.21 B
ATOM 6396 O TYR B 186 -35.185 -8.183-102.139 1.00 34.25 B
ATOM 6397 N LYS B 187 -33.695 -6.965-103.293 1.00 35.08 B
ATOM 6398 CA LYS B 187 -34.402 -5.739-102.973 1.00 37.37 B
ATOM 6399 CB LYS B 187 -33.623 -4.502-103.435 1.00 36.32 B
ATOM 6400 CG LYS B 187 -34.275 -3.171-103.062 1.00 35.98 B
ATOM 6401 CD LYS B 187 -33.280 -2.022-103.192 1.00 38.33 B
ATOM 6402 CE LYS B 187 -33.958 -0.635-103.141 1.00 40.55 B
ATOM 6403 NZ LYS B 187 -34.545 -0.235-101.815 1.00 40.56 B
ATOM 6404 C LYS B 187 -35.751 -5.815-103.664 1.00 38.78 B
ATOM 6405 O LYS B 187 -36.677 -5.105-103.298 1.00 39.33 B
ATOM 6406 N GLN B 188 -35.862 -6.701-104.650 1.00 40.87 B
ATOM 6407 CA GLN B 188 -37.115 -6.869-105.383 1.00 43.68 B
ATOM 6408 CB GLN B 188 -36.859 -7.267-106.838 1.00 47.68 B
ATOM 6409 CG GLN B 188 -36.407 -6.108-107.715 1.00 53.40 B
ATOM 6410 CD GLN B 188 -36.456 -6.448-109.189 1.00 56.48 B
ATOM 6411 OE1 GLN B 188 -37.532 -6.704-109.742 1.00 58.64 B
ATOM 6412 NE2 GLN B 188 -35.291 -6.457-109.839 1.00 57.87 B
ATOM 6413 C GLN B 188 -38.023 -7.892-104.736 1.00 42.78 B
ATOM 6414 O GLN B 188 -39.158 -8.086-105.174 1.00 42.06 B
ATOM 6415 N ASP B 189 -37.513 -8.550-103.699 1.00 42.48 B
ATOM 6416 CA ASP B 189 -38.285 -9.535-102.958 1.00 42.31 B
ATOM 6417 CB ASP B 189 -37.408 -10.723-102.552 1.00 44.31 B
ATOM 6418 CG ASP B 189 -37.279 -11.767-103.663 1.00 46.37 B
ATOM 6419 OD1 ASP B 189 -36.986 -11.387-104.818 1.00 48.84 B
ATOM 6420 OD2 ASP B 189 -37.467 -12.973-103.386 1.00 47.14 B
ATOM 6421 C ASP B 189 -38.839 -8.840-101.729 1.00 41.85 B
ATOM 6422 O ASP B 189 -39.534 -9.448-100.913 1.00 41.67 B

ATOM 6423 N GLY B 190 -38.519 -7.556-101.599 1.00 41.14 B
ATOM 6424 CA GLY B 190 -39.022 -6.786-100.477 1.00 40.66 B
ATOM 6425 C GLY B 190 -38.062 -6.391 -99.370 1.00 40.19 B
ATOM 6426 O GLY B 190 -38.406 -5.538 -98.552 1.00 40.46 B
ATOM 6427 N PHE B 191 -36.869 -6.980 -99.326 1.00 39.41 B
ATOM 6428 CA PHE B 191 -35.913 -6.650 -98.265 1.00 39.16 B
ATOM 6429 CB PHE B 191 -35.064 -7.871 -97.919 1.00 37.34 B
ATOM 6430 CG PHE B 191 -35.846 -9.141 -97.778 1.00 36.52 B
ATOM 6431 CD1 PHE B 191 -36.155 -9.909 -98.894 1.00 36.27 B
ATOM 6432 CD2 PHE B 191 -36.234 -9.597 -96.526 1.00 37.00 B
ATOM 6433 CE1 PHE B 191 -36.830 -11.111 -98.773 1.00 35.30 B
ATOM 6434 CE2 PHE B 191 -36.914 -10.805 -96.393 1.00 36.88 B
ATOM 6435 CZ PHE B 191 -37.210 -11.562 -97.525 1.00 35.73 B
ATOM 6436 C PHE B 191 -34.979 -5.474 -98.596 1.00 39.60 B
ATOM 6437 O PHE B 191 -34.722 -5.185 -99.765 1.00 40.10 B
ATOM 6438 N THR B 192 -34.469 -4.805 -97.561 1.00 39.43 B
ATOM 6439 CA THR B 192 -33.562 -3.677 -97.761 1.00 39.58 B
ATOM 6440 CB THR B 192 -33.189 -3.014 -96.418 1.00 39.81 B
ATOM 6441 OG1 THR B 192 -34.284 -2.215 -95.970 1.00 40.57 B
ATOM 6442 CG2 THR B 192 -31.951 -2.126 -96.565 1.00 40.02 B
ATOM 6443 C THR B 192 -32.279 -4.101 -98.465 1.00 39.75 B
ATOM 6444 O THR B 192 -31.788 -3.394 -99.349 1.00 40.51 B
ATOM 6445 N ASP B 193 -31.738 -5.248 -98.066 1.00 38.79 B
ATOM 6446 CA ASP B 193 -30.516 -5.768 -98.662 1.00 38.64 B
ATOM 6447 CB ASP B 193 -29.300 -5.043 -98.088 1.00 40.83 B
ATOM 6448 CG ASP B 193 -29.242 -5.086 -96.575 1.00 43.65 B
ATOM 6449 OD1 ASP B 193 -28.943 -6.169 -95.999 1.00 44.15 B
ATOM 6450 OD2 ASP B 193 -29.497 -4.020 -95.968 1.00 45.51 B
ATOM 6451 C ASP B 193 -30.405 -7.267 -98.415 1.00 38.55 B
ATOM 6452 O ASP B 193 -31.216 -7.836 -97.680 1.00 38.71 B
ATOM 6453 N THR B 194 -29.419 -7.915 -99.032 1.00 37.22 B
ATOM 6454 CA THR B 194 -29.271 -9.355 -98.852 1.00 35.62 B
ATOM 6455 CB THR B 194 -27.979 -9.887 -99.498 1.00 34.98 B
ATOM 6456 OG1 THR B 194 -28.003 -9.610-100.898 1.00 34.57 B

ATOM 6457 CG2 THR B 194 -27.862 -11.399 -99.301 1.00 34.21 B
ATOM 6458 C THR B 194 -29.251 -9.682 -97.369 1.00 34.80 B
ATOM 6459 O THR B 194 -29.856 -10.659 -96.934 1.00 33.93 B
ATOM 6460 N GLY B 195 -28.564 -8.847 -96.597 1.00 33.67 B
ATOM 6461 CA GLY B 195 -28.470 -9.067 -95.168 1.00 33.04 B
ATOM 6462 C GLY B 195 -29.797 -9.344 -94.494 1.00 32.84 B
ATOM 6463 O GLY B 195 -29.929 -10.276 -93.703 1.00 31.58 B
ATOM 6464 N ALA B 196 -30.797 -8.537 -94.819 1.00 33.00 B
ATOM 6465 CA ALA B 196 -32.109 -8.684 -94.213 1.00 32.24 B
ATOM 6466 CB ALA B 196 -32.977 -7.503 -94.570 1.00 32.31 B
ATOM 6467 C ALA B 196 -32.816 -9.968 -94.584 1.00 31.89 B
ATOM 6468 O ALA B 196 -33.599 -10.483 -93.793 1.00 31.33 B
ATOM 6469 N TYR B 197 -32.505 -10.566 -95.709 1.00 32.56 B
ATOM 6470 CA TYR B 197 -33.135 -11.780 -96.153 1.00 33.18 B
ATOM 6471 CB TYR B 197 -32.936 -12.070 -97.642 1.00 34.14 B
ATOM 6472 CG TYR B 197 -33.461 -13.439 -98.123 1.00 36.36 B
ATOM 6473 CD1 TYR B 197 -34.754 -13.744 -98.125 1.00 36.44 B
ATOM 6474 CE1 TYR B 197 -35.157 -14.935 -98.521 1.00 35.85 B
ATOM 6475 CD2 TYR B 197 -32.623 -14.407 -98.587 1.00 36.83 B
ATOM 6476 CE2 TYR B 197 -33.063 -15.585 -98.950 1.00 35.86 B
ATOM 6477 CZ TYR B 197 -34.313 -15.835 -98.910 1.00 35.59 B
ATOM 6478 OH TYR B 197 -34.721 -17.042 -99.281 1.00 36.67 B
ATOM 6479 C TYR B 197 -32.562 -12.845 -95.381 1.00 34.09 B
ATOM 6480 O TYR B 197 -33.222 -13.683 -94.922 1.00 35.63 B
ATOM 6481 N TRP B 198 -31.287 -12.842 -95.245 1.00 33.00 B
ATOM 6482 CA TRP B 198 -30.622 -13.894 -94.493 1.00 32.25 B
ATOM 6483 CB TRP B 198 -29.110 -13.656 -94.507 1.00 32.05 B
ATOM 6484 CG TRP B 198 -28.447 -14.031 -95.790 1.00 31.14 B
ATOM 6485 CD2 TRP B 198 -27.037 -14.135 -96.029 1.00 30.39 B
ATOM 6486 CE2 TRP B 198 -26.868 -14.478 -97.388 1.00 30.02 B
ATOM 6487 CE3 TRP B 198 -25.900 -13.970 -95.227 1.00 29.21 B
ATOM 6488 CD1 TRP B 198 -29.057 -14.311 -96.977 1.00 31.77 B
ATOM 6489 NE1 TRP B 198 -28.117 -14.581 -97.944 1.00 30.04 B
ATOM 6490 CZ2 TRP B 198 -25.612 -14.656 -97.965 1.00 30.26 B

ATOM 6491 CZ3 TRP B 198 -24.643 -14.147 -95.802 1.00 29.09 B
ATOM 6492 CH2 TRP B 198 -24.512 -14.487 -97.160 1.00 30.14 B
ATOM 6493 C TRP B 198 -31.140 -13.990 -93.042 1.00 31.82 B
ATOM 6494 O TRP B 198 -31.522 -15.065 -92.574 1.00 30.97 B
ATOM 6495 N ARG B 199 -31.161 -12.858 -92.342 1.00 31.66 B
ATOM 6496 CA ARG B 199 -31.626 -12.819 -90.954 1.00 31.94 B
ATOM 6497 CB ARG B 199 -31.486 -11.401 -90.373 1.00 29.67 B
ATOM 6498 CG ARG B 199 -30.057 -10.882 -90.289 1.00 28.31 B
ATOM 6499 CD ARG B 199 -29.983 -9.575 -89.519 1.00 28.29 B
ATOM 6500 NE ARG B 199 -30.568 -8.442 -90.230 1.00 27.75 B
ATOM 6501 CZ ARG B 199 -29.909 -7.681 -91.096 1.00 27.19 B
ATOM 6502 NH1 ARG B 199 -30.520 -6.664 -91.694 1.00 26.48 B
ATOM 6503 NH2 ARG B 199 -28.634 -7.933 -91.363 1.00 27.27 B
ATOM 6504 C ARG B 199 -33.078 -13.277 -90.820 1.00 33.00 B
ATOM 6505 O ARG B 199 -33.416 -14.023 -89.902 1.00 33.95 B
ATOM 6506 N SER B 200 -33.929 -12.843 -91.746 1.00 34.43 B
ATOM 6507 CA SER B 200 -35.349 -13.186 -91.719 1.00 35.08 B
ATOM 6508 CB SER B 200 -36.054 -12.635 -92.961 1.00 35.45 B
ATOM 6509 OG SER B 200 -35.913 -13.512 -94.065 1.00 36.25 B
ATOM 6510 C SER B 200 -35.661 -14.675 -91.591 1.00 35.18 B
ATOM 6511 O SER B 200 -36.807 -15.031 -91.354 1.00 34.04 B
ATOM 6512 N TRP B 201 -34.663 -15.542 -91.750 1.00 36.20 B
ATOM 6513 CA TRP B 201 -34.903 -16.983 -91.627 1.00 37.86 B
ATOM 6514 CB TRP B 201 -33.722 -17.803 -92.143 1.00 38.05 B
ATOM 6515 CG TRP B 201 -33.521 -17.746 -93.585 1.00 38.87 B
ATOM 6516 CD2 TRP B 201 -32.269 -17.766 -94.260 1.00 39.87 B
ATOM 6517 CE2 TRP B 201 -32.542 -17.773 -95.645 1.00 40.25 B
ATOM 6518 CE3 TRP B 201 -30.936 -17.781 -93.831 1.00 40.79 B
ATOM 6519 CD1 TRP B 201 -34.482 -17.738 -94.551 1.00 40.00 B
ATOM 6520 NE1 TRP B 201 -33.904 -17.757 -95.795 1.00 40.01 B
ATOM 6521 CZ2 TRP B 201 -31.532 -17.793 -96.605 1.00 40.89 B
ATOM 6522 CZ3 TRP B 201 -29.931 -17.801 -94.787 1.00 41.80 B
ATOM 6523 CH2 TRP B 201 -30.239 -17.806 -96.160 1.00 42.01 B
ATOM 6524 C TRP B 201 -35.153 -17.409 -90.188 1.00 38.61 B

```
ATOM   6525  O   TRP B 201    -35.530 -18.551 -89.922  1.00 39.72      B
ATOM   6526  N   TYR B 202    -34.922 -16.497 -89.256  1.00 39.16      B
ATOM   6527  CA  TYR B 202    -35.130 -16.813 -87.860  1.00 40.18      B
ATOM   6528  CB  TYR B 202    -33.932 -16.346 -87.041  1.00 39.68      B
ATOM   6529  CG  TYR B 202    -32.645 -17.016 -87.446  1.00 38.95      B
ATOM   6530  CD1 TYR B 202    -31.819 -16.449 -88.413  1.00 37.89      B
ATOM   6531  CE1 TYR B 202    -30.646 -17.072 -88.805  1.00 38.09      B
ATOM   6532  CD2 TYR B 202    -32.263 -18.235 -86.879  1.00 38.68      B
ATOM   6533  CE2 TYR B 202    -31.095 -18.870 -87.266  1.00 38.11      B
ATOM   6534  CZ  TYR B 202    -30.292 -18.279 -88.228  1.00 38.47      B
ATOM   6535  OH  TYR B 202    -29.124 -18.885 -88.605  1.00 39.79      B
ATOM   6536  C   TYR B 202    -36.425 -16.215 -87.318  1.00 41.53      B
ATOM   6537  O   TYR B 202    -36.768 -16.416 -86.150  1.00 42.44      B
ATOM   6538  N   ASN B 203    -37.141 -15.492 -88.174  1.00 42.63      B
ATOM   6539  CA  ASN B 203    -38.412 -14.887 -87.801  1.00 43.66      B
ATOM   6540  CB  ASN B 203    -39.557 -15.891 -87.978  1.00 46.12      B
ATOM   6541  CG  ASN B 203    -39.639 -16.459 -89.399  1.00 49.37      B
ATOM   6542  OD1 ASN B 203    -40.622 -17.114 -89.759  1.00 52.01      B
ATOM   6543  ND2 ASN B 203    -38.602 -16.224 -90.203  1.00 50.79      B
ATOM   6544  C   ASN B 203    -38.453 -14.385 -86.373  1.00 43.57      B
ATOM   6545  O   ASN B 203    -39.097 -14.989 -85.508  1.00 43.53      B
ATOM   6546  N   SER B 204    -37.752 -13.283 -86.133  1.00 42.83      B
ATOM   6547  CA  SER B 204    -37.688 -12.673 -84.814  1.00 41.81      B
ATOM   6548  CB  SER B 204    -36.568 -13.367 -84.029  1.00 43.12      B
ATOM   6549  OG  SER B 204    -36.252 -12.662 -82.839  1.00 43.97      B
ATOM   6550  C   SER B 204    -37.374 -11.196 -84.965  1.00 40.55      B
ATOM   6551  O   SER B 204    -36.304 -10.827 -85.448  1.00 40.94      B
ATOM   6552  N   PRO B 205    -38.304 -10.325 -84.554  1.00 39.19      B
ATOM   6553  CD  PRO B 205    -39.613 -10.630 -83.959  1.00 38.10      B
ATOM   6554  CA  PRO B 205    -38.104  -8.874 -84.657  1.00 38.58      B
ATOM   6555  CB  PRO B 205    -39.441  -8.298 -84.191  1.00 37.69      B
ATOM   6556  CG  PRO B 205    -40.412  -9.430 -84.369  1.00 37.85      B
ATOM   6557  C   PRO B 205    -36.978  -8.434 -83.744  1.00 38.32      B
ATOM   6558  O   PRO B 205    -36.622  -7.263 -83.703  1.00 39.81      B
```

ATOM 6559 N THR B 206 -36.421 -9.400 -83.024 1.00 38.03 B
ATOM 6560 CA THR B 206 -35.373 -9.145 -82.050 1.00 37.88 B
ATOM 6561 CB THR B 206 -35.898 -9.462 -80.627 1.00 36.74 B
ATOM 6562 OG1 THR B 206 -36.626 -10.699 -80.658 1.00 35.80 B
ATOM 6563 CG2 THR B 206 -36.812 -8.349 -80.118 1.00 35.96 B
ATOM 6564 C THR B 206 -34.078 -9.924 -82.259 1.00 38.21 B
ATOM 6565 O THR B 206 -33.137 -9.785 -81.474 1.00 39.10 B
ATOM 6566 N PHE B 207 -34.020 -10.736 -83.308 1.00 37.36 B
ATOM 6567 CA PHE B 207 -32.835 -11.548 -83.572 1.00 36.22 B
ATOM 6568 CB PHE B 207 -32.844 -12.026 -85.025 1.00 33.23 B
ATOM 6569 CG PHE B 207 -31.783 -13.039 -85.335 1.00 31.17 B
ATOM 6570 CD1 PHE B 207 -31.678 -14.202 -84.591 1.00 30.77 B
ATOM 6571 CD2 PHE B 207 -30.894 -12.838 -86.379 1.00 31.77 B
ATOM 6572 CE1 PHE B 207 -30.706 -15.147 -84.881 1.00 30.69 B
ATOM 6573 CE2 PHE B 207 -29.916 -13.786 -86.677 1.00 31.30 B
ATOM 6574 CZ PHE B 207 -29.826 -14.939 -85.925 1.00 30.78 B
ATOM 6575 C PHE B 207 -31.486 -10.884 -83.256 1.00 36.80 B
ATOM 6576 O PHE B 207 -30.686 -11.426 -82.492 1.00 36.56 B
ATOM 6577 N GLU B 208 -31.256 -9.695 -83.749 1.00 37.54 B
ATOM 6578 CA GLU B 208 -29.992 -9.049 -83.584 1.00 39.43 B
ATOM 6579 CB GLU B 208 -29.908 -7.836 -84.484 1.00 40.68 B
ATOM 6580 CG GLU B 208 -29.213 -8.009 -85.822 1.00 42.09 B
ATOM 6581 CD GLU B 208 -29.380 -6.835 -86.731 1.00 43.81 B
ATOM 6582 OE1 GLU B 208 -28.443 -6.065 -86.871 1.00 45.01 B
ATOM 6583 OE2 GLU B 208 -30.456 -6.677 -87.311 1.00 43.27 B
ATOM 6584 C GLU B 208 -29.775 -8.649 -82.170 1.00 40.19 B
ATOM 6585 O GLU B 208 -28.686 -8.735 -81.702 1.00 40.28 B
ATOM 6586 N ASP B 209 -30.815 -8.178 -81.489 1.00 40.82 B
ATOM 6587 CA ASP B 209 -30.739 -7.821 -80.079 1.00 40.77 B
ATOM 6588 CB ASP B 209 -31.986 -7.054 -79.641 1.00 43.28 B
ATOM 6589 CG ASP B 209 -31.907 -5.579 -79.982 1.00 46.34 B
ATOM 6590 OD1 ASP B 209 -32.879 -4.854 -79.677 1.00 48.43 B
ATOM 6591 OD2 ASP B 209 -30.875 -5.140 -80.547 1.00 46.31 B
ATOM 6592 C ASP B 209 -30.571 -9.071 -79.225 1.00 38.98 B

ATOM 6593 O ASP B 209 -29.816 -9.058 -78.261 1.00 39.16 B
ATOM 6594 N ASP B 210 -31.265 -10.151 -79.573 1.00 37.37 B
ATOM 6595 CA ASP B 210 -31.138 -11.391 -78.818 1.00 36.62 B
ATOM 6596 CB ASP B 210 -32.123 -12.444 -79.332 1.00 37.49 B
ATOM 6597 CG ASP B 210 -33.587 -12.061 -79.079 1.00 39.88 B
ATOM 6598 OD1 ASP B 210 -33.859 -11.339 -78.095 1.00 39.31 B
ATOM 6599 OD2 ASP B 210 -34.476 -12.499 -79.849 1.00 40.56 B
ATOM 6600 C ASP B 210 -29.703 -11.934 -78.879 1.00 36.08 B
ATOM 6601 O ASP B 210 -29.190 -12.451 -77.891 1.00 35.99 B
ATOM 6602 N LEU B 211 -29.052 -11.813 -80.029 1.00 35.62 B
ATOM 6603 CA LEU B 211 -27.680 -12.290 -80.169 1.00 36.04 B
ATOM 6604 CB LEU B 211 -27.296 -12.406 -81.643 1.00 37.00 B
ATOM 6605 CG LEU B 211 -27.922 -13.485 -82.528 1.00 35.90 B
ATOM 6606 CD1 LEU B 211 -27.620 -13.132 -83.976 1.00 34.48 B
ATOM 6607 CD2 LEU B 211 -27.382 -14.872 -82.167 1.00 33.46 B
ATOM 6608 C LEU B 211 -26.683 -11.368 -79.477 1.00 36.87 B
ATOM 6609 O LEU B 211 -25.595 -11.796 -79.108 1.00 35.98 B
ATOM 6610 N GLU B 212 -27.036 -10.094 -79.331 1.00 39.18 B
ATOM 6611 CA GLU B 212 -26.143 -9.151 -78.658 1.00 40.45 B
ATOM 6612 CB GLU B 212 -26.628 -7.705 -78.852 1.00 42.04 B
ATOM 6613 CG GLU B 212 -25.745 -6.666 -78.163 1.00 48.37 B
ATOM 6614 CD GLU B 212 -25.378 -5.474 -79.060 1.00 53.52 B
ATOM 6615 OE1 GLU B 212 -24.810 -5.711 -80.153 1.00 56.77 B
ATOM 6616 OE2 GLU B 212 -25.642 -4.302 -78.674 1.00 54.88 B
ATOM 6617 C GLU B 212 -26.104 -9.517 -77.171 1.00 39.50 B
ATOM 6618 O GLU B 212 -25.032 -9.677 -76.594 1.00 39.49 B
ATOM 6619 N HIS B 213 -27.288 -9.666 -76.580 1.00 38.88 B
ATOM 6620 CA HIS B 213 -27.466 -10.038 -75.176 1.00 39.24 B
ATOM 6621 CB HIS B 213 -28.980 -10.139 -74.882 1.00 43.25 B
ATOM 6622 CG HIS B 213 -29.335 -10.486 -73.458 1.00 47.80 B
ATOM 6623 CD2 HIS B 213 -29.975 -9.767 -72.499 1.00 48.56 B
ATOM 6624 ND1 HIS B 213 -29.094 -11.728 -72.900 1.00 48.92 B
ATOM 6625 CE1 HIS B 213 -29.570 -11.760 -71.666 1.00 47.69 B
ATOM 6626 NE2 HIS B 213 -30.109 -10.583 -71.398 1.00 48.16 B

ATOM 6627 C HIS B 213 -26.774 -11.384 -74.953 1.00 37.53 B
ATOM 6628 O HIS B 213 -25.937 -11.537 -74.064 1.00 37.10 B
ATOM 6629 N LEU B 214 -27.117 -12.353 -75.789 1.00 35.78 B
ATOM 6630 CA LEU B 214 -26.557 -13.694 -75.703 1.00 33.70 B
ATOM 6631 CB LEU B 214 -27.016 -14.513 -76.904 1.00 33.63 B
ATOM 6632 CG LEU B 214 -27.573 -15.894 -76.585 1.00 33.44 B
ATOM 6633 CD1 LEU B 214 -28.120 -16.529 -77.856 1.00 33.30 B
ATOM 6634 CD2 LEU B 214 -26.483 -16.742 -75.962 1.00 33.97 B
ATOM 6635 C LEU B 214 -25.041 -13.713 -75.640 1.00 32.47 B
ATOM 6636 O LEU B 214 -24.452 -14.500 -74.895 1.00 32.09 B
ATOM 6637 N TYR B 215 -24.407 -12.854 -76.432 1.00 31.65 B
ATOM 6638 CA TYR B 215 -22.951 -12.819 -76.453 1.00 31.04 B
ATOM 6639 CB TYR B 215 -22.420 -12.111 -77.710 1.00 29.26 B
ATOM 6640 CG TYR B 215 -20.919 -12.238 -77.837 1.00 26.68 B
ATOM 6641 CD1 TYR B 215 -20.326 -13.471 -78.106 1.00 26.92 B
ATOM 6642 CE1 TYR B 215 -18.936 -13.627 -78.089 1.00 26.11 B
ATOM 6643 CD2 TYR B 215 -20.083 -11.157 -77.568 1.00 24.96 B
ATOM 6644 CE2 TYR B 215 -18.698 -11.297 -77.549 1.00 23.59 B
ATOM 6645 CZ TYR B 215 -18.128 -12.536 -77.804 1.00 25.37 B
ATOM 6646 OH TYR B 215 -16.759 -12.688 -77.726 1.00 24.01 B
ATOM 6647 C TYR B 215 -22.416 -12.134 -75.204 1.00 31.50 B
ATOM 6648 O TYR B 215 -21.306 -12.445 -74.750 1.00 31.83 B
ATOM 6649 N GLN B 216 -23.209 -11.208 -74.655 1.00 31.21 B
ATOM 6650 CA GLN B 216 -22.845 -10.483 -73.436 1.00 30.57 B
ATOM 6651 CB GLN B 216 -24.015 -9.621 -72.950 1.00 32.51 B
ATOM 6652 CG GLN B 216 -24.266 -8.317 -73.688 1.00 36.06 B
ATOM 6653 CD GLN B 216 -23.292 -7.212 -73.294 1.00 40.39 B
ATOM 6654 OE1 GLN B 216 -23.049 -6.976 -72.107 1.00 43.78 B
ATOM 6655 NE2 GLN B 216 -22.742 -6.513 -74.290 1.00 42.11 B
ATOM 6656 C GLN B 216 -22.524 -11.520 -72.357 1.00 29.90 B
ATOM 6657 O GLN B 216 -21.517 -11.419 -71.651 1.00 28.79 B
ATOM 6658 N GLN B 217 -23.395 -12.520 -72.244 1.00 28.48 B
ATOM 6659 CA GLN B 217 -23.240 -13.580 -71.265 1.00 27.84 B
ATOM 6660 CB GLN B 217 -24.441 -14.494 -71.286 1.00 28.43 B

ATOM 6661 CG GLN B 217 -25.720 -13.838 -70.914 1.00 31.93 B
ATOM 6662 CD GLN B 217 -26.849 -14.835 -70.889 1.00 35.29 B
ATOM 6663 OE1 GLN B 217 -26.775 -15.847 -70.194 1.00 36.05 B
ATOM 6664 NE2 GLN B 217 -27.904 -14.563 -71.653 1.00 38.08 B
ATOM 6665 C GLN B 217 -22.012 -14.437 -71.474 1.00 28.33 B
ATOM 6666 O GLN B 217 -21.269 -14.712 -70.534 1.00 30.83 B
ATOM 6667 N LEU B 218 -21.796 -14.884 -72.702 1.00 26.83 B
ATOM 6668 CA LEU B 218 -20.653 -15.740 -72.960 1.00 24.72 B
ATOM 6669 CB LEU B 218 -20.897 -16.565 -74.230 1.00 28.13 B
ATOM 6670 CG LEU B 218 -22.214 -17.319 -74.453 1.00 28.53 B
ATOM 6671 CD1 LEU B 218 -22.191 -17.965 -75.826 1.00 28.31 B
ATOM 6672 CD2 LEU B 218 -22.414 -18.377 -73.390 1.00 29.24 B
ATOM 6673 C LEU B 218 -19.302 -15.029 -73.071 1.00 22.06 B
ATOM 6674 O LEU B 218 -18.280 -15.662 -72.846 1.00 20.21 B
ATOM 6675 N GLU B 219 -19.282 -13.735 -73.403 1.00 19.93 B
ATOM 6676 CA GLU B 219 -18.001 -13.022 -73.562 1.00 18.46 B
ATOM 6677 CB GLU B 219 -18.207 -11.518 -73.746 1.00 19.49 B
ATOM 6678 CG GLU B 219 -16.883 -10.761 -73.843 1.00 23.30 B
ATOM 6679 CD GLU B 219 -17.024 -9.332 -74.373 1.00 29.00 B
ATOM 6680 OE1 GLU B 219 -18.027 -8.652 -74.043 1.00 30.52 B
ATOM 6681 OE2 GLU B 219 -16.115 -8.877 -75.111 1.00 31.10 B
ATOM 6682 C GLU B 219 -16.967 -13.243 -72.468 1.00 16.95 B
ATOM 6683 O GLU B 219 -15.777 -13.310 -72.734 1.00 14.27 B
ATOM 6684 N PRO B 220 -17.409 -13.322 -71.209 1.00 18.05 B
ATOM 6685 CD PRO B 220 -18.756 -13.023 -70.687 1.00 17.90 B
ATOM 6686 CA PRO B 220 -16.463 -13.546 -70.113 1.00 17.73 B
ATOM 6687 CB PRO B 220 -17.375 -13.655 -68.902 1.00 17.18 B
ATOM 6688 CG PRO B 220 -18.473 -12.711 -69.243 1.00 17.43 B
ATOM 6689 C PRO B 220 -15.697 -14.842 -70.365 1.00 17.41 B
ATOM 6690 O PRO B 220 -14.480 -14.897 -70.217 1.00 17.73 B
ATOM 6691 N LEU B 221 -16.436 -15.884 -70.738 1.00 16.39 B
ATOM 6692 CA LEU B 221 -15.867 -17.194 -71.039 1.00 15.39 B
ATOM 6693 CB LEU B 221 -16.903 -18.091 -71.717 1.00 15.95 B
ATOM 6694 CG LEU B 221 -17.746 -19.063 -70.900 1.00 14.81 B

ATOM 6695 CD1 LEU B 221 -16.812 -20.045 -70.228 1.00 17.62 B
ATOM 6696 CD2 LEU B 221 -18.589 -18.324 -69.882 1.00 15.20 B
ATOM 6697 C LEU B 221 -14.682 -17.053 -71.973 1.00 15.16 B
ATOM 6698 O LEU B 221 -13.594 -17.545 -71.686 1.00 15.77 B
ATOM 6699 N TYR B 222 -14.897 -16.379 -73.097 1.00 14.56 B
ATOM 6700 CA TYR B 222 -13.831 -16.195 -74.065 1.00 14.22 B
ATOM 6701 CB TYR B 222 -14.339 -15.440 -75.306 1.00 13.46 B
ATOM 6702 CG TYR B 222 -13.325 -15.417 -76.422 1.00 13.47 B
ATOM 6703 CD1 TYR B 222 -12.894 -16.602 -77.014 1.00 14.59 B
ATOM 6704 CE1 TYR B 222 -11.890 -16.606 -77.971 1.00 16.41 B
ATOM 6705 CD2 TYR B 222 -12.729 -14.231 -76.828 1.00 12.82 B
ATOM 6706 CE2 TYR B 222 -11.727 -14.224 -77.786 1.00 14.95 B
ATOM 6707 CZ TYR B 222 -11.311 -15.414 -78.353 1.00 16.92 B
ATOM 6708 OH TYR B 222 -10.327 -15.418 -79.313 1.00 18.74 B
ATOM 6709 C TYR B 222 -12.647 -15.462 -73.448 1.00 13.96 B
ATOM 6710 O TYR B 222 -11.525 -15.957 -73.463 1.00 13.57 B
ATOM 6711 N LEU B 223 -12.906 -14.291 -72.883 1.00 14.43 B
ATOM 6712 CA LEU B 223 -11.846 -13.499 -72.283 1.00 16.42 B
ATOM 6713 CB LEU B 223 -12.421 -12.279 -71.558 1.00 15.35 B
ATOM 6714 CG LEU B 223 -13.233 -11.312 -72.415 1.00 16.60 B
ATOM 6715 CD1 LEU B 223 -13.558 -10.085 -71.588 1.00 17.31 B
ATOM 6716 CD2 LEU B 223 -12.454 -10.931 -73.672 1.00 16.82 B
ATOM 6717 C LEU B 223 -10.975 -14.297 -71.322 1.00 17.23 B
ATOM 6718 O LEU B 223 -9.765 -14.067 -71.250 1.00 17.39 B
ATOM 6719 N ASN B 224 -11.576 -15.231 -70.589 1.00 17.70 B
ATOM 6720 CA ASN B 224 -10.797 -16.028 -69.657 1.00 19.46 B
ATOM 6721 CB ASN B 224 -11.687 -16.632 -68.567 1.00 19.39 B
ATOM 6722 CG ASN B 224 -11.872 -15.686 -67.379 1.00 22.54 B
ATOM 6723 OD1 ASN B 224 -10.904 -15.285 -66.716 1.00 21.26 B
ATOM 6724 ND2 ASN B 224 -13.115 -15.323 -67.109 1.00 23.94 B
ATOM 6725 C ASN B 224 -9.985 -17.105 -70.367 1.00 20.04 B
ATOM 6726 O ASN B 224 -8.826 -17.336 -70.010 1.00 21.39 B
ATOM 6727 N LEU B 225 -10.567 -17.755 -71.377 1.00 19.22 B
ATOM 6728 CA LEU B 225 -9.828 -18.776 -72.115 1.00 19.05 B

ATOM 6729 CB LEU B 225 -10.746 -19.538 -73.077 1.00 17.14 B
ATOM 6730 CG LEU B 225 -10.133 -20.637 -73.961 1.00 15.90 B
ATOM 6731 CD1 LEU B 225 -9.499 -21.709 -73.114 1.00 14.94 B
ATOM 6732 CD2 LEU B 225 -11.212 -21.251 -74.839 1.00 15.69 B
ATOM 6733 C LEU B 225 -8.733 -18.048 -72.895 1.00 20.51 B
ATOM 6734 O LEU B 225 -7.602 -18.528 -73.006 1.00 21.11 B
ATOM 6735 N HIS B 226 -9.052 -16.937 -73.522 1.00 20.72 B
ATOM 6736 CA HIS B 226 -8.094 -16.065 -74.175 1.00 22.02 B
ATOM 6737 CB HIS B 226 -8.821 -14.889 -74.842 1.00 21.22 B
ATOM 6738 CG HIS B 226 -7.942 -13.917 -75.565 1.00 21.61 B
ATOM 6739 CD2 HIS B 226 -7.655 -13.791 -76.861 1.00 21.38 B
ATOM 6740 ND1 HIS B 226 -7.288 -12.898 -74.948 1.00 22.44 B
ATOM 6741 CE1 HIS B 226 -6.598 -12.220 -75.824 1.00 22.02 B
ATOM 6742 NE2 HIS B 226 -6.806 -12.742 -76.993 1.00 22.78 B
ATOM 6743 C HIS B 226 -6.899 -15.618 -73.388 1.00 22.98 B
ATOM 6744 O HIS B 226 -5.840 -15.762 -73.834 1.00 23.84 B
ATOM 6745 N ALA B 227 -7.066 -14.978 -72.258 1.00 23.29 B
ATOM 6746 CA ALA B 227 -5.927 -14.575 -71.444 1.00 22.27 B
ATOM 6747 CB ALA B 227 -6.400 -13.874 -70.210 1.00 22.66 B
ATOM 6748 C ALA B 227 -5.112 -15.797 -71.059 1.00 22.27 B
ATOM 6749 O ALA B 227 -3.874 -15.760 -71.084 1.00 21.04 B
ATOM 6750 N PHE B 228 -5.812 -16.880 -70.712 1.00 22.63 B
ATOM 6751 CA PHE B 228 -5.155 -18.115 -70.306 1.00 22.45 B
ATOM 6752 CB PHE B 228 -6.163 -19.185 -69.923 1.00 22.79 B
ATOM 6753 CG PHE B 228 -5.520 -20.454 -69.410 1.00 24.39 B
ATOM 6754 CD1 PHE B 228 -4.843 -20.461 -68.194 1.00 23.41 B
ATOM 6755 CD2 PHE B 228 -5.576 -21.643 -70.157 1.00 25.34 B
ATOM 6756 CE1 PHE B 228 -4.234 -21.624 -67.731 1.00 23.30 B
ATOM 6757 CE2 PHE B 228 -4.967 -22.816 -69.701 1.00 22.88 B
ATOM 6758 CZ PHE B 228 -4.296 -22.807 -68.489 1.00 22.61 B
ATOM 6759 C PHE B 228 -4.253 -18.678 -71.377 1.00 22.02 B
ATOM 6760 O PHE B 228 -3.134 -19.079 -71.092 1.00 21.51 B
ATOM 6761 N VAL B 229 -4.743 -18.724 -72.609 1.00 22.59 B
ATOM 6762 CA VAL B 229 -3.947 -19.235 -73.722 1.00 22.91 B

ATOM 6763 CB VAL B 229 -4.822 -19.470 -74.974 1.00 23.63 B
ATOM 6764 CG1 VAL B 229 -3.966 -19.920 -76.140 1.00 21.53 B
ATOM 6765 CG2 VAL B 229 -5.884 -20.525 -74.659 1.00 26.20 B
ATOM 6766 C VAL B 229 -2.809 -18.283 -74.089 1.00 22.16 B
ATOM 6767 O VAL B 229 -1.693 -18.737 -74.369 1.00 21.48 B
ATOM 6768 N ARG B 230 -3.083 -16.973 -74.083 1.00 21.06 B
ATOM 6769 CA ARG B 230 -2.071 -15.983 -74.432 1.00 20.67 B
ATOM 6770 CB ARG B 230 -2.615 -14.571 -74.251 1.00 20.76 B
ATOM 6771 CG ARG B 230 -1.617 -13.464 -74.593 1.00 22.09 B
ATOM 6772 CD ARG B 230 -2.286 -12.098 -74.554 1.00 23.42 B
ATOM 6773 NE ARG B 230 -2.971 -11.878 -73.282 1.00 26.06 B
ATOM 6774 CZ ARG B 230 -3.820 -10.886 -73.036 1.00 25.34 B
ATOM 6775 NH1 ARG B 230 -4.110 -10.000 -73.967 1.00 24.93 B
ATOM 6776 NH2 ARG B 230 -4.383 -10.788 -71.848 1.00 27.59 B
ATOM 6777 C ARG B 230 -0.844 -16.192 -73.559 1.00 20.86 B
ATOM 6778 O ARG B 230 0.278 -16.299 -74.066 1.00 20.03 B
ATOM 6779 N ARG B 231 -1.066 -16.268 -72.248 1.00 21.67 B
ATOM 6780 CA ARG B 231 0.019 -16.484 -71.294 1.00 21.51 B
ATOM 6781 CB ARG B 231 -0.553 -16.672 -69.881 1.00 21.39 B
ATOM 6782 CG ARG B 231 0.450 -17.225 -68.870 1.00 21.72 B
ATOM 6783 CD ARG B 231 1.579 -16.250 -68.587 1.00 22.79 B
ATOM 6784 NE ARG B 231 1.388 -15.571 -67.310 1.00 25.85 B
ATOM 6785 CZ ARG B 231 2.318 -15.489 -66.360 1.00 28.16 B
ATOM 6786 NH1 ARG B 231 2.051 -14.859 -65.229 1.00 28.48 B
ATOM 6787 NH2 ARG B 231 3.519 -16.031 -66.535 1.00 27.57 B
ATOM 6788 C ARG B 231 -0.825 -17.720 -71.709 1.00 21.35 B
ATOM 6789 O ARG B 231 2.044 -17.774 -71.542 1.00 21.43 B
ATOM 6790 N ALA B 232 0.136 -18.715 -72.254 1.00 20.76 B
ATOM 6791 CA ALA B 232 0.802 -19.932 -72.690 1.00 20.23 B
ATOM 6792 CB ALA B 232 -0.218 -21.023 -72.974 1.00 20.20 B
ATOM 6793 C ALA B 232 1.622 -19.647 -73.939 1.00 20.04 B
ATOM 6794 O ALA B 232 2.760 -20.103 -74.056 1.00 19.26 B
ATOM 6795 N LEU B 233 1.054 -18.892 -74.873 1.00 19.63 B
ATOM 6796 CA LEU B 233 1.786 -18.582 -76.090 1.00 21.10 B

ATOM 6797 CB LEU B 233 0.873 -17.874 -77.097 1.00 21.92 B
ATOM 6798 CG LEU B 233 -0.255 -18.721 -77.710 1.00 21.31 B
ATOM 6799 CD1 LEU B 233 -1.187 -17.842 -78.524 1.00 20.30 B
ATOM 6800 CD2 LEU B 233 0.339 -19.820 -78.567 1.00 19.80 B
ATOM 6801 C LEU B 233 3.004 -17.725 -75.750 1.00 22.39 B
ATOM 6802 O LEU B 233 4.049 -17.849 -76.386 1.00 21.88 B
ATOM 6803 N HIS B 234 2.869 -16.868 -74.738 1.00 24.08 B
ATOM 6804 CA HIS B 234 3.973 -16.005 -74.299 1.00 25.31 B
ATOM 6805 CB HIS B 234 3.502 -15.044 -73.186 1.00 26.17 B
ATOM 6806 CG HIS B 234 4.584 -14.156 -72.633 1.00 28.56 B
ATOM 6807 CD2 HIS B 234 4.848 -12.840 -72.832 1.00 28.59 B
ATOM 6808 ND1 HIS B 234 5.565 -14.614 -71.778 1.00 30.42 B
ATOM 6809 CE1 HIS B 234 6.387 -13.623 -71.477 1.00 30.15 B
ATOM 6810 NE2 HIS B 234 5.975 -12.536 -72.104 1.00 28.10 B
ATOM 6811 C HIS B 234 5.117 -16.877 -73.786 1.00 26.21 B
ATOM 6812 O HIS B 234 6.287 -16.646 -74.093 1.00 25.87 B
ATOM 6813 N ARG B 235 4.767 -17.890 -73.011 1.00 27.16 B
ATOM 6814 CA ARG B 235 5.754 -18.793 -72.456 1.00 29.03 B
ATOM 6815 CB ARG B 235 5.043 -19.828 -71.586 1.00 30.09 B
ATOM 6816 CG ARG B 235 5.832 -20.326 -70.390 1.00 32.57 B
ATOM 6817 CD ARG B 235 5.022 -20.114 -69.102 1.00 34.97 B
ATOM 6818 NE ARG B 235 3.617 -20.512 -69.243 1.00 36.36 B
ATOM 6819 CZ ARG B 235 2.685 -20.366 -68.296 1.00 36.83 B
ATOM 6820 NH1 ARG B 235 2.990 -19.825 -67.111 1.00 35.93 B
ATOM 6821 NH2 ARG B 235 1.435 -20.761 -68.535 1.00 35.62 B
ATOM 6822 C ARG B 235 6.560 -19.477 -73.577 1.00 30.15 B
ATOM 6823 O ARG B 235 7.784 -19.603 -73.479 1.00 30.63 B
ATOM 6824 N ARG B 236 5.909 -19.906 -74.638 1.00 31.31 B
ATOM 6825 CA ARG B 236 6.548 -20.536 -75.807 1.00 31.43 B
ATOM 6826 CB ARG B 236 5.609 -21.521 -76.445 1.00 31.09 B
ATOM 6827 CG ARG B 236 5.661 -21.683 -77.868 1.00 31.43 B
ATOM 6828 CD ARG B 236 6.548 -22.761 -78.336 1.00 32.54 B
ATOM 6829 NE ARG B 236 6.061 -24.073 -78.041 1.00 34.07 B
ATOM 6830 CZ ARG B 236 6.575 -25.162 -78.513 1.00 32.33 B

ATOM 6831 NH1 ARG B 236 7.577 -25.076 -79.312 1.00 29.15 B
ATOM 6832 NH2 ARG B 236 6.081 -26.325 -78.185 1.00 31.45 B
ATOM 6833 C ARG B 236 7.205 -19.678 -76.837 1.00 31.48 B
ATOM 6834 O ARG B 236 8.304 -19.946 -77.206 1.00 31.93 B
ATOM 6835 N TYR B 237 6.562 -18.613 -77.264 1.00 30.56 B
ATOM 6836 CA TYR B 237 7.156 -17.754 -78.284 1.00 29.73 B
ATOM 6837 CB TYR B 237 6.081 -17.226 -79.240 1.00 28.59 B
ATOM 6838 CG TYR B 237 5.357 -18.320 -79.987 1.00 28.00 B
ATOM 6839 CD1 TYR B 237 4.018 -18.593 -79.729 1.00 29.08 B
ATOM 6840 CE1 TYR B 237 3.350 -19.613 -80.397 1.00 31.20 B
ATOM 6841 CD2 TYR B 237 6.017 -19.096 -80.934 1.00 28.30 B
ATOM 6842 CE2 TYR B 237 5.364 -20.126 -81.614 1.00 29.20 B
ATOM 6843 CZ TYR B 237 4.028 -20.380 -81.342 1.00 30.81 B
ATOM 6844 OH TYR B 237 3.366 -21.392 -82.010 1.00 30.34 B
ATOM 6845 C TYR B 237 7.983 -16.597 -77.750 1.00 29.62 B
ATOM 6846 O TYR B 237 8.791 -16.032 -78.474 1.00 28.77 B
ATOM 6847 N GLY B 238 7.781 -16.231 -76.493 1.00 30.50 B
ATOM 6848 CA GLY B 238 8.573 -15.146 -75.936 1.00 30.96 B
ATOM 6849 C GLY B 238 8.024 -13.734 -75.985 1.00 30.45 B
ATOM 6850 O GLY B 238 7.215 -13.376 -76.831 1.00 30.03 B
ATOM 6851 N ASP B 239 8.508 -12.922 -75.059 1.00 32.37 B
ATOM 6852 CA ASP B 239 8.089 -11.535 -74.923 1.00 34.39 B
ATOM 6853 CB ASP B 239 8.952 -10.856 -73.857 1.00 35.83 B
ATOM 6854 CG ASP B 239 8.254 -9.669 -73.232 1.00 38.01 B
ATOM 6855 OD1 ASP B 239 7.146 -9.875 -72.692 1.00 39.77 B
ATOM 6856 OD2 ASP B 239 8.793 -8.540 -73.280 1.00 39.71 B
ATOM 6857 C ASP B 239 8.119 -10.687 -76.207 1.00 33.63 B
ATOM 6858 O ASP B 239 7.479 -9.639 -76.278 1.00 32.08 B
ATOM 6859 N ARG B 240 8.732 -11.181 -77.251 1.00 33.23 B
ATOM 6860 CA ARG B 240 8.861 -10.442 -78.459 1.00 32.47 B
ATOM 6861 CB ARG B 240 9.966 -10.987 -79.262 1.00 34.01 B
ATOM 6862 CG ARG B 240 10.199 -10.122 -80.379 1.00 38.24 B
ATOM 6863 CD ARG B 240 11.533 -10.254 -80.957 1.00 41.40 B
ATOM 6864 NE ARG B 240 11.984 -9.061 -81.630 1.00 42.59 B

ATOM 6865 CZ ARG B 240 12.127 -8.991 -82.920 1.00 44.09 B
ATOM 6866 NH1 ARG B 240 11.851 -10.033 -83.655 1.00 43.55 B
ATOM 6867 NH2 ARG B 240 12.536 -7.880 -83.483 1.00 43.90 B
ATOM 6868 C ARG B 240 7.696 -10.513 -79.322 1.00 31.55 B
ATOM 6869 O ARG B 240 7.355 -9.577 -79.937 1.00 30.43 B
ATOM 6870 N TYR B 241 7.118 -11.678 -79.405 1.00 30.27 B
ATOM 6871 CA TYR B 241 5.972 -11.905 -80.276 1.00 28.18 B
ATOM 6872 CB TYR B 241 6.199 -13.167 -81.100 1.00 29.74 B
ATOM 6873 CG TYR B 241 7.397 -13.079 -81.991 1.00 31.46 B
ATOM 6874 CD1 TYR B 241 8.491 -13.897 -81.782 1.00 32.92 B
ATOM 6875 CE1 TYR B 241 9.621 -13.807 -82.588 1.00 36.73 B
ATOM 6876 CD2 TYR B 241 7.452 -12.153 -83.036 1.00 33.91 B
ATOM 6877 CE2 TYR B 241 8.581 -12.046 -83.849 1.00 35.38 B
ATOM 6878 CZ TYR B 241 9.662 -12.882 -83.618 1.00 36.91 B
ATOM 6879 OH TYR B 241 10.785 -12.821 -84.408 1.00 38.75 B
ATOM 6880 C TYR B 241 4.600 -11.987 -79.631 1.00 27.03 B
ATOM 6881 O TYR B 241 3.590 -12.088 -80.325 1.00 27.79 B
ATOM 6882 N ILE B 242 4.543 -11.973 -78.312 1.00 25.27 B
ATOM 6883 CA ILE B 242 3.253 -12.021 -77.651 1.00 23.95 B
ATOM 6884 CB ILE B 242 3.076 -13.334 -76.855 1.00 22.69 B
ATOM 6885 CG2 ILE B 242 1.748 -13.329 -76.131 1.00 22.47 B
ATOM 6886 CG1 ILE B 242 3.130 -14.539 -77.794 1.00 21.86 B
ATOM 6887 CD1 ILE B 242 1.899 -14.702 -78.661 1.00 22.55 B
ATOM 6888 C ILE B 242 3.179 -10.845 -76.696 1.00 23.43 B
ATOM 6889 O ILE B 242 4.153 -10.537 -76.021 1.00 24.17 B
ATOM 6890 N ASN B 243 2.049 -10.153 -76.663 1.00 23.08 B
ATOM 6891 CA ASN B 243 1.919 -9.042 -75.727 1.00 22.44 B
ATOM 6892 CB ASN B 243 1.521 -7.742 -76.424 1.00 22.04 B
ATOM 6893 CG ASN B 243 1.353 -6.594 -75.449 1.00 22.02 B
ATOM 6894 OD1 ASN B 243 0.648 -6.713 -74.446 1.00 22.51 B
ATOM 6895 ND2 ASN B 243 2.002 -5.475 -75.736 1.00 22.16 B
ATOM 6896 C ASN B 243 0.845 -9.430 -74.729 1.00 22.08 B
ATOM 6897 O ASN B 243 -0.326 -9.611 -75.098 1.00 22.03 B
ATOM 6898 N LEU B 244 1.257 -9.561 -73.469 1.00 21.01 B

ATOM 6899 CA LEU B 244 0.358 -9.960 -72.392 1.00 20.38 B
ATOM 6900 CB LEU B 244 1.155 -10.181 -71.108 1.00 18.30 B
ATOM 6901 CG LEU B 244 2.049 -11.417 -71.181 1.00 16.14 B
ATOM 6902 CD1 LEU B 244 3.085 -11.410 -70.076 1.00 16.27 B
ATOM 6903 CD2 LEU B 244 1.160 -12.643 -71.106 1.00 15.25 B
ATOM 6904 C LEU B 244 -0.771 -8.987 -72.157 1.00 20.70 B
ATOM 6905 O LEU B 244 -1.719 -9.291 -71.440 1.00 20.34 B
ATOM 6906 N ARG B 245 -0.680 -7.874 -72.794 1.00 22.95 B
ATOM 6907 CA ARG B 245 -1.689 -6.898 -72.663 1.00 26.00 B
ATOM 6908 CB ARG B 245 -1.100 -5.743 -71.973 1.00 27.86 B
ATOM 6909 CG ARG B 245 -1.544 -5.539 -70.588 1.00 31.18 B
ATOM 6910 CD ARG B 245 -0.481 -5.572 -69.604 1.00 35.24 B
ATOM 6911 NE ARG B 245 0.623 -4.739 -69.975 1.00 40.23 B
ATOM 6912 CZ ARG B 245 0.963 -3.664 -69.337 1.00 42.55 B
ATOM 6913 NH1 ARG B 245 0.271 -3.299 -68.303 1.00 44.34 B
ATOM 6914 NH2 ARG B 245 1.994 -2.956 -69.707 1.00 43.15 B
ATOM 6915 C ARG B 245 -2.208 -6.460 -73.964 1.00 26.90 B
ATOM 6916 O ARG B 245 -3.005 -5.651 -73.999 1.00 27.65 B
ATOM 6917 N GLY B 246 -1.789 -7.070 -75.049 1.00 27.24 B
ATOM 6918 CA GLY B 246 -2.246 -6.766 -76.394 1.00 25.95 B
ATOM 6919 C GLY B 246 -2.988 -7.944 -76.979 1.00 24.24 B
ATOM 6920 O GLY B 246 -3.137 -8.949 -76.298 1.00 24.92 B
ATOM 6921 N PRO B 247 -3.477 -7.854 -78.227 1.00 22.68 B
ATOM 6922 CD PRO B 247 -3.479 -6.678 -79.119 1.00 21.66 B
ATOM 6923 CA PRO B 247 -4.201 -8.971 -78.843 1.00 20.46 B
ATOM 6924 CB PRO B 247 -4.923 -8.313 -80.010 1.00 19.56 B
ATOM 6925 CG PRO B 247 -3.962 -7.269 -80.432 1.00 21.20 B
ATOM 6926 C PRO B 247 -3.234 -10.050 -79.286 1.00 19.37 B
ATOM 6927 O PRO B 247 -2.023 -9.841 -79.316 1.00 18.26 B
ATOM 6928 N ILE B 248 -3.765 -11.212 -79.625 1.00 19.87 B
ATOM 6929 CA ILE B 248 -2.909 -12.310 -80.057 1.00 19.37 B
ATOM 6930 CB ILE B 248 -3.523 -13.678 -79.672 1.00 17.70 B
ATOM 6931 CG2 ILE B 248 -2.547 -14.788 -79.979 1.00 17.20 B
ATOM 6932 CG1 ILE B 248 -3.874 -13.702 -78.191 1.00 18.35 B

ATOM 6933 CD1 ILE B 248 -4.509 -14.999 -77.749 1.00 17.39 B
ATOM 6934 C ILE B 248 -2.675 -12.323 -81.565 1.00 18.82 B
ATOM 6935 O ILE B 248 -3.570 -12.005 -82.342 1.00 19.02 B
ATOM 6936 N PRO B 249 -1.456 -12.674 -81.997 1.00 19.42 B
ATOM 6937 CD PRO B 249 -0.233 -12.765 -81.182 1.00 20.56 B
ATOM 6938 CA PRO B 249 -1.131 -12.740 -83.426 1.00 20.44 B
ATOM 6939 CB PRO B 249 0.334 -13.145 -83.420 1.00 21.40 B
ATOM 6940 CG PRO B 249 0.847 -12.464 -82.183 1.00 21.16 B
ATOM 6941 C PRO B 249 -2.023 -13.822 -84.043 1.00 20.41 B
ATOM 6942 O PRO B 249 -1.970 -14.976 -83.626 1.00 20.15 B
ATOM 6943 N ALA B 250 -2.824 -13.443 -85.036 1.00 20.31 B
ATOM 6944 CA ALA B 250 -3.780 -14.346 -85.696 1.00 19.16 B
ATOM 6945 CB ALA B 250 -4.484 -13.596 -86.825 1.00 18.60 B
ATOM 6946 C ALA B 250 -3.319 -15.710 -86.214 1.00 18.37 B
ATOM 6947 O ALA B 250 -4.155 -16.536 -86.560 1.00 19.30 B
ATOM 6948 N HIS B 251 -2.022 -15.971 -86.255 1.00 17.40 B
ATOM 6949 CA HIS B 251 -1.555 -17.248 -86.769 1.00 18.91 B
ATOM 6950 CB HIS B 251 -0.506 -16.986 -87.835 1.00 18.35 B
ATOM 6951 CG HIS B 251 0.744 -16.371 -87.298 1.00 18.22 B
ATOM 6952 CD2 HIS B 251 2.026 -16.805 -87.300 1.00 18.71 B
ATOM 6953 ND1 HIS B 251 0.751 -15.169 -86.635 1.00 19.23 B
ATOM 6954 CE1 HIS B 251 1.982 -14.887 -86.248 1.00 19.78 B
ATOM 6955 NE2 HIS B 251 2.776 -15.864 -86.640 1.00 18.50 B
ATOM 6956 C HIS B 251 -0.961 -18.213 -85.741 1.00 20.76 B
ATOM 6957 O HIS B 251 -0.272 -19.167 -86.113 1.00 22.64 B
ATOM 6958 N LEU B 252 -1.218 -17.989 -84.458 1.00 21.14 B
ATOM 6959 CA LEU B 252 -0.642 -18.847 -83.429 1.00 19.87 B
ATOM 6960 CB LEU B 252 0.027 -17.991 -82.369 1.00 20.54 B
ATOM 6961 CG LEU B 252 1.005 -16.997 -82.981 1.00 21.73 B
ATOM 6962 CD1 LEU B 252 1.535 -16.075 -81.904 1.00 24.85 B
ATOM 6963 CD2 LEU B 252 2.137 -17.751 -83.656 1.00 21.93 B
ATOM 6964 C LEU B 252 -1.616 -19.775 -82.763 1.00 18.66 B
ATOM 6965 O LEU B 252 -1.207 -20.667 -82.035 1.00 17.04 B
ATOM 6966 N LEU B 253 -2.903 -19.578 -83.013 1.00 19.25 B

ATOM 6967 CA LEU B 253 -3.916 -20.414 -82.394 1.00 19.58 B
ATOM 6968 CB LEU B 253 -5.223 -19.635 -82.255 1.00 20.54 B
ATOM 6969 CG LEU B 253 -5.249 -18.512 -81.204 1.00 20.58 B
ATOM 6970 CD1 LEU B 253 -4.605 -18.997 -79.925 1.00 20.51 B
ATOM 6971 CD2 LEU B 253 -4.502 -17.310 -81.703 1.00 21.84 B
ATOM 6972 C LEU B 253 -4.170 -21.745 -83.090 1.00 20.20 B
ATOM 6973 O LEU B 253 -5.237 -22.334 -82.948 1.00 20.57 B
ATOM 6974 N GLY B 254 -3.181 -22.219 -83.839 1.00 21.11 B
ATOM 6975 CA GLY B 254 -3.299 -23.500 -84.516 1.00 22.14 B
ATOM 6976 C GLY B 254 -4.409 -23.686 -85.540 1.00 23.50 B
ATOM 6977 O GLY B 254 -4.887 -24.806 -85.736 1.00 24.00 B
ATOM 6978 N ASP B 255 -4.812 -22.601 -86.197 1.00 23.64 B
ATOM 6979 CA ASP B 255 -5.855 -22.641 -87.213 1.00 23.22 B
ATOM 6980 CB ASP B 255 -7.240 -22.710 -86.574 1.00 24.00 B
ATOM 6981 CG ASP B 255 -8.365 -22.596 -87.600 1.00 27.63 B
ATOM 6982 OD1 ASP B 255 -8.363 -21.614 -88.376 1.00 28.48 B
ATOM 6983 OD2 ASP B 255 -9.258 -23.475 -87.639 1.00 28.83 B
ATOM 6984 C ASP B 255 -5.748 -21.381 -88.054 1.00 23.59 B
ATOM 6985 O ASP B 255 -5.600 -20.287 -87.518 1.00 24.69 B
ATOM 6986 N MET B 256 -5.833 -21.551 -89.372 1.00 23.63 B
ATOM 6987 CA MET B 256 -5.737 -20.449 -90.336 1.00 22.67 B
ATOM 6988 CB MET B 256 -6.225 -20.929 -91.715 1.00 21.60 B
ATOM 6989 CG MET B 256 -6.044 -19.938 -92.855 1.00 18.93 B
ATOM 6990 SD MET B 256 -4.338 -19.351 -93.031 1.00 20.97 B
ATOM 6991 CE MET B 256 -3.478 -20.835 -93.442 1.00 18.41 B
ATOM 6992 C MET B 256 -6.513 -19.203 -89.927 1.00 22.47 B
ATOM 6993 O MET B 256 -6.025 -18.079 -90.066 1.00 20.92 B
ATOM 6994 N TRP B 257 -7.715 -19.417 -89.406 1.00 23.06 B
ATOM 6995 CA TRP B 257 -8.590 -18.330 -88.996 1.00 24.82 B
ATOM 6996 CB TRP B 257 -9.978 -18.598 -89.557 1.00 25.20 B
ATOM 6997 CG TRP B 257 -9.947 -18.801 -91.024 1.00 27.53 B
ATOM 6998 CD2 TRP B 257 -9.763 -20.043 -91.710 1.00 29.46 B
ATOM 6999 CE2 TRP B 257 -9.760 -19.760 -93.094 1.00 29.76 B
ATOM 7000 CE3 TRP B 257 -9.602 -21.370 -91.293 1.00 30.37 B

ATOM 7001 CD1 TRP B 257 -10.040 -17.839 -91.990 1.00 28.93 B
ATOM 7002 NE1 TRP B 257 -9.928 -18.407 -93.237 1.00 29.83 B
ATOM 7003 CZ2 TRP B 257 -9.601 -20.759 -94.059 1.00 29.66 B
ATOM 7004 CZ3 TRP B 257 -9.443 -22.360 -92.255 1.00 28.48 B
ATOM 7005 CH2 TRP B 257 -9.445 -22.047 -93.618 1.00 28.72 B
ATOM 7006 C TRP B 257 -8.679 -18.086 -87.489 1.00 24.55 B
ATOM 7007 O TRP B 257 -9.361 -17.159 -87.050 1.00 24.08 B
ATOM 7008 N ALA B 258 -7.984 -18.909 -86.711 1.00 24.08 B
ATOM 7009 CA ALA B 258 -8.008 -18.795 -85.260 1.00 23.69 B
ATOM 7010 CB ALA B 258 -7.474 -17.437 -84.842 1.00 22.34 B
ATOM 7011 C ALA B 258 -9.442 -18.971 -84.765 1.00 23.31 B
ATOM 7012 O ALA B 258 -9.874 -18.282 -83.854 1.00 23.14 B
ATOM 7013 N GLN B 259 -10.176 -19.901 -85.357 1.00 23.73 B
ATOM 7014 CA GLN B 259 -11.565 -20.088 -84.975 1.00 25.42 B
ATOM 7015 CB GLN B 259 -12.433 -20.220 -86.234 1.00 27.91 B
ATOM 7016 CG GLN B 259 -12.263 -21.499 -87.038 1.00 30.22 B
ATOM 7017 CD GLN B 259 -12.819 -21.349 -88.444 1.00 33.44 B
ATOM 7018 OE1 GLN B 259 -12.125 -20.865 -89.343 1.00 36.51 B
ATOM 7019 NE2 GLN B 259 -14.080 -21.741 -88.639 1.00 32.96 B
ATOM 7020 C GLN B 259 -11.826 -21.245 -84.017 1.00 25.57 B
ATOM 7021 O GLN B 259 -12.933 -21.390 -83.484 1.00 25.13 B
ATOM 7022 N SER B 260 -10.809 -22.077 -83.823 1.00 25.46 B
ATOM 7023 CA SER B 260 -10.882 -23.197 -82.894 1.00 27.10 B
ATOM 7024 CB SER B 260 -11.503 -24.433 -83.549 1.00 24.95 B
ATOM 7025 OG SER B 260 -10.688 -24.928 -84.584 1.00 28.64 B
ATOM 7026 C SER B 260 -9.426 -23.430 -82.494 1.00 28.21 B
ATOM 7027 O SER B 260 -8.534 -23.470 -83.342 1.00 28.47 B
ATOM 7028 N TRP B 261 -9.183 -23.558 -81.195 1.00 29.86 B
ATOM 7029 CA TRP B 261 -7.824 -23.717 -80.696 1.00 31.13 B
ATOM 7030 CB TRP B 261 -7.579 -22.673 -79.596 1.00 30.79 B
ATOM 7031 CG TRP B 261 -7.980 -21.251 -79.985 1.00 29.47 B
ATOM 7032 CD2 TRP B 261 -7.965 -20.097 -79.137 1.00 28.29 B
ATOM 7033 CE2 TRP B 261 -8.357 -18.993 -79.925 1.00 27.16 B
ATOM 7034 CE3 TRP B 261 -7.657 -19.889 -77.787 1.00 27.38 B

ATOM 7035 CD1 TRP B 261 -8.373 -20.806 -81.220 1.00 28.11 B
ATOM 7036 NE1 TRP B 261 -8.600 -19.454 -81.190 1.00 26.68 B
ATOM 7037 CZ2 TRP B 261 -8.448 -17.703 -79.410 1.00 26.96 B
ATOM 7038 CZ3 TRP B 261 -7.748 -18.611 -77.276 1.00 27.41 B
ATOM 7039 CH2 TRP B 261 -8.142 -17.530 -78.088 1.00 27.30 B
ATOM 7040 C TRP B 261 -7.397 -25.097 -80.182 1.00 31.99 B
ATOM 7041 O TRP B 261 -6.308 -25.224 -79.616 1.00 31.88 B
ATOM 7042 N GLU B 262 -8.223 -26.126 -80.381 1.00 32.78 B
ATOM 7043 CA GLU B 262 -7.873 -27.457 -79.893 1.00 34.30 B
ATOM 7044 CB GLU B 262 -8.999 -28.464 -80.153 1.00 36.35 B
ATOM 7045 CG GLU B 262 -9.251 -28.815 -81.599 1.00 42.20 B
ATOM 7046 CD GLU B 262 -9.882 -27.674 -82.365 1.00 47.50 B
ATOM 7047 OE1 GLU B 262 -9.177 -26.664 -82.600 1.00 50.53 B
ATOM 7048 OE2 GLU B 262 -11.083 -27.783 -82.727 1.00 49.30 B
ATOM 7049 C GLU B 262 -6.564 -28.002 -80.452 1.00 33.85 B
ATOM 7050 O GLU B 262 -5.992 -28.937 -79.891 1.00 34.16 B
ATOM 7051 N ASN B 263 -6.083 -27.415 -81.543 1.00 33.98 B
ATOM 7052 CA ASN B 263 -4.831 -27.857 -82.150 1.00 34.54 B
ATOM 7053 CB ASN B 263 -4.761 -27.441 -83.622 1.00 35.87 B
ATOM 7054 CG ASN B 263 -5.538 -28.367 -84.521 1.00 37.79 B
ATOM 7055 OD1 ASN B 263 -5.178 -29.528 -84.692 1.00 39.16 B
ATOM 7056 ND2 ASN B 263 -6.620 -27.862 -85.098 1.00 40.36 B
ATOM 7057 C ASN B 263 -3.598 -27.341 -81.425 1.00 34.03 B
ATOM 7058 O ASN B 263 -2.479 -27.603 -81.844 1.00 33.21 B
ATOM 7059 N ILE B 264 -3.819 -26.794 -80.308 1.00 34.70 B
ATOM 7060 CA ILE B 264 -2.743 -26.212 -79.659 1.00 36.56 B
ATOM 7061 CB ILE B 264 -2.894 -24.861 -79.912 1.00 37.19 B
ATOM 7062 CG2 ILE B 264 -2.985 -24.163 -78.757 1.00 38.17 B
ATOM 7063 CG1 ILE B 264 -1.753 -24.379 -80.653 1.00 37.64 B
ATOM 7064 CD1 ILE B 264 -1.432 -23.227 -80.167 1.00 39.01 B
ATOM 7065 C ILE B 264 -2.918 -26.562 -78.230 1.00 36.94 B
ATOM 7066 O ILE B 264 -2.483 -25.932 -77.377 1.00 36.97 B
ATOM 7067 N TYR B 265 -3.609 -27.653 -78.041 1.00 37.21 B
ATOM 7068 CA TYR B 265 -3.930 -28.245 -76.757 1.00 36.40 B

ATOM 7069 CB TYR B 265 -4.763 -29.512 -76.980 1.00 36.14 B
ATOM 7070 CG TYR B 265 -5.110 -30.246 -75.711 1.00 37.26 B
ATOM 7071 CD1 TYR B 265 -6.010 -29.703 -74.788 1.00 37.55 B
ATOM 7072 CE1 TYR B 265 -6.281 -30.355 -73.575 1.00 37.58 B
ATOM 7073 CD2 TYR B 265 -4.491 -31.462 -75.397 1.00 37.08 B
ATOM 7074 CE2 TYR B 265 -4.750 -32.117 -74.193 1.00 37.28 B
ATOM 7075 CZ TYR B 265 -5.643 -31.559 -73.289 1.00 36.96 B
ATOM 7076 OH TYR B 265 -5.890 -32.203 -72.107 1.00 36.45 B
ATOM 7077 C TYR B 265 -2.643 -28.576 -76.001 1.00 36.26 B
ATOM 7078 O TYR B 265 -2.509 -28.259 -74.818 1.00 36.16 B
ATOM 7079 N ASP B 266 -1.689 -29.188 -76.694 1.00 35.99 B
ATOM 7080 CA ASP B 266 -0.420 -29.567 -76.078 1.00 37.23 B
ATOM 7081 CB ASP B 266 0.428 -30.394 -77.059 1.00 39.84 B
ATOM 7082 CG ASP B 266 -0.841 -29.604 -78.301 1.00 43.75 B
ATOM 7083 OD1 ASP B 266 -0.063 -29.178 -79.056 1.00 46.15 B
ATOM 7084 OD2 ASP B 266 2.065 -29.408 -78.529 1.00 43.83 B
ATOM 7085 C ASP B 266 0.417 -28.400 -75.535 1.00 36.31 B
ATOM 7086 O ASP B 266 1.518 -28.609 -75.023 1.00 36.63 B
ATOM 7087 N MET B 267 -0.090 -27.177 -75.637 1.00 35.12 B
ATOM 7088 CA MET B 267 0.647 -26.028 -75.130 1.00 34.41 B
ATOM 7089 CB MET B 267 0.855 -24.979 -76.210 1.00 34.18 B
ATOM 7090 CG MET B 267 1.494 -25.484 -77.466 1.00 36.61 B
ATOM 7091 SD MET B 267 1.928 -24.091 -78.523 1.00 37.28 B
ATOM 7092 CE MET B 267 3.725 -24.245 -78.528 1.00 34.54 B
ATOM 7093 C MET B 267 -0.108 -25.370 -73.998 1.00 34.79 B
ATOM 7094 O MET B 267 0.429 -24.498 -73.320 1.00 36.35 B
ATOM 7095 N VAL B 268 -1.356 -25.774 -73.800 1.00 33.26 B
ATOM 7096 CA VAL B 268 -2.162 -25.178 -72.755 1.00 32.39 B
ATOM 7097 CB VAL B 268 -3.324 -24.387 -73.365 1.00 31.12 B
ATOM 7098 CG1 VAL B 268 -2.781 -23.229 -74.165 1.00 29.64 B
ATOM 7099 CG2 VAL B 268 -4.161 -25.285 -74.237 1.00 29.68 B
ATOM 7100 C VAL B 268 -2.711 -26.186 -71.757 1.00 33.71 B
ATOM 7101 O VAL B 268 -3.064 -25.831 -70.632 1.00 33.28 B
ATOM 7102 N VAL B 269 -2.773 -27.446 -72.171 1.00 35.08 B

ATOM 7103 CA VAL B 269 -3.287 -28.495 -71.300 1.00 35.68 B
ATOM 7104 CB VAL B 269 -2.841 -29.913 -71.781 1.00 35.61 B
ATOM 7105 CG1 VAL B 269 -1.334 -29.978 -71.942 1.00 35.03 B
ATOM 7106 CG2 VAL B 269 -3.307 -30.963 -70.791 1.00 35.51 B
ATOM 7107 C VAL B 269 -2.821 -28.260 -69.871 1.00 35.58 B
ATOM 7108 O VAL B 269 -1.629 -28.294 -69.578 1.00 34.66 B
ATOM 7109 N PRO B 270 -3.773 -27.985 -68.968 1.00 36.56 B
ATOM 7110 CD PRO B 270 -5.199 -27.827 -69.304 1.00 36.13 B
ATOM 7111 CA PRO B 270 -3.551 -27.727 -67.544 1.00 38.85 B
ATOM 7112 CB PRO B 270 -4.960 -27.764 -66.974 1.00 37.80 B
ATOM 7113 CG PRO B 270 -5.750 -27.135 -68.078 1.00 37.04 B
ATOM 7114 C PRO B 270 -2.624 -28.727 -66.864 1.00 41.69 B
ATOM 7115 O PRO B 270 -1.534 -28.365 -66.419 1.00 42.89 B
ATOM 7116 N PHE B 271 -3.051 -29.984 -66.787 1.00 44.18 B
ATOM 7117 CA PHE B 271 -2.245 -31.016 -66.144 1.00 45.80 B
ATOM 7118 CB PHE B 271 -3.070 -31.708 -65.070 1.00 44.56 B
ATOM 7119 CG PHE B 271 -3.789 -30.750 -64.180 1.00 43.49 B
ATOM 7120 CD1 PHE B 271 -5.166 -30.617 -64.249 1.00 43.20 B
ATOM 7121 CD2 PHE B 271 -3.089 -29.949 -63.298 1.00 42.12 B
ATOM 7122 CE1 PHE B 271 -5.831 -29.700 -63.452 1.00 41.69 B
ATOM 7123 CE2 PHE B 271 -3.748 -29.037 -62.507 1.00 41.07 B
ATOM 7124 CZ PHE B 271 -5.123 -28.913 -62.583 1.00 40.95 B
ATOM 7125 C PHE B 271 -1.734 -32.018 -67.156 1.00 47.68 B
ATOM 7126 O PHE B 271 -2.415 -32.993 -67.487 1.00 47.80 B
ATOM 7127 N PRO B 272 -0.517 -31.781 -67.662 1.00 49.60 B
ATOM 7128 CD PRO B 272 0.295 -30.616 -67.280 1.00 49.61 B
ATOM 7129 CA PRO B 272 0.196 -32.591 -68.651 1.00 52.19 B
ATOM 7130 CB PRO B 272 1.525 -31.853 -68.812 1.00 51.23 B
ATOM 7131 CG PRO B 272 1.175 -30.450 -68.488 1.00 50.69 B
ATOM 7132 C PRO B 272 0.403 -34.026 -68.191 1.00 54.54 B
ATOM 7133 O PRO B 272 0.378 -34.957 -69.005 1.00 54.80 B
ATOM 7134 N ASP B 273 0.608 -34.180 -66.882 1.00 56.81 B
ATOM 7135 CA ASP B 273 0.844 -35.477 -66.252 1.00 59.57 B
ATOM 7136 CB ASP B 273 0.689 -35.351 -64.730 1.00 60.95 B

ATOM 7137 CG ASP B 273 1.456 -36.427 -63.970 1.00 62.77 B
ATOM 7138 OD1 ASP B 273 2.706 -36.445 -64.066 1.00 64.05 B
ATOM 7139 OD2 ASP B 273 0.812 -37.253 -63.280 1.00 63.57 B
ATOM 7140 C ASP B 273 -0.116 -36.538 -66.791 1.00 61.06 B
ATOM 7141 O ASP B 273 0.317 -37.539 -67.380 1.00 61.20 B
ATOM 7142 N LYS B 274 -1.411 -36.318 -66.589 1.00 62.13 B
ATOM 7143 CA LYS B 274 -2.435 -37.140 -67.224 1.00 62.87 B
ATOM 7144 CB LYS B 274 -3.831 -36.674 -66.804 1.00 61.63 B
ATOM 7145 CG LYS B 274 -3.965 -36.375 -65.320 1.00 59.72 B
ATOM 7146 CD LYS B 274 -5.258 -36.943 -64.757 0.00 60.12 B
ATOM 7147 CE LYS B 274 -5.465 -38.384 -65.194 0.00 60.29 B
ATOM 7148 NZ LYS B 274 -6.546 -38.506 -66.211 0.00 59.93 B
ATOM 7149 C LYS B 274 -2.306 -37.105 -68.743 1.00 64.32 B
ATOM 7150 O LYS B 274 -2.020 -36.061 -69.327 1.00 65.21 B
ATOM 7151 N PRO B 275 -2.520 -38.254 -69.376 1.00 65.24 B
ATOM 7152 CD PRO B 275 -2.099 -39.438 -68.607 1.00 65.62 B
ATOM 7153 CA PRO B 275 -2.253 -38.404 -70.810 1.00 66.55 B
ATOM 7154 CB PRO B 275 -1.411 -39.679 -70.874 1.00 66.34 B
ATOM 7155 CG PRO B 275 -1.819 -40.456 -69.674 1.00 65.56 B
ATOM 7156 C PRO B 275 -3.540 -38.585 -71.610 1.00 67.38 B
ATOM 7157 O PRO B 275 -4.622 -38.654 -71.028 1.00 67.20 B
ATOM 7158 N ALA B 276 -3.415 -38.662 -72.931 1.00 68.18 B
ATOM 7159 CA ALA B 276 -3.859 -37.583 -73.805 1.00 68.57 B
ATOM 7160 CB ALA B 276 -2.999 -37.528 -75.059 1.00 68.32 B
ATOM 7161 C ALA B 276 -5.330 -37.743 -74.174 1.00 69.08 B
ATOM 7162 O ALA B 276 -5.852 -38.857 -74.213 1.00 68.14 B
ATOM 7163 N ALA B 277 -5.993 -36.623 -74.443 1.00 70.04 B
ATOM 7164 CA ALA B 277 -7.379 -36.644 -74.897 1.00 71.40 B
ATOM 7165 CB ALA B 277 -8.284 -35.986 -73.866 1.00 70.14 B
ATOM 7166 C ALA B 277 -7.526 -35.958 -76.251 1.00 72.83 B
ATOM 7167 O ALA B 277 -8.562 -35.364 -76.548 1.00 74.35 B
ATOM 7168 N ALA B 278 -6.482 -36.046 -77.069 1.00 73.67 B
ATOM 7169 CA ALA B 278 -6.648 -36.195 -78.510 1.00 74.27 B
ATOM 7170 CB ALA B 278 -5.743 -35.224 -79.252 1.00 74.17 B

ATOM 7171 C ALA B 278 -6.371 -37.628 -78.951 1.00 74.53 B
ATOM 7172 O ALA B 278 -5.247 -38.117 -78.834 1.00 74.53 B
ATOM 7173 N VAL B 279 -7.401 -38.296 -79.460 1.00 74.27 B
ATOM 7174 CA VAL B 279 -7.326 -39.725 -79.739 1.00 73.31 B
ATOM 7175 CB VAL B 279 -8.716 -40.384 -79.685 1.00 73.17 B
ATOM 7176 CG1 VAL B 279 -8.689 -41.740 -80.374 1.00 74.36 B
ATOM 7177 CG2 VAL B 279 -9.186 -40.520 -78.245 1.00 71.95 B
ATOM 7178 C VAL B 279 -6.701 -39.987 -81.106 1.00 73.12 B
ATOM 7179 O VAL B 279 -6.637 -41.129 -81.560 1.00 73.40 B
ATOM 7180 N THR B 280 -6.243 -38.922 -81.756 1.00 72.70 B
ATOM 7181 CA THR B 280 -5.780 -39.008 -83.135 1.00 70.80 B
ATOM 7182 CB THR B 280 -5.066 -37.707 -83.547 1.00 71.20 B
ATOM 7183 OG1 THR B 280 -6.015 -36.635 -83.601 1.00 71.26 B
ATOM 7184 CG2 THR B 280 -4.565 -37.804 -84.980 1.00 70.13 B
ATOM 7185 C THR B 280 -4.850 -40.200 -83.332 1.00 69.48 B
ATOM 7186 O THR B 280 -5.134 -41.097 -84.126 1.00 68.67 B
ATOM 7187 N SER B 281 -3.738 -40.204 -82.604 1.00 68.41 B
ATOM 7188 CA SER B 281 -2.711 -41.226 -82.779 1.00 67.77 B
ATOM 7189 CB SER B 281 -1.479 -40.893 -81.931 1.00 67.08 B
ATOM 7190 OG SER B 281 -1.840 -40.615 -80.596 1.00 68.17 B
ATOM 7191 C SER B 281 -3.226 -42.625 -82.442 1.00 67.28 B
ATOM 7192 O SER B 281 -2.719 -43.620 -82.960 1.00 66.75 B
ATOM 7193 N THR B 282 -4.231 -42.700 -81.575 1.00 67.56 B
ATOM 7194 CA THR B 282 -4.808 -43.986 -81.201 1.00 66.56 B
ATOM 7195 CB THR B 282 -5.818 -43.850 -80.029 1.00 67.21 B
ATOM 7196 OG1 THR B 282 -5.141 -43.381 -78.852 1.00 66.81 B
ATOM 7197 CG2 THR B 282 -6.473 -45.195 -79.731 1.00 67.35 B
ATOM 7198 C THR B 282 -5.539 -44.519 -82.424 1.00 65.98 B
ATOM 7199 O THR B 282 -5.660 -45.729 -82.606 1.00 65.78 B
ATOM 7200 N MET B 283 -6.022 -43.598 -83.258 1.00 65.18 B
ATOM 7201 CA MET B 283 -6.739 -43.956 -84.479 1.00 64.20 B
ATOM 7202 CB MET B 283 -7.462 -42.735 -85.064 1.00 63.25 B
ATOM 7203 CG MET B 283 -8.564 -42.156 -84.194 1.00 61.60 B
ATOM 7204 SD MET B 283 -9.358 -40.705 -84.933 1.00 59.65 B

ATOM 7205 CE MET B 283 -11.017 -41.304 -85.169 1.00 59.91 B
ATOM 7206 C MET B 283 -5.766 -44.503 -85.521 1.00 64.49 B
ATOM 7207 O MET B 283 -5.907 -45.637 -85.983 1.00 64.71 B
ATOM 7208 N LEU B 284 -4.781 -43.690 -85.889 1.00 63.88 B
ATOM 7209 CA LEU B 284 -3.792 -44.094 -86.878 1.00 63.34 B
ATOM 7210 CB LEU B 284 -2.687 -43.035 -87.003 1.00 62.89 B
ATOM 7211 CG LEU B 284 -3.033 -41.677 -87.625 1.00 62.80 B
ATOM 7212 CD1 LEU B 284 -1.790 -40.805 -87.651 1.00 62.34 B
ATOM 7213 CD2 LEU B 284 -3.572 -41.869 -89.037 1.00 63.36 B
ATOM 7214 C LEU B 284 -3.158 -45.443 -86.549 1.00 63.39 B
ATOM 7215 O LEU B 284 -2.931 -46.255 -87.445 1.00 63.72 B
ATOM 7216 N GLN B 285 -3.015 -45.749 -85.278 1.00 63.21 B
ATOM 7217 CA GLN B 285 -2.314 -46.939 -84.835 1.00 62.83 B
ATOM 7218 CB GLN B 285 -1.962 -46.838 -83.372 1.00 62.67 B
ATOM 7219 CG GLN B 285 -0.512 -46.829 -83.018 1.00 62.26 B
ATOM 7220 CD GLN B 285 -0.167 -45.889 -81.872 0.00 62.36 B
ATOM 7221 OE1 GLN B 285 0.531 -44.898 -82.053 0.00 62.34 B
ATOM 7222 NE2 GLN B 285 -0.657 -46.201 -80.695 0.00 62.34 B
ATOM 7223 C GLN B 285 -3.130 -48.157 -84.956 1.00 63.20 B
ATOM 7224 O GLN B 285 -2.742 -49.172 -84.474 1.00 63.50 B
ATOM 7225 N GLN B 286 -4.292 -48.048 -85.542 1.00 63.81 B
ATOM 7226 CA GLN B 286 -5.053 -49.237 -85.800 1.00 65.00 B
ATOM 7227 CB GLN B 286 -6.101 -49.544 -84.750 1.00 64.16 B
ATOM 7228 CG GLN B 286 -6.720 -48.396 -84.001 1.00 63.00 B
ATOM 7229 CD GLN B 286 -7.450 -48.838 -82.801 1.00 62.00 B
ATOM 7230 OE1 GLN B 286 -8.603 -49.156 -82.866 1.00 60.20 B
ATOM 7231 NE2 GLN B 286 -6.769 -48.866 -81.693 1.00 61.54 B
ATOM 7232 C GLN B 286 -5.698 -49.147 -87.118 1.00 66.60 B
ATOM 7233 O GLN B 286 -6.757 -49.697 -87.346 1.00 66.70 B
ATOM 7234 N GLY B 287 -5.051 -48.428 -88.030 1.00 67.72 B
ATOM 7235 CA GLY B 287 -5.440 -48.441 -89.428 1.00 68.48 B
ATOM 7236 C GLY B 287 -6.854 -47.940 -89.645 1.00 69.07 B
ATOM 7237 O GLY B 287 -7.611 -48.509 -90.431 1.00 69.61 B
ATOM 7238 N TRP B 288 -7.212 -46.869 -88.943 1.00 69.05 B

ATOM 7239 CA TRP B 288 -8.532 -46.267 -89.084 1.00 69.17 B
ATOM 7240 CB TRP B 288 -8.744 -45.184 -88.025 1.00 69.47 B
ATOM 7241 CG TRP B 288 -9.540 -45.648 -86.843 1.00 69.17 B
ATOM 7242 CD2 TRP B 288 -10.821 -45.162 -86.425 1.00 68.11 B
ATOM 7243 CE2 TRP B 288 -11.189 -45.883 -85.271 1.00 67.71 B
ATOM 7244 CE3 TRP B 288 -11.699 -44.187 -86.911 1.00 67.90 B
ATOM 7245 CD1 TRP B 288 -9.192 -46.619 -85.949 1.00 69.41 B
ATOM 7246 NE1 TRP B 288 -10.176 -46.767 -85.002 1.00 69.25 B
ATOM 7247 CZ2 TRP B 288 -12.389 -45.661 -84.600 1.00 66.69 B
ATOM 7248 CZ3 TRP B 288 -12.889 -43.968 -86.242 1.00 67.63 B
ATOM 7249 CH2 TRP B 288 -13.222 -44.701 -85.100 1.00 66.67 B
ATOM 7250 C TRP B 288 -8.727 -45.681 -90.479 1.00 69.05 B
ATOM 7251 O TRP B 288 -8.028 -44.748 -90.874 1.00 69.33 B
ATOM 7252 N ASN B 289 -9.827 -46.039 -91.106 1.00 68.68 B
ATOM 7253 CA ASN B 289 -10.122 -45.800 -92.508 1.00 67.30 B
ATOM 7254 CB ASN B 289 -11.088 -46.886 -92.960 1.00 67.20 B
ATOM 7255 CG ASN B 289 -10.628 -47.603 -94.130 1.00 67.35 B
ATOM 7256 OD1 ASN B 289 -11.407 -47.970 -94.945 1.00 67.97 B
ATOM 7257 ND2 ASN B 289 -9.354 -47.837 -94.218 1.00 67.51 B
ATOM 7258 C ASN B 289 -10.891 -44.562 -92.745 1.00 66.19 B
ATOM 7259 O ASN B 289 -11.754 -44.212 -92.008 1.00 66.48 B
ATOM 7260 N ALA B 290 -10.739 -43.990 -93.896 1.00 64.84 B
ATOM 7261 CA ALA B 290 -11.638 -42.882 -94.195 1.00 63.39 B
ATOM 7262 CB ALA B 290 -11.269 -42.243 -95.525 1.00 63.28 B
ATOM 7263 C ALA B 290 -13.093 -43.339 -94.207 1.00 62.02 B
ATOM 7264 O ALA B 290 -13.997 -42.573 -93.875 1.00 61.01 B
ATOM 7265 N THR B 291 -13.311 -44.592 -94.591 1.00 61.38 B
ATOM 7266 CA THR B 291 -14.659 -45.137 -94.702 1.00 60.32 B
ATOM 7267 CB THR B 291 -14.708 -46.241 -95.774 1.00 60.41 B
ATOM 7268 OG1 THR B 291 -13.980 -45.817 -96.933 1.00 59.55 B
ATOM 7269 CG2 THR B 291 -16.126 -46.414 -96.295 1.00 60.90 B
ATOM 7270 C THR B 291 -15.143 -45.685 -93.363 1.00 59.28 B
ATOM 7271 O THR B 291 -16.332 -45.627 -93.050 1.00 59.12 B
ATOM 7272 N HIS B 292 -14.213 -46.216 -92.577 1.00 58.15 B

ATOM 7273 CA HIS B 292 -14.542 -46.783 -91.272 1.00 56.88 B
ATOM 7274 CB HIS B 292 -13.306 -47.440 -90.644 1.00 58.47 B
ATOM 7275 CG HIS B 292 -13.590 -48.193 -89.377 1.00 59.90 B
ATOM 7276 CD2 HIS B 292 -13.101 -48.045 -88.121 1.00 60.26 B
ATOM 7277 ND1 HIS B 292 -14.471 -49.254 -89.322 1.00 60.90 B
ATOM 7278 CE1 HIS B 292 -14.516 -49.725 -88.088 1.00 61.17 B
ATOM 7279 NE2 HIS B 292 -13.694 -49.009 -87.339 1.00 60.99 B
ATOM 7280 C HIS B 292 -15.034 -45.646 -90.388 1.00 55.01 B
ATOM 7281 O HIS B 292 -15.935 -45.826 -89.567 1.00 54.04 B
ATOM 7282 N MET B 293 -14.443 -44.468 -90.570 1.00 53.31 B
ATOM 7283 CA MET B 293 -14.833 -43.294 -89.799 1.00 51.32 B
ATOM 7284 CB MET B 293 -13.961 -42.082 -90.179 1.00 50.39 B
ATOM 7285 CG MET B 293 -12.519 -42.162 -89.659 1.00 50.23 B
ATOM 7286 SD MET B 293 -11.416 -40.803 -90.150 1.00 50.22 B
ATOM 7287 CE MET B 293 -11.988 -39.528 -89.096 1.00 51.58 B
ATOM 7288 C MET B 293 -16.316 -42.986 -90.022 1.00 50.58 B
ATOM 7289 O MET B 293 -17.068 -42.835 -89.057 1.00 51.16 B
ATOM 7290 N PHE B 294 -16.742 -42.915 -91.283 1.00 49.52 B
ATOM 7291 CA PHE B 294 -18.145 -42.628 -91.597 1.00 48.60 B
ATOM 7292 CB PHE B 294 -18.345 -42.399 -93.099 1.00 47.08 B
ATOM 7293 CG PHE B 294 -17.818 -41.086 -93.594 1.00 44.74 B
ATOM 7294 CD1 PHE B 294 -16.475 -40.932 -93.900 1.00 44.44 B
ATOM 7295 CD2 PHE B 294 -18.668 -39.999 -93.752 1.00 43.81 B
ATOM 7296 CE1 PHE B 294 -15.990 -39.717 -94.354 1.00 44.73 B
ATOM 7297 CE2 PHE B 294 -18.190 -38.781 -94.204 1.00 43.84 B
ATOM 7298 CZ PHE B 294 -16.851 -38.639 -94.507 1.00 44.16 B
ATOM 7299 C PHE B 294 -19.103 -43.725 -91.141 1.00 48.75 B
ATOM 7300 O PHE B 294 -20.298 -43.477 -90.970 1.00 47.53 B
ATOM 7301 N ARG B 295 -18.569 -44.910 -90.907 1.00 49.32 B
ATOM 7302 CA ARG B 295 -19.372 -46.040 -90.469 1.00 50.26 B
ATOM 7303 CB ARG B 295 -18.893 -47.370 -91.043 1.00 50.60 B
ATOM 7304 CG ARG B 295 -19.365 -47.673 -92.461 1.00 52.42 B
ATOM 7305 CD ARG B 295 -20.343 -48.803 -92.664 1.00 54.07 B
ATOM 7306 NE ARG B 295 -20.704 -49.076 -94.063 1.00 56.47 B

ATOM 7307 CZ ARG B 295 -19.939 -49.672 -94.997 1.00 57.23 B
ATOM 7308 NH1 ARG B 295 -18.709 -50.071 -94.771 1.00 57.09 B
ATOM 7309 NH2 ARG B 295 -20.412 -49.849 -96.196 1.00 57.74 B
ATOM 7310 C ARG B 295 -19.439 -46.137 -89.003 1.00 50.16 B
ATOM 7311 O ARG B 295 -20.228 -46.868 -88.489 1.00 49.80 B
ATOM 7312 N VAL B 296 -18.608 -45.361 -88.337 1.00 51.02 B
ATOM 7313 CA VAL B 296 -18.615 -45.227 -86.881 1.00 51.29 B
ATOM 7314 CB VAL B 296 -17.257 -44.726 -86.355 1.00 50.60 B
ATOM 7315 CG1 VAL B 296 -17.367 -44.358 -84.887 1.00 49.32 B
ATOM 7316 CG2 VAL B 296 -16.208 -45.795 -86.549 1.00 50.75 B
ATOM 7317 C VAL B 296 -19.672 -44.186 -86.540 1.00 51.85 B
ATOM 7318 O VAL B 296 -20.403 -44.314 -85.555 1.00 52.22 B
ATOM 7319 N ALA B 297 -19.735 -43.146 -87.366 1.00 51.60 B
ATOM 7320 CA ALA B 297 -20.707 -42.085 -87.175 1.00 51.60 B
ATOM 7321 CB ALA B 297 -20.439 -40.938 -88.141 1.00 49.51 B
ATOM 7322 C ALA B 297 -22.075 -42.690 -87.434 1.00 51.83 B
ATOM 7323 O ALA B 297 -23.024 -42.437 -86.694 1.00 51.69 B
ATOM 7324 N GLU B 298 -22.174 -43.502 -88.482 1.00 52.66 B
ATOM 7325 CA GLU B 298 -23.442 -44.138 -88.808 1.00 54.12 B
ATOM 7326 CB GLU B 298 -23.312 -45.027 -90.039 1.00 55.63 B
ATOM 7327 CG GLU B 298 -24.563 -45.860 -90.305 1.00 56.50 B
ATOM 7328 CD GLU B 298 -24.530 -46.547 -91.651 1.00 57.39 B
ATOM 7329 OE1 GLU B 298 -23.608 -47.361 -91.894 1.00 57.90 B
ATOM 7330 OE2 GLU B 298 -25.432 -46.263 -92.468 1.00 58.40 B
ATOM 7331 C GLU B 298 -23.870 -44.985 -87.631 1.00 54.81 B
ATOM 7332 O GLU B 298 -25.013 -44.907 -87.174 1.00 54.55 B
ATOM 7333 N GLU B 299 -22.995 -45.826 -87.167 1.00 55.93 B
ATOM 7334 CA GLU B 299 -23.321 -46.625 -86.023 1.00 57.13 B
ATOM 7335 CB GLU B 299 -22.058 -47.159 -85.468 1.00 59.00 B
ATOM 7336 CG GLU B 299 -22.082 -47.394 -83.998 1.00 63.65 B
ATOM 7337 CD GLU B 299 -20.765 -47.086 -83.321 1.00 66.21 B
ATOM 7338 OE1 GLU B 299 -20.578 -45.954 -82.905 1.00 67.81 B
ATOM 7339 OE2 GLU B 299 -19.921 -47.966 -83.197 1.00 67.52 B
ATOM 7340 C GLU B 299 -24.025 -45.800 -84.995 1.00 56.38 B

ATOM 7341 O GLU B 299 -25.165 -45.986 -84.719 1.00 56.78 B
ATOM 7342 N PHE B 300 -23.346 -44.828 -84.455 1.00 54.34 B
ATOM 7343 CA PHE B 300 -23.951 -44.049 -83.388 1.00 51.53 B
ATOM 7344 CB PHE B 300 -23.119 -42.788 -83.125 1.00 50.38 B
ATOM 7345 CG PHE B 300 -23.412 -42.133 -81.804 1.00 48.99 B
ATOM 7346 CD1 PHE B 300 -22.516 -42.237 -80.751 1.00 48.84 B
ATOM 7347 CD2 PHE B 300 -24.595 -41.428 -81.606 1.00 48.25 B
ATOM 7348 CE1 PHE B 300 -22.796 -41.648 -79.522 1.00 48.35 B
ATOM 7349 CE2 PHE B 300 -24.885 -40.837 -80.382 1.00 46.80 B
ATOM 7350 CZ PHE B 300 -23.987 -40.946 -79.339 1.00 46.90 B
ATOM 7351 C PHE B 300 -25.392 -43.661 -83.727 1.00 50.66 B
ATOM 7352 O PHE B 300 -26.305 -43.918 -82.948 1.00 50.67 B
ATOM 7353 N PHE B 301 -25.595 -43.047 -84.889 1.00 49.87 B
ATOM 7354 CA PHE B 301 -26.928 -42.613 -85.314 1.00 49.03 B
ATOM 7355 CB PHE B 301 -26.888 -42.059 -86.734 1.00 48.30 B
ATOM 7356 CG PHE B 301 -26.547 -40.605 -86.822 1.00 46.96 B
ATOM 7357 CD1 PHE B 301 -25.234 -40.197 -87.028 1.00 46.04 B
ATOM 7358 CD2 PHE B 301 -27.548 -39.641 -86.749 1.00 46.47 B
ATOM 7359 CE1 PHE B 301 -24.922 -38.856 -87.167 1.00 44.67 B
ATOM 7360 CE2 PHE B 301 -27.246 -38.295 -86.887 1.00 45.55 B
ATOM 7361 CZ PHE B 301 -25.930 -37.903 -87.097 1.00 45.08 B
ATOM 7362 C PHE B 301 -28.008 -43.687 -85.277 1.00 48.85 B
ATOM 7363 O PHE B 301 -29.171 -43.397 -84.996 1.00 47.72 B
ATOM 7364 N THR B 302 -27.628 -44.920 -85.596 1.00 49.24 B
ATOM 7365 CA THR B 302 -28.576 -46.031 -85.619 1.00 50.05 B
ATOM 7366 CB THR B 302 -27.995 -47.250 -86.389 1.00 48.64 B
ATOM 7367 OG1 THR B 302 -26.667 -47.525 -85.938 1.00 48.59 B
ATOM 7368 CG2 THR B 302 -27.952 -46.967 -87.875 1.00 48.67 B
ATOM 7369 C THR B 302 -28.984 -46.464 -84.213 1.00 51.24 B
ATOM 7370 O THR B 302 -30.145 -46.803 -83.969 1.00 51.73 B
ATOM 7371 N SER B 303 -28.023 -46.435 -83.294 1.00 51.94 B
ATOM 7372 CA SER B 303 -28.248 -46.818 -81.906 1.00 52.64 B
ATOM 7373 CB SER B 303 -26.941 -46.690 -81.129 1.00 54.20 B
ATOM 7374 OG SER B 303 -25.901 -47.382 -81.813 1.00 57.91 B

ATOM 7375 C SER B 303 -29.340 -45.994 -81.233 1.00 52.02 B
ATOM 7376 O SER B 303 -29.926 -46.432 -80.250 1.00 52.06 B
ATOM 7377 N LEU B 304 -29.606 -44.802 -81.761 1.00 51.35 B
ATOM 7378 CA LEU B 304 -30.650 -43.932 -81.224 1.00 50.47 B
ATOM 7379 CB LEU B 304 -30.291 -42.468 -81.434 1.00 49.84 B
ATOM 7380 CG LEU B 304 -29.000 -42.012 -80.778 1.00 49.70 B
ATOM 7381 CD1 LEU B 304 -28.625 -40.639 -81.296 1.00 50.27 B
ATOM 7382 CD2 LEU B 304 -29.181 -42.017 -79.272 1.00 50.22 B
ATOM 7383 C LEU B 304 -31.898 -44.239 -82.011 1.00 50.40 B
ATOM 7384 O LEU B 304 -32.908 -43.548 -81.900 1.00 49.72 B
ATOM 7385 N GLU B 305 -31.801 -45.285 -82.821 1.00 51.01 B
ATOM 7386 CA GLU B 305 -32.890 -45.733 -83.672 1.00 51.68 B
ATOM 7387 CB GLU B 305 -34.049 -46.270 -82.833 1.00 52.20 B
ATOM 7388 CG GLU B 305 -33.868 -47.726 -82.451 1.00 52.80 B
ATOM 7389 CD GLU B 305 -35.041 -48.276 -81.671 1.00 54.06 B
ATOM 7390 OE1 GLU B 305 -35.197 -47.920 -80.486 1.00 54.47 B
ATOM 7391 OE2 GLU B 305 -35.818 -49.064 -82.250 1.00 55.72 B
ATOM 7392 C GLU B 305 -33.373 -44.664 -84.643 1.00 51.92 B
ATOM 7393 O GLU B 305 -34.556 -44.309 -84.691 1.00 51.00 B
ATOM 7394 N LEU B 306 -32.410 -44.149 -85.399 1.00 52.28 B
ATOM 7395 CA LEU B 306 -32.645 -43.168 -86.447 1.00 52.41 B
ATOM 7396 CB LEU B 306 -31.722 -41.960 -86.274 1.00 51.86 B
ATOM 7397 CG LEU B 306 -31.990 -41.020 -85.096 1.00 50.88 B
ATOM 7398 CD1 LEU B 306 -30.830 -40.065 -84.960 1.00 50.95 B
ATOM 7399 CD2 LEU B 306 -33.290 -40.261 -85.303 1.00 48.98 B
ATOM 7400 C LEU B 306 -32.230 -44.000 -87.664 1.00 52.75 B
ATOM 7401 O LEU B 306 -31.444 -44.947 -87.519 1.00 53.18 B
ATOM 7402 N SER B 307 -32.753 -43.686 -88.848 1.00 52.03 B
ATOM 7403 CA SER B 307 -32.405 -44.467 -90.037 1.00 50.10 B
ATOM 7404 CB SER B 307 -33.274 -44.052 -91.223 1.00 50.33 B
ATOM 7405 OG SER B 307 -33.229 -42.654 -91.426 1.00 50.38 B
ATOM 7406 C SER B 307 -30.932 -44.352 -90.409 1.00 48.48 B
ATOM 7407 O SER B 307 -30.283 -43.343 -90.120 1.00 46.77 B
ATOM 7408 N PRO B 308 -30.378 -45.407 -91.034 1.00 48.01 B

ATOM 7409 CD PRO B 308 -30.974 -46.749 -91.184 1.00 47.11 B
ATOM 7410 CA PRO B 308 -28.971 -45.420 -91.446 1.00 48.04 B
ATOM 7411 CB PRO B 308 -28.630 -46.906 -91.456 1.00 46.53 B
ATOM 7412 CG PRO B 308 -29.894 -47.509 -91.944 1.00 46.92 B
ATOM 7413 C PRO B 308 -28.763 -44.766 -92.810 1.00 48.45 B
ATOM 7414 O PRO B 308 -29.722 -44.399 -93.492 1.00 48.31 B
ATOM 7415 N MET B 309 -27.499 -44.632 -93.196 1.00 49.00 B
ATOM 7416 CA MET B 309 -27.130 -44.018 -94.461 1.00 50.21 B
ATOM 7417 CB MET B 309 -25.643 -43.658 -94.438 1.00 52.23 B
ATOM 7418 CG MET B 309 -25.239 -42.716 -93.306 1.00 54.16 B
ATOM 7419 SD MET B 309 -26.026 -41.079 -93.404 1.00 57.33 B
ATOM 7420 CE MET B 309 -27.391 -41.266 -92.227 1.00 56.32 B
ATOM 7421 C MET B 309 -27.415 -44.940 -95.638 1.00 50.62 B
ATOM 7422 O MET B 309 -26.839 -46.029 -95.724 1.00 51.08 B
ATOM 7423 N PRO B 310 -28.301 -44.509 -96.565 1.00 50.95 B
ATOM 7424 CD PRO B 310 -29.013 -43.229 -96.424 1.00 51.64 B
ATOM 7425 CA PRO B 310 -28.749 -45.199 -97.785 1.00 50.63 B
ATOM 7426 CB PRO B 310 -29.628 -44.161 -98.467 1.00 50.97 B
ATOM 7427 CG PRO B 310 -30.212 -43.436 -97.315 1.00 52.19 B
ATOM 7428 C PRO B 310 -27.632 -45.666 -98.708 1.00 50.75 B
ATOM 7429 O PRO B 310 -26.534 -45.118 -98.702 1.00 49.35 B
ATOM 7430 N PRO B 311 -27.905 -46.697 -99.521 1.00 52.26 B
ATOM 7431 CD PRO B 311 -29.074 -47.597 -99.509 1.00 52.62 B
ATOM 7432 CA PRO B 311 -26.875 -47.196 -100.435 1.00 53.26 B
ATOM 7433 CB PRO B 311 -27.575 -48.361 -101.131 1.00 52.93 B
ATOM 7434 CG PRO B 311 -28.490 -48.883 -100.062 1.00 52.28 B
ATOM 7435 C PRO B 311 -26.414 -46.118 -101.408 1.00 53.82 B
ATOM 7436 O PRO B 311 -25.224 -46.017 -101.711 1.00 53.65 B
ATOM 7437 N GLU B 312 -27.353 -45.309 -101.890 1.00 54.28 B
ATOM 7438 CA GLU B 312 -27.001 -44.248 -102.823 1.00 55.41 B
ATOM 7439 CB GLU B 312 -28.226 -43.412 -103.211 1.00 57.24 B
ATOM 7440 CG GLU B 312 -29.531 -43.769 -102.504 1.00 60.17 B
ATOM 7441 CD GLU B 312 -30.542 -44.445 -103.411 1.00 62.02 B
ATOM 7442 OE1 GLU B 312 -30.492 -45.688 -103.531 1.00 62.26 B

ATOM 7443 OE2 GLU B 312 -31.380 -43.729-104.003 1.00 63.75 B
ATOM 7444 C GLU B 312 -25.956 -43.352-102.186 1.00 55.14 B
ATOM 7445 O GLU B 312 -25.107 -42.788-102.881 1.00 55.72 B
ATOM 7446 N PHE B 313 -26.026 -43.229-100.862 1.00 54.81 B
ATOM 7447 CA PHE B 313 -25.084 -42.415-100.098 1.00 54.20 B
ATOM 7448 CB PHE B 313 -25.501 -42.366 -98.619 1.00 53.56 B
ATOM 7449 CG PHE B 313 -24.461 -41.755 -97.705 1.00 53.96 B
ATOM 7450 CD1 PHE B 313 -24.287 -40.368 -97.640 1.00 53.97 B
ATOM 7451 CD2 PHE B 313 -23.629 -42.572 -96.934 1.00 53.22 B
ATOM 7452 CE1 PHE B 313 -23.298 -39.805 -96.825 1.00 53.34 B
ATOM 7453 CE2 PHE B 313 -22.640 -42.024 -96.117 1.00 52.89 B
ATOM 7454 CZ PHE B 313 -22.472 -40.635 -96.063 1.00 53.40 B
ATOM 7455 C PHE B 313 -23.669 -42.992-100.224 1.00 54.08 B
ATOM 7456 O PHE B 313 -22.724 -42.270-100.543 1.00 54.19 B
ATOM 7457 N TRP B 314 -23.526 -44.292 -99.978 1.00 53.44 B
ATOM 7458 CA TRP B 314 -22.227 -44.941-100.064 1.00 52.83 B
ATOM 7459 CB TRP B 314 -22.295 -46.332 -99.432 1.00 52.29 B
ATOM 7460 CG TRP B 314 -22.616 -46.255 -97.975 1.00 52.93 B
ATOM 7461 CD2 TRP B 314 -21.684 -46.026 -96.909 1.00 53.40 B
ATOM 7462 CE2 TRP B 314 -22.436 -45.871 -95.720 1.00 52.89 B
ATOM 7463 CE3 TRP B 314 -20.285 -45.927 -96.844 1.00 52.73 B
ATOM 7464 CD1 TRP B 314 -23.861 -46.242 -97.404 1.00 52.32 B
ATOM 7465 NE1 TRP B 314 -23.760 -46.010 -96.048 1.00 52.62 B
ATOM 7466 CZ2 TRP B 314 -21.835 -45.621 -94.484 1.00 52.10 B
ATOM 7467 CZ3 TRP B 314 -19.690 -45.679 -95.617 1.00 51.83 B
ATOM 7468 CH2 TRP B 314 -20.465 -45.528 -94.451 1.00 51.78 B
ATOM 7469 C TRP B 314 -21.762 -45.032-101.503 1.00 53.55 B
ATOM 7470 O TRP B 314 -20.566 -45.041-101.780 1.00 53.48 B
ATOM 7471 N GLU B 315 -22.713 -45.061-102.416 1.00 54.70 B
ATOM 7472 CA GLU B 315 -22.417 -45.177-103.839 1.00 55.43 B
ATOM 7473 CB GLU B 315 -23.671 -45.586-104.614 1.00 58.77 B
ATOM 7474 CG GLU B 315 -23.599 -46.978-105.222 1.00 63.61 B
ATOM 7475 CD GLU B 315 -24.781 -47.844-104.834 1.00 65.26 B
ATOM 7476 OE1 GLU B 315 -24.557 -48.969-104.339 1.00 65.06 B

ATOM 7477 OE2 GLU B 315 -25.934 -47.402-105.026 1.00 67.31 B
ATOM 7478 C GLU B 315 -21.860 -43.871-104.395 1.00 53.88 B
ATOM 7479 O GLU B 315 -20.832 -43.890-105.098 1.00 52.60 B
ATOM 7480 N GLY B 316 -22.517 -42.754-104.136 1.00 52.87 B
ATOM 7481 CA GLY B 316 -22.074 -41.474-104.671 1.00 52.06 B
ATOM 7482 C GLY B 316 -21.190 -40.543-103.845 1.00 50.71 B
ATOM 7483 O GLY B 316 -20.387 -39.795-104.400 1.00 50.69 B
ATOM 7484 N SER B 317 -21.332 -40.574-102.529 1.00 49.78 B
ATOM 7485 CA SER B 317 -20.550 -39.709-101.654 1.00 48.80 B
ATOM 7486 CB SER B 317 -20.873 -40.064-100.190 1.00 49.55 B
ATOM 7487 OG SER B 317 -20.389 -39.105 -99.261 1.00 51.22 B
ATOM 7488 C SER B 317 -19.034 -39.791-101.914 1.00 47.89 B
ATOM 7489 O SER B 317 -18.486 -40.867-102.137 1.00 46.70 B
ATOM 7490 N MET B 318 -18.371 -38.637-101.910 1.00 47.79 B
ATOM 7491 CA MET B 318 -16.919 -38.562-102.101 1.00 48.09 B
ATOM 7492 CB MET B 318 -16.541 -37.320-102.927 1.00 47.90 B
ATOM 7493 CG MET B 318 -15.030 -37.128-103.104 1.00 48.25 B
ATOM 7494 SD MET B 318 -14.528 -35.545-103.831 1.00 49.77 B
ATOM 7495 CE MET B 318 -14.076 -34.605-102.388 1.00 49.10 B
ATOM 7496 C MET B 318 -16.319 -38.445-100.696 1.00 48.19 B
ATOM 7497 O MET B 318 -16.215 -37.349-100.156 1.00 48.60 B
ATOM 7498 N LEU B 319 -15.914 -39.568-100.112 1.00 48.43 B
ATOM 7499 CA LEU B 319 -15.379 -39.567 -98.755 1.00 48.44 B
ATOM 7500 CB LEU B 319 -15.832 -40.837 -98.033 1.00 46.97 B
ATOM 7501 CG LEU B 319 -17.301 -41.230 -98.235 1.00 45.66 B
ATOM 7502 CD1 LEU B 319 -17.577 -42.521 -97.493 1.00 44.48 B
ATOM 7503 CD2 LEU B 319 -18.227 -40.119 -97.760 1.00 43.43 B
ATOM 7504 C LEU B 319 -13.868 -39.426 -98.628 1.00 49.96 B
ATOM 7505 O LEU B 319 -13.345 -39.448 -97.522 1.00 50.38 B
ATOM 7506 N GLU B 320 -13.151 -39.179 -99.706 1.00 52.33 B
ATOM 7507 CA GLU B 320 -11.690 -39.134 -99.675 1.00 54.83 B
ATOM 7508 CB GLU B 320 -11.158 -40.470-100.084 1.00 55.60 B
ATOM 7509 CG GLU B 320 -10.435 -41.310 -99.068 1.00 58.16 B
ATOM 7510 CD GLU B 320 -10.738 -42.777 -99.237 1.00 59.94 B

ATOM 7511 OE1 GLU B 320 -11.724 -43.106 -99.884 1.00 61.71 B
ATOM 7512 OE2 GLU B 320 -9.991 -43.603 -98.729 1.00 60.61 B
ATOM 7513 C GLU B 320 -11.289 -38.185-100.760 1.00 56.11 B
ATOM 7514 O GLU B 320 -12.080 -37.927-101.591 1.00 56.81 B
ATOM 7515 N LYS B 321 -10.064 -37.678-100.771 1.00 57.23 B
ATOM 7516 CA LYS B 321 -9.570 -36.774-101.812 1.00 58.16 B
ATOM 7517 CB LYS B 321 -8.406 -35.925-101.289 1.00 58.03 B
ATOM 7518 CG LYS B 321 -7.825 -34.958-102.314 1.00 57.91 B
ATOM 7519 CD LYS B 321 -6.819 -33.998-101.685 1.00 58.23 B
ATOM 7520 CE LYS B 321 -6.193 -33.079-102.725 1.00 59.06 B
ATOM 7521 NZ LYS B 321 -5.283 -32.080-102.106 1.00 58.96 B
ATOM 7522 C LYS B 321 -9.120 -37.610-103.008 1.00 58.96 B
ATOM 7523 O LYS B 321 -8.317 -38.536-102.860 1.00 59.67 B
ATOM 7524 N PRO B 322 -9.635 -37.293-104.208 1.00 59.46 B
ATOM 7525 CD PRO B 322 -10.491 -36.125-104.489 1.00 59.56 B
ATOM 7526 CA PRO B 322 -9.306 -38.005-105.448 1.00 59.46 B
ATOM 7527 CB PRO B 322 -9.776 -37.041-106.525 1.00 59.49 B
ATOM 7528 CG PRO B 322 -10.981 -36.415-105.884 1.00 59.86 B
ATOM 7529 C PRO B 322 -7.830 -38.373-105.598 1.00 59.89 B
ATOM 7530 O PRO B 322 -6.940 -37.625-105.185 1.00 59.41 B
ATOM 7531 N ALA B 323 -7.586 -39.539-106.191 1.00 60.58 B
ATOM 7532 CA ALA B 323 -6.230 -40.035-106.412 1.00 60.84 B
ATOM 7533 CB ALA B 323 -6.239 -41.569-106.488 1.00 61.04 B
ATOM 7534 C ALA B 323 -5.690 -39.445-107.711 1.00 60.86 B
ATOM 7535 O ALA B 323 -4.539 -39.003-107.777 1.00 60.40 B
ATOM 7536 N ASP B 324 -6.545 -39.440-108.734 1.00 60.62 B
ATOM 7537 CA ASP B 324 -6.209 -38.910-110.050 1.00 59.84 B
ATOM 7538 CB ASP B 324 -7.375 -39.140-111.018 1.00 59.77 B
ATOM 7539 CG ASP B 324 -8.681 -38.545-110.517 1.00 60.20 B
ATOM 7540 OD1 ASP B 324 -8.715 -37.315-110.302 1.00 60.26 B
ATOM 7541 OD2 ASP B 324 -9.667 -39.301-110.341 1.00 59.27 B
ATOM 7542 C ASP B 324 -5.864 -37.422-109.982 1.00 59.85 B
ATOM 7543 O ASP B 324 -5.447 -36.825-110.972 1.00 59.68 B
ATOM 7544 N GLY B 325 -6.053 -36.827-108.809 1.00 60.28 B

ATOM 7545 CA GLY B 325 -5.727 -35.426-108.618 1.00 60.00 B
ATOM 7546 C GLY B 325 -6.557 -34.396-109.354 1.00 59.96 B
ATOM 7547 O GLY B 325 -6.014 -33.371-109.772 1.00 61.00 B
ATOM 7548 N ARG B 326 -7.856 -34.647-109.520 1.00 58.60 B
ATOM 7549 CA ARG B 326 -8.737 -33.688-110.192 1.00 57.47 B
ATOM 7550 CB ARG B 326 -9.953 -34.408-110.798 1.00 55.76 B
ATOM 7551 CG ARG B 326 -10.698 -35.377-109.866 1.00 55.90 B
ATOM 7552 CD ARG B 326 -11.919 -36.009-110.564 1.00 55.13 B
ATOM 7553 NE ARG B 326 -12.199 -37.389-110.145 1.00 54.79 B
ATOM 7554 CZ ARG B 326 -13.028 -37.736-109.164 1.00 54.54 B
ATOM 7555 NH1 ARG B 326 -13.676 -36.808-108.478 1.00 53.78 B
ATOM 7556 NH2 ARG B 326 -13.215 -39.016-108.871 1.00 54.53 B
ATOM 7557 C ARG B 326 -9.195 -32.619-109.189 1.00 57.84 B
ATOM 7558 O ARG B 326 -9.927 -32.915-108.248 1.00 58.57 B
ATOM 7559 N GLU B 327 -8.828 -31.391-109.424 1.00 57.58 B
ATOM 7560 CA GLU B 327 -9.151 -30.416-108.463 1.00 57.99 B
ATOM 7561 CB GLU B 327 -8.996 -29.053-109.051 1.00 59.13 B
ATOM 7562 CG GLU B 327 -7.596 -28.780-109.540 1.00 61.73 B
ATOM 7563 CD GLU B 327 -6.680 -28.108-108.533 1.00 62.98 B
ATOM 7564 OE1 GLU B 327 -6.505 -26.907-108.613 1.00 63.20 B
ATOM 7565 OE2 GLU B 327 -6.093 -28.779-107.688 1.00 63.72 B
ATOM 7566 C GLU B 327 -10.530 -30.673-107.961 1.00 57.50 B
ATOM 7567 O GLU B 327 -11.343 -31.154-108.659 1.00 57.30 B
ATOM 7568 N VAL B 328 -10.754 -30.398-106.684 1.00 57.00 B
ATOM 7569 CA VAL B 328 -12.094 -30.443-106.090 1.00 55.19 B
ATOM 7570 CB VAL B 328 -12.460 -31.831-105.508 1.00 53.91 B
ATOM 7571 CG1 VAL B 328 -12.448 -32.876-106.594 1.00 54.28 B
ATOM 7572 CG2 VAL B 328 -11.506 -32.189-104.373 1.00 52.61 B
ATOM 7573 C VAL B 328 -12.206 -29.482-104.930 1.00 54.64 B
ATOM 7574 O VAL B 328 -11.205 -28.972-104.429 1.00 55.42 B
ATOM 7575 N VAL B 329 -13.446 -29.243-104.520 1.00 53.30 B
ATOM 7576 CA VAL B 329 -13.736 -28.391-103.380 1.00 52.31 B
ATOM 7577 CB VAL B 329 -15.174 -27.825-103.459 1.00 51.65 B
ATOM 7578 CG1 VAL B 329 -15.491 -27.015-102.225 1.00 50.64 B

ATOM 7579 CG2 VAL B 329 -15.323 -26.972-104.699 1.00 51.33 B
ATOM 7580 C VAL B 329 -13.627 -29.367-102.207 1.00 52.54 B
ATOM 7581 O VAL B 329 -14.526 -30.189-101.991 1.00 52.36 B
ATOM 7582 N CYS B 330 -12.513 -29.299-101.476 1.00 51.68 B
ATOM 7583 CA CYS B 330 -12.281 -30.186-100.339 1.00 50.73 B
ATOM 7584 C CYS B 330 -13.086 -29.867 -99.073 1.00 49.82 B
ATOM 7585 O CYS B 330 -13.197 -30.711 -98.177 1.00 49.21 B
ATOM 7586 CB CYS B 330 -10.793 -30.214 -99.991 1.00 51.73 B
ATOM 7587 SG CYS B 330 -9.879 -31.608-100.722 1.00 56.85 B
ATOM 7588 N HIS B 331 -13.677 -28.722 -99.015 1.00 48.53 B
ATOM 7589 CA HIS B 331 -14.384 -28.426 -97.857 1.00 47.51 B
ATOM 7590 CB HIS B 331 -15.081 -27.156 -98.028 1.00 47.42 B
ATOM 7591 CG HIS B 331 -15.269 -26.421 -96.761 1.00 48.71 B
ATOM 7592 CD2 HIS B 331 -14.379 -25.859 -95.937 1.00 49.23 B
ATOM 7593 ND1 HIS B 331 -16.496 -26.179 -96.217 1.00 49.51 B
ATOM 7594 CE1 HIS B 331 -16.352 -25.488 -95.116 1.00 50.21 B
ATOM 7595 NE2 HIS B 331 -15.075 -25.282 -94.925 1.00 50.01 B
ATOM 7596 C HIS B 331 -15.419 -29.410 -97.700 1.00 46.60 B
ATOM 7597 O HIS B 331 -16.098 -29.664 -98.597 1.00 47.48 B
ATOM 7598 N ALA B 332 -15.619 -29.888 -96.497 1.00 44.75 B
ATOM 7599 CA ALA B 332 -16.676 -30.834 -96.132 1.00 42.81 B
ATOM 7600 CB ALA B 332 -16.539 -31.213 -94.665 1.00 43.46 B
ATOM 7601 C ALA B 332 -18.090 -30.321 -96.408 1.00 41.54 B
ATOM 7602 O ALA B 332 -18.446 -29.222 -95.992 1.00 41.71 B
ATOM 7603 N SER B 333 -18.896 -31.140 -97.086 1.00 39.95 B
ATOM 7604 CA SER B 333 -20.257 -30.753 -97.430 1.00 39.34 B
ATOM 7605 CB SER B 333 -20.259 -30.102 -98.810 1.00 40.07 B
ATOM 7606 OG SER B 333 -19.181 -29.192 -98.943 1.00 43.13 B
ATOM 7607 C SER B 333 -21.255 -31.916 -97.426 1.00 38.72 B
ATOM 7608 O SER B 333 -20.891 -33.061 -97.680 1.00 38.19 B
ATOM 7609 N ALA B 334 -22.517 -31.596 -97.142 1.00 37.76 B
ATOM 7610 CA ALA B 334 -23.603 -32.570 -97.109 1.00 37.28 B
ATOM 7611 CB ALA B 334 -24.260 -32.577 -95.740 1.00 36.47 B
ATOM 7612 C ALA B 334 -24.609 -32.155 -98.175 1.00 37.54 B

ATOM 7613 O ALA B 334 -25.140 -31.048 -98.145 1.00 37.40 B
ATOM 7614 N TRP B 335 -24.886 -33.062 -99.106 1.00 38.33 B
ATOM 7615 CA TRP B 335 -25.784 -32.766-100.214 1.00 38.41 B
ATOM 7616 CB TRP B 335 -25.072 -33.078-101.528 1.00 36.68 B
ATOM 7617 CG TRP B 335 -23.803 -32.344-101.716 1.00 34.64 B
ATOM 7618 CD2 TRP B 335 -23.491 -31.434-102.776 1.00 33.48 B
ATOM 7619 CE2 TRP B 335 -22.163 -31.004-102.579 1.00 32.92 B
ATOM 7620 CE3 TRP B 335 -24.204 -30.942-103.879 1.00 31.95 B
ATOM 7621 CD1 TRP B 335 -22.690 -32.425-100.937 1.00 34.18 B
ATOM 7622 NE1 TRP B 335 -21.698 -31.622-101.447 1.00 33.45 B
ATOM 7623 CZ2 TRP B 335 -21.531 -30.105-103.446 1.00 30.94 B
ATOM 7624 CZ3 TRP B 335 -23.573 -30.049-104.738 1.00 29.75 B
ATOM 7625 CH2 TRP B 335 -22.252 -29.643-104.515 1.00 29.66 B
ATOM 7626 C TRP B 335 -27.152 -33.430-100.255 1.00 39.18 B
ATOM 7627 O TRP B 335 -27.277 -34.650-100.156 1.00 39.16 B
ATOM 7628 N ASP B 336 -28.174 -32.606-100.439 1.00 39.43 B
ATOM 7629 CA ASP B 336 -29.536 -33.097-100.551 1.00 40.41 B
ATOM 7630 CB ASP B 336 -30.440 -32.406 -99.530 1.00 41.21 B
ATOM 7631 CG ASP B 336 -31.906 -32.718 -99.739 1.00 40.90 B
ATOM 7632 OD1 ASP B 336 -32.222 -33.821-100.238 1.00 41.13 B
ATOM 7633 OD2 ASP B 336 -32.741 -31.858 -99.390 1.00 40.89 B
ATOM 7634 C ASP B 336 -30.034 -32.826-101.971 1.00 40.33 B
ATOM 7635 O ASP B 336 -30.460 -31.710-102.286 1.00 39.58 B
ATOM 7636 N PHE B 337 -29.964 -33.854-102.820 1.00 40.17 B
ATOM 7637 CA PHE B 337 -30.391 -33.765-104.211 1.00 39.82 B
ATOM 7638 CB PHE B 337 -29.944 -35.007-104.977 1.00 39.12 B
ATOM 7639 CG PHE B 337 -28.462 -35.079-105.214 1.00 41.00 B
ATOM 7640 CD1 PHE B 337 -27.590 -35.400-104.183 1.00 41.73 B
ATOM 7641 CD2 PHE B 337 -27.934 -34.845-106.486 1.00 41.52 B
ATOM 7642 CE1 PHE B 337 -26.202 -35.492-104.415 1.00 42.84 B
ATOM 7643 CE2 PHE B 337 -26.551 -34.932-106.730 1.00 41.63 B
ATOM 7644 CZ PHE B 337 -25.686 -35.258-105.694 1.00 42.07 B
ATOM 7645 C PHE B 337 -31.894 -33.561-104.421 1.00 40.14 B
ATOM 7646 O PHE B 337 -32.381 -33.664-105.544 1.00 40.24 B

ATOM 7647 N TYR B 338 -32.623 -33.269-103.348 1.00 40.23 B
ATOM 7648 CA TYR B 338 -34.064 -33.033-103.428 1.00 40.46 B
ATOM 7649 CB TYR B 338 -34.339 -31.613-103.920 1.00 40.63 B
ATOM 7650 CG TYR B 338 -34.168 -30.569-102.852 1.00 42.58 B
ATOM 7651 CD1 TYR B 338 -32.909 -30.059-102.535 1.00 42.35 B
ATOM 7652 CE1 TYR B 338 -32.751 -29.118-101.523 1.00 44.95 B
ATOM 7653 CD2 TYR B 338 -35.268 -30.114-102.129 1.00 44.11 B
ATOM 7654 CE2 TYR B 338 -35.126 -29.181-101.116 1.00 45.97 B
ATOM 7655 CZ TYR B 338 -33.867 -28.682-100.812 1.00 46.67 B
ATOM 7656 OH TYR B 338 -33.741 -27.755 -99.787 1.00 49.64 B
ATOM 7657 C TYR B 338 -34.865 -34.005-104.284 1.00 40.55 B
ATOM 7658 O TYR B 338 -35.784 -33.595-104.988 1.00 39.91 B
ATOM 7659 N ASN B 339 -34.524 -35.288-104.214 1.00 41.22 B
ATOM 7660 CA ASN B 339 -35.222 -36.316-104.978 1.00 40.28 B
ATOM 7661 CB ASN B 339 -34.327 -36.842-106.101 1.00 39.19 B
ATOM 7662 CG ASN B 339 -33.367 -37.923-105.630 1.00 40.19 B
ATOM 7663 OD1 ASN B 339 -32.890 -37.901-104.495 1.00 41.09 B
ATOM 7664 ND2 ASN B 339 -33.067 -38.869-106.511 1.00 40.47 B
ATOM 7665 C ASN B 339 -35.622 -37.473-104.065 1.00 40.95 B
ATOM 7666 O ASN B 339 -35.956 -38.549-104.545 1.00 42.00 B
ATOM 7667 N ARG B 340 -35.569 -37.247-102.751 1.00 40.55 B
ATOM 7668 CA ARG B 340 -35.928 -38.263-101.756 1.00 38.61 B
ATOM 7669 CB ARG B 340 -37.418 -38.598-101.850 1.00 37.99 B
ATOM 7670 CG ARG B 340 -38.348 -37.486-101.432 1.00 38.78 B
ATOM 7671 CD ARG B 340 -39.765 -37.719-101.942 1.00 39.23 B
ATOM 7672 NE ARG B 340 -39.840 -37.605-103.397 1.00 40.32 B
ATOM 7673 CZ ARG B 340 -39.741 -38.620-104.254 1.00 40.18 B
ATOM 7674 NH1 ARG B 340 -39.568 -39.865-103.828 1.00 41.25 B
ATOM 7675 NH2 ARG B 340 -39.803 -38.389-105.556 1.00 41.21 B
ATOM 7676 C ARG B 340 -35.141 -39.559-101.876 1.00 38.04 B
ATOM 7677 O ARG B 340 -35.444 -40.525-101.185 1.00 39.27 B
ATOM 7678 N ALA B 341 -34.135 -39.600-102.741 1.00 37.34 B
ATOM 7679 CA ALA B 341 -33.373 -40.830-102.902 1.00 37.80 B
ATOM 7680 CB ALA B 341 -33.865 -41.595-104.134 1.00 37.33 B

ATOM 7681 C ALA B 341 -31.872 -40.638-102.983 1.00 38.56 B
ATOM 7682 O ALA B 341 -31.129 -41.608-102.932 1.00 38.15 B
ATOM 7683 N ASP B 342 -31.416 -39.399-103.121 1.00 40.06 B
ATOM 7684 CA ASP B 342 -29.979 -39.154-103.190 1.00 41.24 B
ATOM 7685 CB ASP B 342 -29.578 -38.709-104.592 1.00 44.15 B
ATOM 7686 CG ASP B 342 -28.754 -39.755-105.313 1.00 48.05 B
ATOM 7687 OD1 ASP B 342 -27.670 -40.140-104.800 1.00 49.49 B
ATOM 7688 OD2 ASP B 342 -29.203 -40.195-106.394 1.00 50.22 B
ATOM 7689 C ASP B 342 -29.459 -38.150-102.170 1.00 40.07 B
ATOM 7690 O ASP B 342 -29.879 -36.990-102.144 1.00 39.33 B
ATOM 7691 N PHE B 343 -28.548 -38.621-101.320 1.00 39.08 B
ATOM 7692 CA PHE B 343 -27.927 -37.798-100.287 1.00 37.96 B
ATOM 7693 CB PHE B 343 -28.572 -38.005 -98.915 1.00 35.15 B
ATOM 7694 CG PHE B 343 -30.049 -38.169 -98.948 1.00 32.00 B
ATOM 7695 CD1 PHE B 343 -30.615 -39.398 -99.233 1.00 31.15 B
ATOM 7696 CD2 PHE B 343 -30.877 -37.100 -98.692 1.00 30.96 B
ATOM 7697 CE1 PHE B 343 -31.986 -39.559 -99.248 1.00 30.27 B
ATOM 7698 CE2 PHE B 343 -32.248 -37.255 -98.705 1.00 30.76 B
ATOM 7699 CZ PHE B 343 -32.802 -38.485 -98.988 1.00 30.63 B
ATOM 7700 C PHE B 343 -26.485 -38.248-100.189 1.00 38.67 B
ATOM 7701 O PHE B 343 -26.216 -39.438-100.022 1.00 37.95 B
ATOM 7702 N ARG B 344 -25.558 -37.303-100.284 1.00 39.83 B
ATOM 7703 CA ARG B 344 -24.148 -37.640-100.201 1.00 41.22 B
ATOM 7704 CB ARG B 344 -23.547 -37.733-101.606 1.00 42.87 B
ATOM 7705 CG ARG B 344 -24.269 -38.719-102.513 1.00 44.21 B
ATOM 7706 CD ARG B 344 -23.709 -38.691-103.915 1.00 43.81 B
ATOM 7707 NE ARG B 344 -24.775 -38.760-104.906 1.00 44.99 B
ATOM 7708 CZ ARG B 344 -24.606 -38.495-106.198 1.00 45.22 B
ATOM 7709 NH1 ARG B 344 -23.405 -38.148-106.656 1.00 44.57 B
ATOM 7710 NH2 ARG B 344 -25.646 -38.548-107.026 1.00 44.88 B
ATOM 7711 C ARG B 344 -23.389 -36.621 -99.375 1.00 40.59 B
ATOM 7712 O ARG B 344 -23.950 -35.634 -98.913 1.00 39.89 B
ATOM 7713 N ILE B 345 -22.103 -36.881 -99.193 1.00 40.09 B
ATOM 7714 CA ILE B 345 -21.239 -36.004 -98.429 1.00 39.84 B

ATOM 7715 CB ILE B 345 -20.988 -36.572 -96.996 1.00 39.20 B
ATOM 7716 CG2 ILE B 345 -19.737 -35.954 -96.382 1.00 37.70 B
ATOM 7717 CG1 ILE B 345 -22.212 -36.327 -96.105 1.00 38.01 B
ATOM 7718 CD1 ILE B 345 -22.082 -36.915 -94.712 1.00 35.06 B
ATOM 7719 C ILE B 345 -19.912 -35.890 -99.161 1.00 41.09 B
ATOM 7720 O ILE B 345 -19.270 -36.895 -99.448 1.00 40.89 B
ATOM 7721 N LYS B 346 -19.532 -34.698 -99.543 1.00 42.17 B
ATOM 7722 CA LYS B 346 -18.241 -34.408 -100.084 1.00 42.62 B
ATOM 7723 CB LYS B 346 -18.412 -33.216 -100.966 1.00 43.14 B
ATOM 7724 CG LYS B 346 -17.478 -33.017 -102.093 1.00 41.36 B
ATOM 7725 CD LYS B 346 -17.645 -31.641 -102.644 1.00 40.12 B
ATOM 7726 CE LYS B 346 -16.908 -30.643 -101.809 1.00 40.19 B
ATOM 7727 NZ LYS B 346 -17.817 -29.758 -101.032 1.00 40.18 B
ATOM 7728 C LYS B 346 -17.350 -33.982 -98.991 1.00 42.92 B
ATOM 7729 O LYS B 346 -17.640 -33.042 -98.354 1.00 42.56 B
ATOM 7730 N GLN B 347 -16.254 -34.673 -98.773 1.00 43.33 B
ATOM 7731 CA GLN B 347 -15.298 -34.289 -97.739 1.00 44.46 B
ATOM 7732 CB GLN B 347 -15.906 -34.548 -96.360 1.00 44.80 B
ATOM 7733 CG GLN B 347 -15.047 -34.105 -95.183 1.00 44.06 B
ATOM 7734 CD GLN B 347 -15.372 -34.878 -93.917 1.00 42.39 B
ATOM 7735 OE1 GLN B 347 -16.525 -35.221 -93.669 1.00 41.94 B
ATOM 7736 NE2 GLN B 347 -14.356 -35.149 -93.108 1.00 40.77 B
ATOM 7737 C GLN B 347 -13.991 -35.063 -97.863 1.00 45.51 B
ATOM 7738 O GLN B 347 -13.984 -36.289 -97.772 1.00 45.42 B
ATOM 7739 N CYS B 348 -12.890 -34.341 -98.063 1.00 47.24 B
ATOM 7740 CA CYS B 348 -11.572 -34.958 -98.193 1.00 48.99 B
ATOM 7741 C CYS B 348 -11.118 -35.454 -96.818 1.00 48.98 B
ATOM 7742 O CYS B 348 -10.122 -34.984 -96.274 1.00 50.46 B
ATOM 7743 CB CYS B 348 -10.568 -33.940 -98.769 1.00 50.32 B
ATOM 7744 SG CYS B 348 -11.070 -33.243 -100.389 1.00 55.08 B
ATOM 7745 N THR B 349 -11.860 -36.414 -96.272 1.00 48.36 B
ATOM 7746 CA THR B 349 -11.598 -36.986 -94.948 1.00 48.03 B
ATOM 7747 CB THR B 349 -12.613 -38.116 -94.624 1.00 47.41 B
ATOM 7748 OG1 THR B 349 -13.931 -37.569 -94.543 1.00 47.68 B

ATOM 7749 CG2 THR B 349 -12.281 -38.780 -93.305 1.00 46.30 B
ATOM 7750 C THR B 349 -10.200 -37.534 -94.656 1.00 48.19 B
ATOM 7751 O THR B 349 -9.771 -38.512 -95.258 1.00 47.84 B
ATOM 7752 N ALA B 350 -9.505 -36.896 -93.715 1.00 48.96 B
ATOM 7753 CA ALA B 350 -8.178 -37.336 -93.284 1.00 49.73 B
ATOM 7754 CB ALA B 350 -7.247 -36.143 -93.110 1.00 48.06 B
ATOM 7755 C ALA B 350 -8.410 -38.042 -91.940 1.00 50.47 B
ATOM 7756 O ALA B 350 -9.534 -38.042 -91.427 1.00 50.70 B
ATOM 7757 N VAL B 351 -7.379 -38.650 -91.362 1.00 50.83 B
ATOM 7758 CA VAL B 351 -7.578 -39.345 -90.094 1.00 51.04 B
ATOM 7759 CB VAL B 351 -6.838 -40.698 -90.073 1.00 50.51 B
ATOM 7760 CG1 VAL B 351 -7.245 -41.486 -88.839 1.00 49.37 B
ATOM 7761 CG2 VAL B 351 -7.154 -41.485 -91.331 1.00 50.03 B
ATOM 7762 C VAL B 351 -7.130 -38.512 -88.892 1.00 52.13 B
ATOM 7763 O VAL B 351 -5.961 -38.551 -88.502 1.00 52.31 B
ATOM 7764 N THR B 352 -8.080 -37.765 -88.321 1.00 53.15 B
ATOM 7765 CA THR B 352 -7.861 -36.899 -87.154 1.00 52.83 B
ATOM 7766 CB THR B 352 -7.609 -35.426 -87.563 1.00 53.24 B
ATOM 7767 OG1 THR B 352 -6.632 -35.375 -88.608 1.00 53.73 B
ATOM 7768 CG2 THR B 352 -7.100 -34.606 -86.357 1.00 54.03 B
ATOM 7769 C THR B 352 -9.127 -36.911 -86.302 1.00 52.77 B
ATOM 7770 O THR B 352 -10.203 -37.244 -86.796 1.00 52.27 B
ATOM 7771 N MET B 353 -9.008 -36.541 -85.028 1.00 52.71 B
ATOM 7772 CA MET B 353 -10.178 -36.513 -84.165 1.00 53.00 B
ATOM 7773 CB MET B 353 -9.789 -36.292 -82.702 1.00 54.58 B
ATOM 7774 CG MET B 353 -10.969 -36.446 -81.742 1.00 57.20 B
ATOM 7775 SD MET B 353 -10.547 -36.211 -79.998 1.00 61.27 B
ATOM 7776 CE MET B 353 -10.489 -34.369 -79.905 1.00 61.02 B
ATOM 7777 C MET B 353 -11.096 -35.392 -84.636 1.00 52.59 B
ATOM 7778 O MET B 353 -12.305 -35.578 -84.747 1.00 53.03 B
ATOM 7779 N ASP B 354 -10.564 -34.230 -84.896 1.00 52.62 B
ATOM 7780 CA ASP B 354 -11.327 -33.143 -85.480 1.00 52.72 B
ATOM 7781 CB ASP B 354 -10.393 -32.078 -86.034 1.00 55.53 B
ATOM 7782 CG ASP B 354 -10.377 -30.801 -85.232 1.00 58.02 B

DEMANDE OU BREVET VOLUMINEUX

LA PRÉSENTE PARTIE DE CETTE DEMANDE OU CE BREVET COMPREND PLUS D'UN TOME.

CECI EST LE TOME 1 DE 3
CONTENANT LES PAGES 1 À 314

NOTE : Pour les tomes additionels, veuillez contacter le Bureau canadien des brevets

JUMBO APPLICATIONS/PATENTS

THIS SECTION OF THE APPLICATION/PATENT CONTAINS MORE THAN ONE VOLUME

THIS IS VOLUME 1 OF 3
CONTAINING PAGES 1 TO 314

NOTE: For additional volumes, please contact the Canadian Patent Office

NOM DU FICHIER / FILE NAME :

NOTE POUR LE TOME / VOLUME NOTE:

CLAIMS

1. A crystal of the N-domain of ACE protein.

2. A crystal according to claim 1 wherein the N-domain of ACE protein is minimally glycosylated.

3. A crystal according to claim 2 wherein the N-domain of ACE protein is minimally glycosylated at amino acids 25, 45, 117, 289 and 480 of SEQ ID NO: 1.

4. A crystal according to any one of the preceding claims comprising atoms arranged in a spatial relationship represented by at least a portion of the structural co-ordinates set forth in Table A or Table B.

5. A crystal according to any one of the preceding claims wherein the crystal belongs to the space group $C222_1$.

7. A crystal according to any one of the preceding claims having unit cell dimensions of: a=101.12 Å, b=211.32 Å, c=171.27 Å.

8. A crystal according to any one of the preceding claims wherein the crystal is a crystal of the N-domain of human ACE protein.

9. A crystal according to any one of the preceding claims wherein the crystal further comprises a ligand bound to the N-domain of ACE protein or a portion thereof.

10. A crystal according to claim 9 wherein the ligand modulates the activity of N-domain of ACE protein.

11. A crystal according to claim 10 wherein the ligand is an inhibitor of the N-domain of ACE protein.

12. A crystal according to claim 11 wherein the inhibitor is lisinopril or a derivative thereof.

13. A crystal according to claim 12 comprising atoms arranged in a spatial relationship represented by at least a portion of the structural co-ordinates set forth in Table B.

14. A crystal according to claim 13 having unit cell dimensions of: a=101.32 Å, b=211.90 Å, c=171.03 Å.

15. A method of preparing a crystal of the N-domain of ACE protein comprising the steps of:

(a) culturing host cells comprising the N-domain of ACE protein;
(b) purifying the N-domain of ACE protein; and
(c) crystallising the N-domain of ACE protein.

16. A method according to claim 15 wherein the N-domain of ACE protein is crystallised using about 5 mM HEPES and about 0.1 mM PMSF with an equal volume of a reservoir solution containing about 0.2M lithium sulphate, 15 % PEG 4000, about 100 mM $CH_3COONa.3H_2O$ pH 4.9 and about 10 µM $ZnSO_4.7H_2O$.

17. A method according to any of claims 15 or 16 wherein the crystal that is prepared has a structure defined by at least a portion of the structural co-ordinates set forth in Table A.

18. A method according to any of claims 15 to 17 wherein the crystal belongs to the space group $C222_1$.

19. A method according to any of claims 15 to 18 wherein the crystal has the unit cell dimensions: a= 101.12 Å, b=211.32 Å and c=171.27 Å.

20. A method according to any of claims 15 to 19 wherein the N-domain of ACE protein is an N-domain of human ACE protein.

21. A method according to any of claims 15 to 20 wherein the N-domain of ACE protein is crystallised in the presence of a ligand.

22. A method according to claim 21 wherein the ligand is a modulator of the N-domain of ACE protein.

23. A method according to claim 22 wherein the ligand is an inhibitor of the N-domain of ACE protein.

24. A method according to claim 23 wherein the inhibitor of the N-domain of ACE protein is lisinopril or a derivative thereof.

25. A method according to claim 24 wherein the crystal that is prepared has a strusture defined by at least a portion of the structural co-ordinates set forth in Table B.

26. A method according to claim 25 wherein the crystal has unit cell dimensions: a= 101.32 Å, b=211.90 Å and c=171.03 Å.

27. A method according to claim 25 wherein the crystal is crystallised using about 5 mM HEPES and about 0.1 mM PMSF with an equal volume of a reservoir solution containing about 0.2M lithium sulphate, 18 % PEG 4000, about 100 mM $CH_3COONa.3H_2O$ pH 4.9 and about 10 µM $ZnSO_4.7H_2O$.

28. A method of screening for a modulator of the N-domain of ACE protein wherein the method comprises the use of a crystal according to any of claims 1-14.

29. A method according to claim 28 comprising the steps of:

(a) providing at least a portion of the structural co-ordinates set forth in Table A or Table B;

(b) employing at least a portion of the structural co-ordinates set forth in Table A or Table B to design or select or synthesise a putative modulator of the N-domain;

(c) contacting the putative modulator of the N-domain with the N-domain or a mutant, variant, homologue, derivative or fragment thereof in the presence of a substrate; and

(d) screening the putative modulator of the N-domain in an assay for the potential to modulate the N-domain.

30. A method of screening for a modulator of the C-domain of ACE protein wherein the method comprises the use of a crystal according to any of claims 1-14.

31. A method according to claim 30 comprising the steps of:

(a) providing at least a portion of the structural co-ordinates set forth in Table A or Table B;

(b) employing at least a portion of the structural co-ordinates set forth in Table A or Table B to design or select or synthesise a putative modulator of the C-domain of ACE protein;

(c) contacting the putative modulator of the C-domain with the C-domain or a mutant, variant, homologue, derivative or fragment thereof in the presence of a substrate; and

(d) screening the putative modulator of the C-domain in an assay for the potential to selectively modulate the C-domain.

32. A method according to any one of claims 29 or 31 wherein at least a portion of the structural co-ordinates set forth in Table A or Table B and/or the putative modulator of the N-domain of ACE protein or C-domain of ACE protein and/or the substrate are

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

33. A method according to claim 29, claim 31 or claim 32 wherein the putative N-domain modulator or the putative C-domain modulator is selected from a library of compounds.

34. A method according claim 29, claim 31 or claim 32 wherein the putative N-domain modulator or C-domain modulator is selected from a database.

35. A method according to any one of claims claim 28 to 31 wherein the putative N-domain modulator or C-domain modulator is designed *de novo*.

36. A method according to claim 29, claim 31 or claim 32 wherein the putative N-domain modulator or C-domain modulator is designed from a known ACE modulator.

37. A method according to claim 29, claim 31 or claim 32 wherein the design or selection of the putative N-domain modulator or C-domain modulator is performed in conjunction with computer modelling.

38. A method according to any of claims 28 to 37 wherein the selected N-domain modulator or C-domain modulator is useful in the prevention and/or treatment of an ACE protein related disorder.

39. A method according to claim 38 wherein the disorder is hypertension, myocardial infarction or congestive heart failure.

40. A process comprising the steps of:

(a) performing the method according to any of claims 28 to 38;

(b) identifying one or more modulators of the N-domain and/or C-domain; and

(c) preparing a quantity of those one or more N-domain and/or C-domain modulators.

41. A process comprising the steps of:

(a) performing the method according to any of claims 28 to 38;

(b) identifying one or more N-domain and/or C-domain modulators; and

(c) preparing a pharmaceutical composition comprising those one or more identified N-domain modulators.

42. A process comprising the steps of:

(a) performing the method according to any of claims 28 to 38;

(b) identifying one or more N-domain and/or C-domain modulators;

(c) modifying those one or more N-domain and/or C-domain modulators; and

(d) optionally preparing a pharmaceutical composition comprising those one or more N-domain and/or C-domain modulators.

43. A method of obtaining structural information about a molecule or a molecular complex of unknown structure by using at least a portion of the structural co-ordinates set forth in N-domain of ACE protein, comprising the steps of:

(a) generating X-ray diffraction data from a crystallised molecule or molecular complex;

(b) applying at least a portion of the structure co-ordinates of the N-domain to said X-ray diffraction pattern to generate a three dimensional electron density map of at least a portion of the molecule or molecular complex; and

(c) using all or a portion of the structural co-ordinates set forth in N-domain to generate homology models of the N-domain of ACE protein.

44. A method according to claim 43 wherein the structure co-ordinates of the N-domain of ACE protein are used for domain co-operativity studies.

45. The N-domain of ACE protein modulator and/or the C-domain of ACE protein modulator identified by the method of any of claims 28 to 38.

46. The N-domain of ACE protein modulator according to claim 45 wherein the modulator inhibits the N-domain of the ACE protein.

47. The C-domain of ACE protein modulator according to claim 45 wherein the modulator inhibits the C-domain of ACE protein.

48. A pharmaceutical composition comprising the N-domain of ACE protein modulator and/or the C-domain of ACE protein modulator according to any one of claims 45 to 47 and a pharmaceutically acceptable carrier, diluent, excipient or adjuvant or any combination thereof.

49. A method of preventing and/or treating an ACE related disorder comprising administering a modulator of the N-domain and/or C-domain according to any of claims 45 to 47 and/or a pharmaceutical composition according to claim 48 wherein said modulator or said composition is capable of causing a beneficial, preventative and/or therapeutic effect.

50. A computer for producing a three-dimensional representation of N-domain of ACE protein wherein said computer comprises:

(a) a computer-readable data storage medium comprising a data storage material encoded with computer-readable data, wherein said data comprises the structure co-ordinates of the N-domain;

(b) a working memory for storing instructions for processing said computer-readable data;

(c) a central-processing unit coupled to said working memory and to said computer-readable data storage medium for processing said computer-machine readable data into said three-dimensional representation; and

(d) a display coupled to said central-processing unit for displaying said three-dimensional representation.

51. A machine-readable data storage medium comprising a data storage material encoded with machine readable data, wherein the data is defined by at least a portion of the structural co-ordinates of the N-domain of ACE protein set forth in Table A or Table B.

52. Use of the N-domain of ACE protein crystal in the preparation of a medicament to prevent and/or treat an ACE related disorder.

53. Use according to claim 52 wherein the disorder is hypertension, myocardial infarction or congestive heart failure.

54. Use of at least a portion of the structural co-ordinates set forth in Table A or Table B to screen for modulators of the N-domain of ACE protein and/or the C-domain of the ACE protein.

55. Use of at least a portion of the structural co-ordinates set forth in Table A or Table B to solve the structure of the crystalline form of any other protein with significant amino acid sequence homology to any functional domain of the N-domain of ACE protein.

56. Use of at least a portion of the structural co-ordinates set forth in Table A or Table B in molecular design techniques to design, select and synthesise modulators of the N-domain of ACE protein and/or the C-domain of ACE protein.

57. Use of at least a portion of the structural co-ordinates set forth in Table A or Table B in the development of compounds that can isomerise to reaction intermediates in the chemical reaction of a substrate or other compound that binds to the N-domain of ACE protein and/or the C-domain of ACE protein.

58. Use of at least a portion of the structural co-ordinates set forth in Table A or Table B to screen small molecule databases for chemical entities or compounds that modulate the N-domain of ACE protein or the C-domain of ACE protein.

59. Use of at least a portion of the structural co-ordinates set forth in Table A or Table B to solve the structure of the crystalline form of any other domain with significant amino acid sequence homology to any functional domain of the N-domain of ACE protein.

60. Use according to claim 59 wherein the structure of the crystalline form of any other domain with significant amino acid sequence homology to any functional domain of the N-domain of ACE protein is solved using molecular replacement.

61. Use of at least a portion of the structural co-ordinates set forth in Table A or Table B to identify the binding site of any modulator of the N-domain of ACE protein.

62. Use according to claim 61 wherein the binding site is that of lisinopril or derivatives thereof.

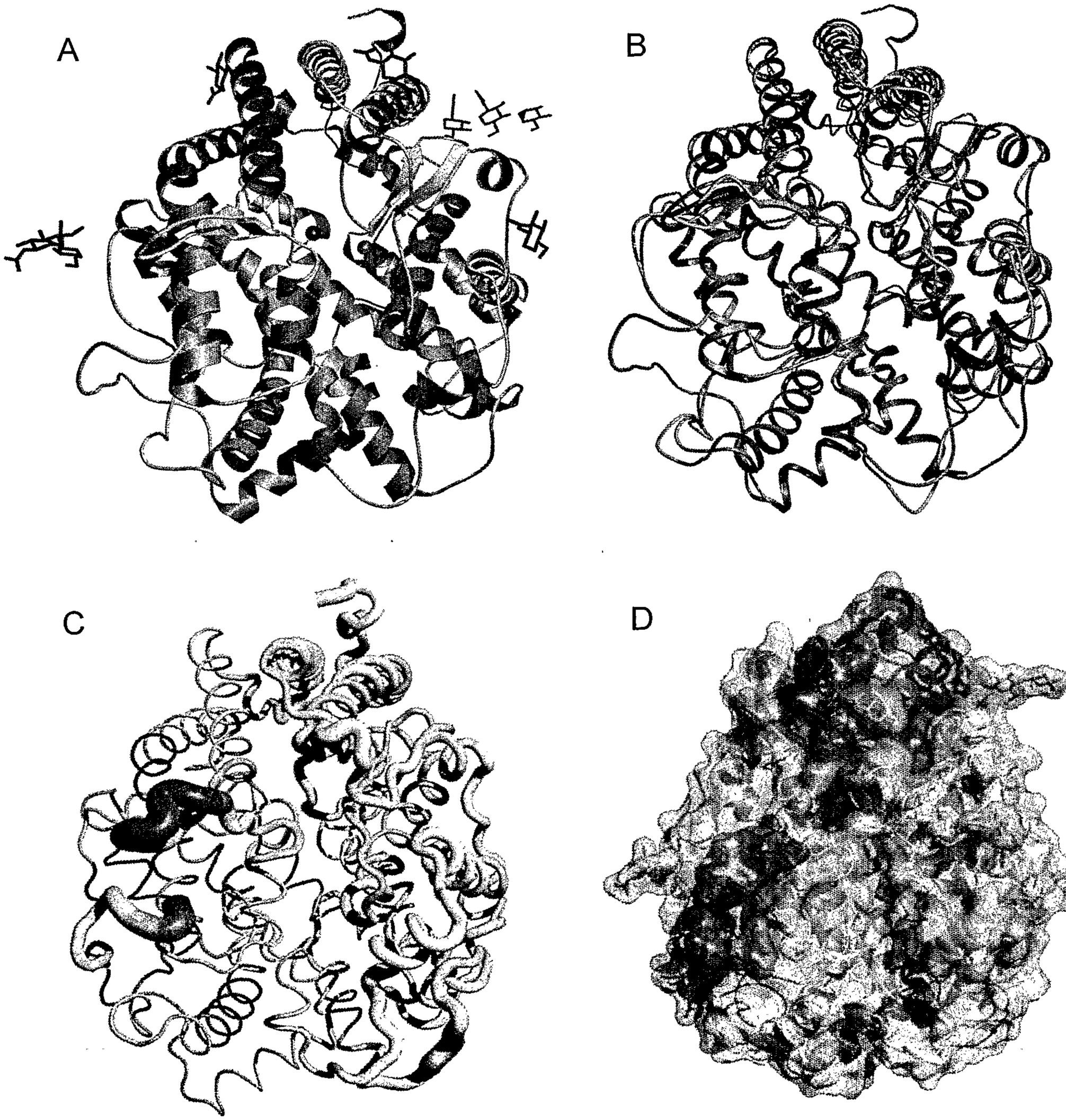


FIG. 1

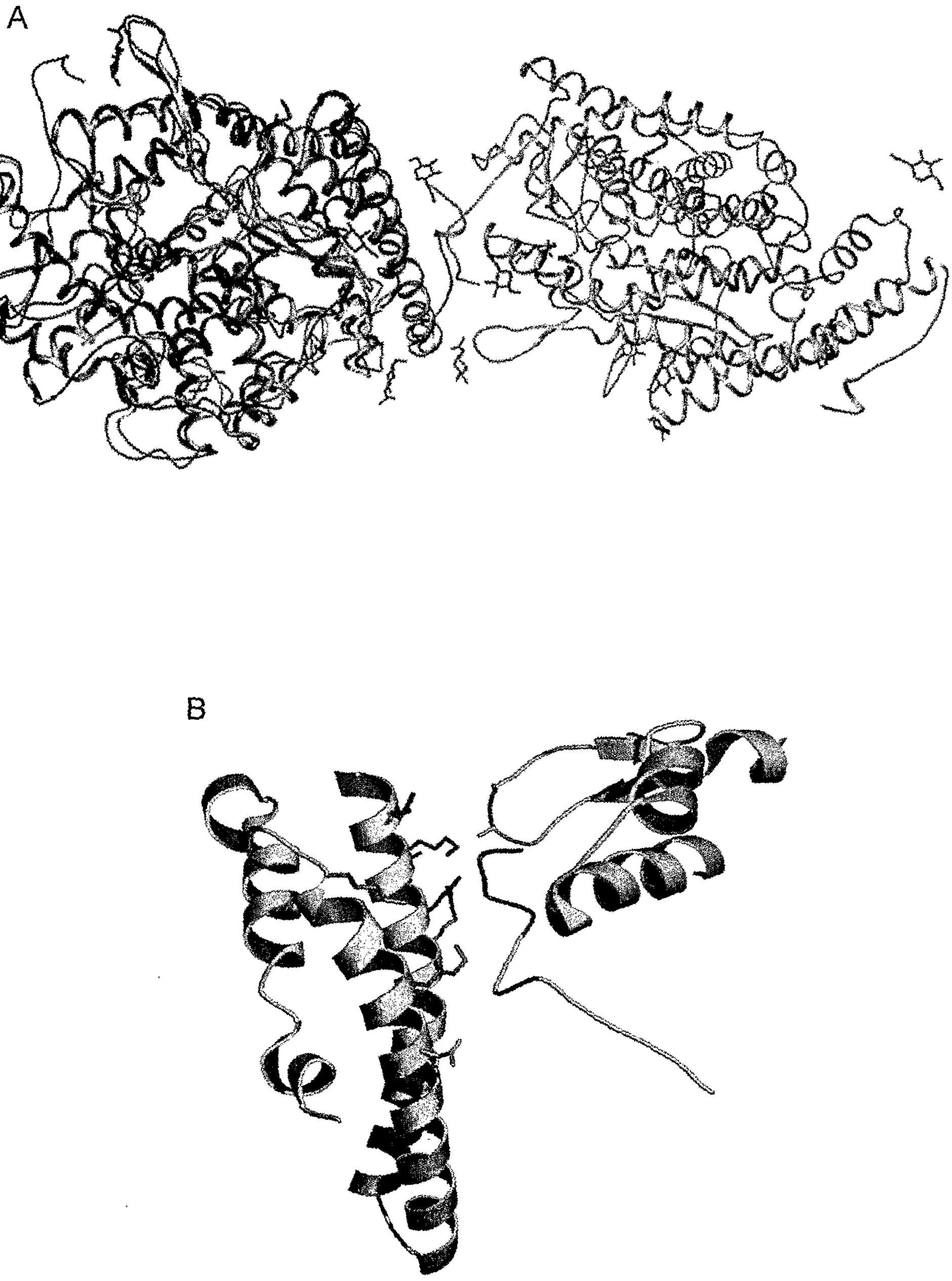


FIG. 2

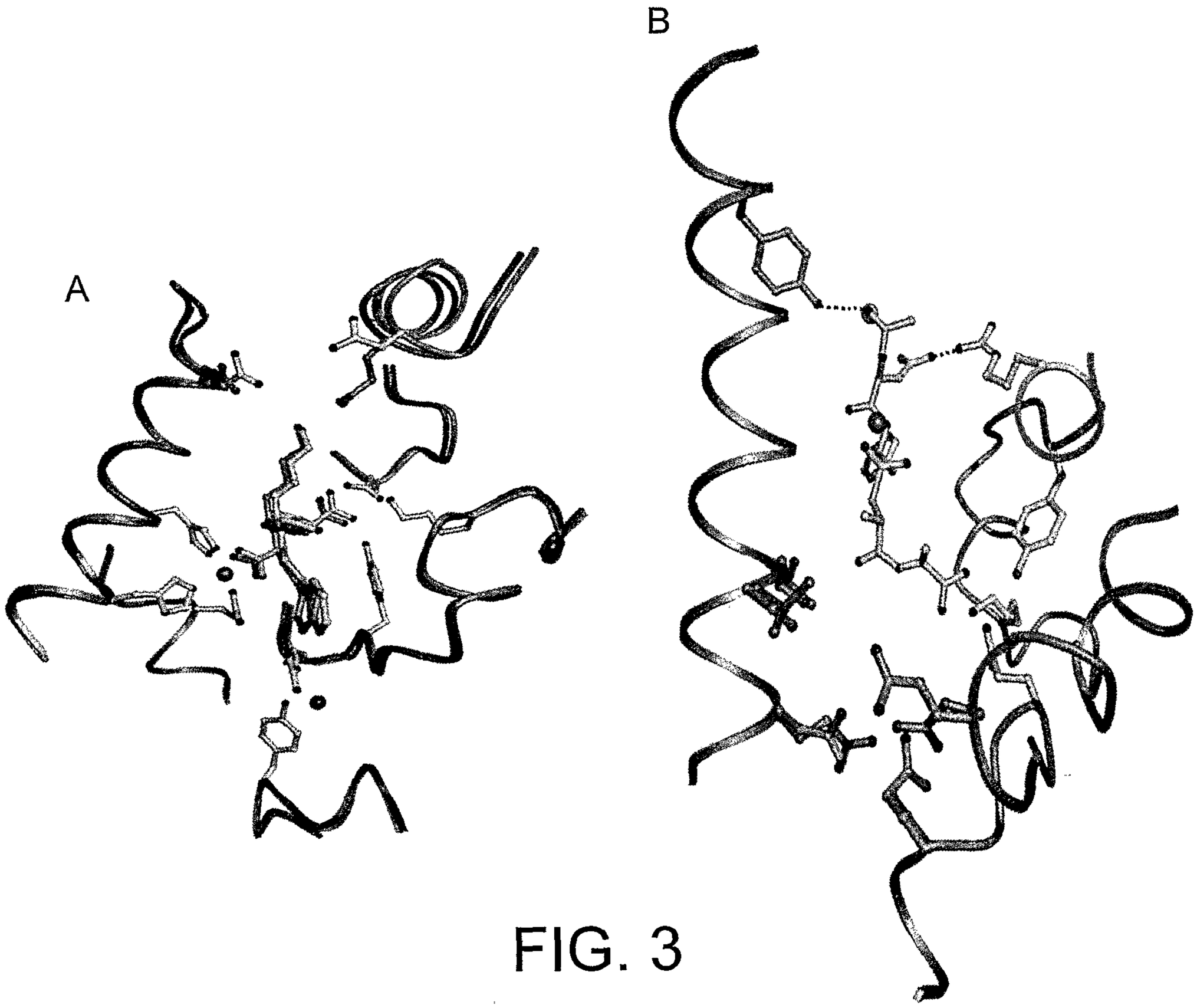


FIG. 3

```
                    H1                                  α2                                                  α3
N domain   1    LDPGLQPGNFSADEAGAQLFAQSYNSSAEQVLFQSVAASWAHDTNITAENARRQEEAALLSQE
tACE       37   ---------LVTDEAEASKFVEEYDRTSQVVWNEYAEANWNYNTNITTETSKILLQKNMQIAN
ACE2       18   ---------QSTIEEQAKTFLDKFNHEAEDLFYQSSLASWNYNTNITEENVQNMNNAGDKWSA

                                        α4              H5              α6
N domain   64   FAEAWGQKAKELYEPIWQNFTDPQLRRIIGAVRTLGSANLPLAKRQQYNALLSNMSRIYSTAK
tACE       91   HTLKYGTQARKEDVNQLQ---NTTLKRIIKKVQDLERAALPAQELEEYNKILLDMETTYSVAI
ACE2       72   FLKEQSTLAQMYPLQETQN---LTVKLQLQALQQNGSSVLSEDKSKRLNTILNTMSTIYSTGK

                  β1          β2          α7                                  α8
N domain   127  VCLPNKTATCWSLDPDLTNILASSRSYAMLLFAWEGWHNAAGIPLKPLYEDFTALSNEAYKQD
tACE       151  VCHPNG--SCLQLEPDLTNVMATSRKYEDLLWAWEGWRDKAGRAILQFYPKYVELINQAARLN
ACE2       132  VCNPDNPQECLLLEPGLNEIMANSLDYNERLWAWESWRSEVGKQLRPLYEEYVVLKNEMARAN

                          α/H9                                  α10
N domain   190  GFTDTGAYWRSWYNSP----------TFEDDLEHLYQQLEPLYLNLHAFVRRALHRRYGDRYI
tACE       212  GYVDAGDSWRSMYETP----------SLEQDLERLFQELQPLYLNLHAYVRRALHRHYGAQHI
ACE2       195  HYEDYGDYWRGDYEVNGVDGYDYSRGQLIEDVEHTFEEIKPLYEHLHAYVRAKLMNAYPS-YI

                          β3                H/α11                H/α12          α13
N domain   243  NLRGPIPAHLLGDMWAQSWENIYDMVVPFPDKPNLDVTSTMLQQGWNATHMFRVAEEFFTSLE
tACE       265  NLEGPIPAHLLGNMWAQTWSNIYDLVVPFPSAPSMDTTEAMLKQGWTPRRMFKEADDFFTSLG
ACE2       257  SPIGCLPAHLLGDMWCRFWTNLYSLTVPFGQKPNIDVTDAMVDQAWDAQRIFKEAEKFFVSVG

                                  α14                     β4          β5              α15
N domain   306  LSPMPPEFWEGSMLEKPADGREVVCHASAWDFYNRKDFRIKQCTRVTMDQLSTVHHEMGHIQY
tACE       328  LLPVPPEFWNKSMLEKPTDGREVVCHASAWDFYNCKDFRIKQCTTVNLEDLVVAHHEMGHIQY
ACE2       320  LPNMTQGFWENSMLTDPGNVQKAVCHPTAWDLGK-GDFRILMCTKVTMDDFLTAHHEMGHIQY

                            H16             α17             α18                 α19
N domain   369  YLQYKDLFVSLRRGANPGPHEAIGDVLALSVSTPEHLHKIGLLDRVTN-DTSSDINYLLKMAL
tACE       391  FMQYKDLPVALREGANPGFHEAIGDVLALSVSTPKHLHSLNLLSSEGG-SDEHDINFLMKMAL
ACE2       382  DMAYAAQPFLLRNGANEGFHEAVGEIMSLSAATPKHLKSIGLLSPDFQEDNETEINFLLKQAL

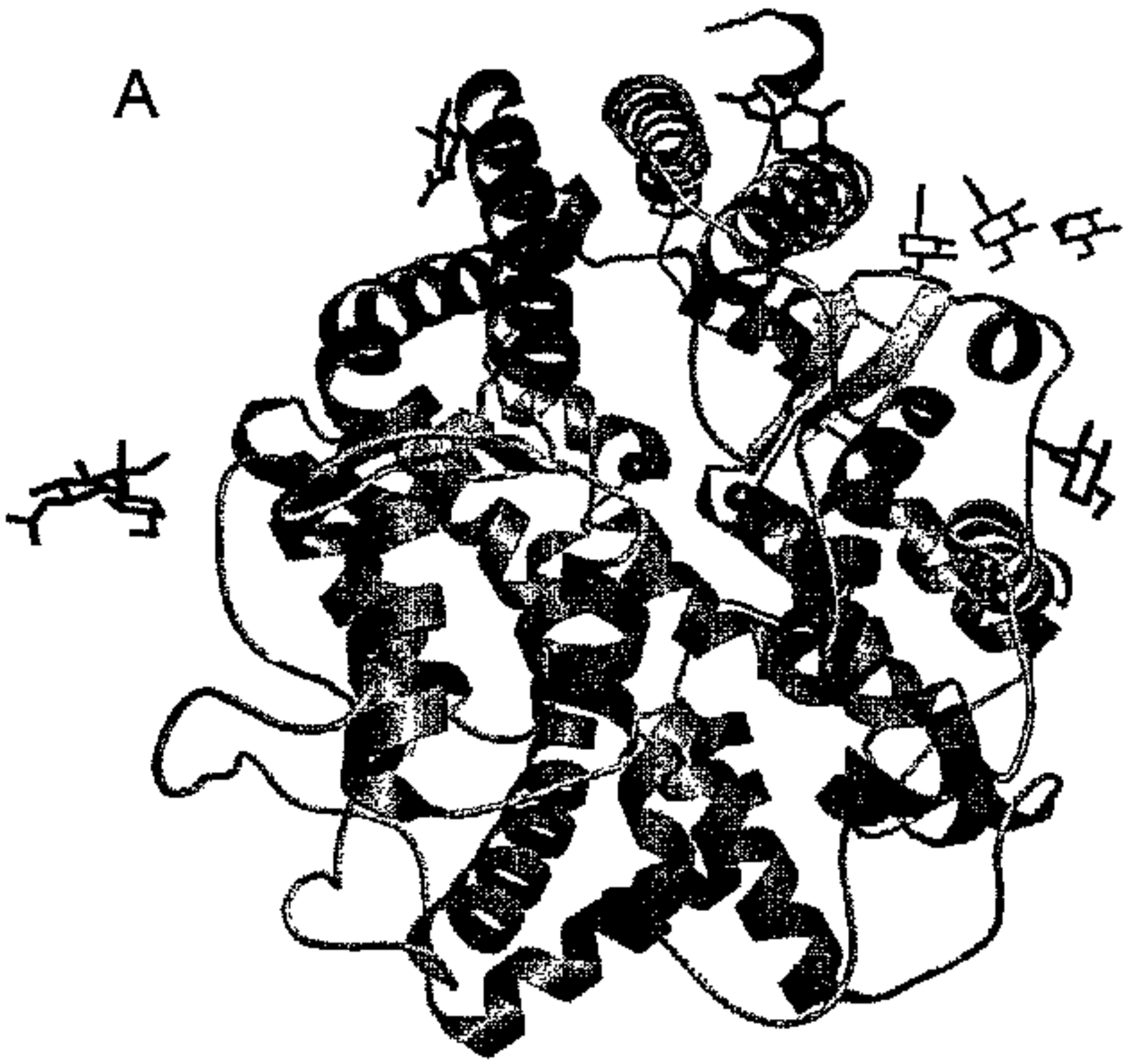
                          α20                         H/α21       β6          H22
N domain   431  EKIAFLPFGYLVDQWRWGVFSGRTPPSRYNFDWWYLRTKYQGICPPVTRNETHFDAGAKFHVP
tACE       453  DKIAFIPFSYLVDQWRWRVFDGSITKENYNQEWWSLRLKYQGLCPPVPRTQGDFDPGAKFHIP
ACE2       445  TIVGTLPFTYMLEKWRWMVFKGEIPKDQWMKKWWEMKREIVGVVEPVPHDETYCDPASLFHVS

                          α23                         H24             α25             α26
N domain   494  NVTPYIRYFVSFVLQFQFHEALCKEAGYEGPLHQCDIYRSTKAGAKLRKVLQAGSSRPWQEVL
tACE       516  SSVPYIRYFVSFIIQFQFHEALCQAAGHTGPLHKCDIYQSKEAGQRLATAMKLGFSRPWPEAM
ACE2       508  NDYSFIRYYTRTLYQFQFQEALCQAAKHEGPLHKCDISNSTEAGQRLFNMLRLGKSEPWTLAL

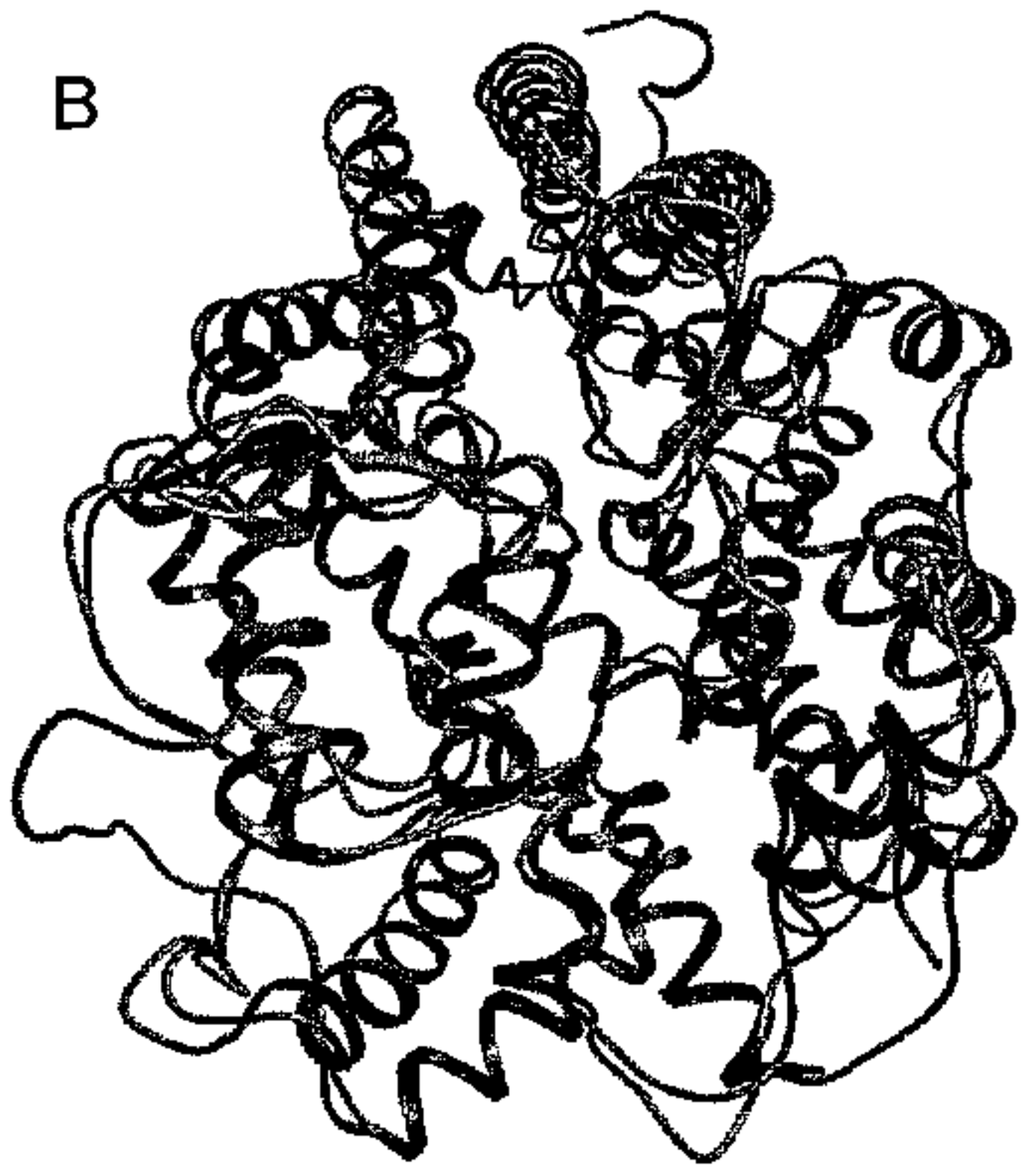
                                  α27
N domain   557  KDMVGLDALDAQPLLKYFQPVTQWLQEQNQQNGEVLGWPEYQWHPPLPDNTPESED      612
tACE       579  QLITGQPNMSASAMLSYFKPLLDWLRTENELHGEKLGWPQYNWTPNS---------      626
ACE2       571  ENVVGAKNMNVRPLLNYFEPLFTWLKDQNKN-SFVGWST-DWSPYAD---------      615
```

FIG. 4

A



B



C



D

