Physiological, structural and functional analysis of the paralogous cation-proton antiporters of NhaP type from *Vibrio cholerae*

by

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Abstract

The genome of *Vibrio cholerae* contains three structural genes for the NhaP-type antiporters paralogues Vc-NhaP1, 2 and 3 supposedly mediating exchange of K^+ and or Na^+ for protons across the membrane. Individual biochemical and physiological properties of these ion exchangers were analyzed in the presented work. Phenotype analysis of engineered chromosomal *Vc-nhaP1, Vc-nhaP2* and *Vc-nhaP3* deletion mutants and complementation of each isoform *in trans* reported in this thesis, has proven that the three NhaP paralogues are essential for maintaining K^+ homeostasis in the cytoplasm of *V. cholerae* in the cell is *in vivo*. Expressed *in trans*, neither of the Vc-NhaP paralogues was able to complement the severe potassium-sensitive phenotype of the triple deletion mutant completely. The wild type *V. cholerae* had much higher survival rates compared to the triple deletion mutant, VcΔNhaP123, when challenged by HCl (pH 3.5). We therefore suggested that Vc-NhaP paralogues might play a role in the Acid Tolerance Response (ATR) of *V. cholerae* as it passes through the gastric acid barrier of the stomach. Comparison of the biochemical properties of Vc-NhaP isoforms revealed that Vc-NhaP2 is the most active among all three paralogues. In the course of extensive mutagenesis experiments, we have identified a number of functionally critical residues. In particular, we found that mutation of Gly159 to Ala renders Vc-NhaP2 able to exchange Li^+ for protons, introducing a completely new activity. A structural analysis of Vc-NhaP2 based on the mutagenesis data combined with the *in silico* structure modelling and Molecular Dynamics Simulations yielded information regarding two important elements in the organization of Vc-NhaP2: (1) a putative cation binding pocket formed by antiparallel extended regions of two transmembrane segments (TMSs V/XII) crossing each other in the middle of the membrane, and (2) a cluster of amino acid residues near the putative cation binding pocket possibly determining the ion selectivity. The detailed structural analysis also

illuminated the possible intra-molecular events comprising the catalytic cycle of Vc-NhaP2 antiporter.

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List of Abbreviations

ATR	Acid Tolerance Response
CPA	Cation Proton Antiporter family
FAD	flavin adenine dinucleotide
MD	Molecular Dynamics simulation
NAD	nicotinamide adenine dinucleotide
TMS	transmembrane segment
BLAST	basic local alignment search tool
BTP	Bis-Tris propane
DTT	1,4-dithiothreitol
NQR	NADH:quinone oxidoreductase
ORF	Open reading frame
PMSF	phenylmethanesulfonyl fluoride
ΔpH	pH difference across the membrane
ΔpK	chemical gradient of K^+ across the membrane
OD	optical density

Chapter 1. Literature review

1.1 Introduction

Cation/proton antiporters are integral membrane proteins found in all domains of life. They are crucial for maintaining cellular homeostasis [1,2], regulation of cellular volume by primarily exchanging monovalent cations such as K^+ (and/or Na^+) for H^+ across the membrane, resistance to elevated levels of cations (Na^+ or K^+) in the medium [3], and the establishment of Na^+ gradient across the membrane [4]. The latter is of great importance in bacterial energetics, as it is a major energy source for the rotation of bacterial flagellum as seen, for example, in a well-studied case of the polar flagellar motor of *V. cholerae* [5-7]. Since Peter Mitchell postulated the presence of 'housekeeping' Na^+/H^+ antiporters in 1961 [8], extensive work has been done on these proposed antiporters. Examples of well and extensively characterized Na^+/H^+ antiporters are the NhaA from *Escherichia coli* (Ec-NhaA), which facilitates the removal of Na^+ and Li^+ from the cells at alkaline pH [9,10]; the NHE (Na^+/H^+ exchangers) in humans that participate in the regulation of cell volume, pH, intracellular sodium concentration and for the reabsorption of Na^+ across renal, intestinal, and other epithelia [11, 12]; NHXs from plants, which are essential for salt tolerance [13] and NhaP1 from archaea that are involved in internal pH homeostasis [14-15].

Bacteria typically possess more than one type of cation/proton antiporter. For example, the genome of *Vibrio cholerae* contains at least eleven open reading frames annotated as structural genes for Na^+/H^+ antiporters [16-17]. The presence of these Na^+/H^+ antiporters in multiple numbers indicates the significance of these membrane proteins. Indeed, they are important in maintaining internal pH homeostasis, ion balance, osmoregulation and are involved in various physiological functions [18,25]. Dysregulation of mammalian Na^+/H^+ exchanger isoform 1 (NHE1) has been shown to be associated with heart disease and cancer [19-20]. It has been shown

that chemical inhibition of NHE1 along with paclitaxel therapy resulted in a significant decrease in the invasive and migratory behavior of breast cancer cells, indicating the potential of using NHE1 as a novel co-adjuvant target in combination with paclitaxel therapy to enhance the efficacy of breast cancer treatment [20]. In bacteria, the sodium motive force generated by the Na^+/H^+ antiporters along with the primary Na^+ pump, Na^+-translocating NADH:ubiquinone oxidoreductase (Na^+-NQR) is believed to influence the virulence traits in *V. cholerae* [6-7]. In this species, the expression of the major virulence factors, cholera toxin (CT) and toxin co-regulated pilus (TCP) is influenced by the fluctuation of Na^+ gradient across the membrane [6-7, 16].

Alongside Na^+/H^+ antiporters, Peter Mitchell also postulated the presence of antiporters mediating K^+/H^+ transmembrane ion exchange. However, the investigated protein systems that are responsible for K^+/H^+ exchange have shown transporting activity only under high levels of stress, such as, when the cell is under elevated hypoosmotic stress or in the event of elevated intracellular K^+ levels [2]. No 'housekeeping' prokaryotic K^+/H^+ antiporters had been discovered in bacteria before 2006. Then in 2006 Radchanko and coworkers reported the first possible K^+/H^+ antiporter [21-22]. This NhaP2 antiporter was identified from the bacterium *Vibrio parahaemolyticus,* which showed a barely detectable activity with K^+ as a translocation substrate. Unfortunately, the authors did not examine whether the chromosomal deletion of the *nhaP2* gene would result in a potassium-sensitive phenotype. Led by this experiment, in 2010 Resch *et al.* carried out a much more extensive study on antiporters of *V. cholerae* that exclusively transport K^+ [23]. The deletion of the *Vc-nhaP2* gene resulted in a potassium sensitive phenotype at acidic pH [23]. Moreover, Vc-NhaP2 was able to catalyze the exchange of K^+, Na^+ and Rb^+ for H^+ *in vitro* [23]. *In vivo,* however, it operates as a true Mitchellian K^+/H^+ antiporter that is able to protect growing cells of *V. cholerae* at pH 6.0 from high K^+ concentrations in the environment [23]. The genome of *V. cholerae* also

contains two other NhaP paralogues, Vc-NhaP1 and NhaP3, which have been extensively characterized biochemically as well as physiologically [24-25].

V. cholerae is the causative agent of the acute life-threatening diarrheal disease, cholera and is considered as an 'emerging and re-emerging' disease [123] with both epidemic and pandemic potential. The cholera toxin (CT), an enterotoxin produced by the pathogenic *V. cholerae,* is responsible for causing acute diarrhea by creating an electrolyte imbalance in infected individuals. Patients (both adult and children) usually die from excessive dehydration [123].

V. cholerae is transmitted by the fecal-oral route and it is exposed to a wide range of environmental challenges. As such, it must adapt efficiently to changes in the ionic composition of its micro-surroundings, especially after being ingested by humans, since it has to pass through the low pH and high potassium [60-61] stomach gastric acid barrier before reaching the small intestine for colonization and secretion of the cholerae toxin [55]. *V. cholerae* possesses an Acid Tolerance Response (ATR) to overcome and survive within this hostile environment [56-59]. This survival system has been shown to be composed of a complex cascade of proteins, among which are several inducible amino acid decarboxylases [56-59]. Our findings suggest that Vc-NhaP1, 2 and 3 might be also involved in the ATR of *V. cholerae* and essential for the survival of *V. cholerae* in the low pH and high potassium condition of the gastric acid barrier ([25], discussed in Chapter 3 of the thesis).

Given the possible role of Vc-NhaP type antiporters in the ATR of *V. cholerae,* we hypothesize that Vc-NhaP type antiporters might be good targets for development of antimicrobials against *V. cholerae*. The structural, functional and dynamics analysis of Vc-NhaP type antiporters will be important for development of prospective antimicrobials targeting these antiporters. As Vc-NhaP2 is the major component among the three Vc-NhaP-type antiporters, we

carried out detailed structural and functional analysis of Vc-NhaP2 by combining *in silico* structure modeling, Molecular Dynamics Simulations and extensive mutagenesis experiments to determine the possible amino acid residues involved in ion transport and determining the ion selectivity ([32, 35], discussed in Chapters 4 and 5 of the thesis). The physiological, structural and functional studies of all the three *V. cholerae* paralogous, Vc-NhaP1,2 and 3 are reviewed in the following section, and this work was published by Mourin, M *et al.* 2019 [26].

Physiological, structural and functional analysis of the paralogues cation-proton antiporters of NhaP type from *Vibrio cholerae*

Authors' contributions

Conceptualization, Dibrov, P. and O'Neil, J.; methodology, O'Neil, J. and Hausner, G.; software, Wai, A; validation, Mourin, M., O'Neil, J. and Hausner, G.; investigation, Mourin, M.; writing—original draft preparation, Mourin, M.; writing—review and editing, Dibrov, P., O'Neil, J. and Mourin, M.; visualization, Mourin, M.; supervision, Dibrov, P.

1.2 Abstract

The transmembrane K^+/H^+ antiporters of NhaP type of *Vibrio cholerae* (Vc-NhaP1, 2, and 3) are critical for maintenance of K^+ homeostasis in the cytoplasm. The entire functional NhaP group is indispensable for the survival of *V. cholerae* at low pHs suggesting their possible role in the Acid Tolerance Response (ATR) of *V. cholerae*. Our findings suggest that the Vc-NhaP123 group, and especially its major component, Vc-NhaP2, might be a promising target for the development of novel antimicrobials by narrowly targeting *V. cholerae* and other NhaP-expressing pathogens. On the basis of Vc-NhaP2 *in silico* structure modeling, Molecular Dynamics Simulations and extensive mutagenesis studies we suggest that the ion-motive module of Vc-NhaP2 is comprised of two functional regions: (i) a putative cation-binding pocket that is formed

by antiparallel unfolded regions of two transmembrane segments (TMSs V/XII) crossing each other in the middle of the membrane, known as the NhaA fold, and (ii) a cluster of amino acids determining the ion selectivity.

1.3 Introduction

Vibrio cholerae encodes for an elaborate set of membrane cation-proton antiporters that are responsible for the circulation of alkali cations Na^+ and K^+ [16,27]. These secondary ion pumps play a key role in ion and pH homeostasis. In particular, *V. cholerae* encodes three NhaP type antiporters, encoded by paralogous structural genes *Vc-nhaP1, 2* and *3*, mediating the exchange of K^+ and Na^+ for protons [17,23]. We found that all three Vc-NhaP-type antiporters exchange K^+ for H^+ *in vivo* and operate in concert to maintain the viability of *V. cholerae* cells in acidic, especially K^+-rich environments [25]. Vc-NhaP2 seems to be a major component of this trio [5]. At the physiological level, the importance of the entire NhaP group for survival of *V. cholerae* at low pHs indicated its possible role at the critical step of the natural infectious process, when ingested *V. cholerae* passes the gastric acid barrier. Therefore, the Vc-NhaP123 group, and especially Vc-NhaP2 might be promising targets for the development of novel antimicrobials by narrowly targeting *V. cholerae* and other NhaP-expressing pathogens [25].

The NhaP type antiporters belong to the phylogenetically diverse cation/proton antiporter superfamily (CPA1) that includes the pharmacologically important NHEs, NHXs from plants, NhaP1 from archaea, and others [11,13-15,17,19-20,29-30]. The structural and functional analysis of prokaryotic antiporters has contributed to the overall understanding of human homologs important in health and disease [28]. For example, the human homolog of NhaP type antiporters, the NHE1 Na^+/H^+ exchangers have been shown to be associated with different

diseases, and a change in the activity of NHE1 plays role in heart failure [19]. Enhanced expression of NHE1 is also an indication of malignant gliomas [67]. Inhibitors against NHE1 significantly decreased the metastasis and enhanced the survival rate in mouse glioma models [67]. A structural model of clinically important human NHE1 was generated using the *E. coli* NhaA (Ec-NhaA) structure as template to predict the binding site of NHE1 inhibitors [68]. In *Arabidopsis thaliana* membrane trafficking, growth, cell expansion and internal pH homeostasis are maintained by NHXs $K^+(Na^+)/H^+$ antiporters [13]. These NHXs antiporters share structural similarity especially in the core ion translocation domain with the bacterial Na^+/H^+ antiporters [13]. The Na^+/H^+ exchanger of *Schizosaccharomyces pombe* (Sp-NHE1) plays an important role in salt stress tolerance and mutation of some conserved acidic and polar amino acid residues located in either a transmembrane segment or an extracellular loop eliminated its ability to confer salt resistance [69]. The archaeal NhaP1 antiporters in *Pyrococcus abyssii* (Pa-NhaP1) and *Methanococcus jannaschii* (Mj-NhaP1) have been crystallized and widely studied [14-15,29-30]. The mammalian CPA1 antiporters are suggested to share sequence homology with the archaeal NhaP1 antiporters [11,70], and hence the crystal structures of Pa-NhaP1 and Mj-NhaP1 could be used as models for the transmembrane parts of NHE1 [14-15].

The extended and diverse NhaP family consists of transporters with different ion selectivities. It includes not only different *bona fide* $Na^+(Li^+)/H^+$ antiporters such as the Mj-NhaP1 from the archeon *Methanococcus jannaschii* [29-30] and Pa-NhaP1 from *Pseudomonas aeruginosa* [30], but also cyanobacterial Syn-NhaP1, which possibly can use Ca^{2+} as another substrate [31], $K^+(Na^+)/H^+$ antiporters Vc-NhaP1,2 [23-24], highly selective K^+/H^+ antiporter Vc-NhaP3 [25], $Ca^{2+}(Na^+,Li^+,K^+)/H^+$ antiporter Yp-NhaP [33] and alkali-activated Aa-NhaP from *Alkalimonas amylolytica*, which can also exchange H^+ for K^+, Ca^{2+} and, possibly, NH_4^+ but not

the smaller Li^+ [34]. Together, therefore, they display a broad substrate specificity that includes the efflux of Li^+, Na^+ and K^+. Of note, the NhaP family provided the first examples of truly Mitchellian K^+/H^+ antiporters in bacteria, which remained unidentified for a long time. Over the years, we have accumulated a considerable amount of biochemical information about Vc-NhaP2 [17,23-25,32,35,51]. Noticeably, the Vc-NhaP2 deletion mutant of *V. cholerae* is highly sensitive to external K^+ at pH 6.0 although its resistance to Na^+ is unaffected [23]. This observation suggests that *in vivo* Vc-NhaP2 acts as a K^+/H^+ antiporter, rather than a Na^+/H^+ antiporter [23]. Kinetic measurements of Vc-NhaP2 activity in the experimental model of everted sub-bacterial vesicles confirmed the ability Vc-NhaP2 to mediate direct K^+/H^+ exchange [23]. Results of the cation competition experiments carried out on Vc-NhaP2 expressing membrane vesicles have also strongly indicated that this antiporter is able to bind Li^+ and countertransport it with Na^+ or K^+ but not H^+ [17,23]. The chromosomal deletion of the *nhaP3* gene showed only minor growth defects at high potassium concentration at acidic pH [25]. Comparison of the biochemical properties of Vc-NhaP isoforms revealed that Vc-NhaP2 is the most active among all three paralogues with apparent K_m values for both K^+ and Na^+ of 1.6 and 1.04 mM respectively, whereas Vc-NhaP1 and Vc-NhaP3 demonstrated much weaker affinity to Na^+ as well as K^+ [23-25].

To explain these experimental data, we have suggested that protons, as well as alkali cations all compete for different subsets of ligands within the common spacious ion-binding site of Vc-NhaP2 [17]. While H^+ requires only one negative ligand for its coordination, the optimal coordination number for Li^+ is 6 [36]. If the subset of ligands for Li^+ happens to include a ligand used for protonation-deprotonation, the Li^+ ion would always outcompete H^+ and prevent direct Li^+/H^+ exchange (Fig. 4 of appendix). Our hypothesis implied that Li^+ may directly or indirectly prevent H^+ from binding to its ligand [17]. The molecular mechanism of this unusual ion selectivity

of Vc-NhaP2 remains incompletely understood. An in-depth structural and functional analysis of Vc-NhaP2 could shed light on this intriguing problem. A detailed structural analysis would also illuminate the intra-molecular events comprising the catalytic cycle of NhaP-type antiporters.

1.4 Structural model Vc-NhaP2

In our most recent study, we have combined homologue-based structure modeling with site-directed mutagenesis and antiport activity measurements to identify and characterize the structural elements responsible for the cation selectivity of Vc-NhaP2 [35]. The structural model for the transmembrane segments of Vc-NhaP2 that comprise the ion-motive functional module of the transporter, was generated by *Phyre*^{2} [37] and Robetta [38]. The *Pyrococcus abyssii* NhaP structure [15] was used as template to generate a structure by *Phyre*^{2}. The Vc-NhaP2 structure generated using Rosetta software [88] on the Robetta server [38,89] was further refined using locPREFMD [121] (frig.bch.msu.edu) (Fig. 1.1 and Supplementary material, data set S3). Antiporters can exist either in cytoplasmic or periplasmic open conformation [14-15, 39-40], where the ion binding pocket is either open to the cytoplasmic side or to the periplasmic side (Fig 3 of Appendix). In the generated model Vc-NhaP2 has an inward-open conformation (Fig. 1.1). The inward-open conformation is also evident from the solvent accessible surface analysis where the solvent accessible surface area (indicated by the purple color) is present at the cytoplasmic side (Fig. 1.1C). A negatively charged cavity which is present in the middle of the membrane (Fig. 1.1B), is accessible to solvent from the cytoplasmic side (Fig. 1.1C). Each protomer of Vc-NhaP2 has 13 transmembrane segments (TMSs) connected by short loops or helices on the membrane surface (Fig. 1.1A). TMSs IV–VII and TMSs XI-XII form a six-helix bundle, while TMSs I–III and TMSs VII–X form the dimer interface. TMS V and TMS XII in the six-helix bundle are

discontinuous [35], forming the distinctive NhaA fold initially identified in Ec-NhaA Na^+/H^+ antiporter [10,39-40]. In the *E. coli* antiporter, the NhaA fold is crucial for the conformational change expected to occur upon ligand binding [39]. The NhaA fold is shared by multiple members of the CPA1 and CPA2 family, *e.g*, the NhaA of *E. coli* (Ec-NhaA) [39], NapA of *T. thermophilus* (Tt-NapA) [40], NhaP of *Pyrococcus abyssii* (Pa-NhaP) [15] and *Methanococcus jannaschii* (Mj-NhaP1) [14]. Besides possessing the NhaA fold, CPA transporters are often classified based on their ion selectivity and electrogenicity [41]. Both Ec-NhaA and Tt-NapA have been suggested to be electrogenic, exchanging one alkali cation for two protons [39-40]. Two conserved aspartates in the ion binding site of Ec-NhaA, Asp163 and Asp164 (so-called "DD motif") located on TMS V have been proposed to be the primary proton carriers [39,41]. According to an alternative antiport mechanism for electrogenic Ec-NhaA, Asp163 forms a salt bridge with Lys300, in its de-protonated form. Ion binding breaks this salt bridge allowing the bound ion to be alternatively transported either to the cytoplasm or periplasm [43]. The conserved DD motif and the salt bridge between Asp163 and Lys300 are essential for electrogenic antiporter function as disruption of the salt bridge renders electrogenic Ec-NhaA electroneutral [39,42].

1.5 Amino acid residues affecting the ion binding and selectivity of Vc-NhaP2

In electroneutral CPA transporters, a highly conserved Asn-Asp motif (ND motif) is present instead of the DD motif and the Lys300 is replaced with an arginine [32,35]. In agreement with this, Vc-NhaP has the conserved ND motif (Asn161-Asp162) in TMS VI and Arg315 in TMS X (Fig. 1.2) [32, 35]. As determinants of ion selectivity, CPA transporters share eight highly conserved amino acid residues located on different transmembrane helices for either K^+ or Na^+ selective transport [41].

Fig. 1.1

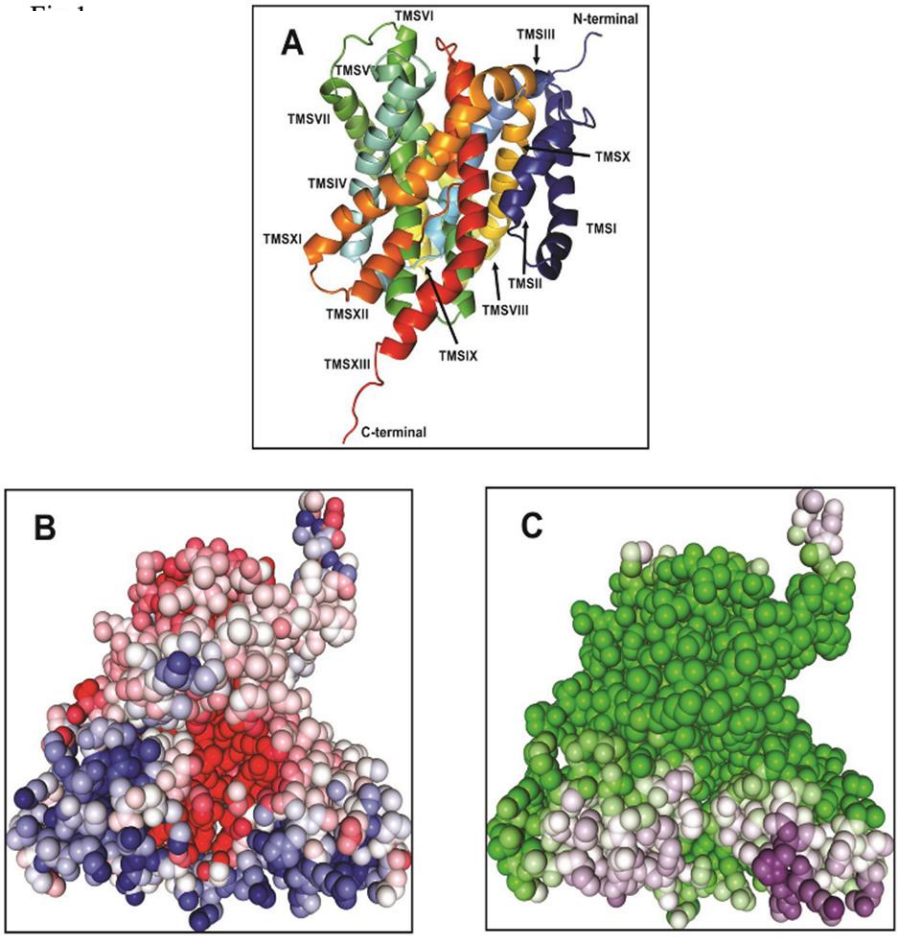

Fig. 1.1. The inward-open view of the structural model of the transmembrane domain of Vc-NhaP2 (**A**). The structure is generated by Robetta and visualized by PyMOL 1.6 [63]. The model is shown in a rainbow of colors with TMSs numbered from I to XIII. The electrostatic surface potential of Vc-NhaP2 (**B**). A highly negatively charged (red colored) cavity is present in the middle of the Vc-NhaP2. The positively charged residues (blue colored) are lining the exterior of the antiporter. The solvent accessible surface of Vc-NhaP2 (**C**). The solvent accessible surface is indicated by the dark purple color. Solvent-inaccessible residues are green. The images for both electrostatic and solvent accessibility surface potential are generated by Protein-Sol (protein-sol.manchester.ac.uk) [64].

These residues form a compact group in the folded tertiary structure of the antiporters [32,41]. In the case of Na^+/H^+ antiporters belonging to CPA1, *e.g.* Ec-NhaA, residues A131, the TD motif (Thr132-Asp133) and I134 on TMS IV together with a tandem Asp162-Asp163 on TMS V and Lys300 on TMS IX are involved in forming a structural motif determining the Na^+ selectivity (Fig. 1.2). In contrast, in CPA2, *e.g.*, Pa-NhaP A128, the TD motif (Thr129-Asp130) and Pro131 on TMS V together with the ND motif (Asn158-Asp159) on TMS VI and a salt bridge formed between Glu154 and Arg337 are involved in Na^+/H^+ exchange (Fig. 1.2). Antiporters showing K^+ selectivity are suggested to contain polar or charged residues instead of the nonpolar residues adjacent to the TD motif [41]. This is also supported by our findings obtained from the combined *in silico* and mutagenesis analysis of the Vc-NhaP2 antiporter. We carried out two rounds of Ala mutagenesis on selected amino acid residues based on our *in silico* model predictions. We found that a cluster of negatively charged and polar residues belonging to TMS V and VI of Vc-NhaP2 forms the cation-binding pocket in the middle of the membrane [35]. Glu155, Asp133, Thr132 and Ser158 from TMS V together with Asp162 and Asn161 from TMS VI, and the possible salt bridge partner of Glu157 and Arg315 are essential for K^+/H^+ transport (Fig. 1.2). Vc-NhaP2 also contains a built-in filter in the vicinity of these conserved amino acid residues determining Na^+, Li^+ or K^+ selectivity [35]. This has also been observed in the case of the eukaryotic antiporter from yeast *Zygosaccharomyces rouxii* (Zr-SOD22) that exports Na^+ and Li^+, but not K^+ [43]. It has been suggested that a hydrophobic filter near the transporter's ion binding site confers cation selectivity [27]. A triple Zr-Sod2-22 mutant Thr141Ser-Ala179Thr-Val375Ile was generated that gained K^+/H^+ transport capacity [43].

Fig. 1.2

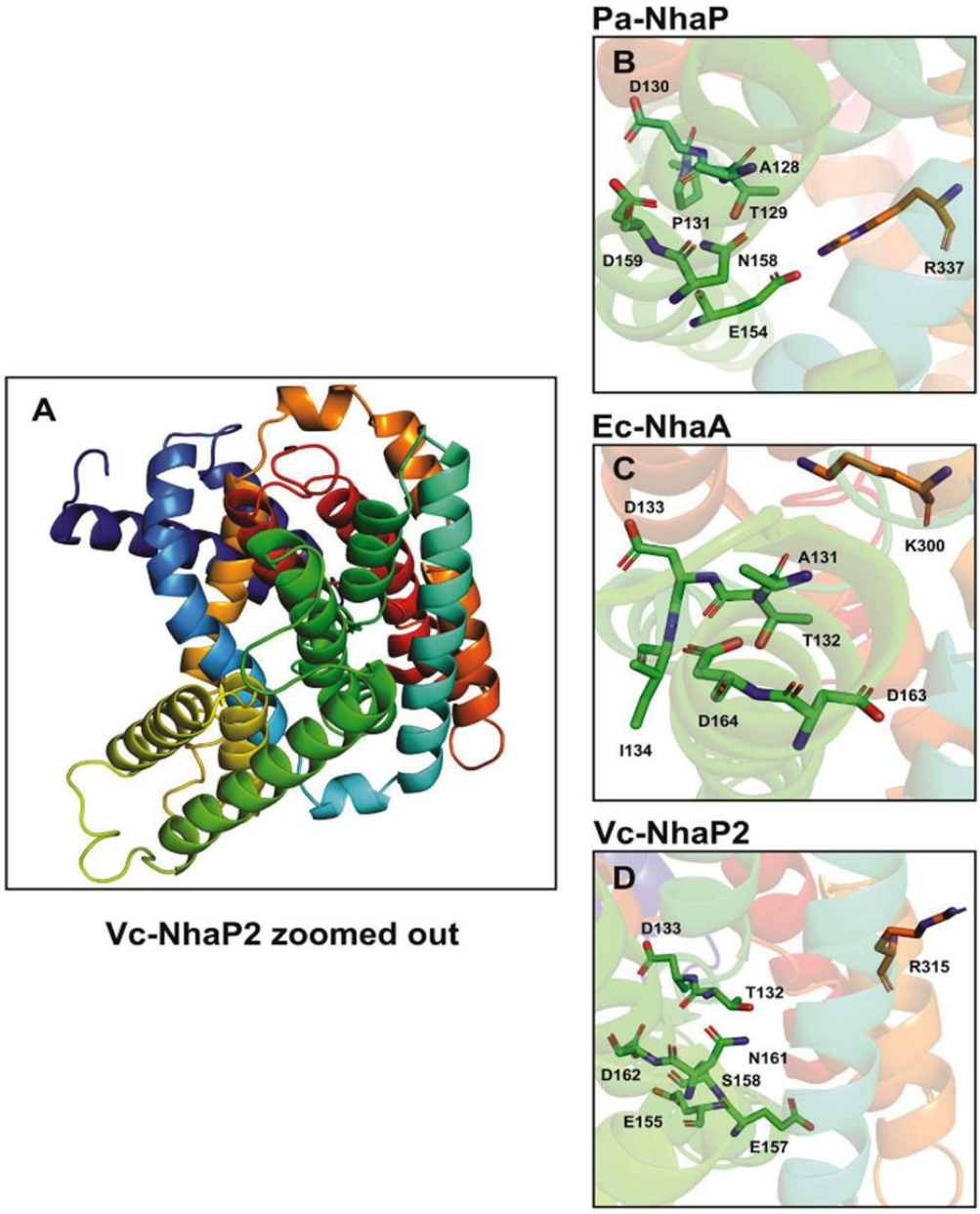

Fig. 1.2 Amino acid residues implicated in ion binding in NhaP-type antiporters. Structural data for proteins from NhaP2 of *V. cholerae* (Vc-NhaP2) (based on data from [8] (**A and D**), *Pyrococcus abyssii* (Pa-NhaP) (PDB accession code: 4CZA) (**B)** and NhaA of *E. coli* (Ec-NhaA) (PDB accession code: 1ZCD) (**C**) were used to generate 3D images with PyMOL 1.6 [63]. Amino acid residues are shown in stick-and-surface representation.

In the case of Vc-NhaP2 nine residues (Tyr251, Leu257, Glu258, Asn259, Asp273, Thr276, Gln280, Leu289, Leu342) from TMS IX, X, and XII form a pathway for translocated ions with a built-in filter determining cation selectivity [35]. Limited Ala-scanning mutagenesis supported these predictions. Thus, mutations Asp162Ala and the nearby Asn161Ala inactivated the antiporter completely [32] (as one would expect after removal of putative ion-coordination ligands), while Asp273Ala, Thr276Ala, Leu289Ala, and Leu342Ala substitutions indeed resulted in drastic restrictive changes in K^+/Na^+ specificity [35]. Furthermore, alanines in positions 251, 257-258, and 280, brought in a completely new type of activity: direct Li^+/H^+ exchange [35]. These experimental results further validate our *in silico* modeling of Vc-NhaP2. We have also identified that mutation of a single Gly159 to alanine, located in the vicinity of the putative cation binding pocket enables Vc-NhaP2 to exchange Li^+ for H^+ directly [32]. Interestingly, any negatively or positively charged residue at the position of G159 allows Li^+ to be exchanged for H^+ [32]. The Gly159Ala mutant variant was also able to protect the antiport deficient *E. coli* strain (highly sensitive to Li^+) against high concentration of Li^+ (upto 250 mM) when expressed *in trans* [32].

This finding supports the idea of "ligand shading" in the active center of Vc-NhaP2, when different alkali cations use overlapping but not identical sets of ligands, thus differently affecting the possibility of protonation of the antiporter during the catalytic cycle [17]. In the future construction of double and triple Ala substitution will be attempted in order to eliminate all the "excess" coordination ligands and thus manipulate the ion selectivity to yield strictly selective Na^+/H^+, K^+/H^+, or Li^+/H^+ antiporters, independently of the residues of TMS IX-XII, which comprise a distant "selectivity filter".

The Na^+/H^+ antiport cycle in *E. coli* NhaA is suggested to follow the "alternating-access" mechanism of secondary active transporters, with the ion binding pocket either open to the

cytoplasm or the periplasm [10,39]. Upon ligand binding a conformational change is induced which involves rearrangement of TMSs IV, V and XI in the core domain, allowing ions to be transported either to the cytoplasm or the periplasm [44]. NapA of *T. thermophilus* (Tt-NapA), NhaP of *M. jannaschii* (Mj-NhaP1) and *P. abyssii* (Pa-NhaP) the alternating access has been suggested to follow a two-domain elevator mechanism for the $Na^{+/}H^{+}$ transport, where the core domain rotates against the fixed dimerization domain with the release of Na^{+} or H^{+} either the cytoplasm or the periplasm [14-15,40]. In case of Mj-NhaP1, only binding of ligand (Na^{+}) has been shown to induce the conformational change and allow the ion binding pocket to alternatively access either to the cytoplasmic or periplasmic side [14]. Recently it has been suggested that a hydrophobic filter on the extracellular side controls ion accessibility to the binding pocket in Pa-NhaP, with the opening and closing of the gate strictly controlled by domain movement [65]. Microsecond MD simulations and transition-state sampling along with mutagenesis experiments revealed that the hydrophobic gate maintains a delicate balance between open and closed structures and without ions (Na^{+} or H^{+}) it remains closed, thus preventing transmembrane cation leakage [65].

In order to probe the conformational changes occurring upon ion binding in Vc-NhaP2, we carried out Molecular Dynamics (MD) simulations and the average fluctuation of the backbone C-alpha carbon for each residue was calculated over an 11 ns time scale. Amino acid residues in TMS IV, V, XI and XII in the core domain and TMS VII and VIII in the dimerization domain showed the highest fluctuations (Fig. 1 of the Appendix). The amino acid residues forming the putative cation binding pocket did not show any significant fluctuation. This is in agreement with the findings that in Ec-NhaA, TMSs III, IV and XI in the core domain showed higher deuterium uptake upon Li^{+} binding in a hydrogen/deuterium exchange mass spectrometry experiment

compared to TMS V containing the ion binding residues [44], suggesting that the conformational change occurring in the core domain alternatively opens the rigid ion binding pocket either to the cytoplasm or to the periplasm. These observations suggest that Vc-NhaP2 might follow the 'alternating access mechanism', where the major conformational change occurs in the core domain, especially in the cross-over region between the extended chains of TMS V and XII, and thus alternatively opens the ion binding pocket either to the cytoplasm or to the periplasm. For the MD simulations, an all-atom Vc-NhaP2 model generated using Robetta [35, 38] was imbedded in the lipid bilayer and the water, lipid and protein components were extensively energy minimized using Charmm-Gui protocols [45-46] and Gromacs 5.1.4 [47]. The total system consisted of about 120,000 atoms in an orthorhombic simulation cell with a free NaCl concentration of 250 mM. Equilibrium MD simulations were performed after energy minimization and 11 ns of equilibration with position restraints. All simulations were carried out under periodic boundary conditions at constant temperature (T = 310°K) and pressure (P = 1 bar). It is still not clear if Vc-NhaP2 follows a two-domain elevator access mechanism as suggested for Tt-NapA or Mj-NhaP1. Longer MD simulations and transition-state sampling will be carried out in the future to analyze the possible ion exchange mechanism and associated conformational changes for Vc-NhaP2.

1.6 Putative role of soluble C-terminus of NhaP2

The NhaP type antiporters from eukaryotes have long C-terminal tails that play an important role in the regulation of ion transport [48-49]. The human Na^+/H^+ exchanger, NHE1 consists of a N-terminal integral membrane domain involved in ion binding and a long C-terminal regulatory domain comprising ~300 cytoplasmic amino acids [49]. A number of signalling molecules are involved in the regulation of the C-terminal region which is linked to the N-terminal

ion binding domain [50]. NHE1 is activated in the presence of increased intracellular Ca^{2+} and calmodulin. NHE1 is activated upon a calmodulin-dependent binding of Ca^{2+} to the NHE1 cytosolic C-terminal region. The NHE1 cytosolic C-terminal binding region has been crystallized in complex with calmodulin and Ca^{2+} [34]. Calmodulin binds to both a high-affinity region and to a low affinity region in the C-terminal domain. In the absence of calmodulin, the high-affinity binding site of NHE1 possibly interacts with the N-terminal transmembrane domain, acting in an auto-inhibitory manner [50]. Recently it has been reported that the extracellular signal-regulated kinase (ERK) mediated phosphorylation of the C-terminal domain that is involved in the structural and functional changes of NHE1 [72].

In contract, the C-terminal cytoplasmic tails in prokaryotic antiporters are much shorter compared to the eukaryotic ones, *e. g.*, the C-terminal tail of Vc-NhaP2 is predicted to consist of only 120 amino acids [51-52]. In prokaryotes, the C-terminal tail has been shown to play a role in the function and/or regulation of these antiporters. In cyanobacterial Syn-NhaP1, deletion of the C-terminal hydrophilic tail resulted in a dramatic decrease in Na^+/H^+ and Li^+/H^+ antiport activity [53]. The C-terminal deletion mutant of Vc-NhaP2 showed diminished K^+/H^+ and Na^+/H^+ antiport activity, with a 5-fold decrease in the affinity for its major substrate K^+ [51-52]. When the truncated C-terminal deletion mutant of Vc-NhaP2 was expressed in an antiport deficient *E. coli* strain, it caused increased sensitivity of the *E. coli* host to Na^+ ions at neutral pH [51-52]. Though the chromosomal C-terminal deletion mutant of Vc-NhaP2 did not affect the ability of *V. cholerae* to grow at high potassium concentrations at acidic pH 6.0, the kinetic analysis clearly indicated that the cytoplasmic portion of Vc-NhaP2 is required for its optimal ion binding and maximal activity [51-52].

Interestingly, the C-terminal tail of Vc-NhaP2 is predicted to contain significant domain structure, including a the Rossman fold that binds to dinucleotide cofactors such as NAD and FAD [52]. The Rossman fold has been found in K^+ channels and is capable of pH induced conformational changes in protein upon cofactors binding [54]. The domain is suggested to be involved in pH-sensitive gating of K^+ channels [54]. Dynamic light scattering experiments at pH 7.0 with FAD indicated that FAD stabilized the C-terminal region of Vc-NhaP2 in an oligomeric form compared to experiments conducted in the absence of FAD [52]. More analysis is needed to fully understand the possible involvement of the C-terminal domain in the regulation of ion transport of Vc-NhaP2. The X-ray structure of the Vc-NhaP2 C-terminal tail, cross-linking and mutagenesis experiments will be the first step towards understanding the possible regulatory role and also the *in situ* role of the C-terminal tail in facilitating the oligomerization of the antiporter.

1.7 NhaP paralogues in Acid Tolerance Response (ATR) of *Vibrio cholerae*

V. cholerae is transmitted by the fecal-oral route. It must pass through the low pH environment of the stomach to reach the small intestine where it colonizes in the intestine and secretes cholerae toxin causing cholera diarrhoeal disease [55]. It possesses an Acid Tolerance Response (ATR) that would increase its survival within these hostile environments [56-59]. ATR is suggested to be a "significant factor in their epidemic proliferation and virulence" [56-59]. This survival system has been shown to be composed of a complex cascade of proteins, among which are several inducible amino acid decarboxylases. An essential component of organic and inorganic ATR in *V. cholerae* is the *cadABC* system. *cadA* encodes an inducible lysine decarboxylase [56-59]. *cadA* was shown to be the second gene in an operon with *cadB*, encoding a lysine/cadaverine antiporter. *cadC*, which belongs to the ToxR-like family of transcriptional regulators positively

regulates transcription of *cadBA*. *CadC* is activated at low pH by AphB, a LysR-type activator by cooperating with the quorum-sensing-regulated activator AphA at the *tcpH* promoter on the *Vibrio* pathogenicity island (VPI) [59].

Our findings suggest how the Vc-NhaP group might boost the chances of survival when ingested *V. cholerae* cells pass the gastric acid barrier in the course of a normal infectious process [25], where the cells face the stressful conditions of low pH and high potassium concentrations [60-61]. The low pH is due to the secretion of H^+ by the parietal cells into the stomach lumen up to 150 mmol/L [60-61]. H^+ is pumped into the lumen *via* the K^+/H^+ ATPase that pump out 1 H^+ in exchange for one K^+ ion and the K^+ is then recycled by K^+ channels [60-61]. Bacteria adopt different survival strategies to overcome the acidity. This is supported by the observation that wild type *V. cholerae* survived better compared to the Vc-NhaP123 triple deletion mutant when exposed to inorganic acid challenge [25]. In these experiments, *V. cholerae* cultures were resuspended in potassium-rich LBK medium adjusted to pH 3.5, 4.0 or 4.5 and incubated for different time intervals. Aliquots of cells were taken at each time point and spread onto LBK agar (pH 7.5) for a standard colony count. Furthermore, introduction of *nhaP*1, 2, and especially 3 genes *in trans* boosted the survival of mutant *V. cholerae* cells under these experimental conditions of inorganic acid challenge (M. Mourin *et al*., unpublished observations).

1.8 Regulation of Vc-NhaP isoforms

In vivo the Vc-NhaP type antiporters function as a whole to maintain potassium homeostasis in the bacterial cytoplasm [25]. All three paralogues are crucial for survival of *V. cholerae* at acidic (pH 6.0) and alkaline (pH 8.0) pHs. Interestingly, the Vc-NhaP1 alone is efficient for the restoration of growth of *V. cholerae* at high and low potassium concentration at

acidic pH 6.0, possibly due to its role in alkalinization of the cytoplasm of *V. cholerae* growing in acidic media [24-25] as it has been shown that the internal pH homeostasis mediated by Vc-NhaP1 is K^+-dependent [24].

It is interesting to note how the three different Vc-NhaP paralogues situated at different locations on the chromosome, are able to function in concert to maintain potassium homeostasis in the bacterial cytoplasm. It is possible that they are regulated in a quorum sensing-dependent manner like the *cadABC* and the *ivr* gene in *V. cholerae* [59]. Both the *cadABC* and *ivr* genes are activated in response to low pH and regulated by a signal transduction event in response to lower cell density. The regulation of the *ivr* gene encoding the Cl^-/H^+ antiporter is finely tuned in response to pH by AphB, which gets activated by AphA in a quorum sensing-dependent manner. At low pH the *ivr* gene is activated and participates in the ATR response of *V. cholerae.* In the small intestine when *V. cholerae* is exposed to alkaline pH, the *ivr* gene is turned off to prevent excessive alkalinisation of the cytoplasm [59]. The regulatory proteins ToxR, ToxT and TcpP that are involved in the virulence genes expression in *V. cholerae* are also regulated in a quorum sensing-dependent manner *via* AphB and AphA [62]. It is possible that Vc-NhaP paralogues are also regulated in a pH and quorum sensing dependent manner. The role of *AphB* and *AphA* in the regulation of Vc-NhaP paralogues is a subject for future investigation.

1.9 Perspective and expected impact of the Vc-NhaP paralogues research

Cation/proton antiporters are ubiquitous membrane transporters and the most universal transporting component in all living organisms studied so far. This is particularly evident when looking at the NhaP type antiporters due to their vast diversity in both eukaryotes and prokaryotes. This group of antiporters has evolved to play a role in a variety of physiological functions of all

organisms due to their ability to mediate rapid cation/H^+ exchange that makes them very efficient in enhancing the survival potential of the microorganism at different stressful environmental conditions as well as in the human body. Studying the NhaP type antiporters in the dangerous human pathogen *V. cholerae* not only helps us to understand the physiology, structure and dynamics of other prokaryotic homologous but also has shed light on the possible structures and functions of its eukaryotic homologues.

Antiporters of the Vc-NhaP type emerge as molecules that might be important in the early stages of infections caused by *Vibrios*. Therefore, all of these antiporters, but especially Vc-NhaP2, are prospective targets for the development of novel antimicrobials targeting this specific group of pathogens. The potential of cation-proton antiporters in general and NhaP type antiporters in particular as targets for antimicrobials remains virtually uninvestigated. We however feel that this potential is quite significant. Noticeably, in the dangerous human pathogen *Yersinia pestis*, elimination of genes encoding NhaA and NhaB sodium-proton antiporters resulted in complete loss of virulence in an *in vivo* model of plague; introduction of the *nhaA* or *nhaB* genes *in trans* restored the virulence of the *Y. pestis* mutant [66]. The *Y. pestis* strain with the deleted *nhaA* and *nhaB* genes survived very poorly in blood and blood serum *ex vivo*, as well as in artificial growth media containing Na^+ levels and pH values similar to those of blood [66]. Thus, the Na^+/H^+ antiport is crucial for the survival of *Y. pestis* in the bloodstream of infected organisms and thus appears to be a promising drug target not only for *Y. pestis* but possibly other blood-borne bacterial pathogens. Given the possible role of Vc-NhaP2 in the ATR of *V. cholerae* outlined above, we hypothesize that the inhibition of Vc-NhaP2 alone (or, perhaps, of all three Vc-NhaP paralogues) might disrupt the infectious process caused by this pathogen as it attempts to cross the gastric acid barrier. One could also mention that the inhibition of antiporters of NhaP type (which are not widely

represented in the genomes of benign gut microflora) is not as indiscriminative as application of conventional antibiotics and thus should be less damaging to human microbiota in a real clinical setting. Future studies of Vc-NhaP-deficient strains in the *in vivo* models of cholera will further clarify a potential value of NhaP type antiporters as drug targets. One may expect that such novel remedies will be especially valuable against strains resistant to currently used antibiotics. This would have immediate medical applications (*V. cholerae, V. parahaemolyticus,* etc.) as well as industrial ones, *e.g.*, in fish farming, where infections caused by a number of *Vibrio* species are among the most long-standing problems [72]. Results of studies focused on the 3D-structure and functioning of the NhaP-type antiporters will be important for the future development of inhibitors targeting these ion exchangers. The Vc-NhaP trio of antiporters represents a compact phylogenetic entity undergoing rapid divergent evolution. Using model-assisted scanning mutagenesis, we intend to investigate if the accumulation of seemingly neutral mutations, such as G159A, might be a mechanism of such divergent evolution. Having identified novel mutations in Vc-NhaP2 that manipulate the selectivity of ion translocation [32,35], we hope to be able to shed new light on the events in the active site of NhaP-type antiporters. In particular, this is expected to guide an extensive experimental testing of the available *in silico* tools for the structural analysis. On a more general note, one could expect that the results of experimental probing of the applicability of the *Phyre*^{2} [37] and Robetta [38] models to cation-proton antiporters would be especially valuable for researchers studying this class of hard-to-crystallize proteins. From a methodological point of view, the reviewed studies would permit evaluation of the potential of comparative *in silico* modelling for structural analysis of ion transporters whose actual structures are not readily available (*e.g.*, proteins that are important for practical applications but are hard to express and/or crystallize).

1.10 Research Objectives

The major research objectives are **(i)** to compare all three Vc-NhaP antiporters physiologically by expressing each antiporter in the triple Δ*nhaP1*Δ*nhaP2*Δ*nhaP3* deletion mutant of *V. cholerae*; and **(ii)** identification of molecular determinants of cation specificity in Vc-NhaP isoforms. Conserved amino acid residues associated within putative transmembrane segments, especially charged and polar ones, are of special interest, as these residues may form a part of the cation-binding site. As NhaP2 is the most active among all three isoforms, the goal is to identify the potential amino acid residues in the Vc-NhaP2 isoform that are critical for transport activity by combining homology modelling based on the available crystallography data on NhaP homologues with Molecular Dynamics (MD) simulations of lipid bilayer-embedded Vc-NhaP2 and alanine-scanning mutagenesis analysis.

In this thesis, the physiology of the Vc-NhaP paralogous group of cation-proton antiporters in *Vibrio cholerae* is discussed in Chapter 3. The structural and functional analysis of Vc-NhaP2 are discussed in Chapters 4 and 5.

Chapter 2: Materials and methods

2.1 Bacterial strains and culture conditions

The Na^+/H^+ antiporter-deficient strain of *E. coli* TO114 (Fl IN (*rrnD-rrnE*) *nhaA*::Km^R *nhaB*::Em^R *chaA*::Cm^R) was kindly offered by Dr. T. Nakamura (Niigata University of Pharmacy and Applied Life Sciences, Niigata, Japan) [22]. The *Vibrio cholerae* strain used in this study was O395N1 [73], which is the classical Ogawa strain with partial deletion of the *ctx*AB operon (O1 classical biotype; Sm^R, Δ*ctxA*1). Unless indicated otherwise, TO114 cells were grown aerobically at 37°C in LBK medium (modified L broth in which NaCl is replaced by KCl [74]) supplemented with 100 µg/ml ampicillin, 30 µg/ml kanamycin, 34 µg/ml chloramphenicol, 100 µg/ml erythromycin and 0.05% (w/v) arabinose. *V. cholerae* cells were grown aerobically at 37°C in LB supplemented with 100 µg/ml carbenicillin, 100 µg/ml streptomycin and 0.0005% (w/v) arabinose.

All bacterial strains and plasmids used in this study are listed in Table 2.1. All strains were maintained in 20% glycerol stocks at -80°C until use.

2.2 Cloning of *Vc-nhaP3*

Sequence data for *V. cholerae* were obtained from the Institute of Genomic Research (http://www.jcvi.org). Cloning of *Vc-nhaP3* was performed as described previously for *Vc-nhaP1* and *Vc-nhaP2* [23-24]. The *Vc-nhaP3* ORF was amplified by high-fidelity PCR with chromosomal DNA of *V. cholerae* O395N1 as a template and cloned into the pBAD-TOPO vector (Invitrogen) under the arabinose-induced promoter (pBAD), yielding pVc-NhaP3. The forward primer VcNhaP3expF and reverse primer VcNhaP3expR were used for cloning (Table 2.2). The forward primer allowed for the expression of the encoded antiporter without addition of the N-terminal leader sequence introduced by this vector. It contained an in-frame stop codon and a translation re initiation sequence, which consists of a ribosome-binding site and the first ATG of the protein. In the reverse primer, the native stop codon of *Vc-nhaP3* was maintained. The *nhaP3* ORF was amplified by PCR as described in [23-24] with 1 unit of Platinum PCR Supermix High-Fidelity DNA polymerase (Invitrogen). The sequence of the obtained construct was validated by DNA sequencing.

2.3 Construction of *V. cholerae* strain carrying deletions of *nhaP1, 2* and *3*

Genomic DNA from *V. cholerae* O395N1 was isolated using the DNeasy Blood and Tissue kit (Qiagen). Oligonucleotide primers used for construction are listed in Table 2.2. Each of the Δ*nhaP1,* Δ*nhaP2,* and Δ*nhaP3* deletions was constructed as described below, and the deletion mutant obtained at each step was used to introduce the next mutation after verification the junction of deletion by PCR on a single colony. To introduce the Δ*nhaP1,* Δ*nhaP2,* or Δ*nhaP3* deletions into the chromosome of O395N1 *V. cholerae*, overlap extension PCR was used as previously described [76]. PCR was used to amplify regions 1 kb upstream (primers 1 and 2) and downstream (primers

3 and 4) of the targeted locus (Table 2.2). Primers 2 and 3 have complementary *Bgl*II sites engineered into the primers to allow the two fragments to anneal. The final PCR product results from combining the two PCR products and adding primers 1 and 4, creating a fusion PCR product containing the flanking regions of the desired gene. The fragment was cloned into pWM91 [75], containing the R6K origin of replication that requires the product of the *pir* gene for replication and the *sacB* genes for sucrose counter-selection. The mutated allele was introduced into the chromosome of the *V. cholerae* O395N1 following sucrose selection as described in [77].

2.4 Cloning and expression of Vc-NhaP2 mutant variants

The full-length *Vc-nhaP2* gene was amplified from the genomic DNA of *V. cholerae* O395-N1 by high-fidelity PCR and cloned into the pBAD-TOPO vector (Invitrogen) under the arabinose-induced promotor (pBAD) as described in [4], but with a slight primer modification to eliminate the native stop-codon. The following primers were used for cloning: forward primer VcNhaP2expF 5 ’-GAGGAATAATAAGTGGACGCCGTTACGATTAAC-3’ and the new reverse primer VcNhaP2expR-STOPgone 5’-TTTCTCCGCGCCTTCTTGTAGCTC-3’. This modification extended the reading frame through the C-terminal tags (V5 and His) provided by the pBAD-TOPO vector. The resulting translation product, Vc-NhaP2, contained the entire ORF-encoded antiporter (including C-terminal V5 and 6×His tags) expressed from the arabinose-inducible pBAD promoter. Genes encoding Vc-NhaP2 variants were constructed by site-directed mutagenesis using that QuikChange Lightning Site-Directed Mutagenesis Kit (Agilent Technologies). This method uses a high fidelity Pfu Fusion-based DNA polymerase, two synthetic oligonucleotide primers with the desired mutations and the supercoiled double-stranded DNA template. After amplification, the PCR product was digested with 2 U of the restriction endonuclease *Dpn*I at 37°C for 60 min to eliminate

the methylated and hemimethylated template. Mutated ssDNA was either chemically transformed into XL10 Gold ultracompetent cells or electrocompetent *E. coli* KNabc as follows. 45 µl of XL10 Gold cells were thawed and gently mixed with 2 µl of β-ME and incubated on ice for 2 min. Then, 2 µl of DNA was added and again incubated on ice for 30 min, after which the cell mix was heat shocked for 30 sec at 42°C and then cooled for 2 min on ice before being mixed with 500 µl of SOC medium (Super Optimal broth with Catabolite repression) (Hanahan, 1983). Alternatively, the DNA was introduced into electrocompetent *E.coli* KNabc with a GenePulsar 1 (1,600V, 25 mF and 400 Ohm; Bio-Rad), before being mixed with 1 ml of SOC. In both preparations, the cells were then incubated for 60 min at 37°C and shaking, before being selected on several pre-warmed LBK agar plates supplemented with 100 µg/ml ampicillin overnight at 37°C. Successful transformants were cultured, the plasmids isolated and submitted for sequencing at the Oregon State University Center for Genome Research and Biocomputing. For confirmation of the correct mutation and absence of amplification mistakes the entire gene and V5 tag were sequenced. Mutant variants were named for their targeted amino acid, followed by its location in the amino acid sequence and the amino acid it got mutated into, for example D162A means, that the aspartic acid located in position 162 of the amino acid sequence was replaced by alanine.

2.5 Growth phenotype assays

For growth analysis of *V. cholerae* ΔNhaP1, 2 and 3, LBB medium (non-cationic adjusted L broth) was supplemented with antibiotics, 0.0005% arabinose, and varying concentrations of KCl, LiCl or NaCl. The initial pH was adjusted to pH 6.0, pH 7.2, pH 8.0 and pH 8.5 by the addition of 60mM Bis-Tris-Propane (BTP)-HCl. Cells were inoculated at a starting optical density at 600 nm (O.D. (600nm)) of 0.05 into 200 µl of liquid media placed in 96 deep-well plates (Whatman) and

grown at 37°C for 18 hours with vigorous aeration. Growth was then measured as the O.D. of the bacterial suspension at 600 nm by scanning the plates on the Biotek Instruments plate reader using the Gen5 program. For growth analysis of the triple mutant *V. cholerae* ΔNhaP123, cells were grown in 2 ml of the same media in test tubes, using the same procedure as above. All experiments were repeated at least three times in triplicate. The O.D. of the bacterial suspension at 600 nm was measured with an Ultraspec 3000 spectrophotometer (Pharmicia Biotech). A Biotek Instruments plate reader with the Gen5 program was used for scanning the plates. Data were directly exported to an Excel® file for statistical analysis. For each strain at a given condition set, an average of 8 replicates were measured and standard deviations were calculated and the results plotted.

2.6 Isolation of membrane vesicles and assays of antiporter activity

Inside-out membrane vesicles from TO114 cells transformed with pVc-NhaP1, 2 or 3 or pBAD24 ("empty" control) were isolated from cells grown in LBK medium supplemented with 100 µg/ml ampicillin, 30 µg/ml kanamycin, 34 µg/ml chloramphenicol, 100 µg/ml erythromycin and 0.05% arabinose. Cells were harvested at an O.D. (600nm) of 1.0 to 1.2 and washed three times in buffer containing 140 mM choline-chloride, 10% (w/v) glycerol and 20 mM Tris-HCl, pH 7.5, and then resuspended in the same buffer containing 1 mM 1,4-dithiothreitol (DTT), 1 µg/ml pepstatin-A, 0.1 mM phenylmethylsulfonyl fluoride (PMSF) and approximately 5 mg/L DNase. The bacterial suspension was then passed twice through a French Press (Aminco), the unbroken cells were pelleted at 12,000 × *g* for 10 min at 4°C, and the supernatant was ultracentrifuged at 184,000 × *g* for 90 min at 4°C. The resulting membrane pellets were then resuspended and stored in the same buffer until assay for cation/proton antiport activity.

For measuring antiport activity, aliquots of vesicles (200 µg of protein) were added to 2 ml of buffer containing 140 mM choline chloride, 5 mM $MgCl_2$, 10% (w/v) glycerol, 4 µM acridine orange and 50 mM BTP-Cl adjusted to the indicated pH. The cation/H^+ antiport activity was measured using the acridine orange fluorescence quenching/dequenching assay [51]. Acridine Orange (AO) is a fluorescent pH indicator. Being a weak amine, AO easily penetrates membranes in its uncharged form. Energization (ΔpH formation, acid inside) of the membrane leads to AO uptake and quenching of its fluorescence. Addition of a substrate cation leads to cation/H^+ antiport, so ΔpH drops, and some AO diffuses back into the medium leading to fluorescence dequenching. The fluorescence dequenching/ quenching ratio serves as a relative measure of antiport activity. Respiration-dependent generation of ΔpH was initiated by the addition of 20 mM Tris-lactate and the resulting quenching of acridine orange fluorescence was monitored in a Shimadzu RF-1501 spectrofluorophotometer (excitation at 492 nm and emission at 528 nm). Antiport activity was calculated based on its ability to dissipate the established ΔpH in response to the addition of 10 mM KCl. The antiport activities are expressed as percent restoration of lactate-induced fluorescence quenching. Each experiment was carried out in duplicate on at least five separate isolations of membrane vesicles.

2.7 Immunodetection of Vc-NhaP isoforms and Vc-NhaP2 mutant variants in sub-bacterial vesicles

The TO114 cells were transformed with the expression plasmid pBAD-TOPO, containing *Vc-nhaP1, 2,* or *3* ORF cloned in-frame with the downstream V5 epitope for immunogenic

detection (constructs pVc-NhaP1T, pVc-NhaP2T, and pVc-NhaP3T). To this end, site-directed mutagenesis was carried out to replace the stop codons of *nhaP* genes with alanine-encoding triplets. Mutagenic primers (listed in Table 2.2) were designed employing the QuikChange Primer Design Program (Agilent Technologies). The Quick Change Lightning Site-Directed Mutagenesis Kit was used according to the manufacturer's protocol with minor modifications. Briefly, at least 30 ng/µl of plasmid pBAD-TOPO containing cloned *Vc-nhaP1, 2,* or *3* ORF were used as a PCR template and the template DNA was afterwards digested using *Dpn*I for 60 min at 37 °C. Instead of the chemically competent cells included in the kit, the plasmid was transformed into the electrocompetent *E. coli* TO114 cells. Selected transformant colonies were propagated, plasmid DNA was isolated, and the validity of constructs was confirmed by DNA sequencing. Membrane vesicles from each transformant were isolated as described above. Samples of membranes for electrophoresis were taken at the last step of isolating the membrane vesicles. Prior to electrophoresis, protein content in the samples was determined using a Detergent Compatible (DC) Protein Assay Kit (Bio-Rad) following the manufacturer's instructions, and volumes were adjusted with the buffer used for isolation of vesicles to equalize protein content in all samples. For immunodetection of Vc-NhaP2 mutant variants the TO114 cells were transformed with the expression plasmid pBAD-TOPO, containing Vc-NhaP2 mutant variants with the C-terminal V5 epitope for immunogenic detection. Membrane vesicles were isolated from each transformant as described above.

Aliquots of membranes were mixed with standard SDS PAGE loading buffer and incubated at 85 °C for 5 min. For electrophoresis, 20 µl (~50 µg of total protein) of sample was loaded per lane. Proteins were resolved on a 10% polyacrylamide gel according to [78] and transferred onto an Amersham Hybond ECL nitrocellulose membrane (GE Healthcare) by semi-dry

transfer at 250 mA for 35 min. The membrane was blocked overnight at room temperature in TBS (pH 7.5) containing 10% skimmed milk powder. Further, the membrane was incubated with Anti-V5-HRP antibody (Novex) at a dilution of 1:5000 in TBS containing 1% skimmed milk powder. The blot was then rinsed four times for 10 min each with TBS, and incubated for 5 min in 5 ml of Luminata Forte Western Horseradish peroxidase Substrate (Millipore). The resulting signal from immunoreactive proteins was detected using a Fluoro ChemTM 8900 (ProteinSimple). For quantitation (Fig. 3.3; inset), the band densities for each individual Vc-NhaP isoform obtained in four independent assays were integrated using the built-in FluorChemTM 8900 densitometry software. Mean values (in arbitrary density units) were plotted together with bars showing standard deviation.

2.8 Acid tolerance response (ATR) tests

One colony of each strain was inoculated in 35 ml LBK and incubated overnight at 37°C with shaking until an OD600 of 0.6 to 0.8 was reached. The cells were pelleted in a bucket rotor at 3600×g for 5 min at 4 °C, re-suspended in 1 ml of LBK, and divided into two Eppendorf tubes. The cells were then re-pelleted in a tabletop centrifuge at 4000×g for 60 s. The supernatant was removed once more and one pellet underwent acid treatment with 1 ml of HCl-adjusted LBK (pH 3.5, 4.0, or 4.5) and the other was re-suspended in neutral pH LBK (negative control) and incubated at room temperature. At 15, 60, and 90 min, the cells were washed in neutral pH LBK and counted using a plating technique developed by Chen *et al.* [79]. After overnight incubation of the plates at 37 °C, cell survival was calculated and analyzed with GraphPad PRISM (v.6.07). A two-way ANOVA and a subsequent Sidak's multiple-comparisons test were used to evaluate the

results. For all strains, three biological replicates with each three technical replicates were analyzed unless otherwise noted. The threshold for significance was $P < 0.05$.

2.9 Protein determination

Protein content in preparations of sub-bacterial vesicles was measured with a DC Protein Assay Kit (Bio-Rad) following the manufacturer's instructions.

2.10 *In Silico* Analyses of Vc-NhaP Proteins

The sequences of NhaP proteins from *V. cholerae* and *V. parahaemolyticus* were aligned using a BLASTP (https://blast.ncbi.nlm.nih.gov). The number and intramolecular distribution of putative transmembrane segments in the Vc-NhaP antiporters was deduced using the computer assisted program MEMSAT-SVM [80-82] on the PSIPRED Server, Bioinformatics Group, University College, London [83-84].

2.11 Generation of *in silico* structural models of Vc-NhaP2

Vc-NhaP2 consists of 581 amino acids, where 391 amino acids comprise the main transmembrane segments and the rest belong to the cytoplasmic tail. We have already reported that deletion of the cytoplasmic tail did not have any significant impact on the Vc-NhaP2 antiport function [51]. Therefore, to generate the model by *Phyre*^{2} [37] we used only the "catalytically competent" 391 amino acid sequence consisting of the main transmembrane domain of the protein. Furthermore, Rosetta [88] independently determined that residues 1-391 form the transmembrane domain and residues 400 – 581 form the cytoplasmic domain. The structural models of Vc-NhaP2 were generated using *Phyre*^{2} [37] and Rosetta [88] software using the Robetta server [38,89] (http://robetta.bakerlab.org) and visualized by

PyMOL [63]. The Rosetta-generated structure has a Template Model-score of 0.865 with respect to PDB ID: 4czb, the Na^+-H^+ antiporter Pa-NhaP from archeon *Pyrococcus abyssi* [15]. The Template Model-score is a measure of the similarity between two protein structures with different tertiary structures. The Ramachandran plots for the structural model of Vc-NhaP2 and the template used for the *Phyre*^{2} model were generated by Rampage (http://www cryst.bioc.cam.ac.uk/rampage) [90] (Fig. 2A and B of the Appendix). The sizes and positions of alpha-helices and residues of the template and our protein of interest are very similar (Supplementary material, data set S1 and S2). According to the Ramachandran plot values, 78% amino acid residues are involved in α helices formation in our protein of interest which is very similar to the template. In Pa-NhaP, about 76% amino acid residues form α helices. The length of each TMS is similar in both Pa-NhaP and Vc-NhaP2 except TMS XII. The TMS XII of Vc-NhaP2 is shorter (consists of 27 amino acid residues) than that of Pa-NhaP (consists of 34 amino acid residues).

For individual cation ligands (K^+), the structure was adjusted by changing the van der Waals radius of Ta^+ of the template model [15] to that of K^+ [36] when applying PyMOL. As an initial template for the modeling by *Phyre*^{2}, the sequence for the Pa-NhaP was used because its X-ray diffraction data were available [15]. We then validated the obtained structure by independently generating a structure using Rosetta [88] software on the Robetta server [38,89] (http://robetta.bakerlab.org). Superimposition of the two structures generated by *Phyre*^{2} and Rosetta using PyMOL showed that they are nearly identical with a root-mean-square deviation (RMSD) value with respect to alpha carbons of the TMSs of 1.6 A°. The surface potential of Vc-NhaP2 was calculated by Adaptive Poisson-Boltzmann Solver (APBS) [91].

The Vc-NhaP2 structure generated using Rosetta software [88] on the Robetta server [38,89] was further refined using locPREFMD [121] (frig.bch.msu.edu) (Fig. 1.1 and Supplementary material, data set S3). The quality of the generated structure was checked using SWISS-MODEL (swissmodel.expasy.org) [122]. locPREFMD refines protein structure via molecular-dynamics simulations [121]. The refined model has a MolProbity-score of 1.0 with 0 clash score and bad bonds and 95% of residues are in the favored Ramachandran region (Fig. 2C of the Appendix). Based on all-atom contact analysis, hydrogen placement, backbone torsion angle and steric clashes, MolProbity score provides a single number representing the protein quality statistics [125]. Poor structure quality is strongly indicated with unfavorable steric clashes, whereas with clashes reduced nearly to zero indicates the structure is well-ordered [126].

For the MD simulations the structure generated using Rosetta software [88] was embedded in a lipid bilayer membrane composed of mixed 1-palmitoyl 2oleoylphosphatidylethanolamine (POPE) (80%)/1-palmitoyl-2oleoylphosphatidylglycerol (POPG) bilayer (20%) [125] and the water, lipid and protein components were extensively energy minimized using Charmm-Gui protocols [45-46] and Gromacs 5.1.4 [47]. The total system consisted of about 120,000 atoms in an orthorhombic simulation cell with a free NaCl concentration of 250 mM. Equilibrium MD simulations were performed after energy minimization and 11 ns of equilibration with position restraints. All simulations were carried out under periodic boundary conditions at constant temperature (T = 310°K) and pressure (P = 1 bar).

Table 2.1 Bacterial strains and plasmids used in this study

Strains	Description	Reference or Source
Vibrio cholerae		
O395N1	O1 classical biotype; Sm^R, Δ*ctxA*1	[73]
VcΔNhaP123	O395N1 (Δ *nhaP1* Δ *nhaP2* Δ *nhaP3*)	This study (chapter 3)
Escherichia coli		
TO114	F l IN (*rrnD-rrnE*) *nhaA*::Km^R *nhaB*::Em^R *chaA*::Cm^R	[21]
TOP10	Cloning strain	Invitrogen
Plasmids		
pBAD-TOPO	Cloning vector, Amp^+	Invitrogen
pBAD24	Cloning vector with PBAD promoter; Amp^+	Invitrogen
pWM91	Suicidal vector; R6K origin of replication	Metcalf *et al.* [75]
pVc-NhaP1	Vc-*nhaP1* ORF cloned into pBAD24 under the PBAD	Quinn *et al*. [24]
pVc-NhaP2	Vc-*nhaP2* ORF cloned into pBAD24 under the PBAD	Resch *et al*. [23]
pVc-NhaP3	Vc-*nhaP3* ORF cloned into pBAD24 under the PBAD	This study (chapter 3)
pVc-NhaP1T	Vc-*nhaP1* ORF + V5 epitope tag in pBAD-TOPO	This study (chapter 3)
pVc-NhaP2T	Vc-*nhaP2* ORF + V5 epitope tag in pBAD-TOPO	This study (chapter 3)
pVc-NhaP3T	Vc-*nhaP3* ORF + V5 epitope tag in pBAD-TOPO	This study (chapter 3)

Table 2.2 Oligonucleotide primers used in this study

Name	Sequence	Task
VcNhaP3expF	5′-GAG GAA TAA TAA TGA TGC ACG AAG AGT CTA TTGC-3′	*Vc-nhaP3* cloning
VcNhaP3expR	5′-CTA TGG GCT CTC GTG ACT TTT GAT CAG-3′	
VcNhaP1-FT	5′-CTT CAA GCT CGC CCT TTT TGT GTT GTT GTT CTT GCT G-3′	Vc-NhaP1 immunodetection
VcNhaP1-RT	5′-CAG CAA GAA CAA CAA CAC AAA AAG GGC GAG CTT GAA G-3′	
VcNhaP2-FT	5′-CAA GCT CGC CCT TTT TCT CCG CGC CTT CTT G-3′	Vc-NhaP2 immunodetection
VcNhaP2-RT	5′-CAA GAA GGC GCG GAG AAA AAG GGC GAG CTT G-3′	
VcNhaP3-FT	5′-CAA GCT CGC CCT TTT TCT CCG CGC CTT CTT G-3′	Vc-NhaP3 immunodetection
VcNhaP3-RT	5′-CAA GAA GGC GCG GAG AAA AAG GGC GAG CTT G-3′	
NhaP1-1	5′-GGG GGG GAT CCG CAT TCT GAA ATG CGT GAA AG-3	VcΔNhaP123 construction
NhaP1-2	5′-GAC TGA CTG ACT GAC TGA CTG ACT CAT TCT CTT CTC AGT GTG TGT AAC AAT TTG -3′	
NhaP1-3	5′-AGT CAG TCA GTC AGT CAG TCA GTC TAA TCT CCG TTG TTT AAT CGA CAA AC-3′	
NhaP1-4	5′-GGG GGG AGC TCA AGT TCG GAA TTG ATA AGC GC-3′	
NhaP2-1	5′-GGG GGA CTA GTG GTT CTG GAG TAG TAA CGA TCT CCG -3′	
NhaP2-2	5′-GAC TGA CTG ACT GAC TGA CTG ACT CAC TCT ACC TCC CAG TCT GCG ATT AACG-3′	
NhaP2-3	5′-AGT CAG TCA GTC AGT CAG TCA GTC TAA CGA TCG TTT GCG CCT TGA CGT TGAGG-3′	
NhaP2-4	5′-GGG GGG AGC TCG GAA CGC GCA AGG CGA GCC AGT ACC G-3′	
NhaP3-1	5′-GGG GGG ATC CCC AAC CAG AAG CAG CAA CAC AATGG-3′	
NhaP3-2	5′-GAC TGA CTG ACT GAC TGA CTG ACT CAT GAT TGC ACC TCT TAT CGG-3′	
NhaP3-3	5′-AGT CAG TCA GTC AGT CAG TCA GTC TAG GGC TCT CGT TTT GCT CTGGC-3′	
NhaP3-4	5′-GGG GGG AGC TCG CGA GTC TTG GCG TGA TTT AC-3′	

Chapter 3.

Physiology of the Vc-NhaP paralogous group of cation-proton antiporters in *Vibrio cholerae*

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Author contributions

Mourin, M., Schubiger, C.B. and Resch C.T., performed most of the experiments, contributed to data organization and manuscript review; Mourin, M. performed most of the growth experiments as well as all membrane isolation and antiport measurements in vesicles; Schubiger, C.B. performed a crucial part of the molecular cloning, as well as some growth experiments and reviewed the manuscript; Resch C.T designed some experiments, contributed to the activity measurements in vesicles and Western blot analysis; critically reviewed data and contributed to the writing of the manuscript; Häse C.C. and Dibrov, P. designed all the experiments, critically reviewed and edited the data and PD wrote and reviewed manuscript.

3.1 Abstract

The genome of *Vibrio cholerae* encodes three cation-proton antiporters of the NhaP type, Vc-NhaP1, 2 and 3. To examine the physiological roles of the Vc-NhaP antiporters, triple Δ*nhaP1*Δ*nhaP2*Δ*nhaP3* and single Δ*nhaP3* deletion mutants of *V. cholerae* were constructed and characterized. Vc-NhaP3 was, for the first time, cloned, functionally expressed in the antiport-deficient *Escherichia coli* strain TO114, and biochemically characterized. Activity measurements

in the inside-out membrane vesicles experimental model defined Vc-NhaP3 as a potassium-specific cation-proton antiporter. While elimination of functional Vc-NhaP3 resulted in only a minor growth defect in potassium-rich medium at pH 6.0, the triple Vc-NhaP mutant demonstrated severe growth defects at both low and high [K^+] at pH 6.0 and failed to grow at high [K^+] in alkaline (pH 8.0 and 8.5) media, as well. Expressed *in trans*, neither of the Vc-NhaP paralogues was able to complement the severe potassium-sensitive phenotype of the triple deletion mutant completely. Vc-NhaP1 provided much better complementation at acidic pH compared to Vc-NhaP2, despite the fact that Vc-NhaP2 showed much higher antiport activity in sub-bacterial vesicles. In alkaline pH only Vc-NhaP2 complemented the potassium-sensitive phenotype of the triple deletion mutant. Taken together, these data suggest that *in vivo* all three isoforms operate in concert, contributing to K^+ resistance of *V. cholerae*. We suggest that the Vc-NhaP paralogue group might play a role in passing of the gastric acid barrier by ingested *V. cholerae* cells.

3.2 Introduction

The genome of the dangerous human pathogen *Vibrio cholerae* contains three structural genes encoding paralogues Vc-NhaP1, 2 and 3, belonging to the CPA-1 family and initially annotated as sodium-proton antiporters [7,17]. Since expression of major virulence factors in *V. cholerae* is strictly dependent upon transmembrane circulation and homeostasis of alkali cations, primarily Na^+ [6-7, 92], we undertook a systematic analysis of these membrane ion transporters. Previously, we already reported the detailed biochemical characterization of the Vc-NhaP2 isoform [23,51]. The Vc-NhaP2 deletion mutant of *V. cholerae* was found to be very sensitive to high concentrations of K^+ at pH 6.0 while its resistance to Na^+ remained unaffected [23]. Such an unexpected phenotype suggested that *in vivo* Vc-NhaP2 actually acted as a K^+/H^+ antiporter. Kinetic

analysis of Vc-NhaP2 operating in sub-bacterial vesicles confirmed this suggestion: electroneutral K^+/H^+ antiport was found to be a predominant type of Vc-NhaP2 activity [23]. These findings looked especially interesting because, despite the widely recognized importance of housekeeping K^+/H^+ antiporters for bacterial ion/pH homeostasis [2,21], genes for such transporters had not been confidently identified in bacteria at that time (discussed in [23]). The experiments with Vc-NhaP2 have also revealed a unique feature of this antiporter: its ability to bind Li^+ and exchange it for other alkali cations but not for H^+ [23]. Further, the Vc-NhaP1 isoform has been cloned and characterized, as well [24]. When assayed in inside-out sub-bacterial vesicles derived from an antiporterless *E. coli* strain, Vc-NhaP1 acted as an electroneutral antiporter, exchanging K^+ or Na^+ ions for protons equally well within a broad pH range (7.25 to 9.0). Of note, unlike Vc-NhaP2, Vp-NhaP1 was unable to bind Li^+ [24]. The phenotype of Δ*nhaP1* mutant of *V. cholerae* suggested that Vc-NhaP1 is required for the cytoplasmic pH homeostasis and growth in acidic environments especially at low (below 100 mM) and high (above 300 mM) potassium concentration [24].

Here we report, for the first time, basic biochemical properties of the third isoform, Vc-NhaP3, functionally expressed in the antiport-deficient *E. coli* strain TO114 and the physiological consequences of the chromosomal deletion of the *nhaP3* gene. At last, we were able to compare all three Vc-NhaP antiporters functionally as well as physiologically, by expressing each antiporter in the triple Δ*nhaP1*Δ*nhaP2*Δ*nhaP3* deletion mutant of *V. cholerae*. Taken together with previously reported findings, the results obtained in this study suggest that (i) all three Vc-NhaP paralogues are chemiosmotically active and function *in vivo* primarily as K^+/H^+ antiporters; (ii) all three antiporters are needed for the maximal growth of *V. cholerae* at acidic external pH in media with either high (in excess of 300 mM) or lowered (lower than 100 mM) concentrations of potassium; (iii) without functional Vc-NhaP1, 2 and 3 *V. cholerae* cannot grow at elevated (app. 300 mM) concentrations

of potassium also in alkaline (pH 8.0 and pH 8.5) media. Therefore, the Vc-NhaP paralogue group in the membrane of *V. cholerae* functions as a whole to maintain the K^+ homeostasis in the bacterial cytoplasm.

3.3 Results

3.3.1 Vc-NhaP3 activity measured in the inside-out membrane vesicles

The gene encoding Vc-NhaP3 was cloned into the standard expression vector pBAD-TOPO as described in "Materials and Methods" and expressed in the antiport-deficient (Δ*nhaA*, Δ*nhaB*, Δ*chaA*) *E. coli* strain TO114. Inside-out membrane vesicles from TO114/pVc-NhaP3 and "empty" TO114/pBAD24 cells were then obtained, and the cloned antiporter was analyzed for cation/H^+ exchange activities by the standard acridine orange (AO) fluorescence dequenching technique. The results were expressed as percent restoration of lactate-induced AO fluorescence quenching. When assayed by the addition of 10 mM of KCl, Vc-NhaP3 demonstrated modest ion exchange activity, which reached its maximal level of app. 15% at pH 7.5 (Fig. 3.1, squares). No K^+/H^+ antiport was registered at pH 6.5 or 8.5 and above (Fig. 3.1).

To assess the affinity of Vc-NhaP3 for transported potassium, the AO dequenching in vesicles isolated from TO114/pVc-NhaP3 was initiated by varying concentrations of K^+ at pH 7.5. These measurements yielded the concentration of K^+ required for half-maximal response (Fig. 3.2). By convention, the easily assessable half-maximal concentrations are universally used as a measure of affinity of cation-proton antiporters (see, for example, [93-96,23] and references therein), although they are only indirectly related to the actual K_m value of the antiport. These parameters are termed "apparent K_m" for the corresponding cation (often, just "K_m for a given cation"), and we shall use this convenient term here. For Vc-NhaP3, $[K^+]_{1/2}$ was found to be 8.3 mM (Fig. 3.2),

which is a relatively high value suggesting that Vc-NhaP3 is a low-affinity K^+/H^+ antiporter. Noticeably, Vc-NhaP3 did not show any measurable Na^+/H^+ or Li^+/H^+ antiport activity at any tested pH (Fig. 3.1, triangles and circles). This differentiates it from two other Vc-NhaP isoforms which can exchange K^+ or Na^+ for H^+ and defines Vc-NhaP3 as a truly potassium-specific cation-proton antiporter.

Fig 3.1

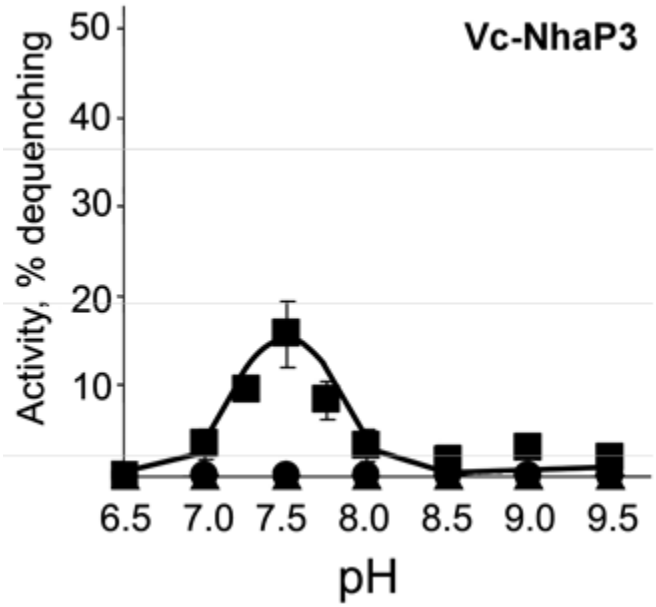

Fig 3.1 pH profile of Vc-NhaP3 activity. Inside-out membrane vesicles were isolated from TO114 cells transformed with pVc-NhaP3 or "empty" pBAD24 and assayed with 10 mM of KCl (squares), NaCl (circles), or LiCl (triangles) in standard choline chloride buffer (140 mM choline chloride, 5 mM $MgCl_2$, 10% glycerol) adjusted to the indicated pH with 50 mM BTP-HCl. In each case, the residual non-specific activity measured in "empty" vesicles was subtracted from that registered in Vc-NhaP3-containing vesicles and the resulting Vc-NhaP3-dependent activity was plotted as a function of pH. Plotted are the averages of six measurements (taken in duplicate with three separate isolations of vesicles). Error bars indicate standard deviation.

Fig 3.2

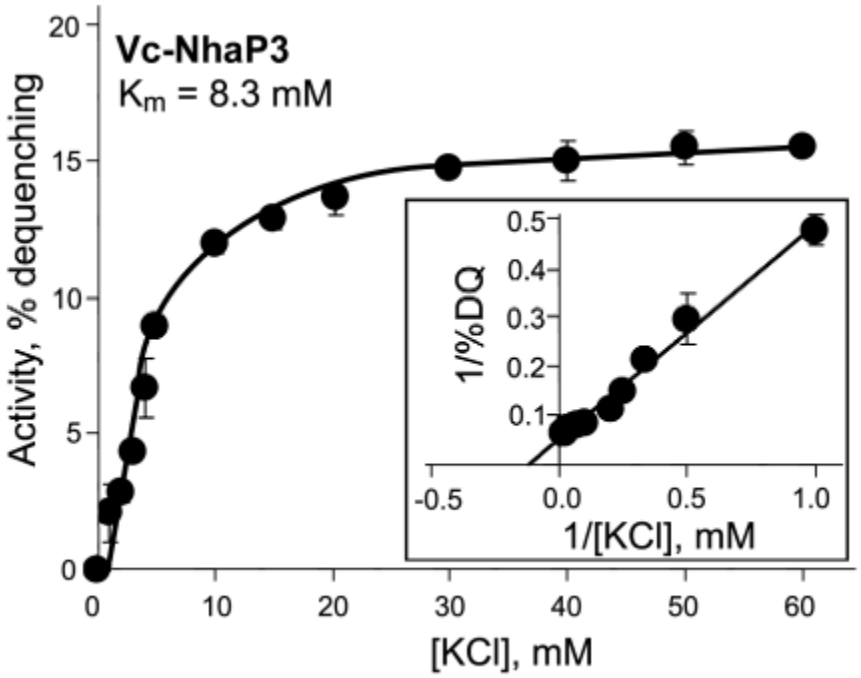

Fig 3.2 Determination of the kinetic parameters of Vc-NhaP3. Inside-out membrane vesicles were isolated from TO114/pVc-NhaP3 transformants and assayed in standard choline chloride buffer adjusted to pH 7.5 with the final concentration of added KCl varying from 0.05 to 50 mM. Each point represents the average of four measurements (taken in duplicate with two separate isolations of vesicles). Inset, double-reciprocal plot.

3.3.2 Comparative biochemistry of Vc-NhaP paralogues

The above measurements allow for the direct comparison of K^+/H^+ antiport activities of all three Vc-NhaP paralogues. For these experiments, we used Vc-NhaP1 and Vc-NhaP2 cloned into pBAD-TOPO plasmid and functionally expressed in the antiport-deficient *E. coli* TO114 as described previously [23-24]. The inside-out membrane vesicles were isolated, and K^+/H^+ antiport activities of all three antiporters were assessed at different pHs according to a standard protocol with 10 mM KCl, as described in "Materials and Methods".

Fig 3.3

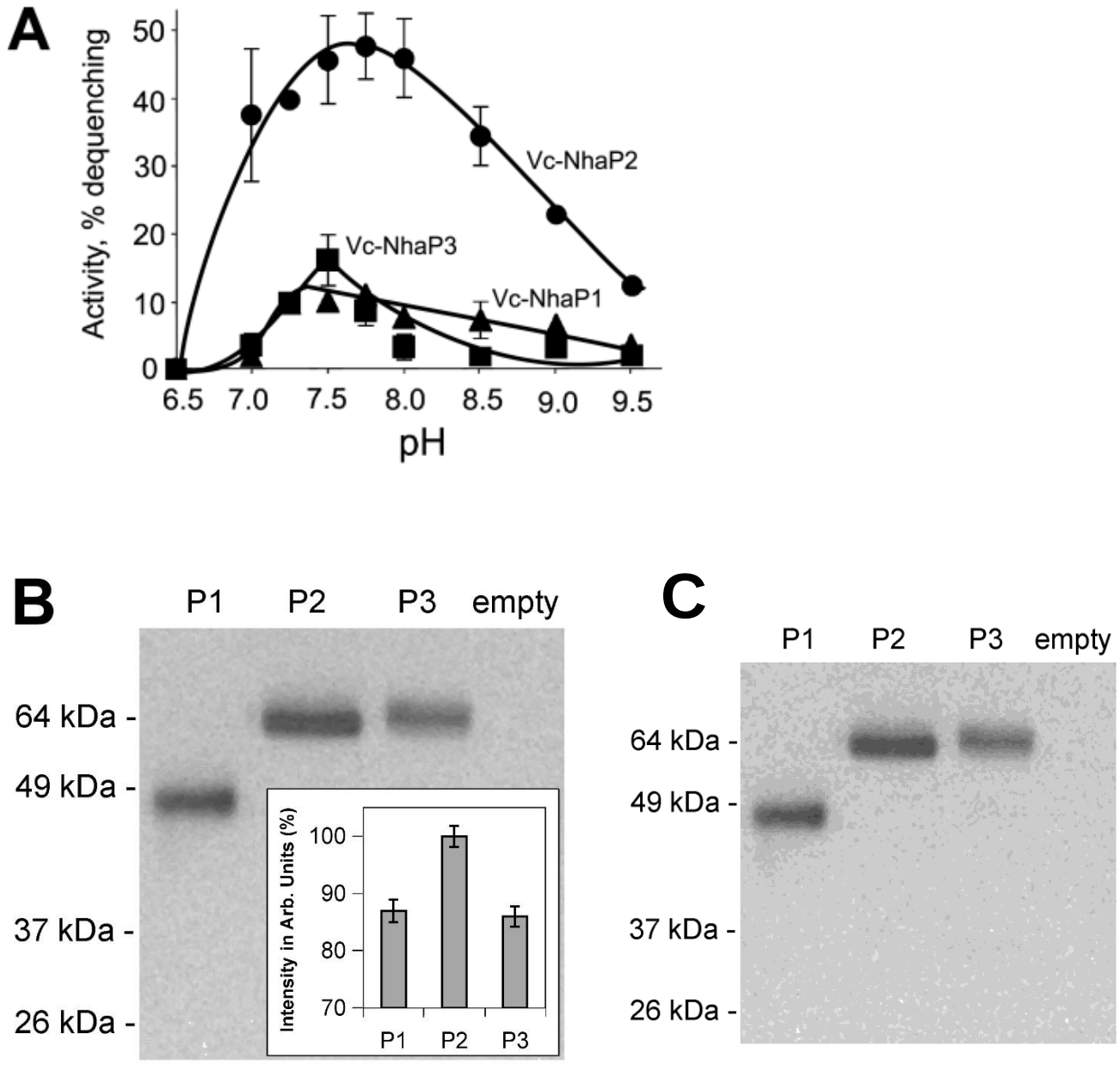

Fig 3.3 The direct comparison of K^+/H^+ antiport activities of all three Vc-NhaP paralogues. All three antiporters were cloned and functionally expressed in the antiport-deficient *E. coli* TO114 (see the text for details). The K^+/H^+ antiport activities were assessed at different pHs according to a standard protocol with 10 mM KCl added, as described in "Materials and Methods" and specified in the

legend for Fig. 3.1. **Panel A:** pH-profiles of the K^+/H^+ antiport mediated by Vc-NhaP1 (triangles), Vc-NhaP2 (circles), and NhaP3 (squares). Plotted are the averages of five different experiments. **Panel B and C:** Expression of three Vc-NhaP isoforms in *E. coli* TO114. Proteins of membrane vesicles were resolved by SDS PAGE in 10% polyacrylamide gel, and Western blot analysis was performed as described in "Materials and Methods". P1, Vc-NhaP1; P2, Vc-NhaP2; P3, Vc-NhaP3; "empty", negative control (vesicles isolated from the TO114 cells transformed with pBAD-TOPO).

Vc-NhaP2 was by far the most active K^+/H^+ exchanger among the three paralogues, showing approximately 50% of AO dequenching at pH 7.5 to 8.0 (Fig. 3.3A, circles), while maximal activities of Vc-NhaP1 and 3 were below 20% (Fig. 3.3A, triangles and squares). The activity profile of Vc-NhaP3 resembled that of Vc-NhaP2, having the maximum at pH close to 7.5 (Fig. 3.3A, squares), while Vc-NhaP1 demonstrated much broader "window of activity" from pH 7.25 to pH 9.0 (Fig. 3.3A, triangles).

To examine whether these differences in activity reflect the differences in representation of the three antiporters in the bacterial membrane, Western blot analysis of membrane proteins from the TO114 vesicles expressing either antiporter was performed (Fig. 3.3B). For this assay, cells of TO114 were transformed with either *Vc-nhaP* gene cloned into pBAD-TOPO plasmid in frame with the downstream V5 epitope for immunodetection. Separate control measurements of the activity of the tagged antiporters yielded results nearly identical to those obtained when the *Vc-nhaP* genes were cloned into pBAD24 without any ORF extensions (data not shown). We therefore assumed that the addition of the relatively compact C-terminal immunoreactive tags did not affect either expression/targeting or functional properties of the cloned antiporters. Levels of heterologously expressed Vc-NhaP proteins were similar (Fig. 3.3B). Of note, while the amounts of Vc-NhaP1 and

Vc-NhaP3 in the membranes are apparently close, the level of Vc-NhaP2 seems to be somewhat higher (Fig. 3.3B, "P2" lane). Such differences in expression could in part account for the observed levels of activity of heterologously-expressed Vc-NhaP3 (Fig. 3.). Indeed, Vc-NhaP2 is undoubtedly much more active than the equally expressed Vc-NhaP1 or Vc-NhaP3 (Fig. 3.3A, B). It should be stressed here, that in their native host, actual levels of expression of Vc-NhaP paralogues could be very different from those observed here in the model heterologous expression system (Fig. 3.3B). It is conceivable that their expression *in vivo* could be regulated by as yet unknown mechanisms.

3.3.3 K_m values and ion specificities of Vc-NhaP paralogues

Results of the side-to-side comparison of activities of Vc-NhaP isoforms in membrane vesicles are given in Table 3.3. Neither antiporter was able to mediate Li^+/H^+ exchange, but Vc-NhaP2 actually can bind Li^+ ion and exchange it for other alkali cations [23]. Whereas Vc-NhaP1 shows comparable activities with both Na^+ and K^+, Vc-NhaP2 prefers K^+ as a substrate and retains the ability to mediate modest Na^+/H^+ antiport. In contrast, the third isoform Vc-NhaP3 completely lost its ability to mediate Na^+/H^+ exchange, showing absolute specificity for K^+. Among all the paralogues, Vc-NhaP2 is the most active showing much higher affinity for both K^+ and Na^+, with apparent K_m of 1.62 and 1.04 mM respectively, whereas Vc-NhaP1 demonstrated lower affinity to Na^+ (apparent K_m = 9.09 mM) as well as K^+ (apparent K_m = 12.5 mM). The above comparative kinetic data in conjunction with sequence alignment (Fig. 3.4) help to recognize potential amino acid residues that may determine ion specificity and selectivity in NhaP-type antiporters from *V. cholerae* and, possibly, in other homologous ion exchangers from different microorganisms.

Table 3.1 Biochemical properties of Vc-NhaP proteins measured in inside-out sub-bacterial vesicles

Protein	[a] Apparent K_m,mM			Reference
	Na^+	Li^+	K^+	
NhaP1	9.09 (pH8.00)	–	12.5 (pH 7.75)	[24]
NhaP2	1.04 (pH7.50)	–	1.62 (pH 7.50)	[23]
NhaP3	–	–	8.3 (pH 7.50)	This work

[a] - measured as a concentration of substrate cation required for the half-maximal AO dequenching

Fig 3.4

```
Vc-NhaP1        91  PNLKDQ (12) LFSTF (27) LISPTDPIAVLAIVKKL--KAPKRISTQIEGESLFNDGF  177
Vc-NhaP2        83  ASFRVA (12) AVTTL (22) IVGSTDAAAVFSLLKGR--SLNERVGATLEIESGTNDPM  164
Vc-NhaP3        82  KEIRGV (12) LVSWG (22) LTVVTGPTVIVPLLRTV--RPTARLANILRWEGILIDPL  163
Vp-NhaP1        91  PNLKDQ (12) LFSTF (27) LISPTDPIAVLAIVKKL--DAPKRISTQIEGESLFNDGF  177
Vp-NhaP2        83  ASFRVA (12) AITTL (22) IVGSTDAAAVFSLLKGR--SLNERVGSTLEIESGTNDPM  164
Vp-NhaP3        81  KEIRGV (12) IISWA (22) LTVVTGPTVIVPLLRTV--RPNSTLANILRWEGILIDPL  162

Vc-NhaP1       178  GLV (73) HV--SGP (9) IGN-WT (15) FWELV (37) CGRYL (26) GLRG--G  365
Vc-NhaP2       165  AVF (75) GG--SGI (9) LGN--- (10) VLDGM (37) FARPI (23) GLR----  343
Vc-NhaP3       164  GAL (71) ESE-SGL (9) LAN--- (10) FKEHL (37) LARPA (22) APRGIVA  342
Vp-NhaP1       178  GLV (73) HV--SGP (9) IGN-WT (15) FWELV (37) ASRYL (26) GLRG--G  365
Vp-NhaP2       165  AVF (75) GG--SGI (9) LGN--- (10) VLDGM (37) FARPI (23) GLR----  343
Vp-NhaP3       163  GAL (71) ESE-AGL (9) LAN--- (10) FKEHL (37) VSRPL (22) APRGIVA  341

Vc-NhaP1       366  LALAMALSIP (25) VFSILVQGSTITPMIEK-------- 417
Vc-NhaP2       344  GAVPIILAVF (20) MVSLVVQGGTLTKAMSLAKVELPPK 398
Vc-NhaP3       343  ASISSLLAIK (20) IGTVVLQSATARPMALALKVSEPAP 397
Vp-NhaP1       366  LALAMALSIP (25) VFSILIQGSTITPMIEK-------- 417
Vp-NhaP2       344  GAVPIILAVF (20) MVSLIVQGGTLTKAMSLAKVELPPK 398
Vp-NhaP3       342  ASISSLFAIK (20) IGTVVLQSATARPMAIALGVAEPAP 396
```

Fig 3.4. Partial alignments of NhaP-type proteins from *V. cholerae* (Vc) and *V. parahaemolyticus* (Vp). The sequences were aligned using a BLASTP. The highly conserved same polar/charged residues located in or associated with putative TMSs are shadowed in dark grey. All the other charged/polar residues are shadowed in light grey. The accession numbers are: Vc-NhaP1, NP_230043.1; Vp-NhaP1, NP_799097.1; Vc-NhaP2, NP_232330.1; Vp-NhaP2, NP_799246.1; Vc-NhaP3, NP_230338.1; Vp-NhaP3, NP_799787.1.

Charged and polar conserved residues associated with putative transmembrane segments (TMSs) always are of special interest because such residues were shown to be important for function in different Na^+/H^+ antiporters studied to date [10,93-96], including those of the NhaP-type [53,97]. Sequence alignment of the NhaP-type proteins from two *Vibrio* species immediately identifies a number of such conserved potentially interesting residues (Fig. 3.4). In Fig. 3.5, selected charged/polar residues are shown in the "topographical Vc-NhaP context". Although topologies presented in Fig. 3.5 remain putative at this moment, they still are useful instruments of comparative analysis. As Fig. 3.5 shows, both general membrane topography as well as the distribution of the selected residues in all three Vc-NhaP isoforms seems to be generally conserved, as one would expect for a group of closely related paralogues.

However, it appears that Vc-NhaP3 lost one characteristic charged residue, corresponding to D133 in TMS V of Vc-NhaP2 or D146 in Vc-NhaP1 (Fig. 3.5, lower panel). Since Vc-NhaP3 also lost the ability to exchange Na^+ for H^+ (Fig. 3.1), one may suggest that these residues are crucial for binding of sodium ion and thus are playing a role of determinants of the cation specificity for a given antiporter type. In line with this assumption is the fact that mutation of the analog of D133 of Vc-NhaP2, D138 from a cyanobacterial NhaP antiporter into either Glu or Tyr, abolished Na^+/H^+ and Li^+/H^+ exchange activity [53]. Furthermore, the analogous D132 from the evolutionary distant Mj-NhaP1 was also found to be essential for activity [97]. It should be noted here that, although TMS V and XII are distant in the diagrams presented in Fig. 3.5, they could be very close in the actual three-dimensional structure, as it happens with discontinuous TMS IV and XI of NhaA from *Escherichia coli*, where Asp and Thr residues from both TMSs participate in the formation of common cation-binding site [10,96]. Another loss of polar/charged residue Vc-NhaP3 is substitution of the polar asparagine in position 161 of Vc-NhaP2 (position 174 in Vc-NhaP1) by neutral

isoleucine in TMS VI of Vc-NhaP3 (Fig. 3.4). There are a number of less obvious variations, as well, such as inversion of charge, with positive arginine replacing negative glutamate in the position of 154 of Vc-NhaP3 (Fig. 3.4). Mutational analysis of conserved residues in the Vc-NhaP group of antiporters is currently under way in our group.

Fig 3.5

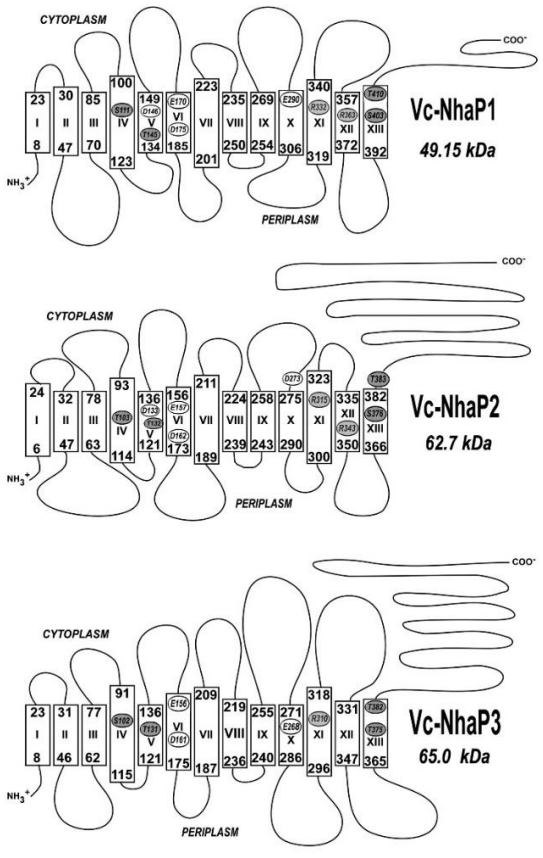

Figure 3.5 Predicted membrane topologies of Vc-NhaP paralogues. Topologies were deduced by the computer-assisted program MEMSAT-SVM (PSIPRED Server, Bioinformatics Group, University College London). Selected conserved residues associated with transmembrane segments and possibly participating in binding/translocation of substrate cations are shown. Negatively charged residues (empty circles), positively charged residues (light grey), polar residues (dark grey).

Mammalian Na^+/H^+ antiporters typically possess extended cytoplasmic soluble C-terminal modules ("tails") which are up to a few hundreds of amino acid residues in length and play an important role in regulation of the antiport activity by hormones, growth factors and Ca^{2+} levels [98-99]. Interestingly, many NhaP-type antiporters from prokaryotes also have such C-terminal tails [17,100], including Vc-NhaP proteins (Fig. 3.5). Recently, we reported that the truncated version of Vc-NhaP2 devoid of its cytoplasmic "tail" was still fully functional and, being expressed *in trans*, able to complement the growth phenotype in the *V. cholerae* mutant bearing chromosomal *nhaP2* deletion [51]. However, the truncated variant of Vc-NhaP2 had lowered antiport activity and affinity to K^+ ions, suggesting that the "tail", while not directly involved in the ion translocation, is still needed for optimal activity, possibly influencing the conformation of the Vc-NhaP2 molecule in the membrane and/or its oligomeric state [51].

3.3.4 Phenotypical effect of the deletion of Vc-NhaP3

Relatively low K^+/H^+ antiport activity of Vc-NhaP3 in the heterologous expression system (Fig. 3.3) apparently reflects a modest *in vivo* contribution of this antiporter to the overall ion homeostasis of *V. cholerae*. Indeed, the chromosomal deletion of *Vc-nhaP3* only has a minor phenotypical manifestation (Fig. 3.6). The growth of the ΔVc-NhaP3 mutant was inhibited (but not completely arrested) only in the presence of really high (500 mM) K^+ at pH 6.0 (Fig. 3.6, empty circles); introduction of the deleted gene on plasmid complemented the phenotype entirely (Fig. 3.6, closed circles). Growth of the mutant at pH 6.0 in the presence of different concentrations of NaCl or LiCl, as well as the growth at any other tested pH (7.2 and 8.0) and salt load was unaffected by the deletion (data not shown).

Fig 3.6

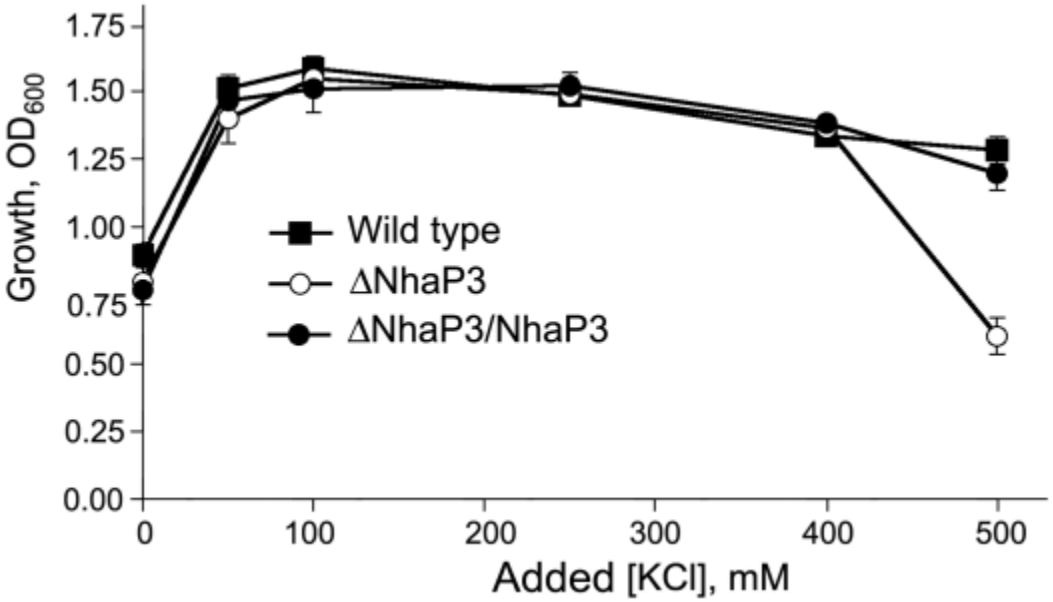

Fig 3.6 Growth phenotype of the VcΔ*nhaP3* deletion mutant of *V. cholerae*. Wild-type *V. cholerae* (closed squares), the chromosomal Δ*Vc-nhaP3* mutant (open circles) and the mutant expressing Vc-NhaP3 *in trans* (closed circles) were grown in LB-based media at pH 6.0 with increasing concentration of added K^+. Cultures were grown aerobically for 18 hrs, then OD_{600} was measured. Plotted are the averages of three separate experiments performed in triplicate.

3.3.5 Physiological consequences of the triple deletion of Vc-NhaP1, 2 and 3

The triple deletion mutant of *V. cholerae,* VcΔNhaP123 was constructed as described in Materials and Methods. VcΔNhaP123 expressing either Vc-NhaP1, 2 or 3 *in trans* (or harboring empty expression vector) was then used to analyze the physiological role of all three Vc-NhaP antiporters as a group. Growth of each strain was analyzed in LBB-based media containing increasing concentrations of KCl, NaCl and LiCl (up to 500 mM) at four different pH values (6.0,

7.2, 8.0 and 8.5). The triple NhaP deletion did not affect the growth of *V. cholerae* in NaCl- or LiCl-media at any pH tested (data not shown), indicating that the Vc-NhaP group is not involved in the homeostasis of these cations *in vivo*.

In contrast, elimination of the entire Vc-NhaP group of antiporters caused severe growth defects in media with varying [K^+], pointing at a seriously impared K^+ ion and/or pH homeostasis in the VcΔNhaP123 strain (Fig. 3.7, empty circles *vs.* closed squares). In the acidic (pH 6.0) medium, growth of the triple mutant was considerably suppressed at both low (<150 mM) and high (>350 mM) added KCl (Fig. 3.7A), and even within a "comfortable" range of 150 to 300 mM (apparently mimicking typical cytoplasmic K^+ content of marine *Vibrio* species, see [102] and Refs. therein) the growth yield of VcΔNhaP123 was lower than that of the parental wild type strain (Fig. 3.7A). Of note, at pH 7.2 (Fig. 3.7B) deletion of NhaP antiporters did not affect the growth in the presence of 50-500 mM of added KCl. It is possible that other, yet unidentified, cation transporting system(s) is able to regulate the internal potassium contents in *V. cholerae* growing at this pH. However, further alkalinization of the growth media revealed the inability of the VcΔNhaP123 strain to cope with high K^+ loads. As it is evident from Fig. 3.7C-D, at the external pH of 8.0 and 8.5, the triple deletion mutant was unable to grow when [KCl] in the medium exceeded 250 mM.

3.3.6 Partial complementation of the triple deletion by individual *Vc-nhaP* paralogous

In order to analyze physiological contributions of individual Vc-NhaP antiporters, genes encoding them were introduced *in trans* into the VcΔNhaP123 cells, and growth yield of the obtained transformants was documented at different pH and potassium loads. Functional Vc-NhaP1 completely rescued the growth of the VcΔNhaP123 cells at acidic pH in the presence of both low (below 150 mM) and high (above 250 mM) potassium concentrations (Fig. 3.7A, closed triangles).

Fig 3.7

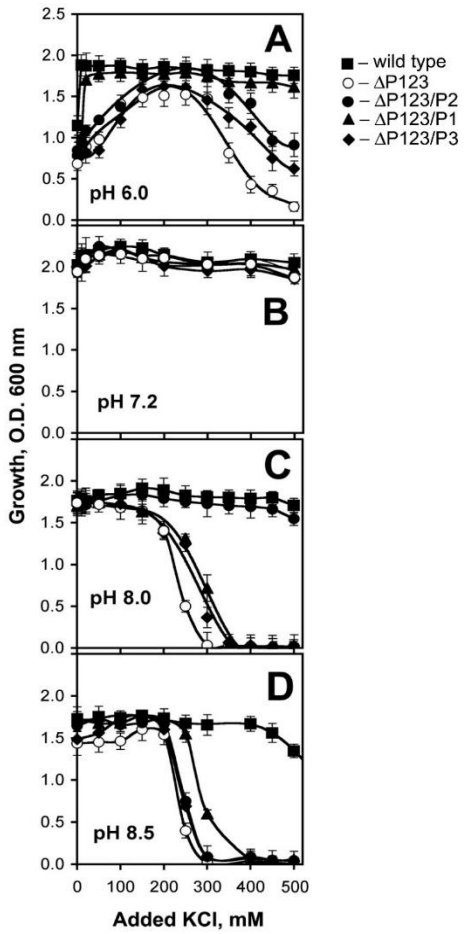

Fig 3.7 Growth phenotype of the Δ*nhaP123* deletion mutant of *V. cholerae*. The triple mutant *V. cholerae* strain VcΔNhaP123 was transformed with the pVc-NhaP1 (closed triangles), pVc-NhaP2 (closed circles) and pVc-NhaP3 (closed diamonds). Wild-type cells (closed squares) and triple mutant VcΔNhaP123 (empty circles) were transformed with empty pBAD24. Cells were grown aerobically for 18 h in 2 ml media in test tubes. In all cases, the LBB medium, adjusted to the desirable pH, was supplemented with 0.0002%(w/v) arabinose and the indicated concentrations of KCl. Growth yield for 18 hours was measured as the OD_{600} of the bacterial suspension. The starting OD_{600} was approximately 0.05 in all cases. Plotted are the averages of three separate experiments, each performed in triplicate.

This finding is in full accord with the previous observation about Vc-NhaP1 protecting cytoplasmic pH homeostasis and growth of *V. cholerae* in acidic media with limited and excessive concentrations of potassium ions [24]. At higher pHs, Vc-NhaP1 only provided a partial complementation at 250-300 mM of added KCl (Fig. 3.7C-D, closed triangles). Remarkably, although Vc-NhaP1 has lower affinity to both K^+ and Na^+ (Table 3.1) and shows better cation/proton antiport activity with Na^+ then K^+ [24], it was the only Vc-NhaP paralogue that completely rescued the growth of the triple mutant at elevated concentrations of K^+ in acidic growth environments (Fig. 3.7A). As to Vc-NhaP2 and 3, these antiporters complemented the growth at pH 6.0 only partially at [KCl] of 350 mM and higher (Fig. 3.7A, closed circles and diamonds).

At external pH of 8.0 and 8.5, the growth of the triple mutant was markedly inhibited at 250 mM of K^+ and completely arrested at higher potassium concentrations (Fig. 3.7C-D, open circles). Introduction of the high-affinity Vc-NhaP2, the most active K^+/H^+ antiporter of the group (Table 3.1, Fig. 3.3A), *in trans* resulted in complete restoration of growth of the VcΔNhaP123 cells at pH 8.0 (Fig. 3.7C, closed circles). Vc-NhaP3 offered a partial protection of growth at 250-300 mM of added KCl at pH 8.0 but not 8.5 (Fig. 3.7C-D, closed diamonds), while Vc-NhaP3 was the only Vc-NhaP isoform that partially protected the growth at pH 8.5 (Fig. 3.7C-D, closed triangles).

3.3.7 Vc-NhaP antiporters and acid resistance

Extrapolating the data shown in Fig. 3.7A, one could suppose that the Vc-NhaP group might boost the chances of survival when ingested *V. cholerae* cells pass the gastric acid barrier [60-61] in the course of a normal infectious process. In order to check such a possibility, acid tolerance response (ATR) tests were carried out. *V. cholerae* cells were challenged by HCl for 15,

60, and 90 min at pH 3.0, 3.5, 4.0, and 4.5. Neither the wild-type parental strain, *V. cholerae* O395N1, nor VcΔNhaP123 survived at pH 3.0 even after 15 min of incubation (data not shown). At pH 3.5, the triple mutant died at a much higher rate than the isogenic wildtype strain (Fig. 3.8, upper panel). The difference in survival exceeded two orders of magnitude at 15 min ($P < 0.0001$) and was still measurable at 60 min of incubation with acid. At 90 min, both survival rates were extremely low (5.0 × 10−6 percent or lower) and no statistically significant difference between the two strains could be detected. Therefore, we are inclined to consider this point as a tolerance limit for *V. cholerae* O395N1 for the survival in acid. Upon milder acid challenge at pH 4.0, the wild type still survived better than the VcΔNhaP123 at all time points. At 15, 60, and 90 min, the wild type had a higher average percentage of survival by 11.5, 8.0, and 11.55 percent, respectively, compared to the triple mutant (Fig. 3.8, middle panel). This trend was less pronounced at pH 4.5, although even under these conditions the deletion of Vc-NhaP antiporters resulted in somewhat lower survival rates at all time points (Fig. 3.8, lower panel).

3.4 Discussion

The presence of three fairly similar NhaP paralogues operating in the same bacterial membrane offers a rare opportunity to assess the biochemical and physiological results of divergent evolution of secondary ion transporters at its relatively early stages. Experiments presented in this communication revealed (i) striking differences in transport properties as well as physiological roles among the three Vc-NhaP isoforms, and (ii) necessity of all three antiporters for the maximal K^+ resistance of *V. cholerae* cells over the pH range 6.0 to 8.5. The latter observation indicates a coordinated co-evolution of three Vc-NhaP isoforms rather than absolutely independent divergence due to the random mutational process. As to the individual roles of Vc-NhaP1, 2 and 3, the data

summarized in Fig. 3.7 pose a few intriguing questions: **(1)** While it seems obvious how electroneutral K^+/H^+ antiporters could protect cells growing in acidic media from excessive external potassium (when ΔpH on the membrane can drive efflux of cytoplasmic K^+ mediated by NhaP-type proteins), the ΔpH on the membrane of marine vibrions is expected to be close to zero when external pH exceeds 8.0 [101]. If so, what drives K^+ efflux *via* Vc-NhaP proteins at high pH (Fig. 3.7C-D)? **(2)** It is not immediately clear why a relatively weak Vc-NhaP1 isoform offers much better complementation than the most active Vc-NhaP2 (Fig. 3.3A and Fig. 3.7A)? **(3)** How could different Vc-NhaP isoforms interact at the molecular level, so that only their simultaneous presence is ensuring the maximal K^+ resistance at all external pHs? Trying to answer question **(1)**, one could suggest that the internal pH in cells of *V. cholerae* growing at pH 8.0 is higher than measured earlier in cells of the closely related species *Vibrio alginolyticus* [101], so that the residual ΔpH is still sufficient to energize the NhaP antiporters. In accord with this suggestion, the most active Vc-NhaP2 provides full complementation at this pH, while Vc-NhaP1 and 3 protect the growth of the VcΔNhaP123 strain only partially (Fig. 3.7C). In addition, Vc-NhaP1 and Vc-NhaP2 (but not Vc-NhaP3) are $K^+(Na^+)/H^+$ antiporters able to mediate heterologous Na^+/K^+ exchange (ref [23-24]; Fig. 3.1 of this work), so that in the absence of ΔpH, Vc-NhaP 1 and 2 could expel internal K^+ at the expense of ΔpNa maintained on the membrane by NQR and powerful Na^+/H^+ antiporters, such as alkali-activated Vc-NhaA and Vc-Mrp residing in the same membrane [7,102-103]. Of note, Vc-NhaP3, being a "pure" K^+/H^+ antiporter (Fig. 3.1), failed to rescue the growth of VcΔNhaP123 at an external pH of 8.5 (Fig. 3.7D, closed diamonds), where ΔpH must be negligible, while Vc-NhaP1, whose preferred substrate is Na^+ [24], still protected the growth at 250-300 mM of KCl (Fig. 3.7D, closed triangles).

Fig 3.8

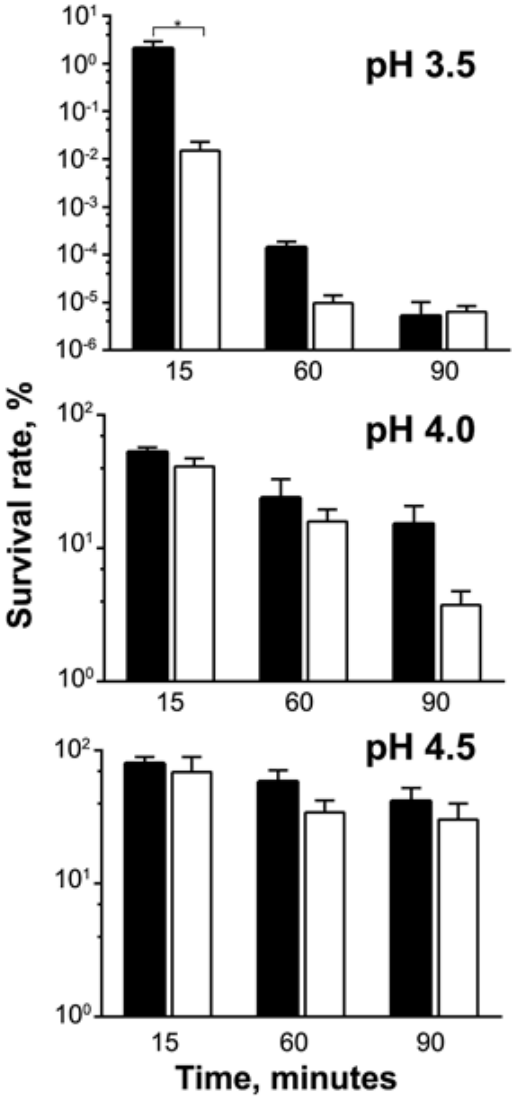

Fig 3.8 Acid tolerance response of the wild-type strain and the triple deletion mutant. The triple mutant *V. cholerae* strain VcΔNhaP123 (*open bars*) and the wild-type isogenic strain (*closed bars*) were both transformed with empty pBAD24 plasmids and exposed to LBK adjusted to pH 3.5, 4.0, and 4.5 with HCl for 15, 60, or 90 min. Aliquots of the treated cell suspensions were plated on LBK-Amp agar plates. After overnight incubation at 37 °C, the colony counts were compared to those of non-acid treated suspensions and plotted as percent of survival. Bars show standard error margins and the *asterisk* is for $P < 0.05$

Any substantive answer to question **(2)** apparently should take into account the role of Vc-NhaP1 in the pH homeostasis of *V. cholerae*. It has been shown that the K^+ (but not Na^+) transport mediated by Vc-NhaP1 leads to *alkalinization* of the cytoplasm of *V. cholerae* growing in acidic, low-K^+ media [24]. This experimental observation (Vc-NhaP1 moving H^+ out and K^+ into the cell against both ΔpH and ΔpK^+) clearly defies thermodynamic expectations and hints at possible functional coupling between Vc-NhaP1 and other (yet unidentified) energy transducer(s). However, regardless of a precise molecular mechanism, it seems to be clear that the growth defects of VcΔNhaP123 at pH 6.0 are largely due to impaired Vc-NhaP1-dependent pH regulation. This conclusion is supported by the following facts: (*a*) the growth phenotype of a single *Vc-nhaP1* deletion mutant is very similar to that of the triple VcΔNhaP123 mutant reported here [24]; (b) introduction of Vc-NhaP2 and 3 failed to rescue the growth in low-K^+ media at pH 6.0 and improved it only slightly at elevated concentrations of added KCl (Fig.3.7A).

As to the question **(3)**, it is worth mentioning that bacterial cation-proton antiporters of different architectures form dimers in the membrane [104,96], including those of the NhaP type [29,15]. It is conceivable that Vc-NhaP isoforms could form hetero-dimers, which are more efficient than "pure" antiporters. Alternatively, dimers formed by each isoform could co-exist in the membrane, functioning in concert to provide maximal resistance of growth. Indeed, neither of Vc-NhaP isoforms alone was able to complement the growth defect of the VcΔNhaP123 strain at pH 8.5, but the wild type parental strain, possessing all three antiporters, demonstrated a robust growth up to 500 mM of added KCl (Fig. 3.7D). Alterations in expression of *Vc-nhaP1*, *Vc-nhaP2* and *Vc-nhaP3* genes at various external pHs could hardly explain the observed different contributions of individual antiporters into the growth phenotypes of *V. cholerae*, because in this work they were expressed *in trans* from the same arabinose-induced pBAD promoter. However,

a pH-regulated expression of chromosomal *Vc-nhaP* genes *in vivo* could not be excluded at present. Investigation of such a regulation appears to be an interesting line of future work. Last but not least, our pilot data shown in Fig. 8 indicate that the Vc-NhaP group of cation–proton antiporters indeed contributes to the survival of *V. cholerae* at extremely acidic external pH values upon inorganic acid challenge. Therefore, the Vc-NhaP group might boost the chances of survival when ingested *V. cholerae* cells pass a potassium-rich gastric acid barrier [60-61] in the course of normal infectious process. The acid tolerance response (ATR) in *V. cholerae* was discovered more than 15 years ago [56] and its biochemistry has been studied since in a great deal of detail [56-59,105]. However, to the best of our knowledge, nothing was ever reported about a possible involvement of any cation–proton antiporter(s) in the ATR, the important physiological reaction, which enhances both the infectivity and epidemiological spread of *V. cholerae* [56]. Although the data presented in Fig. 3.8 are rather preliminary indications, Vc-NhaP123 paralogues appear to be potentially important for the actual infectious process at the stage of passing the gastric acid barrier by ingested *V. cholerae* cells. We are currently conducting the experiments to investigate this intriguing possibility in more detail.

Chapter 4.

Mutations of a single glycine in Vc-NhaP2, a cation-proton antiporter in *Vibrio cholerae*, confer the ability to exchange Li^+ for H^+

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Authors contribution

Mourin, M., performed all the experiments, contributed to data organization, manuscript writing and review; Schubiger, C.B. performed crucial part of the molecular cloning; Häse C.C. and Dibrov, P. critically reviewed and edited data and reviewed manuscript.

4.1 Abstract

The cation/proton antiporter Vc-NhaP2 from the important human pathogen *Vibrio cholerae* acts as a K^+/H^+ exchanger *in vivo*, contributing to the survival of *V. cholerae* at low pH and possibly enhancing the chances of the ingested *V. cholerae* cells to pass the acidic gastric barrier. Vc-NhaP2 is also able to exchange Na^+ but not Li^+ ions for H^+. We attempted to identify the amino acids responsible for the cation specificity of Vc-NhaP2 by limited alanine-scanning mutagenesis. Here we report a novel mutation, Gly159Ala, which enables Vc-NhaP2 to exchange Li^+ for H^+. Substitutions of Gly159 with Leu, Asp, or Lys, but not Ser had the same effect. Alanine substitution of the highly conserved Asn161 or Asp162 residues located nearby resulted in total inactivation of the antiporter. In the course of alanine-scanning mutagenesis, two distant residues, Asp273 and Leu289 that control the K^+ /Na^+ selectivity of Vc-NhaP2 were also identified. These findings

support the idea of "ligand shading" in the active site of Vc- NhaP2, where different alkali cations are coordinated by overlapping but not identical sets of ligands, thus differently affecting the probability of protonation of the antiporter during the catalytic cycle. In a phylogenetic context, our results demonstrate one of the mechanisms underlying rapid divergent evolution of paralogous membrane transporters through the accumulation of seemingly insignificant single-point mutations (such as Gly-to-Ala) that might, nevertheless, have an immediate adaptive value.

4.2 Introduction

Bacterial alkali cation/proton antiporters of the NhaP type form a surprisingly diverse group of membrane transporters [17] that contribute to the control of cytoplasmic pH and ion homeostasis by exchanging either monovalent cations such as sodium and/or potassium for protons [106,21,23-25] or K^+ for Na^+ through a heterological ion exchange [23]. The resulting transmembrane ion gradients can also serve as a direct energy source for a number of functions, such as the proton motive force buffering by ΔpK^+ [107], Na^+-substrate symports [108,7], or rotation of the Na^+-dependent polar flagellar motors [109]. The first NhaP type antiporter was identified in *Pseudomonas aeruginosa* in 1998 [106]. Presently, the NhaP family is considered as a part of the extended monovalent cation-proton antiporter 1 (CPA1) superfamily [17,100].

Of note, despite broad variations in Na^+-K^+ selectivity among the NhaP-type antiporters, Li^+ is a poor substrate for most of them [17]. This seems paradoxical, as Na^+ and Li^+ ions have similarly small ionic radii (1.16 and 0.90 Å, respectively) while K^+ is much bulkier (1.52 Å) and could be expected to require larger coordination sphere [110]. Indeed, in the majority of Na^+/H^+ antiporters of different types studied to date, Na^+ and Li^+ are equally good substrates while K^+ is not transported

at all [111]. Defying these expectations, the Vc-NhaP2 antiporter from the dangerous pathogen *Vibrio cholerae,* uses K^+ as a preferred substrate both *in vitro* [23] and *in vivo* [25].

In vivo, Vc-NhaP2 acts as a K^+/H^+ exchanger, contributing to the survival of *V. cholerae* at low pH and possibly enhancing the chances of the ingested *V. cholerae* cells to pass the acidic gastric barrier [25]. In the absence of K^+, Vc-NhaP2 was also able to exchange Na^+ for H^+ [25]. Ion competition assays in the inside-out membrane vesicles containing Vc-NhaP2, indicated that the antiporter can bind Li^+ and exchange it for other alkali cations [23]. Nevertheless, direct Vc-NhaP2-mediated Li^+/H^+ exchange was undetectable [23]. Here we report an unusual mutation, Gly159Ala, which enables Vc-NhaP2 to exchange Li^+ for H^+ directly. Furthermore, substitutions of Gly159 with Leu, Asp, or Lys (but not Ser) also resulted in this new function, i.e., the direct Li^+/H^+ exchange. Alanine substitutions of the highly conserved Asn161 or Asp162 residues located nearby resulted in total inactivation of the antiporter. In addition, alanine substitution of two distant residues, Asp273 and Leu289, affected the K^+/Na^+ selectivity of Vc-NhaP2 without altering its Li^+ discrimination. Together, these findings support our previously proposed idea of "ligand shading" in the active site of Vc-NhaP2, where different alkali cations use overlapping but not identical sets of ligands, thus differently affecting the probability of protonation of the antiporter during the catalytic cycle [17]. Our findings also indicate that in the actual 3D-structure of Vc-NhaP2, these two distant groups of residues (in positions 159-162 and 273-289) might be located in close proximity, contributing to the coordination of translocated cations.

4.3 Results

4.3.1 Selection of targets for site-directed mutagenesis

When crystallographic data are not available, mutational analysis remains a powerful tool of structural examination of membrane transporters. Here we applied it to probe amino acid residues that might determine the ion selectivity of Vc-NhaP2. A multiple sequence alignment of NhaP-type antiporters revealed a significant number of highly conserved amino acid residues (Fig. 4.1). Charged and polar amino acid residues associated with putative transmembrane segments are of special interest, as these residues were shown to form cation-binding pocket in Na^+/H^+ antiporters [10]. In particular, a ND motif (Asn158/Asp159) is present in NhaP1 from *Methanococcus jannaschii* [14] and in NhaP from *Pyrococcus abyssi*, where it was shown to be essential for antiport activity [15]. This ND motif is highly conserved in NhaP-type antiporters (Fig. 4.1) as well as throughout the entire CPA1 family. It is also present in Vc-NhaP2, corresponding to Asn161 and Asp162 there, indicating the possibility of their involvement in cation binding. In this study, these two residues together with several others have been chosen for mutagenesis. Conserved polar/charged as well as some nearby residues were selected. All targeted residues were mutagenized to alanine and the resulting phenotype was documented (Table 4.1).

4.3.2 Mutations inactivating Vc-NhaP2 completely

As one can see from Table 4.1, ten of the analyzed alanine substitutions resulted in complete inactivation of Vc-NhaP2. This kind of phenotype is exemplified by the Asp162Ala variant (Fig. 4.2A). The other mutant variants with abolished antiport activity showed the same pattern of activity with all alkali cations checked (data not shown). It has been reported that the mutation to alanine of Asp159 (an analog of Asp162 in Vc-NhaP2) and Asn158 (an analog of

Asn161 in Vc-NhaP2) in Pa-NhaP resulted in complete loss of activity by the protein from *P. abyssi* [15]. Our results strongly confirm that this ND motif, which is conserved in the CPA-1 family, is also critical for the antiport activity of Vc-NhaP2. Of note, residues with aliphatic, positively charged and polar side chains turned out to be important for the activity of Vc-NhaP2, as well: Leu154 and Leu287, Arg315 and Arg343, Ser376 and Thr383 (Table 4.1). In all cases, the absence of activity cannot be attributed to affected expression and/or targeting of modified antiporter, as confirmed by Western blotting (Fig. 4.2E).

4.3.3 Mutations suppressing the Vc-NhaP2-mediated Na^+/H^+ antiport

In NhaP-type antiporters, a negatively charged side chain is generally conserved in the position occupied by Asp273 in Vc- NhaP2, as well as a non-polar one at the position corresponding to Leu289, excluding two cases where non-polar methionine residues are present (Fig. 4.1). Noticeably, in the *V. cholerae* paralogous variants, Vc-NhaP1 and Vc-NhaP3, there is either methionine or alanine in this position, which makes Leu289 an interesting residue to modify. Mutations of Asp273 or Leu289 to alanine both resulted in a restrictive change in K^+/Na^+ specificity of Vc-NhaP2, converting it into an exclusive K^+/H^+ antiporter (Fig. 4.2, Panels B and C, respectively). Whereas the Asp273Ala substitution changed the pH profile of remaining K^+/H^+ antiport only slightly, resulting in measurable activity at pH 6.5, where the wild type antiporter is inactive (compare Fig. 4.2B to Fig. 4.2D), the mutation of Leu289 to alanine caused a significant change in the pH profile (Fig. 4.2C).

Table 4.1 Effects of mutagenesis on the activity of Vc-NhaP2.

Targeted Residue	Wild Type	Mutant Variant	Observed Phenotype
154	L	A	Abolished antiport activity
157	E	A	Abolished antiport activity
159	G	A	Ion selectivity change
159	G	D	Ion selectivity change
159	G	K	pH profile and selectivity change
159	G	L	Ion selectivity change
159	G	S	pH profile change
161	N	A	Abolished antiport activity
162	D	A	Abolished antiport activity
273	D	A	K^+/Na^+ selectivity change
287	L	A	Abolished antiport activity
289	L	A	K^+/Na^+ selectivity change
315	R	A	Abolished antiport activity
341	G	A	Abolished antiport activity
343	R	A	Abolished antiport activity
376	S	A	Abolished antiport activity
383	T	A	Abolished antiport activity

Activity of the Leu289Ala mutant variant gradually rose as pH increased from 6.9 to 9.5, reaching the maximal levels (approx 35% dequenching) at pH 9.5 (Fig. 4.2C), while in case of the wild type NhaP2 it was below 20% at pH 9.5 (Fig. 4.2D). Like the wild type Vc-NhaP2, both Asp273Ala and Leu289Ala variants showed absolutely no activity with Li^+ at any pH examined (Fig. 4.2, Panels B-D). Immunodetection again confirmed similar levels of these mutant variants in membranes of sub-bacterial vesicles (Fig. 4.2E).

4.3.4 A new activity caused by Gly159Ala substitution: Direct Li^+/H^+ exchange

Gly159 is located in close vicinity of the highly conserved ND motif (Fig. 4.1). Its substitution with alanine caused drastic changes in the ion selectivity of the antiporter.

Fig. 4.1

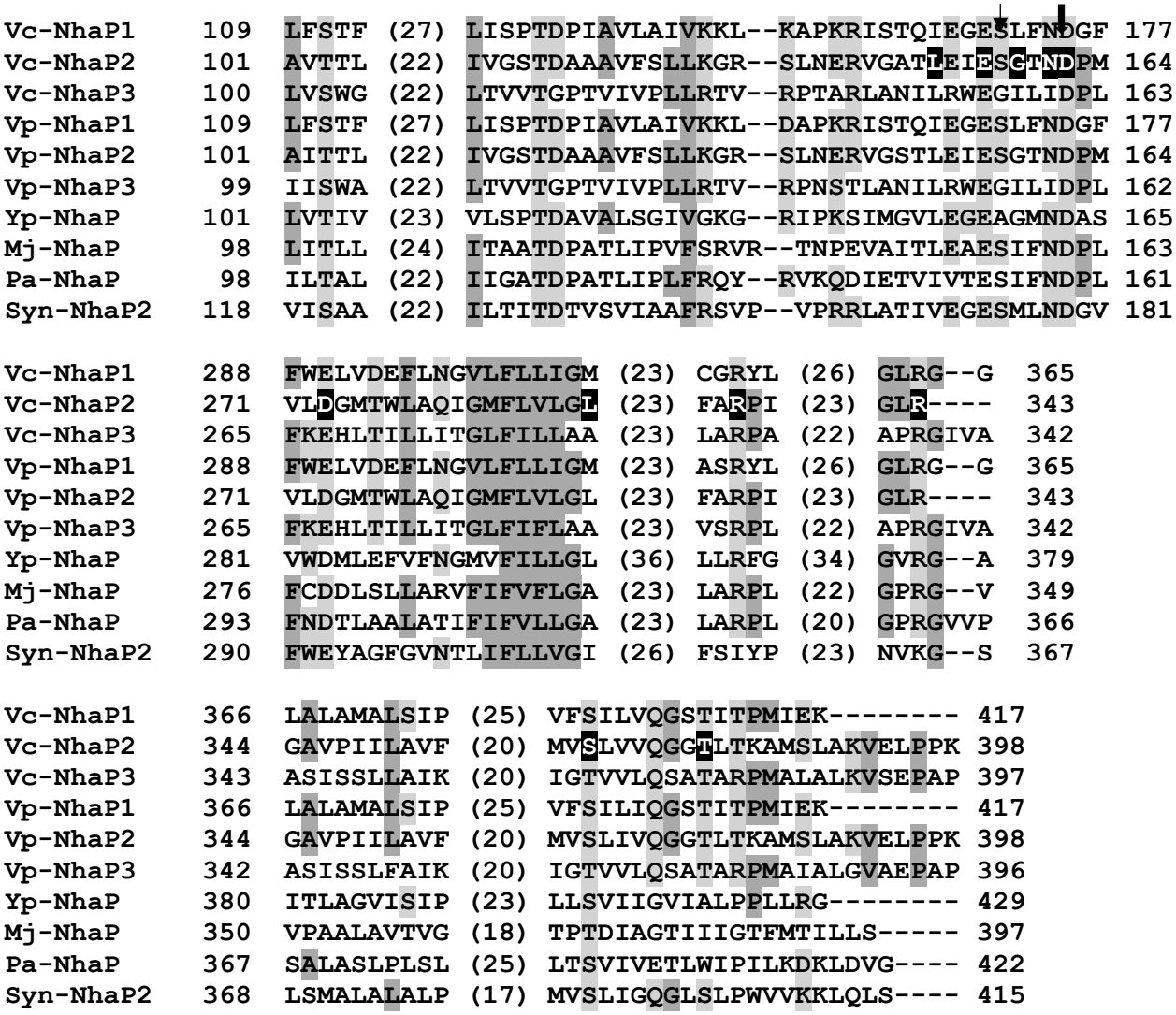


Fig 4.1 Selected conserved amino acid residues of representative members of NhaP subfamily. Conserved charged and polar residues are shadowed light grey, non-polar residues are shadowed dark grey, and those targeted for mutagenesis are shadowed black. The bold arrow indicates a functionally important ND motif (positions 161-162 in Vc-NhaP2). The regular arrow indicates an upstream glycine (G159) that was found to affect ion selectivity of Vc-NhaP2 (see the text for details). Protein sequences were aligned using MAFFT (http://mafft.cbrc.jp/alignment/ server/). The following accession numbers refer to the cation/H^+ antiporters shown: Vc-NhaP1 (*Vibrio cholerae*), NP_230043.1; Vc-NhaP2 (*V. cholerae*), NP_232330.1; Vc-NhaP3 (*V. cholerae*),

NP_230338.1;Vp-NhaP1 (*Vibrio parahaemolyticus*), NP_799097.1; Vp-NhaP2 (*V. parahaemolyticus*), NP_799246.1; Vp- NhaP3 (*V. parahaemolyticus*), NP_799787.1; Yp-NhaP1 (*Yersinia pestis*), NP_667581.1; Mj-NhaP (*Methanoccus jannaschii*), WP_010869549.1; Pa-NhaP (*Pyrococcus abyssii*), WP_010868413.1; Syn-NhaP2 (Synechocystis species PCC 6803), NP_441812.1.

Interestingly, introduction of a methyl group as the side chain at position 159 resulted in inverted ion preferences of Vc-NhaP2: now Na^+/H^+ antiport prevailed over K^+/H^+ antiport, reaching approx 30% dequenching at pH 8.0 (Fig. 4.3A, circles). But, most importantly, the Gly159Ala variant also exhibited a new type of activity, which was absent in the wild type Vc-NhaP2, namely, direct Li^+/H^+ antiport. This modest but measurable Li^+/H^+ exchange peaked at approx 10% dequenching at pH 8.0 (Fig. 4.3, triangles). Direct Li^+/H^+ exchange has never been observed in any of NhaP paralogues in *V. cholerae* [25].

4.3.5 Substitution of Gly159 with Aspartate, Lysine, Leucine and Serine

The presence of the bulkier alanine residue in place of glycine in the vicinity of a putative cation-binding residue altered the substrate selectivity of Vc-NhaP2. This raised a new question, namely whether a charged or a polar residue at this position would modify it even further, for example, by providing an additional ligand for Li^+ binding. To test such a possibility, Gly159 was mutated to the negatively charged aspartate, positively charged lysine, polar serine and much bulkier non-polar leucine. However, none of these substitutions altered K^+/Na^+ selectivity of Vc-NhaP, leaving K^+ as the preferable substrate (Fig. 4.3B-E).

Fig. 4.2

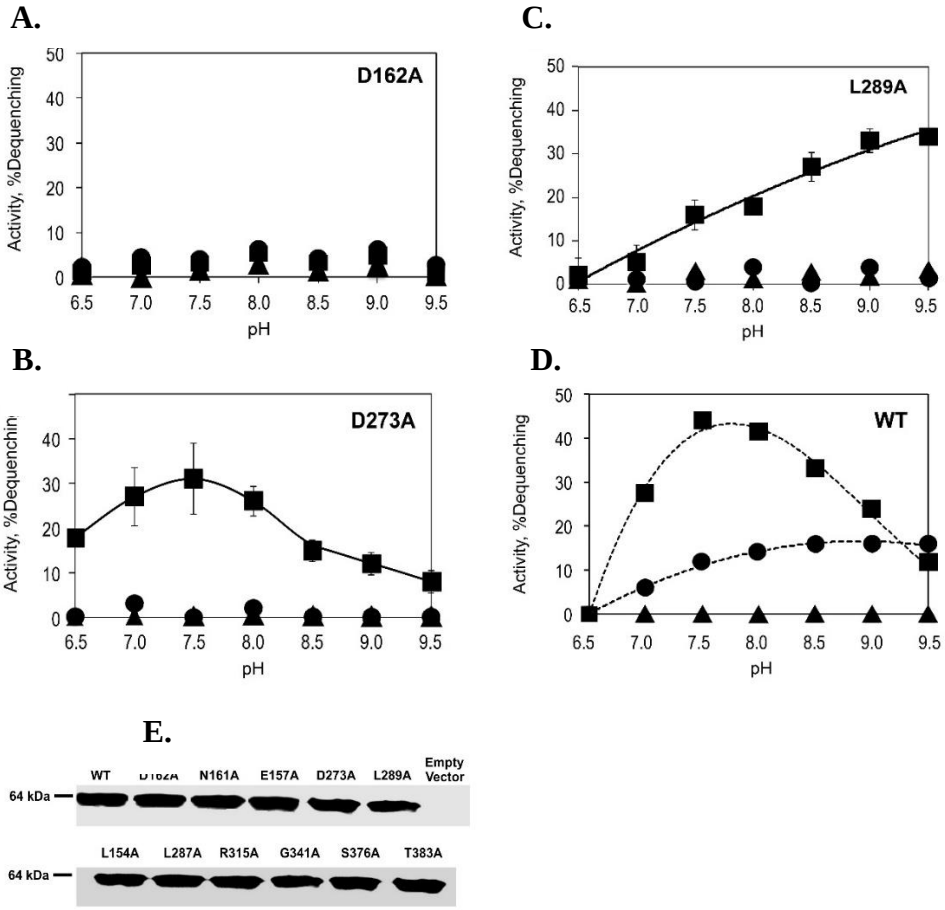


Fig 4.2 The complete inactivation of antiport activity (Panel A) or changes in K^+/Na^+ selectivity (Panel B and C) caused by mutagenesis. Only one of ten Ala substitutions that inactivate Vc-NhaP2 completely, D162A, is shown. Inside-out membrane vesicles were isolated and assayed for antiport activity with 10 mM NaCl (circles), KCl (squares) or LiCl (triangles) as described in "Materials and Methods". The pH profile of activity of the non-mutated Vc-NhaP2 is shown for comparison (Panel D). Plotted are the averages of three independent measurements. Bars show the standard deviation. Immunodetection of all the mutant variants of Vc-NhaP2 (Panel E) was carried out as described in "Materials and Methods". For the negative control, 'empty' vesicles isolated from the TO114 cells transformed with pBAD-TOPO were used.

The Asp159, Lys159 and Leu159 variants were all able to mediate direct Li^+/H^+ exchange (Fig. 4.3B, D, and E). Li^+/H^+ exchange in the Gly159Asp mutant variant showed a sharp maximum (approx. 12% dequenching) at pH 7.5, whereas the variant possessing the positively charged lysine at this position, exhibited a gradual rise of Li^+/H^+ exchange from pH 7.5 to the maximal activities (approx. 10% dequenching) at alkaline pH 9.0 and higher. Of note, the pH control of both K^+/H^+ and Na^+/H^+ antiport was somewhat altered in this variant (Fig. 4.3E, squares and circles). The bulkier side chain of leucine at position 159 led to slightly decreased Li^+/H^+ exchange activity compared to the Gly159Ala variant, showing >10% dequenching (Fig. 4.3B, triangles). The Ser159 variant showed no Li^+/H^+ exchange, behaving similarly to the wild type NhaP2, with minor alkaline shifts in pH profiles of K^+/H^+ and Na^+/H^+ antiport (Fig. 4.3C). Therefore, introduction of a charge or polar group at position 159 had no potentiating effect on Li^+/H^+ exchange. Again, immunodetection assays of Gly159Ala, Gly159Asp, Gly159Leu, Gly159Ser and Gly159Lys mutant variants in sub bacterial vesicles confirmed that all of them were expressed and targeted to the membrane properly (Fig. 4.3F).

4.3.6 Effect of Gly159Ala mutation on bacterial growth

In the next series of experiments, a possible physiological effect of the G159A substitution was analyzed, by testing the possibility of whether it enhances protection of bacterial growth against toxic external Li^+ *in vivo*. For these experiments, *E. coli* EP432, which is highly sensitive to environmental Li^+ [111], was used. Similar to previous studies, at pH 6.0, its growth was markedly inhibited when 50 mM of LiCl was added to the medium and almost completely arrested at 150 mM (Fig. 4.4A, filled diamonds). EP432 cells expressing wild type Vc-NhaP2 from a plasmid, exhibited a somewhat higher Li^+ resistance (Fig. 4.4A, filled circles).

Fig. 4.3

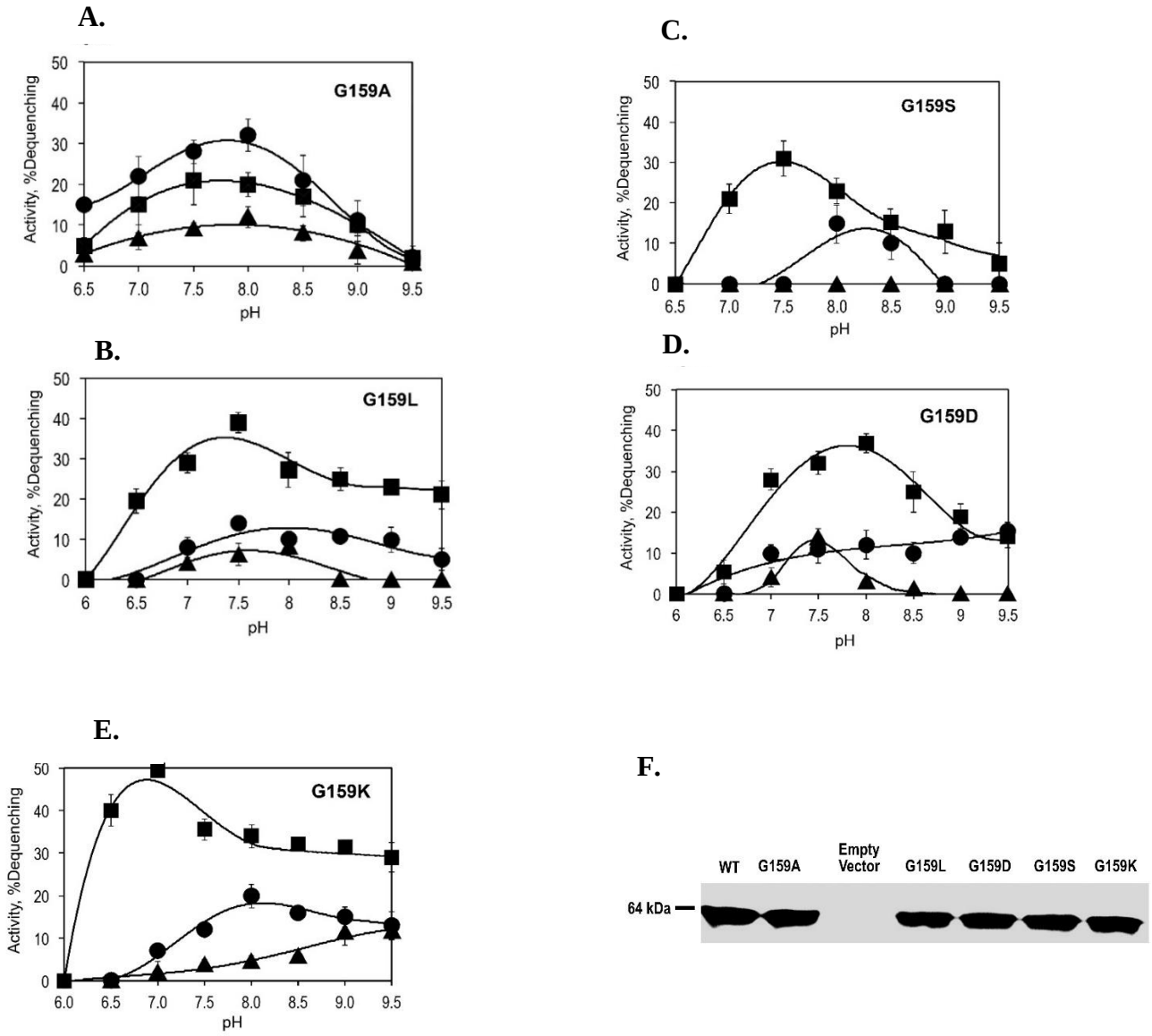


Fig 4.3 Effects of the substitutions of Gly159 by residues with different side chains (Panels A-E). Inside-out membrane vesicles were isolated and assayed for antiport activity with 10 mM NaCl (circles), KCl (squares) or LiCl (triangles) as described in "Materials and Methods". Plotted are the average values of three independent measurements. Immunodetection control (Panel F) was performed as described in the legend for Fig. 4.2.

Such an effect was expected due to the ability of Vc-NhaP2 to exchange Li^+ for Na^+ (or K^+) [23], which likely provided this protection against external Li^+. As shown in Fig. 4.4, transformation of *E. coli* EP432 with a plasmid containing the Gly159Ala variant resulted in markedly increased protection against high external LiCl concentrations. A normal growth yield was observed up to 200 mM of added LiCl, and a marginal growth ability was still registered in the presence of as much as 400 mM of LiCl (Fig. 4.4A, empty circles). Remarkably, the Gly159 mutated variant of Vc-NhaP2 was able to exchange external protons for cytoplasmic Li^+ ions. It suggests the possibility of detoxifying the cells by expelling Li^+. However, at pH 7.0 and 8.0, wild type Vc-NhaP2 was as effective in conferring Li^+ resistance as its Gly159Ala variant (Fig. 4.4B and 4.4C, filled and empty circles). Such a phenotype was not surprising, because Vc-NhaP2 is an electroneutral cation-proton antiporter, and the transmembrane pH difference (ΔpH) is the sole driving force for the exchange of any substrate cation for proton [23]. Therefore, direct Li^+/H^+ exchange through the Gly159Ala variant, was expected to occur (and contribute to the overall Li^+ resistance) only at sufficiently acidic external pH, where sizable ΔpH exists on the cell membrane [111].

4.4 Discussion

The data reported in this communication offer several new clues about the functional organization of the NhaP-type of antiporters, and in particluar the Vc-NhaP2 protein. First, while the Gly159, Asn161 and Asp162 residues are located in the putative transmembrane segment VI (TMS VI) of Vc-NhaP2, the Asp273 and Leu289 residues are both associated with the distant putative TMS X [25]. Nevertheless, mutation of either of them into alanine resulted in dramatic changes in the substrate specificity or abolished the antiport altogether (Asn161 and Asp162). Therefore, one may suggest that in an actual three-dimensional structure, TMS VI and TMS X are

close to one another, contributing to the formation of a cation-binding site of the antiporter. Such an arrangement indeed exists in the Na^+/H^+ antiporter from *Escherichia coli*, Ec-NhaA [74], belonging to the CPA-2 branch of the CPA family. In Ec-NhaA, unwound stretches of the discontinuous TMS IV and XI form a cation-binding cavity in the middle of the membrane [10]. Additional antiporters from CPA-2 also demonstrate a similar architectural theme. In Pa-NhaP, a Na^+/H^+ antiporter from a hyperthermophilic archaeon *Pyrococcus abyssi*, three negative/polar residues from three different TMSs (III, V and VI) participate in ion-binding [15,112]. Mj-NhaP from another thermophilic archaeon, *Methanococcoccus* employs acidic residues from TMS V and VI to bind substrate ions [14]. The Asn161-Asp162 dyad, predicted to represent an ND motif that is conserved in all antiporters belonging to the CPA-1 branch of the CPA family, predictably turned out essential for the activity of Vc-NhaP2, as well (Fig. 4.2A). Of note, the electrogenic CPA-2 transporters have in the same place a conserved Asp-Asp motif with an additional negative charge [14,112]. Both residues were proposed to bind protons during the electrogenic antiport cycle [10], however N-to-D substitution in this motif did not affect Na^+:H^+ stoichiometry of Mj-NhaP [14]. Nevertheless, our alanine mutagenesis of Asn161 in Vc-NhaP2, together with the previously reported phenotypes for Mj-NhaP [14], indicates that the side chain of asparagine is still involved in ion translocation, albeit indirectly. In contrast, the negatively charged component of the motif (corresponds to Asp162 in Vc-NhaP2) seems to coordinate translocated cations directly in the archaeal NhaP-type antiporters mentioned above [14-15,112]. Therefore, we suggest that Asp162 of the ND motif of Vc-NhaP2 is most probably directly involved in the coordination of translocated cations. However, further experiments will be needed to verify this prediction.

Fig. 4.4

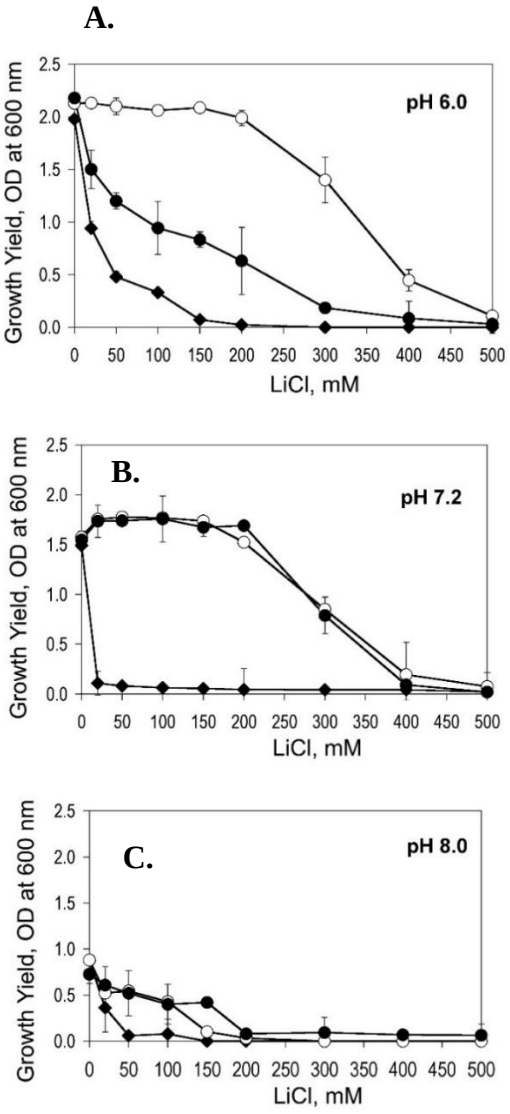


Fig 4.4 Physiological effect of the Gly159Ala substitution in Vc-NhaP2. Cells of *E. coli* EP432 transformed with the "empty" pBAD-TOPO vector (closed diamonds), *E.coli* EP432 expressing the G159A mutant variant of Vc-NhaP2 cloned into the same vector (open circles), and expressing the non-mutated Vc-NhaP2 (filled circles) were grown aerobically in non-cationic LB media supplemented with increasing concentrations of added Li^+ at indicated pHs. After 18 hours, growth yield was measured as light absorbance at 600 nm. Plotted are the averages of three separate experiments. Bars show standard deviation.

Another remarkable result was the acquisition of a new activity, namely direct Li^+/H^+ antiport, as a consequence of the substitution of Gly159 (located in the vicinity of the conserved Asn161-Asp162 motif) by another neutral, negatively or positively charged residue (Fig. 4.3). To the best of our knowledge, mutations of aliphatic residues having such an effect have never been reported before. These findings are in accord with our previously suggested idea of "ligand shading" in the active site of Vc-NhaP2, where different alkali cations use overlapping but not identical sets of ligands, thus differently affecting the probability of protonation of the antiporter during the catalytic cycle [17]. As the electrical properties of the side chain were not important for this effect, one may conclude that the substitutions of Gly159 affected the delicately balanced overall conformation of the ion-coordinating pocket by insertion of a bulky side chain in place of single –H rather than providing or eliminating ligands for coordination of substrate cations. As a result, binding of Li^+ by the mutated Vc-NhaP2 did no longer prevent its protonation and, therefore, allowed for the direct Li^+/H^+ exchange. In all tested substitutions of Gly159, the acquired Li^+/H^+ antiport remained minor compared to the K^+/H^+ and Na^+/H^+ antiport mediated by the mutated Vc-NhaP2 (Fig. 4.3). Thus, it was important to determine, whether such a modest additional activity brought into existence by a "neutral" mutation of a single glycine into alanine, could be of any physiological significance. It turned out that the ability of the mutated Vc-NhaP2 antiporter to exchange Li^+ for H^+ directly resulted in a considerably enhanced lithium resistance of the test strain, *E. coli* EP432, expressing the Gly159Ala variant of Vc-NhaP2 in acidic growth medium (Fig. 4.4A). This result demonstrates how accumulation of seemingly insignificant mutations may drive a rapid divergent evolution of proteins encoded by paralogous genes, as exemplified by Vc-NhaP1, NhaP2 and NhaP3 co-existing in the membrane of *V. cholerae* [25].

Chapter 5

A pathway leading to cation binding pocket determines the selectivity of NhaP2 antiporter in *Vibrio cholerae*

Authors contribution

Mourin, M. performed most of the experiments, contributed to data organization, manuscript writing and review; Mourin, M. performed all the mutant variants analysis experiments, contributed to the activity measurements in vesicles, Western blot analysis and *in silico* analysis; Wai, A. and O'Neil, J. helped in *in silico* analysis; Schubiger, C. B. constructed the mutant variants. O'Neil, J., Häse C.C. and Dibrov, P. critically reviewed manuscript.

5.1 Abstract

The Vc-NhaP2 antiporter from *Vibrio cholerae* exchanges H^+ for K^+ or Na^+ but not for the smaller Li^+. The molecular basis of this unusual selectivity remains unknown. *Phyre*^{2} and Rosetta software were used to generate a structural model of the Vc-NhaP2. The obtained model suggested that a cluster of residues from different transmembrane segments (TMSs) forms a putative cation-binding pocket in the middle of the membrane: D133 and T132 from TMS V together with D162 and E157 of TMS VI. The model also suggested that L257, G258,

and Y251 from TMS IX together with T276, D273, Q280 and L289 from TMS X as well as L342 from TMS XII form a pathway for translocated ions with a built-in filter determining cation selectivity. Alanine-scanning mutagenesis of the identified residues verified the model by showing that structural modifications of the pathway resulted in altered cation selectivity and transport activity. In particular, L257A, G258A, Q280A, and Y251A variants gained Li^+/H^+ antiport capacity that was absent in the nonmutated antiporter. T276A, D273A, and L289A variants exclusively exchanged K^+ for H^+, while a L342A variant mediated Na^+/H^+ exchange only, thus maintaining strict alkali cation selectivity

5.2 Introduction

Cation-proton antiporters are ubiquitous membrane ion pumps that play a key role in the ion and pH homeostasis of all living cells. In *Vibrio cholerae,* as in all marine-borne bacteria, both the survival and dissemination in diverse ecological niches is strictly dependent upon the circulation of alkali cations, primarily Na^+ and K^+ [7,16,27,111]. The membrane of *V. cholerae* contains a trio of cation-proton antiporters of a specific type, NhaP, that are responsible for the transport of K^+ and Na^+ [17,23]. They are encoded by three paralogous structural genes, *Vc-nhaP1, 2* and *3*. Physiological analysis of the *nhaP123* triple deletion mutant of *V. cholerae* indicated that Vc-NhaP2 plays a major role in the survival of bacterial cells challenged by inorganic acid, HCl [25]. Thus Vc-NhaP2 might be a new, previously unknown, component of the Acid Tolerance Response (ATR) [25] enhancing the chances of survival when ingested *V. cholerae* cells pass a K^+-rich gastric acid barrier [61] in the course of a normal infectious process. Therefore, the Vc-NhaP123 group seems to be a promising potential target for the development of novel antimicrobials narrowly targeting *V. cholerae*.

Among the three NhaP paralogues the Vc-NhaP2 antiporter acts as a K^+/H^+ exchanger *in vivo*, contributing to the survival of *V. cholerae* at low pH [23]. Kinetic experiments with Vc-NhaP2 have also revealed a unique feature of this antiporter: its ability to bind Li^+ and exchange it for other alkali cations but not for H^+ [23,25]. Of note, all Na^+/H^+ antiporters characterized until the discovery of the NhaP family in 1998, could transport Li^+ in place of Na^+. This seemed natural, given the smaller ion radius of Li^+ (0.76 Å for Li^+ *vs.* 1.02 Å for Na^+, see [115]). To resolve this paradox, we have suggested a hypothesis of "ligand shading" [17]. It states that protons, alkali and alkali earth cations all compete for different subsets of ligands within the common spacious ion-binding site of Vc-NhaP2. While H^+ requires only one negative ligand (X^-), the optimal coordination number for Li^+ is six [36]. If the subset of ligands for Li^+ happens to include X^-, the Li^+ ion would outcompete H^+, thus preventing Li^+/H^+ exchange. We named this situation "ligand shading", implying that the Li^+ ion directly (by actual binding to X^-) or indirectly (by affecting its position in the ion-binding site) prevents H^+ from binding to its ligand. Na^+ and K^+, however, could bind to their own subsets of ligands that do not include/affect X^-. Both ions require six to eight ligands for optimal coordination [36], so, unlike H^+, they should easily displace Li^+ from the ion-binding site. This would make possible Na^+/Li^+ or K^+/Li^+ exchange, as well as the exchange of both Na^+ and K^+ with H^+, but not direct Li^+/H^+ exchange.

Importantly, in the case of Vc-NhaP2, binding of Na^+ might result in a "partial shading" of X^-, not preventing the protonation of X^- completely but making it less efficient: having very similar affinities for K^+ and Na^+, Vc-NhaP2 nevertheless is "kinetically incompetent" when exchanging H^+ for Na^+ in the presence of K^+ [17]. Another critical advantage of Vc-NhaP2 as an experimental subject is that direct Li^+/H^+ exchange could be

activated here by a single “neutral” amino acid substitution, G159A [32]. This opens a unique opportunity for modelling-guided Ala-scanning mutagenesis aimed at the identification of all possible substitutions having the same effect. In conjunction with the *in silico* structural analysis, this would seriously facilitate a fine mapping of the cation-binding site in Vc-NhaP2.

In the present study, we combined protein structure modeling with the site-directed mutagenesis and antiport activity measurements to localize and characterize the structural element(s) responsible for cation selectivity of Vc-NhaP2. Our *in silico* analysis suggests that a cluster of negatively charged and polar residues belonging to different transmembrane segments (TMSs) forms a putative cation binding pocket in the middle of the membrane. The model also proposes that a number of amino acid residues from TMS IX, TMS X as well as TMS XII, form a pathway for substrate ions. The limited Ala-scanning mutagenesis of identified residues supports the idea that this pathway contains a built-in filter determining the cation selectivity.

Another aim of this work was to evaluate *in silico* homolog-based structural modeling as a guiding tool for the selective, precisely targeted mutagenesis. The presented data allow us to conclude that this approach, despite of its inherent limitations, is a valuable tool for identification of potential functionally important amino acid residues in membrane transporters lacking a high-resolution structure.

5.3 Results

5.3.1 Structural model of Vc-NhaP2 reveals a putative cation-binding site

In the present study we intended to use *in silico* modelling as a guiding tool for targeted mutagenic analysis. An *in silico* high-resolution structural model of Vc-NhaP2 was developed based on the available crystallography data on the NhaP-type protein from *Pyrococcus abyssi*

(Pa-NhaP) [15]. Pa-NhaP (NCBI accession number, WP_010868413.1) and Vc-NhaP2 (NCBI accession number, NP_232330.1) have 27% of identical and 83% similar amino acid residues. The protein sequences were aligned using MAFFT (http://mafft.cbrc.jp/alignment/server/). Since Pa-NhaP and Vc-NhaP2 are close homologs, they may be subjected to the homologue-based modelling [28,43]. The generated model of Vc-NhaP2 has an inward-open conformation (Fig. 5.1). This is very similar to the 3D-structure of the "template" antiporter, Pa-NhaP [14]. Like Pa-NhaP, Vc-NhaP2 is present as a dimer in the *Phyre*^{2}-generated structure (not shown). Each protomer of Vc-NhaP2 has 13 transmembrane segments (TMSs) connected by short loops or helices on the membrane surface. TMS IV-VI and TMS XI-XIII form a 6-helix bundle, while TMS I-III and TMS VII-X form the dimer interface. TMS I-VI and TMSs VIII-XIII are two halves of an inverted 6-helix repeat, connected by TMS VII. TMS V and TMS XII in the 6-helix bundle are discontinuous. Their cytoplasmic and extracellular halves are connected by unwound stretches with an antiparallel orientation, which cross one another in the center of the protomer (Fig. 5.1). The Vc-NhaP2 surface potential modeling revealed that a highly negatively charged (red colored) cavity is present in the middle of the antiporter (Fig. 5.2A). Three lines of experimental evidence suggest that this is where the putative cation-binding pocket is located: (i) in the "template" antiporter, Pa-NhaP, the charged and polar amino acid residues present in this negatively lined cavity (specifically, D159, D130, T129 and S155) are directly involved in cation binding [14]; (ii) In Vc-NhaP2, we previously conducted substitution of D162 which corresponds to D159 of Pa-NhaP, and it completely inactivated the Vc-NhaP2 [32]; (iii) In this work, further alanine substitutions of three selected amino acid residues suggested by the model, inactivated Vc-NhaP2, as well (see Fig. 5.3 and below). Taken together, the model predictions and results of two rounds of Ala mutagenesis

strongly indicate that in Vc-NhaP2 a cluster of negatively charged and polar residues belonging to TMS V and VI likely forms the cation-binding pocket in the middle of the membrane where D133 and T132 from TMS V are in close proximity to D162 and E157 of TMS VI are located (Fig. 5.2B).

Fig 5.1

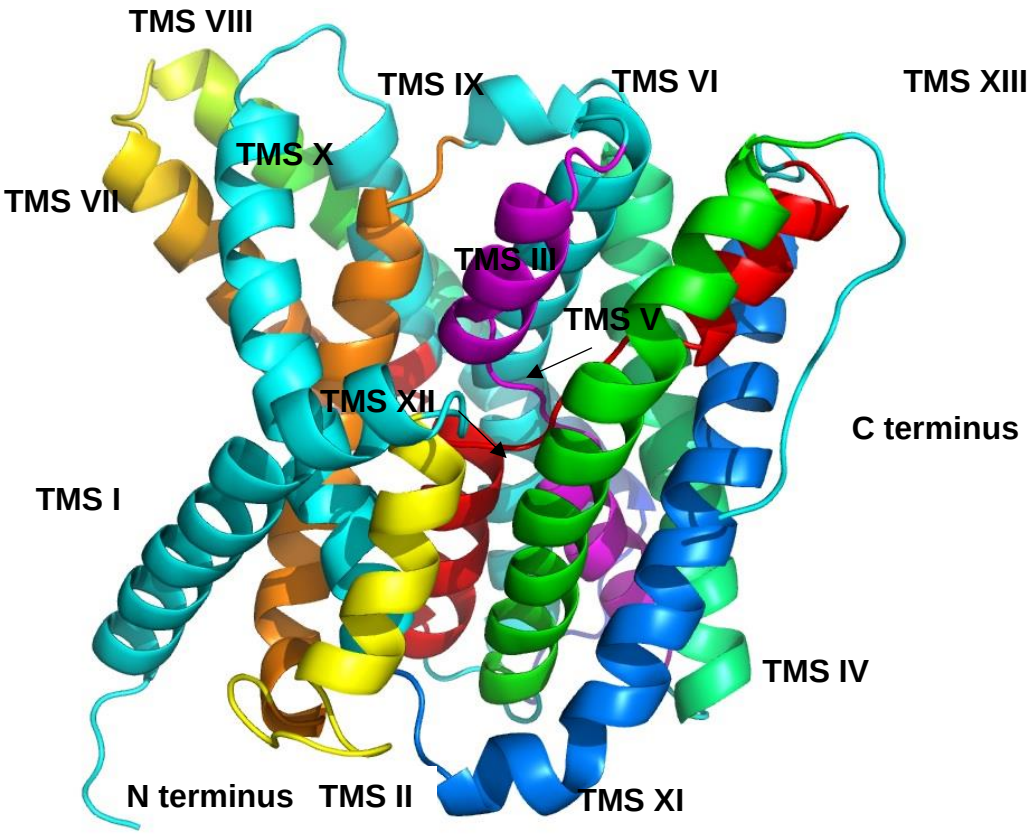


Fig 5.1 Inward-open view of the 3D model of the transmembrane part of Vc-NhaP2. The model was generated by Rosetta and visualized with PyMOL 1.6 as described in "Materials and Methods". The model is shown in a rainbow of colors from blue for the N-terminal methionyl residue to red for the C-terminal isoleucine residue of the protein. TMSs are numbered from 1 to 13. TMS V (Magenta) and TMS XII (red) are indicated with arrows.

Fig 5.2

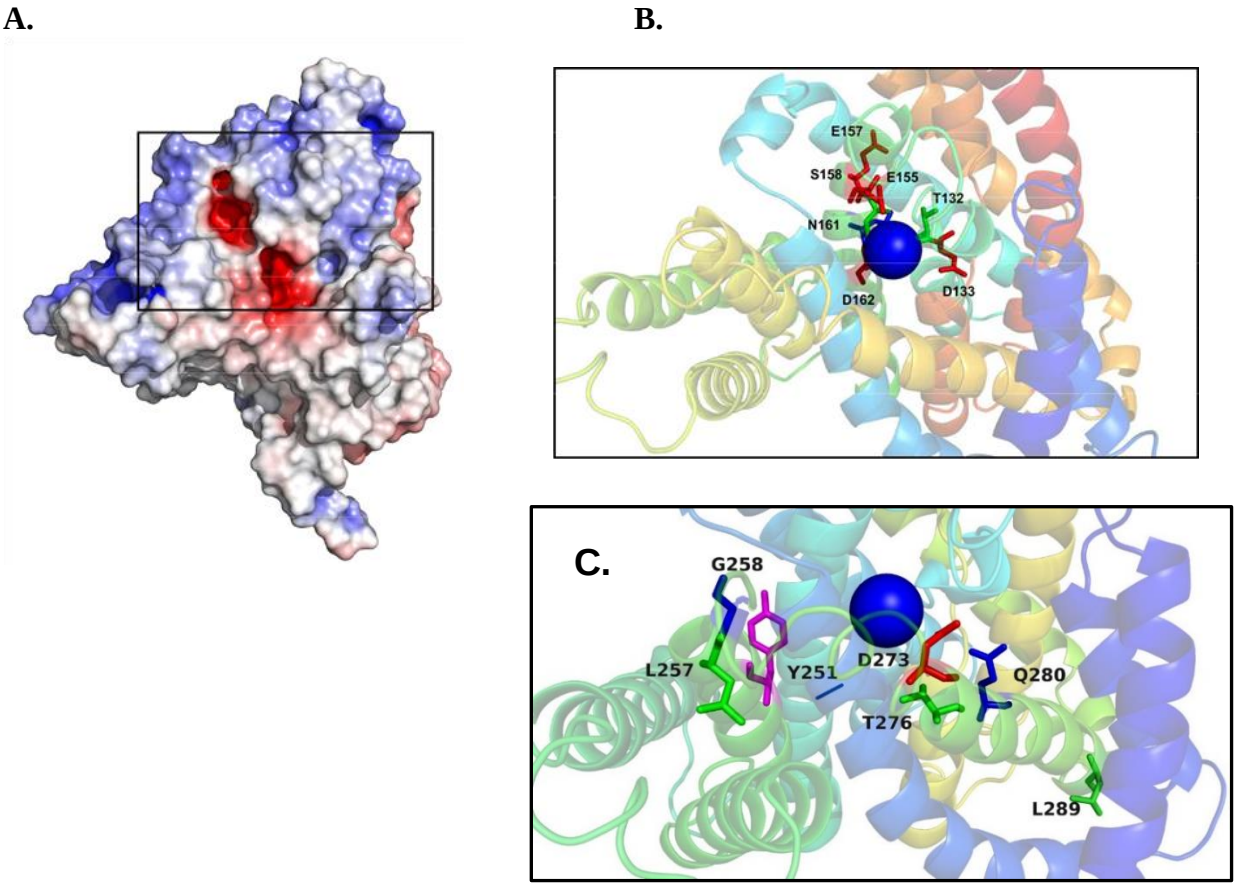


Fig 5.2 Identification of the putative cation-binding pocket and cation selectivity elements in Vc-NhaP2. (A) The surface potential of Vc-NhaP2. A highly negatively charged (red colored) cavity is present in the middle of the antiporter. The charged and polar amino acid residues present in this negatively lined cavity are indicated in panel B. The blue color indicates the positively charged residues lining the exterior of the antiporter. (B) Amino acid residues forming the putative cation-binding pocket. D133 and T132 from TMS V located in close proximity to D162 and E157 of TMS VI are shown in a stick-and-surface representation. For K^+ cation ligand (blue sphere) the structure was adjusted by changing the van der Waals radius to the appropriate value (see "Materials and Methods"). (C) Detailed view of supposed cation selectivity filter. Residues from TMSs IX, X and XII presumably form a transmembrane

pathway determining the cation selectivity. L257, G258, and Y251 from TMS IX together with T276, D273, Q280 and L289 from TMS X as well as L342 from TMS XII, are shown as stick-and-surface representation.

5.3.2 Model suggests a pathway determining cation selectivity

Based on mutagenesis analysis we identified a number of amino acid residues that were changing the activity of Vc-NhaP2 antiporter with different cations or even creating new activity, Li^+/H^+ exchange. We interpreted these observations as changes in ion selectivity. We have assumed that a pathway formed by Y251, L257 and G258 from TMS IX together with T276, D273, Q280 and L289 from TMS X as well as L342 from TMS XII, extending from the cytoplasmic side to the putative cation binding pocket might exist that determines the cation selectivity of Vc-NhaP2 (Fig. 5.2C). Further *in silico* structural model suggested that mutation of these amino acid residues might create a conformational change affecting the delicately balanced overall conformation of the ion-coordinating pocket and thus allowing different ions to be translocated. This indicates the indirect involvement of this cluster of amino acid residues in determining the ion selectivity of Vc-NhaP2 as seen in Zr-Sod2-22[43]. It has also been experimentally shown that all the cations usually competitively bind to the same binding pocket but binding of specific ions only allow them to be exchanged for protons either to the cytoplasmic or the periplasmic side. Certain ions bind in a functional way allowing a conformational change to occur that permits those ions to be exchanged for protons [127]. This finding supports the idea of "ligand shading" in the active center of Vc-NhaP2 [17]. This explanation is also supported by the observation that changes in the side-chain size of the Gly159 located near the putative cation binding pocket caused drastic changes in the ion

selectivity of the antiporter [32]. Introduction of a simple methyl group or a charged group at the side chain at position 159 resulted in Li^+ selectivity. As the side chain characteristics was not important for this effect, it can be assumed that the substitutions of Gly159 affected the delicately balanced overall conformation of the ion-coordinating pocket by introducing a bulky side chain in place of single –H rather than providing or eliminating ligands for coordination of substrate cations. As a result, binding of Li^+ by the mutated Vc-NhaP2 did no longer prevent its protonation and, therefore, allowed for the direct Li^+/H^+ exchange. A recent study showed that such a selectivity filter exists in the vicinity of the cation binding core of the *Zygosaccharomyces rouxii* Sod2-22 antiporter [43]. The cation specificity of Sod2-22 antiporter may be determined by a combination of the size of the filter, its hydrophobicity and the position of the filter relative to the aspartic residue 176 (corresponding to Asp162 in Vc-NhaP2) [43]. Despite the fact that Vc-NhaP2 is evolutionary distant from Zr-Sod2-22, the mechanism of ion selectivity might be conserved. Another possible explanation is that the binding sites in the selectivity filter are not able to pay for the energetic cost of Li^+ dehydration or simply providing geometric constraints against Li^+ ion. Ions usually lose their hydration shell while entering the antiporter [15]. This is also evident from ion selectivity of K^+ channel which is highly selective to only K^+ and not Na^+ [128]. In case of K^+ channel the K^+ ions in the filter is surrounded by the oxygen atoms that are arranged like the water molecules that encircle hydrated K^+ ions in the cavity of the channel. Dehydration energy can not be compensated while Na^+ binds due to its small size compared to K^+ and thus the filter selects only K^+ ion [128].

5.3.3 Mutations that inactivate Vc-NhaP2 completely

The analyzed alanine substitutions of the selected amino acid residues presumably involved in direct cation binding (Fig. 5.2B) indeed resulted in complete inactivation of Vc-NhaP2. Three mutant variants (D162, N161 and E157) characterized previously [32] showed absence of activity with all alkali cations tested. In this work, the same effect was observed with the D133A substitution (Fig. 5.3A). All the above residues are highly conserved through the entire CPA-1 family [32]. Furthermore, a residue with a polar side chain, T132, turned out to be critical for the activity of Vc-NhaP2, as well (Fig. 5.3A). However, changing S158 or E155 to alanine had no significant effect on the activity of Vc- NhaP2 (data not shown). In all cases, the absence of activity cannot be attributed to low expression levels and/or impaired targeting of modified antiporter proteins, as the amounts of the Vc-NhaP2 variants in the membrane vesicles was nearly the same in all constructs, as confirmed by Western blotting (Fig. 5.3D).

5.3.4 K^+ and Na^+ selectivity changes caused by mutations

A pathway formed by amino acid residues from TMSs IX, X and XII which is leading to the cation binding pocket (Fig. 5.2C), presumably determines the selectivity of Vc-NhaP2. In accord with this idea, mutation of D273 or L289 of TMS X into alanine converted Vc-NhaP2 into a K^+/H^+ antiporter, abolishing its ability to conduct Na^+/H^+ exchange [32]. Noticeably, the T276A substitution within the same TMS, also causes a restrictive change in the K^+/Na^+ specificity of Vc-NhaP2, although some residual Na^+/H^+ antiport activity remains detectable in this variant (Fig. 5.3B). On the other hand, the T276A substitution drastically enhances K^+/H^+ antiport, which in this variant reached approximately 70% of dequenching at

pH 8.5 (Fig. 5.3B), while in the wild type Vc-NhaP2 it never exceeded 46% [23]. In addition, the T276A substitution broadened the pH profile of K^+/H^+ antiport activity, maintaining it at approximately 50% at pH 9.5, while in the wild-type Vc-NhaP2 it was below 20% at this alkaline pH [23]. Thus, mutation of D273, T276 as well as Leu289 from TMS X to alanine converts Vc-NhaP2 into a highly selective K^+/H^+ antiporter. Like the wild type Vc-NhaP2, T276A, D273A and L289A variants showed no activity with Li^+ at any pH tested.

Interestingly, mutation Leu342Ala resulted in the opposite effect: it converts Vc-NhaP2 into a Na^+/H^+ antiporter with a minor (below 10% dequenching) K^+/H^+ exchange activity (Fig. 5.3C). The L342A variant exhibited a pH profile of Na^+/H^+ antiport activity with a maximum (about 42% dequenching) at pH 7.0 to 8.0 (Fig. 5.3C). Like the wild type Vc-NhaP2, it showed no activity with Li^+ at any pH tested. Immunodetection of these mutant variants confirmed that they all had similar levels of expression in the membranes of sub-bacterial vesicles (Fig. 5.3D).

5.3.5 Mutations causing a new activity: Li^+/H^+ antiport

Direct Li^+/H^+ exchange has never been observed in any NhaP paralogues in *V. cholerae* [17]. We found that L257, G258 and Y251 from TMS IX as well as Q280 from TMS X determine Li^+ selectivity, as alanine mutant variants of these residues gained Li^+/H^+ antiport capacity that was absent in the wild type Vc-NhaP2 (Fig. 5.4). The L257A variant exhibited direct Li^+/H^+ antiport activity at very alkaline pHs, reaching maximal activity (~24% dequenching) only at pH 9.5 (Fig. 5.4A). The G258A mutant variant gained Li^+/H^+ antiport activity at moderately alkaline pHs (8.0-8.5) with maximum (~27% dequenching) at pH 8.5 (Fig. 5.4B). The Q280A variant only showed moderate (13% dequenching) Li^+/H^+ antiport at

nearly neutral pH 7.5 (Fig. 5.4C). In contrast, the Y251A variant exhibited direct Li^+/H^+ antiport within the wide pH range (Fig. 5.4D). It was detectable from pH 6.5 to 9.5, showing nearly equal activity (~13% dequenching) at pH 7.0 up to 9.0 (Fig. 5.4D). Of note, the appearance of direct Li^+/H^+ antiport activity was accompanied by the deformations of pH profiles for both K^+/H^+ and Na^+/H^+ antiport in all four mutant variants (Fig. 5.4). Again, all these mutant variants were present in the membranes of sub-bacterial vesicles at nearly the same levels (Fig. 5.4E).

5.4 Discussion

The family of NhaP type antiporters consists of transporters with broad substrate specificity that mediate the efflux of Li^+, Na^+ and K^+, but the NhaP2 antiporter from *Vibrio cholerae* does not exchange Li^+ ions for protons across the membrane [23]. This peculiar ion selectivity remains not fully understood. In this study, we have combined *in silico* modeling and experimental approaches to analyze the determinants of cation specificity of the Vc-NhaP2 antiporter. We found that there is a pathway positioned in close proximity to the cation binding site in the core of the putative cationic pathway determining the ability of the antiporter to recognize and transport particular cations. The known 3D structures of the bacterial Na^+/H^+ antiporters, NhaA from *E. coli* [10] and NhaP from *P. abyssi* and *M. jannaschi* [14,15] show that the two funnel-shaped domains narrowing towards the center of the membrane form the ion translocation pathway. They lead to a cluster of conserved negatively charged residues forming the cation-binding site.

Fig 5.3

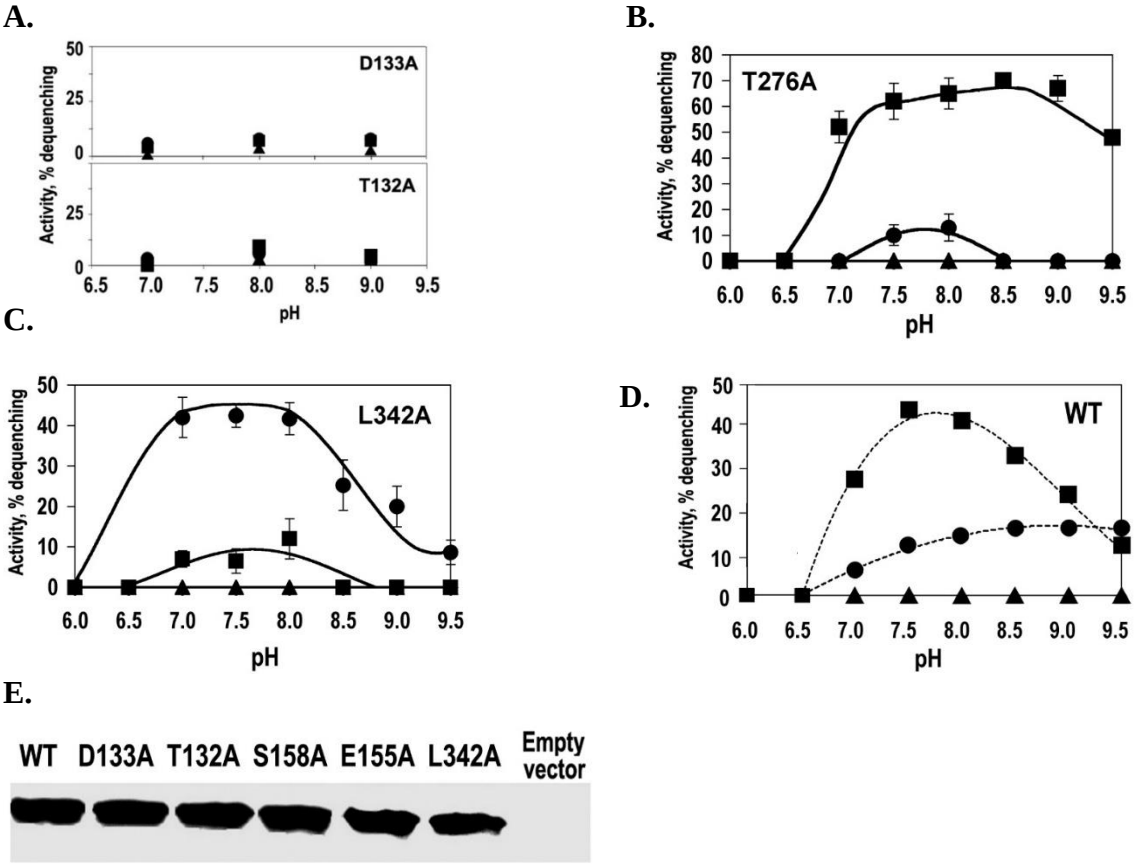


Fig 5.3. Mutations causing the inactivation of Vc-NhaP2 (Panel **A**) or changes in K^+/Na^+ selectivity (Panels **B** and **C**). Inside-out membrane vesicles were isolated and assayed for antiport activity with 10 mM NaCl (circles), KCl (squares) or LiCl (triangles) as described in "Materials and Methods". Plotted are the averages of three independent measurements. Bars show the standard deviation. The pH profile of activity of the non-mutated Vc-NhaP2 is shown for comparison (Panel **D**). Immunodetection of all the mutant variants of Vc-NhaP2 (Panel **E**) was carried out as described in "Materials and Methods". For negative control, 'empty' vesicles isolated from the TO114 cells transformed with pBAD-TOPO plasmid were used.

Fig 5.4

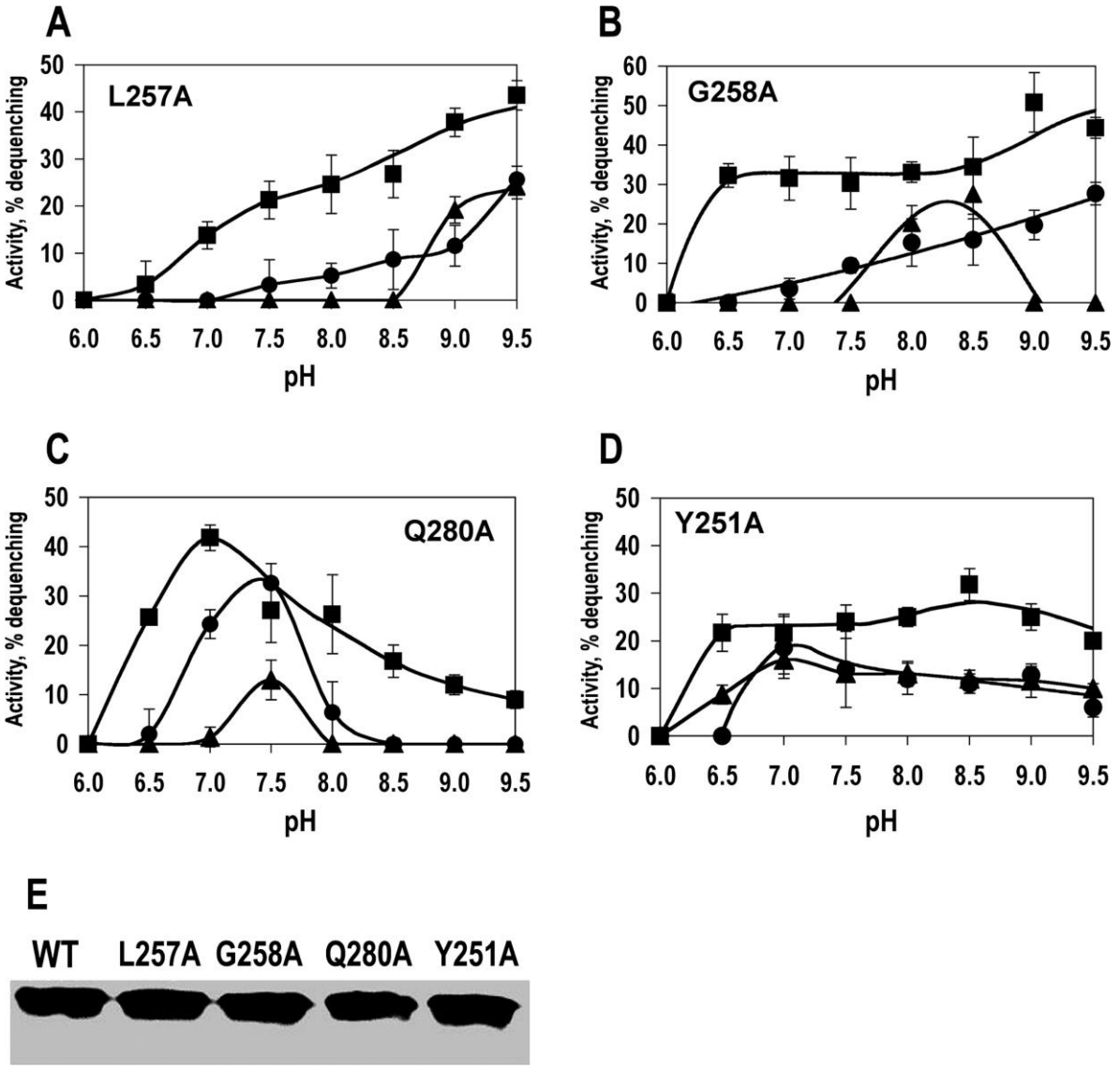


Fig.5.4 Mutations introducing direct Li^+/H^+ antiport. (Panel A to D): Ala substitutions of four residues unlock direct Li^+/H^+ antiport with distinct pH profiles. See the text for further details. Inside-out membrane vesicles were isolated and assayed for antiport activity with 10 mM NaCl (circles), KCl (squares) or LiCl (triangles) as described in "Materials and Methods". Plotted are the averages of three independent measurements. Bars show the standard deviation. (Panel E) Immunodetection of Vc-NhaP2 in vesicular membranes was performed as described in Fig. 5.3.

Recently, it was proposed that the mechanism whereby the Na^+/H^+ antiporter exchanges cations, involves a large movement of the core domain against the fixed dimerization domain, facilitating ion movement either to the periplasmic or the cytosolic side [40]. Due to the similarity of the protein structure and transport mechanism in Na^+/H^+ antiporters from different organisms [114], the crystal structure of *E. coli* NhaA was successfully used as a template to generate a 3D model of the plasma-membrane Sod2-22 antiporter from *Z. rouxii* [43]. Following the same rationale, we used the 3D structure of Pa-NhaP as a template to generate an *in silico* model of Vc-NhaP2 antiporter by a homologue-based software, *Phyre*^{2}. Taking into account limitations inherent to this solely homologue-based structural modelling (violations of Ramachandran restraints, inaccuracies in prediction of extramembrane loop conformations, especially when the percentage of identity is not high), we have also validated the obtained structure using Rosetta software on the Robetta server. In Robetta, sequences submitted to the server are parsed into putative domains and models are generated using either comparative modeling or de novo structure prediction methods [89]. The structures generated by *Phyre*^{2} and Rosetta are nearly identical with a C-alpha RMSD value of TMSs of 1.6 A°. According to the generated model, all residues that we identified previously (D162 and E157) [32] and D133 and T132 (this work) are likely to be directly involved in cation binding (Fig. 5.3A, B). The crucial role of these residues was confirmed by alanine scanning mutagenesis. In NhaP-type antiporters, a tandem of highly conserved negatively charged aspartate residues is thought to bind translocated cations [15]. In Vc-NhaP2 these aspartate residues (D162 and D133) are also evolutionarily conserved. The structural modeling also revealed that L257, G258, and Y251 from TMS IX together with T276, D273, Q280 and L289 from TMS X as well as L342 from TMS XII are located close to each other

and, may form a pathway through which substrate cations can be translocated in a highly selective manner (Fig. 5.2C). Substitutions of these residues with Ala indeed changed K^+, Na^+ or Li^+ selectivity (Fig. 5.3 and 5.4).

Changes in the side-chain size of the residues near the cation binding pocket may create conformational changes which may influence the accessibility of the binding aspartate and affect the ion selectivity of the Vc-NhaP2 [32]. Substitution of G159 present in TMS VI located in close vicinity of the highly conserved ND motif in TMS VI (N161 and D162 in Vc-NhaP2) to alanine caused drastic changes in the ion selectivity of the antiporter [32]. Introduction of a simple methyl group at the side chain at position 159 resulted in Li^+ selectivity. This is similar to the observation that the length of the side chains in the center of the molecule was shown to be an important determinant of substrate specificity for a glucose transporter [116]. The Gly159, Asn161 and Asp162 residues located in the TMS VI of Vc-NhaP2, are in close proximity to the Asp273 and Leu289 in TMS X (Fig 5.1, 5.2B and 5.2C), suggesting that the TMS VI and TMS X are close to one another and contributing to the formation of a putative cation-binding site of the antiporter. Mutation of either of Asn161 or Asp162 into alanine resulted in dramatic changes in the substrate specificity or abolished the antiport altogether [32]. The major findings of this study combining protein modeling and experimental analysis are two-fold: (1) Residues presumably forming the transmembrane cation pathway in close proximity to the putative cation binding site can determine the cation selectivity of the NhaP-type antiporter. (2) Experimental results confirmed that amino acid residues identified through the *in silico* modeling, play important roles in the determination of cation selectivity in the Vc-NhaP2 antiporter. This therefore validates the use of homologue-based *in silico* modeling as a tool for revealing the general features of a 3D structure, despite

the inherent limitations of this methodology mentioned above. In conjunction with other tools, such as Robetta, they could successfully guide targeted mutagenic analysis of antiporters. There are several other computational techniques that can be used for prediction of ion binding site in secondary transporters [117,118]. For example, homology modelling combined with molecular dynamics simulations and grand canonical Monte Carlo and free energy simulations were used to identify a third sodium-binding site in glutamate transporters [113]. Employing such strategies may have a considerable impact on the time and labor costs of experimental characterization of ion transporters. One may hope that this approach will be helpful in studies of the ion transport mechanism in other members of the CPA family. Models generated in this way (and verified experimentally) could be used for further *in silico* exploration of high prediction potential, such as through molecular dynamics simulations. From the practical point of view, cost/time effective approaches combining the *in silico* and experimental procedures may be important in the screening of ion transporters as potential targets for the development of novel antimicrobials. For example, the significance of Vc-NhaP- type antiporters in bacterial survival when ingested *V. cholerae* cells pass a K^+-rich gastric acid barrier [61] in the course of a normal infectious process makes these antiporters worth considering [25].

Chapter 6. Conclusions and future perspectives

Cation-proton antiporters are ubiquitous secondary ion pumps that play a key role in the ion and pH homeostasis of all living cells. Typically, bacteria are exposed to a wide range of environmental challenges and have to adapt efficiently to changes in the ionic composition of their micro-surroundings. In *Vibrio cholerae*, as in all marine-borne bacteria, both survival and dissemination in diverse ecological niches is strictly dependent upon the circulation of two alkali cations, Na^+ and K^+ [5-7,16,27]. *V. cholerae* faces many environmental challenges during the free-living phase of its life cycle. *V. cholerae* is usually a marine organism found in sea water, but during its life time it is also found in estuarine water where it faces massive fluctuations in pH and Na^+ or K^+ ion concentrations. To adapt to these stressful conditions *V. cholerae* possesses several survival mechanisms [18]. During the infectious process, after being transmitted by the fecal-oral route and after being ingested the *V. cholerae* passes through the low pH and high potassium [60-61] environment of the stomach to reach the small intestine, where the pH is alkaline. It then colonizes in the small intestine and secretes cholerae toxin causing cholera diarrhoeal disease [55]. Bacteria adopt different survival strategies to overcome the acidity. *V. cholerae* possesses an Acid Tolerance Response (ATR) that increases its survival within these hostile environments [56-59].

The membrane of *V. cholerae* contains a trio of cation-proton antiporters of a specific type, NhaP, that, as we showed, are responsible for the transport of both K^+ and Na^+ [23-25]. They are encoded by three paralogous structural genes, *Vc-nhaP1*, *2* and *3*. Our phenotypical analysis of deletion mutants suggests that these antiporters play an essential role in bacterial physiology [23-25], and we hypothesized that they could comprise a novel mechanism of the Acid Tolerance Response (ATR). Preliminary ATR tests conducted with the wild-type parental strain, *V. cholerae* O395N1 and its triple deletion mutant, VcΔNhaP123, showed that, being challenged by HCl (pH

3.5), the triple mutant died at a much higher rate than the isogenic wild type strain [25]. Considering the possible physiological role of Vc-NhaP isoforms in the ATR of *V. cholerae*, we hypothesize that the inhibition of Vc-NhaP paralogues might inhibit the infectious process caused by this pathogen when it crosses the gastric acid barrier. Future studies with the VcΔNhaP123 *V. cholerae* cells carrying the wild-type as well as mutated Vc-NhaP2 variants expressed from plasmids will evaluate the exact contribution of Vc-NhaP isoforms to the ATR response as well as their potentiality to become possible targets for future drug development.

The combination of an *in silico* approach and targeted mutagenesis experiments has allowed us to identify the putative active site for ion translocation and putative amino acid residues determining the ion selectivity in Vc-NhaP2 [31,35]. The obtained results allow us to conclude that the *in silico* modeling approach might be a valuable tool for identification of functionally important amino acid residues in the membrane transporters. It has also allowed us to use the generated *in silico* model in Molecular Dynamics (MD) simulations of lipid bilayer-embedded Vc-NhaP2. We carried out MD simulations for the direct visualization of phenomena related to the transmembrane ion movements mediated by cation antiporters. We probed the conformational changes presumably occurring upon ion binding in Vc-NhaP2 by MD simulations over an 11 ns time scale and calculated the average fluctuation of the backbone C-alpha carbon for each residue (Fig. 1 of the Appendix). We found that the positions of the amino acid residues supposedly forming the putative cation binding pocket did not show any significant fluctuation compared to the residues present in the core domain. This agrees with the previously reported findings that in Ec-NhaA, the core domain showed higher flexibility compared to the rigid ion binding pocket [44], suggesting that the conformational change occurring in the core domain alternatively opens the rigid ion binding pocket either to the cytoplasm or to the periplasm. Our observations suggest

that Vc-NhaP2 might follow this 'alternating access mechanism', where the major conformational change occurs in the core domain and thus alternatively opens the ion binding pocket either to the cytoplasm or to the periplasm. In the literature, two possible mechanisms are suggested for 'alternating access' of ions: (1) In the case of antiporters, the rigid ion binding pocket opens either to the cytoplasm or to the periplasm, with the movement of core domain relative to the dimerization domain [10-11,44]; (2) the ion binding pocket moves to open up alternatively to the cytoplasm or the periplasm by a large rotation of the core domain against the dimerization domain, named 'two-domain elevator access mechanism' [14-15,40]. Ec-NhaA follows the first mechanism [10,11,44] whereas a number of experiments suggested that Pa-NhaP, Tt-NapA and Mj-NhaP follow the second one [14-15,40]. In Tt-NapA strictly conserved Asp157 and Asp156 (equivalent to Asp163 and 164 in Ec-NhaA) present at the bottom of a negatively charged ion funnel is alternatively getting exposed to the cytoplasm or the periplasm with a large 20° rotation of the core domain against the dimerization interface [40]. During this process, these two aspartate residues also move 10 Å to coordinate either Na^+ or H^+, which are competing for binding the antiporter. The 'two-domain elevator access mechanism' has also been suggested for the glutamate transporter (GltPh) [124].

The MD simulation results suggested that Vc-NhaP2 might follow the 'alternating access' mechanism for ion transport, like Ec-NhaA (Fig. 3 of Appendix) [26]. In the generated structural model, Vc-NhaP2 has an inward-open conformation (Fig. 1.1A). It is also evident from the solvent accessibility surface analysis where the most solvent accessible area (indicated with the dark purple colour) is located at the cytoplasmic site (Fig. 1.1C). Ions possibly enter from the cytoplasmic site and bind to the amino acid residues present in the highly negatively charged cavity in the middle of Vc-NhaP2 (Fig. 1.1B and Fig. 3 of Appendix). A cluster of amino acid

residues from different TMSs extending from the cytoplasmic side to the putative cation binding pocket might exist that determines the cation selectivity of Vc-NhaP2 (Fig. 5.2C). Binding of specific ions (K^+ or Na^+) possibly induces a conformational change affecting the overall balanced conformation of the ion binding pocket and thus allowing those ions to be exchanged for protons. While binding of Li^+ to the cation binding pocket does not allow a conformational change required for the exchange of Li^+ for proton across the membrane [127]. Asp162, Asp133, Thr132 and Ser158 forming the putative ion binding pocket (Fig. 1.2C and Fig. 3 of Appendix). As these residues coordinate K^+ or Na^+, a conformational change possibly occurs in the extended chain regions of TMSs V and XII (Fig. 1 and 3 of Appendix) which closes the cytoplasmic side and alternatively opens the putative cation binding pocket to the periplasmic side. The translocated ion is then released into the periplasmic side. Protonation of the negatively charged residues (Asp162, Asp133, Thr132 and Ser158) in the putative cation binding pocket possibly brings the antiporter back to the cytoplasmic open conformation (Fig. 3 of Appendix).
Longer MD simulations and transition-state sampling need to be carried out to determine if there is a rotation of the core against the dimer interface for 'alternating access' of the cation binding site either to the cytoplasm or to the periplasm in Vc-NhaP2. But to these ends, a high-resolution structure of the antiporter would also be very helpful.

A detailed understanding of ion antiport mechanism requires high-resolution structures of antiporters co-crystallized with different substrate ions. Co-crystallization of Vc-NhaP2 with different substrate ions will also verify the idea of 'Ligand shading' which will help us to clearly understand the differences in ion selectivity of Vc-NhaP2. Ion transporters are difficult to purify and crystallize, but in recent years considerable progress has been achieved not only with NhaA from *E. coli* [9-11,39], but also with the full-length antiporters of NhaP-type from

hyperthermophilic archaeons *Methanococcus jannaschii* [14] and *Pyrococcus abyssi* [15]. Immediate goals for further study are: construction of His-tagged versions of Vc-NhaP2 and their over-expression and purification for subsequent in-depth characterization, including standard biophysical tests for their folding status (Circular Dichroism, Trp fluorescence), reconstitution into proteoliopsomes, NMR assays (including fast magic-angle spinning solid-state NMR), and crystallization trials. NMR studies of membrane proteins embedded into phospholipids bilayers will give important structural information and shed a light on the dynamics of protein [119]. Structural and dynamics analysis of Vc-NhaP2 using magic angle spinning solid state NMR, with proton detection under high spinning frequency will give sufficient data to resolve and assign resonances associated with each amino acid residue, measure distance restraints and calculate the three-dimensional structure of the protein [120]. The structural data will provide great insight into the ligand binding site as well as the details of the mechanism of ion translocation.

Appendix

Fig. 1

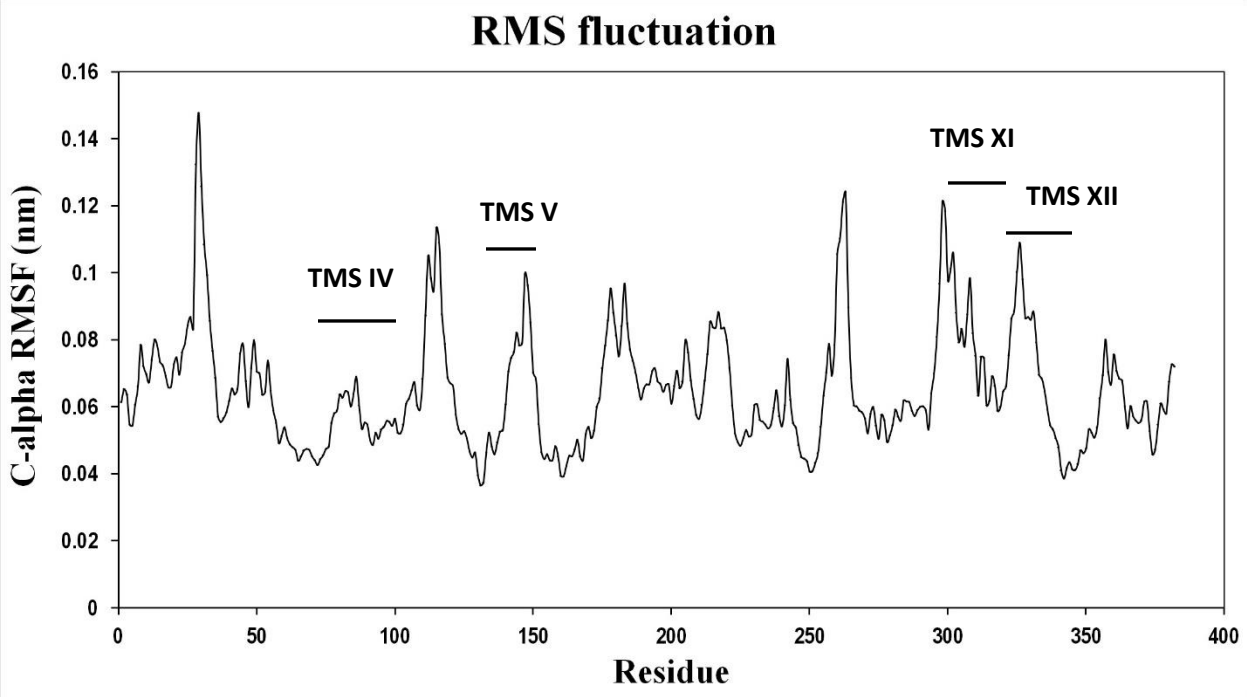


Fig. 1 The root-mean-square fluctuations (RMSFs) of the backbone C-alpha coordinatea are shown as a function of residue number over the 11 ns simulation. Residues 90-109, 129-142, 307-317 and 333-342 are located in the TMS IV, V, XI and XII respectively. Residues 187-212 and 226-241 are located in the TMS VII and VIII respectively. All the other residues showing significant fluctuations are present in the loop regions. TMSs IV, V, XI and XII form the core domain, whereas TMSs VII and VIII are a part of the dimerization domain.

Fig. 2

A.

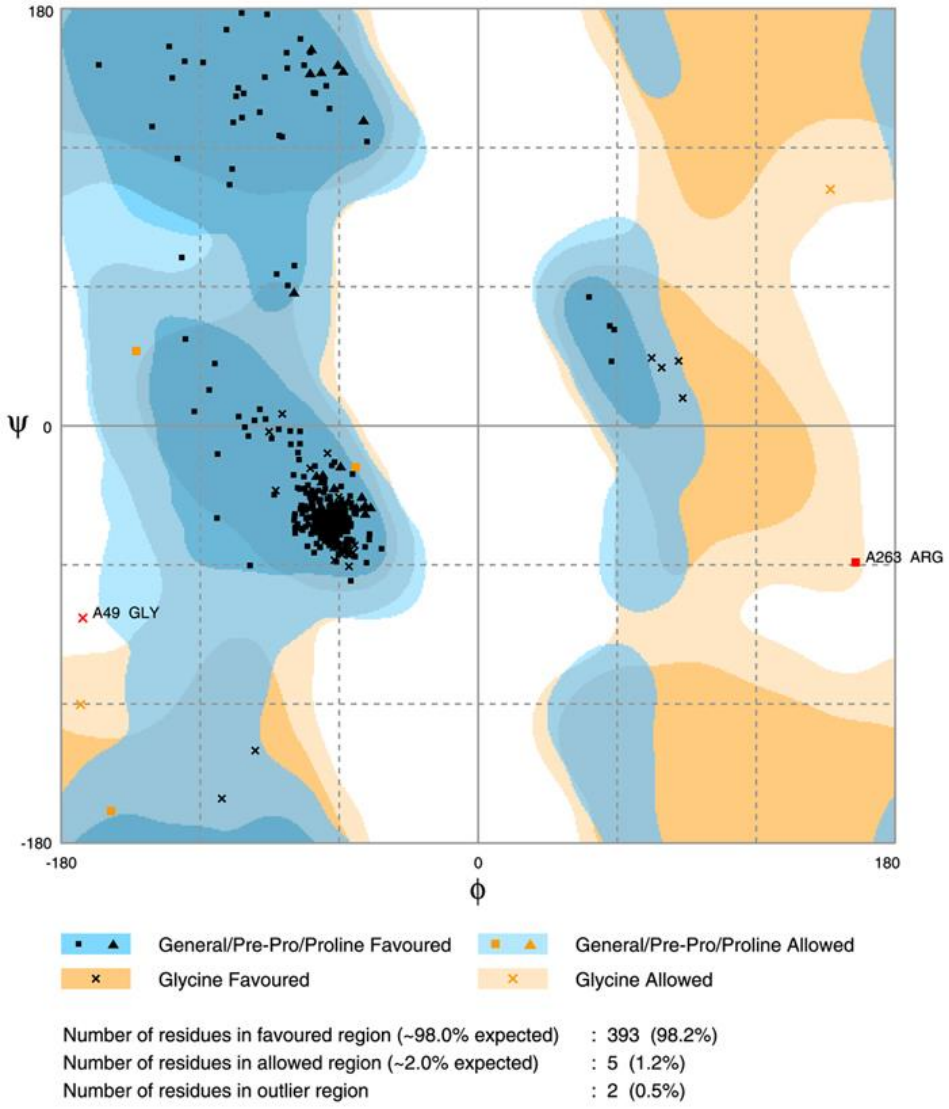


Fig. 2A Ramachandran plot for Vc-NhaP2. The structure of Vc-NhaP2 was generated using *Phyre*^{2} [37]. Amino acid residues are within the favourable zone for Vc-NhaP2.

Fig. 2

B.

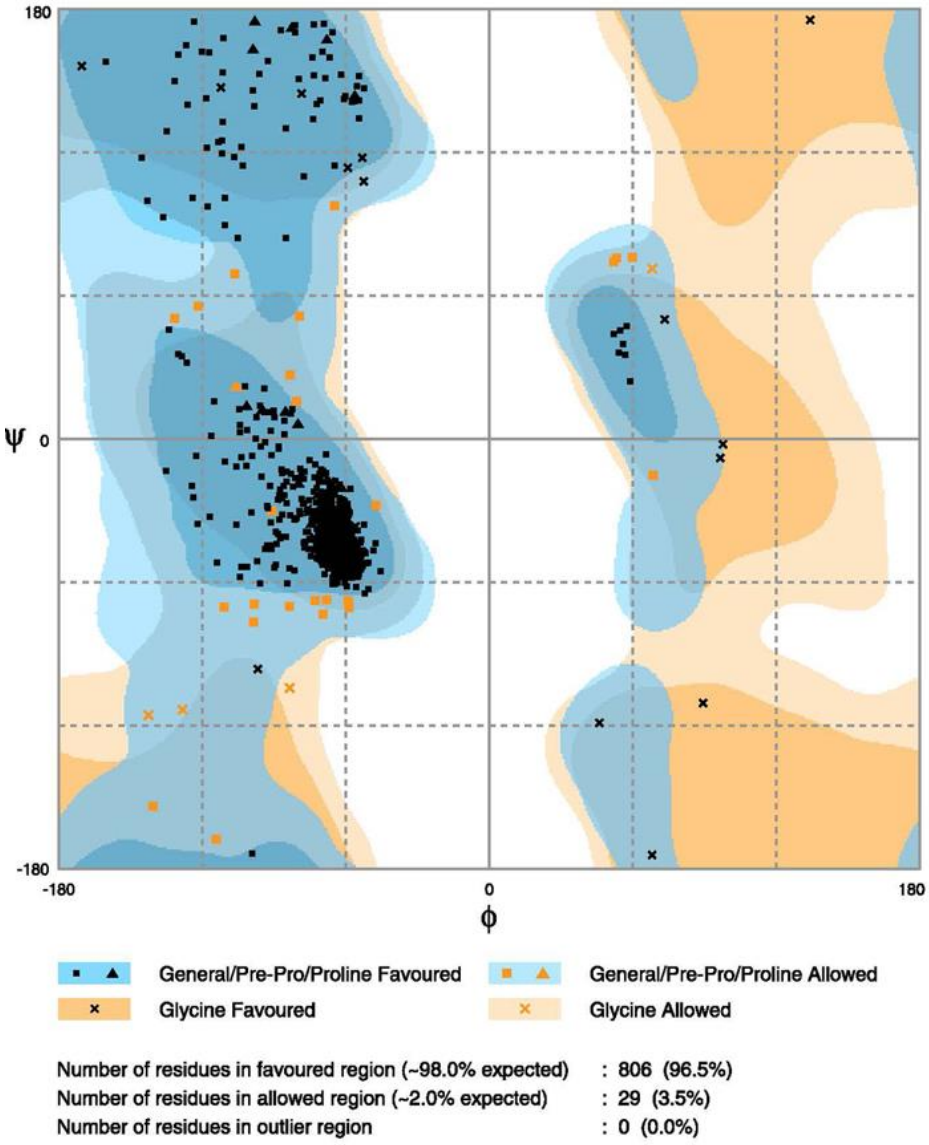
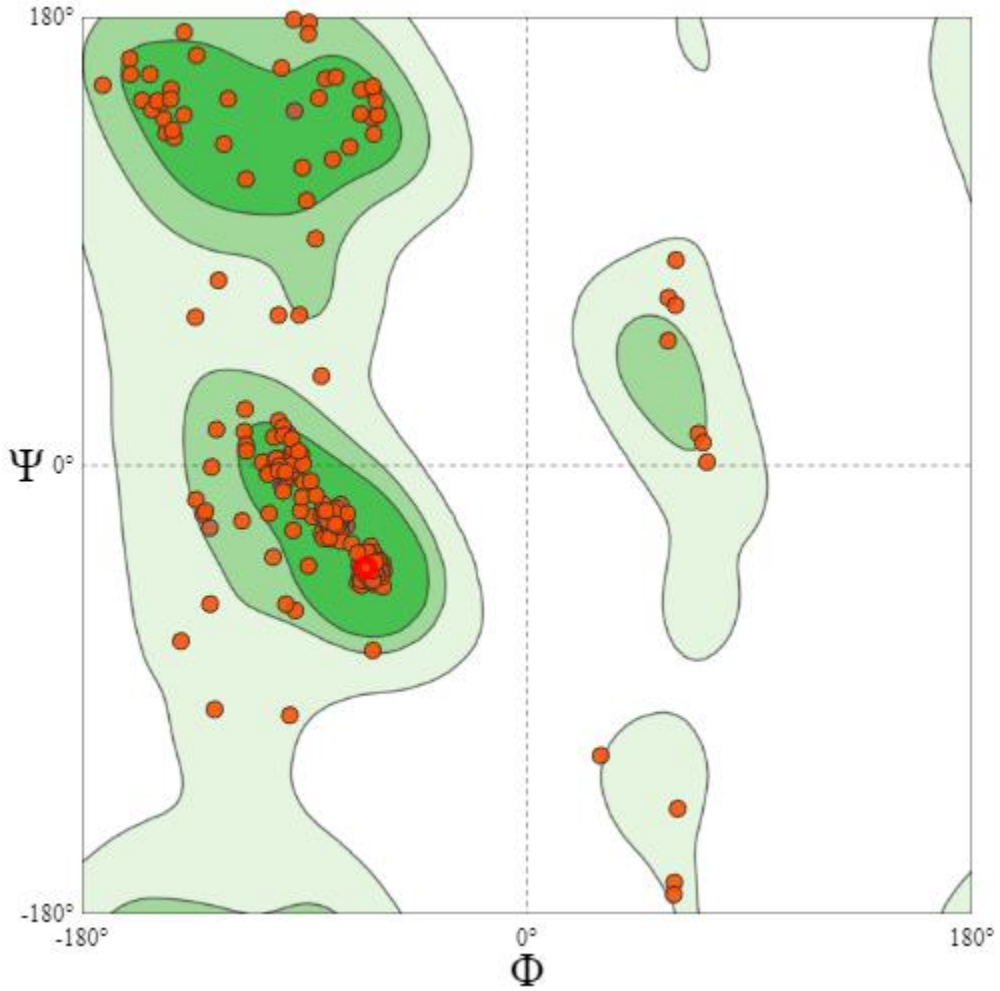


Fig. 2B Ramachandran plot for Pa-NhaP (PDB accession code: 4CZA). The structure was crystallized with a resolution of 3.2 A°. Amino acid residues are within the favourable zone for Pa-NhaP.

Fig. 2

C.



Number of residues in favoured region (~98.0% expected) : 361 (95.0%)
Number of residues in allowed region (~2.0% expected) : 17 (4.5%)
Number of residues in outlier region : 2 (0.5%)

Fig. 2C Ramachandran plot for refined Vc-NhaP2 structure. The structure was generated using Rosetta software [88] on the Robetta server [38,89] and further refined using locPREFMD. Amino acid residues are within the favourable zone for Vc-NhaP2.

Fig. 3

A. **B.**

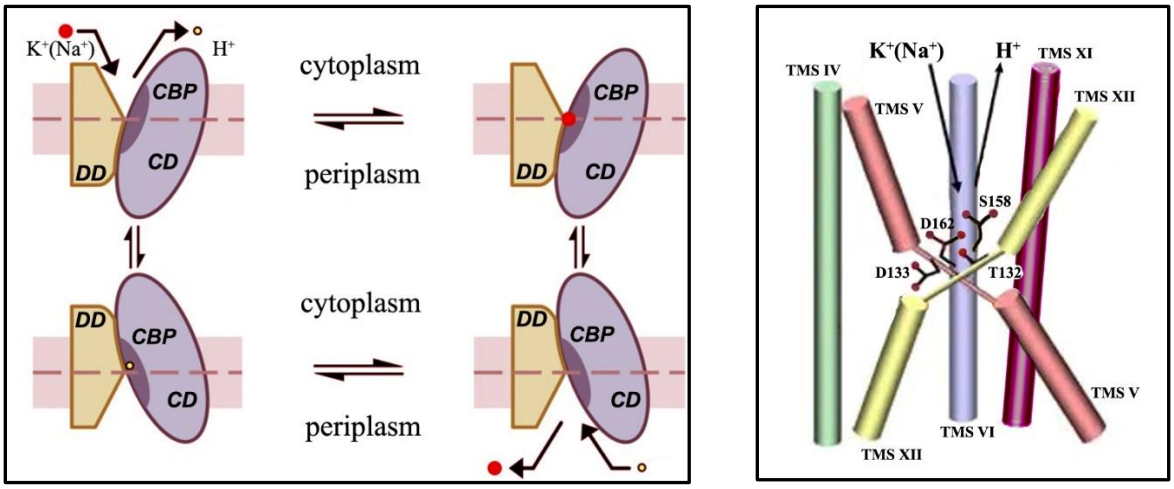


Fig. 3 Alternating-access mechanism of Vc-NhaP2. **(A)** Schematic representation of Vc-NhaP2 viewed parallel to the membrane. Modelled after Fig. 5 from ref [44]. The core domain (CD) and the dimerization domain (DD) are indicated as purple and brown segment respectively. The cation binding pocket (CBP) is shown in dark purple color. The membrane is indicated as pink and, the dashed line represents its center. In the cytoplasmic open conformation Vc-NhaP2 binds to Na^+/K^+ and releases one H^+. Conformational change occurring in the transmembrane segments (TMSs) IV, V, XI and XII closes the cytoplasmic side and opens the CBP to the periplasmic side. TMS VI including the CBP remains rigid throughout the ion translocation process. Na^+/K^+ is released into the periplasm, H^+ can bind and a new cycle begins. **(B)** Schematic representation of the core domain (CD) and the cation binding pocket (CBP) of Vc-NhaP2.

Fig. 4

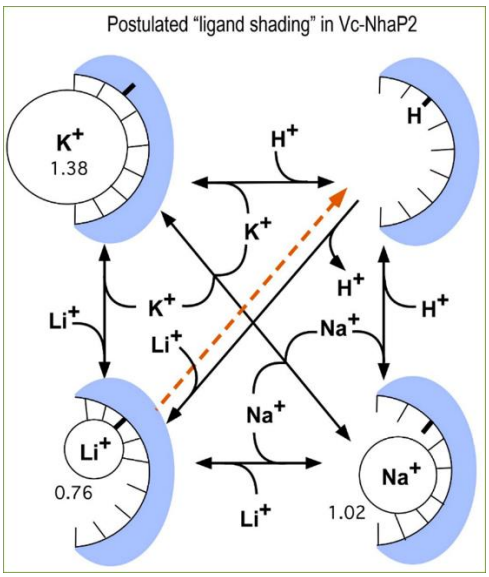


Fig. 4. Proposed 'Ligand shading' hypothesis. Li^+ shares ligand with H^+, but Li^+ binds stronger. H^+ is "shaded", cannot bind active site, cannot induce conformational change. Binding of K^+ does not shade H^+, K^+/H^+ antiport can occur. Na^+ partially shades H^+, leading to kinetic inefficiency, preference for K^+/H^+ antiport.

Supplementary material

S1 Data Set (Pa-NhaP used as a template)

```
c4czbB_ (1)     GLU            176.955 -59.366 106.489
c4czbB_ (1)     LEU     H      -175.550        -61.223 -42.415
c4czbB_ (1)     MET     H      178.732 -62.012 -36.741
c4czbB_ (1)     MET     H      176.688 -62.951 -49.268
c4czbB_ (1)     ALA     H      177.463 -55.520 -46.421
c4czbB_ (1)     ILE     H      177.271 -60.173 -37.572
c4czbB_ (1)     TYR     H      179.756 -61.241 -44.239
c4czbB_ (1)     LEU     H      175.572 -59.640 -36.925
c4czbB_ (1)     LEU     H      179.262 -57.889 -42.897
c4czbB_ (1)     ALA     H      178.241 -57.858 -46.270
c4czbB_ (1)     LEU     H      -179.475        -67.669 -43.109
c4czbB_ (1)     VAL     H      178.988 -63.219 -67.010
c4czbB_ (1)     LEU     H      -177.515        -58.434 -38.423
c4czbB_ (1)     SER     H      178.811 -58.490 -44.052
c4czbB_ (1)     LEU     H      175.994 -56.504 -51.789
c4czbB_ (1)     VAL     H      178.829 -54.706 -50.455
c4czbB_ (1)     ALA     H      -179.555        -62.635 -37.256
c4czbB_ (1)     LYS     H      175.351 -61.205 -47.458
c4czbB_ (1)     ILE     H      176.247 -58.091 -40.666
c4czbB_ (1)     ALA     H      178.708 -60.634 -41.830
c4czbB_ (1)     GLU     H      176.431 -67.179 -36.082
c4czbB_ (1)     LYS     H      -179.184        -69.896 -11.538
c4czbB_ (1)     LEU            -179.516        -125.359        12.540
c4czbB_ (1)     LYS            -179.762        56.229  21.403
c4czbB_ (1)     ILE            177.287 -90.880 139.635
c4czbB_ (1)     PRO            173.466 -55.955 137.642
c4czbB_ (1)     ASP            -177.319        -69.914 -39.381
c4czbB_ (1)     ILE     H      -174.670        -44.198 -56.448
c4czbB_ (1)     PRO     H      -175.703        -67.272 -30.512
c4czbB_ (1)     LEU     H      178.368 -68.210 -42.079
c4czbB_ (1)     LEU     H      175.296 -60.089 -44.307
c4czbB_ (1)     LEU     H      178.746 -62.448 -43.447
c4czbB_ (1)     LEU     H      176.416 -58.522 -46.940
c4czbB_ (1)     LEU     H      176.508 -56.607 -45.491
c4czbB_ (1)     LEU     H      176.365 -65.230 -41.295
c4czbB_ (1)     ILE     H      178.795 -58.352 -61.939
c4czbB_ (1)     ILE     H      -178.849        -74.179 -9.065
c4czbB_ (1)     PRO            -177.861        -65.118 -39.585
c4czbB_ (1)     PHE            -172.694        -62.784 -46.004
c4czbB_ (1)     LEU            -178.458        -103.074        -14.980
c4czbB_ (1)     GLN            -178.653        54.755  30.552
c4czbB_ (1)     ILE            172.406 -68.212 -45.952
c4czbB_ (1)     ILE            175.784 -116.862        112.766
c4czbB_ (1)     PRO            179.769 -66.228 162.824
c4czbB_ (1)     SER     H      -176.765        -66.544 -60.608
c4czbB_ (1)     ASP     H      -177.522        -50.302 -42.472
c4czbB_ (1)     SER     H      177.543 -59.974 -49.786
c4czbB_ (1)     ALA     H      178.255 -58.445 -37.099
c4czbB_ (1)     MET     H      178.186 -65.160 -43.609
c4czbB_ (1)     GLU     H      -179.386        -69.197 -37.253
c4czbB_ (1)     ILE     H      174.816 -63.775 -48.831
c4czbB_ (1)     PHE     H      -179.542        -63.215 -25.698
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c4czbB_ (1)     GLU     H       178.734 -62.476 -27.392
c4czbB_ (1)     TYR             178.715 -98.776 -53.832
c4czbB_ (1)     ALA             -174.599        -79.788 3.702
c4czbB_ (1)     PRO     H       -179.872        -54.461 -38.307
c4czbB_ (1)     ILE     H       178.738 -56.376 -52.905
c4czbB_ (1)     LEU     H       179.923 -65.049 -32.530
c4czbB_ (1)     ILE     H       179.147 -71.064 -23.288
c4czbB_ (1)     PHE     H       179.514 -73.740 -51.325
c4czbB_ (1)     ILE     H       -177.717        -57.558 -44.160
c4czbB_ (1)     LEU     H       177.842 -59.537 -44.033
c4czbB_ (1)     LEU     H       175.844 -61.104 -60.602
c4czbB_ (1)     ALA     H       -178.833        -91.337 -19.459
c4czbB_ (1)     PHE     H       -179.349        -101.516        -17.780
c4czbB_ (1)     THR             -177.670        -60.353 -32.448
c4czbB_ (1)     MET             175.744 -143.057        166.662
c4czbB_ (1)     ARG             -173.235        -120.707        165.736
c4czbB_ (1)     ILE             -175.993        -103.309        8.421
c4czbB_ (1)     SER             177.716 -79.207 -7.508
c4czbB_ (1)     LEU             -176.045        -112.913        6.239
c4czbB_ (1)     LEU             -174.992        -90.474 -11.002
c4czbB_ (1)     LYS             -173.954        -54.965 -23.482
c4czbB_ (1)     ARG             179.558 -71.760 -49.122
c4czbB_ (1)     VAL             -169.381        -122.206        15.515
c4czbB_ (1)     ILE     H       -174.932        -54.770 -28.296
c4czbB_ (1)     LYS     H       179.142 -66.819 -57.267
c4czbB_ (1)     THR     H       175.299 -53.258 -40.309
c4czbB_ (1)     VAL     H       176.078 -55.510 -57.229
c4czbB_ (1)     VAL     H       -178.568        -57.841 -50.602
c4czbB_ (1)     ARG     H       -178.819        -59.999 -46.174
c4czbB_ (1)     LEU     H       178.695 -65.086 -28.697
c4czbB_ (1)     ASP     H       -174.894        -87.972 -19.158
c4czbB_ (1)     THR     H       -179.297        -107.041        -65.635
c4czbB_ (1)     ILE     H       -174.246        -64.005 -55.147
c4czbB_ (1)     THR     H       176.451 -54.761 -39.809
c4czbB_ (1)     PHE     H       177.386 -56.017 -62.951
c4czbB_ (1)     LEU     H       -179.105        -55.583 -49.083
c4czbB_ (1)     ILE     H       178.356 -56.494 -50.102
c4czbB_ (1)     THR     H       178.151 -54.537 -49.939
c4czbB_ (1)     LEU     H       -179.993        -63.000 -34.391
c4czbB_ (1)     LEU     H       178.463 -64.980 -57.812
c4czbB_ (1)     ILE     H       179.256 -57.768 -43.517
c4czbB_ (1)     SER     H       175.661 -58.225 -35.281
c4czbB_ (1)     PHE     H       175.742 -51.429 -50.235
c4czbB_ (1)     ILE     H       179.103 -58.740 -54.286
c4czbB_ (1)     PHE     H       -177.725        -55.514 -40.099
c4czbB_ (1)     ASN     H       176.296 -67.086 -49.216
c4czbB_ (1)     MET     H       -176.034        -66.638 -18.787
c4czbB_ (1)     VAL             -179.796        -82.947 -50.000
c4czbB_ (1)     LEU             -174.790        -90.086 20.518
c4czbB_ (1)     ASN             -178.311        60.545  10.918
c4czbB_ (1)     LEU             175.900 -70.686 148.075
c4czbB_ (1)     PRO             178.435 -60.394 153.751
c4czbB_ (1)     TYR             -176.876        -71.309 -7.781
c4czbB_ (1)     THR             177.878 -103.564        6.686
c4czbB_ (1)     SER             179.580 -68.172 120.129
c4czbB_ (1)     PRO             179.319 -64.247 -16.336
c4czbB_ (1)     VAL     H       177.102 -57.274 -57.280
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c4czbB_ (1)	TYR	H	-179.185	-67.473	-32.067	
c4czbB_ (1)	LEU	H	174.522	-65.951	-47.179	
c4czbB_ (1)	PHE	H	177.662	-54.135	-51.793	
c4czbB_ (1)	ALA	H	178.521	-58.628	-35.596	
c4czbB_ (1)	ILE	H	176.870	-72.953	-49.466	
c4czbB_ (1)	THR	H	-176.080	-80.275	-2.262	
c4czbB_ (1)	ALA		-177.639	-67.228	-32.916	
c4czbB_ (1)	ALA		-179.926	-76.982	140.182	
c4czbB_ (1)	THR		178.817	-97.625	173.974	
c4czbB_ (1)	ASP		-179.712	-114.979	118.785	
c4czbB_ (1)	PRO		-179.354	-69.518	-56.415	
c4czbB_ (1)	ALA	H	-176.874	-57.305	-21.684	
c4czbB_ (1)	THR		175.452	-66.947	-48.455	
c4czbB_ (1)	LEU		-179.042	-89.662	2.362	
c4czbB_ (1)	ILE		-179.781	-66.172	-46.792	
c4czbB_ (1)	PRO	H	176.098	-69.919	-39.968	
c4czbB_ (1)	VAL	H	-173.048	-68.929	-11.164	
c4czbB_ (1)	PHE	H	175.221	-107.058	-33.897	
c4czbB_ (1)	SER	H	-178.974	-66.055	-48.582	
c4czbB_ (1)	ARG	H	177.240	-59.835	-29.914	
c4czbB_ (1)	VAL	H	177.076	-82.738	-40.997	
c4czbB_ (1)	ARG		-173.106	52.307	49.804	
c4czbB_ (1)	THR		-174.765	-62.101	-175.790	
c4czbB_ (1)	ASN		176.919	-51.178	108.057	
c4czbB_ (1)	PRO		-169.401	-42.788	-37.404	
c4czbB_ (1)	GLU	H	174.646	-51.205	-61.331	
c4czbB_ (1)	VAL	H	178.545	-52.529	-53.119	
c4czbB_ (1)	ALA	H	-178.742	-52.852	-64.815	
c4czbB_ (1)	ILE	H	-177.689	-62.769	-27.201	
c4czbB_ (1)	THR	H	175.538	-63.107	-52.034	
c4czbB_ (1)	LEU	H	179.479	-60.638	-46.769	
c4czbB_ (1)	GLU	H	177.297	-56.286	-50.804	
c4czbB_ (1)	ALA	H	179.314	-57.640	-48.496	
c4czbB_ (1)	GLU	H	178.782	-57.705	-47.368	
c4czbB_ (1)	SER	H	-179.708	-59.650	-61.290	
c4czbB_ (1)	ILE	H	-178.952	-54.695	-39.689	
c4czbB_ (1)	PHE	H	-178.934	-77.744	-21.551	
c4czbB_ (1)	ASN	H	177.824	-90.665	-18.891	
c4czbB_ (1)	ASP	H	172.589	-50.810	-46.202	
c4czbB_ (1)	PRO	H	178.604	-75.298	-49.741	
c4czbB_ (1)	LEU	H	-175.906	-52.171	-36.762	
c4czbB_ (1)	ILE	H	174.986	-60.858	-49.951	
c4czbB_ (1)	VAL	H	178.956	-55.955	-50.748	
c4czbB_ (1)	SER	H	176.722	-56.286	-48.281	
c4czbB_ (1)	THR	H	176.979	-61.733	-40.596	
c4czbB_ (1)	SER	H	179.958	-61.430	-43.097	
c4czbB_ (1)	VAL	H	179.435	-64.888	-51.207	
c4czbB_ (1)	ILE	H	-177.407	-60.732	-35.857	
c4czbB_ (1)	LEU	H	178.659	-57.225	-29.191	
c4czbB_ (1)	LEU	H	178.770	-64.568	-30.815	
c4czbB_ (1)	PHE		-179.428	-74.444	-9.335	
c4czbB_ (1)	LEU		177.990	-156.411	-171.963	
c4czbB_ (1)	PHE		-178.029	-69.143	-18.887	
c4czbB_ (1)	SER		-178.383	-148.257	-94.578	
c4czbB_ (1)	SER		-178.136	56.916	43.266	
c4czbB_ (1)	SER		177.219	-61.680	-50.916	
c4czbB_ (1)	ASN		177.761	-142.024	129.136	

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c4czbB_ (1)     PRO            -175.784        -62.100 -38.573
c4czbB_ (1)     LEU     H      -179.413        -61.972 -41.791
c4czbB_ (1)     ILE     H      179.409 -58.636 -52.930
c4czbB_ (1)     ASP     H      179.780 -68.601 -23.610
c4czbB_ (1)     LEU     H      175.887 -69.210 -48.341
c4czbB_ (1)     ILE     H      176.802 -62.305 -42.421
c4czbB_ (1)     THR     H      -179.469        -61.841 -50.023
c4czbB_ (1)     LEU     H      -179.586        -64.681 -55.781
c4czbB_ (1)     ALA     H      -179.745        -58.336 -61.729
c4czbB_ (1)     ALA     H      179.256 -62.955 -41.162
c4czbB_ (1)     ILE     H      175.444 -59.301 -56.745
c4czbB_ (1)     VAL     H      -178.515        -57.196 -64.052
c4czbB_ (1)     VAL     H      -177.133        -60.306 -47.084
c4czbB_ (1)     LEU     H      179.881 -72.411 -29.917
c4czbB_ (1)     LEU     H      175.893 -61.538 -59.722
c4czbB_ (1)     LEU     H      179.194 -62.350 -26.263
c4czbB_ (1)     ALA     H      175.943 -65.627 -46.501
c4czbB_ (1)     LYS     H      176.276 -62.915 -44.991
c4czbB_ (1)     ILE     H      178.477 -54.610 -55.871
c4czbB_ (1)     TYR     H      178.729 -60.717 -36.379
c4czbB_ (1)     GLU     H      177.080 -56.761 -62.630
c4czbB_ (1)     LYS     H      -179.514        -59.498 -31.814
c4czbB_ (1)     ILE     H      -176.904        -77.774 -24.337
c4czbB_ (1)     ILE     H      179.290 -89.114 -42.044
c4czbB_ (1)     ILE     H      -179.254        -57.739 -44.526
c4czbB_ (1)     HIS            -176.004        -67.746 -6.425
c4czbB_ (1)     CYS            179.845 -140.744        -175.977
c4czbB_ (1)     ASP            174.739 -124.460        75.772
c4czbB_ (1)     PHE            -178.383        -57.005 -37.865
c4czbB_ (1)     HIS            -177.002        54.815  -118.841
c4czbB_ (1)     GLU            -175.834        -59.553 -26.215
c4czbB_ (1)     TYR     H      -176.559        -83.973 13.884
c4czbB_ (1)     VAL     H      175.070 -74.228 -42.981
c4czbB_ (1)     ALA     H      -178.046        -47.427 -51.127
c4czbB_ (1)     PRO     H      -179.468        -69.872 -21.249
c4czbB_ (1)     LEU     H      -178.634        -69.741 -55.917
c4czbB_ (1)     VAL     H      -177.656        -71.714 -44.618
c4czbB_ (1)     LEU     H      -178.910        -56.758 -57.572
c4czbB_ (1)     ALA     H      175.088 -70.456 -37.172
c4czbB_ (1)     MET     H      178.892 -60.909 -39.703
c4czbB_ (1)     LEU     H      176.613 -59.761 -35.409
c4czbB_ (1)     LEU     H      -178.286        -63.138 -26.096
c4czbB_ (1)     LEU     H      -179.850        -77.656 -48.456
c4czbB_ (1)     TYR     H      175.687 -55.163 -59.250
c4czbB_ (1)     VAL     H      177.595 -61.760 -29.220
c4czbB_ (1)     ASP     H      -171.388        -110.934        -39.690
c4czbB_ (1)     ASP     H      -177.147        -88.278 -59.703
c4czbB_ (1)     LEU     H      -171.702        -66.490 -61.998
c4czbB_ (1)     LEU     H      -173.278        -51.138 -40.784
c4czbB_ (1)     PRO     H      176.708 -62.100 -30.715
c4czbB_ (1)     SER     H      -179.778        -60.113 -28.385
c4czbB_ (1)     ILE     H      -178.445        -106.269        -12.739
c4czbB_ (1)     CYS            -174.728        -141.129        -14.279
c4czbB_ (1)     TYR            177.308 -86.983 -172.662
c4czbB_ (1)     PHE            179.705 -130.476        160.935
c4czbB_ (1)     SER            175.452 -75.082 113.499
c4czbB_ (1)     TYR     H      -179.823        -64.671 -51.324
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c4czbB_ (1)     MET     H       178.126 -61.872 -37.244
c4czbB_ (1)     ALA     H       175.573 -59.667 -42.145
c4czbB_ (1)     VAL     H       175.851 -61.050 -48.886
c4czbB_ (1)     ALA     H       179.683 -57.477 -49.482
c4czbB_ (1)     ILE     H       177.934 -59.632 -52.972
c4czbB_ (1)     MET     H       179.968 -53.468 -55.345
c4czbB_ (1)     LEU     H       178.654 -63.964 -59.468
c4czbB_ (1)     TYR     H       179.553 -59.120 -31.941
c4czbB_ (1)     LEU     H       179.175 -68.169 -43.355
c4czbB_ (1)     ASP     H       179.733 -66.343 -23.224
c4czbB_ (1)     ALA     H       178.285 -83.722 -26.576
c4czbB_ (1)     LEU     H       176.093 -87.315 -0.204
c4czbB_ (1)     PHE             176.083 -113.656        -31.814
c4czbB_ (1)     ARG             172.074 -66.751 -57.149
c4czbB_ (1)     ALA             163.048 -78.187 152.265
c4czbB_ (1)     ASP             -176.154        -113.997        93.803
c4czbB_ (1)     ASP             174.797 -102.465        139.757
c4czbB_ (1)     ILE             179.739 -72.509 -16.635
c4czbB_ (1)     ASP     H       178.194 -60.650 -22.452
c4czbB_ (1)     TYR     H       -178.215        -57.173 -53.181
c4czbB_ (1)     LYS     H       -169.793        -57.420 -26.361
c4czbB_ (1)     TYR     H       177.251 -67.468 -51.679
c4czbB_ (1)     ILE     H       -176.835        -50.976 -54.425
c4czbB_ (1)     VAL     H       178.523 -53.494 -55.305
c4czbB_ (1)     SER     H       177.976 -61.872 -32.966
c4czbB_ (1)     PHE     H       177.110 -69.225 -59.720
c4czbB_ (1)     CYS     H       -176.673        -62.216 -38.114
c4czbB_ (1)     ASP     H       -179.948        -59.947 -43.501
c4czbB_ (1)     ASP     H       174.749 -69.203 -35.111
c4czbB_ (1)     LEU     H       178.584 -72.021 -36.830
c4czbB_ (1)     SER     H       176.880 -64.304 -36.161
c4czbB_ (1)     LEU     H       -176.519        -64.507 -34.314
c4czbB_ (1)     LEU     H       175.530 -60.331 -59.780
c4czbB_ (1)     ALA     H       179.654 -55.356 -35.944
c4czbB_ (1)     ARG     H       176.765 -58.263 -56.153
c4czbB_ (1)     VAL     H       178.170 -63.712 -44.393
c4czbB_ (1)     PHE     H       -178.216        -59.772 -48.690
c4czbB_ (1)     ILE     H       -175.843        -65.365 -52.694
c4czbB_ (1)     PHE     H       -177.064        -55.180 -45.759
c4czbB_ (1)     VAL     H       177.458 -61.519 -51.542
c4czbB_ (1)     PHE     H       -179.802        -63.455 -28.683
c4czbB_ (1)     LEU             172.419 -61.288 -42.907
c4czbB_ (1)     ALA             179.383 -97.336 -33.241
c4czbB_ (1)     CYS             -179.084        -67.336 -11.243
c4czbB_ (1)     ILE             176.332 -68.452 136.886
c4czbB_ (1)     LYS             172.947 -97.314 126.561
c4czbB_ (1)     LEU     H       -175.800        -49.819 -46.477
c4czbB_ (1)     SER     H       177.236 -62.685 -51.213
c4czbB_ (1)     MET     H       178.476 -58.894 -39.674
c4czbB_ (1)     LEU     H       177.718 -58.268 -53.682
c4czbB_ (1)     GLU     H       178.881 -60.859 -30.443
c4czbB_ (1)     ASN             -178.573        -74.978 -39.226
c4czbB_ (1)     TYR             -176.136        -119.708        29.045
c4czbB_ (1)     PHE             176.592 -65.261 -70.316
c4czbB_ (1)     ILE     H       -178.936        -50.434 -49.881
c4czbB_ (1)     PRO     H       -177.755        -61.711 -50.027
c4czbB_ (1)     LEU     H       177.066 -57.873 -42.968
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c4czbB_ (1)	LEU	H	179.688	-68.555	-38.258			
c4czbB_ (1)	VAL	H	175.542	-59.491	-45.920			
c4czbB_ (1)	ALA	H	177.321	-54.595	-47.416			
c4czbB_ (1)	LEU	H	177.146	-57.375	-41.580			
c4czbB_ (1)	SER	H	178.966	-66.723	-51.631			
c4czbB_ (1)	ILE	H	-175.743		-68.031	-48.492		
c4czbB_ (1)	PHE	H	-170.715		-90.999	-26.012		
c4czbB_ (1)	LEU	H	-176.801		-111.669		-61.050	
c4czbB_ (1)	ALA	H	-177.275		-55.381	-66.539		
c4czbB_ (1)	ARG	H	-178.909		-49.165	-52.405		
c4czbB_ (1)	PRO	H	-179.095		-63.954	-45.131		
c4czbB_ (1)	LEU	H	177.888	-55.864	-49.887			
c4czbB_ (1)	VAL	H	177.066	-62.569	-52.430			
c4czbB_ (1)	PHE	H	179.815	-58.547	-49.974			
c4czbB_ (1)	LEU	H	-177.250		-66.292	-30.410		
c4czbB_ (1)	LEU		-177.075		-120.540		45.377	
c4czbB_ (1)	ILE		-178.681		-79.188	-18.307		
c4czbB_ (1)	SER		-176.192		-102.273		165.007	
c4czbB_ (1)	LYS		176.958	-95.707	18.984			
c4czbB_ (1)	HIS		-176.625		-99.052	147.542		
c4czbB_ (1)	SER		178.694	-69.566	160.618			
c4czbB_ (1)	PHE	H	174.770	-61.947	-38.992			
c4czbB_ (1)	LYS	H	178.068	-66.609	-31.458			
c4czbB_ (1)	GLU	H	178.381	-71.108	-47.812			
c4czbB_ (1)	LYS	H	176.945	-59.711	-39.469			
c4czbB_ (1)	LEU	H	177.059	-65.653	-35.059			
c4czbB_ (1)	TYR	H	175.609	-60.338	-56.564			
c4czbB_ (1)	PHE	H	178.994	-54.865	-34.012			
c4czbB_ (1)	ALA	H	179.611	-64.079	-58.646			
c4czbB_ (1)	LEU		-175.313		-84.325	17.447		
c4czbB_ (1)	GLU		-177.761		-101.737		-82.213	
c4czbB_ (1)	PRO		178.099	-94.914	168.404			
c4czbB_ (1)	ARG		177.400	-92.172	173.395			
c4czbB_ (1)	VAL		-169.481		-70.803	-41.508		
c4czbB_ (1)	VAL	H	178.699	-57.459	-48.726			
c4czbB_ (1)	PRO	H	176.309	-62.708	-28.883			
c4czbB_ (1)	ALA	H	177.809	-67.787	-57.256			
c4czbB_ (1)	ALA	H	177.549	-52.474	-47.864			
c4czbB_ (1)	LEU	H	178.190	-61.645	-37.558			
c4czbB_ (1)	ALA	H	179.168	-62.809	-53.925			
c4czbB_ (1)	VAL	H	179.606	-62.146	-44.548			
c4czbB_ (1)	THR	H	178.934	-58.681	-42.080			
c4czbB_ (1)	VAL	H	176.049	-63.010	-45.499			
c4czbB_ (1)	ILE	H	-179.065		-65.808	-38.454		
c4czbB_ (1)	GLU	H	-179.020		-67.045	-37.583		
c4czbB_ (1)	ILE	H	175.576	-66.737	-54.764			
c4czbB_ (1)	LEU	H	-178.393		-57.554	-36.276		
c4czbB_ (1)	LYS	H	-178.584		-81.735	-35.219		
c4czbB_ (1)	ASN	H	-175.249		-105.274		-46.818	
c4czbB_ (1)	ALA	H	-177.473		-67.655	-16.726		
c4czbB_ (1)	ASP	H	173.123	-60.745	-35.677			
c4czbB_ (1)	LYS	H	177.072	-88.181	-38.933			
c4czbB_ (1)	ILE		179.656	-123.247		82.558		
c4czbB_ (1)	PRO		174.726	-95.857	128.593			
c4czbB_ (1)	ALA		174.185	-64.075	133.103			
c4czbB_ (1)	SER	H	-173.343		-54.011	-56.477		
c4czbB_ (1)	ILE	H	178.791	-54.137	-41.976			

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c4czbB_ (1)     THR     H       179.344 -74.694 -31.418
c4czbB_ (1)     LYS     H       -176.156        -63.905 -15.061
c4czbB_ (1)     TYR             174.594 -61.460 -30.206
c4czbB_ (1)     ILE             169.179 -103.684        129.511
c4czbB_ (1)     THR             179.359 -55.615 126.996
c4czbB_ (1)     PRO     H       176.297 -54.234 -27.670
c4czbB_ (1)     THR     H       172.682 -52.642 -56.717
c4czbB_ (1)     ASP     H       -179.357        -75.058 -17.508
c4czbB_ (1)     ILE     H       172.923 -66.319 -58.111
c4czbB_ (1)     ALA     H       177.580 -59.009 -41.398
c4czbB_ (1)     THR     H       -179.779        -62.038 -43.206
c4czbB_ (1)     ILE     H       178.057 -61.588 -49.846
c4czbB_ (1)     ILE     H       -176.972        -64.327 -51.657
c4czbB_ (1)     ILE     H       -179.960        -66.793 -37.522
c4czbB_ (1)     THR     H       175.221 -59.813 -39.455
c4czbB_ (1)     PHE     H       179.780 -57.303 -59.661
c4czbB_ (1)     MET     H       179.503 -62.018 -30.205
c4czbB_ (1)     THR     H       175.999 -63.988 -53.452
c4czbB_ (1)     ILE     H       176.108 -52.557 -58.609
c4czbB_ (1)     LEU     H       179.786 -47.631 -64.525
c4czbB_ (1)     LEU     H       -176.072        -56.244 -47.938
c4czbB_ (1)     SER     H       -179.948        -59.794 -45.696
c4czbB_ (1)     VAL     H       -179.973        -63.027 -51.813
c4czbB_ (1)     ILE     H       179.111 -61.828 -42.135
c4czbB_ (1)     LEU     H       176.872 -57.362 -42.321
c4czbB_ (1)     GLU     H       174.660 -60.863 -44.238
c4czbB_ (1)     ALA     H       -178.935        -59.950 -30.122
c4czbB_ (1)     SER     H       176.282 -94.594 -13.323
c4czbB_ (1)     TRP     H       -175.607        -84.297 -50.415
c4czbB_ (1)     ALA     H       -167.847        -29.497 -79.054
c4czbB_ (1)     MET     H       -179.233        -48.995 -51.928
c4czbB_ (1)     LEU     H       -177.103        -66.361 -43.449
c4czbB_ (1)     ALA     H       -179.195        -59.104 -44.034
c4czbB_ (1)     LEU     H       176.698 -67.865 -52.521
c4czbB_ (1)     LYS     H       -172.818        -70.291 -7.294
c4czbB_ (1)     LEU             -176.769        -122.332        -3.060
c4czbB_ (1)     LEU             -179.010        -108.909        26.564
c4czbB_ (1)     GLU             -171.666        -69.509 -73.037
c4czbB_ (1)     TYR             -170.251        41.577  73.105
c4czbB_ (1)     LYS             -179.012        -65.790 131.728
c4czbB_ (1)     PRO             176.961 -92.539 127.892
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S2 Data Set (Vc-NhaP2, protein of interest)

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robettastr2     ASP             -179.343        -96.508 2.340
robettastr2     ALA             -178.140        -65.589 146.601
robettastr2     VAL             175.864 -84.583 124.600
robettastr2     THR     H       -175.581        -68.589 -32.796
robettastr2     ILE     H       178.264 -70.332 -31.159
robettastr2     ASN     H       179.438 -69.171 -36.978
robettastr2     SER     H       177.535 -62.818 -42.881
robettastr2     PHE     H       177.557 -56.858 -50.599
robettastr2     PHE     H       -178.249        -63.322 -41.026
robettastr2     MET     H       179.969 -68.139 -39.175
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robettastr2    ILE    H      176.613 -62.124 -45.905
robettastr2    GLY    H      177.808 -53.295 -51.597
robettastr2    ALA    H      -179.216        -57.693 -40.587
robettastr2    LEU    H      179.978 -74.637 -34.677
robettastr2    LEU    H      -178.244        -60.378 -41.237
robettastr2    ILE    H      -178.067        -75.758 -45.012
robettastr2    GLY    H      -179.289        -57.739 -38.464
robettastr2    ILE    H      179.617 -61.108 -49.378
robettastr2    SER    H      -177.520        -77.900 -26.776
robettastr2    VAL    H      177.477 -62.577 -43.836
robettastr2    LEU    H      177.656 -66.848 -38.342
robettastr2    LEU    H      179.542 -61.166 -36.043
robettastr2    SER    H      -177.611        -48.174 -59.068
robettastr2    PRO    H      178.823 -67.413 -23.805
robettastr2    VAL    H      176.888 -68.016 -48.458
robettastr2    SER    H      -178.418        -66.624 -28.826
robettastr2    SER    H      179.455 -66.804 -42.560
robettastr2    LYS    H      178.858 -69.660 -36.724
robettastr2    LEU    H      179.480 -72.460 -30.909
robettastr2    GLY           -176.655        86.570  27.959
robettastr2    ILE           -178.257        -105.729        130.873
robettastr2    PRO           179.426 -49.450 131.963
robettastr2    ILE    H      -177.323        -61.474 -27.588
robettastr2    LEU    H      -177.992        -74.843 -27.016
robettastr2    LEU    H      -179.112        -72.074 -46.665
robettastr2    VAL    H      -179.467        -68.894 -27.949
robettastr2    PHE    H      177.425 -59.007 -43.125
robettastr2    LEU    H      178.825 -70.498 -39.946
robettastr2    ALA    H      -178.301        -63.409 -43.851
robettastr2    VAL    H      -178.749        -73.489 -25.563
robettastr2    GLY    H      175.970 -56.994 -51.717
robettastr2    MET    H      -179.722        -60.081 -41.415
robettastr2    LEU    H      -177.552        -71.324 -35.270
robettastr2    ALA    H      179.264 -75.200 -21.992
robettastr2    GLY           178.890 -96.196 -140.125
robettastr2    GLU           -170.330        -76.864 -2.428
robettastr2    ASP           175.078 -91.784 2.855
robettastr2    GLY           -178.796        -170.628        -82.943
robettastr2    ILE           -174.199        -68.390 -45.928
robettastr2    GLY           -179.051        79.225  25.082
robettastr2    GLN           -179.048        -67.498 -42.210
robettastr2    ILE           178.982 -129.779        115.225
robettastr2    ALA           -177.016        -91.059 177.495
robettastr2    PHE           177.158 -52.804 -17.918
robettastr2    ASP    H      177.974 -54.208 -20.844
robettastr2    ASN    H      177.821 -63.158 -17.166
robettastr2    TYR    H      179.830 -41.732 -53.020
robettastr2    PRO    H      179.174 -66.986 -21.008
robettastr2    VAL    H      178.557 -74.414 -43.596
robettastr2    ALA    H      -179.871        -57.932 -36.357
robettastr2    TYR    H      177.740 -56.595 -53.466
robettastr2    LEU    H      -177.411        -68.703 -39.054
robettastr2    VAL    H      -179.771        -66.137 -45.161
robettastr2    SER    H      -177.954        -64.424 -42.748
robettastr2    ASN    H      179.914 -67.103 -46.767
robettastr2    LEU    H      -179.075        -66.516 -46.291
robettastr2    ALA    H      -178.894        -59.853 -37.470
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robettastr2    LEU    H       -178.207       -64.057 -43.845
robettastr2    ALA    H       -179.444       -63.019 -44.052
robettastr2    ILE    H       -178.566       -67.759 -47.884
robettastr2    ILE    H       -176.044       -62.556 -43.585
robettastr2    LEU    H       178.490 -65.986 -43.531
robettastr2    LEU    H       -179.836       -54.853 -42.320
robettastr2    ASP    H       176.855 -61.955 -49.569
robettastr2    GLY    H       -178.959       -57.706 -37.376
robettastr2    GLY    H       177.629 -62.024 -58.005
robettastr2    MET    H       -179.726       -59.840 -34.919
robettastr2    ARG            -178.564       -60.654 -33.436
robettastr2    THR            -175.558       -102.078       178.079
robettastr2    ARG            178.398 -140.727       129.083
robettastr2    VAL            -176.189       -60.831 -37.402
robettastr2    ALA            179.176 -54.766 -33.344
robettastr2    SER            -177.230       -76.932 -7.787
robettastr2    PHE            -178.953       -79.685 -21.234
robettastr2    ARG    H       -170.472       -47.008 -49.091
robettastr2    VAL            -176.042       -62.021 -15.688
robettastr2    ALA            177.753 -147.565       32.203
robettastr2    PHE            -176.093       -60.256 -55.572
robettastr2    TRP    H       -176.682       -65.626 -41.472
robettastr2    PRO    H       172.009 -56.015 -32.372
robettastr2    SER    H       179.187 -74.235 -40.079
robettastr2    VAL    H       179.542 -64.942 -46.002
robettastr2    SER    H       -179.077       -69.008 -43.797
robettastr2    LEU    H       177.230 -61.108 -44.931
robettastr2    ALA    H       179.286 -66.394 -41.377
robettastr2    THR    H       -176.563       -70.835 -54.730
robettastr2    LEU    H       -178.278       -76.664 -35.753
robettastr2    GLY    H       178.887 -58.862 -55.437
robettastr2    VAL    H       -179.382       -66.566 -44.325
robettastr2    ALA    H       -178.683       -60.210 -42.378
robettastr2    VAL    H       -179.801       -74.528 -43.594
robettastr2    THR    H       179.608 -59.626 -44.199
robettastr2    THR    H       179.820 -55.488 -49.099
robettastr2    LEU    H       178.037 -64.758 -50.243
robettastr2    LEU    H       -173.817       -66.238 -41.738
robettastr2    THR    H       -179.181       -71.677 -30.376
robettastr2    GLY    H       176.229 -62.465 -52.531
robettastr2    LEU    H       -178.903       -59.889 -38.909
robettastr2    LEU    H       179.326 -61.682 -42.475
robettastr2    ALA    H       179.945 -65.737 -39.544
robettastr2    MET    H       -174.942       -73.098 -35.627
robettastr2    TRP    H       179.627 -64.711 -39.854
robettastr2    LEU    H       179.964 -70.283 -41.499
robettastr2    PHE    H       -177.230       -100.728       -0.643
robettastr2    ASN            179.869 58.702  41.473
robettastr2    LEU            -179.951       -108.623       170.874
robettastr2    SER            -175.469       -72.484 161.054
robettastr2    LEU    H       178.462 -59.555 -44.415
robettastr2    LEU    H       179.817 -61.505 -34.816
robettastr2    GLN    H       176.240 -62.694 -36.829
robettastr2    GLY    H       177.961 -61.084 -52.453
robettastr2    VAL    H       -177.276       -58.287 -40.541
robettastr2    LEU    H       174.186 -62.811 -46.993
robettastr2    VAL    H       179.202 -56.879 -43.246
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robettastr2    GLY     H       -179.947        -60.431 -45.503
robettastr2    ALA     H       -178.868        -59.556 -37.906
robettastr2    ILE     H       -178.787        -68.257 -52.433
robettastr2    VAL     H       -178.651        -77.780 -11.574
robettastr2    GLY             177.210 -72.468 -18.393
robettastr2    SER             179.886 -82.650 160.921
robettastr2    THR             176.494 -133.388        163.635
robettastr2    ASP             177.695 -107.256        103.959
robettastr2    ALA     H       -177.265        -59.031 -31.802
robettastr2    ALA     H       -176.741        -69.870 -40.854
robettastr2    ALA     H       -179.925        -62.738 -44.727
robettastr2    VAL     H       -177.771        -69.734 -50.802
robettastr2    PHE     H       -178.888        -54.489 -49.616
robettastr2    SER     H       -176.612        -59.919 -44.192
robettastr2    LEU     H       -178.419        -71.676 -31.439
robettastr2    LEU     H       -178.112        -77.911 -42.364
robettastr2    LYS     H       -177.651        -67.994 -34.805
robettastr2    GLY             179.986 -65.022 -11.871
robettastr2    ARG             179.066 -116.095        15.499
robettastr2    SER             179.525 56.842  43.070
robettastr2    LEU             176.356 -64.184 136.774
robettastr2    ASN             175.943 -47.968 122.579
robettastr2    GLU     H       -177.685        -49.651 -35.549
robettastr2    ARG     H       -178.453        -58.847 -42.092
robettastr2    VAL     H       -176.181        -78.700 -43.693
robettastr2    GLY     H       179.964 -55.675 -54.096
robettastr2    ALA     H       179.799 -59.732 -39.801
robettastr2    THR     H       179.471 -58.708 -45.696
robettastr2    LEU     H       -179.504        -66.028 -37.550
robettastr2    GLU     H       178.088 -66.033 -46.683
robettastr2    ILE     H       -177.437        -64.647 -44.929
robettastr2    GLU     H       178.092 -54.199 -49.518
robettastr2    SER     H       -178.867        -64.896 -40.797
robettastr2    GLY     H       178.464 -60.288 -38.271
robettastr2    THR     H       -179.832        -73.117 -39.730
robettastr2    ASN     H       -179.512        -57.452 -34.500
robettastr2    ASP     H       -177.957        -54.985 -66.869
robettastr2    PRO     H       -178.471        -62.173 -26.761
robettastr2    MET     H       178.732 -68.157 -52.285
robettastr2    ALA     H       -178.424        -62.512 -34.735
robettastr2    VAL     H       178.686 -63.620 -44.726
robettastr2    PHE     H       178.439 -60.891 -39.991
robettastr2    LEU     H       -178.480        -64.736 -44.090
robettastr2    THR     H       -179.519        -61.079 -46.442
robettastr2    VAL     H       -177.322        -64.205 -45.898
robettastr2    THR     H       -178.710        -72.697 -29.865
robettastr2    LEU     H       176.426 -69.237 -39.201
robettastr2    ILE     H       175.664 -61.303 -43.635
robettastr2    ALA     H       179.749 -58.477 -43.757
robettastr2    VAL     H       179.912 -70.496 -17.392
robettastr2    LEU     H       175.575 -103.374        3.998
robettastr2    GLY             -171.527        -84.568 5.113
robettastr2    SER             -177.648        -163.773        155.700
robettastr2    ALA             170.891 -58.734 -33.859
robettastr2    GLU             -177.516        -86.957 65.401
robettastr2    THR             -176.219        -126.351        37.428
robettastr2    ASN             177.053 -79.348 69.084
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robettastr2    LEU           -173.215       -103.550       145.726
robettastr2    SER           174.711 -82.350 154.202
robettastr2    ALA           173.520 -55.249 -30.259
robettastr2    GLY    H      179.626 -58.854 -34.137
robettastr2    PHE    H      178.770 -62.376 -50.175
robettastr2    LEU    H      -176.900       -62.391 -49.685
robettastr2    LEU    H      -178.153       -65.323 -40.199
robettastr2    LEU    H      178.926 -65.075 -42.199
robettastr2    SER    H      -179.394       -59.609 -42.565
robettastr2    PHE    H      178.080 -56.669 -48.941
robettastr2    ILE    H      -177.674       -62.179 -45.566
robettastr2    GLN    H      -179.955       -65.061 -37.254
robettastr2    GLN    H      178.328 -64.398 -36.989
robettastr2    PHE    H      -179.965       -65.652 -47.280
robettastr2    GLY    H      -179.169       -54.000 -54.661
robettastr2    VAL    H      -179.531       -62.463 -46.497
robettastr2    GLY    H      -177.738       -58.215 -54.454
robettastr2    ALA    H      -177.956       -60.888 -40.557
robettastr2    LEU    H      -177.546       -76.416 -44.296
robettastr2    LEU    H      -178.906       -69.652 -44.029
robettastr2    GLY    H      -178.048       -55.496 -55.819
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robettastr2    ALA    H      178.616 -63.540 -43.776
robettastr2    GLY    H      -178.417       -61.959 -49.944
robettastr2    GLY    H      179.953 -56.122 -52.871
robettastr2    TRP    H      -179.438       -63.298 -45.514
robettastr2    ILE    H      -177.407       -61.690 -44.630
robettastr2    LEU    H      179.105 -64.431 -46.335
robettastr2    TRP    H      176.818 -48.758 -52.260
robettastr2    TRP    H      -179.823       -61.248 -49.058
robettastr2    LEU    H      -179.460       -63.250 -37.883
robettastr2    ILE    H      179.685 -63.777 -44.654
robettastr2    ASN    H      178.741 -70.487 -45.163
robettastr2    ARG    H      -177.687       -55.725 -42.833
robettastr2    ASN    H      -178.191       -94.218 7.148
robettastr2    GLN           -179.824       47.898  55.519
robettastr2    LEU           -173.938       -75.138 155.533
robettastr2    PRO           169.899 -60.514 155.841
robettastr2    GLU    H      177.678 -59.149 -33.576
robettastr2    GLY    H      178.476 -58.841 -35.295
robettastr2    LEU    H      -178.560       -76.331 -34.396
robettastr2    TYR    H      -178.978       -59.196 -42.194
robettastr2    SER    H      -178.769       -68.620 -45.818
robettastr2    ILE    H      -179.164       -62.873 -48.793
robettastr2    LEU    H      -176.685       -69.083 -39.552
robettastr2    ALA    H      -179.794       -67.478 -41.675
robettastr2    VAL    H      179.859 -69.509 -46.105
robettastr2    SER    H      -179.957       -62.929 -40.725
robettastr2    GLY    H      -179.569       -56.026 -55.532
robettastr2    GLY    H      -179.791       -61.007 -41.500
robettastr2    LEU    H      -177.863       -71.946 -33.499
robettastr2    MET    H      -179.602       -79.100 -38.070
robettastr2    ILE    H      -179.315       -68.069 -31.874
robettastr2    PHE    H      173.886 -58.987 -53.352
robettastr2    ALA    H      179.270 -59.714 -39.579
robettastr2    LEU    H      -179.336       -67.978 -48.102
robettastr2    SER    H      179.681 -60.137 -39.011
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robettastr2    ASN    H      179.915 -63.284 -40.946
robettastr2    ALA    H      178.155 -60.879 -34.007
robettastr2    LEU    H      -179.204        -81.130 -2.266
robettastr2    GLY           -179.297        88.308  11.945
robettastr2    GLY           -179.299        -110.613        -160.842
robettastr2    SER           179.620 -106.197        110.777
robettastr2    GLY    H      178.418 -60.154 -30.787
robettastr2    ILE    H      -178.756        -68.098 -42.485
robettastr2    LEU    H      175.298 -64.266 -41.330
robettastr2    SER    H      -179.225        -57.380 -42.307
robettastr2    ILE    H      177.641 -63.039 -44.328
robettastr2    TYR    H      -179.939        -55.971 -49.512
robettastr2    LEU    H      -176.818        -71.368 -33.151
robettastr2    THR    H      177.313 -63.039 -46.934
robettastr2    GLY    H      179.677 -59.110 -51.146
robettastr2    LEU    H      -179.355        -60.992 -41.632
robettastr2    LEU    H      179.042 -66.398 -40.589
robettastr2    LEU    H      178.200 -66.297 -23.830
robettastr2    GLY    H      178.536 -90.223 -2.591
robettastr2    ASN           -177.898        -99.192 -4.401
robettastr2    ARG           -176.838        -71.095 143.651
robettastr2    PRO           -179.455        -79.440 57.676
robettastr2    THR           -176.669        -158.401        -166.216
robettastr2    ARG           -59.405 162.995 -58.946
robettastr2    SER           170.525 -59.136 -26.190
robettastr2    ARG    H      179.138 -55.746 -39.854
robettastr2    HIS    H      -177.081        -75.917 -37.862
robettastr2    ALA    H      178.914 -61.512 -43.544
robettastr2    ILE    H      -179.129        -67.457 -47.799
robettastr2    LEU    H      -177.992        -65.011 -41.319
robettastr2    ASN    H      -179.567        -61.266 -39.460
robettastr2    VAL    H      176.826 -65.919 -43.872
robettastr2    LEU    H      178.961 -63.651 -33.069
robettastr2    ASP    H      178.983 -59.576 -47.023
robettastr2    GLY    H      178.052 -60.339 -51.524
robettastr2    MET    H      -178.903        -58.065 -41.897
robettastr2    THR    H      -178.723        -66.464 -44.862
robettastr2    TRP    H      -179.119        -61.787 -47.054
robettastr2    LEU    H      179.531 -64.962 -37.287
robettastr2    ALA    H      178.052 -62.124 -42.221
robettastr2    GLN    H      178.229 -66.270 -37.976
robettastr2    ILE    H      177.410 -61.949 -49.433
robettastr2    GLY    H      -177.881        -55.754 -60.685
robettastr2    MET    H      -177.115        -58.887 -45.419
robettastr2    PHE    H      179.595 -70.588 -42.606
robettastr2    LEU    H      -176.901        -65.786 -42.272
robettastr2    VAL    H      176.819 -56.357 -45.690
robettastr2    LEU    H      -179.106        -56.241 -51.844
robettastr2    GLY    H      -176.646        -57.580 -37.069
robettastr2    LEU    H      179.411 -67.680 -23.741
robettastr2    LEU           -178.773        -86.076 -1.508
robettastr2    VAL           -178.353        -85.842 125.196
robettastr2    THR           -179.441        -101.912        132.945
robettastr2    PRO    H      177.500 -46.366 -35.013
robettastr2    SER    H      -179.950        -62.608 -39.927
robettastr2    GLU    H      -176.867        -74.448 -36.538
robettastr2    LEU    H      179.822 -65.988 -39.120
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robettastr2	MET	H	179.243	-64.272	-34.707		
robettastr2	GLU		178.446	-79.033	-44.064		
robettastr2	ILE		-175.546		-122.549		6.161
robettastr2	ALA		179.668	-61.190	-38.848		
robettastr2	LEU	H	-179.795		-61.216	-49.802	
robettastr2	PRO	H	176.768	-69.793	-21.452		
robettastr2	GLY	H	174.457	-61.644	-51.508		
robettastr2	LEU	H	178.377	-64.521	-38.293		
robettastr2	ALA	H	179.077	-59.891	-41.583		
robettastr2	LEU	H	178.548	-70.750	-37.604		
robettastr2	ALA	H	179.158	-57.581	-39.167		
robettastr2	VAL	H	178.268	-64.228	-51.684		
robettastr2	GLY	H	-178.587		-61.027	-51.008	
robettastr2	MET	H	-177.931		-59.514	-43.484	
robettastr2	ILE	H	-177.482		-78.993	-46.308	
robettastr2	LEU	H	-177.331		-71.315	-44.364	
robettastr2	PHE	H	-178.265		-98.471	-60.288	
robettastr2	ALA	H	-168.669		-63.395	-45.240	
robettastr2	ARG	H	179.950	-53.091	-56.492		
robettastr2	PRO	H	176.065	-52.537	-35.167		
robettastr2	ILE	H	-179.698		-71.199	-43.638	
robettastr2	ALA	H	-179.632		-61.117	-40.189	
robettastr2	VAL	H	177.497	-65.056	-45.737		
robettastr2	TRP	H	-178.713		-61.095	-40.135	
robettastr2	ILE	H	177.424	-62.806	-43.482		
robettastr2	GLY	H	177.967	-61.448	-34.560		
robettastr2	LEU	H	-177.599		-88.025	-29.740	
robettastr2	ALA	H	-175.901		-53.497	-37.494	
robettastr2	PRO		177.808	-59.347	-17.337		
robettastr2	PHE		-177.139		-112.708		-39.846
robettastr2	LYS		-176.810		57.582	27.761	
robettastr2	SER		179.893	-89.117	-5.468		
robettastr2	PHE		-178.524		-104.462		142.101
robettastr2	THR		176.605	-76.715	166.873		
robettastr2	ALA	H	178.657	-59.029	-38.229		
robettastr2	ARG	H	-178.789		-65.695	-40.605	
robettastr2	GLU	H	177.777	-67.172	-35.939		
robettastr2	LYS	H	178.185	-62.543	-39.895		
robettastr2	TRP	H	177.984	-68.925	-40.150		
robettastr2	PHE	H	179.883	-61.811	-48.512		
robettastr2	VAL	H	-179.283		-61.796	-40.086	
robettastr2	SER	H	177.396	-61.789	-37.595		
robettastr2	TRP	H	179.252	-74.260	-28.951		
robettastr2	VAL		-178.966		-94.291	135.292	
robettastr2	GLY		178.390	152.066	101.961		
robettastr2	LEU		-177.253		-101.231		143.358
robettastr2	ARG		174.236	-92.059	150.391		
robettastr2	GLY		-179.110		-171.597		-120.253
robettastr2	ALA	H	-174.526		-54.994	-43.371	
robettastr2	VAL	H	-175.795		-73.673	-51.999	
robettastr2	PRO	H	173.769	-48.703	-37.769		
robettastr2	ILE	H	179.169	-66.688	-46.712		
robettastr2	ILE	H	178.119	-61.948	-44.432		
robettastr2	LEU	H	-177.209		-71.730	-27.892	
robettastr2	ALA	H	176.581	-65.116	-39.281		
robettastr2	VAL	H	179.071	-72.956	-39.367		
robettastr2	PHE	H	-177.253		-46.864	-46.723	

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robettastr2    PRO    H      175.372 -50.214 -30.515
robettastr2    MET    H      -179.736        -79.410 -40.711
robettastr2    MET    H      -177.638        -65.088 -31.548
robettastr2    ALA    H      178.764 -77.311 -14.610
robettastr2    GLY           -177.498        74.910  29.268
robettastr2    LEU           -178.346        -70.338 143.406
robettastr2    PRO           176.096 -48.764 -34.058
robettastr2    ASN           -179.915        -113.673        26.838
robettastr2    ALA    H      -177.009        -52.798 -38.004
robettastr2    GLN    H      -179.514        -65.993 -27.069
robettastr2    LEU    H      -179.346        -79.290 -39.098
robettastr2    TYR    H      -178.845        -63.254 -40.607
robettastr2    PHE    H      178.704 -61.181 -58.660
robettastr2    ASN    H      -177.552        -76.901 -27.276
robettastr2    LEU    H      -178.673        -73.303 -42.550
robettastr2    ALA    H      178.335 -62.556 -36.726
robettastr2    PHE    H      178.011 -54.786 -49.513
robettastr2    PHE    H      179.368 -70.353 -28.901
robettastr2    VAL    H      176.108 -64.865 -42.122
robettastr2    VAL    H      179.524 -63.376 -49.758
robettastr2    MET    H      -176.532        -63.425 -41.191
robettastr2    VAL    H      -179.676        -66.914 -44.496
robettastr2    SER    H      -177.652        -63.974 -30.586
robettastr2    LEU    H      179.025 -68.955 -38.549
robettastr2    VAL    H      177.524 -67.972 -45.913
robettastr2    VAL    H      -177.104        -63.929 -47.668
robettastr2    GLN    H      -178.996        -73.853 -39.647
robettastr2    GLY    H      179.045 -57.749 -35.651
robettastr2    GLY    H      179.496 -87.364 -27.942
robettastr2    THR    H      -176.302        -112.464        -12.170
robettastr2    LEU    H      -179.045        -54.539 -35.295
robettastr2    THR    H      179.576 -59.655 -40.706
robettastr2    LYS    H      -178.721        -70.503 -39.782
robettastr2    ALA    H      179.732 -61.621 -44.418
robettastr2    MET    H      179.030 -66.261 -49.802
robettastr2    SER    H      -177.186        -58.307 -40.291
robettastr2    LEU    H      177.831 -65.268 -49.485
robettastr2    ALA    H      -176.769        -55.278 -33.280
robettastr2    LYS           -178.294        -80.883 -7.991
robettastr2    VAL           -175.815        -126.685        157.216
robettastr2    GLU           -179.617        -82.195 60.524
robettastr2    LEU           179.313 -118.730        156.712
robettastr2    PRO           169.309 -58.252 153.165
robettastr2    PRO           -177.890        -67.679 152.724
robettastr2    LYS           179.947 -127.912        72.592
robettastr2    PRO           178.727 -72.484 152.263
robettastr2    GLU           176.318 -132.030        150.057
robettastr2    PRO           175.843 -71.899 162.600
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S3 Data Set (Vc-NhaP2 refined structure)

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REMARK initial molprobity 1.556
REMARK initial/complete molprobity 1.590
REMARK final molprobity 1.002000
REMARK CA-RMSD from-initial 0.164900
REMARK SC-RMSD from-initial 3.621500
ATOM      1  N   MET A   1      39.641  47.694  23.385  1.00  0.00
ATOM      2  HT1 MET A   1      39.620  48.714  23.589  1.00  0.00
ATOM      3  HT2 MET A   1      40.323  47.224  24.016  1.00  0.00
ATOM      4  HT3 MET A   1      38.697  47.285  23.536  1.00  0.00
ATOM      5  CA  MET A   1      40.058  47.480  21.972  1.00  0.00
ATOM      6  HA  MET A   1      39.296  47.935  21.354  1.00  0.00
ATOM      7  CB  MET A   1      41.425  48.166  21.674  1.00  0.00
ATOM      8  HB1 MET A   1      42.056  48.213  22.588  1.00  0.00
ATOM      9  HB2 MET A   1      42.005  47.576  20.926  1.00  0.00
ATOM     10  CG  MET A   1      41.280  49.570  21.052  1.00  0.00
ATOM     11  HG1 MET A   1      42.297  49.924  20.769  1.00  0.00
ATOM     12  HG2 MET A   1      40.697  49.473  20.110  1.00  0.00
ATOM     13  SD  MET A   1      40.498  50.803  22.139  1.00  0.00
ATOM     14  CE  MET A   1      40.557  52.161  20.934  1.00  0.00
ATOM     15  HE1 MET A   1      40.116  53.088  21.359  1.00  0.00
ATOM     16  HE2 MET A   1      41.604  52.386  20.638  1.00  0.00
ATOM     17  HE3 MET A   1      39.988  51.903  20.014  1.00  0.00
ATOM     18  C   MET A   1      40.096  46.018  21.615  1.00  0.00
ATOM     19  O   MET A   1      40.119  45.153  22.491  1.00  0.00
ATOM     20  N   ASP A   2      40.081  45.725  20.314  1.00  0.00
ATOM     21  HN  ASP A   2      40.074  46.434  19.610  1.00  0.00
ATOM     22  CA  ASP A   2      39.996  44.385  19.777  1.00  0.00
ATOM     23  HA  ASP A   2      39.707  43.702  20.564  1.00  0.00
ATOM     24  CB  ASP A   2      38.887  44.325  18.673  1.00  0.00
ATOM     25  HB1 ASP A   2      38.807  43.289  18.282  1.00  0.00
ATOM     26  HB2 ASP A   2      37.913  44.593  19.135  1.00  0.00
ATOM     27  CG  ASP A   2      39.132  45.281  17.488  1.00  0.00
ATOM     28  OD1 ASP A   2      40.070  46.119  17.525  1.00  0.00
ATOM     29  OD2 ASP A   2      38.319  45.196  16.529  1.00  0.00
ATOM     30  C   ASP A   2      41.326  43.902  19.238  1.00  0.00
ATOM     31  O   ASP A   2      41.437  42.756  18.804  1.00  0.00
ATOM     32  N   ALA A   3      42.354  44.756  19.278  1.00  0.00
ATOM     33  HN  ALA A   3      42.223  45.682  19.618  1.00  0.00
ATOM     34  CA  ALA A   3      43.695  44.447  18.823  1.00  0.00
ATOM     35  HA  ALA A   3      43.626  44.138  17.789  1.00  0.00
ATOM     36  CB  ALA A   3      44.607  45.687  18.917  1.00  0.00
ATOM     37  HB1 ALA A   3      44.695  46.040  19.966  1.00  0.00
ATOM     38  HB2 ALA A   3      44.180  46.513  18.309  1.00  0.00
ATOM     39  HB3 ALA A   3      45.624  45.463  18.528  1.00  0.00
ATOM     40  C   ALA A   3      44.332  43.326  19.609  1.00  0.00
ATOM     41  O   ALA A   3      44.929  42.414  19.039  1.00  0.00
ATOM     42  N   VAL A   4      44.188  43.373  20.932  1.00  0.00
ATOM     43  HN  VAL A   4      43.698  44.122  21.372  1.00  0.00
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ATOM     44  CA  VAL A   4      44.665  42.350  21.823  1.00  0.00
ATOM     45  HA  VAL A   4      44.460  41.385  21.378  1.00  0.00
ATOM     46  CB  VAL A   4      46.165  42.477  22.115  1.00  0.00
ATOM     47  HB  VAL A   4      46.703  42.352  21.146  1.00  0.00
ATOM     48  CG1 VAL A   4      46.517  43.886  22.645  1.00  0.00
ATOM     49 HG11 VAL A   4      45.977  44.103  23.590  1.00  0.00
ATOM     50 HG12 VAL A   4      46.259  44.669  21.902  1.00  0.00
ATOM     51 HG13 VAL A   4      47.608  43.951  22.844  1.00  0.00
ATOM     52  CG2 VAL A   4      46.662  41.345  23.042  1.00  0.00
ATOM     53 HG21 VAL A   4      46.378  40.354  22.632  1.00  0.00
ATOM     54 HG22 VAL A   4      46.237  41.449  24.060  1.00  0.00
ATOM     55 HG23 VAL A   4      47.769  41.385  23.129  1.00  0.00
ATOM     56  C   VAL A   4      43.793  42.492  23.044  1.00  0.00
ATOM     57  O   VAL A   4      43.359  43.594  23.384  1.00  0.00
ATOM     58  N   THR A   5      43.496  41.375  23.712  1.00  0.00
ATOM     59  HN  THR A   5      43.831  40.487  23.407  1.00  0.00
ATOM     60  CA  THR A   5      42.695  41.348  24.918  1.00  0.00
ATOM     61  HA  THR A   5      41.959  42.139  24.858  1.00  0.00
ATOM     62  CB  THR A   5      41.943  40.037  25.126  1.00  0.00
ATOM     63  HB  THR A   5      41.501  39.982  26.147  1.00  0.00
ATOM     64  OG1 THR A   5      42.792  38.910  24.931  1.00  0.00
ATOM     65  HG1 THR A   5      43.525  39.017  25.540  1.00  0.00
ATOM     66  CG2 THR A   5      40.785  39.969  24.109  1.00  0.00
ATOM     67 HG21 THR A   5      41.170  39.984  23.068  1.00  0.00
ATOM     68 HG22 THR A   5      40.100  40.832  24.246  1.00  0.00
ATOM     69 HG23 THR A   5      40.201  39.035  24.254  1.00  0.00
ATOM     70  C   THR A   5      43.574  41.637  26.108  1.00  0.00
ATOM     71  O   THR A   5      44.744  41.259  26.137  1.00  0.00
ATOM     72  N   ILE A   6      43.010  42.291  27.128  1.00  0.00
ATOM     73  HN  ILE A   6      42.066  42.606  27.078  1.00  0.00
ATOM     74  CA  ILE A   6      43.693  42.599  28.373  1.00  0.00
ATOM     75  HA  ILE A   6      44.693  42.921  28.129  1.00  0.00
ATOM     76  CB  ILE A   6      43.005  43.711  29.167  1.00  0.00
ATOM     77  HB  ILE A   6      43.599  43.914  30.090  1.00  0.00
ATOM     78  CG2 ILE A   6      41.581  43.291  29.606  1.00  0.00
ATOM     79 HG21 ILE A   6      41.608  42.409  30.280  1.00  0.00
ATOM     80 HG22 ILE A   6      40.948  43.053  28.727  1.00  0.00
ATOM     81 HG23 ILE A   6      41.100  44.124  30.162  1.00  0.00
ATOM     82  CG1 ILE A   6      42.963  45.037  28.362  1.00  0.00
ATOM     83 HG11 ILE A   6      42.466  45.804  28.998  1.00  0.00
ATOM     84 HG12 ILE A   6      42.333  44.904  27.456  1.00  0.00
ATOM     85  CD1 ILE A   6      44.337  45.574  27.945  1.00  0.00
ATOM     86  HD1 ILE A   6      44.826  44.893  27.218  1.00  0.00
ATOM     87  HD2 ILE A   6      44.997  45.682  28.831  1.00  0.00
ATOM     88  HD3 ILE A   6      44.229  46.570  27.465  1.00  0.00
ATOM     89  C   ILE A   6      43.833  41.347  29.209  1.00  0.00
ATOM     90  O   ILE A   6      44.710  41.254  30.066  1.00  0.00
ATOM     91  N   ASN A   7      42.998  40.347  28.918  1.00  0.00
ATOM     92  HN  ASN A   7      42.288  40.495  28.234  1.00  0.00
ATOM     93  CA  ASN A   7      43.026  39.008  29.454  1.00  0.00
ATOM     94  HA  ASN A   7      42.959  39.084  30.531  1.00  0.00
ATOM     95  CB  ASN A   7      41.828  38.192  28.901  1.00  0.00
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ATOM     96  HB1 ASN A   7      41.797  37.183  29.364  1.00  0.00
ATOM     97  HB2 ASN A   7      41.921  38.070  27.800  1.00  0.00
ATOM     98  CG  ASN A   7      40.502  38.913  29.183  1.00  0.00
ATOM     99  OD1 ASN A   7      39.805  39.324  28.249  1.00  0.00
ATOM    100  ND2 ASN A   7      40.168  39.082  30.495  1.00  0.00
ATOM    101 HD21 ASN A   7      39.315  39.549  30.727  1.00  0.00
ATOM    102 HD22 ASN A   7      40.767  38.733  31.214  1.00  0.00
ATOM    103  C   ASN A   7      44.305  38.284  29.111  1.00  0.00
ATOM    104  O   ASN A   7      44.806  37.510  29.919  1.00  0.00
ATOM    105  N   SER A   8      44.836  38.505  27.903  1.00  0.00
ATOM    106  HN  SER A   8      44.422  39.167  27.283  1.00  0.00
ATOM    107  CA  SER A   8      46.045  37.862  27.421  1.00  0.00
ATOM    108  HA  SER A   8      45.895  36.795  27.506  1.00  0.00
ATOM    109  CB  SER A   8      46.273  38.220  25.925  1.00  0.00
ATOM    110  HB1 SER A   8      46.472  39.307  25.810  1.00  0.00
ATOM    111  HB2 SER A   8      45.355  37.975  25.350  1.00  0.00
ATOM    112  OG  SER A   8      47.357  37.497  25.349  1.00  0.00
ATOM    113  HG  SER A   8      47.089  36.574  25.330  1.00  0.00
ATOM    114  C   SER A   8      47.273  38.228  28.236  1.00  0.00
ATOM    115  O   SER A   8      48.032  37.351  28.645  1.00  0.00
ATOM    116  N   PHE A   9      47.455  39.524  28.513  1.00  0.00
ATOM    117  HN  PHE A   9      46.834  40.214  28.150  1.00  0.00
ATOM    118  CA  PHE A   9      48.504  40.039  29.376  1.00  0.00
ATOM    119  HA  PHE A   9      49.456  39.684  29.004  1.00  0.00
ATOM    120  CB  PHE A   9      48.477  41.591  29.402  1.00  0.00
ATOM    121  HB1 PHE A   9      49.237  41.984  30.114  1.00  0.00
ATOM    122  HB2 PHE A   9      47.479  41.962  29.724  1.00  0.00
ATOM    123  CG  PHE A   9      48.787  42.172  28.051  1.00  0.00
ATOM    124  CD1 PHE A   9      50.120  42.377  27.657  1.00  0.00
ATOM    125  HD1 PHE A   9      50.921  42.106  28.327  1.00  0.00
ATOM    126  CE1 PHE A   9      50.419  42.939  26.410  1.00  0.00
ATOM    127  HE1 PHE A   9      51.449  43.078  26.118  1.00  0.00
ATOM    128  CZ  PHE A   9      49.383  43.317  25.548  1.00  0.00
ATOM    129  HZ  PHE A   9      49.610  43.753  24.587  1.00  0.00
ATOM    130  CD2 PHE A   9      47.756  42.565  27.183  1.00  0.00
ATOM    131  HD2 PHE A   9      46.728  42.430  27.479  1.00  0.00
ATOM    132  CE2 PHE A   9      48.050  43.135  25.941  1.00  0.00
ATOM    133  HE2 PHE A   9      47.245  43.437  25.293  1.00  0.00
ATOM    134  C   PHE A   9      48.348  39.577  30.801  1.00  0.00
ATOM    135  O   PHE A   9      49.316  39.178  31.444  1.00  0.00
ATOM    136  N   PHE A  10      47.111  39.625  31.303  1.00  0.00
ATOM    137  HN  PHE A  10      46.358  39.963  30.741  1.00  0.00
ATOM    138  CA  PHE A  10      46.731  39.244  32.642  1.00  0.00
ATOM    139  HA  PHE A  10      47.339  39.823  33.323  1.00  0.00
ATOM    140  CB  PHE A  10      45.233  39.612  32.878  1.00  0.00
ATOM    141  HB1 PHE A  10      44.610  39.154  32.081  1.00  0.00
ATOM    142  HB2 PHE A  10      45.110  40.715  32.818  1.00  0.00
ATOM    143  CG  PHE A  10      44.717  39.150  34.223  1.00  0.00
ATOM    144  CD1 PHE A  10      43.812  38.077  34.316  1.00  0.00
ATOM    145  HD1 PHE A  10      43.485  37.571  33.419  1.00  0.00
ATOM    146  CE1 PHE A  10      43.345  37.645  35.563  1.00  0.00
ATOM    147  HE1 PHE A  10      42.656  36.815  35.624  1.00  0.00
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ATOM    148  CZ  PHE A  10      43.771  38.289  36.731  1.00  0.00
ATOM    149  HZ  PHE A  10      43.411  37.957  37.694  1.00  0.00
ATOM    150  CD2 PHE A  10      45.131  39.794  35.401  1.00  0.00
ATOM    151  HD2 PHE A  10      45.822  40.623  35.344  1.00  0.00
ATOM    152  CE2 PHE A  10      44.664  39.365  36.650  1.00  0.00
ATOM    153  HE2 PHE A  10      44.992  39.864  37.550  1.00  0.00
ATOM    154  C   PHE A  10      47.004  37.784  32.928  1.00  0.00
ATOM    155  O   PHE A  10      47.511  37.445  33.991  1.00  0.00
ATOM    156  N   MET A  11      46.674  36.912  31.975  1.00  0.00
ATOM    157  HN  MET A  11      46.251  37.228  31.126  1.00  0.00
ATOM    158  CA  MET A  11      46.837  35.481  32.070  1.00  0.00
ATOM    159  HA  MET A  11      46.294  35.153  32.947  1.00  0.00
ATOM    160  CB  MET A  11      46.210  34.798  30.823  1.00  0.00
ATOM    161  HB1 MET A  11      46.575  35.333  29.916  1.00  0.00
ATOM    162  HB2 MET A  11      45.108  34.939  30.866  1.00  0.00
ATOM    163  CG  MET A  11      46.521  33.299  30.625  1.00  0.00
ATOM    164  HG1 MET A  11      47.609  33.172  30.445  1.00  0.00
ATOM    165  HG2 MET A  11      46.011  32.972  29.692  1.00  0.00
ATOM    166  SD  MET A  11      45.990  32.232  32.001  1.00  0.00
ATOM    167  CE  MET A  11      46.761  30.727  31.337  1.00  0.00
ATOM    168  HE1 MET A  11      47.856  30.866  31.209  1.00  0.00
ATOM    169  HE2 MET A  11      46.330  30.463  30.348  1.00  0.00
ATOM    170  HE3 MET A  11      46.604  29.866  32.021  1.00  0.00
ATOM    171  C   MET A  11      48.266  35.045  32.244  1.00  0.00
ATOM    172  O   MET A  11      48.564  34.224  33.107  1.00  0.00
ATOM    173  N   ILE A  12      49.178  35.618  31.454  1.00  0.00
ATOM    174  HN  ILE A  12      48.926  36.302  30.773  1.00  0.00
ATOM    175  CA  ILE A  12      50.576  35.240  31.492  1.00  0.00
ATOM    176  HA  ILE A  12      50.631  34.188  31.731  1.00  0.00
ATOM    177  CB  ILE A  12      51.299  35.433  30.158  1.00  0.00
ATOM    178  HB  ILE A  12      52.342  35.047  30.256  1.00  0.00
ATOM    179  CG2 ILE A  12      51.394  36.926  29.774  1.00  0.00
ATOM    180 HG21 ILE A  12      51.981  37.501  30.520  1.00  0.00
ATOM    181 HG22 ILE A  12      50.386  37.378  29.688  1.00  0.00
ATOM    182 HG23 ILE A  12      51.904  37.021  28.792  1.00  0.00
ATOM    183  CG1 ILE A  12      50.628  34.612  29.024  1.00  0.00
ATOM    184 HG11 ILE A  12      51.212  34.783  28.091  1.00  0.00
ATOM    185 HG12 ILE A  12      49.600  34.995  28.845  1.00  0.00
ATOM    186  CD1 ILE A  12      50.567  33.103  29.288  1.00  0.00
ATOM    187  HD1 ILE A  12      49.896  32.876  30.143  1.00  0.00
ATOM    188  HD2 ILE A  12      51.579  32.711  29.522  1.00  0.00
ATOM    189  HD3 ILE A  12      50.180  32.572  28.393  1.00  0.00
ATOM    190  C   ILE A  12      51.299  35.955  32.606  1.00  0.00
ATOM    191  O   ILE A  12      52.352  35.504  33.047  1.00  0.00
ATOM    192  N   GLY A  13      50.726  37.050  33.111  1.00  0.00
ATOM    193  HN  GLY A  13      49.883  37.415  32.720  1.00  0.00
ATOM    194  CA  GLY A  13      51.249  37.760  34.257  1.00  0.00
ATOM    195  HA1 GLY A  13      50.743  38.713  34.295  1.00  0.00
ATOM    196  HA2 GLY A  13      52.323  37.849  34.164  1.00  0.00
ATOM    197  C   GLY A  13      50.929  37.010  35.516  1.00  0.00
ATOM    198  O   GLY A  13      51.810  36.748  36.328  1.00  0.00
ATOM    199  N   ALA A  14      49.661  36.626  35.682  1.00  0.00
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ATOM    200  HN  ALA A  14      48.971  36.862  34.998  1.00  0.00
ATOM    201  CA  ALA A  14      49.152  35.871  36.805  1.00  0.00
ATOM    202  HA  ALA A  14      49.390  36.424  37.703  1.00  0.00
ATOM    203  CB  ALA A  14      47.623  35.695  36.713  1.00  0.00
ATOM    204  HB1 ALA A  14      47.341  35.141  35.791  1.00  0.00
ATOM    205  HB2 ALA A  14      47.131  36.691  36.678  1.00  0.00
ATOM    206  HB3 ALA A  14      47.230  35.146  37.596  1.00  0.00
ATOM    207  C   ALA A  14      49.782  34.507  36.914  1.00  0.00
ATOM    208  O   ALA A  14      50.152  34.077  38.005  1.00  0.00
ATOM    209  N   LEU A  15      49.927  33.819  35.779  1.00  0.00
ATOM    210  HN  LEU A  15      49.592  34.189  34.914  1.00  0.00
ATOM    211  CA  LEU A  15      50.559  32.522  35.683  1.00  0.00
ATOM    212  HA  LEU A  15      50.038  31.857  36.358  1.00  0.00
ATOM    213  CB  LEU A  15      50.433  31.985  34.232  1.00  0.00
ATOM    214  HB1 LEU A  15      50.858  32.742  33.536  1.00  0.00
ATOM    215  HB2 LEU A  15      49.350  31.887  33.998  1.00  0.00
ATOM    216  CG  LEU A  15      51.110  30.624  33.929  1.00  0.00
ATOM    217  HG  LEU A  15      52.204  30.720  34.119  1.00  0.00
ATOM    218  CD1 LEU A  15      50.578  29.490  34.827  1.00  0.00
ATOM    219 HD11 LEU A  15      49.485  29.362  34.679  1.00  0.00
ATOM    220 HD12 LEU A  15      50.768  29.712  35.898  1.00  0.00
ATOM    221 HD13 LEU A  15      51.083  28.533  34.576  1.00  0.00
ATOM    222  CD2 LEU A  15      50.954  30.265  32.439  1.00  0.00
ATOM    223 HD21 LEU A  15      51.381  31.067  31.801  1.00  0.00
ATOM    224 HD22 LEU A  15      49.881  30.141  32.183  1.00  0.00
ATOM    225 HD23 LEU A  15      51.484  29.315  32.213  1.00  0.00
ATOM    226  C   LEU A  15      52.011  32.551  36.084  1.00  0.00
ATOM    227  O   LEU A  15      52.466  31.689  36.829  1.00  0.00
ATOM    228  N   LEU A  16      52.759  33.550  35.610  1.00  0.00
ATOM    229  HN  LEU A  16      52.373  34.272  35.038  1.00  0.00
ATOM    230  CA  LEU A  16      54.195  33.581  35.784  1.00  0.00
ATOM    231  HA  LEU A  16      54.555  32.568  35.669  1.00  0.00
ATOM    232  CB  LEU A  16      54.827  34.463  34.680  1.00  0.00
ATOM    233  HB1 LEU A  16      54.604  35.534  34.875  1.00  0.00
ATOM    234  HB2 LEU A  16      54.333  34.189  33.720  1.00  0.00
ATOM    235  CG  LEU A  16      56.342  34.271  34.433  1.00  0.00
ATOM    236  HG  LEU A  16      56.881  34.496  35.381  1.00  0.00
ATOM    237  CD1 LEU A  16      56.689  32.826  34.022  1.00  0.00
ATOM    238 HD11 LEU A  16      56.090  32.523  33.138  1.00  0.00
ATOM    239 HD12 LEU A  16      56.486  32.118  34.852  1.00  0.00
ATOM    240 HD13 LEU A  16      57.765  32.750  33.756  1.00  0.00
ATOM    241  CD2 LEU A  16      56.841  35.262  33.362  1.00  0.00
ATOM    242 HD21 LEU A  16      56.633  36.307  33.671  1.00  0.00
ATOM    243 HD22 LEU A  16      56.329  35.072  32.394  1.00  0.00
ATOM    244 HD23 LEU A  16      57.935  35.149  33.211  1.00  0.00
ATOM    245  C   LEU A  16      54.577  34.055  37.169  1.00  0.00
ATOM    246  O   LEU A  16      55.585  33.616  37.723  1.00  0.00
ATOM    247  N   ILE A  17      53.740  34.905  37.774  1.00  0.00
ATOM    248  HN  ILE A  17      52.966  35.290  37.274  1.00  0.00
ATOM    249  CA  ILE A  17      53.785  35.254  39.184  1.00  0.00
ATOM    250  HA  ILE A  17      54.803  35.538  39.409  1.00  0.00
ATOM    251  CB  ILE A  17      52.869  36.434  39.531  1.00  0.00
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ATOM    252  HB  ILE A  17      51.865  36.228  39.091  1.00  0.00
ATOM    253  CG2 ILE A  17      52.670  36.597  41.059  1.00  0.00
ATOM    254 HG21 ILE A  17      53.649  36.652  41.581  1.00  0.00
ATOM    255 HG22 ILE A  17      52.088  35.753  41.484  1.00  0.00
ATOM    256 HG23 ILE A  17      52.107  37.531  41.267  1.00  0.00
ATOM    257  CG1 ILE A  17      53.385  37.753  38.888  1.00  0.00
ATOM    258 HG11 ILE A  17      52.577  38.513  38.974  1.00  0.00
ATOM    259 HG12 ILE A  17      53.574  37.594  37.806  1.00  0.00
ATOM    260  CD1 ILE A  17      54.659  38.332  39.513  1.00  0.00
ATOM    261  HD1 ILE A  17      55.494  37.605  39.440  1.00  0.00
ATOM    262  HD2 ILE A  17      54.505  38.594  40.580  1.00  0.00
ATOM    263  HD3 ILE A  17      54.956  39.254  38.971  1.00  0.00
ATOM    264  C   ILE A  17      53.484  34.045  40.038  1.00  0.00
ATOM    265  O   ILE A  17      54.153  33.806  41.037  1.00  0.00
ATOM    266  N   GLY A  18      52.494  33.243  39.636  1.00  0.00
ATOM    267  HN  GLY A  18      51.967  33.459  38.815  1.00  0.00
ATOM    268  CA  GLY A  18      52.067  32.052  40.346  1.00  0.00
ATOM    269  HA1 GLY A  18      51.218  31.659  39.807  1.00  0.00
ATOM    270  HA2 GLY A  18      51.830  32.333  41.363  1.00  0.00
ATOM    271  C   GLY A  18      53.125  30.987  40.379  1.00  0.00
ATOM    272  O   GLY A  18      53.320  30.344  41.405  1.00  0.00
ATOM    273  N   ILE A  19      53.834  30.795  39.264  1.00  0.00
ATOM    274  HN  ILE A  19      53.600  31.296  38.432  1.00  0.00
ATOM    275  CA  ILE A  19      54.991  29.930  39.149  1.00  0.00
ATOM    276  HA  ILE A  19      54.701  28.965  39.535  1.00  0.00
ATOM    277  CB  ILE A  19      55.428  29.756  37.689  1.00  0.00
ATOM    278  HB  ILE A  19      55.480  30.770  37.224  1.00  0.00
ATOM    279  CG2 ILE A  19      56.839  29.131  37.560  1.00  0.00
ATOM    280 HG21 ILE A  19      56.904  28.185  38.137  1.00  0.00
ATOM    281 HG22 ILE A  19      57.623  29.827  37.924  1.00  0.00
ATOM    282 HG23 ILE A  19      57.057  28.909  36.494  1.00  0.00
ATOM    283  CG1 ILE A  19      54.376  28.943  36.882  1.00  0.00
ATOM    284 HG11 ILE A  19      54.674  28.972  35.810  1.00  0.00
ATOM    285 HG12 ILE A  19      53.385  29.432  36.959  1.00  0.00
ATOM    286  CD1 ILE A  19      54.217  27.475  37.302  1.00  0.00
ATOM    287  HD1 ILE A  19      53.875  27.396  38.355  1.00  0.00
ATOM    288  HD2 ILE A  19      55.174  26.923  37.196  1.00  0.00
ATOM    289  HD3 ILE A  19      53.460  26.978  36.658  1.00  0.00
ATOM    290  C   ILE A  19      56.132  30.395  40.028  1.00  0.00
ATOM    291  O   ILE A  19      56.757  29.588  40.709  1.00  0.00
ATOM    292  N   SER A  20      56.399  31.705  40.055  1.00  0.00
ATOM    293  HN  SER A  20      55.879  32.346  39.495  1.00  0.00
ATOM    294  CA  SER A  20      57.426  32.286  40.904  1.00  0.00
ATOM    295  HA  SER A  20      58.360  31.793  40.671  1.00  0.00
ATOM    296  CB  SER A  20      57.578  33.803  40.624  1.00  0.00
ATOM    297  HB1 SER A  20      58.342  34.241  41.302  1.00  0.00
ATOM    298  HB2 SER A  20      56.621  34.339  40.786  1.00  0.00
ATOM    299  OG  SER A  20      58.010  34.037  39.289  1.00  0.00
ATOM    300  HG  SER A  20      57.265  33.822  38.718  1.00  0.00
ATOM    301  C   SER A  20      57.158  32.086  42.379  1.00  0.00
ATOM    302  O   SER A  20      58.059  31.722  43.128  1.00  0.00
ATOM    303  N   VAL A  21      55.903  32.284  42.792  1.00  0.00
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ATOM    304  HN  VAL A  21      55.218  32.608  42.140  1.00  0.00
ATOM    305  CA  VAL A  21      55.377  32.046  44.124  1.00  0.00
ATOM    306  HA  VAL A  21      56.005  32.592  44.814  1.00  0.00
ATOM    307  CB  VAL A  21      53.948  32.577  44.265  1.00  0.00
ATOM    308  HB  VAL A  21      53.345  32.246  43.389  1.00  0.00
ATOM    309  CG1 VAL A  21      54.009  34.119  44.263  1.00  0.00
ATOM    310 HG11 VAL A  21      54.493  34.510  43.347  1.00  0.00
ATOM    311 HG12 VAL A  21      54.591  34.475  45.137  1.00  0.00
ATOM    312 HG13 VAL A  21      52.985  34.544  44.325  1.00  0.00
ATOM    313  CG2 VAL A  21      53.244  32.070  45.545  1.00  0.00
ATOM    314 HG21 VAL A  21      53.865  32.283  46.440  1.00  0.00
ATOM    315 HG22 VAL A  21      53.046  30.979  45.494  1.00  0.00
ATOM    316 HG23 VAL A  21      52.267  32.585  45.667  1.00  0.00
ATOM    317  C   VAL A  21      55.473  30.588  44.516  1.00  0.00
ATOM    318  O   VAL A  21      55.797  30.260  45.655  1.00  0.00
ATOM    319  N   LEU A  22      55.210  29.686  43.568  1.00  0.00
ATOM    320  HN  LEU A  22      54.941  29.978  42.651  1.00  0.00
ATOM    321  CA  LEU A  22      55.225  28.254  43.773  1.00  0.00
ATOM    322  HA  LEU A  22      54.687  28.044  44.687  1.00  0.00
ATOM    323  CB  LEU A  22      54.517  27.559  42.580  1.00  0.00
ATOM    324  HB1 LEU A  22      55.037  27.841  41.639  1.00  0.00
ATOM    325  HB2 LEU A  22      53.483  27.964  42.521  1.00  0.00
ATOM    326  CG  LEU A  22      54.410  26.014  42.628  1.00  0.00
ATOM    327  HG  LEU A  22      55.440  25.589  42.638  1.00  0.00
ATOM    328  CD1 LEU A  22      53.681  25.514  43.890  1.00  0.00
ATOM    329 HD11 LEU A  22      52.653  25.930  43.931  1.00  0.00
ATOM    330 HD12 LEU A  22      54.226  25.821  44.807  1.00  0.00
ATOM    331 HD13 LEU A  22      53.615  24.405  43.880  1.00  0.00
ATOM    332  CD2 LEU A  22      53.727  25.484  41.352  1.00  0.00
ATOM    333 HD21 LEU A  22      54.288  25.807  40.450  1.00  0.00
ATOM    334 HD22 LEU A  22      52.689  25.873  41.281  1.00  0.00
ATOM    335 HD23 LEU A  22      53.689  24.374  41.367  1.00  0.00
ATOM    336  C   LEU A  22      56.636  27.725  43.919  1.00  0.00
ATOM    337  O   LEU A  22      56.861  26.700  44.560  1.00  0.00
ATOM    338  N   LEU A  23      57.615  28.449  43.371  1.00  0.00
ATOM    339  HN  LEU A  23      57.413  29.276  42.850  1.00  0.00
ATOM    340  CA  LEU A  23      59.007  28.079  43.445  1.00  0.00
ATOM    341  HA  LEU A  23      59.101  27.019  43.630  1.00  0.00
ATOM    342  CB  LEU A  23      59.724  28.439  42.118  1.00  0.00
ATOM    343  HB1 LEU A  23      60.827  28.344  42.228  1.00  0.00
ATOM    344  HB2 LEU A  23      59.497  29.501  41.873  1.00  0.00
ATOM    345  CG  LEU A  23      59.319  27.556  40.912  1.00  0.00
ATOM    346  HG  LEU A  23      58.207  27.536  40.846  1.00  0.00
ATOM    347  CD1 LEU A  23      59.841  28.164  39.596  1.00  0.00
ATOM    348 HD11 LEU A  23      60.951  28.200  39.601  1.00  0.00
ATOM    349 HD12 LEU A  23      59.454  29.197  39.468  1.00  0.00
ATOM    350 HD13 LEU A  23      59.510  27.553  38.730  1.00  0.00
ATOM    351  CD2 LEU A  23      59.790  26.097  41.074  1.00  0.00
ATOM    352 HD21 LEU A  23      59.341  25.635  41.977  1.00  0.00
ATOM    353 HD22 LEU A  23      60.896  26.058  41.168  1.00  0.00
ATOM    354 HD23 LEU A  23      59.489  25.497  40.190  1.00  0.00
ATOM    355  C   LEU A  23      59.708  28.799  44.571  1.00  0.00
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ATOM    356  O   LEU A  23      60.855  28.489  44.868  1.00  0.00
ATOM    357  N   SER A  24      59.031  29.733  45.246  1.00  0.00
ATOM    358  HN  SER A  24      58.113  30.010  44.971  1.00  0.00
ATOM    359  CA  SER A  24      59.550  30.367  46.449  1.00  0.00
ATOM    360  HA  SER A  24      60.506  30.793  46.176  1.00  0.00
ATOM    361  CB  SER A  24      58.645  31.542  46.907  1.00  0.00
ATOM    362  HB1 SER A  24      59.029  31.971  47.858  1.00  0.00
ATOM    363  HB2 SER A  24      57.604  31.206  47.073  1.00  0.00
ATOM    364  OG  SER A  24      58.649  32.591  45.947  1.00  0.00
ATOM    365  HG  SER A  24      58.058  33.270  46.283  1.00  0.00
ATOM    366  C   SER A  24      59.817  29.442  47.628  1.00  0.00
ATOM    367  O   SER A  24      60.888  29.595  48.216  1.00  0.00
ATOM    368  N   PRO A  25      58.985  28.462  48.036  1.00  0.00
ATOM    369  CD  PRO A  25      57.561  28.358  47.703  1.00  0.00
ATOM    370  HD1 PRO A  25      57.385  28.383  46.611  1.00  0.00
ATOM    371  HD2 PRO A  25      57.017  29.190  48.201  1.00  0.00
ATOM    372  CA  PRO A  25      59.329  27.554  49.121  1.00  0.00
ATOM    373  HA  PRO A  25      59.739  28.122  49.944  1.00  0.00
ATOM    374  CB  PRO A  25      58.013  26.855  49.506  1.00  0.00
ATOM    375  HB1 PRO A  25      57.551  27.412  50.352  1.00  0.00
ATOM    376  HB2 PRO A  25      58.139  25.796  49.808  1.00  0.00
ATOM    377  CG  PRO A  25      57.118  27.011  48.275  1.00  0.00
ATOM    378  HG1 PRO A  25      57.347  26.206  47.542  1.00  0.00
ATOM    379  HG2 PRO A  25      56.038  26.988  48.524  1.00  0.00
ATOM    380  C   PRO A  25      60.379  26.575  48.659  1.00  0.00
ATOM    381  O   PRO A  25      61.190  26.158  49.482  1.00  0.00
ATOM    382  N   VAL A  26      60.364  26.182  47.383  1.00  0.00
ATOM    383  HN  VAL A  26      59.660  26.519  46.762  1.00  0.00
ATOM    384  CA  VAL A  26      61.346  25.303  46.779  1.00  0.00
ATOM    385  HA  VAL A  26      61.366  24.393  47.362  1.00  0.00
ATOM    386  CB  VAL A  26      60.984  24.955  45.335  1.00  0.00
ATOM    387  HB  VAL A  26      60.984  25.872  44.704  1.00  0.00
ATOM    388  CG1 VAL A  26      59.558  24.363  45.303  1.00  0.00
ATOM    389 HG11 VAL A  26      58.799  25.110  45.615  1.00  0.00
ATOM    390 HG12 VAL A  26      59.489  23.481  45.973  1.00  0.00
ATOM    391 HG13 VAL A  26      59.306  24.039  44.270  1.00  0.00
ATOM    392  CG2 VAL A  26      62.006  23.960  44.740  1.00  0.00
ATOM    393 HG21 VAL A  26      62.082  23.056  45.379  1.00  0.00
ATOM    394 HG22 VAL A  26      63.012  24.418  44.647  1.00  0.00
ATOM    395 HG23 VAL A  26      61.681  23.646  43.725  1.00  0.00
ATOM    396  C   VAL A  26      62.728  25.929  46.839  1.00  0.00
ATOM    397  O   VAL A  26      63.701  25.277  47.211  1.00  0.00
ATOM    398  N   SER A  27      62.814  27.224  46.523  1.00  0.00
ATOM    399  HN  SER A  27      62.001  27.713  46.212  1.00  0.00
ATOM    400  CA  SER A  27      64.015  28.030  46.593  1.00  0.00
ATOM    401  HA  SER A  27      64.765  27.540  45.987  1.00  0.00
ATOM    402  CB  SER A  27      63.761  29.450  46.034  1.00  0.00
ATOM    403  HB1 SER A  27      64.662  30.088  46.167  1.00  0.00
ATOM    404  HB2 SER A  27      62.907  29.933  46.555  1.00  0.00
ATOM    405  OG  SER A  27      63.483  29.403  44.642  1.00  0.00
ATOM    406  HG  SER A  27      62.607  29.009  44.557  1.00  0.00
ATOM    407  C   SER A  27      64.573  28.161  47.982  1.00  0.00
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ATOM    408  O   SER A  27      65.785  28.134  48.164  1.00  0.00
ATOM    409  N   SER A  28      63.696  28.301  48.979  1.00  0.00
ATOM    410  HN  SER A  28      62.718  28.334  48.785  1.00  0.00
ATOM    411  CA  SER A  28      64.055  28.371  50.385  1.00  0.00
ATOM    412  HA  SER A  28      64.760  29.183  50.500  1.00  0.00
ATOM    413  CB  SER A  28      62.805  28.661  51.251  1.00  0.00
ATOM    414  HB1 SER A  28      63.095  28.738  52.322  1.00  0.00
ATOM    415  HB2 SER A  28      62.050  27.855  51.151  1.00  0.00
ATOM    416  OG  SER A  28      62.207  29.897  50.877  1.00  0.00
ATOM    417  HG  SER A  28      61.848  29.776  49.992  1.00  0.00
ATOM    418  C   SER A  28      64.722  27.104  50.876  1.00  0.00
ATOM    419  O   SER A  28      65.670  27.159  51.656  1.00  0.00
ATOM    420  N   LYS A  29      64.247  25.947  50.404  1.00  0.00
ATOM    421  HN  LYS A  29      63.476  25.931  49.770  1.00  0.00
ATOM    422  CA  LYS A  29      64.782  24.648  50.759  1.00  0.00
ATOM    423  HA  LYS A  29      64.960  24.638  51.824  1.00  0.00
ATOM    424  CB  LYS A  29      63.764  23.536  50.401  1.00  0.00
ATOM    425  HB1 LYS A  29      64.234  22.533  50.525  1.00  0.00
ATOM    426  HB2 LYS A  29      63.474  23.642  49.332  1.00  0.00
ATOM    427  CG  LYS A  29      62.488  23.539  51.264  1.00  0.00
ATOM    428  HG1 LYS A  29      61.795  22.769  50.856  1.00  0.00
ATOM    429  HG2 LYS A  29      61.980  24.523  51.183  1.00  0.00
ATOM    430  CD  LYS A  29      62.737  23.235  52.751  1.00  0.00
ATOM    431  HD1 LYS A  29      63.362  24.046  53.185  1.00  0.00
ATOM    432  HD2 LYS A  29      63.309  22.282  52.823  1.00  0.00
ATOM    433  CE  LYS A  29      61.435  23.112  53.555  1.00  0.00
ATOM    434  HE1 LYS A  29      60.811  22.284  53.157  1.00  0.00
ATOM    435  HE2 LYS A  29      60.859  24.060  53.507  1.00  0.00
ATOM    436  NZ  LYS A  29      61.714  22.822  54.982  1.00  0.00
ATOM    437  HZ1 LYS A  29      62.276  23.596  55.389  1.00  0.00
ATOM    438  HZ2 LYS A  29      62.246  21.932  55.057  1.00  0.00
ATOM    439  HZ3 LYS A  29      60.817  22.734  55.502  1.00  0.00
ATOM    440  C   LYS A  29      66.102  24.329  50.091  1.00  0.00
ATOM    441  O   LYS A  29      66.865  23.505  50.591  1.00  0.00
ATOM    442  N   LEU A  30      66.401  24.996  48.974  1.00  0.00
ATOM    443  HN  LEU A  30      65.758  25.646  48.575  1.00  0.00
ATOM    444  CA  LEU A  30      67.648  24.820  48.257  1.00  0.00
ATOM    445  HA  LEU A  30      68.108  23.877  48.515  1.00  0.00
ATOM    446  CB  LEU A  30      67.385  24.889  46.730  1.00  0.00
ATOM    447  HB1 LEU A  30      68.348  24.878  46.172  1.00  0.00
ATOM    448  HB2 LEU A  30      66.870  25.851  46.503  1.00  0.00
ATOM    449  CG  LEU A  30      66.515  23.736  46.173  1.00  0.00
ATOM    450  HG  LEU A  30      65.596  23.654  46.797  1.00  0.00
ATOM    451  CD1 LEU A  30      66.054  24.046  44.736  1.00  0.00
ATOM    452 HD11 LEU A  30      66.930  24.139  44.060  1.00  0.00
ATOM    453 HD12 LEU A  30      65.484  25.000  44.712  1.00  0.00
ATOM    454 HD13 LEU A  30      65.397  23.234  44.358  1.00  0.00
ATOM    455  CD2 LEU A  30      67.236  22.376  46.244  1.00  0.00
ATOM    456 HD21 LEU A  30      67.490  22.122  47.294  1.00  0.00
ATOM    457 HD22 LEU A  30      68.172  22.404  45.648  1.00  0.00
ATOM    458 HD23 LEU A  30      66.582  21.574  45.839  1.00  0.00
ATOM    459  C   LEU A  30      68.611  25.932  48.610  1.00  0.00
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ATOM    460  O   LEU A  30      69.785  25.882  48.247  1.00  0.00
ATOM    461  N   GLY A  31      68.131  26.934  49.352  1.00  0.00
ATOM    462  HN  GLY A  31      67.171  26.930  49.624  1.00  0.00
ATOM    463  CA  GLY A  31      68.886  28.070  49.834  1.00  0.00
ATOM    464  HA1 GLY A  31      69.738  27.691  50.382  1.00  0.00
ATOM    465  HA2 GLY A  31      68.212  28.644  50.453  1.00  0.00
ATOM    466  C   GLY A  31      69.395  28.982  48.750  1.00  0.00
ATOM    467  O   GLY A  31      70.454  29.586  48.905  1.00  0.00
ATOM    468  N   ILE A  32      68.661  29.106  47.641  1.00  0.00
ATOM    469  HN  ILE A  32      67.790  28.629  47.545  1.00  0.00
ATOM    470  CA  ILE A  32      69.056  29.935  46.520  1.00  0.00
ATOM    471  HA  ILE A  32      70.126  30.042  46.563  1.00  0.00
ATOM    472  CB  ILE A  32      68.739  29.328  45.148  1.00  0.00
ATOM    473  HB  ILE A  32      69.174  29.986  44.360  1.00  0.00
ATOM    474  CG2 ILE A  32      67.217  29.242  44.894  1.00  0.00
ATOM    475 HG21 ILE A  32      66.750  30.248  44.874  1.00  0.00
ATOM    476 HG22 ILE A  32      66.728  28.633  45.680  1.00  0.00
ATOM    477 HG23 ILE A  32      67.023  28.761  43.912  1.00  0.00
ATOM    478  CG1 ILE A  32      69.385  27.926  44.983  1.00  0.00
ATOM    479 HG11 ILE A  32      69.139  27.556  43.963  1.00  0.00
ATOM    480 HG12 ILE A  32      68.923  27.222  45.708  1.00  0.00
ATOM    481  CD1 ILE A  32      70.907  27.895  45.158  1.00  0.00
ATOM    482  HD1 ILE A  32      71.191  28.148  46.201  1.00  0.00
ATOM    483  HD2 ILE A  32      71.392  28.620  44.470  1.00  0.00
ATOM    484  HD3 ILE A  32      71.297  26.879  44.933  1.00  0.00
ATOM    485  C   ILE A  32      68.402  31.296  46.700  1.00  0.00
ATOM    486  O   ILE A  32      67.270  31.346  47.184  1.00  0.00
ATOM    487  N   PRO A  33      69.050  32.430  46.370  1.00  0.00
ATOM    488  CD  PRO A  33      70.484  32.512  46.085  1.00  0.00
ATOM    489  HD1 PRO A  33      70.660  32.144  45.052  1.00  0.00
ATOM    490  HD2 PRO A  33      71.078  31.922  46.818  1.00  0.00
ATOM    491  CA  PRO A  33      68.426  33.747  46.312  1.00  0.00
ATOM    492  HA  PRO A  33      68.143  34.008  47.322  1.00  0.00
ATOM    493  CB  PRO A  33      69.519  34.676  45.761  1.00  0.00
ATOM    494  HB1 PRO A  33      69.428  35.708  46.156  1.00  0.00
ATOM    495  HB2 PRO A  33      69.500  34.706  44.649  1.00  0.00
ATOM    496  CG  PRO A  33      70.821  34.000  46.198  1.00  0.00
ATOM    497  HG1 PRO A  33      71.686  34.294  45.572  1.00  0.00
ATOM    498  HG2 PRO A  33      71.029  34.254  47.261  1.00  0.00
ATOM    499  C   PRO A  33      67.182  33.793  45.459  1.00  0.00
ATOM    500  O   PRO A  33      67.250  33.401  44.295  1.00  0.00
ATOM    501  N   ILE A  34      66.064  34.282  46.000  1.00  0.00
ATOM    502  HN  ILE A  34      66.039  34.597  46.945  1.00  0.00
ATOM    503  CA  ILE A  34      64.801  34.325  45.292  1.00  0.00
ATOM    504  HA  ILE A  34      64.712  33.400  44.738  1.00  0.00
ATOM    505  CB  ILE A  34      63.595  34.395  46.229  1.00  0.00
ATOM    506  HB  ILE A  34      62.666  34.366  45.611  1.00  0.00
ATOM    507  CG2 ILE A  34      63.585  35.707  47.049  1.00  0.00
ATOM    508 HG21 ILE A  34      63.533  36.595  46.387  1.00  0.00
ATOM    509 HG22 ILE A  34      64.493  35.785  47.682  1.00  0.00
ATOM    510 HG23 ILE A  34      62.696  35.736  47.714  1.00  0.00
ATOM    511  CG1 ILE A  34      63.574  33.133  47.129  1.00  0.00
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ATOM    512 HG11 ILE A  34      64.395  33.190  47.875  1.00  0.00
ATOM    513 HG12 ILE A  34      63.766  32.248  46.482  1.00  0.00
ATOM    514  CD1 ILE A  34      62.243  32.909  47.855  1.00  0.00
ATOM    515  HD1 ILE A  34      61.409  32.853  47.123  1.00  0.00
ATOM    516  HD2 ILE A  34      62.036  33.735  48.567  1.00  0.00
ATOM    517  HD3 ILE A  34      62.275  31.957  48.427  1.00  0.00
ATOM    518  C   ILE A  34      64.771  35.448  44.280  1.00  0.00
ATOM    519  O   ILE A  34      64.048  35.372  43.291  1.00  0.00
ATOM    520  N   LEU A  35      65.598  36.478  44.486  1.00  0.00
ATOM    521  HN  LEU A  35      66.170  36.498  45.302  1.00  0.00
ATOM    522  CA  LEU A  35      65.770  37.605  43.593  1.00  0.00
ATOM    523  HA  LEU A  35      64.803  38.067  43.455  1.00  0.00
ATOM    524  CB  LEU A  35      66.740  38.628  44.243  1.00  0.00
ATOM    525  HB1 LEU A  35      67.725  38.158  44.449  1.00  0.00
ATOM    526  HB2 LEU A  35      66.289  38.882  45.230  1.00  0.00
ATOM    527  CG  LEU A  35      66.960  39.964  43.483  1.00  0.00
ATOM    528  HG  LEU A  35      66.025  40.195  42.922  1.00  0.00
ATOM    529  CD1 LEU A  35      67.179  41.120  44.480  1.00  0.00
ATOM    530 HD11 LEU A  35      68.074  40.922  45.107  1.00  0.00
ATOM    531 HD12 LEU A  35      66.293  41.231  45.141  1.00  0.00
ATOM    532 HD13 LEU A  35      67.334  42.075  43.937  1.00  0.00
ATOM    533  CD2 LEU A  35      68.127  39.920  42.475  1.00  0.00
ATOM    534 HD21 LEU A  35      67.936  39.188  41.666  1.00  0.00
ATOM    535 HD22 LEU A  35      69.071  39.643  42.990  1.00  0.00
ATOM    536 HD23 LEU A  35      68.264  40.917  42.005  1.00  0.00
ATOM    537  C   LEU A  35      66.284  37.168  42.243  1.00  0.00
ATOM    538  O   LEU A  35      65.799  37.618  41.205  1.00  0.00
ATOM    539  N   LEU A  36      67.259  36.255  42.244  1.00  0.00
ATOM    540  HN  LEU A  36      67.616  35.890  43.100  1.00  0.00
ATOM    541  CA  LEU A  36      67.878  35.740  41.046  1.00  0.00
ATOM    542  HA  LEU A  36      68.027  36.558  40.357  1.00  0.00
ATOM    543  CB  LEU A  36      69.245  35.094  41.390  1.00  0.00
ATOM    544  HB1 LEU A  36      69.705  34.684  40.463  1.00  0.00
ATOM    545  HB2 LEU A  36      69.078  34.247  42.093  1.00  0.00
ATOM    546  CG  LEU A  36      70.277  36.054  42.039  1.00  0.00
ATOM    547  HG  LEU A  36      69.835  36.461  42.978  1.00  0.00
ATOM    548  CD1 LEU A  36      71.555  35.292  42.438  1.00  0.00
ATOM    549 HD11 LEU A  36      72.051  34.882  41.534  1.00  0.00
ATOM    550 HD12 LEU A  36      71.312  34.449  43.117  1.00  0.00
ATOM    551 HD13 LEU A  36      72.264  35.973  42.956  1.00  0.00
ATOM    552  CD2 LEU A  36      70.629  37.254  41.137  1.00  0.00
ATOM    553 HD21 LEU A  36      69.730  37.866  40.925  1.00  0.00
ATOM    554 HD22 LEU A  36      71.055  36.901  40.174  1.00  0.00
ATOM    555 HD23 LEU A  36      71.380  37.901  41.638  1.00  0.00
ATOM    556  C   LEU A  36      67.005  34.715  40.358  1.00  0.00
ATOM    557  O   LEU A  36      67.089  34.537  39.145  1.00  0.00
ATOM    558  N   VAL A  37      66.128  34.050  41.118  1.00  0.00
ATOM    559  HN  VAL A  37      66.101  34.194  42.105  1.00  0.00
ATOM    560  CA  VAL A  37      65.119  33.145  40.602  1.00  0.00
ATOM    561  HA  VAL A  37      65.630  32.449  39.951  1.00  0.00
ATOM    562  CB  VAL A  37      64.453  32.313  41.700  1.00  0.00
ATOM    563  HB  VAL A  37      64.144  32.977  42.536  1.00  0.00
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ATOM    564  CG1 VAL A  37      63.193  31.563  41.206  1.00  0.00
ATOM    565 HG11 VAL A  37      63.432  30.948  40.314  1.00  0.00
ATOM    566 HG12 VAL A  37      62.375  32.268  40.951  1.00  0.00
ATOM    567 HG13 VAL A  37      62.819  30.889  42.006  1.00  0.00
ATOM    568  CG2 VAL A  37      65.503  31.313  42.227  1.00  0.00
ATOM    569 HG21 VAL A  37      66.419  31.830  42.573  1.00  0.00
ATOM    570 HG22 VAL A  37      65.788  30.597  41.427  1.00  0.00
ATOM    571 HG23 VAL A  37      65.087  30.738  43.079  1.00  0.00
ATOM    572  C   VAL A  37      64.110  33.863  39.732  1.00  0.00
ATOM    573  O   VAL A  37      63.736  33.361  38.678  1.00  0.00
ATOM    574  N   PHE A  38      63.677  35.061  40.138  1.00  0.00
ATOM    575  HN  PHE A  38      63.984  35.453  41.003  1.00  0.00
ATOM    576  CA  PHE A  38      62.722  35.865  39.387  1.00  0.00
ATOM    577  HA  PHE A  38      61.850  35.250  39.211  1.00  0.00
ATOM    578  CB  PHE A  38      62.308  37.131  40.193  1.00  0.00
ATOM    579  HB1 PHE A  38      61.515  37.691  39.653  1.00  0.00
ATOM    580  HB2 PHE A  38      63.193  37.793  40.321  1.00  0.00
ATOM    581  CG  PHE A  38      61.761  36.792  41.565  1.00  0.00
ATOM    582  CD1 PHE A  38      60.999  35.630  41.811  1.00  0.00
ATOM    583  HD1 PHE A  38      60.759  34.951  41.007  1.00  0.00
ATOM    584  CE1 PHE A  38      60.567  35.315  43.105  1.00  0.00
ATOM    585  HE1 PHE A  38      60.003  34.410  43.281  1.00  0.00
ATOM    586  CZ  PHE A  38      60.868  36.170  44.170  1.00  0.00
ATOM    587  HZ  PHE A  38      60.538  35.925  45.169  1.00  0.00
ATOM    588  CD2 PHE A  38      62.019  37.660  42.644  1.00  0.00
ATOM    589  HD2 PHE A  38      62.589  38.563  42.480  1.00  0.00
ATOM    590  CE2 PHE A  38      61.582  37.351  43.937  1.00  0.00
ATOM    591  HE2 PHE A  38      61.810  38.014  44.758  1.00  0.00
ATOM    592  C   PHE A  38      63.243  36.273  38.025  1.00  0.00
ATOM    593  O   PHE A  38      62.511  36.227  37.037  1.00  0.00
ATOM    594  N   LEU A  39      64.527  36.639  37.949  1.00  0.00
ATOM    595  HN  LEU A  39      65.088  36.692  38.772  1.00  0.00
ATOM    596  CA  LEU A  39      65.226  36.909  36.706  1.00  0.00
ATOM    597  HA  LEU A  39      64.683  37.686  36.187  1.00  0.00
ATOM    598  CB  LEU A  39      66.677  37.387  36.995  1.00  0.00
ATOM    599  HB1 LEU A  39      67.238  37.497  36.040  1.00  0.00
ATOM    600  HB2 LEU A  39      67.192  36.610  37.601  1.00  0.00
ATOM    601  CG  LEU A  39      66.792  38.735  37.753  1.00  0.00
ATOM    602  HG  LEU A  39      66.125  38.695  38.645  1.00  0.00
ATOM    603  CD1 LEU A  39      68.226  38.959  38.272  1.00  0.00
ATOM    604 HD11 LEU A  39      68.936  39.037  37.421  1.00  0.00
ATOM    605 HD12 LEU A  39      68.541  38.114  38.917  1.00  0.00
ATOM    606 HD13 LEU A  39      68.279  39.896  38.866  1.00  0.00
ATOM    607  CD2 LEU A  39      66.352  39.927  36.884  1.00  0.00
ATOM    608 HD21 LEU A  39      65.315  39.784  36.522  1.00  0.00
ATOM    609 HD22 LEU A  39      67.018  40.029  36.001  1.00  0.00
ATOM    610 HD23 LEU A  39      66.393  40.869  37.469  1.00  0.00
ATOM    611  C   LEU A  39      65.290  35.699  35.794  1.00  0.00
ATOM    612  O   LEU A  39      65.060  35.810  34.592  1.00  0.00
ATOM    613  N   ALA A  40      65.589  34.529  36.366  1.00  0.00
ATOM    614  HN  ALA A  40      65.779  34.485  37.345  1.00  0.00
ATOM    615  CA  ALA A  40      65.666  33.253  35.682  1.00  0.00
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ATOM    616  HA  ALA A  40      66.363  33.375  34.865  1.00  0.00
ATOM    617  CB  ALA A  40      66.200  32.145  36.611  1.00  0.00
ATOM    618  HB1 ALA A  40      65.508  31.963  37.460  1.00  0.00
ATOM    619  HB2 ALA A  40      67.184  32.448  37.028  1.00  0.00
ATOM    620  HB3 ALA A  40      66.338  31.193  36.055  1.00  0.00
ATOM    621  C   ALA A  40      64.346  32.800  35.096  1.00  0.00
ATOM    622  O   ALA A  40      64.301  32.281  33.985  1.00  0.00
ATOM    623  N   VAL A  41      63.253  32.998  35.837  1.00  0.00
ATOM    624  HN  VAL A  41      63.339  33.382  36.756  1.00  0.00
ATOM    625  CA  VAL A  41      61.889  32.720  35.426  1.00  0.00
ATOM    626  HA  VAL A  41      61.871  31.701  35.065  1.00  0.00
ATOM    627  CB  VAL A  41      60.913  32.803  36.603  1.00  0.00
ATOM    628  HB  VAL A  41      61.081  33.755  37.156  1.00  0.00
ATOM    629  CG1 VAL A  41      61.190  31.617  37.553  1.00  0.00
ATOM    630 HG11 VAL A  41      62.245  31.595  37.888  1.00  0.00
ATOM    631 HG12 VAL A  41      60.969  30.657  37.040  1.00  0.00
ATOM    632 HG13 VAL A  41      60.540  31.690  38.451  1.00  0.00
ATOM    633  CG2 VAL A  41      59.439  32.758  36.148  1.00  0.00
ATOM    634 HG21 VAL A  41      59.255  31.855  35.529  1.00  0.00
ATOM    635 HG22 VAL A  41      59.169  33.658  35.560  1.00  0.00
ATOM    636 HG23 VAL A  41      58.768  32.715  37.032  1.00  0.00
ATOM    637  C   VAL A  41      61.476  33.594  34.254  1.00  0.00
ATOM    638  O   VAL A  41      60.786  33.142  33.341  1.00  0.00
ATOM    639  N   GLY A  42      61.922  34.854  34.245  1.00  0.00
ATOM    640  HN  GLY A  42      62.464  35.208  35.005  1.00  0.00
ATOM    641  CA  GLY A  42      61.693  35.781  33.152  1.00  0.00
ATOM    642  HA1 GLY A  42      62.068  36.741  33.475  1.00  0.00
ATOM    643  HA2 GLY A  42      60.634  35.796  32.933  1.00  0.00
ATOM    644  C   GLY A  42      62.436  35.392  31.899  1.00  0.00
ATOM    645  O   GLY A  42      61.901  35.483  30.797  1.00  0.00
ATOM    646  N   MET A  43      63.680  34.932  32.047  1.00  0.00
ATOM    647  HN  MET A  43      64.104  34.916  32.951  1.00  0.00
ATOM    648  CA  MET A  43      64.503  34.396  30.981  1.00  0.00
ATOM    649  HA  MET A  43      64.558  35.150  30.208  1.00  0.00
ATOM    650  CB  MET A  43      65.936  34.138  31.515  1.00  0.00
ATOM    651  HB1 MET A  43      65.867  33.494  32.419  1.00  0.00
ATOM    652  HB2 MET A  43      66.360  35.113  31.844  1.00  0.00
ATOM    653  CG  MET A  43      66.928  33.468  30.544  1.00  0.00
ATOM    654  HG1 MET A  43      66.543  32.468  30.248  1.00  0.00
ATOM    655  HG2 MET A  43      67.867  33.289  31.114  1.00  0.00
ATOM    656  SD  MET A  43      67.319  34.451  29.062  1.00  0.00
ATOM    657  CE  MET A  43      68.636  33.335  28.497  1.00  0.00
ATOM    658  HE1 MET A  43      68.236  32.319  28.292  1.00  0.00
ATOM    659  HE2 MET A  43      69.437  33.243  29.261  1.00  0.00
ATOM    660  HE3 MET A  43      69.103  33.712  27.563  1.00  0.00
ATOM    661  C   MET A  43      63.906  33.149  30.357  1.00  0.00
ATOM    662  O   MET A  43      63.903  32.993  29.137  1.00  0.00
ATOM    663  N   LEU A  44      63.364  32.263  31.199  1.00  0.00
ATOM    664  HN  LEU A  44      63.410  32.434  32.182  1.00  0.00
ATOM    665  CA  LEU A  44      62.695  31.026  30.848  1.00  0.00
ATOM    666  HA  LEU A  44      63.393  30.453  30.254  1.00  0.00
ATOM    667  CB  LEU A  44      62.350  30.239  32.139  1.00  0.00
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ATOM    668  HB1 LEU A  44      61.663  30.848  32.763  1.00  0.00
ATOM    669  HB2 LEU A  44      63.290  30.106  32.719  1.00  0.00
ATOM    670  CG  LEU A  44      61.713  28.841  31.947  1.00  0.00
ATOM    671  HG  LEU A  44      60.765  28.960  31.374  1.00  0.00
ATOM    672  CD1 LEU A  44      62.625  27.888  31.150  1.00  0.00
ATOM    673 HD11 LEU A  44      63.597  27.760  31.672  1.00  0.00
ATOM    674 HD12 LEU A  44      62.818  28.287  30.133  1.00  0.00
ATOM    675 HD13 LEU A  44      62.145  26.892  31.048  1.00  0.00
ATOM    676  CD2 LEU A  44      61.336  28.227  33.310  1.00  0.00
ATOM    677 HD21 LEU A  44      60.636  28.896  33.853  1.00  0.00
ATOM    678 HD22 LEU A  44      62.245  28.085  33.933  1.00  0.00
ATOM    679 HD23 LEU A  44      60.846  27.241  33.168  1.00  0.00
ATOM    680  C   LEU A  44      61.451  31.251  30.013  1.00  0.00
ATOM    681  O   LEU A  44      61.162  30.477  29.102  1.00  0.00
ATOM    682  N   ALA A  45      60.709  32.322  30.314  1.00  0.00
ATOM    683  HN  ALA A  45      60.976  32.912  31.073  1.00  0.00
ATOM    684  CA  ALA A  45      59.503  32.739  29.625  1.00  0.00
ATOM    685  HA  ALA A  45      58.805  31.916  29.682  1.00  0.00
ATOM    686  CB  ALA A  45      58.867  33.970  30.298  1.00  0.00
ATOM    687  HB1 ALA A  45      59.539  34.851  30.244  1.00  0.00
ATOM    688  HB2 ALA A  45      58.667  33.751  31.368  1.00  0.00
ATOM    689  HB3 ALA A  45      57.904  34.235  29.812  1.00  0.00
ATOM    690  C   ALA A  45      59.731  33.051  28.161  1.00  0.00
ATOM    691  O   ALA A  45      58.876  32.764  27.323  1.00  0.00
ATOM    692  N   GLY A  46      60.887  33.646  27.845  1.00  0.00
ATOM    693  HN  GLY A  46      61.542  33.863  28.566  1.00  0.00
ATOM    694  CA  GLY A  46      61.339  33.961  26.502  1.00  0.00
ATOM    695  HA1 GLY A  46      62.264  34.506  26.617  1.00  0.00
ATOM    696  HA2 GLY A  46      60.565  34.544  26.024  1.00  0.00
ATOM    697  C   GLY A  46      61.621  32.756  25.635  1.00  0.00
ATOM    698  O   GLY A  46      61.281  31.623  25.972  1.00  0.00
ATOM    699  N   GLU A  47      62.277  33.002  24.496  1.00  0.00
ATOM    700  HN  GLU A  47      62.547  33.935  24.270  1.00  0.00
ATOM    701  CA  GLU A  47      62.703  32.014  23.520  1.00  0.00
ATOM    702  HA  GLU A  47      63.087  32.580  22.685  1.00  0.00
ATOM    703  CB  GLU A  47      63.864  31.143  24.081  1.00  0.00
ATOM    704  HB1 GLU A  47      64.159  30.392  23.313  1.00  0.00
ATOM    705  HB2 GLU A  47      63.512  30.585  24.975  1.00  0.00
ATOM    706  CG  GLU A  47      65.130  31.938  24.470  1.00  0.00
ATOM    707  HG1 GLU A  47      65.914  31.236  24.825  1.00  0.00
ATOM    708  HG2 GLU A  47      64.894  32.637  25.301  1.00  0.00
ATOM    709  CD  GLU A  47      65.679  32.725  23.279  1.00  0.00
ATOM    710  OE1 GLU A  47      65.668  33.984  23.343  1.00  0.00
ATOM    711  OE2 GLU A  47      66.118  32.076  22.293  1.00  0.00
ATOM    712  C   GLU A  47      61.583  31.158  22.962  1.00  0.00
ATOM    713  O   GLU A  47      61.521  29.955  23.215  1.00  0.00
ATOM    714  N   ASP A  48      60.685  31.786  22.194  1.00  0.00
ATOM    715  HN  ASP A  48      60.798  32.757  22.004  1.00  0.00
ATOM    716  CA  ASP A  48      59.537  31.190  21.526  1.00  0.00
ATOM    717  HA  ASP A  48      58.976  32.016  21.114  1.00  0.00
ATOM    718  CB  ASP A  48      59.986  30.269  20.349  1.00  0.00
ATOM    719  HB1 ASP A  48      59.102  29.795  19.870  1.00  0.00
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ATOM    720  HB2 ASP A  48      60.650  29.466  20.731  1.00  0.00
ATOM    721  CG  ASP A  48      60.728  31.054  19.259  1.00  0.00
ATOM    722  OD1 ASP A  48      61.284  30.381  18.350  1.00  0.00
ATOM    723  OD2 ASP A  48      60.702  32.313  19.276  1.00  0.00
ATOM    724  C   ASP A  48      58.589  30.478  22.465  1.00  0.00
ATOM    725  O   ASP A  48      58.198  29.334  22.234  1.00  0.00
ATOM    726  N   GLY A  49      58.199  31.167  23.539  1.00  0.00
ATOM    727  HN  GLY A  49      58.551  32.084  23.704  1.00  0.00
ATOM    728  CA  GLY A  49      57.252  30.687  24.518  1.00  0.00
ATOM    729  HA1 GLY A  49      57.787  30.599  25.453  1.00  0.00
ATOM    730  HA2 GLY A  49      56.794  29.763  24.193  1.00  0.00
ATOM    731  C   GLY A  49      56.168  31.710  24.669  1.00  0.00
ATOM    732  O   GLY A  49      55.691  32.282  23.690  1.00  0.00
ATOM    733  N   ILE A  50      55.741  31.925  25.915  1.00  0.00
ATOM    734  HN  ILE A  50      56.178  31.451  26.675  1.00  0.00
ATOM    735  CA  ILE A  50      54.661  32.804  26.314  1.00  0.00
ATOM    736  HA  ILE A  50      53.804  32.498  25.729  1.00  0.00
ATOM    737  CB  ILE A  50      54.275  32.648  27.786  1.00  0.00
ATOM    738  HB  ILE A  50      53.465  33.372  28.037  1.00  0.00
ATOM    739  CG2 ILE A  50      53.679  31.232  27.964  1.00  0.00
ATOM    740 HG21 ILE A  50      54.451  30.453  27.790  1.00  0.00
ATOM    741 HG22 ILE A  50      52.844  31.071  27.250  1.00  0.00
ATOM    742 HG23 ILE A  50      53.281  31.102  28.992  1.00  0.00
ATOM    743  CG1 ILE A  50      55.465  32.917  28.744  1.00  0.00
ATOM    744 HG11 ILE A  50      55.921  33.900  28.493  1.00  0.00
ATOM    745 HG12 ILE A  50      56.246  32.140  28.597  1.00  0.00
ATOM    746  CD1 ILE A  50      55.067  32.950  30.225  1.00  0.00
ATOM    747  HD1 ILE A  50      54.675  31.966  30.554  1.00  0.00
ATOM    748  HD2 ILE A  50      54.287  33.721  30.401  1.00  0.00
ATOM    749  HD3 ILE A  50      55.950  33.197  30.852  1.00  0.00
ATOM    750  C   ILE A  50      54.897  34.265  25.984  1.00  0.00
ATOM    751  O   ILE A  50      56.034  34.733  25.938  1.00  0.00
ATOM    752  N   GLY A  51      53.805  34.997  25.745  1.00  0.00
ATOM    753  HN  GLY A  51      52.903  34.575  25.770  1.00  0.00
ATOM    754  CA  GLY A  51      53.808  36.411  25.434  1.00  0.00
ATOM    755  HA1 GLY A  51      54.753  36.857  25.714  1.00  0.00
ATOM    756  HA2 GLY A  51      52.967  36.845  25.954  1.00  0.00
ATOM    757  C   GLY A  51      53.607  36.608  23.964  1.00  0.00
ATOM    758  O   GLY A  51      53.830  35.701  23.164  1.00  0.00
ATOM    759  N   GLN A  52      53.163  37.809  23.587  1.00  0.00
ATOM    760  HN  GLN A  52      52.980  38.525  24.257  1.00  0.00
ATOM    761  CA  GLN A  52      52.846  38.149  22.216  1.00  0.00
ATOM    762  HA  GLN A  52      53.168  37.360  21.550  1.00  0.00
ATOM    763  CB  GLN A  52      51.309  38.367  22.055  1.00  0.00
ATOM    764  HB1 GLN A  52      50.801  37.464  22.461  1.00  0.00
ATOM    765  HB2 GLN A  52      51.084  38.398  20.965  1.00  0.00
ATOM    766  CG  GLN A  52      50.657  39.626  22.689  1.00  0.00
ATOM    767  HG1 GLN A  52      49.564  39.605  22.491  1.00  0.00
ATOM    768  HG2 GLN A  52      51.063  40.536  22.198  1.00  0.00
ATOM    769  CD  GLN A  52      50.897  39.757  24.199  1.00  0.00
ATOM    770  OE1 GLN A  52      51.777  40.509  24.627  1.00  0.00
ATOM    771  NE2 GLN A  52      50.104  39.010  25.020  1.00  0.00
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ATOM    772 HE21 GLN A  52      50.232  39.073  26.009  1.00  0.00
ATOM    773 HE22 GLN A  52      49.386  38.427  24.638  1.00  0.00
ATOM    774  C   GLN A  52      53.580  39.412  21.828  1.00  0.00
ATOM    775  O   GLN A  52      53.491  39.857  20.684  1.00  0.00
ATOM    776  N   ILE A  53      54.347  39.987  22.757  1.00  0.00
ATOM    777  HN  ILE A  53      54.417  39.616  23.680  1.00  0.00
ATOM    778  CA  ILE A  53      55.183  41.135  22.500  1.00  0.00
ATOM    779  HA  ILE A  53      55.718  40.947  21.579  1.00  0.00
ATOM    780  CB  ILE A  53      54.416  42.462  22.402  1.00  0.00
ATOM    781  HB  ILE A  53      53.479  42.254  21.833  1.00  0.00
ATOM    782  CG2 ILE A  53      55.222  43.469  21.548  1.00  0.00
ATOM    783 HG21 ILE A  53      55.517  43.007  20.582  1.00  0.00
ATOM    784 HG22 ILE A  53      56.135  43.804  22.080  1.00  0.00
ATOM    785 HG23 ILE A  53      54.605  44.365  21.326  1.00  0.00
ATOM    786  CG1 ILE A  53      53.991  43.045  23.772  1.00  0.00
ATOM    787 HG11 ILE A  53      54.879  43.469  24.288  1.00  0.00
ATOM    788 HG12 ILE A  53      53.594  42.222  24.400  1.00  0.00
ATOM    789  CD1 ILE A  53      52.907  44.123  23.662  1.00  0.00
ATOM    790  HD1 ILE A  53      52.003  43.714  23.164  1.00  0.00
ATOM    791  HD2 ILE A  53      53.272  44.996  23.081  1.00  0.00
ATOM    792  HD3 ILE A  53      52.621  44.476  24.674  1.00  0.00
ATOM    793  C   ILE A  53      56.176  41.106  23.635  1.00  0.00
ATOM    794  O   ILE A  53      55.975  40.401  24.624  1.00  0.00
ATOM    795  N   ALA A  54      57.285  41.837  23.491  1.00  0.00
ATOM    796  HN  ALA A  54      57.410  42.429  22.700  1.00  0.00
ATOM    797  CA  ALA A  54      58.414  41.743  24.384  1.00  0.00
ATOM    798  HA  ALA A  54      58.395  40.787  24.890  1.00  0.00
ATOM    799  CB  ALA A  54      59.749  41.835  23.610  1.00  0.00
ATOM    800  HB1 ALA A  54      59.806  42.764  23.004  1.00  0.00
ATOM    801  HB2 ALA A  54      59.829  40.973  22.912  1.00  0.00
ATOM    802  HB3 ALA A  54      60.619  41.794  24.301  1.00  0.00
ATOM    803  C   ALA A  54      58.329  42.822  25.442  1.00  0.00
ATOM    804  O   ALA A  54      57.628  42.662  26.439  1.00  0.00
ATOM    805  N   PHE A  55      59.078  43.913  25.269  1.00  0.00
ATOM    806  HN  PHE A  55      59.628  44.029  24.446  1.00  0.00
ATOM    807  CA  PHE A  55      59.233  44.956  26.265  1.00  0.00
ATOM    808  HA  PHE A  55      59.506  44.472  27.193  1.00  0.00
ATOM    809  CB  PHE A  55      60.364  45.939  25.846  1.00  0.00
ATOM    810  HB1 PHE A  55      60.557  46.674  26.657  1.00  0.00
ATOM    811  HB2 PHE A  55      60.065  46.493  24.929  1.00  0.00
ATOM    812  CG  PHE A  55      61.670  45.225  25.576  1.00  0.00
ATOM    813  CD1 PHE A  55      62.178  44.262  26.471  1.00  0.00
ATOM    814  HD1 PHE A  55      61.638  44.018  27.373  1.00  0.00
ATOM    815  CE1 PHE A  55      63.387  43.608  26.205  1.00  0.00
ATOM    816  HE1 PHE A  55      63.763  42.869  26.895  1.00  0.00
ATOM    817  CZ  PHE A  55      64.118  43.924  25.054  1.00  0.00
ATOM    818  HZ  PHE A  55      65.056  43.427  24.856  1.00  0.00
ATOM    819  CD2 PHE A  55      62.419  45.534  24.425  1.00  0.00
ATOM    820  HD2 PHE A  55      62.054  46.276  23.731  1.00  0.00
ATOM    821  CE2 PHE A  55      63.636  44.891  24.166  1.00  0.00
ATOM    822  HE2 PHE A  55      64.203  45.143  23.282  1.00  0.00
ATOM    823  C   PHE A  55      57.983  45.758  26.548  1.00  0.00
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ATOM    824  O   PHE A  55      57.660  46.028  27.704  1.00  0.00
ATOM    825  N   ASP A  56      57.265  46.152  25.492  1.00  0.00
ATOM    826  HN  ASP A  56      57.529  45.880  24.571  1.00  0.00
ATOM    827  CA  ASP A  56      56.120  47.039  25.554  1.00  0.00
ATOM    828  HA  ASP A  56      56.456  47.950  26.032  1.00  0.00
ATOM    829  CB  ASP A  56      55.625  47.342  24.108  1.00  0.00
ATOM    830  HB1 ASP A  56      55.176  46.435  23.653  1.00  0.00
ATOM    831  HB2 ASP A  56      56.501  47.639  23.491  1.00  0.00
ATOM    832  CG  ASP A  56      54.623  48.500  24.069  1.00  0.00
ATOM    833  OD1 ASP A  56      54.756  49.437  24.899  1.00  0.00
ATOM    834  OD2 ASP A  56      53.780  48.509  23.133  1.00  0.00
ATOM    835  C   ASP A  56      55.008  46.425  26.386  1.00  0.00
ATOM    836  O   ASP A  56      54.691  45.250  26.224  1.00  0.00
ATOM    837  N   ASN A  57      54.433  47.213  27.300  1.00  0.00
ATOM    838  HN  ASN A  57      54.730  48.161  27.389  1.00  0.00
ATOM    839  CA  ASN A  57      53.328  46.843  28.171  1.00  0.00
ATOM    840  HA  ASN A  57      53.067  47.745  28.702  1.00  0.00
ATOM    841  CB  ASN A  57      52.077  46.392  27.356  1.00  0.00
ATOM    842  HB1 ASN A  57      51.223  46.217  28.047  1.00  0.00
ATOM    843  HB2 ASN A  57      52.278  45.441  26.825  1.00  0.00
ATOM    844  CG  ASN A  57      51.645  47.490  26.374  1.00  0.00
ATOM    845  OD1 ASN A  57      51.463  48.646  26.772  1.00  0.00
ATOM    846  ND2 ASN A  57      51.490  47.121  25.070  1.00  0.00
ATOM    847 HD21 ASN A  57      51.272  47.817  24.386  1.00  0.00
ATOM    848 HD22 ASN A  57      51.666  46.177  24.793  1.00  0.00
ATOM    849  C   ASN A  57      53.670  45.821  29.241  1.00  0.00
ATOM    850  O   ASN A  57      52.774  45.278  29.887  1.00  0.00
ATOM    851  N   TYR A  58      54.961  45.561  29.459  1.00  0.00
ATOM    852  HN  TYR A  58      55.669  46.001  28.911  1.00  0.00
ATOM    853  CA  TYR A  58      55.421  44.603  30.442  1.00  0.00
ATOM    854  HA  TYR A  58      54.603  44.289  31.078  1.00  0.00
ATOM    855  CB  TYR A  58      56.055  43.364  29.748  1.00  0.00
ATOM    856  HB1 TYR A  58      56.698  43.681  28.898  1.00  0.00
ATOM    857  HB2 TYR A  58      56.686  42.787  30.459  1.00  0.00
ATOM    858  CG  TYR A  58      55.001  42.407  29.248  1.00  0.00
ATOM    859  CD1 TYR A  58      54.703  42.288  27.880  1.00  0.00
ATOM    860  HD1 TYR A  58      55.202  42.923  27.164  1.00  0.00
ATOM    861  CE1 TYR A  58      53.782  41.336  27.428  1.00  0.00
ATOM    862  HE1 TYR A  58      53.577  41.248  26.373  1.00  0.00
ATOM    863  CZ  TYR A  58      53.136  40.494  28.341  1.00  0.00
ATOM    864  OH  TYR A  58      52.206  39.538  27.877  1.00  0.00
ATOM    865  HH  TYR A  58      51.891  39.043  28.636  1.00  0.00
ATOM    866  CD2 TYR A  58      54.337  41.563  30.158  1.00  0.00
ATOM    867  HD2 TYR A  58      54.560  41.636  31.212  1.00  0.00
ATOM    868  CE2 TYR A  58      53.407  40.614  29.711  1.00  0.00
ATOM    869  HE2 TYR A  58      52.910  39.976  30.426  1.00  0.00
ATOM    870  C   TYR A  58      56.446  45.221  31.354  1.00  0.00
ATOM    871  O   TYR A  58      56.278  45.212  32.572  1.00  0.00
ATOM    872  N   VAL A  59      57.524  45.770  30.785  1.00  0.00
ATOM    873  HN  VAL A  59      57.631  45.804  29.793  1.00  0.00
ATOM    874  CA  VAL A  59      58.670  46.223  31.556  1.00  0.00
ATOM    875  HA  VAL A  59      58.675  45.717  32.511  1.00  0.00
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ATOM    876  CB  VAL A  59      60.010  45.923  30.867  1.00  0.00
ATOM    877  HB  VAL A  59      60.820  46.033  31.626  1.00  0.00
ATOM    878  CG1 VAL A  59      60.022  44.453  30.398  1.00  0.00
ATOM    879 HG11 VAL A  59      61.038  44.175  30.043  1.00  0.00
ATOM    880 HG12 VAL A  59      59.749  43.780  31.235  1.00  0.00
ATOM    881 HG13 VAL A  59      59.311  44.289  29.562  1.00  0.00
ATOM    882  CG2 VAL A  59      60.338  46.883  29.699  1.00  0.00
ATOM    883 HG21 VAL A  59      61.243  46.524  29.163  1.00  0.00
ATOM    884 HG22 VAL A  59      59.502  46.932  28.977  1.00  0.00
ATOM    885 HG23 VAL A  59      60.550  47.909  30.063  1.00  0.00
ATOM    886  C   VAL A  59      58.558  47.707  31.821  1.00  0.00
ATOM    887  O   VAL A  59      59.450  48.315  32.412  1.00  0.00
ATOM    888  N   ALA A  60      57.446  48.306  31.399  1.00  0.00
ATOM    889  HN  ALA A  60      56.701  47.772  31.008  1.00  0.00
ATOM    890  CA  ALA A  60      57.263  49.729  31.354  1.00  0.00
ATOM    891  HA  ALA A  60      57.959  50.217  32.023  1.00  0.00
ATOM    892  CB  ALA A  60      57.433  50.280  29.922  1.00  0.00
ATOM    893  HB1 ALA A  60      58.451  50.036  29.548  1.00  0.00
ATOM    894  HB2 ALA A  60      56.695  49.821  29.230  1.00  0.00
ATOM    895  HB3 ALA A  60      57.313  51.383  29.891  1.00  0.00
ATOM    896  C   ALA A  60      55.872  50.025  31.830  1.00  0.00
ATOM    897  O   ALA A  60      55.080  49.116  32.079  1.00  0.00
ATOM    898  N   TYR A  61      55.571  51.318  31.972  1.00  0.00
ATOM    899  HN  TYR A  61      56.261  52.003  31.754  1.00  0.00
ATOM    900  CA  TYR A  61      54.312  51.877  32.422  1.00  0.00
ATOM    901  HA  TYR A  61      54.461  52.946  32.456  1.00  0.00
ATOM    902  CB  TYR A  61      53.159  51.562  31.415  1.00  0.00
ATOM    903  HB1 TYR A  61      52.288  52.226  31.599  1.00  0.00
ATOM    904  HB2 TYR A  61      52.833  50.504  31.523  1.00  0.00
ATOM    905  CG  TYR A  61      53.586  51.763  29.979  1.00  0.00
ATOM    906  CD1 TYR A  61      53.422  50.713  29.061  1.00  0.00
ATOM    907  HD1 TYR A  61      52.979  49.784  29.386  1.00  0.00
ATOM    908  CE1 TYR A  61      53.843  50.847  27.736  1.00  0.00
ATOM    909  HE1 TYR A  61      53.711  50.022  27.055  1.00  0.00
ATOM    910  CZ  TYR A  61      54.428  52.041  27.303  1.00  0.00
ATOM    911  OH  TYR A  61      54.871  52.156  25.967  1.00  0.00
ATOM    912  HH  TYR A  61      54.745  51.299  25.540  1.00  0.00
ATOM    913  CD2 TYR A  61      54.146  52.973  29.529  1.00  0.00
ATOM    914  HD2 TYR A  61      54.269  53.797  30.216  1.00  0.00
ATOM    915  CE2 TYR A  61      54.572  53.110  28.200  1.00  0.00
ATOM    916  HE2 TYR A  61      55.016  54.038  27.870  1.00  0.00
ATOM    917  C   TYR A  61      53.975  51.427  33.827  1.00  0.00
ATOM    918  O   TYR A  61      54.836  51.423  34.704  1.00  0.00
ATOM    919  N   LEU A  62      52.707  51.082  34.061  1.00  0.00
ATOM    920  HN  LEU A  62      52.055  51.045  33.309  1.00  0.00
ATOM    921  CA  LEU A  62      52.126  50.876  35.366  1.00  0.00
ATOM    922  HA  LEU A  62      52.230  51.811  35.897  1.00  0.00
ATOM    923  CB  LEU A  62      50.617  50.549  35.211  1.00  0.00
ATOM    924  HB1 LEU A  62      50.510  49.611  34.622  1.00  0.00
ATOM    925  HB2 LEU A  62      50.150  51.366  34.617  1.00  0.00
ATOM    926  CG  LEU A  62      49.808  50.397  36.525  1.00  0.00
ATOM    927  HG  LEU A  62      50.253  49.568  37.123  1.00  0.00
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ATOM    928  CD1 LEU A  62      49.850  51.672  37.390  1.00  0.00
ATOM    929 HD11 LEU A  62      49.429  52.532  36.828  1.00  0.00
ATOM    930 HD12 LEU A  62      50.891  51.915  37.684  1.00  0.00
ATOM    931 HD13 LEU A  62      49.251  51.529  38.314  1.00  0.00
ATOM    932  CD2 LEU A  62      48.352  49.990  36.224  1.00  0.00
ATOM    933 HD21 LEU A  62      48.327  49.042  35.647  1.00  0.00
ATOM    934 HD22 LEU A  62      47.846  50.781  35.630  1.00  0.00
ATOM    935 HD23 LEU A  62      47.789  49.843  37.170  1.00  0.00
ATOM    936  C   LEU A  62      52.791  49.805  36.198  1.00  0.00
ATOM    937  O   LEU A  62      53.019  50.006  37.386  1.00  0.00
ATOM    938  N   VAL A  63      53.118  48.664  35.586  1.00  0.00
ATOM    939  HN  VAL A  63      52.973  48.555  34.606  1.00  0.00
ATOM    940  CA  VAL A  63      53.612  47.482  36.270  1.00  0.00
ATOM    941  HA  VAL A  63      52.868  47.206  37.005  1.00  0.00
ATOM    942  CB  VAL A  63      53.777  46.316  35.290  1.00  0.00
ATOM    943  HB  VAL A  63      54.461  46.615  34.462  1.00  0.00
ATOM    944  CG1 VAL A  63      52.398  45.991  34.674  1.00  0.00
ATOM    945 HG11 VAL A  63      52.002  46.844  34.087  1.00  0.00
ATOM    946 HG12 VAL A  63      51.670  45.738  35.474  1.00  0.00
ATOM    947 HG13 VAL A  63      52.485  45.118  33.992  1.00  0.00
ATOM    948  CG2 VAL A  63      54.374  45.064  35.977  1.00  0.00
ATOM    949 HG21 VAL A  63      53.772  44.788  36.868  1.00  0.00
ATOM    950 HG22 VAL A  63      55.426  45.231  36.290  1.00  0.00
ATOM    951 HG23 VAL A  63      54.367  44.207  35.269  1.00  0.00
ATOM    952  C   VAL A  63      54.912  47.717  37.012  1.00  0.00
ATOM    953  O   VAL A  63      55.050  47.327  38.171  1.00  0.00
ATOM    954  N   SER A  64      55.869  48.387  36.368  1.00  0.00
ATOM    955  HN  SER A  64      55.738  48.741  35.445  1.00  0.00
ATOM    956  CA  SER A  64      57.189  48.572  36.931  1.00  0.00
ATOM    957  HA  SER A  64      57.428  47.727  37.563  1.00  0.00
ATOM    958  CB  SER A  64      58.251  48.618  35.798  1.00  0.00
ATOM    959  HB1 SER A  64      58.293  47.615  35.320  1.00  0.00
ATOM    960  HB2 SER A  64      59.259  48.845  36.208  1.00  0.00
ATOM    961  OG  SER A  64      57.927  49.564  34.784  1.00  0.00
ATOM    962  HG  SER A  64      58.570  49.432  34.080  1.00  0.00
ATOM    963  C   SER A  64      57.264  49.811  37.786  1.00  0.00
ATOM    964  O   SER A  64      57.875  49.789  38.852  1.00  0.00
ATOM    965  N   ASN A  65      56.627  50.901  37.347  1.00  0.00
ATOM    966  HN  ASN A  65      56.147  50.894  36.472  1.00  0.00
ATOM    967  CA  ASN A  65      56.610  52.165  38.062  1.00  0.00
ATOM    968  HA  ASN A  65      57.636  52.445  38.260  1.00  0.00
ATOM    969  CB  ASN A  65      55.925  53.268  37.207  1.00  0.00
ATOM    970  HB1 ASN A  65      54.914  52.929  36.896  1.00  0.00
ATOM    971  HB2 ASN A  65      55.819  54.201  37.803  1.00  0.00
ATOM    972  CG  ASN A  65      56.765  53.607  35.965  1.00  0.00
ATOM    973  OD1 ASN A  65      57.920  53.192  35.822  1.00  0.00
ATOM    974  ND2 ASN A  65      56.148  54.394  35.034  1.00  0.00
ATOM    975 HD21 ASN A  65      56.643  54.650  34.205  1.00  0.00
ATOM    976 HD22 ASN A  65      55.210  54.702  35.184  1.00  0.00
ATOM    977  C   ASN A  65      55.909  52.085  39.397  1.00  0.00
ATOM    978  O   ASN A  65      56.407  52.611  40.391  1.00  0.00
ATOM    979  N   LEU A  66      54.753  51.414  39.443  1.00  0.00
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ATOM    980  HN  LEU A  66      54.362  50.998  38.623  1.00  0.00
ATOM    981  CA  LEU A  66      53.994  51.211  40.661  1.00  0.00
ATOM    982  HA  LEU A  66      53.847  52.186  41.104  1.00  0.00
ATOM    983  CB  LEU A  66      52.615  50.582  40.346  1.00  0.00
ATOM    984  HB1 LEU A  66      52.115  51.221  39.585  1.00  0.00
ATOM    985  HB2 LEU A  66      52.764  49.576  39.895  1.00  0.00
ATOM    986  CG  LEU A  66      51.646  50.439  41.547  1.00  0.00
ATOM    987  HG  LEU A  66      52.122  49.774  42.305  1.00  0.00
ATOM    988  CD1 LEU A  66      51.351  51.789  42.233  1.00  0.00
ATOM    989 HD11 LEU A  66      50.634  51.646  43.069  1.00  0.00
ATOM    990 HD12 LEU A  66      52.280  52.233  42.648  1.00  0.00
ATOM    991 HD13 LEU A  66      50.909  52.502  41.506  1.00  0.00
ATOM    992  CD2 LEU A  66      50.339  49.752  41.109  1.00  0.00
ATOM    993 HD21 LEU A  66      49.665  49.610  41.980  1.00  0.00
ATOM    994 HD22 LEU A  66      49.813  50.372  40.352  1.00  0.00
ATOM    995 HD23 LEU A  66      50.555  48.758  40.663  1.00  0.00
ATOM    996  C   LEU A  66      54.738  50.356  41.655  1.00  0.00
ATOM    997  O   LEU A  66      54.739  50.646  42.849  1.00  0.00
ATOM    998  N   ALA A  67      55.399  49.300  41.171  1.00  0.00
ATOM    999  HN  ALA A  67      55.381  49.085  40.197  1.00  0.00
ATOM   1000  CA  ALA A  67      56.192  48.407  41.986  1.00  0.00
ATOM   1001  HA  ALA A  67      55.545  48.015  42.759  1.00  0.00
ATOM   1002  CB  ALA A  67      56.747  47.225  41.166  1.00  0.00
ATOM   1003  HB1 ALA A  67      57.419  47.578  40.355  1.00  0.00
ATOM   1004  HB2 ALA A  67      55.909  46.665  40.700  1.00  0.00
ATOM   1005  HB3 ALA A  67      57.310  46.522  41.817  1.00  0.00
ATOM   1006  C   ALA A  67      57.346  49.112  42.658  1.00  0.00
ATOM   1007  O   ALA A  67      57.551  48.953  43.857  1.00  0.00
ATOM   1008  N   LEU A  68      58.072  49.946  41.909  1.00  0.00
ATOM   1009  HN  LEU A  68      57.883  50.044  40.933  1.00  0.00
ATOM   1010  CA  LEU A  68      59.149  50.777  42.411  1.00  0.00
ATOM   1011  HA  LEU A  68      59.864  50.129  42.896  1.00  0.00
ATOM   1012  CB  LEU A  68      59.835  51.528  41.242  1.00  0.00
ATOM   1013  HB1 LEU A  68      60.481  52.351  41.624  1.00  0.00
ATOM   1014  HB2 LEU A  68      59.046  51.986  40.605  1.00  0.00
ATOM   1015  CG  LEU A  68      60.733  50.629  40.360  1.00  0.00
ATOM   1016  HG  LEU A  68      60.170  49.697  40.125  1.00  0.00
ATOM   1017  CD1 LEU A  68      61.055  51.311  39.016  1.00  0.00
ATOM   1018 HD11 LEU A  68      61.620  52.252  39.186  1.00  0.00
ATOM   1019 HD12 LEU A  68      60.118  51.551  38.470  1.00  0.00
ATOM   1020 HD13 LEU A  68      61.670  50.637  38.381  1.00  0.00
ATOM   1021  CD2 LEU A  68      62.026  50.225  41.094  1.00  0.00
ATOM   1022 HD21 LEU A  68      61.795  49.642  42.009  1.00  0.00
ATOM   1023 HD22 LEU A  68      62.604  51.128  41.385  1.00  0.00
ATOM   1024 HD23 LEU A  68      62.664  49.601  40.435  1.00  0.00
ATOM   1025  C   LEU A  68      58.697  51.782  43.437  1.00  0.00
ATOM   1026  O   LEU A  68      59.373  51.986  44.444  1.00  0.00
ATOM   1027  N   ALA A  69      57.544  52.413  43.200  1.00  0.00
ATOM   1028  HN  ALA A  69      57.026  52.240  42.364  1.00  0.00
ATOM   1029  CA  ALA A  69      56.955  53.372  44.106  1.00  0.00
ATOM   1030  HA  ALA A  69      57.681  54.158  44.263  1.00  0.00
ATOM   1031  CB  ALA A  69      55.672  53.997  43.521  1.00  0.00
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ATOM   1032  HB1 ALA A  69      54.889  53.228  43.353  1.00  0.00
ATOM   1033  HB2 ALA A  69      55.899  54.474  42.544  1.00  0.00
ATOM   1034  HB3 ALA A  69      55.267  54.778  44.199  1.00  0.00
ATOM   1035  C   ALA A  69      56.625  52.760  45.449  1.00  0.00
ATOM   1036  O   ALA A  69      56.968  53.322  46.482  1.00  0.00
ATOM   1037  N   ILE A  70      56.004  51.577  45.445  1.00  0.00
ATOM   1038  HN  ILE A  70      55.736  51.157  44.579  1.00  0.00
ATOM   1039  CA  ILE A  70      55.679  50.798  46.627  1.00  0.00
ATOM   1040  HA  ILE A  70      55.152  51.457  47.301  1.00  0.00
ATOM   1041  CB  ILE A  70      54.754  49.625  46.269  1.00  0.00
ATOM   1042  HB  ILE A  70      55.190  49.109  45.380  1.00  0.00
ATOM   1043  CG2 ILE A  70      54.660  48.563  47.392  1.00  0.00
ATOM   1044 HG21 ILE A  70      54.386  49.031  48.360  1.00  0.00
ATOM   1045 HG22 ILE A  70      55.623  48.025  47.513  1.00  0.00
ATOM   1046 HG23 ILE A  70      53.888  47.808  47.134  1.00  0.00
ATOM   1047  CG1 ILE A  70      53.346  50.131  45.848  1.00  0.00
ATOM   1048 HG11 ILE A  70      52.782  49.262  45.438  1.00  0.00
ATOM   1049 HG12 ILE A  70      53.445  50.872  45.028  1.00  0.00
ATOM   1050  CD1 ILE A  70      52.512  50.757  46.975  1.00  0.00
ATOM   1051  HD1 ILE A  70      53.021  51.647  47.400  1.00  0.00
ATOM   1052  HD2 ILE A  70      52.332  50.026  47.791  1.00  0.00
ATOM   1053  HD3 ILE A  70      51.526  51.081  46.580  1.00  0.00
ATOM   1054  C   ILE A  70      56.911  50.333  47.384  1.00  0.00
ATOM   1055  O   ILE A  70      56.970  50.441  48.609  1.00  0.00
ATOM   1056  N   ILE A  71      57.919  49.836  46.659  1.00  0.00
ATOM   1057  HN  ILE A  71      57.834  49.772  45.665  1.00  0.00
ATOM   1058  CA  ILE A  71      59.167  49.313  47.190  1.00  0.00
ATOM   1059  HA  ILE A  71      58.903  48.551  47.911  1.00  0.00
ATOM   1060  CB  ILE A  71      60.019  48.634  46.103  1.00  0.00
ATOM   1061  HB  ILE A  71      59.998  49.283  45.198  1.00  0.00
ATOM   1062  CG2 ILE A  71      61.503  48.461  46.514  1.00  0.00
ATOM   1063 HG21 ILE A  71      61.569  47.877  47.455  1.00  0.00
ATOM   1064 HG22 ILE A  71      62.006  49.438  46.658  1.00  0.00
ATOM   1065 HG23 ILE A  71      62.067  47.920  45.727  1.00  0.00
ATOM   1066  CG1 ILE A  71      59.395  47.263  45.731  1.00  0.00
ATOM   1067 HG11 ILE A  71      58.294  47.373  45.637  1.00  0.00
ATOM   1068 HG12 ILE A  71      59.579  46.548  46.563  1.00  0.00
ATOM   1069  CD1 ILE A  71      59.933  46.670  44.422  1.00  0.00
ATOM   1070  HD1 ILE A  71      61.015  46.437  44.503  1.00  0.00
ATOM   1071  HD2 ILE A  71      59.786  47.382  43.582  1.00  0.00
ATOM   1072  HD3 ILE A  71      59.397  45.729  44.179  1.00  0.00
ATOM   1073  C   ILE A  71      59.955  50.355  47.953  1.00  0.00
ATOM   1074  O   ILE A  71      60.502  50.071  49.016  1.00  0.00
ATOM   1075  N   LEU A  72      60.015  51.580  47.432  1.00  0.00
ATOM   1076  HN  LEU A  72      59.556  51.810  46.575  1.00  0.00
ATOM   1077  CA  LEU A  72      60.851  52.609  48.008  1.00  0.00
ATOM   1078  HA  LEU A  72      61.616  52.165  48.631  1.00  0.00
ATOM   1079  CB  LEU A  72      61.548  53.410  46.883  1.00  0.00
ATOM   1080  HB1 LEU A  72      62.177  54.208  47.335  1.00  0.00
ATOM   1081  HB2 LEU A  72      60.769  53.888  46.249  1.00  0.00
ATOM   1082  CG  LEU A  72      62.466  52.576  45.955  1.00  0.00
ATOM   1083  HG  LEU A  72      61.868  51.741  45.522  1.00  0.00
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ATOM   1084  CD1 LEU A  72      62.958  53.428  44.767  1.00  0.00
ATOM   1085 HD11 LEU A  72      63.575  54.277  45.130  1.00  0.00
ATOM   1086 HD12 LEU A  72      62.094  53.833  44.199  1.00  0.00
ATOM   1087 HD13 LEU A  72      63.573  52.810  44.079  1.00  0.00
ATOM   1088  CD2 LEU A  72      63.655  51.951  46.712  1.00  0.00
ATOM   1089 HD21 LEU A  72      63.300  51.277  47.519  1.00  0.00
ATOM   1090 HD22 LEU A  72      64.286  52.745  47.165  1.00  0.00
ATOM   1091 HD23 LEU A  72      64.281  51.357  46.015  1.00  0.00
ATOM   1092  C   LEU A  72      60.051  53.548  48.884  1.00  0.00
ATOM   1093  O   LEU A  72      60.623  54.394  49.571  1.00  0.00
ATOM   1094  N   LEU A  73      58.724  53.376  48.932  1.00  0.00
ATOM   1095  HN  LEU A  73      58.265  52.723  48.333  1.00  0.00
ATOM   1096  CA  LEU A  73      57.875  54.055  49.894  1.00  0.00
ATOM   1097  HA  LEU A  73      58.242  55.061  50.035  1.00  0.00
ATOM   1098  CB  LEU A  73      56.409  54.103  49.388  1.00  0.00
ATOM   1099  HB1 LEU A  73      56.059  53.071  49.169  1.00  0.00
ATOM   1100  HB2 LEU A  73      56.405  54.673  48.434  1.00  0.00
ATOM   1101  CG  LEU A  73      55.375  54.794  50.316  1.00  0.00
ATOM   1102  HG  LEU A  73      55.317  54.219  51.269  1.00  0.00
ATOM   1103  CD1 LEU A  73      55.775  56.242  50.661  1.00  0.00
ATOM   1104 HD11 LEU A  73      55.863  56.851  49.737  1.00  0.00
ATOM   1105 HD12 LEU A  73      56.747  56.266  51.195  1.00  0.00
ATOM   1106 HD13 LEU A  73      55.007  56.704  51.317  1.00  0.00
ATOM   1107  CD2 LEU A  73      53.967  54.758  49.688  1.00  0.00
ATOM   1108 HD21 LEU A  73      53.664  53.712  49.471  1.00  0.00
ATOM   1109 HD22 LEU A  73      53.954  55.333  48.738  1.00  0.00
ATOM   1110 HD23 LEU A  73      53.224  55.205  50.382  1.00  0.00
ATOM   1111  C   LEU A  73      57.935  53.330  51.214  1.00  0.00
ATOM   1112  O   LEU A  73      57.756  53.933  52.269  1.00  0.00
ATOM   1113  N   ASP A  74      58.261  52.033  51.177  1.00  0.00
ATOM   1114  HN  ASP A  74      58.359  51.563  50.302  1.00  0.00
ATOM   1115  CA  ASP A  74      58.578  51.226  52.336  1.00  0.00
ATOM   1116  HA  ASP A  74      57.736  51.287  53.012  1.00  0.00
ATOM   1117  CB  ASP A  74      58.808  49.748  51.892  1.00  0.00
ATOM   1118  HB1 ASP A  74      59.719  49.676  51.268  1.00  0.00
ATOM   1119  HB2 ASP A  74      57.941  49.420  51.281  1.00  0.00
ATOM   1120  CG  ASP A  74      58.952  48.791  53.081  1.00  0.00
ATOM   1121  OD1 ASP A  74      59.555  47.700  52.890  1.00  0.00
ATOM   1122  OD2 ASP A  74      58.408  49.094  54.175  1.00  0.00
ATOM   1123  C   ASP A  74      59.804  51.784  53.037  1.00  0.00
ATOM   1124  O   ASP A  74      59.828  51.910  54.258  1.00  0.00
ATOM   1125  N   GLY A  75      60.812  52.184  52.255  1.00  0.00
ATOM   1126  HN  GLY A  75      60.752  52.069  51.266  1.00  0.00
ATOM   1127  CA  GLY A  75      62.029  52.814  52.728  1.00  0.00
ATOM   1128  HA1 GLY A  75      62.677  52.918  51.871  1.00  0.00
ATOM   1129  HA2 GLY A  75      62.453  52.194  53.505  1.00  0.00
ATOM   1130  C   GLY A  75      61.791  54.189  53.295  1.00  0.00
ATOM   1131  O   GLY A  75      62.468  54.607  54.233  1.00  0.00
ATOM   1132  N   GLY A  76      60.806  54.908  52.750  1.00  0.00
ATOM   1133  HN  GLY A  76      60.282  54.540  51.986  1.00  0.00
ATOM   1134  CA  GLY A  76      60.425  56.239  53.176  1.00  0.00
ATOM   1135  HA1 GLY A  76      59.745  56.619  52.428  1.00  0.00
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ATOM   1136  HA2 GLY A  76      61.320  56.838  53.276  1.00  0.00
ATOM   1137  C   GLY A  76      59.703  56.239  54.498  1.00  0.00
ATOM   1138  O   GLY A  76      59.677  57.253  55.193  1.00  0.00
ATOM   1139  N   MET A  77      59.114  55.101  54.871  1.00  0.00
ATOM   1140  HN  MET A  77      59.134  54.301  54.276  1.00  0.00
ATOM   1141  CA  MET A  77      58.405  54.926  56.119  1.00  0.00
ATOM   1142  HA  MET A  77      58.084  55.888  56.496  1.00  0.00
ATOM   1143  CB  MET A  77      57.161  54.028  55.896  1.00  0.00
ATOM   1144  HB1 MET A  77      56.720  53.726  56.872  1.00  0.00
ATOM   1145  HB2 MET A  77      57.475  53.101  55.367  1.00  0.00
ATOM   1146  CG  MET A  77      56.040  54.705  55.082  1.00  0.00
ATOM   1147  HG1 MET A  77      55.274  53.929  54.867  1.00  0.00
ATOM   1148  HG2 MET A  77      56.444  55.045  54.106  1.00  0.00
ATOM   1149  SD  MET A  77      55.247  56.103  55.932  1.00  0.00
ATOM   1150  CE  MET A  77      53.927  56.308  54.707  1.00  0.00
ATOM   1151  HE1 MET A  77      53.376  55.356  54.558  1.00  0.00
ATOM   1152  HE2 MET A  77      54.337  56.626  53.725  1.00  0.00
ATOM   1153  HE3 MET A  77      53.197  57.074  55.043  1.00  0.00
ATOM   1154  C   MET A  77      59.285  54.292  57.173  1.00  0.00
ATOM   1155  O   MET A  77      58.849  54.071  58.302  1.00  0.00
ATOM   1156  N   ARG A  78      60.548  54.022  56.834  1.00  0.00
ATOM   1157  HN  ARG A  78      60.876  54.198  55.907  1.00  0.00
ATOM   1158  CA  ARG A  78      61.527  53.470  57.746  1.00  0.00
ATOM   1159  HA  ARG A  78      61.045  53.114  58.645  1.00  0.00
ATOM   1160  CB  ARG A  78      62.260  52.278  57.080  1.00  0.00
ATOM   1161  HB1 ARG A  78      63.157  51.977  57.666  1.00  0.00
ATOM   1162  HB2 ARG A  78      62.605  52.595  56.071  1.00  0.00
ATOM   1163  CG  ARG A  78      61.371  51.030  56.941  1.00  0.00
ATOM   1164  HG1 ARG A  78      60.372  51.347  56.570  1.00  0.00
ATOM   1165  HG2 ARG A  78      61.217  50.582  57.947  1.00  0.00
ATOM   1166  CD  ARG A  78      61.961  49.983  55.985  1.00  0.00
ATOM   1167  HD1 ARG A  78      62.883  49.519  56.393  1.00  0.00
ATOM   1168  HD2 ARG A  78      62.203  50.455  55.009  1.00  0.00
ATOM   1169  NE  ARG A  78      60.919  48.941  55.718  1.00  0.00
ATOM   1170  HE  ARG A  78      60.234  49.134  55.010  1.00  0.00
ATOM   1171  CZ  ARG A  78      60.703  47.849  56.486  1.00  0.00
ATOM   1172  NH1 ARG A  78      61.504  47.523  57.518  1.00  0.00
ATOM   1173 HH11 ARG A  78      62.281  48.108  57.741  1.00  0.00
ATOM   1174 HH12 ARG A  78      61.302  46.716  58.070  1.00  0.00
ATOM   1175  NH2 ARG A  78      59.641  47.070  56.192  1.00  0.00
ATOM   1176 HH21 ARG A  78      59.035  47.346  55.441  1.00  0.00
ATOM   1177 HH22 ARG A  78      59.427  46.274  56.754  1.00  0.00
ATOM   1178  C   ARG A  78      62.545  54.504  58.157  1.00  0.00
ATOM   1179  O   ARG A  78      63.451  54.202  58.932  1.00  0.00
ATOM   1180  N   THR A  79      62.399  55.739  57.671  1.00  0.00
ATOM   1181  HN  THR A  79      61.632  55.978  57.079  1.00  0.00
ATOM   1182  CA  THR A  79      63.356  56.796  57.918  1.00  0.00
ATOM   1183  HA  THR A  79      64.109  56.436  58.606  1.00  0.00
ATOM   1184  CB  THR A  79      64.068  57.258  56.642  1.00  0.00
ATOM   1185  HB  THR A  79      64.306  56.354  56.035  1.00  0.00
ATOM   1186  OG1 THR A  79      65.314  57.873  56.950  1.00  0.00
ATOM   1187  HG1 THR A  79      65.884  57.176  57.284  1.00  0.00
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ATOM   1188  CG2 THR A  79      63.218  58.208  55.770  1.00  0.00
ATOM   1189 HG21 THR A  79      63.034  59.174  56.284  1.00  0.00
ATOM   1190 HG22 THR A  79      62.243  57.741  55.522  1.00  0.00
ATOM   1191 HG23 THR A  79      63.749  58.431  54.821  1.00  0.00
ATOM   1192  C   THR A  79      62.626  57.918  58.609  1.00  0.00
ATOM   1193  O   THR A  79      61.436  58.133  58.383  1.00  0.00
ATOM   1194  N   ARG A  80      63.335  58.629  59.490  1.00  0.00
ATOM   1195  HN  ARG A  80      64.283  58.387  59.674  1.00  0.00
ATOM   1196  CA  ARG A  80      62.895  59.861  60.111  1.00  0.00
ATOM   1197  HA  ARG A  80      61.823  59.960  60.024  1.00  0.00
ATOM   1198  CB  ARG A  80      63.316  59.921  61.607  1.00  0.00
ATOM   1199  HB1 ARG A  80      63.337  60.983  61.946  1.00  0.00
ATOM   1200  HB2 ARG A  80      64.350  59.526  61.701  1.00  0.00
ATOM   1201  CG  ARG A  80      62.412  59.186  62.624  1.00  0.00
ATOM   1202  HG1 ARG A  80      61.430  59.705  62.688  1.00  0.00
ATOM   1203  HG2 ARG A  80      62.904  59.314  63.617  1.00  0.00
ATOM   1204  CD  ARG A  80      62.212  57.673  62.419  1.00  0.00
ATOM   1205  HD1 ARG A  80      61.974  57.189  63.391  1.00  0.00
ATOM   1206  HD2 ARG A  80      63.124  57.208  61.985  1.00  0.00
ATOM   1207  NE  ARG A  80      61.044  57.454  61.511  1.00  0.00
ATOM   1208  HE  ARG A  80      60.522  58.250  61.199  1.00  0.00
ATOM   1209  CZ  ARG A  80      60.677  56.243  61.033  1.00  0.00
ATOM   1210  NH1 ARG A  80      61.315  55.111  61.386  1.00  0.00
ATOM   1211 HH11 ARG A  80      62.101  55.154  61.999  1.00  0.00
ATOM   1212 HH12 ARG A  80      61.032  54.239  60.993  1.00  0.00
ATOM   1213  NH2 ARG A  80      59.646  56.184  60.165  1.00  0.00
ATOM   1214 HH21 ARG A  80      59.206  57.032  59.872  1.00  0.00
ATOM   1215 HH22 ARG A  80      59.383  55.313  59.747  1.00  0.00
ATOM   1216  C   ARG A  80      63.544  60.986  59.347  1.00  0.00
ATOM   1217  O   ARG A  80      64.524  60.773  58.639  1.00  0.00
ATOM   1218  N   VAL A  81      62.987  62.195  59.446  1.00  0.00
ATOM   1219  HN  VAL A  81      62.191  62.337  60.031  1.00  0.00
ATOM   1220  CA  VAL A  81      63.369  63.344  58.642  1.00  0.00
ATOM   1221  HA  VAL A  81      63.275  63.022  57.616  1.00  0.00
ATOM   1222  CB  VAL A  81      62.393  64.510  58.822  1.00  0.00
ATOM   1223  HB  VAL A  81      61.370  64.124  58.592  1.00  0.00
ATOM   1224  CG1 VAL A  81      62.687  65.640  57.809  1.00  0.00
ATOM   1225 HG11 VAL A  81      62.707  65.238  56.774  1.00  0.00
ATOM   1226 HG12 VAL A  81      63.661  66.126  58.023  1.00  0.00
ATOM   1227 HG13 VAL A  81      61.894  66.415  57.868  1.00  0.00
ATOM   1228  CG2 VAL A  81      62.369  65.019  60.280  1.00  0.00
ATOM   1229 HG21 VAL A  81      63.346  65.460  60.567  1.00  0.00
ATOM   1230 HG22 VAL A  81      62.117  64.203  60.988  1.00  0.00
ATOM   1231 HG23 VAL A  81      61.605  65.815  60.384  1.00  0.00
ATOM   1232  C   VAL A  81      64.815  63.773  58.805  1.00  0.00
ATOM   1233  O   VAL A  81      65.492  64.064  57.821  1.00  0.00
ATOM   1234  N   ALA A  82      65.321  63.776  60.040  1.00  0.00
ATOM   1235  HN  ALA A  82      64.767  63.509  60.824  1.00  0.00
ATOM   1236  CA  ALA A  82      66.655  64.246  60.344  1.00  0.00
ATOM   1237  HA  ALA A  82      67.006  64.905  59.561  1.00  0.00
ATOM   1238  CB  ALA A  82      66.669  65.009  61.682  1.00  0.00
ATOM   1239  HB1 ALA A  82      66.341  64.355  62.518  1.00  0.00
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ATOM   1240  HB2 ALA A  82      65.975  65.875  61.627  1.00  0.00
ATOM   1241  HB3 ALA A  82      67.685  65.397  61.910  1.00  0.00
ATOM   1242  C   ALA A  82      67.608  63.084  60.453  1.00  0.00
ATOM   1243  O   ALA A  82      68.809  63.276  60.636  1.00  0.00
ATOM   1244  N   SER A  83      67.095  61.861  60.296  1.00  0.00
ATOM   1245  HN  SER A  83      66.118  61.731  60.146  1.00  0.00
ATOM   1246  CA  SER A  83      67.905  60.665  60.268  1.00  0.00
ATOM   1247  HA  SER A  83      68.833  60.825  60.801  1.00  0.00
ATOM   1248  CB  SER A  83      67.121  59.489  60.910  1.00  0.00
ATOM   1249  HB1 SER A  83      66.218  59.245  60.310  1.00  0.00
ATOM   1250  HB2 SER A  83      66.792  59.797  61.926  1.00  0.00
ATOM   1251  OG  SER A  83      67.922  58.319  61.044  1.00  0.00
ATOM   1252  HG  SER A  83      67.376  57.655  61.472  1.00  0.00
ATOM   1253  C   SER A  83      68.207  60.341  58.820  1.00  0.00
ATOM   1254  O   SER A  83      69.228  59.726  58.518  1.00  0.00
ATOM   1255  N   PHE A  84      67.332  60.777  57.904  1.00  0.00
ATOM   1256  HN  PHE A  84      66.502  61.255  58.182  1.00  0.00
ATOM   1257  CA  PHE A  84      67.461  60.572  56.478  1.00  0.00
ATOM   1258  HA  PHE A  84      67.596  59.509  56.336  1.00  0.00
ATOM   1259  CB  PHE A  84      66.150  61.019  55.750  1.00  0.00
ATOM   1260  HB1 PHE A  84      65.965  62.096  55.950  1.00  0.00
ATOM   1261  HB2 PHE A  84      65.291  60.441  56.146  1.00  0.00
ATOM   1262  CG  PHE A  84      66.194  60.791  54.248  1.00  0.00
ATOM   1263  CD1 PHE A  84      66.687  59.587  53.705  1.00  0.00
ATOM   1264  HD1 PHE A  84      67.032  58.798  54.356  1.00  0.00
ATOM   1265  CE1 PHE A  84      66.752  59.400  52.319  1.00  0.00
ATOM   1266  HE1 PHE A  84      67.140  58.478  51.916  1.00  0.00
ATOM   1267  CZ  PHE A  84      66.311  60.408  51.454  1.00  0.00
ATOM   1268  HZ  PHE A  84      66.362  60.262  50.385  1.00  0.00
ATOM   1269  CD2 PHE A  84      65.720  61.779  53.365  1.00  0.00
ATOM   1270  HD2 PHE A  84      65.308  62.695  53.760  1.00  0.00
ATOM   1271  CE2 PHE A  84      65.786  61.594  51.977  1.00  0.00
ATOM   1272  HE2 PHE A  84      65.433  62.366  51.309  1.00  0.00
ATOM   1273  C   PHE A  84      68.682  61.261  55.911  1.00  0.00
ATOM   1274  O   PHE A  84      69.436  60.659  55.151  1.00  0.00
ATOM   1275  N   ARG A  85      68.912  62.513  56.308  1.00  0.00
ATOM   1276  HN  ARG A  85      68.314  62.975  56.957  1.00  0.00
ATOM   1277  CA  ARG A  85      70.052  63.261  55.842  1.00  0.00
ATOM   1278  HA  ARG A  85      70.859  62.577  55.612  1.00  0.00
ATOM   1279  CB  ARG A  85      69.711  64.098  54.575  1.00  0.00
ATOM   1280  HB1 ARG A  85      69.298  63.398  53.817  1.00  0.00
ATOM   1281  HB2 ARG A  85      70.671  64.498  54.174  1.00  0.00
ATOM   1282  CG  ARG A  85      68.739  65.293  54.693  1.00  0.00
ATOM   1283  HG1 ARG A  85      68.774  65.825  53.715  1.00  0.00
ATOM   1284  HG2 ARG A  85      69.105  66.010  55.456  1.00  0.00
ATOM   1285  CD  ARG A  85      67.278  64.899  54.964  1.00  0.00
ATOM   1286  HD1 ARG A  85      67.160  64.392  55.942  1.00  0.00
ATOM   1287  HD2 ARG A  85      66.930  64.215  54.163  1.00  0.00
ATOM   1288  NE  ARG A  85      66.398  66.111  54.932  1.00  0.00
ATOM   1289  HE  ARG A  85      65.847  66.273  54.116  1.00  0.00
ATOM   1290  CZ  ARG A  85      66.260  66.965  55.974  1.00  0.00
ATOM   1291  NH1 ARG A  85      66.968  66.825  57.112  1.00  0.00
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ATOM   1292 HH11 ARG A  85      67.621  66.073  57.198  1.00  0.00
ATOM   1293 HH12 ARG A  85      66.842  67.470  57.863  1.00  0.00
ATOM   1294  NH2 ARG A  85      65.383  67.985  55.868  1.00  0.00
ATOM   1295 HH21 ARG A  85      64.847  68.095  55.034  1.00  0.00
ATOM   1296 HH22 ARG A  85      65.265  68.622  56.628  1.00  0.00
ATOM   1297  C   ARG A  85      70.509  64.153  56.954  1.00  0.00
ATOM   1298  O   ARG A  85      69.703  64.817  57.609  1.00  0.00
ATOM   1299  N   VAL A  86      71.823  64.165  57.196  1.00  0.00
ATOM   1300  HN  VAL A  86      72.432  63.551  56.700  1.00  0.00
ATOM   1301  CA  VAL A  86      72.493  65.095  58.079  1.00  0.00
ATOM   1302  HA  VAL A  86      71.950  65.112  59.014  1.00  0.00
ATOM   1303  CB  VAL A  86      73.934  64.665  58.358  1.00  0.00
ATOM   1304  HB  VAL A  86      74.504  64.597  57.403  1.00  0.00
ATOM   1305  CG1 VAL A  86      74.648  65.678  59.281  1.00  0.00
ATOM   1306 HG11 VAL A  86      74.069  65.823  60.217  1.00  0.00
ATOM   1307 HG12 VAL A  86      74.777  66.662  58.784  1.00  0.00
ATOM   1308 HG13 VAL A  86      75.657  65.298  59.548  1.00  0.00
ATOM   1309  CG2 VAL A  86      73.914  63.259  59.000  1.00  0.00
ATOM   1310 HG21 VAL A  86      73.497  62.500  58.306  1.00  0.00
ATOM   1311 HG22 VAL A  86      73.303  63.268  59.927  1.00  0.00
ATOM   1312 HG23 VAL A  86      74.947  62.949  59.263  1.00  0.00
ATOM   1313  C   VAL A  86      72.458  66.490  57.494  1.00  0.00
ATOM   1314  O   VAL A  86      72.103  67.453  58.171  1.00  0.00
ATOM   1315  N   ALA A  87      72.789  66.598  56.207  1.00  0.00
ATOM   1316  HN  ALA A  87      73.055  65.798  55.673  1.00  0.00
ATOM   1317  CA  ALA A  87      72.819  67.842  55.487  1.00  0.00
ATOM   1318  HA  ALA A  87      71.856  68.326  55.586  1.00  0.00
ATOM   1319  CB  ALA A  87      73.969  68.784  55.907  1.00  0.00
ATOM   1320  HB1 ALA A  87      74.951  68.275  55.814  1.00  0.00
ATOM   1321  HB2 ALA A  87      73.840  69.091  56.967  1.00  0.00
ATOM   1322  HB3 ALA A  87      73.981  69.704  55.284  1.00  0.00
ATOM   1323  C   ALA A  87      73.033  67.457  54.054  1.00  0.00
ATOM   1324  O   ALA A  87      73.611  66.410  53.762  1.00  0.00
ATOM   1325  N   PHE A  88      72.560  68.294  53.131  1.00  0.00
ATOM   1326  HN  PHE A  88      72.071  69.126  53.381  1.00  0.00
ATOM   1327  CA  PHE A  88      72.701  68.048  51.715  1.00  0.00
ATOM   1328  HA  PHE A  88      72.596  66.987  51.525  1.00  0.00
ATOM   1329  CB  PHE A  88      71.605  68.817  50.927  1.00  0.00
ATOM   1330  HB1 PHE A  88      71.742  68.678  49.831  1.00  0.00
ATOM   1331  HB2 PHE A  88      71.661  69.906  51.146  1.00  0.00
ATOM   1332  CG  PHE A  88      70.220  68.323  51.269  1.00  0.00
ATOM   1333  CD1 PHE A  88      69.375  69.056  52.124  1.00  0.00
ATOM   1334  HD1 PHE A  88      69.729  69.972  52.571  1.00  0.00
ATOM   1335  CE1 PHE A  88      68.068  68.621  52.383  1.00  0.00
ATOM   1336  HE1 PHE A  88      67.426  69.197  53.033  1.00  0.00
ATOM   1337  CZ  PHE A  88      67.589  67.449  51.785  1.00  0.00
ATOM   1338  HZ  PHE A  88      66.579  67.118  51.974  1.00  0.00
ATOM   1339  CD2 PHE A  88      69.731  67.138  50.690  1.00  0.00
ATOM   1340  HD2 PHE A  88      70.363  66.566  50.026  1.00  0.00
ATOM   1341  CE2 PHE A  88      68.425  66.703  50.947  1.00  0.00
ATOM   1342  HE2 PHE A  88      68.058  65.796  50.490  1.00  0.00
ATOM   1343  C   PHE A  88      74.041  68.486  51.178  1.00  0.00
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ATOM   1344  O   PHE A  88      74.515  67.931  50.191  1.00  0.00
ATOM   1345  N   TRP A  89      74.671  69.480  51.813  1.00  0.00
ATOM   1346  HN  TRP A  89      74.293  69.882  52.642  1.00  0.00
ATOM   1347  CA  TRP A  89      75.868  70.120  51.291  1.00  0.00
ATOM   1348  HA  TRP A  89      75.595  70.454  50.299  1.00  0.00
ATOM   1349  CB  TRP A  89      76.196  71.415  52.095  1.00  0.00
ATOM   1350  HB1 TRP A  89      76.511  71.172  53.128  1.00  0.00
ATOM   1351  HB2 TRP A  89      75.248  71.993  52.180  1.00  0.00
ATOM   1352  CG  TRP A  89      77.235  72.303  51.472  1.00  0.00
ATOM   1353  CD1 TRP A  89      76.972  73.383  50.669  1.00  0.00
ATOM   1354  HD1 TRP A  89      75.983  73.747  50.429  1.00  0.00
ATOM   1355  NE1 TRP A  89      78.145  73.915  50.207  1.00  0.00
ATOM   1356  HE1 TRP A  89      78.225  74.689  49.618  1.00  0.00
ATOM   1357  CE2 TRP A  89      79.198  73.199  50.696  1.00  0.00
ATOM   1358  CD2 TRP A  89      78.669  72.172  51.512  1.00  0.00
ATOM   1359  CE3 TRP A  89      79.541  71.292  52.152  1.00  0.00
ATOM   1360  HE3 TRP A  89      79.176  70.506  52.795  1.00  0.00
ATOM   1361  CZ3 TRP A  89      80.915  71.432  51.946  1.00  0.00
ATOM   1362  HZ3 TRP A  89      81.599  70.748  52.430  1.00  0.00
ATOM   1363  CZ2 TRP A  89      80.565  73.345  50.497  1.00  0.00
ATOM   1364  HZ2 TRP A  89      80.969  74.126  49.871  1.00  0.00
ATOM   1365  CH2 TRP A  89      81.418  72.441  51.131  1.00  0.00
ATOM   1366  HH2 TRP A  89      82.487  72.529  50.989  1.00  0.00
ATOM   1367  C   TRP A  89      77.075  69.207  51.100  1.00  0.00
ATOM   1368  O   TRP A  89      77.684  69.322  50.037  1.00  0.00
ATOM   1369  N   PRO A  90      77.474  68.273  51.986  1.00  0.00
ATOM   1370  CD  PRO A  90      77.070  68.214  53.395  1.00  0.00
ATOM   1371  HD1 PRO A  90      76.233  67.488  53.483  1.00  0.00
ATOM   1372  HD2 PRO A  90      76.760  69.199  53.796  1.00  0.00
ATOM   1373  CA  PRO A  90      78.639  67.431  51.746  1.00  0.00
ATOM   1374  HA  PRO A  90      79.458  68.058  51.416  1.00  0.00
ATOM   1375  CB  PRO A  90      78.928  66.747  53.095  1.00  0.00
ATOM   1376  HB1 PRO A  90      80.015  66.605  53.257  1.00  0.00
ATOM   1377  HB2 PRO A  90      78.417  65.762  53.180  1.00  0.00
ATOM   1378  CG  PRO A  90      78.308  67.694  54.125  1.00  0.00
ATOM   1379  HG1 PRO A  90      78.061  67.186  55.079  1.00  0.00
ATOM   1380  HG2 PRO A  90      79.006  68.537  54.321  1.00  0.00
ATOM   1381  C   PRO A  90      78.338  66.411  50.684  1.00  0.00
ATOM   1382  O   PRO A  90      79.235  66.078  49.915  1.00  0.00
ATOM   1383  N   SER A  91      77.111  65.884  50.668  1.00  0.00
ATOM   1384  HN  SER A  91      76.429  66.190  51.328  1.00  0.00
ATOM   1385  CA  SER A  91      76.652  64.902  49.709  1.00  0.00
ATOM   1386  HA  SER A  91      77.328  64.059  49.753  1.00  0.00
ATOM   1387  CB  SER A  91      75.221  64.424  50.067  1.00  0.00
ATOM   1388  HB1 SER A  91      74.894  63.644  49.347  1.00  0.00
ATOM   1389  HB2 SER A  91      74.497  65.265  50.030  1.00  0.00
ATOM   1390  OG  SER A  91      75.183  63.846  51.367  1.00  0.00
ATOM   1391  HG  SER A  91      75.300  64.564  51.994  1.00  0.00
ATOM   1392  C   SER A  91      76.655  65.429  48.291  1.00  0.00
ATOM   1393  O   SER A  91      77.101  64.746  47.372  1.00  0.00
ATOM   1394  N   VAL A  92      76.172  66.661  48.103  1.00  0.00
ATOM   1395  HN  VAL A  92      75.784  67.169  48.870  1.00  0.00
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ATOM   1396  CA  VAL A  92      76.165  67.381  46.842  1.00  0.00
ATOM   1397  HA  VAL A  92      75.713  66.730  46.106  1.00  0.00
ATOM   1398  CB  VAL A  92      75.310  68.648  46.927  1.00  0.00
ATOM   1399  HB  VAL A  92      75.560  69.197  47.863  1.00  0.00
ATOM   1400  CG1 VAL A  92      75.540  69.609  45.737  1.00  0.00
ATOM   1401 HG11 VAL A  92      75.385  69.079  44.775  1.00  0.00
ATOM   1402 HG12 VAL A  92      76.562  70.039  45.752  1.00  0.00
ATOM   1403 HG13 VAL A  92      74.819  70.452  45.790  1.00  0.00
ATOM   1404  CG2 VAL A  92      73.826  68.219  46.988  1.00  0.00
ATOM   1405 HG21 VAL A  92      73.636  67.537  47.841  1.00  0.00
ATOM   1406 HG22 VAL A  92      73.540  67.694  46.053  1.00  0.00
ATOM   1407 HG23 VAL A  92      73.175  69.111  47.103  1.00  0.00
ATOM   1408  C   VAL A  92      77.565  67.672  46.354  1.00  0.00
ATOM   1409  O   VAL A  92      77.868  67.476  45.179  1.00  0.00
ATOM   1410  N   SER A  93      78.443  68.119  47.258  1.00  0.00
ATOM   1411  HN  SER A  93      78.160  68.270  48.203  1.00  0.00
ATOM   1412  CA  SER A  93      79.832  68.424  46.973  1.00  0.00
ATOM   1413  HA  SER A  93      79.841  69.129  46.154  1.00  0.00
ATOM   1414  CB  SER A  93      80.485  69.094  48.211  1.00  0.00
ATOM   1415  HB1 SER A  93      79.880  69.977  48.509  1.00  0.00
ATOM   1416  HB2 SER A  93      80.498  68.386  49.067  1.00  0.00
ATOM   1417  OG  SER A  93      81.814  69.535  47.950  1.00  0.00
ATOM   1418  HG  SER A  93      81.743  70.247  47.310  1.00  0.00
ATOM   1419  C   SER A  93      80.614  67.198  46.543  1.00  0.00
ATOM   1420  O   SER A  93      81.395  67.250  45.596  1.00  0.00
ATOM   1421  N   LEU A  94      80.389  66.071  47.223  1.00  0.00
ATOM   1422  HN  LEU A  94      79.775  66.074  48.011  1.00  0.00
ATOM   1423  CA  LEU A  94      80.950  64.777  46.901  1.00  0.00
ATOM   1424  HA  LEU A  94      82.024  64.891  46.874  1.00  0.00
ATOM   1425  CB  LEU A  94      80.569  63.756  48.006  1.00  0.00
ATOM   1426  HB1 LEU A  94      80.965  64.135  48.974  1.00  0.00
ATOM   1427  HB2 LEU A  94      79.461  63.722  48.097  1.00  0.00
ATOM   1428  CG  LEU A  94      81.080  62.307  47.812  1.00  0.00
ATOM   1429  HG  LEU A  94      80.667  61.921  46.854  1.00  0.00
ATOM   1430  CD1 LEU A  94      82.614  62.226  47.712  1.00  0.00
ATOM   1431 HD11 LEU A  94      82.934  61.173  47.563  1.00  0.00
ATOM   1432 HD12 LEU A  94      82.988  62.828  46.858  1.00  0.00
ATOM   1433 HD13 LEU A  94      83.074  62.607  48.647  1.00  0.00
ATOM   1434  CD2 LEU A  94      80.553  61.382  48.926  1.00  0.00
ATOM   1435 HD21 LEU A  94      80.873  60.334  48.742  1.00  0.00
ATOM   1436 HD22 LEU A  94      80.944  61.705  49.914  1.00  0.00
ATOM   1437 HD23 LEU A  94      79.443  61.409  48.958  1.00  0.00
ATOM   1438  C   LEU A  94      80.498  64.278  45.549  1.00  0.00
ATOM   1439  O   LEU A  94      81.293  63.748  44.777  1.00  0.00
ATOM   1440  N   ALA A  95      79.211  64.452  45.245  1.00  0.00
ATOM   1441  HN  ALA A  95      78.585  64.867  45.903  1.00  0.00
ATOM   1442  CA  ALA A  95      78.610  64.073  43.988  1.00  0.00
ATOM   1443  HA  ALA A  95      78.819  63.024  43.841  1.00  0.00
ATOM   1444  CB  ALA A  95      77.083  64.248  44.032  1.00  0.00
ATOM   1445  HB1 ALA A  95      76.660  63.658  44.874  1.00  0.00
ATOM   1446  HB2 ALA A  95      76.801  65.311  44.181  1.00  0.00
ATOM   1447  HB3 ALA A  95      76.621  63.883  43.091  1.00  0.00
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ATOM   1448  C   ALA A  95      79.174  64.821  42.800  1.00  0.00
ATOM   1449  O   ALA A  95      79.483  64.219  41.776  1.00  0.00
ATOM   1450  N   THR A  96      79.345  66.142  42.924  1.00  0.00
ATOM   1451  HN  THR A  96      79.068  66.627  43.753  1.00  0.00
ATOM   1452  CA  THR A  96      79.964  66.964  41.896  1.00  0.00
ATOM   1453  HA  THR A  96      79.453  66.737  40.970  1.00  0.00
ATOM   1454  CB  THR A  96      79.816  68.469  42.121  1.00  0.00
ATOM   1455  HB  THR A  96      80.455  69.046  41.413  1.00  0.00
ATOM   1456  OG1 THR A  96      80.151  68.852  43.450  1.00  0.00
ATOM   1457  HG1 THR A  96      81.063  68.586  43.593  1.00  0.00
ATOM   1458  CG2 THR A  96      78.350  68.863  41.854  1.00  0.00
ATOM   1459 HG21 THR A  96      77.666  68.334  42.550  1.00  0.00
ATOM   1460 HG22 THR A  96      78.067  68.606  40.812  1.00  0.00
ATOM   1461 HG23 THR A  96      78.213  69.957  41.992  1.00  0.00
ATOM   1462  C   THR A  96      81.420  66.615  41.667  1.00  0.00
ATOM   1463  O   THR A  96      81.868  66.509  40.526  1.00  0.00
ATOM   1464  N   LEU A  97      82.167  66.421  42.757  1.00  0.00
ATOM   1465  HN  LEU A  97      81.759  66.501  43.665  1.00  0.00
ATOM   1466  CA  LEU A  97      83.577  66.094  42.763  1.00  0.00
ATOM   1467  HA  LEU A  97      84.090  66.857  42.195  1.00  0.00
ATOM   1468  CB  LEU A  97      84.092  66.106  44.229  1.00  0.00
ATOM   1469  HB1 LEU A  97      83.467  65.408  44.830  1.00  0.00
ATOM   1470  HB2 LEU A  97      83.928  67.127  44.639  1.00  0.00
ATOM   1471  CG  LEU A  97      85.578  65.734  44.461  1.00  0.00
ATOM   1472  HG  LEU A  97      85.751  64.702  44.078  1.00  0.00
ATOM   1473  CD1 LEU A  97      86.540  66.678  43.713  1.00  0.00
ATOM   1474 HD11 LEU A  97      86.395  67.725  44.056  1.00  0.00
ATOM   1475 HD12 LEU A  97      86.361  66.635  42.619  1.00  0.00
ATOM   1476 HD13 LEU A  97      87.593  66.385  43.907  1.00  0.00
ATOM   1477  CD2 LEU A  97      85.896  65.703  45.970  1.00  0.00
ATOM   1478 HD21 LEU A  97      85.230  64.982  46.490  1.00  0.00
ATOM   1479 HD22 LEU A  97      85.746  66.709  46.416  1.00  0.00
ATOM   1480 HD23 LEU A  97      86.950  65.394  46.136  1.00  0.00
ATOM   1481  C   LEU A  97      83.883  64.756  42.133  1.00  0.00
ATOM   1482  O   LEU A  97      84.827  64.625  41.356  1.00  0.00
ATOM   1483  N   GLY A  98      83.084  63.744  42.468  1.00  0.00
ATOM   1484  HN  GLY A  98      82.308  63.894  43.080  1.00  0.00
ATOM   1485  CA  GLY A  98      83.337  62.368  42.117  1.00  0.00
ATOM   1486  HA1 GLY A  98      82.921  61.767  42.912  1.00  0.00
ATOM   1487  HA2 GLY A  98      84.399  62.209  41.990  1.00  0.00
ATOM   1488  C   GLY A  98      82.644  61.992  40.846  1.00  0.00
ATOM   1489  O   GLY A  98      83.296  61.665  39.857  1.00  0.00
ATOM   1490  N   VAL A  99      81.308  61.974  40.870  1.00  0.00
ATOM   1491  HN  VAL A  99      80.809  62.314  41.663  1.00  0.00
ATOM   1492  CA  VAL A  99      80.479  61.380  39.840  1.00  0.00
ATOM   1493  HA  VAL A  99      80.801  60.353  39.751  1.00  0.00
ATOM   1494  CB  VAL A  99      78.999  61.345  40.226  1.00  0.00
ATOM   1495  HB  VAL A  99      78.602  62.376  40.351  1.00  0.00
ATOM   1496  CG1 VAL A  99      78.155  60.647  39.138  1.00  0.00
ATOM   1497 HG11 VAL A  99      77.127  60.476  39.522  1.00  0.00
ATOM   1498 HG12 VAL A  99      78.079  61.266  38.221  1.00  0.00
ATOM   1499 HG13 VAL A  99      78.602  59.669  38.866  1.00  0.00
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ATOM   1500  CG2 VAL A  99      78.857  60.608  41.572  1.00  0.00
ATOM   1501 HG21 VAL A  99      77.782  60.496  41.826  1.00  0.00
ATOM   1502 HG22 VAL A  99      79.312  59.597  41.517  1.00  0.00
ATOM   1503 HG23 VAL A  99      79.343  61.178  42.389  1.00  0.00
ATOM   1504  C   VAL A  99      80.624  62.007  38.473  1.00  0.00
ATOM   1505  O   VAL A  99      80.803  61.300  37.486  1.00  0.00
ATOM   1506  N   ALA A 100      80.581  63.339  38.395  1.00  0.00
ATOM   1507  HN  ALA A 100      80.455  63.902  39.209  1.00  0.00
ATOM   1508  CA  ALA A 100      80.675  64.054  37.136  1.00  0.00
ATOM   1509  HA  ALA A 100      79.902  63.668  36.485  1.00  0.00
ATOM   1510  CB  ALA A 100      80.438  65.564  37.334  1.00  0.00
ATOM   1511  HB1 ALA A 100      79.443  65.729  37.801  1.00  0.00
ATOM   1512  HB2 ALA A 100      81.210  66.005  37.999  1.00  0.00
ATOM   1513  HB3 ALA A 100      80.456  66.100  36.361  1.00  0.00
ATOM   1514  C   ALA A 100      82.007  63.854  36.453  1.00  0.00
ATOM   1515  O   ALA A 100      82.067  63.612  35.248  1.00  0.00
ATOM   1516  N   VAL A 101      83.090  63.928  37.231  1.00  0.00
ATOM   1517  HN  VAL A 101      82.994  64.129  38.203  1.00  0.00
ATOM   1518  CA  VAL A 101      84.452  63.716  36.790  1.00  0.00
ATOM   1519  HA  VAL A 101      84.624  64.371  35.947  1.00  0.00
ATOM   1520  CB  VAL A 101      85.445  64.079  37.894  1.00  0.00
ATOM   1521  HB  VAL A 101      85.234  63.477  38.807  1.00  0.00
ATOM   1522  CG1 VAL A 101      86.901  63.803  37.456  1.00  0.00
ATOM   1523 HG11 VAL A 101      87.120  64.314  36.495  1.00  0.00
ATOM   1524 HG12 VAL A 101      87.085  62.716  37.338  1.00  0.00
ATOM   1525 HG13 VAL A 101      87.605  64.184  38.226  1.00  0.00
ATOM   1526  CG2 VAL A 101      85.255  65.570  38.252  1.00  0.00
ATOM   1527 HG21 VAL A 101      84.246  65.763  38.673  1.00  0.00
ATOM   1528 HG22 VAL A 101      85.396  66.205  37.352  1.00  0.00
ATOM   1529 HG23 VAL A 101      86.003  65.873  39.015  1.00  0.00
ATOM   1530  C   VAL A 101      84.669  62.296  36.314  1.00  0.00
ATOM   1531  O   VAL A 101      85.245  62.076  35.252  1.00  0.00
ATOM   1532  N   THR A 102      84.178  61.315  37.078  1.00  0.00
ATOM   1533  HN  THR A 102      83.711  61.530  37.935  1.00  0.00
ATOM   1534  CA  THR A 102      84.315  59.898  36.784  1.00  0.00
ATOM   1535  HA  THR A 102      85.372  59.732  36.628  1.00  0.00
ATOM   1536  CB  THR A 102      83.909  59.000  37.959  1.00  0.00
ATOM   1537  HB  THR A 102      84.429  59.368  38.872  1.00  0.00
ATOM   1538  OG1 THR A 102      82.511  59.021  38.228  1.00  0.00
ATOM   1539  HG1 THR A 102      82.277  59.943  38.363  1.00  0.00
ATOM   1540  CG2 THR A 102      84.355  57.542  37.718  1.00  0.00
ATOM   1541 HG21 THR A 102      85.446  57.501  37.515  1.00  0.00
ATOM   1542 HG22 THR A 102      83.818  57.095  36.855  1.00  0.00
ATOM   1543 HG23 THR A 102      84.144  56.922  38.616  1.00  0.00
ATOM   1544  C   THR A 102      83.622  59.512  35.494  1.00  0.00
ATOM   1545  O   THR A 102      84.176  58.764  34.695  1.00  0.00
ATOM   1546  N   THR A 103      82.422  60.052  35.264  1.00  0.00
ATOM   1547  HN  THR A 103      82.006  60.650  35.947  1.00  0.00
ATOM   1548  CA  THR A 103      81.622  59.844  34.071  1.00  0.00
ATOM   1549  HA  THR A 103      81.512  58.775  33.956  1.00  0.00
ATOM   1550  CB  THR A 103      80.209  60.416  34.234  1.00  0.00
ATOM   1551  HB  THR A 103      80.275  61.435  34.676  1.00  0.00
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ATOM   1552  OG1 THR A 103      79.496  60.525  33.008  1.00  0.00
ATOM   1553  HG1 THR A 103      78.677  60.982  33.215  1.00  0.00
ATOM   1554  CG2 THR A 103      79.403  59.498  35.175  1.00  0.00
ATOM   1555 HG21 THR A 103      79.922  59.361  36.145  1.00  0.00
ATOM   1556 HG22 THR A 103      79.270  58.499  34.710  1.00  0.00
ATOM   1557 HG23 THR A 103      78.398  59.929  35.374  1.00  0.00
ATOM   1558  C   THR A 103      82.324  60.335  32.815  1.00  0.00
ATOM   1559  O   THR A 103      82.315  59.662  31.784  1.00  0.00
ATOM   1560  N   LEU A 104      82.958  61.508  32.893  1.00  0.00
ATOM   1561  HN  LEU A 104      82.935  62.052  33.729  1.00  0.00
ATOM   1562  CA  LEU A 104      83.754  62.052  31.813  1.00  0.00
ATOM   1563  HA  LEU A 104      83.123  62.082  30.937  1.00  0.00
ATOM   1564  CB  LEU A 104      84.195  63.496  32.166  1.00  0.00
ATOM   1565  HB1 LEU A 104      84.771  63.480  33.116  1.00  0.00
ATOM   1566  HB2 LEU A 104      83.276  64.096  32.349  1.00  0.00
ATOM   1567  CG  LEU A 104      85.044  64.232  31.097  1.00  0.00
ATOM   1568  HG  LEU A 104      85.995  63.667  30.954  1.00  0.00
ATOM   1569  CD1 LEU A 104      84.339  64.306  29.728  1.00  0.00
ATOM   1570 HD11 LEU A 104      83.368  64.836  29.824  1.00  0.00
ATOM   1571 HD12 LEU A 104      84.151  63.290  29.324  1.00  0.00
ATOM   1572 HD13 LEU A 104      84.972  64.856  29.000  1.00  0.00
ATOM   1573  CD2 LEU A 104      85.433  65.639  31.589  1.00  0.00
ATOM   1574 HD21 LEU A 104      85.988  65.573  32.549  1.00  0.00
ATOM   1575 HD22 LEU A 104      84.524  66.257  31.747  1.00  0.00
ATOM   1576 HD23 LEU A 104      86.080  66.145  30.840  1.00  0.00
ATOM   1577  C   LEU A 104      84.961  61.195  31.489  1.00  0.00
ATOM   1578  O   LEU A 104      85.230  60.904  30.325  1.00  0.00
ATOM   1579  N   LEU A 105      85.681  60.749  32.523  1.00  0.00
ATOM   1580  HN  LEU A 105      85.432  61.000  33.457  1.00  0.00
ATOM   1581  CA  LEU A 105      86.854  59.907  32.406  1.00  0.00
ATOM   1582  HA  LEU A 105      87.537  60.408  31.735  1.00  0.00
ATOM   1583  CB  LEU A 105      87.537  59.730  33.785  1.00  0.00
ATOM   1584  HB1 LEU A 105      88.310  58.931  33.734  1.00  0.00
ATOM   1585  HB2 LEU A 105      86.770  59.410  34.524  1.00  0.00
ATOM   1586  CG  LEU A 105      88.245  61.002  34.316  1.00  0.00
ATOM   1587  HG  LEU A 105      87.523  61.849  34.279  1.00  0.00
ATOM   1588  CD1 LEU A 105      88.658  60.818  35.789  1.00  0.00
ATOM   1589 HD11 LEU A 105      89.387  59.986  35.884  1.00  0.00
ATOM   1590 HD12 LEU A 105      87.769  60.584  36.412  1.00  0.00
ATOM   1591 HD13 LEU A 105      89.127  61.747  36.176  1.00  0.00
ATOM   1592  CD2 LEU A 105      89.459  61.406  33.455  1.00  0.00
ATOM   1593 HD21 LEU A 105      89.149  61.638  32.416  1.00  0.00
ATOM   1594 HD22 LEU A 105      90.204  60.583  33.429  1.00  0.00
ATOM   1595 HD23 LEU A 105      89.945  62.309  33.880  1.00  0.00
ATOM   1596  C   LEU A 105      86.581  58.555  31.796  1.00  0.00
ATOM   1597  O   LEU A 105      87.363  58.086  30.976  1.00  0.00
ATOM   1598  N   THR A 106      85.466  57.920  32.171  1.00  0.00
ATOM   1599  HN  THR A 106      84.857  58.319  32.857  1.00  0.00
ATOM   1600  CA  THR A 106      85.038  56.631  31.652  1.00  0.00
ATOM   1601  HA  THR A 106      85.875  55.958  31.784  1.00  0.00
ATOM   1602  CB  THR A 106      83.856  56.009  32.395  1.00  0.00
ATOM   1603  HB  THR A 106      83.421  55.160  31.826  1.00  0.00
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ATOM   1604  OG1 THR A 106      82.813  56.943  32.634  1.00  0.00
ATOM   1605  HG1 THR A 106      82.554  57.296  31.779  1.00  0.00
ATOM   1606  CG2 THR A 106      84.354  55.463  33.751  1.00  0.00
ATOM   1607 HG21 THR A 106      84.774  56.277  34.378  1.00  0.00
ATOM   1608 HG22 THR A 106      85.145  54.700  33.595  1.00  0.00
ATOM   1609 HG23 THR A 106      83.518  54.987  34.306  1.00  0.00
ATOM   1610  C   THR A 106      84.758  56.653  30.165  1.00  0.00
ATOM   1611  O   THR A 106      85.044  55.688  29.458  1.00  0.00
ATOM   1612  N   GLY A 107      84.199  57.761  29.669  1.00  0.00
ATOM   1613  HN  GLY A 107      83.981  58.534  30.261  1.00  0.00
ATOM   1614  CA  GLY A 107      83.896  57.938  28.266  1.00  0.00
ATOM   1615  HA1 GLY A 107      83.317  58.846  28.188  1.00  0.00
ATOM   1616  HA2 GLY A 107      83.361  57.064  27.922  1.00  0.00
ATOM   1617  C   GLY A 107      85.125  58.102  27.417  1.00  0.00
ATOM   1618  O   GLY A 107      85.194  57.577  26.306  1.00  0.00
ATOM   1619  N   LEU A 108      86.124  58.827  27.927  1.00  0.00
ATOM   1620  HN  LEU A 108      86.044  59.255  28.826  1.00  0.00
ATOM   1621  CA  LEU A 108      87.364  59.069  27.221  1.00  0.00
ATOM   1622  HA  LEU A 108      87.145  59.203  26.171  1.00  0.00
ATOM   1623  CB  LEU A 108      88.037  60.354  27.763  1.00  0.00
ATOM   1624  HB1 LEU A 108      89.017  60.505  27.258  1.00  0.00
ATOM   1625  HB2 LEU A 108      88.226  60.233  28.853  1.00  0.00
ATOM   1626  CG  LEU A 108      87.195  61.640  27.553  1.00  0.00
ATOM   1627  HG  LEU A 108      86.205  61.495  28.043  1.00  0.00
ATOM   1628  CD1 LEU A 108      87.849  62.854  28.240  1.00  0.00
ATOM   1629 HD11 LEU A 108      88.842  63.063  27.790  1.00  0.00
ATOM   1630 HD12 LEU A 108      87.983  62.658  29.325  1.00  0.00
ATOM   1631 HD13 LEU A 108      87.209  63.754  28.122  1.00  0.00
ATOM   1632  CD2 LEU A 108      86.919  61.935  26.064  1.00  0.00
ATOM   1633 HD21 LEU A 108      86.338  61.112  25.599  1.00  0.00
ATOM   1634 HD22 LEU A 108      87.873  62.055  25.511  1.00  0.00
ATOM   1635 HD23 LEU A 108      86.330  62.871  25.962  1.00  0.00
ATOM   1636  C   LEU A 108      88.305  57.889  27.327  1.00  0.00
ATOM   1637  O   LEU A 108      89.122  57.663  26.436  1.00  0.00
ATOM   1638  N   LEU A 109      88.170  57.093  28.392  1.00  0.00
ATOM   1639  HN  LEU A 109      87.540  57.341  29.126  1.00  0.00
ATOM   1640  CA  LEU A 109      88.847  55.825  28.581  1.00  0.00
ATOM   1641  HA  LEU A 109      89.909  56.003  28.484  1.00  0.00
ATOM   1642  CB  LEU A 109      88.547  55.270  29.999  1.00  0.00
ATOM   1643  HB1 LEU A 109      87.447  55.266  30.153  1.00  0.00
ATOM   1644  HB2 LEU A 109      88.979  55.975  30.741  1.00  0.00
ATOM   1645  CG  LEU A 109      89.067  53.845  30.322  1.00  0.00
ATOM   1646  HG  LEU A 109      88.583  53.125  29.620  1.00  0.00
ATOM   1647  CD1 LEU A 109      90.593  53.716  30.148  1.00  0.00
ATOM   1648 HD11 LEU A 109      91.119  54.417  30.830  1.00  0.00
ATOM   1649 HD12 LEU A 109      90.891  53.945  29.104  1.00  0.00
ATOM   1650 HD13 LEU A 109      90.917  52.680  30.383  1.00  0.00
ATOM   1651  CD2 LEU A 109      88.640  53.423  31.742  1.00  0.00
ATOM   1652 HD21 LEU A 109      87.537  53.488  31.846  1.00  0.00
ATOM   1653 HD22 LEU A 109      89.107  54.090  32.498  1.00  0.00
ATOM   1654 HD23 LEU A 109      88.954  52.378  31.944  1.00  0.00
ATOM   1655  C   LEU A 109      88.446  54.815  27.534  1.00  0.00
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ATOM   1656  O   LEU A 109      89.291  54.118  26.981  1.00  0.00
ATOM   1657  N   ALA A 110      87.147  54.741  27.233  1.00  0.00
ATOM   1658  HN  ALA A 110      86.482  55.306  27.716  1.00  0.00
ATOM   1659  CA  ALA A 110      86.594  53.880  26.210  1.00  0.00
ATOM   1660  HA  ALA A 110      86.897  52.868  26.439  1.00  0.00
ATOM   1661  CB  ALA A 110      85.055  53.946  26.199  1.00  0.00
ATOM   1662  HB1 ALA A 110      84.698  54.970  25.959  1.00  0.00
ATOM   1663  HB2 ALA A 110      84.660  53.672  27.201  1.00  0.00
ATOM   1664  HB3 ALA A 110      84.632  53.237  25.456  1.00  0.00
ATOM   1665  C   ALA A 110      87.102  54.218  24.828  1.00  0.00
ATOM   1666  O   ALA A 110      87.433  53.328  24.048  1.00  0.00
ATOM   1667  N   MET A 111      87.183  55.517  24.521  1.00  0.00
ATOM   1668  HN  MET A 111      86.897  56.203  25.186  1.00  0.00
ATOM   1669  CA  MET A 111      87.667  56.057  23.265  1.00  0.00
ATOM   1670  HA  MET A 111      87.083  55.607  22.474  1.00  0.00
ATOM   1671  CB  MET A 111      87.448  57.594  23.262  1.00  0.00
ATOM   1672  HB1 MET A 111      86.475  57.777  23.777  1.00  0.00
ATOM   1673  HB2 MET A 111      88.225  58.117  23.859  1.00  0.00
ATOM   1674  CG  MET A 111      87.310  58.236  21.865  1.00  0.00
ATOM   1675  HG1 MET A 111      86.561  57.650  21.288  1.00  0.00
ATOM   1676  HG2 MET A 111      86.881  59.253  22.010  1.00  0.00
ATOM   1677  SD  MET A 111      88.851  58.387  20.909  1.00  0.00
ATOM   1678  CE  MET A 111      88.071  59.148  19.456  1.00  0.00
ATOM   1679  HE1 MET A 111      88.826  59.361  18.670  1.00  0.00
ATOM   1680  HE2 MET A 111      87.302  58.475  19.019  1.00  0.00
ATOM   1681  HE3 MET A 111      87.577  60.106  19.726  1.00  0.00
ATOM   1682  C   MET A 111      89.128  55.704  23.056  1.00  0.00
ATOM   1683  O   MET A 111      89.527  55.299  21.967  1.00  0.00
ATOM   1684  N   TRP A 112      89.939  55.829  24.111  1.00  0.00
ATOM   1685  HN  TRP A 112      89.588  56.190  24.973  1.00  0.00
ATOM   1686  CA  TRP A 112      91.334  55.437  24.137  1.00  0.00
ATOM   1687  HA  TRP A 112      91.824  55.943  23.317  1.00  0.00
ATOM   1688  CB  TRP A 112      91.983  55.936  25.472  1.00  0.00
ATOM   1689  HB1 TRP A 112      92.092  57.040  25.405  1.00  0.00
ATOM   1690  HB2 TRP A 112      91.254  55.738  26.288  1.00  0.00
ATOM   1691  CG  TRP A 112      93.304  55.343  25.875  1.00  0.00
ATOM   1692  CD1 TRP A 112      93.538  54.542  26.963  1.00  0.00
ATOM   1693  HD1 TRP A 112      92.803  54.292  27.714  1.00  0.00
ATOM   1694  NE1 TRP A 112      94.828  54.087  26.935  1.00  0.00
ATOM   1695  HE1 TRP A 112      95.235  53.486  27.587  1.00  0.00
ATOM   1696  CE2 TRP A 112      95.461  54.573  25.826  1.00  0.00
ATOM   1697  CD2 TRP A 112      94.530  55.375  25.126  1.00  0.00
ATOM   1698  CE3 TRP A 112      94.912  55.983  23.931  1.00  0.00
ATOM   1699  HE3 TRP A 112      94.223  56.594  23.367  1.00  0.00
ATOM   1700  CZ3 TRP A 112      96.211  55.782  23.458  1.00  0.00
ATOM   1701  HZ3 TRP A 112      96.516  56.244  22.529  1.00  0.00
ATOM   1702  CZ2 TRP A 112      96.754  54.375  25.358  1.00  0.00
ATOM   1703  HZ2 TRP A 112      97.463  53.757  25.888  1.00  0.00
ATOM   1704  CH2 TRP A 112      97.117  54.992  24.160  1.00  0.00
ATOM   1705  HH2 TRP A 112      98.115  54.850  23.770  1.00  0.00
ATOM   1706  C   TRP A 112      91.573  53.949  23.939  1.00  0.00
ATOM   1707  O   TRP A 112      92.459  53.550  23.185  1.00  0.00
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ATOM   1708  N   LEU A 113      90.797  53.116  24.633  1.00  0.00
ATOM   1709  HN  LEU A 113      90.048  53.463  25.195  1.00  0.00
ATOM   1710  CA  LEU A 113      91.103  51.713  24.807  1.00  0.00
ATOM   1711  HA  LEU A 113      92.178  51.605  24.852  1.00  0.00
ATOM   1712  CB  LEU A 113      90.477  51.232  26.145  1.00  0.00
ATOM   1713  HB1 LEU A 113      89.368  51.272  26.065  1.00  0.00
ATOM   1714  HB2 LEU A 113      90.775  51.962  26.932  1.00  0.00
ATOM   1715  CG  LEU A 113      90.897  49.832  26.654  1.00  0.00
ATOM   1716  HG  LEU A 113      90.632  49.077  25.880  1.00  0.00
ATOM   1717  CD1 LEU A 113      92.415  49.738  26.909  1.00  0.00
ATOM   1718 HD11 LEU A 113      92.727  50.496  27.658  1.00  0.00
ATOM   1719 HD12 LEU A 113      92.983  49.911  25.971  1.00  0.00
ATOM   1720 HD13 LEU A 113      92.679  48.731  27.295  1.00  0.00
ATOM   1721  CD2 LEU A 113      90.108  49.458  27.925  1.00  0.00
ATOM   1722 HD21 LEU A 113      89.017  49.469  27.718  1.00  0.00
ATOM   1723 HD22 LEU A 113      90.321  50.182  28.740  1.00  0.00
ATOM   1724 HD23 LEU A 113      90.392  48.442  28.270  1.00  0.00
ATOM   1725  C   LEU A 113      90.583  50.855  23.678  1.00  0.00
ATOM   1726  O   LEU A 113      91.077  49.751  23.453  1.00  0.00
ATOM   1727  N   PHE A 114      89.599  51.359  22.934  1.00  0.00
ATOM   1728  HN  PHE A 114      89.247  52.279  23.096  1.00  0.00
ATOM   1729  CA  PHE A 114      88.917  50.607  21.906  1.00  0.00
ATOM   1730  HA  PHE A 114      89.476  49.718  21.644  1.00  0.00
ATOM   1731  CB  PHE A 114      87.469  50.251  22.350  1.00  0.00
ATOM   1732  HB1 PHE A 114      86.938  49.682  21.556  1.00  0.00
ATOM   1733  HB2 PHE A 114      86.907  51.187  22.553  1.00  0.00
ATOM   1734  CG  PHE A 114      87.442  49.399  23.596  1.00  0.00
ATOM   1735  CD1 PHE A 114      86.687  49.790  24.719  1.00  0.00
ATOM   1736  HD1 PHE A 114      86.147  50.725  24.704  1.00  0.00
ATOM   1737  CE1 PHE A 114      86.614  48.970  25.852  1.00  0.00
ATOM   1738  HE1 PHE A 114      86.020  49.272  26.702  1.00  0.00
ATOM   1739  CZ  PHE A 114      87.302  47.752  25.880  1.00  0.00
ATOM   1740  HZ  PHE A 114      87.244  47.119  26.752  1.00  0.00
ATOM   1741  CD2 PHE A 114      88.125  48.170  23.638  1.00  0.00
ATOM   1742  HD2 PHE A 114      88.700  47.845  22.783  1.00  0.00
ATOM   1743  CE2 PHE A 114      88.062  47.353  24.774  1.00  0.00
ATOM   1744  HE2 PHE A 114      88.592  46.412  24.794  1.00  0.00
ATOM   1745  C   PHE A 114      88.829  51.476  20.687  1.00  0.00
ATOM   1746  O   PHE A 114      89.031  52.686  20.754  1.00  0.00
ATOM   1747  N   ASN A 115      88.522  50.866  19.539  1.00  0.00
ATOM   1748  HN  ASN A 115      88.386  49.879  19.499  1.00  0.00
ATOM   1749  CA  ASN A 115      88.294  51.575  18.298  1.00  0.00
ATOM   1750  HA  ASN A 115      88.915  52.460  18.261  1.00  0.00
ATOM   1751  CB  ASN A 115      88.589  50.655  17.082  1.00  0.00
ATOM   1752  HB1 ASN A 115      88.404  51.199  16.132  1.00  0.00
ATOM   1753  HB2 ASN A 115      87.933  49.757  17.107  1.00  0.00
ATOM   1754  CG  ASN A 115      90.045  50.167  17.100  1.00  0.00
ATOM   1755  OD1 ASN A 115      90.299  48.958  17.093  1.00  0.00
ATOM   1756  ND2 ASN A 115      91.012  51.129  17.143  1.00  0.00
ATOM   1757 HD21 ASN A 115      91.973  50.858  17.162  1.00  0.00
ATOM   1758 HD22 ASN A 115      90.757  52.095  17.159  1.00  0.00
ATOM   1759  C   ASN A 115      86.845  51.992  18.297  1.00  0.00
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ATOM   1760  O   ASN A 115      85.967  51.245  17.869  1.00  0.00
ATOM   1761  N   LEU A 116      86.582  53.192  18.811  1.00  0.00
ATOM   1762  HN  LEU A 116      87.317  53.781  19.141  1.00  0.00
ATOM   1763  CA  LEU A 116      85.256  53.705  19.028  1.00  0.00
ATOM   1764  HA  LEU A 116      84.554  53.250  18.344  1.00  0.00
ATOM   1765  CB  LEU A 116      84.832  53.527  20.513  1.00  0.00
ATOM   1766  HB1 LEU A 116      83.937  54.146  20.731  1.00  0.00
ATOM   1767  HB2 LEU A 116      85.656  53.895  21.165  1.00  0.00
ATOM   1768  CG  LEU A 116      84.485  52.082  20.944  1.00  0.00
ATOM   1769  HG  LEU A 116      85.381  51.446  20.764  1.00  0.00
ATOM   1770  CD1 LEU A 116      84.174  52.031  22.453  1.00  0.00
ATOM   1771 HD11 LEU A 116      83.266  52.630  22.679  1.00  0.00
ATOM   1772 HD12 LEU A 116      85.022  52.446  23.037  1.00  0.00
ATOM   1773 HD13 LEU A 116      83.999  50.984  22.778  1.00  0.00
ATOM   1774  CD2 LEU A 116      83.318  51.480  20.137  1.00  0.00
ATOM   1775 HD21 LEU A 116      83.563  51.435  19.056  1.00  0.00
ATOM   1776 HD22 LEU A 116      82.402  52.093  20.269  1.00  0.00
ATOM   1777 HD23 LEU A 116      83.104  50.448  20.487  1.00  0.00
ATOM   1778  C   LEU A 116      85.308  55.176  18.741  1.00  0.00
ATOM   1779  O   LEU A 116      86.347  55.816  18.898  1.00  0.00
ATOM   1780  N   SER A 117      84.178  55.730  18.301  1.00  0.00
ATOM   1781  HN  SER A 117      83.350  55.188  18.181  1.00  0.00
ATOM   1782  CA  SER A 117      84.042  57.128  17.967  1.00  0.00
ATOM   1783  HA  SER A 117      84.998  57.496  17.618  1.00  0.00
ATOM   1784  CB  SER A 117      83.009  57.318  16.819  1.00  0.00
ATOM   1785  HB1 SER A 117      83.345  56.717  15.945  1.00  0.00
ATOM   1786  HB2 SER A 117      82.963  58.381  16.501  1.00  0.00
ATOM   1787  OG  SER A 117      81.700  56.885  17.177  1.00  0.00
ATOM   1788  HG  SER A 117      81.162  56.971  16.385  1.00  0.00
ATOM   1789  C   SER A 117      83.655  57.924  19.191  1.00  0.00
ATOM   1790  O   SER A 117      83.476  57.379  20.279  1.00  0.00
ATOM   1791  N   LEU A 118      83.541  59.245  19.023  1.00  0.00
ATOM   1792  HN  LEU A 118      83.708  59.650  18.128  1.00  0.00
ATOM   1793  CA  LEU A 118      83.208  60.201  20.055  1.00  0.00
ATOM   1794  HA  LEU A 118      83.965  60.121  20.822  1.00  0.00
ATOM   1795  CB  LEU A 118      83.229  61.631  19.451  1.00  0.00
ATOM   1796  HB1 LEU A 118      82.510  61.671  18.603  1.00  0.00
ATOM   1797  HB2 LEU A 118      84.243  61.811  19.030  1.00  0.00
ATOM   1798  CG  LEU A 118      82.900  62.797  20.418  1.00  0.00
ATOM   1799  HG  LEU A 118      81.883  62.632  20.844  1.00  0.00
ATOM   1800  CD1 LEU A 118      83.891  62.879  21.596  1.00  0.00
ATOM   1801 HD11 LEU A 118      84.924  63.036  21.218  1.00  0.00
ATOM   1802 HD12 LEU A 118      83.868  61.946  22.195  1.00  0.00
ATOM   1803 HD13 LEU A 118      83.626  63.728  22.261  1.00  0.00
ATOM   1804  CD2 LEU A 118      82.842  64.135  19.655  1.00  0.00
ATOM   1805 HD21 LEU A 118      82.083  64.085  18.846  1.00  0.00
ATOM   1806 HD22 LEU A 118      83.829  64.365  19.203  1.00  0.00
ATOM   1807 HD23 LEU A 118      82.567  64.961  20.345  1.00  0.00
ATOM   1808  C   LEU A 118      81.863  59.944  20.695  1.00  0.00
ATOM   1809  O   LEU A 118      81.735  60.003  21.915  1.00  0.00
ATOM   1810  N   LEU A 119      80.852  59.629  19.880  1.00  0.00
ATOM   1811  HN  LEU A 119      80.998  59.580  18.895  1.00  0.00
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ATOM   1812  CA  LEU A 119      79.501  59.333  20.315  1.00  0.00
ATOM   1813  HA  LEU A 119      79.173  60.174  20.910  1.00  0.00
ATOM   1814  CB  LEU A 119      78.569  59.175  19.086  1.00  0.00
ATOM   1815  HB1 LEU A 119      78.960  58.365  18.433  1.00  0.00
ATOM   1816  HB2 LEU A 119      78.610  60.121  18.503  1.00  0.00
ATOM   1817  CG  LEU A 119      77.082  58.874  19.411  1.00  0.00
ATOM   1818  HG  LEU A 119      77.031  57.897  19.946  1.00  0.00
ATOM   1819  CD1 LEU A 119      76.456  59.939  20.335  1.00  0.00
ATOM   1820 HD11 LEU A 119      76.443  60.929  19.833  1.00  0.00
ATOM   1821 HD12 LEU A 119      77.023  60.029  21.284  1.00  0.00
ATOM   1822 HD13 LEU A 119      75.416  59.656  20.594  1.00  0.00
ATOM   1823  CD2 LEU A 119      76.257  58.707  18.121  1.00  0.00
ATOM   1824 HD21 LEU A 119      76.692  57.909  17.483  1.00  0.00
ATOM   1825 HD22 LEU A 119      76.246  59.656  17.545  1.00  0.00
ATOM   1826 HD23 LEU A 119      75.210  58.430  18.366  1.00  0.00
ATOM   1827  C   LEU A 119      79.424  58.097  21.181  1.00  0.00
ATOM   1828  O   LEU A 119      78.652  58.039  22.136  1.00  0.00
ATOM   1829  N   GLN A 120      80.244  57.091  20.870  1.00  0.00
ATOM   1830  HN  GLN A 120      80.874  57.152  20.099  1.00  0.00
ATOM   1831  CA  GLN A 120      80.294  55.861  21.628  1.00  0.00
ATOM   1832  HA  GLN A 120      79.284  55.554  21.858  1.00  0.00
ATOM   1833  CB  GLN A 120      80.999  54.756  20.803  1.00  0.00
ATOM   1834  HB1 GLN A 120      81.041  53.827  21.417  1.00  0.00
ATOM   1835  HB2 GLN A 120      82.040  55.072  20.584  1.00  0.00
ATOM   1836  CG  GLN A 120      80.315  54.401  19.464  1.00  0.00
ATOM   1837  HG1 GLN A 120      80.725  53.444  19.080  1.00  0.00
ATOM   1838  HG2 GLN A 120      80.546  55.192  18.723  1.00  0.00
ATOM   1839  CD  GLN A 120      78.795  54.262  19.627  1.00  0.00
ATOM   1840  OE1 GLN A 120      78.320  53.374  20.343  1.00  0.00
ATOM   1841  NE2 GLN A 120      78.022  55.163  18.950  1.00  0.00
ATOM   1842 HE21 GLN A 120      77.027  55.109  19.025  1.00  0.00
ATOM   1843 HE22 GLN A 120      78.452  55.865  18.385  1.00  0.00
ATOM   1844  C   GLN A 120      81.019  56.047  22.943  1.00  0.00
ATOM   1845  O   GLN A 120      80.814  55.280  23.879  1.00  0.00
ATOM   1846  N   GLY A 121      81.836  57.100  23.050  1.00  0.00
ATOM   1847  HN  GLY A 121      82.012  57.688  22.263  1.00  0.00
ATOM   1848  CA  GLY A 121      82.449  57.518  24.292  1.00  0.00
ATOM   1849  HA1 GLY A 121      82.831  56.648  24.810  1.00  0.00
ATOM   1850  HA2 GLY A 121      83.221  58.229  24.035  1.00  0.00
ATOM   1851  C   GLY A 121      81.455  58.216  25.184  1.00  0.00
ATOM   1852  O   GLY A 121      81.449  58.006  26.395  1.00  0.00
ATOM   1853  N   VAL A 122      80.576  59.042  24.602  1.00  0.00
ATOM   1854  HN  VAL A 122      80.625  59.212  23.620  1.00  0.00
ATOM   1855  CA  VAL A 122      79.495  59.731  25.290  1.00  0.00
ATOM   1856  HA  VAL A 122      79.941  60.280  26.108  1.00  0.00
ATOM   1857  CB  VAL A 122      78.768  60.739  24.395  1.00  0.00
ATOM   1858  HB  VAL A 122      78.464  60.244  23.446  1.00  0.00
ATOM   1859  CG1 VAL A 122      79.746  61.884  24.056  1.00  0.00
ATOM   1860 HG11 VAL A 122      80.656  61.506  23.550  1.00  0.00
ATOM   1861 HG12 VAL A 122      80.055  62.412  24.983  1.00  0.00
ATOM   1862 HG13 VAL A 122      79.255  62.617  23.382  1.00  0.00
ATOM   1863  CG2 VAL A 122      77.494  61.309  25.066  1.00  0.00
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ATOM   1864 HG21 VAL A 122      77.741  61.746  26.056  1.00  0.00
ATOM   1865 HG22 VAL A 122      76.718  60.527  25.203  1.00  0.00
ATOM   1866 HG23 VAL A 122      77.058  62.108  24.430  1.00  0.00
ATOM   1867  C   VAL A 122      78.528  58.747  25.904  1.00  0.00
ATOM   1868  O   VAL A 122      78.105  58.921  27.043  1.00  0.00
ATOM   1869  N   LEU A 123      78.207  57.679  25.169  1.00  0.00
ATOM   1870  HN  LEU A 123      78.585  57.581  24.250  1.00  0.00
ATOM   1871  CA  LEU A 123      77.303  56.619  25.563  1.00  0.00
ATOM   1872  HA  LEU A 123      76.341  57.074  25.750  1.00  0.00
ATOM   1873  CB  LEU A 123      77.167  55.606  24.394  1.00  0.00
ATOM   1874  HB1 LEU A 123      76.702  56.137  23.534  1.00  0.00
ATOM   1875  HB2 LEU A 123      78.188  55.300  24.077  1.00  0.00
ATOM   1876  CG  LEU A 123      76.359  54.313  24.668  1.00  0.00
ATOM   1877  HG  LEU A 123      76.867  53.747  25.484  1.00  0.00
ATOM   1878  CD1 LEU A 123      74.917  54.599  25.128  1.00  0.00
ATOM   1879 HD11 LEU A 123      74.406  53.651  25.397  1.00  0.00
ATOM   1880 HD12 LEU A 123      74.904  55.257  26.021  1.00  0.00
ATOM   1881 HD13 LEU A 123      74.346  55.092  24.314  1.00  0.00
ATOM   1882  CD2 LEU A 123      76.372  53.399  23.426  1.00  0.00
ATOM   1883 HD21 LEU A 123      77.417  53.169  23.126  1.00  0.00
ATOM   1884 HD22 LEU A 123      75.861  53.895  22.575  1.00  0.00
ATOM   1885 HD23 LEU A 123      75.852  52.444  23.645  1.00  0.00
ATOM   1886  C   LEU A 123      77.729  55.906  26.828  1.00  0.00
ATOM   1887  O   LEU A 123      76.902  55.630  27.691  1.00  0.00
ATOM   1888  N   VAL A 124      79.028  55.625  26.965  1.00  0.00
ATOM   1889  HN  VAL A 124      79.673  55.866  26.243  1.00  0.00
ATOM   1890  CA  VAL A 124      79.621  54.978  28.124  1.00  0.00
ATOM   1891  HA  VAL A 124      79.092  54.046  28.267  1.00  0.00
ATOM   1892  CB  VAL A 124      81.095  54.646  27.890  1.00  0.00
ATOM   1893  HB  VAL A 124      81.625  55.552  27.518  1.00  0.00
ATOM   1894  CG1 VAL A 124      81.165  53.555  26.802  1.00  0.00
ATOM   1895 HG11 VAL A 124      80.697  53.894  25.858  1.00  0.00
ATOM   1896 HG12 VAL A 124      80.632  52.645  27.141  1.00  0.00
ATOM   1897 HG13 VAL A 124      82.221  53.286  26.591  1.00  0.00
ATOM   1898  CG2 VAL A 124      81.808  54.165  29.175  1.00  0.00
ATOM   1899 HG21 VAL A 124      81.261  53.310  29.626  1.00  0.00
ATOM   1900 HG22 VAL A 124      81.889  54.979  29.924  1.00  0.00
ATOM   1901 HG23 VAL A 124      82.838  53.831  28.927  1.00  0.00
ATOM   1902  C   VAL A 124      79.425  55.784  29.397  1.00  0.00
ATOM   1903  O   VAL A 124      79.118  55.231  30.453  1.00  0.00
ATOM   1904  N   GLY A 125      79.565  57.109  29.310  1.00  0.00
ATOM   1905  HN  GLY A 125      79.807  57.544  28.445  1.00  0.00
ATOM   1906  CA  GLY A 125      79.362  57.999  30.436  1.00  0.00
ATOM   1907  HA1 GLY A 125      79.802  58.947  30.162  1.00  0.00
ATOM   1908  HA2 GLY A 125      79.819  57.570  31.317  1.00  0.00
ATOM   1909  C   GLY A 125      77.900  58.243  30.722  1.00  0.00
ATOM   1910  O   GLY A 125      77.518  58.522  31.858  1.00  0.00
ATOM   1911  N   ALA A 126      77.054  58.146  29.696  1.00  0.00
ATOM   1912  HN  ALA A 126      77.384  57.880  28.791  1.00  0.00
ATOM   1913  CA  ALA A 126      75.677  58.577  29.741  1.00  0.00
ATOM   1914  HA  ALA A 126      75.553  59.320  30.518  1.00  0.00
ATOM   1915  CB  ALA A 126      75.278  59.201  28.390  1.00  0.00
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ATOM   1916  HB1 ALA A 126      75.425  58.470  27.566  1.00  0.00
ATOM   1917  HB2 ALA A 126      75.917  60.085  28.181  1.00  0.00
ATOM   1918  HB3 ALA A 126      74.221  59.536  28.385  1.00  0.00
ATOM   1919  C   ALA A 126      74.717  57.445  30.016  1.00  0.00
ATOM   1920  O   ALA A 126      73.508  57.662  30.076  1.00  0.00
ATOM   1921  N   ILE A 127      75.230  56.228  30.216  1.00  0.00
ATOM   1922  HN  ILE A 127      76.211  56.061  30.140  1.00  0.00
ATOM   1923  CA  ILE A 127      74.402  55.071  30.500  1.00  0.00
ATOM   1924  HA  ILE A 127      73.371  55.307  30.270  1.00  0.00
ATOM   1925  CB  ILE A 127      74.784  53.868  29.631  1.00  0.00
ATOM   1926  HB  ILE A 127      74.861  54.252  28.586  1.00  0.00
ATOM   1927  CG2 ILE A 127      76.167  53.297  30.019  1.00  0.00
ATOM   1928 HG21 ILE A 127      76.139  52.826  31.024  1.00  0.00
ATOM   1929 HG22 ILE A 127      76.932  54.098  30.023  1.00  0.00
ATOM   1930 HG23 ILE A 127      76.484  52.526  29.287  1.00  0.00
ATOM   1931  CG1 ILE A 127      73.669  52.789  29.609  1.00  0.00
ATOM   1932 HG11 ILE A 127      72.682  53.301  29.586  1.00  0.00
ATOM   1933 HG12 ILE A 127      73.719  52.187  30.540  1.00  0.00
ATOM   1934  CD1 ILE A 127      73.744  51.852  28.398  1.00  0.00
ATOM   1935  HD1 ILE A 127      74.702  51.291  28.395  1.00  0.00
ATOM   1936  HD2 ILE A 127      73.669  52.433  27.453  1.00  0.00
ATOM   1937  HD3 ILE A 127      72.908  51.121  28.424  1.00  0.00
ATOM   1938  C   ILE A 127      74.468  54.753  31.979  1.00  0.00
ATOM   1939  O   ILE A 127      73.783  53.853  32.466  1.00  0.00
ATOM   1940  N   VAL A 128      75.261  55.524  32.733  1.00  0.00
ATOM   1941  HN  VAL A 128      75.814  56.238  32.311  1.00  0.00
ATOM   1942  CA  VAL A 128      75.356  55.448  34.180  1.00  0.00
ATOM   1943  HA  VAL A 128      75.595  54.425  34.435  1.00  0.00
ATOM   1944  CB  VAL A 128      76.469  56.351  34.709  1.00  0.00
ATOM   1945  HB  VAL A 128      76.343  57.382  34.305  1.00  0.00
ATOM   1946  CG1 VAL A 128      77.815  55.792  34.196  1.00  0.00
ATOM   1947 HG11 VAL A 128      77.871  55.827  33.088  1.00  0.00
ATOM   1948 HG12 VAL A 128      77.946  54.739  34.525  1.00  0.00
ATOM   1949 HG13 VAL A 128      78.658  56.388  34.601  1.00  0.00
ATOM   1950  CG2 VAL A 128      76.453  56.437  36.252  1.00  0.00
ATOM   1951 HG21 VAL A 128      76.470  55.419  36.693  1.00  0.00
ATOM   1952 HG22 VAL A 128      75.555  56.973  36.623  1.00  0.00
ATOM   1953 HG23 VAL A 128      77.346  56.994  36.608  1.00  0.00
ATOM   1954  C   VAL A 128      74.030  55.774  34.832  1.00  0.00
ATOM   1955  O   VAL A 128      73.560  55.023  35.683  1.00  0.00
ATOM   1956  N   GLY A 129      73.384  56.854  34.380  1.00  0.00
ATOM   1957  HN  GLY A 129      73.802  57.412  33.667  1.00  0.00
ATOM   1958  CA  GLY A 129      72.081  57.319  34.819  1.00  0.00
ATOM   1959  HA1 GLY A 129      71.353  56.645  34.390  1.00  0.00
ATOM   1960  HA2 GLY A 129      71.984  58.326  34.446  1.00  0.00
ATOM   1961  C   GLY A 129      71.852  57.380  36.311  1.00  0.00
ATOM   1962  O   GLY A 129      72.772  57.604  37.096  1.00  0.00
ATOM   1963  N   SER A 130      70.588  57.216  36.705  1.00  0.00
ATOM   1964  HN  SER A 130      69.867  57.034  36.041  1.00  0.00
ATOM   1965  CA  SER A 130      70.115  57.278  38.070  1.00  0.00
ATOM   1966  HA  SER A 130      70.744  57.963  38.622  1.00  0.00
ATOM   1967  CB  SER A 130      68.662  57.816  38.105  1.00  0.00
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ATOM   1968  HB1 SER A 130      68.679  58.877  37.780  1.00  0.00
ATOM   1969  HB2 SER A 130      68.239  57.781  39.129  1.00  0.00
ATOM   1970  OG  SER A 130      67.801  57.104  37.220  1.00  0.00
ATOM   1971  HG  SER A 130      66.970  57.587  37.212  1.00  0.00
ATOM   1972  C   SER A 130      70.190  55.933  38.751  1.00  0.00
ATOM   1973  O   SER A 130      70.513  54.922  38.132  1.00  0.00
ATOM   1974  N   THR A 131      69.906  55.910  40.057  1.00  0.00
ATOM   1975  HN  THR A 131      69.675  56.754  40.543  1.00  0.00
ATOM   1976  CA  THR A 131      69.865  54.712  40.866  1.00  0.00
ATOM   1977  HA  THR A 131      70.527  53.971  40.438  1.00  0.00
ATOM   1978  CB  THR A 131      70.247  54.951  42.333  1.00  0.00
ATOM   1979  HB  THR A 131      69.432  55.468  42.885  1.00  0.00
ATOM   1980  OG1 THR A 131      71.385  55.799  42.447  1.00  0.00
ATOM   1981  HG1 THR A 131      71.115  56.667  42.120  1.00  0.00
ATOM   1982  CG2 THR A 131      70.567  53.611  43.025  1.00  0.00
ATOM   1983 HG21 THR A 131      71.398  53.090  42.504  1.00  0.00
ATOM   1984 HG22 THR A 131      69.682  52.948  43.022  1.00  0.00
ATOM   1985 HG23 THR A 131      70.868  53.783  44.080  1.00  0.00
ATOM   1986  C   THR A 131      68.436  54.225  40.801  1.00  0.00
ATOM   1987  O   THR A 131      67.513  54.936  41.193  1.00  0.00
ATOM   1988  N   ASP A 132      68.229  53.006  40.291  1.00  0.00
ATOM   1989  HN  ASP A 132      68.984  52.455  39.941  1.00  0.00
ATOM   1990  CA  ASP A 132      66.953  52.309  40.336  1.00  0.00
ATOM   1991  HA  ASP A 132      66.212  52.980  39.925  1.00  0.00
ATOM   1992  CB  ASP A 132      66.978  51.024  39.433  1.00  0.00
ATOM   1993  HB1 ASP A 132      67.168  51.330  38.386  1.00  0.00
ATOM   1994  HB2 ASP A 132      65.980  50.538  39.468  1.00  0.00
ATOM   1995  CG  ASP A 132      68.050  49.987  39.822  1.00  0.00
ATOM   1996  OD1 ASP A 132      67.850  48.804  39.432  1.00  0.00
ATOM   1997  OD2 ASP A 132      69.108  50.347  40.399  1.00  0.00
ATOM   1998  C   ASP A 132      66.531  51.996  41.758  1.00  0.00
ATOM   1999  O   ASP A 132      65.371  52.183  42.123  1.00  0.00
ATOM   2000  N   ALA A 133      67.492  51.551  42.568  1.00  0.00
ATOM   2001  HN  ALA A 133      68.387  51.362  42.167  1.00  0.00
ATOM   2002  CA  ALA A 133      67.438  51.363  43.997  1.00  0.00
ATOM   2003  HA  ALA A 133      68.457  51.147  44.278  1.00  0.00
ATOM   2004  CB  ALA A 133      67.026  52.637  44.770  1.00  0.00
ATOM   2005  HB1 ALA A 133      65.967  52.900  44.568  1.00  0.00
ATOM   2006  HB2 ALA A 133      67.662  53.490  44.454  1.00  0.00
ATOM   2007  HB3 ALA A 133      67.154  52.498  45.865  1.00  0.00
ATOM   2008  C   ALA A 133      66.613  50.183  44.459  1.00  0.00
ATOM   2009  O   ALA A 133      66.518  49.930  45.656  1.00  0.00
ATOM   2010  N   ALA A 134      66.042  49.416  43.525  1.00  0.00
ATOM   2011  HN  ALA A 134      66.113  49.657  42.561  1.00  0.00
ATOM   2012  CA  ALA A 134      65.315  48.195  43.813  1.00  0.00
ATOM   2013  HA  ALA A 134      64.542  48.434  44.532  1.00  0.00
ATOM   2014  CB  ALA A 134      64.658  47.624  42.540  1.00  0.00
ATOM   2015  HB1 ALA A 134      65.422  47.371  41.773  1.00  0.00
ATOM   2016  HB2 ALA A 134      63.971  48.378  42.103  1.00  0.00
ATOM   2017  HB3 ALA A 134      64.066  46.713  42.771  1.00  0.00
ATOM   2018  C   ALA A 134      66.202  47.126  44.407  1.00  0.00
ATOM   2019  O   ALA A 134      65.841  46.474  45.386  1.00  0.00
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ATOM   2020  N   ALA A 135      67.393  46.950  43.828  1.00  0.00
ATOM   2021  HN  ALA A 135      67.664  47.494  43.038  1.00  0.00
ATOM   2022  CA  ALA A 135      68.344  45.950  44.253  1.00  0.00
ATOM   2023  HA  ALA A 135      67.811  45.054  44.542  1.00  0.00
ATOM   2024  CB  ALA A 135      69.327  45.608  43.115  1.00  0.00
ATOM   2025  HB1 ALA A 135      69.899  46.506  42.798  1.00  0.00
ATOM   2026  HB2 ALA A 135      68.766  45.228  42.235  1.00  0.00
ATOM   2027  HB3 ALA A 135      70.045  44.821  43.432  1.00  0.00
ATOM   2028  C   ALA A 135      69.148  46.428  45.432  1.00  0.00
ATOM   2029  O   ALA A 135      69.562  45.631  46.268  1.00  0.00
ATOM   2030  N   VAL A 136      69.352  47.744  45.538  1.00  0.00
ATOM   2031  HN  VAL A 136      69.013  48.364  44.835  1.00  0.00
ATOM   2032  CA  VAL A 136      70.011  48.387  46.658  1.00  0.00
ATOM   2033  HA  VAL A 136      70.966  47.899  46.798  1.00  0.00
ATOM   2034  CB  VAL A 136      70.255  49.873  46.397  1.00  0.00
ATOM   2035  HB  VAL A 136      69.285  50.399  46.248  1.00  0.00
ATOM   2036  CG1 VAL A 136      70.982  50.531  47.591  1.00  0.00
ATOM   2037 HG11 VAL A 136      71.914  49.978  47.831  1.00  0.00
ATOM   2038 HG12 VAL A 136      70.339  50.555  48.494  1.00  0.00
ATOM   2039 HG13 VAL A 136      71.252  51.579  47.337  1.00  0.00
ATOM   2040  CG2 VAL A 136      71.084  50.022  45.102  1.00  0.00
ATOM   2041 HG21 VAL A 136      70.531  49.650  44.215  1.00  0.00
ATOM   2042 HG22 VAL A 136      72.039  49.463  45.189  1.00  0.00
ATOM   2043 HG23 VAL A 136      71.324  51.093  44.927  1.00  0.00
ATOM   2044  C   VAL A 136      69.201  48.196  47.923  1.00  0.00
ATOM   2045  O   VAL A 136      69.746  47.885  48.979  1.00  0.00
ATOM   2046  N   PHE A 137      67.877  48.346  47.815  1.00  0.00
ATOM   2047  HN  PHE A 137      67.467  48.609  46.943  1.00  0.00
ATOM   2048  CA  PHE A 137      66.932  48.182  48.898  1.00  0.00
ATOM   2049  HA  PHE A 137      67.289  48.793  49.714  1.00  0.00
ATOM   2050  CB  PHE A 137      65.531  48.700  48.464  1.00  0.00
ATOM   2051  HB1 PHE A 137      65.100  48.055  47.668  1.00  0.00
ATOM   2052  HB2 PHE A 137      65.636  49.728  48.056  1.00  0.00
ATOM   2053  CG  PHE A 137      64.569  48.790  49.629  1.00  0.00
ATOM   2054  CD1 PHE A 137      64.799  49.725  50.655  1.00  0.00
ATOM   2055  HD1 PHE A 137      65.671  50.362  50.614  1.00  0.00
ATOM   2056  CE1 PHE A 137      63.905  49.847  51.726  1.00  0.00
ATOM   2057  HE1 PHE A 137      64.096  50.570  52.506  1.00  0.00
ATOM   2058  CZ  PHE A 137      62.762  49.041  51.778  1.00  0.00
ATOM   2059  HZ  PHE A 137      62.066  49.142  52.598  1.00  0.00
ATOM   2060  CD2 PHE A 137      63.422  47.979  49.698  1.00  0.00
ATOM   2061  HD2 PHE A 137      63.230  47.257  48.919  1.00  0.00
ATOM   2062  CE2 PHE A 137      62.521  48.106  50.763  1.00  0.00
ATOM   2063  HE2 PHE A 137      61.634  47.491  50.797  1.00  0.00
ATOM   2064  C   PHE A 137      66.867  46.754  49.391  1.00  0.00
ATOM   2065  O   PHE A 137      66.709  46.520  50.585  1.00  0.00
ATOM   2066  N   SER A 138      67.016  45.781  48.486  1.00  0.00
ATOM   2067  HN  SER A 138      67.122  46.004  47.520  1.00  0.00
ATOM   2068  CA  SER A 138      67.080  44.366  48.814  1.00  0.00
ATOM   2069  HA  SER A 138      66.171  44.117  49.345  1.00  0.00
ATOM   2070  CB  SER A 138      67.150  43.522  47.513  1.00  0.00
ATOM   2071  HB1 SER A 138      68.098  43.712  46.970  1.00  0.00
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ATOM   2072  HB2 SER A 138      66.306  43.812  46.850  1.00  0.00
ATOM   2073  OG  SER A 138      67.049  42.126  47.778  1.00  0.00
ATOM   2074  HG  SER A 138      67.082  41.685  46.925  1.00  0.00
ATOM   2075  C   SER A 138      68.261  44.060  49.722  1.00  0.00
ATOM   2076  O   SER A 138      68.143  43.282  50.667  1.00  0.00
ATOM   2077  N   LEU A 139      69.406  44.700  49.465  1.00  0.00
ATOM   2078  HN  LEU A 139      69.476  45.329  48.693  1.00  0.00
ATOM   2079  CA  LEU A 139      70.615  44.548  50.248  1.00  0.00
ATOM   2080  HA  LEU A 139      70.752  43.498  50.465  1.00  0.00
ATOM   2081  CB  LEU A 139      71.832  45.074  49.446  1.00  0.00
ATOM   2082  HB1 LEU A 139      72.755  44.992  50.061  1.00  0.00
ATOM   2083  HB2 LEU A 139      71.673  46.151  49.216  1.00  0.00
ATOM   2084  CG  LEU A 139      72.104  44.334  48.115  1.00  0.00
ATOM   2085  HG  LEU A 139      71.153  44.264  47.545  1.00  0.00
ATOM   2086  CD1 LEU A 139      73.087  45.136  47.239  1.00  0.00
ATOM   2087 HD11 LEU A 139      74.077  45.204  47.735  1.00  0.00
ATOM   2088 HD12 LEU A 139      72.703  46.165  47.070  1.00  0.00
ATOM   2089 HD13 LEU A 139      73.215  44.644  46.253  1.00  0.00
ATOM   2090  CD2 LEU A 139      72.593  42.892  48.347  1.00  0.00
ATOM   2091 HD21 LEU A 139      71.846  42.312  48.927  1.00  0.00
ATOM   2092 HD22 LEU A 139      73.553  42.895  48.906  1.00  0.00
ATOM   2093 HD23 LEU A 139      72.752  42.379  47.376  1.00  0.00
ATOM   2094  C   LEU A 139      70.563  45.291  51.567  1.00  0.00
ATOM   2095  O   LEU A 139      71.206  44.886  52.533  1.00  0.00
ATOM   2096  N   LEU A 140      69.762  46.358  51.643  1.00  0.00
ATOM   2097  HN  LEU A 140      69.274  46.687  50.837  1.00  0.00
ATOM   2098  CA  LEU A 140      69.516  47.097  52.869  1.00  0.00
ATOM   2099  HA  LEU A 140      70.444  47.199  53.412  1.00  0.00
ATOM   2100  CB  LEU A 140      68.933  48.500  52.545  1.00  0.00
ATOM   2101  HB1 LEU A 140      68.503  48.967  53.458  1.00  0.00
ATOM   2102  HB2 LEU A 140      68.104  48.376  51.815  1.00  0.00
ATOM   2103  CG  LEU A 140      69.955  49.513  51.970  1.00  0.00
ATOM   2104  HG  LEU A 140      70.545  49.003  51.174  1.00  0.00
ATOM   2105  CD1 LEU A 140      69.244  50.714  51.316  1.00  0.00
ATOM   2106 HD11 LEU A 140      68.617  51.243  52.065  1.00  0.00
ATOM   2107 HD12 LEU A 140      68.593  50.377  50.483  1.00  0.00
ATOM   2108 HD13 LEU A 140      69.989  51.430  50.911  1.00  0.00
ATOM   2109  CD2 LEU A 140      70.943  50.001  53.046  1.00  0.00
ATOM   2110 HD21 LEU A 140      71.496  49.147  53.483  1.00  0.00
ATOM   2111 HD22 LEU A 140      70.398  50.523  53.861  1.00  0.00
ATOM   2112 HD23 LEU A 140      71.676  50.708  52.604  1.00  0.00
ATOM   2113  C   LEU A 140      68.539  46.359  53.758  1.00  0.00
ATOM   2114  O   LEU A 140      68.482  46.594  54.961  1.00  0.00
ATOM   2115  N   LYS A 141      67.777  45.432  53.181  1.00  0.00
ATOM   2116  HN  LYS A 141      67.830  45.273  52.197  1.00  0.00
ATOM   2117  CA  LYS A 141      66.811  44.621  53.883  1.00  0.00
ATOM   2118  HA  LYS A 141      66.574  45.066  54.840  1.00  0.00
ATOM   2119  CB  LYS A 141      65.510  44.518  53.039  1.00  0.00
ATOM   2120  HB1 LYS A 141      64.832  43.741  53.449  1.00  0.00
ATOM   2121  HB2 LYS A 141      65.798  44.199  52.011  1.00  0.00
ATOM   2122  CG  LYS A 141      64.728  45.846  52.928  1.00  0.00
ATOM   2123  HG1 LYS A 141      64.079  45.803  52.027  1.00  0.00
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ATOM   2124  HG2 LYS A 141      65.446  46.679  52.766  1.00  0.00
ATOM   2125  CD  LYS A 141      63.861  46.200  54.154  1.00  0.00
ATOM   2126  HD1 LYS A 141      63.550  47.266  54.077  1.00  0.00
ATOM   2127  HD2 LYS A 141      64.490  46.107  55.067  1.00  0.00
ATOM   2128  CE  LYS A 141      62.604  45.330  54.328  1.00  0.00
ATOM   2129  HE1 LYS A 141      62.091  45.583  55.278  1.00  0.00
ATOM   2130  HE2 LYS A 141      62.865  44.252  54.342  1.00  0.00
ATOM   2131  NZ  LYS A 141      61.632  45.547  53.227  1.00  0.00
ATOM   2132  HZ1 LYS A 141      62.107  45.405  52.314  1.00  0.00
ATOM   2133  HZ2 LYS A 141      61.247  46.515  53.268  1.00  0.00
ATOM   2134  HZ3 LYS A 141      60.847  44.872  53.316  1.00  0.00
ATOM   2135  C   LYS A 141      67.370  43.240  54.144  1.00  0.00
ATOM   2136  O   LYS A 141      66.686  42.390  54.713  1.00  0.00
ATOM   2137  N   GLY A 142      68.629  43.010  53.757  1.00  0.00
ATOM   2138  HN  GLY A 142      69.145  43.725  53.293  1.00  0.00
ATOM   2139  CA  GLY A 142      69.323  41.749  53.928  1.00  0.00
ATOM   2140  HA1 GLY A 142      69.735  41.490  52.963  1.00  0.00
ATOM   2141  HA2 GLY A 142      68.656  40.992  54.318  1.00  0.00
ATOM   2142  C   GLY A 142      70.463  41.908  54.888  1.00  0.00
ATOM   2143  O   GLY A 142      70.883  40.939  55.518  1.00  0.00
ATOM   2144  N   ARG A 143      70.981  43.129  55.024  1.00  0.00
ATOM   2145  HN  ARG A 143      70.638  43.896  54.487  1.00  0.00
ATOM   2146  CA  ARG A 143      72.035  43.463  55.950  1.00  0.00
ATOM   2147  HA  ARG A 143      72.290  42.615  56.571  1.00  0.00
ATOM   2148  CB  ARG A 143      73.282  43.995  55.191  1.00  0.00
ATOM   2149  HB1 ARG A 143      74.068  44.272  55.929  1.00  0.00
ATOM   2150  HB2 ARG A 143      73.003  44.915  54.629  1.00  0.00
ATOM   2151  CG  ARG A 143      73.895  43.001  54.182  1.00  0.00
ATOM   2152  HG1 ARG A 143      74.743  43.513  53.672  1.00  0.00
ATOM   2153  HG2 ARG A 143      73.138  42.753  53.405  1.00  0.00
ATOM   2154  CD  ARG A 143      74.410  41.711  54.839  1.00  0.00
ATOM   2155  HD1 ARG A 143      73.574  41.158  55.319  1.00  0.00
ATOM   2156  HD2 ARG A 143      75.184  41.957  55.600  1.00  0.00
ATOM   2157  NE  ARG A 143      75.025  40.828  53.794  1.00  0.00
ATOM   2158  HE  ARG A 143      74.991  41.113  52.837  1.00  0.00
ATOM   2159  CZ  ARG A 143      75.573  39.626  54.089  1.00  0.00
ATOM   2160  NH1 ARG A 143      75.634  39.174  55.357  1.00  0.00
ATOM   2161 HH11 ARG A 143      75.264  39.719  56.105  1.00  0.00
ATOM   2162 HH12 ARG A 143      76.045  38.273  55.537  1.00  0.00
ATOM   2163  NH2 ARG A 143      76.072  38.849  53.105  1.00  0.00
ATOM   2164 HH21 ARG A 143      76.071  39.164  52.156  1.00  0.00
ATOM   2165 HH22 ARG A 143      76.457  37.956  53.339  1.00  0.00
ATOM   2166  C   ARG A 143      71.469  44.554  56.814  1.00  0.00
ATOM   2167  O   ARG A 143      70.932  45.539  56.310  1.00  0.00
ATOM   2168  N   SER A 144      71.568  44.386  58.134  1.00  0.00
ATOM   2169  HN  SER A 144      72.022  43.586  58.515  1.00  0.00
ATOM   2170  CA  SER A 144      70.933  45.250  59.110  1.00  0.00
ATOM   2171  HA  SER A 144      70.048  45.694  58.674  1.00  0.00
ATOM   2172  CB  SER A 144      70.520  44.434  60.361  1.00  0.00
ATOM   2173  HB1 SER A 144      70.019  45.091  61.105  1.00  0.00
ATOM   2174  HB2 SER A 144      71.411  43.966  60.834  1.00  0.00
ATOM   2175  OG  SER A 144      69.611  43.400  60.004  1.00  0.00
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ATOM   2176  HG  SER A 144      69.372  42.953  60.820  1.00  0.00
ATOM   2177  C   SER A 144      71.873  46.356  59.518  1.00  0.00
ATOM   2178  O   SER A 144      72.229  46.494  60.687  1.00  0.00
ATOM   2179  N   LEU A 145      72.282  47.168  58.544  1.00  0.00
ATOM   2180  HN  LEU A 145      71.976  47.012  57.607  1.00  0.00
ATOM   2181  CA  LEU A 145      73.171  48.292  58.718  1.00  0.00
ATOM   2182  HA  LEU A 145      73.494  48.352  59.749  1.00  0.00
ATOM   2183  CB  LEU A 145      74.436  48.138  57.823  1.00  0.00
ATOM   2184  HB1 LEU A 145      75.083  47.392  58.341  1.00  0.00
ATOM   2185  HB2 LEU A 145      75.015  49.084  57.791  1.00  0.00
ATOM   2186  CG  LEU A 145      74.242  47.601  56.379  1.00  0.00
ATOM   2187  HG  LEU A 145      73.742  46.608  56.441  1.00  0.00
ATOM   2188  CD1 LEU A 145      73.372  48.496  55.478  1.00  0.00
ATOM   2189 HD11 LEU A 145      73.793  49.521  55.422  1.00  0.00
ATOM   2190 HD12 LEU A 145      72.332  48.556  55.862  1.00  0.00
ATOM   2191 HD13 LEU A 145      73.334  48.074  54.452  1.00  0.00
ATOM   2192  CD2 LEU A 145      75.611  47.354  55.716  1.00  0.00
ATOM   2193 HD21 LEU A 145      76.216  46.647  56.323  1.00  0.00
ATOM   2194 HD22 LEU A 145      76.172  48.307  55.620  1.00  0.00
ATOM   2195 HD23 LEU A 145      75.476  46.919  54.703  1.00  0.00
ATOM   2196  C   LEU A 145      72.420  49.567  58.427  1.00  0.00
ATOM   2197  O   LEU A 145      73.019  50.590  58.112  1.00  0.00
ATOM   2198  N   ASN A 146      71.090  49.522  58.537  1.00  0.00
ATOM   2199  HN  ASN A 146      70.653  48.672  58.825  1.00  0.00
ATOM   2200  CA  ASN A 146      70.158  50.583  58.200  1.00  0.00
ATOM   2201  HA  ASN A 146      70.269  50.791  57.145  1.00  0.00
ATOM   2202  CB  ASN A 146      68.708  50.124  58.500  1.00  0.00
ATOM   2203  HB1 ASN A 146      67.981  50.937  58.280  1.00  0.00
ATOM   2204  HB2 ASN A 146      68.606  49.847  59.572  1.00  0.00
ATOM   2205  CG  ASN A 146      68.352  48.900  57.652  1.00  0.00
ATOM   2206  OD1 ASN A 146      68.289  47.776  58.162  1.00  0.00
ATOM   2207  ND2 ASN A 146      68.111  49.139  56.331  1.00  0.00
ATOM   2208 HD21 ASN A 146      67.930  48.364  55.723  1.00  0.00
ATOM   2209 HD22 ASN A 146      68.148  50.072  55.974  1.00  0.00
ATOM   2210  C   ASN A 146      70.386  51.872  58.950  1.00  0.00
ATOM   2211  O   ASN A 146      70.260  52.953  58.381  1.00  0.00
ATOM   2212  N   GLU A 147      70.728  51.775  60.235  1.00  0.00
ATOM   2213  HN  GLU A 147      70.830  50.885  60.672  1.00  0.00
ATOM   2214  CA  GLU A 147      70.913  52.919  61.099  1.00  0.00
ATOM   2215  HA  GLU A 147      70.432  53.789  60.673  1.00  0.00
ATOM   2216  CB  GLU A 147      70.277  52.637  62.483  1.00  0.00
ATOM   2217  HB1 GLU A 147      70.466  53.505  63.155  1.00  0.00
ATOM   2218  HB2 GLU A 147      70.749  51.737  62.936  1.00  0.00
ATOM   2219  CG  GLU A 147      68.750  52.423  62.391  1.00  0.00
ATOM   2220  HG1 GLU A 147      68.527  51.522  61.781  1.00  0.00
ATOM   2221  HG2 GLU A 147      68.279  53.302  61.901  1.00  0.00
ATOM   2222  CD  GLU A 147      68.140  52.254  63.783  1.00  0.00
ATOM   2223  OE1 GLU A 147      68.203  53.228  64.579  1.00  0.00
ATOM   2224  OE2 GLU A 147      67.597  51.152  64.063  1.00  0.00
ATOM   2225  C   GLU A 147      72.387  53.226  61.251  1.00  0.00
ATOM   2226  O   GLU A 147      72.793  53.945  62.162  1.00  0.00
ATOM   2227  N   ARG A 148      73.209  52.699  60.341  1.00  0.00
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ATOM   2228  HN  ARG A 148      72.851  52.114  59.616  1.00  0.00
ATOM   2229  CA  ARG A 148      74.632  52.920  60.310  1.00  0.00
ATOM   2230  HA  ARG A 148      74.915  53.695  61.008  1.00  0.00
ATOM   2231  CB  ARG A 148      75.386  51.597  60.628  1.00  0.00
ATOM   2232  HB1 ARG A 148      76.466  51.707  60.386  1.00  0.00
ATOM   2233  HB2 ARG A 148      74.978  50.777  59.996  1.00  0.00
ATOM   2234  CG  ARG A 148      75.274  51.137  62.096  1.00  0.00
ATOM   2235  HG1 ARG A 148      75.763  50.141  62.190  1.00  0.00
ATOM   2236  HG2 ARG A 148      74.200  51.003  62.353  1.00  0.00
ATOM   2237  CD  ARG A 148      75.908  52.100  63.114  1.00  0.00
ATOM   2238  HD1 ARG A 148      75.809  51.694  64.143  1.00  0.00
ATOM   2239  HD2 ARG A 148      75.418  53.096  63.058  1.00  0.00
ATOM   2240  NE  ARG A 148      77.368  52.234  62.798  1.00  0.00
ATOM   2241  HE  ARG A 148      77.785  51.570  62.169  1.00  0.00
ATOM   2242  CZ  ARG A 148      78.155  53.216  63.293  1.00  0.00
ATOM   2243  NH1 ARG A 148      77.674  54.152  64.135  1.00  0.00
ATOM   2244 HH11 ARG A 148      76.714  54.124  64.406  1.00  0.00
ATOM   2245 HH12 ARG A 148      78.278  54.865  64.485  1.00  0.00
ATOM   2246  NH2 ARG A 148      79.454  53.258  62.932  1.00  0.00
ATOM   2247 HH21 ARG A 148      79.823  52.551  62.317  1.00  0.00
ATOM   2248 HH22 ARG A 148      80.052  53.970  63.291  1.00  0.00
ATOM   2249  C   ARG A 148      74.986  53.418  58.937  1.00  0.00
ATOM   2250  O   ARG A 148      74.837  54.603  58.643  1.00  0.00
ATOM   2251  N   VAL A 149      75.450  52.514  58.072  1.00  0.00
ATOM   2252  HN  VAL A 149      75.556  51.565  58.355  1.00  0.00
ATOM   2253  CA  VAL A 149      75.832  52.769  56.703  1.00  0.00
ATOM   2254  HA  VAL A 149      76.541  53.583  56.717  1.00  0.00
ATOM   2255  CB  VAL A 149      76.501  51.557  56.064  1.00  0.00
ATOM   2256  HB  VAL A 149      75.775  50.721  55.951  1.00  0.00
ATOM   2257  CG1 VAL A 149      77.648  51.070  56.979  1.00  0.00
ATOM   2258 HG11 VAL A 149      77.267  50.680  57.945  1.00  0.00
ATOM   2259 HG12 VAL A 149      78.357  51.900  57.182  1.00  0.00
ATOM   2260 HG13 VAL A 149      78.207  50.249  56.481  1.00  0.00
ATOM   2261  CG2 VAL A 149      77.046  51.942  54.674  1.00  0.00
ATOM   2262 HG21 VAL A 149      77.725  52.816  54.760  1.00  0.00
ATOM   2263 HG22 VAL A 149      76.228  52.191  53.969  1.00  0.00
ATOM   2264 HG23 VAL A 149      77.621  51.097  54.247  1.00  0.00
ATOM   2265  C   VAL A 149      74.645  53.214  55.887  1.00  0.00
ATOM   2266  O   VAL A 149      74.754  54.141  55.092  1.00  0.00
ATOM   2267  N   GLY A 150      73.492  52.575  56.109  1.00  0.00
ATOM   2268  HN  GLY A 150      73.453  51.864  56.811  1.00  0.00
ATOM   2269  CA  GLY A 150      72.255  52.760  55.382  1.00  0.00
ATOM   2270  HA1 GLY A 150      71.540  52.078  55.815  1.00  0.00
ATOM   2271  HA2 GLY A 150      72.453  52.550  54.342  1.00  0.00
ATOM   2272  C   GLY A 150      71.682  54.140  55.486  1.00  0.00
ATOM   2273  O   GLY A 150      71.093  54.631  54.527  1.00  0.00
ATOM   2274  N   ALA A 151      71.849  54.798  56.636  1.00  0.00
ATOM   2275  HN  ALA A 151      72.309  54.366  57.407  1.00  0.00
ATOM   2276  CA  ALA A 151      71.410  56.159  56.865  1.00  0.00
ATOM   2277  HA  ALA A 151      70.346  56.198  56.675  1.00  0.00
ATOM   2278  CB  ALA A 151      71.682  56.596  58.318  1.00  0.00
ATOM   2279  HB1 ALA A 151      72.768  56.561  58.549  1.00  0.00
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ATOM   2280  HB2 ALA A 151      71.159  55.912  59.019  1.00  0.00
ATOM   2281  HB3 ALA A 151      71.310  57.627  58.497  1.00  0.00
ATOM   2282  C   ALA A 151      72.097  57.118  55.923  1.00  0.00
ATOM   2283  O   ALA A 151      71.457  57.979  55.323  1.00  0.00
ATOM   2284  N   THR A 152      73.412  56.946  55.754  1.00  0.00
ATOM   2285  HN  THR A 152      73.893  56.242  56.269  1.00  0.00
ATOM   2286  CA  THR A 152      74.223  57.660  54.791  1.00  0.00
ATOM   2287  HA  THR A 152      74.005  58.712  54.918  1.00  0.00
ATOM   2288  CB  THR A 152      75.721  57.440  55.020  1.00  0.00
ATOM   2289  HB  THR A 152      76.039  56.424  54.697  1.00  0.00
ATOM   2290  OG1 THR A 152      76.498  58.405  54.316  1.00  0.00
ATOM   2291  HG1 THR A 152      76.429  58.204  53.377  1.00  0.00
ATOM   2292  CG2 THR A 152      76.044  57.586  56.523  1.00  0.00
ATOM   2293 HG21 THR A 152      75.585  56.769  57.118  1.00  0.00
ATOM   2294 HG22 THR A 152      75.676  58.561  56.907  1.00  0.00
ATOM   2295 HG23 THR A 152      77.142  57.538  56.684  1.00  0.00
ATOM   2296  C   THR A 152      73.854  57.270  53.368  1.00  0.00
ATOM   2297  O   THR A 152      73.721  58.125  52.499  1.00  0.00
ATOM   2298  N   LEU A 153      73.687  55.968  53.119  1.00  0.00
ATOM   2299  HN  LEU A 153      73.762  55.308  53.865  1.00  0.00
ATOM   2300  CA  LEU A 153      73.530  55.374  51.805  1.00  0.00
ATOM   2301  HA  LEU A 153      74.395  55.668  51.227  1.00  0.00
ATOM   2302  CB  LEU A 153      73.517  53.826  51.941  1.00  0.00
ATOM   2303  HB1 LEU A 153      72.531  53.447  52.276  1.00  0.00
ATOM   2304  HB2 LEU A 153      74.244  53.590  52.750  1.00  0.00
ATOM   2305  CG  LEU A 153      74.015  53.018  50.715  1.00  0.00
ATOM   2306  HG  LEU A 153      74.889  53.565  50.292  1.00  0.00
ATOM   2307  CD1 LEU A 153      74.534  51.639  51.165  1.00  0.00
ATOM   2308 HD11 LEU A 153      73.707  51.031  51.584  1.00  0.00
ATOM   2309 HD12 LEU A 153      75.315  51.756  51.945  1.00  0.00
ATOM   2310 HD13 LEU A 153      74.981  51.093  50.309  1.00  0.00
ATOM   2311  CD2 LEU A 153      72.968  52.847  49.600  1.00  0.00
ATOM   2312 HD21 LEU A 153      72.675  53.825  49.172  1.00  0.00
ATOM   2313 HD22 LEU A 153      72.061  52.344  49.996  1.00  0.00
ATOM   2314 HD23 LEU A 153      73.385  52.229  48.777  1.00  0.00
ATOM   2315  C   LEU A 153      72.290  55.832  51.076  1.00  0.00
ATOM   2316  O   LEU A 153      72.346  56.165  49.896  1.00  0.00
ATOM   2317  N   GLU A 154      71.152  55.864  51.773  1.00  0.00
ATOM   2318  HN  GLU A 154      71.132  55.602  52.737  1.00  0.00
ATOM   2319  CA  GLU A 154      69.867  56.208  51.199  1.00  0.00
ATOM   2320  HA  GLU A 154      69.735  55.571  50.335  1.00  0.00
ATOM   2321  CB  GLU A 154      68.730  55.851  52.188  1.00  0.00
ATOM   2322  HB1 GLU A 154      67.760  56.237  51.804  1.00  0.00
ATOM   2323  HB2 GLU A 154      68.936  56.334  53.169  1.00  0.00
ATOM   2324  CG  GLU A 154      68.595  54.318  52.357  1.00  0.00
ATOM   2325  HG1 GLU A 154      69.562  53.880  52.679  1.00  0.00
ATOM   2326  HG2 GLU A 154      68.331  53.866  51.377  1.00  0.00
ATOM   2327  CD  GLU A 154      67.538  53.934  53.394  1.00  0.00
ATOM   2328  OE1 GLU A 154      67.585  54.479  54.528  1.00  0.00
ATOM   2329  OE2 GLU A 154      66.676  53.074  53.065  1.00  0.00
ATOM   2330  C   GLU A 154      69.784  57.629  50.686  1.00  0.00
ATOM   2331  O   GLU A 154      69.275  57.864  49.589  1.00  0.00
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ATOM   2332  N   ILE A 155      70.318  58.594  51.445  1.00  0.00
ATOM   2333  HN  ILE A 155      70.702  58.395  52.344  1.00  0.00
ATOM   2334  CA  ILE A 155      70.471  59.963  50.980  1.00  0.00
ATOM   2335  HA  ILE A 155      69.520  60.220  50.534  1.00  0.00
ATOM   2336  CB  ILE A 155      70.691  61.003  52.081  1.00  0.00
ATOM   2337  HB  ILE A 155      69.796  60.960  52.742  1.00  0.00
ATOM   2338  CG2 ILE A 155      71.919  60.659  52.950  1.00  0.00
ATOM   2339 HG21 ILE A 155      72.854  60.699  52.355  1.00  0.00
ATOM   2340 HG22 ILE A 155      71.816  59.649  53.396  1.00  0.00
ATOM   2341 HG23 ILE A 155      72.008  61.388  53.783  1.00  0.00
ATOM   2342  CG1 ILE A 155      70.777  62.459  51.546  1.00  0.00
ATOM   2343 HG11 ILE A 155      71.620  62.562  50.832  1.00  0.00
ATOM   2344 HG12 ILE A 155      71.024  63.122  52.401  1.00  0.00
ATOM   2345  CD1 ILE A 155      69.479  62.958  50.900  1.00  0.00
ATOM   2346  HD1 ILE A 155      68.632  62.882  51.614  1.00  0.00
ATOM   2347  HD2 ILE A 155      69.232  62.363  49.995  1.00  0.00
ATOM   2348  HD3 ILE A 155      69.591  64.020  50.596  1.00  0.00
ATOM   2349  C   ILE A 155      71.493  60.098  49.868  1.00  0.00
ATOM   2350  O   ILE A 155      71.266  60.832  48.911  1.00  0.00
ATOM   2351  N   GLU A 156      72.613  59.369  49.956  1.00  0.00
ATOM   2352  HN  GLU A 156      72.782  58.779  50.743  1.00  0.00
ATOM   2353  CA  GLU A 156      73.668  59.379  48.955  1.00  0.00
ATOM   2354  HA  GLU A 156      74.013  60.399  48.860  1.00  0.00
ATOM   2355  CB  GLU A 156      74.868  58.504  49.400  1.00  0.00
ATOM   2356  HB1 GLU A 156      75.472  58.201  48.514  1.00  0.00
ATOM   2357  HB2 GLU A 156      74.482  57.575  49.870  1.00  0.00
ATOM   2358  CG  GLU A 156      75.826  59.233  50.366  1.00  0.00
ATOM   2359  HG1 GLU A 156      75.274  59.596  51.256  1.00  0.00
ATOM   2360  HG2 GLU A 156      76.261  60.117  49.852  1.00  0.00
ATOM   2361  CD  GLU A 156      76.970  58.324  50.826  1.00  0.00
ATOM   2362  OE1 GLU A 156      77.025  57.140  50.401  1.00  0.00
ATOM   2363  OE2 GLU A 156      77.815  58.818  51.619  1.00  0.00
ATOM   2364  C   GLU A 156      73.205  58.945  47.586  1.00  0.00
ATOM   2365  O   GLU A 156      73.595  59.539  46.584  1.00  0.00
ATOM   2366  N   SER A 157      72.336  57.933  47.529  1.00  0.00
ATOM   2367  HN  SER A 157      72.077  57.440  48.360  1.00  0.00
ATOM   2368  CA  SER A 157      71.696  57.473  46.314  1.00  0.00
ATOM   2369  HA  SER A 157      72.474  57.171  45.627  1.00  0.00
ATOM   2370  CB  SER A 157      70.790  56.252  46.604  1.00  0.00
ATOM   2371  HB1 SER A 157      70.236  55.951  45.687  1.00  0.00
ATOM   2372  HB2 SER A 157      70.056  56.493  47.402  1.00  0.00
ATOM   2373  OG  SER A 157      71.573  55.138  47.017  1.00  0.00
ATOM   2374  HG  SER A 157      70.954  54.442  47.250  1.00  0.00
ATOM   2375  C   SER A 157      70.880  58.547  45.639  1.00  0.00
ATOM   2376  O   SER A 157      70.923  58.690  44.421  1.00  0.00
ATOM   2377  N   GLY A 158      70.153  59.344  46.427  1.00  0.00
ATOM   2378  HN  GLY A 158      70.142  59.214  47.416  1.00  0.00
ATOM   2379  CA  GLY A 158      69.379  60.460  45.927  1.00  0.00
ATOM   2380  HA1 GLY A 158      68.777  60.813  46.751  1.00  0.00
ATOM   2381  HA2 GLY A 158      68.785  60.121  45.088  1.00  0.00
ATOM   2382  C   GLY A 158      70.246  61.602  45.467  1.00  0.00
ATOM   2383  O   GLY A 158      69.988  62.204  44.431  1.00  0.00
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ATOM   2384  N   THR A 159      71.294  61.933  46.222  1.00  0.00
ATOM   2385  HN  THR A 159      71.511  61.413  47.048  1.00  0.00
ATOM   2386  CA  THR A 159      72.085  63.128  46.001  1.00  0.00
ATOM   2387  HA  THR A 159      71.407  63.918  45.706  1.00  0.00
ATOM   2388  CB  THR A 159      72.770  63.600  47.291  1.00  0.00
ATOM   2389  HB  THR A 159      73.313  62.744  47.751  1.00  0.00
ATOM   2390  OG1 THR A 159      73.703  64.661  47.094  1.00  0.00
ATOM   2391  HG1 THR A 159      74.327  64.354  46.430  1.00  0.00
ATOM   2392  CG2 THR A 159      71.696  64.110  48.271  1.00  0.00
ATOM   2393 HG21 THR A 159      70.926  63.335  48.458  1.00  0.00
ATOM   2394 HG22 THR A 159      71.194  65.010  47.859  1.00  0.00
ATOM   2395 HG23 THR A 159      72.159  64.383  49.244  1.00  0.00
ATOM   2396  C   THR A 159      73.081  62.979  44.863  1.00  0.00
ATOM   2397  O   THR A 159      73.517  63.978  44.292  1.00  0.00
ATOM   2398  N   ASN A 160      73.449  61.744  44.505  1.00  0.00
ATOM   2399  HN  ASN A 160      73.094  60.934  44.967  1.00  0.00
ATOM   2400  CA  ASN A 160      74.474  61.534  43.500  1.00  0.00
ATOM   2401  HA  ASN A 160      75.107  62.407  43.480  1.00  0.00
ATOM   2402  CB  ASN A 160      75.422  60.361  43.929  1.00  0.00
ATOM   2403  HB1 ASN A 160      75.441  60.258  45.031  1.00  0.00
ATOM   2404  HB2 ASN A 160      76.453  60.630  43.610  1.00  0.00
ATOM   2405  CG  ASN A 160      75.089  59.014  43.267  1.00  0.00
ATOM   2406  OD1 ASN A 160      75.886  58.523  42.462  1.00  0.00
ATOM   2407  ND2 ASN A 160      73.912  58.421  43.612  1.00  0.00
ATOM   2408 HD21 ASN A 160      73.646  57.559  43.183  1.00  0.00
ATOM   2409 HD22 ASN A 160      73.307  58.854  44.279  1.00  0.00
ATOM   2410  C   ASN A 160      73.872  61.413  42.109  1.00  0.00
ATOM   2411  O   ASN A 160      74.572  61.598  41.113  1.00  0.00
ATOM   2412  N   ASP A 161      72.567  61.138  42.027  1.00  0.00
ATOM   2413  HN  ASP A 161      72.022  60.990  42.849  1.00  0.00
ATOM   2414  CA  ASP A 161      71.838  61.032  40.777  1.00  0.00
ATOM   2415  HA  ASP A 161      72.389  60.329  40.165  1.00  0.00
ATOM   2416  CB  ASP A 161      70.413  60.447  41.008  1.00  0.00
ATOM   2417  HB1 ASP A 161      69.796  60.554  40.089  1.00  0.00
ATOM   2418  HB2 ASP A 161      69.902  60.974  41.839  1.00  0.00
ATOM   2419  CG  ASP A 161      70.467  58.954  41.345  1.00  0.00
ATOM   2420  OD1 ASP A 161      69.381  58.392  41.650  1.00  0.00
ATOM   2421  OD2 ASP A 161      71.561  58.336  41.254  1.00  0.00
ATOM   2422  C   ASP A 161      71.787  62.301  39.939  1.00  0.00
ATOM   2423  O   ASP A 161      71.967  62.152  38.732  1.00  0.00
ATOM   2424  N   PRO A 162      71.603  63.549  40.419  1.00  0.00
ATOM   2425  CD  PRO A 162      70.992  63.840  41.718  1.00  0.00
ATOM   2426  HD1 PRO A 162      71.807  64.036  42.443  1.00  0.00
ATOM   2427  HD2 PRO A 162      70.348  63.015  42.078  1.00  0.00
ATOM   2428  CA  PRO A 162      71.511  64.708  39.534  1.00  0.00
ATOM   2429  HA  PRO A 162      70.820  64.474  38.738  1.00  0.00
ATOM   2430  CB  PRO A 162      70.983  65.835  40.438  1.00  0.00
ATOM   2431  HB1 PRO A 162      70.369  66.566  39.874  1.00  0.00
ATOM   2432  HB2 PRO A 162      71.813  66.372  40.951  1.00  0.00
ATOM   2433  CG  PRO A 162      70.164  65.099  41.494  1.00  0.00
ATOM   2434  HG1 PRO A 162      70.023  65.689  42.422  1.00  0.00
ATOM   2435  HG2 PRO A 162      69.172  64.819  41.075  1.00  0.00
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ATOM   2436  C   PRO A 162      72.840  65.120  38.935  1.00  0.00
ATOM   2437  O   PRO A 162      72.866  66.101  38.194  1.00  0.00
ATOM   2438  N   MET A 163      73.922  64.395  39.225  1.00  0.00
ATOM   2439  HN  MET A 163      73.858  63.605  39.832  1.00  0.00
ATOM   2440  CA  MET A 163      75.247  64.696  38.739  1.00  0.00
ATOM   2441  HA  MET A 163      75.245  65.624  38.185  1.00  0.00
ATOM   2442  CB  MET A 163      76.239  64.797  39.926  1.00  0.00
ATOM   2443  HB1 MET A 163      77.218  65.176  39.558  1.00  0.00
ATOM   2444  HB2 MET A 163      76.408  63.788  40.366  1.00  0.00
ATOM   2445  CG  MET A 163      75.746  65.711  41.067  1.00  0.00
ATOM   2446  HG1 MET A 163      76.563  65.784  41.815  1.00  0.00
ATOM   2447  HG2 MET A 163      74.886  65.219  41.573  1.00  0.00
ATOM   2448  SD  MET A 163      75.286  67.395  40.564  1.00  0.00
ATOM   2449  CE  MET A 163      74.588  67.840  42.179  1.00  0.00
ATOM   2450  HE1 MET A 163      75.342  67.709  42.985  1.00  0.00
ATOM   2451  HE2 MET A 163      73.712  67.201  42.424  1.00  0.00
ATOM   2452  HE3 MET A 163      74.253  68.899  42.188  1.00  0.00
ATOM   2453  C   MET A 163      75.682  63.581  37.814  1.00  0.00
ATOM   2454  O   MET A 163      76.856  63.490  37.457  1.00  0.00
ATOM   2455  N   ALA A 164      74.738  62.733  37.399  1.00  0.00
ATOM   2456  HN  ALA A 164      73.803  62.806  37.737  1.00  0.00
ATOM   2457  CA  ALA A 164      75.002  61.632  36.503  1.00  0.00
ATOM   2458  HA  ALA A 164      75.996  61.708  36.083  1.00  0.00
ATOM   2459  CB  ALA A 164      74.840  60.284  37.235  1.00  0.00
ATOM   2460  HB1 ALA A 164      75.539  60.232  38.093  1.00  0.00
ATOM   2461  HB2 ALA A 164      73.809  60.168  37.634  1.00  0.00
ATOM   2462  HB3 ALA A 164      75.060  59.430  36.559  1.00  0.00
ATOM   2463  C   ALA A 164      74.011  61.614  35.365  1.00  0.00
ATOM   2464  O   ALA A 164      74.273  61.009  34.326  1.00  0.00
ATOM   2465  N   VAL A 165      72.864  62.280  35.530  1.00  0.00
ATOM   2466  HN  VAL A 165      72.667  62.795  36.360  1.00  0.00
ATOM   2467  CA  VAL A 165      71.761  62.152  34.595  1.00  0.00
ATOM   2468  HA  VAL A 165      71.874  61.232  34.040  1.00  0.00
ATOM   2469  CB  VAL A 165      70.390  62.090  35.272  1.00  0.00
ATOM   2470  HB  VAL A 165      69.586  62.016  34.501  1.00  0.00
ATOM   2471  CG1 VAL A 165      70.301  60.793  36.102  1.00  0.00
ATOM   2472 HG11 VAL A 165      69.313  60.735  36.606  1.00  0.00
ATOM   2473 HG12 VAL A 165      70.407  59.909  35.439  1.00  0.00
ATOM   2474 HG13 VAL A 165      71.092  60.748  36.876  1.00  0.00
ATOM   2475  CG2 VAL A 165      70.115  63.359  36.110  1.00  0.00
ATOM   2476 HG21 VAL A 165      69.150  63.255  36.651  1.00  0.00
ATOM   2477 HG22 VAL A 165      70.917  63.519  36.855  1.00  0.00
ATOM   2478 HG23 VAL A 165      70.050  64.259  35.465  1.00  0.00
ATOM   2479  C   VAL A 165      71.741  63.275  33.592  1.00  0.00
ATOM   2480  O   VAL A 165      70.951  63.243  32.652  1.00  0.00
ATOM   2481  N   PHE A 166      72.629  64.265  33.731  1.00  0.00
ATOM   2482  HN  PHE A 166      73.277  64.298  34.488  1.00  0.00
ATOM   2483  CA  PHE A 166      72.692  65.341  32.761  1.00  0.00
ATOM   2484  HA  PHE A 166      71.682  65.589  32.463  1.00  0.00
ATOM   2485  CB  PHE A 166      73.285  66.635  33.400  1.00  0.00
ATOM   2486  HB1 PHE A 166      72.703  66.896  34.310  1.00  0.00
ATOM   2487  HB2 PHE A 166      73.179  67.475  32.680  1.00  0.00
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ATOM   2488  CG  PHE A 166      74.746  66.526  33.776  1.00  0.00
ATOM   2489  CD1 PHE A 166      75.141  66.137  35.069  1.00  0.00
ATOM   2490  HD1 PHE A 166      74.393  65.862  35.798  1.00  0.00
ATOM   2491  CE1 PHE A 166      76.495  66.143  35.432  1.00  0.00
ATOM   2492  HE1 PHE A 166      76.793  65.870  36.431  1.00  0.00
ATOM   2493  CZ  PHE A 166      77.469  66.524  34.503  1.00  0.00
ATOM   2494  HZ  PHE A 166      78.513  66.525  34.784  1.00  0.00
ATOM   2495  CD2 PHE A 166      75.737  66.913  32.855  1.00  0.00
ATOM   2496  HD2 PHE A 166      75.451  67.232  31.863  1.00  0.00
ATOM   2497  CE2 PHE A 166      77.090  66.909  33.213  1.00  0.00
ATOM   2498  HE2 PHE A 166      77.840  67.207  32.495  1.00  0.00
ATOM   2499  C   PHE A 166      73.433  64.880  31.520  1.00  0.00
ATOM   2500  O   PHE A 166      73.188  65.380  30.423  1.00  0.00
ATOM   2501  N   LEU A 167      74.309  63.880  31.671  1.00  0.00
ATOM   2502  HN  LEU A 167      74.523  63.528  32.579  1.00  0.00
ATOM   2503  CA  LEU A 167      74.919  63.156  30.577  1.00  0.00
ATOM   2504  HA  LEU A 167      75.336  63.878  29.889  1.00  0.00
ATOM   2505  CB  LEU A 167      76.033  62.204  31.088  1.00  0.00
ATOM   2506  HB1 LEU A 167      76.431  61.648  30.206  1.00  0.00
ATOM   2507  HB2 LEU A 167      75.612  61.452  31.791  1.00  0.00
ATOM   2508  CG  LEU A 167      77.261  62.875  31.760  1.00  0.00
ATOM   2509  HG  LEU A 167      78.091  62.138  31.662  1.00  0.00
ATOM   2510  CD1 LEU A 167      77.742  64.144  31.030  1.00  0.00
ATOM   2511 HD11 LEU A 167      76.978  64.946  31.091  1.00  0.00
ATOM   2512 HD12 LEU A 167      77.937  63.922  29.959  1.00  0.00
ATOM   2513 HD13 LEU A 167      78.681  64.519  31.490  1.00  0.00
ATOM   2514  CD2 LEU A 167      77.076  63.104  33.275  1.00  0.00
ATOM   2515 HD21 LEU A 167      76.800  62.154  33.778  1.00  0.00
ATOM   2516 HD22 LEU A 167      76.280  63.851  33.468  1.00  0.00
ATOM   2517 HD23 LEU A 167      78.020  63.479  33.724  1.00  0.00
ATOM   2518  C   LEU A 167      73.906  62.335  29.815  1.00  0.00
ATOM   2519  O   LEU A 167      73.934  62.288  28.587  1.00  0.00
ATOM   2520  N   THR A 168      72.987  61.686  30.536  1.00  0.00
ATOM   2521  HN  THR A 168      73.004  61.720  31.533  1.00  0.00
ATOM   2522  CA  THR A 168      71.914  60.882  29.976  1.00  0.00
ATOM   2523  HA  THR A 168      72.371  60.137  29.341  1.00  0.00
ATOM   2524  CB  THR A 168      71.092  60.168  31.046  1.00  0.00
ATOM   2525  HB  THR A 168      70.449  60.886  31.602  1.00  0.00
ATOM   2526  OG1 THR A 168      71.953  59.562  32.001  1.00  0.00
ATOM   2527  HG1 THR A 168      71.381  59.220  32.691  1.00  0.00
ATOM   2528  CG2 THR A 168      70.209  59.077  30.405  1.00  0.00
ATOM   2529 HG21 THR A 168      70.834  58.350  29.845  1.00  0.00
ATOM   2530 HG22 THR A 168      69.473  59.522  29.704  1.00  0.00
ATOM   2531 HG23 THR A 168      69.646  58.525  31.187  1.00  0.00
ATOM   2532  C   THR A 168      70.998  61.733  29.125  1.00  0.00
ATOM   2533  O   THR A 168      70.637  61.354  28.013  1.00  0.00
ATOM   2534  N   VAL A 169      70.654  62.924  29.623  1.00  0.00
ATOM   2535  HN  VAL A 169      70.952  63.190  30.538  1.00  0.00
ATOM   2536  CA  VAL A 169      69.864  63.919  28.928  1.00  0.00
ATOM   2537  HA  VAL A 169      68.950  63.431  28.617  1.00  0.00
ATOM   2538  CB  VAL A 169      69.474  65.084  29.839  1.00  0.00
ATOM   2539  HB  VAL A 169      70.371  65.436  30.397  1.00  0.00
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ATOM   2540  CG1 VAL A 169      68.431  64.562  30.847  1.00  0.00
ATOM   2541 HG11 VAL A 169      68.832  63.731  31.460  1.00  0.00
ATOM   2542 HG12 VAL A 169      67.527  64.199  30.313  1.00  0.00
ATOM   2543 HG13 VAL A 169      68.125  65.385  31.524  1.00  0.00
ATOM   2544  CG2 VAL A 169      68.889  66.287  29.064  1.00  0.00
ATOM   2545 HG21 VAL A 169      68.025  65.967  28.444  1.00  0.00
ATOM   2546 HG22 VAL A 169      69.646  66.760  28.406  1.00  0.00
ATOM   2547 HG23 VAL A 169      68.537  67.059  29.781  1.00  0.00
ATOM   2548  C   VAL A 169      70.536  64.400  27.662  1.00  0.00
ATOM   2549  O   VAL A 169      69.880  64.538  26.631  1.00  0.00
ATOM   2550  N   THR A 170      71.853  64.636  27.715  1.00  0.00
ATOM   2551  HN  THR A 170      72.359  64.513  28.567  1.00  0.00
ATOM   2552  CA  THR A 170      72.627  65.111  26.580  1.00  0.00
ATOM   2553  HA  THR A 170      72.123  66.006  26.242  1.00  0.00
ATOM   2554  CB  THR A 170      74.063  65.524  26.944  1.00  0.00
ATOM   2555  HB  THR A 170      74.042  66.095  27.897  1.00  0.00
ATOM   2556  OG1 THR A 170      74.965  64.436  27.120  1.00  0.00
ATOM   2557  HG1 THR A 170      74.556  63.835  27.752  1.00  0.00
ATOM   2558  CG2 THR A 170      74.626  66.448  25.843  1.00  0.00
ATOM   2559 HG21 THR A 170      73.956  67.319  25.687  1.00  0.00
ATOM   2560 HG22 THR A 170      74.727  65.905  24.879  1.00  0.00
ATOM   2561 HG23 THR A 170      75.629  66.827  26.136  1.00  0.00
ATOM   2562  C   THR A 170      72.595  64.128  25.423  1.00  0.00
ATOM   2563  O   THR A 170      72.392  64.523  24.278  1.00  0.00
ATOM   2564  N   LEU A 171      72.752  62.833  25.716  1.00  0.00
ATOM   2565  HN  LEU A 171      72.904  62.537  26.657  1.00  0.00
ATOM   2566  CA  LEU A 171      72.730  61.775  24.730  1.00  0.00
ATOM   2567  HA  LEU A 171      73.488  62.002  23.993  1.00  0.00
ATOM   2568  CB  LEU A 171      73.067  60.423  25.415  1.00  0.00
ATOM   2569  HB1 LEU A 171      72.338  60.250  26.238  1.00  0.00
ATOM   2570  HB2 LEU A 171      74.072  60.513  25.883  1.00  0.00
ATOM   2571  CG  LEU A 171      73.067  59.170  24.501  1.00  0.00
ATOM   2572  HG  LEU A 171      72.081  59.103  23.986  1.00  0.00
ATOM   2573  CD1 LEU A 171      74.158  59.238  23.414  1.00  0.00
ATOM   2574 HD11 LEU A 171      75.165  59.284  23.879  1.00  0.00
ATOM   2575 HD12 LEU A 171      74.111  58.338  22.765  1.00  0.00
ATOM   2576 HD13 LEU A 171      74.020  60.136  22.776  1.00  0.00
ATOM   2577  CD2 LEU A 171      73.200  57.881  25.334  1.00  0.00
ATOM   2578 HD21 LEU A 171      74.186  57.846  25.840  1.00  0.00
ATOM   2579 HD22 LEU A 171      73.107  56.991  24.678  1.00  0.00
ATOM   2580 HD23 LEU A 171      72.402  57.834  26.106  1.00  0.00
ATOM   2581  C   LEU A 171      71.401  61.664  24.020  1.00  0.00
ATOM   2582  O   LEU A 171      71.352  61.572  22.795  1.00  0.00
ATOM   2583  N   ILE A 172      70.307  61.699  24.786  1.00  0.00
ATOM   2584  HN  ILE A 172      70.395  61.781  25.777  1.00  0.00
ATOM   2585  CA  ILE A 172      68.941  61.609  24.304  1.00  0.00
ATOM   2586  HA  ILE A 172      68.896  60.740  23.662  1.00  0.00
ATOM   2587  CB  ILE A 172      67.950  61.370  25.455  1.00  0.00
ATOM   2588  HB  ILE A 172      68.377  61.819  26.382  1.00  0.00
ATOM   2589  CG2 ILE A 172      66.570  62.040  25.230  1.00  0.00
ATOM   2590 HG21 ILE A 172      65.887  61.781  26.067  1.00  0.00
ATOM   2591 HG22 ILE A 172      66.658  63.145  25.200  1.00  0.00
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ATOM   2592 HG23 ILE A 172      66.110  61.682  24.285  1.00  0.00
ATOM   2593  CG1 ILE A 172      67.745  59.849  25.708  1.00  0.00
ATOM   2594 HG11 ILE A 172      67.039  59.737  26.561  1.00  0.00
ATOM   2595 HG12 ILE A 172      67.251  59.417  24.809  1.00  0.00
ATOM   2596  CD1 ILE A 172      69.002  59.026  26.013  1.00  0.00
ATOM   2597  HD1 ILE A 172      68.726  57.967  26.206  1.00  0.00
ATOM   2598  HD2 ILE A 172      69.709  59.044  25.158  1.00  0.00
ATOM   2599  HD3 ILE A 172      69.518  59.417  26.913  1.00  0.00
ATOM   2600  C   ILE A 172      68.583  62.780  23.412  1.00  0.00
ATOM   2601  O   ILE A 172      67.965  62.596  22.366  1.00  0.00
ATOM   2602  N   ALA A 173      68.984  63.994  23.805  1.00  0.00
ATOM   2603  HN  ALA A 173      69.477  64.110  24.666  1.00  0.00
ATOM   2604  CA  ALA A 173      68.753  65.216  23.061  1.00  0.00
ATOM   2605  HA  ALA A 173      67.688  65.299  22.897  1.00  0.00
ATOM   2606  CB  ALA A 173      69.231  66.447  23.857  1.00  0.00
ATOM   2607  HB1 ALA A 173      68.706  66.489  24.835  1.00  0.00
ATOM   2608  HB2 ALA A 173      70.323  66.395  24.056  1.00  0.00
ATOM   2609  HB3 ALA A 173      69.013  67.388  23.307  1.00  0.00
ATOM   2610  C   ALA A 173      69.437  65.232  21.711  1.00  0.00
ATOM   2611  O   ALA A 173      68.835  65.611  20.707  1.00  0.00
ATOM   2612  N   VAL A 174      70.699  64.795  21.673  1.00  0.00
ATOM   2613  HN  VAL A 174      71.148  64.502  22.516  1.00  0.00
ATOM   2614  CA  VAL A 174      71.530  64.703  20.488  1.00  0.00
ATOM   2615  HA  VAL A 174      71.492  65.670  20.006  1.00  0.00
ATOM   2616  CB  VAL A 174      72.994  64.433  20.842  1.00  0.00
ATOM   2617  HB  VAL A 174      73.047  63.586  21.564  1.00  0.00
ATOM   2618  CG1 VAL A 174      73.559  65.703  21.517  1.00  0.00
ATOM   2619 HG11 VAL A 174      72.955  66.007  22.394  1.00  0.00
ATOM   2620 HG12 VAL A 174      73.567  66.547  20.795  1.00  0.00
ATOM   2621 HG13 VAL A 174      74.601  65.522  21.857  1.00  0.00
ATOM   2622  CG2 VAL A 174      73.853  64.076  19.608  1.00  0.00
ATOM   2623 HG21 VAL A 174      73.768  64.871  18.837  1.00  0.00
ATOM   2624 HG22 VAL A 174      73.546  63.110  19.161  1.00  0.00
ATOM   2625 HG23 VAL A 174      74.919  63.987  19.904  1.00  0.00
ATOM   2626  C   VAL A 174      70.978  63.712  19.480  1.00  0.00
ATOM   2627  O   VAL A 174      71.012  63.954  18.274  1.00  0.00
ATOM   2628  N   LEU A 175      70.426  62.597  19.963  1.00  0.00
ATOM   2629  HN  LEU A 175      70.394  62.426  20.946  1.00  0.00
ATOM   2630  CA  LEU A 175      69.904  61.533  19.128  1.00  0.00
ATOM   2631  HA  LEU A 175      70.408  61.530  18.172  1.00  0.00
ATOM   2632  CB  LEU A 175      70.099  60.156  19.836  1.00  0.00
ATOM   2633  HB1 LEU A 175      69.287  59.438  19.582  1.00  0.00
ATOM   2634  HB2 LEU A 175      70.048  60.316  20.934  1.00  0.00
ATOM   2635  CG  LEU A 175      71.414  59.412  19.487  1.00  0.00
ATOM   2636  HG  LEU A 175      71.479  58.539  20.182  1.00  0.00
ATOM   2637  CD1 LEU A 175      71.380  58.834  18.057  1.00  0.00
ATOM   2638 HD11 LEU A 175      71.323  59.651  17.308  1.00  0.00
ATOM   2639 HD12 LEU A 175      70.497  58.173  17.929  1.00  0.00
ATOM   2640 HD13 LEU A 175      72.297  58.241  17.860  1.00  0.00
ATOM   2641  CD2 LEU A 175      72.681  60.254  19.707  1.00  0.00
ATOM   2642 HD21 LEU A 175      72.723  60.639  20.747  1.00  0.00
ATOM   2643 HD22 LEU A 175      72.700  61.111  19.003  1.00  0.00
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ATOM   2644 HD23 LEU A 175      73.579  59.632  19.518  1.00  0.00
ATOM   2645  C   LEU A 175      68.424  61.719  18.862  1.00  0.00
ATOM   2646  O   LEU A 175      67.802  60.885  18.206  1.00  0.00
ATOM   2647  N   GLY A 176      67.844  62.823  19.340  1.00  0.00
ATOM   2648  HN  GLY A 176      68.376  63.500  19.845  1.00  0.00
ATOM   2649  CA  GLY A 176      66.418  63.059  19.273  1.00  0.00
ATOM   2650  HA1 GLY A 176      66.123  63.405  20.253  1.00  0.00
ATOM   2651  HA2 GLY A 176      65.888  62.165  18.974  1.00  0.00
ATOM   2652  C   GLY A 176      66.093  64.145  18.296  1.00  0.00
ATOM   2653  O   GLY A 176      64.997  64.165  17.739  1.00  0.00
ATOM   2654  N   SER A 177      67.030  65.063  18.056  1.00  0.00
ATOM   2655  HN  SER A 177      67.913  65.043  18.520  1.00  0.00
ATOM   2656  CA  SER A 177      66.841  66.138  17.111  1.00  0.00
ATOM   2657  HA  SER A 177      66.154  65.841  16.330  1.00  0.00
ATOM   2658  CB  SER A 177      66.368  67.434  17.825  1.00  0.00
ATOM   2659  HB1 SER A 177      66.318  68.280  17.107  1.00  0.00
ATOM   2660  HB2 SER A 177      67.076  67.697  18.639  1.00  0.00
ATOM   2661  OG  SER A 177      65.082  67.271  18.409  1.00  0.00
ATOM   2662  HG  SER A 177      64.477  67.088  17.685  1.00  0.00
ATOM   2663  C   SER A 177      68.176  66.426  16.501  1.00  0.00
ATOM   2664  O   SER A 177      69.192  66.454  17.194  1.00  0.00
ATOM   2665  N   ALA A 178      68.190  66.672  15.189  1.00  0.00
ATOM   2666  HN  ALA A 178      67.357  66.622  14.644  1.00  0.00
ATOM   2667  CA  ALA A 178      69.364  67.115  14.477  1.00  0.00
ATOM   2668  HA  ALA A 178      70.226  66.583  14.857  1.00  0.00
ATOM   2669  CB  ALA A 178      69.261  66.884  12.957  1.00  0.00
ATOM   2670  HB1 ALA A 178      68.382  67.414  12.533  1.00  0.00
ATOM   2671  HB2 ALA A 178      69.147  65.799  12.747  1.00  0.00
ATOM   2672  HB3 ALA A 178      70.177  67.243  12.439  1.00  0.00
ATOM   2673  C   ALA A 178      69.526  68.588  14.742  1.00  0.00
ATOM   2674  O   ALA A 178      68.600  69.367  14.516  1.00  0.00
ATOM   2675  N   GLU A 179      70.689  68.966  15.279  1.00  0.00
ATOM   2676  HN  GLU A 179      71.391  68.281  15.454  1.00  0.00
ATOM   2677  CA  GLU A 179      71.078  70.314  15.644  1.00  0.00
ATOM   2678  HA  GLU A 179      72.117  70.240  15.929  1.00  0.00
ATOM   2679  CB  GLU A 179      71.018  71.279  14.426  1.00  0.00
ATOM   2680  HB1 GLU A 179      71.326  72.296  14.764  1.00  0.00
ATOM   2681  HB2 GLU A 179      69.979  71.360  14.044  1.00  0.00
ATOM   2682  CG  GLU A 179      71.971  70.862  13.286  1.00  0.00
ATOM   2683  HG1 GLU A 179      71.699  69.851  12.915  1.00  0.00
ATOM   2684  HG2 GLU A 179      73.015  70.829  13.662  1.00  0.00
ATOM   2685  CD  GLU A 179      71.893  71.858  12.127  1.00  0.00
ATOM   2686  OE1 GLU A 179      72.241  73.049  12.345  1.00  0.00
ATOM   2687  OE2 GLU A 179      71.489  71.438  11.010  1.00  0.00
ATOM   2688  C   GLU A 179      70.356  70.862  16.859  1.00  0.00
ATOM   2689  O   GLU A 179      70.522  72.031  17.199  1.00  0.00
ATOM   2690  N   THR A 180      69.603  70.005  17.560  1.00  0.00
ATOM   2691  HN  THR A 180      69.483  69.071  17.231  1.00  0.00
ATOM   2692  CA  THR A 180      68.994  70.283  18.848  1.00  0.00
ATOM   2693  HA  THR A 180      68.384  69.413  19.036  1.00  0.00
ATOM   2694  CB  THR A 180      69.986  70.314  20.018  1.00  0.00
ATOM   2695  HB  THR A 180      70.772  71.078  19.823  1.00  0.00
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ATOM   2696  OG1 THR A 180      69.372  70.638  21.266  1.00  0.00
ATOM   2697  HG1 THR A 180      69.069  71.547  21.187  1.00  0.00
ATOM   2698  CG2 THR A 180      70.652  68.927  20.147  1.00  0.00
ATOM   2699 HG21 THR A 180      71.213  68.669  19.225  1.00  0.00
ATOM   2700 HG22 THR A 180      69.886  68.143  20.325  1.00  0.00
ATOM   2701 HG23 THR A 180      71.366  68.919  20.998  1.00  0.00
ATOM   2702  C   THR A 180      68.018  71.444  18.841  1.00  0.00
ATOM   2703  O   THR A 180      68.367  72.571  19.191  1.00  0.00
ATOM   2704  N   ASN A 181      66.777  71.178  18.428  1.00  0.00
ATOM   2705  HN  ASN A 181      66.523  70.251  18.166  1.00  0.00
ATOM   2706  CA  ASN A 181      65.718  72.160  18.264  1.00  0.00
ATOM   2707  HA  ASN A 181      66.158  73.080  17.903  1.00  0.00
ATOM   2708  CB  ASN A 181      64.674  71.640  17.232  1.00  0.00
ATOM   2709  HB1 ASN A 181      63.938  72.434  16.987  1.00  0.00
ATOM   2710  HB2 ASN A 181      64.128  70.767  17.651  1.00  0.00
ATOM   2711  CG  ASN A 181      65.351  71.177  15.929  1.00  0.00
ATOM   2712  OD1 ASN A 181      65.128  70.044  15.488  1.00  0.00
ATOM   2713  ND2 ASN A 181      66.208  72.053  15.330  1.00  0.00
ATOM   2714 HD21 ASN A 181      66.691  71.773  14.500  1.00  0.00
ATOM   2715 HD22 ASN A 181      66.366  72.954  15.730  1.00  0.00
ATOM   2716  C   ASN A 181      65.011  72.460  19.576  1.00  0.00
ATOM   2717  O   ASN A 181      63.800  72.679  19.604  1.00  0.00
ATOM   2718  N   LEU A 182      65.757  72.468  20.682  1.00  0.00
ATOM   2719  HN  LEU A 182      66.744  72.330  20.633  1.00  0.00
ATOM   2720  CA  LEU A 182      65.225  72.651  22.007  1.00  0.00
ATOM   2721  HA  LEU A 182      64.344  73.275  21.956  1.00  0.00
ATOM   2722  CB  LEU A 182      64.899  71.267  22.635  1.00  0.00
ATOM   2723  HB1 LEU A 182      65.825  70.649  22.638  1.00  0.00
ATOM   2724  HB2 LEU A 182      64.169  70.758  21.966  1.00  0.00
ATOM   2725  CG  LEU A 182      64.304  71.268  24.065  1.00  0.00
ATOM   2726  HG  LEU A 182      65.041  71.743  24.751  1.00  0.00
ATOM   2727  CD1 LEU A 182      62.989  72.067  24.156  1.00  0.00
ATOM   2728 HD11 LEU A 182      62.226  71.627  23.479  1.00  0.00
ATOM   2729 HD12 LEU A 182      63.145  73.127  23.870  1.00  0.00
ATOM   2730 HD13 LEU A 182      62.596  72.040  25.195  1.00  0.00
ATOM   2731  CD2 LEU A 182      64.100  69.826  24.571  1.00  0.00
ATOM   2732 HD21 LEU A 182      65.057  69.266  24.538  1.00  0.00
ATOM   2733 HD22 LEU A 182      63.358  69.297  23.936  1.00  0.00
ATOM   2734 HD23 LEU A 182      63.730  69.833  25.618  1.00  0.00
ATOM   2735  C   LEU A 182      66.270  73.360  22.828  1.00  0.00
ATOM   2736  O   LEU A 182      67.466  73.122  22.661  1.00  0.00
ATOM   2737  N   SER A 183      65.813  74.226  23.739  1.00  0.00
ATOM   2738  HN  SER A 183      64.831  74.384  23.796  1.00  0.00
ATOM   2739  CA  SER A 183      66.576  74.974  24.722  1.00  0.00
ATOM   2740  HA  SER A 183      65.850  75.604  25.215  1.00  0.00
ATOM   2741  CB  SER A 183      67.164  73.994  25.780  1.00  0.00
ATOM   2742  HB1 SER A 183      68.065  73.482  25.378  1.00  0.00
ATOM   2743  HB2 SER A 183      66.403  73.217  26.005  1.00  0.00
ATOM   2744  OG  SER A 183      67.490  74.630  27.012  1.00  0.00
ATOM   2745  HG  SER A 183      66.655  74.871  27.422  1.00  0.00
ATOM   2746  C   SER A 183      67.628  75.895  24.121  1.00  0.00
ATOM   2747  O   SER A 183      67.614  76.189  22.926  1.00  0.00
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ATOM   2748  N   ALA A 184      68.527  76.406  24.964  1.00  0.00
ATOM   2749  HN  ALA A 184      68.515  76.150  25.929  1.00  0.00
ATOM   2750  CA  ALA A 184      69.572  77.322  24.586  1.00  0.00
ATOM   2751  HA  ALA A 184      69.813  77.190  23.540  1.00  0.00
ATOM   2752  CB  ALA A 184      69.215  78.794  24.873  1.00  0.00
ATOM   2753  HB1 ALA A 184      68.973  78.942  25.947  1.00  0.00
ATOM   2754  HB2 ALA A 184      68.326  79.086  24.274  1.00  0.00
ATOM   2755  HB3 ALA A 184      70.055  79.467  24.598  1.00  0.00
ATOM   2756  C   ALA A 184      70.766  76.938  25.407  1.00  0.00
ATOM   2757  O   ALA A 184      70.659  76.760  26.618  1.00  0.00
ATOM   2758  N   GLY A 185      71.927  76.803  24.760  1.00  0.00
ATOM   2759  HN  GLY A 185      71.979  76.963  23.778  1.00  0.00
ATOM   2760  CA  GLY A 185      73.171  76.388  25.381  1.00  0.00
ATOM   2761  HA1 GLY A 185      73.451  77.158  26.086  1.00  0.00
ATOM   2762  HA2 GLY A 185      73.889  76.270  24.583  1.00  0.00
ATOM   2763  C   GLY A 185      73.082  75.070  26.111  1.00  0.00
ATOM   2764  O   GLY A 185      72.497  74.107  25.617  1.00  0.00
ATOM   2765  N   PHE A 186      73.677  75.014  27.304  1.00  0.00
ATOM   2766  HN  PHE A 186      74.133  75.815  27.682  1.00  0.00
ATOM   2767  CA  PHE A 186      73.762  73.826  28.128  1.00  0.00
ATOM   2768  HA  PHE A 186      73.635  72.949  27.507  1.00  0.00
ATOM   2769  CB  PHE A 186      75.168  73.745  28.807  1.00  0.00
ATOM   2770  HB1 PHE A 186      75.946  73.703  28.014  1.00  0.00
ATOM   2771  HB2 PHE A 186      75.254  72.816  29.411  1.00  0.00
ATOM   2772  CG  PHE A 186      75.465  74.940  29.696  1.00  0.00
ATOM   2773  CD1 PHE A 186      75.214  74.880  31.080  1.00  0.00
ATOM   2774  HD1 PHE A 186      74.800  73.979  31.509  1.00  0.00
ATOM   2775  CE1 PHE A 186      75.484  75.976  31.907  1.00  0.00
ATOM   2776  HE1 PHE A 186      75.278  75.918  32.965  1.00  0.00
ATOM   2777  CZ  PHE A 186      76.026  77.146  31.361  1.00  0.00
ATOM   2778  HZ  PHE A 186      76.237  77.992  31.998  1.00  0.00
ATOM   2779  CD2 PHE A 186      76.031  76.115  29.165  1.00  0.00
ATOM   2780  HD2 PHE A 186      76.252  76.175  28.110  1.00  0.00
ATOM   2781  CE2 PHE A 186      76.303  77.214  29.990  1.00  0.00
ATOM   2782  HE2 PHE A 186      76.729  78.113  29.569  1.00  0.00
ATOM   2783  C   PHE A 186      72.656  73.826  29.170  1.00  0.00
ATOM   2784  O   PHE A 186      72.688  73.040  30.116  1.00  0.00
ATOM   2785  N   LEU A 187      71.665  74.711  29.013  1.00  0.00
ATOM   2786  HN  LEU A 187      71.647  75.306  28.212  1.00  0.00
ATOM   2787  CA  LEU A 187      70.601  74.954  29.968  1.00  0.00
ATOM   2788  HA  LEU A 187      71.080  75.237  30.896  1.00  0.00
ATOM   2789  CB  LEU A 187      69.728  76.146  29.500  1.00  0.00
ATOM   2790  HB1 LEU A 187      69.233  75.912  28.537  1.00  0.00
ATOM   2791  HB2 LEU A 187      70.436  76.986  29.310  1.00  0.00
ATOM   2792  CG  LEU A 187      68.665  76.657  30.509  1.00  0.00
ATOM   2793  HG  LEU A 187      69.023  76.412  31.535  1.00  0.00
ATOM   2794  CD1 LEU A 187      68.540  78.192  30.435  1.00  0.00
ATOM   2795 HD11 LEU A 187      68.199  78.502  29.425  1.00  0.00
ATOM   2796 HD12 LEU A 187      69.520  78.672  30.641  1.00  0.00
ATOM   2797 HD13 LEU A 187      67.806  78.556  31.185  1.00  0.00
ATOM   2798  CD2 LEU A 187      67.276  76.012  30.318  1.00  0.00
ATOM   2799 HD21 LEU A 187      67.321  74.910  30.426  1.00  0.00
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ATOM   2800 HD22 LEU A 187      66.879  76.252  29.309  1.00  0.00
ATOM   2801 HD23 LEU A 187      66.566  76.405  31.076  1.00  0.00
ATOM   2802  C   LEU A 187      69.745  73.746  30.256  1.00  0.00
ATOM   2803  O   LEU A 187      69.379  73.513  31.403  1.00  0.00
ATOM   2804  N   LEU A 188      69.430  72.957  29.225  1.00  0.00
ATOM   2805  HN  LEU A 188      69.728  73.194  28.304  1.00  0.00
ATOM   2806  CA  LEU A 188      68.664  71.727  29.326  1.00  0.00
ATOM   2807  HA  LEU A 188      67.706  71.978  29.759  1.00  0.00
ATOM   2808  CB  LEU A 188      68.469  71.126  27.910  1.00  0.00
ATOM   2809  HB1 LEU A 188      69.466  70.937  27.454  1.00  0.00
ATOM   2810  HB2 LEU A 188      67.963  71.889  27.284  1.00  0.00
ATOM   2811  CG  LEU A 188      67.635  69.823  27.819  1.00  0.00
ATOM   2812  HG  LEU A 188      68.145  69.037  28.421  1.00  0.00
ATOM   2813  CD1 LEU A 188      66.213  69.995  28.387  1.00  0.00
ATOM   2814 HD11 LEU A 188      65.668  70.784  27.827  1.00  0.00
ATOM   2815 HD12 LEU A 188      66.248  70.279  29.459  1.00  0.00
ATOM   2816 HD13 LEU A 188      65.647  69.044  28.298  1.00  0.00
ATOM   2817  CD2 LEU A 188      67.589  69.306  26.368  1.00  0.00
ATOM   2818 HD21 LEU A 188      68.617  69.124  25.989  1.00  0.00
ATOM   2819 HD22 LEU A 188      67.095  70.052  25.709  1.00  0.00
ATOM   2820 HD23 LEU A 188      67.020  68.353  26.315  1.00  0.00
ATOM   2821  C   LEU A 188      69.332  70.696  30.206  1.00  0.00
ATOM   2822  O   LEU A 188      68.682  70.021  31.003  1.00  0.00
ATOM   2823  N   LEU A 189      70.653  70.563  30.074  1.00  0.00
ATOM   2824  HN  LEU A 189      71.153  71.122  29.417  1.00  0.00
ATOM   2825  CA  LEU A 189      71.474  69.673  30.865  1.00  0.00
ATOM   2826  HA  LEU A 189      71.045  68.683  30.797  1.00  0.00
ATOM   2827  CB  LEU A 189      72.923  69.648  30.313  1.00  0.00
ATOM   2828  HB1 LEU A 189      73.466  68.803  30.792  1.00  0.00
ATOM   2829  HB2 LEU A 189      73.457  70.586  30.581  1.00  0.00
ATOM   2830  CG  LEU A 189      73.035  69.485  28.775  1.00  0.00
ATOM   2831  HG  LEU A 189      72.669  70.426  28.300  1.00  0.00
ATOM   2832  CD1 LEU A 189      74.508  69.322  28.356  1.00  0.00
ATOM   2833 HD11 LEU A 189      74.930  68.389  28.786  1.00  0.00
ATOM   2834 HD12 LEU A 189      75.110  70.182  28.716  1.00  0.00
ATOM   2835 HD13 LEU A 189      74.592  69.271  27.250  1.00  0.00
ATOM   2836  CD2 LEU A 189      72.171  68.331  28.229  1.00  0.00
ATOM   2837 HD21 LEU A 189      71.091  68.539  28.374  1.00  0.00
ATOM   2838 HD22 LEU A 189      72.418  67.385  28.752  1.00  0.00
ATOM   2839 HD23 LEU A 189      72.349  68.200  27.141  1.00  0.00
ATOM   2840  C   LEU A 189      71.491  70.084  32.317  1.00  0.00
ATOM   2841  O   LEU A 189      71.400  69.252  33.219  1.00  0.00
ATOM   2842  N   SER A 190      71.572  71.394  32.557  1.00  0.00
ATOM   2843  HN  SER A 190      71.624  72.040  31.797  1.00  0.00
ATOM   2844  CA  SER A 190      71.637  71.981  33.873  1.00  0.00
ATOM   2845  HA  SER A 190      72.330  71.403  34.469  1.00  0.00
ATOM   2846  CB  SER A 190      72.151  73.443  33.758  1.00  0.00
ATOM   2847  HB1 SER A 190      71.418  74.072  33.209  1.00  0.00
ATOM   2848  HB2 SER A 190      73.101  73.438  33.182  1.00  0.00
ATOM   2849  OG  SER A 190      72.412  74.026  35.031  1.00  0.00
ATOM   2850  HG  SER A 190      72.742  74.913  34.864  1.00  0.00
ATOM   2851  C   SER A 190      70.280  71.958  34.546  1.00  0.00
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ATOM   2852  O   SER A 190      70.193  72.003  35.769  1.00  0.00
ATOM   2853  N   PHE A 191      69.200  71.869  33.763  1.00  0.00
ATOM   2854  HN  PHE A 191      69.290  71.842  32.769  1.00  0.00
ATOM   2855  CA  PHE A 191      67.843  71.858  34.265  1.00  0.00
ATOM   2856  HA  PHE A 191      67.726  72.751  34.865  1.00  0.00
ATOM   2857  CB  PHE A 191      66.824  71.938  33.086  1.00  0.00
ATOM   2858  HB1 PHE A 191      66.979  71.090  32.390  1.00  0.00
ATOM   2859  HB2 PHE A 191      66.979  72.882  32.521  1.00  0.00
ATOM   2860  CG  PHE A 191      65.387  71.896  33.565  1.00  0.00
ATOM   2861  CD1 PHE A 191      64.636  70.707  33.493  1.00  0.00
ATOM   2862  HD1 PHE A 191      65.084  69.816  33.079  1.00  0.00
ATOM   2863  CE1 PHE A 191      63.327  70.658  33.986  1.00  0.00
ATOM   2864  HE1 PHE A 191      62.768  69.735  33.943  1.00  0.00
ATOM   2865  CZ  PHE A 191      62.746  71.806  34.539  1.00  0.00
ATOM   2866  HZ  PHE A 191      61.736  71.770  34.921  1.00  0.00
ATOM   2867  CD2 PHE A 191      64.787  73.045  34.109  1.00  0.00
ATOM   2868  HD2 PHE A 191      65.350  73.965  34.168  1.00  0.00
ATOM   2869  CE2 PHE A 191      63.474  73.001  34.596  1.00  0.00
ATOM   2870  HE2 PHE A 191      63.026  73.888  35.018  1.00  0.00
ATOM   2871  C   PHE A 191      67.556  70.679  35.168  1.00  0.00
ATOM   2872  O   PHE A 191      66.995  70.855  36.244  1.00  0.00
ATOM   2873  N   ILE A 192      67.968  69.473  34.764  1.00  0.00
ATOM   2874  HN  ILE A 192      68.441  69.339  33.896  1.00  0.00
ATOM   2875  CA  ILE A 192      67.709  68.284  35.552  1.00  0.00
ATOM   2876  HA  ILE A 192      66.721  68.384  35.983  1.00  0.00
ATOM   2877  CB  ILE A 192      67.691  66.985  34.749  1.00  0.00
ATOM   2878  HB  ILE A 192      67.497  66.142  35.457  1.00  0.00
ATOM   2879  CG2 ILE A 192      69.049  66.721  34.056  1.00  0.00
ATOM   2880 HG21 ILE A 192      69.880  66.686  34.789  1.00  0.00
ATOM   2881 HG22 ILE A 192      69.268  67.508  33.305  1.00  0.00
ATOM   2882 HG23 ILE A 192      69.023  65.740  33.536  1.00  0.00
ATOM   2883  CG1 ILE A 192      66.509  66.995  33.747  1.00  0.00
ATOM   2884 HG11 ILE A 192      66.847  67.429  32.782  1.00  0.00
ATOM   2885 HG12 ILE A 192      65.703  67.652  34.142  1.00  0.00
ATOM   2886  CD1 ILE A 192      65.902  65.606  33.522  1.00  0.00
ATOM   2887  HD1 ILE A 192      65.477  65.214  34.471  1.00  0.00
ATOM   2888  HD2 ILE A 192      66.671  64.891  33.165  1.00  0.00
ATOM   2889  HD3 ILE A 192      65.086  65.656  32.770  1.00  0.00
ATOM   2890  C   ILE A 192      68.665  68.164  36.714  1.00  0.00
ATOM   2891  O   ILE A 192      68.347  67.528  37.716  1.00  0.00
ATOM   2892  N   GLN A 193      69.841  68.793  36.614  1.00  0.00
ATOM   2893  HN  GLN A 193      70.099  69.278  35.783  1.00  0.00
ATOM   2894  CA  GLN A 193      70.760  68.899  37.724  1.00  0.00
ATOM   2895  HA  GLN A 193      70.910  67.907  38.123  1.00  0.00
ATOM   2896  CB  GLN A 193      72.130  69.422  37.225  1.00  0.00
ATOM   2897  HB1 GLN A 193      71.988  70.374  36.669  1.00  0.00
ATOM   2898  HB2 GLN A 193      72.515  68.667  36.503  1.00  0.00
ATOM   2899  CG  GLN A 193      73.162  69.652  38.346  1.00  0.00
ATOM   2900  HG1 GLN A 193      73.210  68.753  38.996  1.00  0.00
ATOM   2901  HG2 GLN A 193      72.868  70.520  38.973  1.00  0.00
ATOM   2902  CD  GLN A 193      74.548  69.930  37.753  1.00  0.00
ATOM   2903  OE1 GLN A 193      75.038  71.064  37.796  1.00  0.00
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ATOM   2904  NE2 GLN A 193      75.189  68.863  37.192  1.00  0.00
ATOM   2905 HE21 GLN A 193      76.094  68.991  36.787  1.00  0.00
ATOM   2906 HE22 GLN A 193      74.750  67.966  37.188  1.00  0.00
ATOM   2907  C   GLN A 193      70.215  69.766  38.839  1.00  0.00
ATOM   2908  O   GLN A 193      70.207  69.370  40.003  1.00  0.00
ATOM   2909  N   GLN A 194      69.707  70.947  38.480  1.00  0.00
ATOM   2910  HN  GLN A 194      69.742  71.238  37.525  1.00  0.00
ATOM   2911  CA  GLN A 194      69.070  71.888  39.373  1.00  0.00
ATOM   2912  HA  GLN A 194      69.754  72.075  40.190  1.00  0.00
ATOM   2913  CB  GLN A 194      68.814  73.227  38.636  1.00  0.00
ATOM   2914  HB1 GLN A 194      68.159  73.882  39.255  1.00  0.00
ATOM   2915  HB2 GLN A 194      68.277  73.007  37.686  1.00  0.00
ATOM   2916  CG  GLN A 194      70.110  74.013  38.349  1.00  0.00
ATOM   2917  HG1 GLN A 194      70.845  73.388  37.802  1.00  0.00
ATOM   2918  HG2 GLN A 194      70.572  74.324  39.310  1.00  0.00
ATOM   2919  CD  GLN A 194      69.797  75.270  37.527  1.00  0.00
ATOM   2920  OE1 GLN A 194      69.829  76.390  38.048  1.00  0.00
ATOM   2921  NE2 GLN A 194      69.484  75.069  36.213  1.00  0.00
ATOM   2922 HE21 GLN A 194      69.512  74.143  35.836  1.00  0.00
ATOM   2923 HE22 GLN A 194      69.265  75.852  35.634  1.00  0.00
ATOM   2924  C   GLN A 194      67.777  71.399  39.977  1.00  0.00
ATOM   2925  O   GLN A 194      67.538  71.583  41.168  1.00  0.00
ATOM   2926  N   PHE A 195      66.926  70.771  39.161  1.00  0.00
ATOM   2927  HN  PHE A 195      67.152  70.624  38.199  1.00  0.00
ATOM   2928  CA  PHE A 195      65.588  70.373  39.547  1.00  0.00
ATOM   2929  HA  PHE A 195      65.181  71.129  40.206  1.00  0.00
ATOM   2930  CB  PHE A 195      64.701  70.244  38.272  1.00  0.00
ATOM   2931  HB1 PHE A 195      64.957  69.336  37.686  1.00  0.00
ATOM   2932  HB2 PHE A 195      64.889  71.127  37.622  1.00  0.00
ATOM   2933  CG  PHE A 195      63.222  70.233  38.595  1.00  0.00
ATOM   2934  CD1 PHE A 195      62.486  71.432  38.548  1.00  0.00
ATOM   2935  HD1 PHE A 195      62.985  72.356  38.297  1.00  0.00
ATOM   2936  CE1 PHE A 195      61.112  71.440  38.816  1.00  0.00
ATOM   2937  HE1 PHE A 195      60.559  72.367  38.774  1.00  0.00
ATOM   2938  CZ  PHE A 195      60.455  70.246  39.140  1.00  0.00
ATOM   2939  HZ  PHE A 195      59.396  70.251  39.348  1.00  0.00
ATOM   2940  CD2 PHE A 195      62.545  69.040  38.905  1.00  0.00
ATOM   2941  HD2 PHE A 195      63.089  68.108  38.933  1.00  0.00
ATOM   2942  CE2 PHE A 195      61.174  69.046  39.190  1.00  0.00
ATOM   2943  HE2 PHE A 195      60.668  68.124  39.433  1.00  0.00
ATOM   2944  C   PHE A 195      65.640  69.050  40.282  1.00  0.00
ATOM   2945  O   PHE A 195      64.732  68.714  41.038  1.00  0.00
ATOM   2946  N   GLY A 196      66.725  68.292  40.106  1.00  0.00
ATOM   2947  HN  GLY A 196      67.448  68.569  39.475  1.00  0.00
ATOM   2948  CA  GLY A 196      66.936  67.030  40.781  1.00  0.00
ATOM   2949  HA1 GLY A 196      67.755  66.541  40.276  1.00  0.00
ATOM   2950  HA2 GLY A 196      66.019  66.460  40.747  1.00  0.00
ATOM   2951  C   GLY A 196      67.324  67.241  42.217  1.00  0.00
ATOM   2952  O   GLY A 196      66.866  66.526  43.107  1.00  0.00
ATOM   2953  N   VAL A 197      68.152  68.257  42.476  1.00  0.00
ATOM   2954  HN  VAL A 197      68.542  68.801  41.736  1.00  0.00
ATOM   2955  CA  VAL A 197      68.508  68.682  43.816  1.00  0.00
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ATOM   2956  HA  VAL A 197      68.636  67.804  44.433  1.00  0.00
ATOM   2957  CB  VAL A 197      69.816  69.475  43.826  1.00  0.00
ATOM   2958  HB  VAL A 197      69.731  70.349  43.141  1.00  0.00
ATOM   2959  CG1 VAL A 197      70.163  69.990  45.242  1.00  0.00
ATOM   2960 HG11 VAL A 197      70.166  69.151  45.969  1.00  0.00
ATOM   2961 HG12 VAL A 197      69.438  70.758  45.582  1.00  0.00
ATOM   2962 HG13 VAL A 197      71.172  70.455  45.238  1.00  0.00
ATOM   2963  CG2 VAL A 197      70.947  68.560  43.306  1.00  0.00
ATOM   2964 HG21 VAL A 197      70.765  68.246  42.259  1.00  0.00
ATOM   2965 HG22 VAL A 197      71.032  67.652  43.940  1.00  0.00
ATOM   2966 HG23 VAL A 197      71.916  69.101  43.337  1.00  0.00
ATOM   2967  C   VAL A 197      67.360  69.495  44.391  1.00  0.00
ATOM   2968  O   VAL A 197      67.150  69.543  45.601  1.00  0.00
ATOM   2969  N   GLY A 198      66.555  70.100  43.515  1.00  0.00
ATOM   2970  HN  GLY A 198      66.745  70.040  42.537  1.00  0.00
ATOM   2971  CA  GLY A 198      65.413  70.914  43.864  1.00  0.00
ATOM   2972  HA1 GLY A 198      65.104  71.414  42.958  1.00  0.00
ATOM   2973  HA2 GLY A 198      65.708  71.602  44.645  1.00  0.00
ATOM   2974  C   GLY A 198      64.251  70.101  44.357  1.00  0.00
ATOM   2975  O   GLY A 198      63.462  70.588  45.160  1.00  0.00
ATOM   2976  N   ALA A 199      64.113  68.858  43.890  1.00  0.00
ATOM   2977  HN  ALA A 199      64.734  68.516  43.186  1.00  0.00
ATOM   2978  CA  ALA A 199      63.122  67.902  44.342  1.00  0.00
ATOM   2979  HA  ALA A 199      62.149  68.360  44.231  1.00  0.00
ATOM   2980  CB  ALA A 199      63.173  66.611  43.499  1.00  0.00
ATOM   2981  HB1 ALA A 199      64.169  66.125  43.576  1.00  0.00
ATOM   2982  HB2 ALA A 199      62.992  66.853  42.430  1.00  0.00
ATOM   2983  HB3 ALA A 199      62.395  65.888  43.826  1.00  0.00
ATOM   2984  C   ALA A 199      63.312  67.536  45.794  1.00  0.00
ATOM   2985  O   ALA A 199      62.351  67.476  46.560  1.00  0.00
ATOM   2986  N   LEU A 200      64.569  67.317  46.194  1.00  0.00
ATOM   2987  HN  LEU A 200      65.319  67.366  45.539  1.00  0.00
ATOM   2988  CA  LEU A 200      64.968  67.043  47.557  1.00  0.00
ATOM   2989  HA  LEU A 200      64.421  66.175  47.885  1.00  0.00
ATOM   2990  CB  LEU A 200      66.491  66.748  47.618  1.00  0.00
ATOM   2991  HB1 LEU A 200      66.835  66.723  48.674  1.00  0.00
ATOM   2992  HB2 LEU A 200      67.034  67.574  47.112  1.00  0.00
ATOM   2993  CG  LEU A 200      66.922  65.410  46.968  1.00  0.00
ATOM   2994  HG  LEU A 200      66.384  65.296  45.999  1.00  0.00
ATOM   2995  CD1 LEU A 200      68.429  65.406  46.650  1.00  0.00
ATOM   2996 HD11 LEU A 200      69.014  65.530  47.585  1.00  0.00
ATOM   2997 HD12 LEU A 200      68.684  66.236  45.961  1.00  0.00
ATOM   2998 HD13 LEU A 200      68.721  64.447  46.171  1.00  0.00
ATOM   2999  CD2 LEU A 200      66.564  64.207  47.862  1.00  0.00
ATOM   3000 HD21 LEU A 200      65.477  64.188  48.075  1.00  0.00
ATOM   3001 HD22 LEU A 200      67.110  64.269  48.827  1.00  0.00
ATOM   3002 HD23 LEU A 200      66.847  63.257  47.362  1.00  0.00
ATOM   3003  C   LEU A 200      64.656  68.182  48.496  1.00  0.00
ATOM   3004  O   LEU A 200      64.173  67.968  49.604  1.00  0.00
ATOM   3005  N   LEU A 201      64.917  69.414  48.056  1.00  0.00
ATOM   3006  HN  LEU A 201      65.304  69.563  47.149  1.00  0.00
ATOM   3007  CA  LEU A 201      64.725  70.603  48.856  1.00  0.00
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ATOM   3008  HA  LEU A 201      64.995  70.383  49.879  1.00  0.00
ATOM   3009  CB  LEU A 201      65.627  71.742  48.319  1.00  0.00
ATOM   3010  HB1 LEU A 201      65.418  72.688  48.867  1.00  0.00
ATOM   3011  HB2 LEU A 201      65.387  71.908  47.245  1.00  0.00
ATOM   3012  CG  LEU A 201      67.147  71.461  48.438  1.00  0.00
ATOM   3013  HG  LEU A 201      67.360  70.469  47.979  1.00  0.00
ATOM   3014  CD1 LEU A 201      67.965  72.500  47.647  1.00  0.00
ATOM   3015 HD11 LEU A 201      67.798  73.518  48.057  1.00  0.00
ATOM   3016 HD12 LEU A 201      67.665  72.493  46.577  1.00  0.00
ATOM   3017 HD13 LEU A 201      69.049  72.265  47.709  1.00  0.00
ATOM   3018  CD2 LEU A 201      67.617  71.391  49.904  1.00  0.00
ATOM   3019 HD21 LEU A 201      67.088  70.582  50.447  1.00  0.00
ATOM   3020 HD22 LEU A 201      67.418  72.355  50.420  1.00  0.00
ATOM   3021 HD23 LEU A 201      68.707  71.184  49.948  1.00  0.00
ATOM   3022  C   LEU A 201      63.286  71.071  48.858  1.00  0.00
ATOM   3023  O   LEU A 201      62.869  71.799  49.756  1.00  0.00
ATOM   3024  N   GLY A 202      62.503  70.643  47.864  1.00  0.00
ATOM   3025  HN  GLY A 202      62.870  70.046  47.153  1.00  0.00
ATOM   3026  CA  GLY A 202      61.141  71.087  47.659  1.00  0.00
ATOM   3027  HA1 GLY A 202      60.914  70.912  46.618  1.00  0.00
ATOM   3028  HA2 GLY A 202      61.057  72.129  47.938  1.00  0.00
ATOM   3029  C   GLY A 202      60.173  70.291  48.479  1.00  0.00
ATOM   3030  O   GLY A 202      59.173  70.825  48.955  1.00  0.00
ATOM   3031  N   LEU A 203      60.459  69.004  48.683  1.00  0.00
ATOM   3032  HN  LEU A 203      61.268  68.583  48.275  1.00  0.00
ATOM   3033  CA  LEU A 203      59.608  68.120  49.449  1.00  0.00
ATOM   3034  HA  LEU A 203      58.607  68.523  49.514  1.00  0.00
ATOM   3035  CB  LEU A 203      59.558  66.723  48.782  1.00  0.00
ATOM   3036  HB1 LEU A 203      58.993  66.011  49.423  1.00  0.00
ATOM   3037  HB2 LEU A 203      60.596  66.341  48.679  1.00  0.00
ATOM   3038  CG  LEU A 203      58.912  66.698  47.373  1.00  0.00
ATOM   3039  HG  LEU A 203      59.472  67.407  46.721  1.00  0.00
ATOM   3040  CD1 LEU A 203      59.052  65.301  46.740  1.00  0.00
ATOM   3041 HD11 LEU A 203      58.527  64.541  47.357  1.00  0.00
ATOM   3042 HD12 LEU A 203      60.124  65.024  46.667  1.00  0.00
ATOM   3043 HD13 LEU A 203      58.615  65.293  45.719  1.00  0.00
ATOM   3044  CD2 LEU A 203      57.437  67.146  47.387  1.00  0.00
ATOM   3045 HD21 LEU A 203      57.345  68.189  47.753  1.00  0.00
ATOM   3046 HD22 LEU A 203      56.839  66.481  48.045  1.00  0.00
ATOM   3047 HD23 LEU A 203      57.013  67.099  46.361  1.00  0.00
ATOM   3048  C   LEU A 203      60.137  67.988  50.857  1.00  0.00
ATOM   3049  O   LEU A 203      59.494  67.376  51.710  1.00  0.00
ATOM   3050  N   ALA A 204      61.278  68.625  51.140  1.00  0.00
ATOM   3051  HN  ALA A 204      61.808  69.069  50.422  1.00  0.00
ATOM   3052  CA  ALA A 204      61.784  68.787  52.483  1.00  0.00
ATOM   3053  HA  ALA A 204      61.342  68.052  53.143  1.00  0.00
ATOM   3054  CB  ALA A 204      63.318  68.656  52.541  1.00  0.00
ATOM   3055  HB1 ALA A 204      63.804  69.405  51.879  1.00  0.00
ATOM   3056  HB2 ALA A 204      63.621  67.643  52.200  1.00  0.00
ATOM   3057  HB3 ALA A 204      63.691  68.801  53.576  1.00  0.00
ATOM   3058  C   ALA A 204      61.415  70.163  52.979  1.00  0.00
ATOM   3059  O   ALA A 204      61.527  70.441  54.170  1.00  0.00
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ATOM   3060  N   GLY A 205      60.919  71.018  52.079  1.00  0.00
ATOM   3061  HN  GLY A 205      60.879  70.765  51.116  1.00  0.00
ATOM   3062  CA  GLY A 205      60.391  72.330  52.389  1.00  0.00
ATOM   3063  HA1 GLY A 205      60.560  72.949  51.520  1.00  0.00
ATOM   3064  HA2 GLY A 205      60.856  72.717  53.285  1.00  0.00
ATOM   3065  C   GLY A 205      58.915  72.231  52.611  1.00  0.00
ATOM   3066  O   GLY A 205      58.343  73.005  53.376  1.00  0.00
ATOM   3067  N   GLY A 206      58.274  71.254  51.962  1.00  0.00
ATOM   3068  HN  GLY A 206      58.765  70.673  51.317  1.00  0.00
ATOM   3069  CA  GLY A 206      56.868  70.951  52.119  1.00  0.00
ATOM   3070  HA1 GLY A 206      56.606  70.255  51.336  1.00  0.00
ATOM   3071  HA2 GLY A 206      56.305  71.874  52.077  1.00  0.00
ATOM   3072  C   GLY A 206      56.612  70.287  53.440  1.00  0.00
ATOM   3073  O   GLY A 206      55.532  70.418  54.010  1.00  0.00
ATOM   3074  N   TRP A 207      57.614  69.564  53.950  1.00  0.00
ATOM   3075  HN  TRP A 207      58.469  69.471  53.446  1.00  0.00
ATOM   3076  CA  TRP A 207      57.584  68.886  55.226  1.00  0.00
ATOM   3077  HA  TRP A 207      56.703  68.262  55.228  1.00  0.00
ATOM   3078  CB  TRP A 207      58.835  67.976  55.369  1.00  0.00
ATOM   3079  HB1 TRP A 207      59.753  68.595  55.462  1.00  0.00
ATOM   3080  HB2 TRP A 207      58.931  67.389  54.428  1.00  0.00
ATOM   3081  CG  TRP A 207      58.755  67.016  56.517  1.00  0.00
ATOM   3082  CD1 TRP A 207      58.220  65.755  56.466  1.00  0.00
ATOM   3083  HD1 TRP A 207      57.868  65.271  55.566  1.00  0.00
ATOM   3084  NE1 TRP A 207      58.162  65.227  57.727  1.00  0.00
ATOM   3085  HE1 TRP A 207      57.778  64.359  57.955  1.00  0.00
ATOM   3086  CE2 TRP A 207      58.663  66.129  58.624  1.00  0.00
ATOM   3087  CD2 TRP A 207      59.067  67.271  57.896  1.00  0.00
ATOM   3088  CE3 TRP A 207      59.628  68.354  58.573  1.00  0.00
ATOM   3089  HE3 TRP A 207      59.952  69.240  58.047  1.00  0.00
ATOM   3090  CZ3 TRP A 207      59.762  68.285  59.961  1.00  0.00
ATOM   3091  HZ3 TRP A 207      60.191  69.120  60.498  1.00  0.00
ATOM   3092  CZ2 TRP A 207      58.774  66.070  60.006  1.00  0.00
ATOM   3093  HZ2 TRP A 207      58.440  65.213  60.566  1.00  0.00
ATOM   3094  CH2 TRP A 207      59.332  67.165  60.667  1.00  0.00
ATOM   3095  HH2 TRP A 207      59.444  67.137  61.742  1.00  0.00
ATOM   3096  C   TRP A 207      57.459  69.853  56.385  1.00  0.00
ATOM   3097  O   TRP A 207      56.762  69.574  57.360  1.00  0.00
ATOM   3098  N   ILE A 208      58.126  71.007  56.282  1.00  0.00
ATOM   3099  HN  ILE A 208      58.673  71.197  55.470  1.00  0.00
ATOM   3100  CA  ILE A 208      58.133  72.069  57.272  1.00  0.00
ATOM   3101  HA  ILE A 208      58.471  71.624  58.197  1.00  0.00
ATOM   3102  CB  ILE A 208      59.081  73.211  56.897  1.00  0.00
ATOM   3103  HB  ILE A 208      58.760  73.641  55.919  1.00  0.00
ATOM   3104  CG2 ILE A 208      60.495  72.625  56.696  1.00  0.00
ATOM   3105 HG21 ILE A 208      60.516  71.928  55.836  1.00  0.00
ATOM   3106 HG22 ILE A 208      60.829  72.079  57.602  1.00  0.00
ATOM   3107 HG23 ILE A 208      61.220  73.441  56.490  1.00  0.00
ATOM   3108  CG1 ILE A 208      59.098  74.381  57.922  1.00  0.00
ATOM   3109 HG11 ILE A 208      58.102  74.872  57.950  1.00  0.00
ATOM   3110 HG12 ILE A 208      59.818  75.146  57.553  1.00  0.00
ATOM   3111  CD1 ILE A 208      59.501  73.983  59.347  1.00  0.00
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ATOM   3112  HD1 ILE A 208      60.537  73.585  59.370  1.00  0.00
ATOM   3113  HD2 ILE A 208      58.816  73.208  59.748  1.00  0.00
ATOM   3114  HD3 ILE A 208      59.456  74.867  60.019  1.00  0.00
ATOM   3115  C   ILE A 208      56.741  72.611  57.504  1.00  0.00
ATOM   3116  O   ILE A 208      56.359  72.885  58.639  1.00  0.00
ATOM   3117  N   LEU A 209      55.958  72.751  56.430  1.00  0.00
ATOM   3118  HN  LEU A 209      56.293  72.511  55.522  1.00  0.00
ATOM   3119  CA  LEU A 209      54.594  73.239  56.472  1.00  0.00
ATOM   3120  HA  LEU A 209      54.614  74.224  56.916  1.00  0.00
ATOM   3121  CB  LEU A 209      54.007  73.322  55.038  1.00  0.00
ATOM   3122  HB1 LEU A 209      52.999  73.794  55.087  1.00  0.00
ATOM   3123  HB2 LEU A 209      53.878  72.297  54.626  1.00  0.00
ATOM   3124  CG  LEU A 209      54.858  74.123  54.020  1.00  0.00
ATOM   3125  HG  LEU A 209      55.849  73.623  53.926  1.00  0.00
ATOM   3126  CD1 LEU A 209      54.212  74.084  52.621  1.00  0.00
ATOM   3127 HD11 LEU A 209      53.218  74.577  52.642  1.00  0.00
ATOM   3128 HD12 LEU A 209      54.081  73.033  52.286  1.00  0.00
ATOM   3129 HD13 LEU A 209      54.855  74.611  51.885  1.00  0.00
ATOM   3130  CD2 LEU A 209      55.111  75.574  54.472  1.00  0.00
ATOM   3131 HD21 LEU A 209      55.664  75.597  55.434  1.00  0.00
ATOM   3132 HD22 LEU A 209      54.147  76.110  54.602  1.00  0.00
ATOM   3133 HD23 LEU A 209      55.715  76.112  53.711  1.00  0.00
ATOM   3134  C   LEU A 209      53.687  72.367  57.311  1.00  0.00
ATOM   3135  O   LEU A 209      52.921  72.875  58.128  1.00  0.00
ATOM   3136  N   TRP A 210      53.794  71.044  57.147  1.00  0.00
ATOM   3137  HN  TRP A 210      54.414  70.664  56.465  1.00  0.00
ATOM   3138  CA  TRP A 210      53.088  70.070  57.956  1.00  0.00
ATOM   3139  HA  TRP A 210      52.033  70.304  57.901  1.00  0.00
ATOM   3140  CB  TRP A 210      53.321  68.635  57.418  1.00  0.00
ATOM   3141  HB1 TRP A 210      52.873  67.897  58.121  1.00  0.00
ATOM   3142  HB2 TRP A 210      54.414  68.430  57.379  1.00  0.00
ATOM   3143  CG  TRP A 210      52.725  68.378  56.072  1.00  0.00
ATOM   3144  CD1 TRP A 210      53.395  68.143  54.903  1.00  0.00
ATOM   3145  HD1 TRP A 210      54.468  68.163  54.802  1.00  0.00
ATOM   3146  NE1 TRP A 210      52.501  67.887  53.899  1.00  0.00
ATOM   3147  HE1 TRP A 210      52.728  67.696  52.969  1.00  0.00
ATOM   3148  CE2 TRP A 210      51.230  67.956  54.390  1.00  0.00
ATOM   3149  CD2 TRP A 210      51.326  68.281  55.762  1.00  0.00
ATOM   3150  CE3 TRP A 210      50.163  68.426  56.515  1.00  0.00
ATOM   3151  HE3 TRP A 210      50.202  68.679  57.564  1.00  0.00
ATOM   3152  CZ3 TRP A 210      48.931  68.209  55.896  1.00  0.00
ATOM   3153  HZ3 TRP A 210      48.025  68.295  56.476  1.00  0.00
ATOM   3154  CZ2 TRP A 210      50.003  67.750  53.770  1.00  0.00
ATOM   3155  HZ2 TRP A 210      49.929  67.491  52.725  1.00  0.00
ATOM   3156  CH2 TRP A 210      48.851  67.873  54.548  1.00  0.00
ATOM   3157  HH2 TRP A 210      47.882  67.707  54.097  1.00  0.00
ATOM   3158  C   TRP A 210      53.477  70.108  59.413  1.00  0.00
ATOM   3159  O   TRP A 210      52.622  70.042  60.289  1.00  0.00
ATOM   3160  N   TRP A 211      54.776  70.225  59.692  1.00  0.00
ATOM   3161  HN  TRP A 211      55.452  70.273  58.958  1.00  0.00
ATOM   3162  CA  TRP A 211      55.313  70.287  61.034  1.00  0.00
ATOM   3163  HA  TRP A 211      54.965  69.407  61.556  1.00  0.00
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ATOM   3164  CB  TRP A 211      56.869  70.231  60.978  1.00  0.00
ATOM   3165  HB1 TRP A 211      57.235  71.033  60.302  1.00  0.00
ATOM   3166  HB2 TRP A 211      57.143  69.263  60.504  1.00  0.00
ATOM   3167  CG  TRP A 211      57.588  70.351  62.290  1.00  0.00
ATOM   3168  CD1 TRP A 211      57.911  69.328  63.143  1.00  0.00
ATOM   3169  HD1 TRP A 211      57.698  68.285  62.962  1.00  0.00
ATOM   3170  NE1 TRP A 211      58.510  69.834  64.266  1.00  0.00
ATOM   3171  HE1 TRP A 211      58.817  69.315  65.033  1.00  0.00
ATOM   3172  CE2 TRP A 211      58.586  71.195  64.172  1.00  0.00
ATOM   3173  CD2 TRP A 211      58.016  71.564  62.933  1.00  0.00
ATOM   3174  CE3 TRP A 211      57.959  72.913  62.582  1.00  0.00
ATOM   3175  HE3 TRP A 211      57.527  73.232  61.646  1.00  0.00
ATOM   3176  CZ3 TRP A 211      58.459  73.866  63.471  1.00  0.00
ATOM   3177  HZ3 TRP A 211      58.413  74.914  63.209  1.00  0.00
ATOM   3178  CZ2 TRP A 211      59.087  72.141  65.058  1.00  0.00
ATOM   3179  HZ2 TRP A 211      59.515  71.860  66.008  1.00  0.00
ATOM   3180  CH2 TRP A 211      59.014  73.486  64.690  1.00  0.00
ATOM   3181  HH2 TRP A 211      59.391  74.243  65.364  1.00  0.00
ATOM   3182  C   TRP A 211      54.828  71.493  61.817  1.00  0.00
ATOM   3183  O   TRP A 211      54.499  71.382  62.997  1.00  0.00
ATOM   3184  N   LEU A 212      54.789  72.652  61.157  1.00  0.00
ATOM   3185  HN  LEU A 212      55.033  72.679  60.189  1.00  0.00
ATOM   3186  CA  LEU A 212      54.527  73.949  61.741  1.00  0.00
ATOM   3187  HA  LEU A 212      55.266  74.091  62.516  1.00  0.00
ATOM   3188  CB  LEU A 212      54.710  75.043  60.658  1.00  0.00
ATOM   3189  HB1 LEU A 212      53.981  74.866  59.837  1.00  0.00
ATOM   3190  HB2 LEU A 212      55.728  74.924  60.226  1.00  0.00
ATOM   3191  CG  LEU A 212      54.574  76.510  61.135  1.00  0.00
ATOM   3192  HG  LEU A 212      53.547  76.658  61.541  1.00  0.00
ATOM   3193  CD1 LEU A 212      55.576  76.855  62.255  1.00  0.00
ATOM   3194 HD11 LEU A 212      56.617  76.690  61.905  1.00  0.00
ATOM   3195 HD12 LEU A 212      55.398  76.224  63.151  1.00  0.00
ATOM   3196 HD13 LEU A 212      55.467  77.919  62.554  1.00  0.00
ATOM   3197  CD2 LEU A 212      54.728  77.481  59.947  1.00  0.00
ATOM   3198 HD21 LEU A 212      53.970  77.258  59.167  1.00  0.00
ATOM   3199 HD22 LEU A 212      55.739  77.381  59.498  1.00  0.00
ATOM   3200 HD23 LEU A 212      54.592  78.530  60.285  1.00  0.00
ATOM   3201  C   LEU A 212      53.165  74.075  62.385  1.00  0.00
ATOM   3202  O   LEU A 212      53.037  74.632  63.474  1.00  0.00
ATOM   3203  N   ILE A 213      52.134  73.539  61.729  1.00  0.00
ATOM   3204  HN  ILE A 213      52.271  73.072  60.858  1.00  0.00
ATOM   3205  CA  ILE A 213      50.755  73.627  62.173  1.00  0.00
ATOM   3206  HA  ILE A 213      50.670  74.391  62.933  1.00  0.00
ATOM   3207  CB  ILE A 213      49.816  74.005  61.025  1.00  0.00
ATOM   3208  HB  ILE A 213      48.783  74.117  61.430  1.00  0.00
ATOM   3209  CG2 ILE A 213      49.789  72.906  59.935  1.00  0.00
ATOM   3210 HG21 ILE A 213      49.418  71.943  60.340  1.00  0.00
ATOM   3211 HG22 ILE A 213      50.800  72.743  59.511  1.00  0.00
ATOM   3212 HG23 ILE A 213      49.110  73.201  59.108  1.00  0.00
ATOM   3213  CG1 ILE A 213      50.234  75.388  60.458  1.00  0.00
ATOM   3214 HG11 ILE A 213      51.187  75.286  59.894  1.00  0.00
ATOM   3215 HG12 ILE A 213      50.419  76.075  61.313  1.00  0.00
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ATOM   3216  CD1 ILE A 213      49.179  76.030  59.551  1.00  0.00
ATOM   3217  HD1 ILE A 213      48.216  76.141  60.093  1.00  0.00
ATOM   3218  HD2 ILE A 213      49.007  75.413  58.644  1.00  0.00
ATOM   3219  HD3 ILE A 213      49.516  77.038  59.226  1.00  0.00
ATOM   3220  C   ILE A 213      50.341  72.315  62.804  1.00  0.00
ATOM   3221  O   ILE A 213      49.163  72.089  63.080  1.00  0.00
ATOM   3222  N   ASN A 214      51.321  71.443  63.056  1.00  0.00
ATOM   3223  HN  ASN A 214      52.260  71.715  62.858  1.00  0.00
ATOM   3224  CA  ASN A 214      51.204  70.075  63.511  1.00  0.00
ATOM   3225  HA  ASN A 214      52.219  69.706  63.482  1.00  0.00
ATOM   3226  CB  ASN A 214      50.688  70.039  64.985  1.00  0.00
ATOM   3227  HB1 ASN A 214      51.114  70.909  65.532  1.00  0.00
ATOM   3228  HB2 ASN A 214      49.583  70.129  65.017  1.00  0.00
ATOM   3229  CG  ASN A 214      51.125  68.759  65.715  1.00  0.00
ATOM   3230  OD1 ASN A 214      50.291  67.928  66.088  1.00  0.00
ATOM   3231  ND2 ASN A 214      52.468  68.601  65.906  1.00  0.00
ATOM   3232 HD21 ASN A 214      52.804  67.788  66.379  1.00  0.00
ATOM   3233 HD22 ASN A 214      53.104  69.305  65.591  1.00  0.00
ATOM   3234  C   ASN A 214      50.399  69.208  62.545  1.00  0.00
ATOM   3235  O   ASN A 214      50.088  69.608  61.427  1.00  0.00
ATOM   3236  N   ARG A 215      50.097  67.975  62.946  1.00  0.00
ATOM   3237  HN  ARG A 215      50.292  67.685  63.880  1.00  0.00
ATOM   3238  CA  ARG A 215      49.562  66.941  62.092  1.00  0.00
ATOM   3239  HA  ARG A 215      49.834  67.165  61.070  1.00  0.00
ATOM   3240  CB  ARG A 215      50.195  65.575  62.472  1.00  0.00
ATOM   3241  HB1 ARG A 215      50.065  65.443  63.571  1.00  0.00
ATOM   3242  HB2 ARG A 215      49.690  64.719  61.976  1.00  0.00
ATOM   3243  CG  ARG A 215      51.700  65.486  62.138  1.00  0.00
ATOM   3244  HG1 ARG A 215      52.147  66.503  62.103  1.00  0.00
ATOM   3245  HG2 ARG A 215      52.201  64.939  62.969  1.00  0.00
ATOM   3246  CD  ARG A 215      52.041  64.731  60.839  1.00  0.00
ATOM   3247  HD1 ARG A 215      53.138  64.782  60.660  1.00  0.00
ATOM   3248  HD2 ARG A 215      51.725  63.668  60.926  1.00  0.00
ATOM   3249  NE  ARG A 215      51.328  65.338  59.669  1.00  0.00
ATOM   3250  HE  ARG A 215      50.639  66.042  59.833  1.00  0.00
ATOM   3251  CZ  ARG A 215      51.517  64.906  58.400  1.00  0.00
ATOM   3252  NH1 ARG A 215      50.744  65.391  57.408  1.00  0.00
ATOM   3253 HH11 ARG A 215      50.872  65.067  56.472  1.00  0.00
ATOM   3254 HH12 ARG A 215      50.019  66.050  57.605  1.00  0.00
ATOM   3255  NH2 ARG A 215      52.460  63.991  58.100  1.00  0.00
ATOM   3256 HH21 ARG A 215      52.606  63.729  57.143  1.00  0.00
ATOM   3257 HH22 ARG A 215      53.052  63.636  58.818  1.00  0.00
ATOM   3258  C   ARG A 215      48.056  66.871  62.133  1.00  0.00
ATOM   3259  O   ARG A 215      47.405  67.624  62.857  1.00  0.00
ATOM   3260  N   ASN A 216      47.494  65.946  61.348  1.00  0.00
ATOM   3261  HN  ASN A 216      48.078  65.393  60.761  1.00  0.00
ATOM   3262  CA  ASN A 216      46.088  65.602  61.254  1.00  0.00
ATOM   3263  HA  ASN A 216      46.023  64.870  60.461  1.00  0.00
ATOM   3264  CB  ASN A 216      45.584  64.931  62.566  1.00  0.00
ATOM   3265  HB1 ASN A 216      44.513  64.653  62.459  1.00  0.00
ATOM   3266  HB2 ASN A 216      45.681  65.643  63.413  1.00  0.00
ATOM   3267  CG  ASN A 216      46.374  63.647  62.875  1.00  0.00
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ATOM   3268  OD1 ASN A 216      47.082  63.086  62.030  1.00  0.00
ATOM   3269  ND2 ASN A 216      46.254  63.179  64.153  1.00  0.00
ATOM   3270 HD21 ASN A 216      46.740  62.348  64.421  1.00  0.00
ATOM   3271 HD22 ASN A 216      45.679  63.664  64.810  1.00  0.00
ATOM   3272  C   ASN A 216      45.197  66.742  60.828  1.00  0.00
ATOM   3273  O   ASN A 216      44.325  67.190  61.572  1.00  0.00
ATOM   3274  N   GLN A 217      45.405  67.214  59.599  1.00  0.00
ATOM   3275  HN  GLN A 217      46.130  66.829  59.028  1.00  0.00
ATOM   3276  CA  GLN A 217      44.589  68.214  58.950  1.00  0.00
ATOM   3277  HA  GLN A 217      44.269  68.935  59.692  1.00  0.00
ATOM   3278  CB  GLN A 217      45.391  68.962  57.849  1.00  0.00
ATOM   3279  HB1 GLN A 217      44.695  69.491  57.161  1.00  0.00
ATOM   3280  HB2 GLN A 217      45.936  68.202  57.247  1.00  0.00
ATOM   3281  CG  GLN A 217      46.388  70.041  58.342  1.00  0.00
ATOM   3282  HG1 GLN A 217      45.805  70.914  58.710  1.00  0.00
ATOM   3283  HG2 GLN A 217      47.005  70.385  57.485  1.00  0.00
ATOM   3284  CD  GLN A 217      47.330  69.540  59.445  1.00  0.00
ATOM   3285  OE1 GLN A 217      48.164  68.659  59.205  1.00  0.00
ATOM   3286  NE2 GLN A 217      47.187  70.110  60.677  1.00  0.00
ATOM   3287 HE21 GLN A 217      47.800  69.832  61.417  1.00  0.00
ATOM   3288 HE22 GLN A 217      46.491  70.809  60.831  1.00  0.00
ATOM   3289  C   GLN A 217      43.354  67.578  58.360  1.00  0.00
ATOM   3290  O   GLN A 217      43.333  66.383  58.072  1.00  0.00
ATOM   3291  N   LEU A 218      42.294  68.373  58.193  1.00  0.00
ATOM   3292  HN  LEU A 218      42.342  69.338  58.438  1.00  0.00
ATOM   3293  CA  LEU A 218      41.003  67.933  57.704  1.00  0.00
ATOM   3294  HA  LEU A 218      40.693  67.145  58.377  1.00  0.00
ATOM   3295  CB  LEU A 218      39.959  69.076  57.858  1.00  0.00
ATOM   3296  HB1 LEU A 218      40.319  69.981  57.328  1.00  0.00
ATOM   3297  HB2 LEU A 218      39.903  69.339  58.937  1.00  0.00
ATOM   3298  CG  LEU A 218      38.520  68.780  57.364  1.00  0.00
ATOM   3299  HG  LEU A 218      38.566  68.494  56.288  1.00  0.00
ATOM   3300  CD1 LEU A 218      37.863  67.618  58.133  1.00  0.00
ATOM   3301 HD11 LEU A 218      37.794  67.862  59.214  1.00  0.00
ATOM   3302 HD12 LEU A 218      38.451  66.684  58.019  1.00  0.00
ATOM   3303 HD13 LEU A 218      36.838  67.433  57.748  1.00  0.00
ATOM   3304  CD2 LEU A 218      37.645  70.047  57.444  1.00  0.00
ATOM   3305 HD21 LEU A 218      38.095  70.867  56.845  1.00  0.00
ATOM   3306 HD22 LEU A 218      37.556  70.387  58.498  1.00  0.00
ATOM   3307 HD23 LEU A 218      36.628  69.840  57.051  1.00  0.00
ATOM   3308  C   LEU A 218      40.999  67.311  56.310  1.00  0.00
ATOM   3309  O   LEU A 218      40.327  66.289  56.173  1.00  0.00
ATOM   3310  N   PRO A 219      41.690  67.778  55.250  1.00  0.00
ATOM   3311  CD  PRO A 219      42.232  69.135  55.135  1.00  0.00
ATOM   3312  HD1 PRO A 219      43.318  69.089  55.365  1.00  0.00
ATOM   3313  HD2 PRO A 219      41.732  69.863  55.803  1.00  0.00
ATOM   3314  CA  PRO A 219      41.631  67.125  53.943  1.00  0.00
ATOM   3315  HA  PRO A 219      40.596  66.909  53.716  1.00  0.00
ATOM   3316  CB  PRO A 219      42.239  68.161  52.975  1.00  0.00
ATOM   3317  HB1 PRO A 219      41.759  68.121  51.977  1.00  0.00
ATOM   3318  HB2 PRO A 219      43.338  68.020  52.857  1.00  0.00
ATOM   3319  CG  PRO A 219      42.014  69.503  53.671  1.00  0.00
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ATOM   3320  HG1 PRO A 219      42.709  70.291  53.317  1.00  0.00
ATOM   3321  HG2 PRO A 219      40.963  69.833  53.520  1.00  0.00
ATOM   3322  C   PRO A 219      42.428  65.841  53.853  1.00  0.00
ATOM   3323  O   PRO A 219      42.554  65.327  52.742  1.00  0.00
ATOM   3324  N   GLU A 220      42.954  65.302  54.956  1.00  0.00
ATOM   3325  HN  GLU A 220      42.842  65.722  55.854  1.00  0.00
ATOM   3326  CA  GLU A 220      43.694  64.065  54.924  1.00  0.00
ATOM   3327  HA  GLU A 220      44.180  63.958  53.963  1.00  0.00
ATOM   3328  CB  GLU A 220      44.798  64.046  56.016  1.00  0.00
ATOM   3329  HB1 GLU A 220      45.276  63.038  56.004  1.00  0.00
ATOM   3330  HB2 GLU A 220      44.348  64.199  57.021  1.00  0.00
ATOM   3331  CG  GLU A 220      45.897  65.104  55.775  1.00  0.00
ATOM   3332  HG1 GLU A 220      45.495  66.124  55.951  1.00  0.00
ATOM   3333  HG2 GLU A 220      46.235  65.042  54.718  1.00  0.00
ATOM   3334  CD  GLU A 220      47.101  64.862  56.688  1.00  0.00
ATOM   3335  OE1 GLU A 220      47.086  65.348  57.851  1.00  0.00
ATOM   3336  OE2 GLU A 220      48.060  64.179  56.237  1.00  0.00
ATOM   3337  C   GLU A 220      42.738  62.918  55.112  1.00  0.00
ATOM   3338  O   GLU A 220      42.236  62.682  56.209  1.00  0.00
ATOM   3339  N   GLY A 221      42.472  62.192  54.022  1.00  0.00
ATOM   3340  HN  GLY A 221      42.872  62.447  53.146  1.00  0.00
ATOM   3341  CA  GLY A 221      41.654  60.999  53.995  1.00  0.00
ATOM   3342  HA1 GLY A 221      41.334  60.863  52.973  1.00  0.00
ATOM   3343  HA2 GLY A 221      40.835  61.110  54.692  1.00  0.00
ATOM   3344  C   GLY A 221      42.477  59.811  54.401  1.00  0.00
ATOM   3345  O   GLY A 221      43.410  59.919  55.196  1.00  0.00
ATOM   3346  N   LEU A 222      42.145  58.638  53.853  1.00  0.00
ATOM   3347  HN  LEU A 222      41.368  58.558  53.235  1.00  0.00
ATOM   3348  CA  LEU A 222      42.905  57.422  54.043  1.00  0.00
ATOM   3349  HA  LEU A 222      42.973  57.242  55.108  1.00  0.00
ATOM   3350  CB  LEU A 222      42.205  56.212  53.374  1.00  0.00
ATOM   3351  HB1 LEU A 222      42.824  55.307  53.577  1.00  0.00
ATOM   3352  HB2 LEU A 222      42.169  56.351  52.275  1.00  0.00
ATOM   3353  CG  LEU A 222      40.770  55.918  53.879  1.00  0.00
ATOM   3354  HG  LEU A 222      40.689  56.299  54.924  1.00  0.00
ATOM   3355  CD1 LEU A 222      39.682  56.610  53.030  1.00  0.00
ATOM   3356 HD11 LEU A 222      39.733  56.255  51.979  1.00  0.00
ATOM   3357 HD12 LEU A 222      39.804  57.711  53.037  1.00  0.00
ATOM   3358 HD13 LEU A 222      38.675  56.371  53.431  1.00  0.00
ATOM   3359  CD2 LEU A 222      40.508  54.400  53.936  1.00  0.00
ATOM   3360 HD21 LEU A 222      41.244  53.905  54.604  1.00  0.00
ATOM   3361 HD22 LEU A 222      40.594  53.955  52.922  1.00  0.00
ATOM   3362 HD23 LEU A 222      39.488  54.199  54.326  1.00  0.00
ATOM   3363  C   LEU A 222      44.301  57.563  53.488  1.00  0.00
ATOM   3364  O   LEU A 222      44.504  58.164  52.437  1.00  0.00
ATOM   3365  N   TYR A 223      45.291  57.031  54.205  1.00  0.00
ATOM   3366  HN  TYR A 223      45.110  56.532  55.049  1.00  0.00
ATOM   3367  CA  TYR A 223      46.688  57.260  53.904  1.00  0.00
ATOM   3368  HA  TYR A 223      46.816  58.306  53.666  1.00  0.00
ATOM   3369  CB  TYR A 223      47.555  56.912  55.144  1.00  0.00
ATOM   3370  HB1 TYR A 223      48.627  57.132  54.953  1.00  0.00
ATOM   3371  HB2 TYR A 223      47.445  55.834  55.389  1.00  0.00
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ATOM   3372  CG  TYR A 223      47.127  57.721  56.346  1.00  0.00
ATOM   3373  CD1 TYR A 223      46.677  57.095  57.522  1.00  0.00
ATOM   3374  HD1 TYR A 223      46.659  56.017  57.584  1.00  0.00
ATOM   3375  CE1 TYR A 223      46.225  57.856  58.608  1.00  0.00
ATOM   3376  HE1 TYR A 223      45.876  57.360  59.503  1.00  0.00
ATOM   3377  CZ  TYR A 223      46.223  59.255  58.531  1.00  0.00
ATOM   3378  OH  TYR A 223      45.771  60.026  59.623  1.00  0.00
ATOM   3379  HH  TYR A 223      45.794  60.950  59.362  1.00  0.00
ATOM   3380  CD2 TYR A 223      47.157  59.126  56.298  1.00  0.00
ATOM   3381  HD2 TYR A 223      47.523  59.626  55.414  1.00  0.00
ATOM   3382  CE2 TYR A 223      46.688  59.890  57.373  1.00  0.00
ATOM   3383  HE2 TYR A 223      46.695  60.968  57.305  1.00  0.00
ATOM   3384  C   TYR A 223      47.150  56.472  52.703  1.00  0.00
ATOM   3385  O   TYR A 223      48.072  56.884  52.000  1.00  0.00
ATOM   3386  N   SER A 224      46.482  55.351  52.423  1.00  0.00
ATOM   3387  HN  SER A 224      45.760  55.025  53.029  1.00  0.00
ATOM   3388  CA  SER A 224      46.614  54.604  51.191  1.00  0.00
ATOM   3389  HA  SER A 224      47.661  54.389  51.044  1.00  0.00
ATOM   3390  CB  SER A 224      45.855  53.255  51.303  1.00  0.00
ATOM   3391  HB1 SER A 224      46.380  52.632  52.059  1.00  0.00
ATOM   3392  HB2 SER A 224      45.867  52.708  50.336  1.00  0.00
ATOM   3393  OG  SER A 224      44.509  53.427  51.743  1.00  0.00
ATOM   3394  HG  SER A 224      44.118  52.549  51.765  1.00  0.00
ATOM   3395  C   SER A 224      46.147  55.380  49.975  1.00  0.00
ATOM   3396  O   SER A 224      46.814  55.388  48.945  1.00  0.00
ATOM   3397  N   ILE A 225      45.001  56.058  50.093  1.00  0.00
ATOM   3398  HN  ILE A 225      44.486  56.018  50.946  1.00  0.00
ATOM   3399  CA  ILE A 225      44.404  56.889  49.063  1.00  0.00
ATOM   3400  HA  ILE A 225      44.380  56.292  48.162  1.00  0.00
ATOM   3401  CB  ILE A 225      42.963  57.276  49.400  1.00  0.00
ATOM   3402  HB  ILE A 225      42.950  57.773  50.397  1.00  0.00
ATOM   3403  CG2 ILE A 225      42.136  55.973  49.515  1.00  0.00
ATOM   3404 HG21 ILE A 225      42.518  55.319  50.325  1.00  0.00
ATOM   3405 HG22 ILE A 225      42.172  55.401  48.565  1.00  0.00
ATOM   3406 HG23 ILE A 225      41.076  56.215  49.741  1.00  0.00
ATOM   3407  CG1 ILE A 225      42.310  58.267  48.395  1.00  0.00
ATOM   3408 HG11 ILE A 225      42.865  59.229  48.401  1.00  0.00
ATOM   3409 HG12 ILE A 225      41.282  58.488  48.761  1.00  0.00
ATOM   3410  CD1 ILE A 225      42.206  57.754  46.952  1.00  0.00
ATOM   3411  HD1 ILE A 225      41.579  56.840  46.899  1.00  0.00
ATOM   3412  HD2 ILE A 225      43.209  57.520  46.539  1.00  0.00
ATOM   3413  HD3 ILE A 225      41.739  58.528  46.306  1.00  0.00
ATOM   3414  C   ILE A 225      45.259  58.099  48.758  1.00  0.00
ATOM   3415  O   ILE A 225      45.436  58.465  47.600  1.00  0.00
ATOM   3416  N   LEU A 226      45.841  58.712  49.793  1.00  0.00
ATOM   3417  HN  LEU A 226      45.658  58.408  50.727  1.00  0.00
ATOM   3418  CA  LEU A 226      46.764  59.826  49.678  1.00  0.00
ATOM   3419  HA  LEU A 226      46.276  60.589  49.090  1.00  0.00
ATOM   3420  CB  LEU A 226      47.095  60.402  51.079  1.00  0.00
ATOM   3421  HB1 LEU A 226      47.944  61.119  51.010  1.00  0.00
ATOM   3422  HB2 LEU A 226      47.412  59.565  51.738  1.00  0.00
ATOM   3423  CG  LEU A 226      45.919  61.158  51.751  1.00  0.00
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ATOM   3424  HG  LEU A 226      45.009  60.520  51.691  1.00  0.00
ATOM   3425  CD1 LEU A 226      46.198  61.402  53.246  1.00  0.00
ATOM   3426 HD11 LEU A 226      47.117  62.010  53.379  1.00  0.00
ATOM   3427 HD12 LEU A 226      46.326  60.435  53.771  1.00  0.00
ATOM   3428 HD13 LEU A 226      45.347  61.937  53.715  1.00  0.00
ATOM   3429  CD2 LEU A 226      45.590  62.486  51.040  1.00  0.00
ATOM   3430 HD21 LEU A 226      45.298  62.308  49.984  1.00  0.00
ATOM   3431 HD22 LEU A 226      46.472  63.160  51.057  1.00  0.00
ATOM   3432 HD23 LEU A 226      44.747  62.996  51.553  1.00  0.00
ATOM   3433  C   LEU A 226      48.033  59.458  48.941  1.00  0.00
ATOM   3434  O   LEU A 226      48.599  60.279  48.222  1.00  0.00
ATOM   3435  N   ALA A 227      48.473  58.204  49.080  1.00  0.00
ATOM   3436  HN  ALA A 227      47.994  57.559  49.672  1.00  0.00
ATOM   3437  CA  ALA A 227      49.643  57.675  48.418  1.00  0.00
ATOM   3438  HA  ALA A 227      50.429  58.415  48.493  1.00  0.00
ATOM   3439  CB  ALA A 227      50.135  56.381  49.098  1.00  0.00
ATOM   3440  HB1 ALA A 227      49.378  55.573  49.018  1.00  0.00
ATOM   3441  HB2 ALA A 227      50.324  56.572  50.176  1.00  0.00
ATOM   3442  HB3 ALA A 227      51.083  56.027  48.640  1.00  0.00
ATOM   3443  C   ALA A 227      49.409  57.385  46.949  1.00  0.00
ATOM   3444  O   ALA A 227      50.364  57.237  46.190  1.00  0.00
ATOM   3445  N   VAL A 228      48.144  57.330  46.524  1.00  0.00
ATOM   3446  HN  VAL A 228      47.387  57.440  47.165  1.00  0.00
ATOM   3447  CA  VAL A 228      47.764  57.132  45.139  1.00  0.00
ATOM   3448  HA  VAL A 228      48.570  56.645  44.611  1.00  0.00
ATOM   3449  CB  VAL A 228      46.517  56.260  44.995  1.00  0.00
ATOM   3450  HB  VAL A 228      45.699  56.652  45.640  1.00  0.00
ATOM   3451  CG1 VAL A 228      46.870  54.835  45.474  1.00  0.00
ATOM   3452 HG11 VAL A 228      47.209  54.837  46.529  1.00  0.00
ATOM   3453 HG12 VAL A 228      47.680  54.408  44.845  1.00  0.00
ATOM   3454 HG13 VAL A 228      45.980  54.176  45.397  1.00  0.00
ATOM   3455  CG2 VAL A 228      46.014  56.226  43.533  1.00  0.00
ATOM   3456 HG21 VAL A 228      46.828  55.902  42.851  1.00  0.00
ATOM   3457 HG22 VAL A 228      45.644  57.220  43.206  1.00  0.00
ATOM   3458 HG23 VAL A 228      45.173  55.506  43.442  1.00  0.00
ATOM   3459  C   VAL A 228      47.561  58.493  44.517  1.00  0.00
ATOM   3460  O   VAL A 228      48.221  58.839  43.538  1.00  0.00
ATOM   3461  N   SER A 229      46.649  59.284  45.090  1.00  0.00
ATOM   3462  HN  SER A 229      46.157  58.971  45.902  1.00  0.00
ATOM   3463  CA  SER A 229      46.200  60.568  44.589  1.00  0.00
ATOM   3464  HA  SER A 229      45.801  60.403  43.597  1.00  0.00
ATOM   3465  CB  SER A 229      45.078  61.129  45.495  1.00  0.00
ATOM   3466  HB1 SER A 229      44.757  62.135  45.149  1.00  0.00
ATOM   3467  HB2 SER A 229      45.433  61.209  46.546  1.00  0.00
ATOM   3468  OG  SER A 229      43.940  60.277  45.460  1.00  0.00
ATOM   3469  HG  SER A 229      43.293  60.662  46.056  1.00  0.00
ATOM   3470  C   SER A 229      47.277  61.613  44.474  1.00  0.00
ATOM   3471  O   SER A 229      47.304  62.355  43.495  1.00  0.00
ATOM   3472  N   GLY A 230      48.162  61.694  45.471  1.00  0.00
ATOM   3473  HN  GLY A 230      48.106  61.082  46.258  1.00  0.00
ATOM   3474  CA  GLY A 230      49.222  62.680  45.509  1.00  0.00
ATOM   3475  HA1 GLY A 230      49.125  63.193  46.454  1.00  0.00
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ATOM   3476  HA2 GLY A 230      49.159  63.354  44.664  1.00  0.00
ATOM   3477  C   GLY A 230      50.579  62.044  45.480  1.00  0.00
ATOM   3478  O   GLY A 230      51.546  62.676  45.058  1.00  0.00
ATOM   3479  N   GLY A 231      50.695  60.795  45.938  1.00  0.00
ATOM   3480  HN  GLY A 231      49.897  60.284  46.250  1.00  0.00
ATOM   3481  CA  GLY A 231      51.976  60.154  46.155  1.00  0.00
ATOM   3482  HA1 GLY A 231      51.796  59.298  46.786  1.00  0.00
ATOM   3483  HA2 GLY A 231      52.647  60.866  46.616  1.00  0.00
ATOM   3484  C   GLY A 231      52.611  59.663  44.888  1.00  0.00
ATOM   3485  O   GLY A 231      53.833  59.695  44.754  1.00  0.00
ATOM   3486  N   LEU A 232      51.805  59.211  43.924  1.00  0.00
ATOM   3487  HN  LEU A 232      50.816  59.162  44.048  1.00  0.00
ATOM   3488  CA  LEU A 232      52.311  58.767  42.643  1.00  0.00
ATOM   3489  HA  LEU A 232      53.236  58.229  42.795  1.00  0.00
ATOM   3490  CB  LEU A 232      51.285  57.836  41.946  1.00  0.00
ATOM   3491  HB1 LEU A 232      51.670  57.545  40.942  1.00  0.00
ATOM   3492  HB2 LEU A 232      50.332  58.391  41.798  1.00  0.00
ATOM   3493  CG  LEU A 232      50.969  56.528  42.714  1.00  0.00
ATOM   3494  HG  LEU A 232      50.563  56.812  43.709  1.00  0.00
ATOM   3495  CD1 LEU A 232      49.871  55.719  41.997  1.00  0.00
ATOM   3496 HD11 LEU A 232      50.225  55.390  40.997  1.00  0.00
ATOM   3497 HD12 LEU A 232      48.961  56.341  41.866  1.00  0.00
ATOM   3498 HD13 LEU A 232      49.603  54.821  42.592  1.00  0.00
ATOM   3499  CD2 LEU A 232      52.219  55.658  42.960  1.00  0.00
ATOM   3500 HD21 LEU A 232      52.966  56.205  43.572  1.00  0.00
ATOM   3501 HD22 LEU A 232      52.688  55.373  41.995  1.00  0.00
ATOM   3502 HD23 LEU A 232      51.938  54.732  43.504  1.00  0.00
ATOM   3503  C   LEU A 232      52.602  59.932  41.734  1.00  0.00
ATOM   3504  O   LEU A 232      53.421  59.822  40.825  1.00  0.00
ATOM   3505  N   MET A 233      51.942  61.067  41.970  1.00  0.00
ATOM   3506  HN  MET A 233      51.286  61.127  42.718  1.00  0.00
ATOM   3507  CA  MET A 233      52.118  62.279  41.203  1.00  0.00
ATOM   3508  HA  MET A 233      52.023  62.016  40.158  1.00  0.00
ATOM   3509  CB  MET A 233      51.013  63.301  41.562  1.00  0.00
ATOM   3510  HB1 MET A 233      51.109  64.196  40.907  1.00  0.00
ATOM   3511  HB2 MET A 233      51.134  63.637  42.615  1.00  0.00
ATOM   3512  CG  MET A 233      49.590  62.729  41.404  1.00  0.00
ATOM   3513  HG1 MET A 233      48.868  63.528  41.681  1.00  0.00
ATOM   3514  HG2 MET A 233      49.457  61.908  42.141  1.00  0.00
ATOM   3515  SD  MET A 233      49.198  62.116  39.735  1.00  0.00
ATOM   3516  CE  MET A 233      47.668  61.263  40.215  1.00  0.00
ATOM   3517  HE1 MET A 233      46.934  61.974  40.650  1.00  0.00
ATOM   3518  HE2 MET A 233      47.871  60.476  40.973  1.00  0.00
ATOM   3519  HE3 MET A 233      47.193  60.776  39.337  1.00  0.00
ATOM   3520  C   MET A 233      53.475  62.902  41.385  1.00  0.00
ATOM   3521  O   MET A 233      54.100  63.323  40.415  1.00  0.00
ATOM   3522  N   ILE A 234      53.965  62.945  42.629  1.00  0.00
ATOM   3523  HN  ILE A 234      53.440  62.603  43.405  1.00  0.00
ATOM   3524  CA  ILE A 234      55.267  63.501  42.942  1.00  0.00
ATOM   3525  HA  ILE A 234      55.393  64.385  42.334  1.00  0.00
ATOM   3526  CB  ILE A 234      55.419  63.923  44.406  1.00  0.00
ATOM   3527  HB  ILE A 234      56.456  64.301  44.573  1.00  0.00
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ATOM   3528  CG2 ILE A 234      55.196  62.729  45.361  1.00  0.00
ATOM   3529 HG21 ILE A 234      55.938  61.923  45.186  1.00  0.00
ATOM   3530 HG22 ILE A 234      54.176  62.311  45.243  1.00  0.00
ATOM   3531 HG23 ILE A 234      55.306  63.066  46.414  1.00  0.00
ATOM   3532  CG1 ILE A 234      54.461  65.090  44.762  1.00  0.00
ATOM   3533 HG11 ILE A 234      54.576  65.303  45.849  1.00  0.00
ATOM   3534 HG12 ILE A 234      53.409  64.772  44.598  1.00  0.00
ATOM   3535  CD1 ILE A 234      54.727  66.388  43.991  1.00  0.00
ATOM   3536  HD1 ILE A 234      54.516  66.259  42.909  1.00  0.00
ATOM   3537  HD2 ILE A 234      55.786  66.700  44.112  1.00  0.00
ATOM   3538  HD3 ILE A 234      54.075  67.202  44.375  1.00  0.00
ATOM   3539  C   ILE A 234      56.377  62.563  42.530  1.00  0.00
ATOM   3540  O   ILE A 234      57.454  63.014  42.150  1.00  0.00
ATOM   3541  N   PHE A 235      56.119  61.252  42.558  1.00  0.00
ATOM   3542  HN  PHE A 235      55.245  60.915  42.899  1.00  0.00
ATOM   3543  CA  PHE A 235      57.021  60.235  42.064  1.00  0.00
ATOM   3544  HA  PHE A 235      57.981  60.395  42.534  1.00  0.00
ATOM   3545  CB  PHE A 235      56.483  58.833  42.482  1.00  0.00
ATOM   3546  HB1 PHE A 235      55.465  58.676  42.068  1.00  0.00
ATOM   3547  HB2 PHE A 235      56.409  58.789  43.590  1.00  0.00
ATOM   3548  CG  PHE A 235      57.377  57.699  42.033  1.00  0.00
ATOM   3549  CD1 PHE A 235      58.618  57.487  42.658  1.00  0.00
ATOM   3550  HD1 PHE A 235      58.945  58.159  43.438  1.00  0.00
ATOM   3551  CE1 PHE A 235      59.426  56.403  42.290  1.00  0.00
ATOM   3552  HE1 PHE A 235      60.372  56.243  42.786  1.00  0.00
ATOM   3553  CZ  PHE A 235      59.006  55.528  41.281  1.00  0.00
ATOM   3554  HZ  PHE A 235      59.629  54.693  40.995  1.00  0.00
ATOM   3555  CD2 PHE A 235      56.965  56.811  41.022  1.00  0.00
ATOM   3556  HD2 PHE A 235      56.011  56.957  40.537  1.00  0.00
ATOM   3557  CE2 PHE A 235      57.777  55.734  40.645  1.00  0.00
ATOM   3558  HE2 PHE A 235      57.451  55.059  39.867  1.00  0.00
ATOM   3559  C   PHE A 235      57.215  60.346  40.563  1.00  0.00
ATOM   3560  O   PHE A 235      58.341  60.327  40.073  1.00  0.00
ATOM   3561  N   ALA A 236      56.113  60.505  39.826  1.00  0.00
ATOM   3562  HN  ALA A 236      55.214  60.506  40.262  1.00  0.00
ATOM   3563  CA  ALA A 236      56.080  60.673  38.388  1.00  0.00
ATOM   3564  HA  ALA A 236      56.611  59.837  37.954  1.00  0.00
ATOM   3565  CB  ALA A 236      54.632  60.670  37.859  1.00  0.00
ATOM   3566  HB1 ALA A 236      54.046  61.506  38.297  1.00  0.00
ATOM   3567  HB2 ALA A 236      54.133  59.718  38.137  1.00  0.00
ATOM   3568  HB3 ALA A 236      54.612  60.759  36.752  1.00  0.00
ATOM   3569  C   ALA A 236      56.753  61.942  37.928  1.00  0.00
ATOM   3570  O   ALA A 236      57.509  61.936  36.957  1.00  0.00
ATOM   3571  N   LEU A 237      56.500  63.045  38.639  1.00  0.00
ATOM   3572  HN  LEU A 237      55.859  63.007  39.405  1.00  0.00
ATOM   3573  CA  LEU A 237      57.075  64.352  38.405  1.00  0.00
ATOM   3574  HA  LEU A 237      56.831  64.647  37.394  1.00  0.00
ATOM   3575  CB  LEU A 237      56.481  65.361  39.425  1.00  0.00
ATOM   3576  HB1 LEU A 237      56.741  65.028  40.454  1.00  0.00
ATOM   3577  HB2 LEU A 237      55.372  65.325  39.342  1.00  0.00
ATOM   3578  CG  LEU A 237      56.910  66.839  39.266  1.00  0.00
ATOM   3579  HG  LEU A 237      58.021  66.891  39.204  1.00  0.00
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ATOM   3580  CD1 LEU A 237      56.334  67.460  37.980  1.00  0.00
ATOM   3581 HD11 LEU A 237      55.224  67.414  37.995  1.00  0.00
ATOM   3582 HD12 LEU A 237      56.700  66.917  37.084  1.00  0.00
ATOM   3583 HD13 LEU A 237      56.638  68.525  37.896  1.00  0.00
ATOM   3584  CD2 LEU A 237      56.498  67.660  40.504  1.00  0.00
ATOM   3585 HD21 LEU A 237      56.958  67.233  41.420  1.00  0.00
ATOM   3586 HD22 LEU A 237      55.394  67.648  40.624  1.00  0.00
ATOM   3587 HD23 LEU A 237      56.833  68.713  40.399  1.00  0.00
ATOM   3588  C   LEU A 237      58.576  64.321  38.557  1.00  0.00
ATOM   3589  O   LEU A 237      59.311  64.877  37.743  1.00  0.00
ATOM   3590  N   SER A 238      59.043  63.645  39.608  1.00  0.00
ATOM   3591  HN  SER A 238      58.403  63.217  40.244  1.00  0.00
ATOM   3592  CA  SER A 238      60.433  63.467  39.945  1.00  0.00
ATOM   3593  HA  SER A 238      60.879  64.452  39.979  1.00  0.00
ATOM   3594  CB  SER A 238      60.540  62.827  41.347  1.00  0.00
ATOM   3595  HB1 SER A 238      60.156  61.784  41.340  1.00  0.00
ATOM   3596  HB2 SER A 238      59.920  63.424  42.048  1.00  0.00
ATOM   3597  OG  SER A 238      61.867  62.841  41.856  1.00  0.00
ATOM   3598  HG  SER A 238      62.374  62.228  41.310  1.00  0.00
ATOM   3599  C   SER A 238      61.188  62.650  38.928  1.00  0.00
ATOM   3600  O   SER A 238      62.322  62.977  38.599  1.00  0.00
ATOM   3601  N   ASN A 239      60.576  61.582  38.408  1.00  0.00
ATOM   3602  HN  ASN A 239      59.671  61.300  38.723  1.00  0.00
ATOM   3603  CA  ASN A 239      61.161  60.770  37.353  1.00  0.00
ATOM   3604  HA  ASN A 239      62.128  60.419  37.689  1.00  0.00
ATOM   3605  CB  ASN A 239      60.234  59.566  37.013  1.00  0.00
ATOM   3606  HB1 ASN A 239      60.645  59.004  36.145  1.00  0.00
ATOM   3607  HB2 ASN A 239      59.219  59.933  36.750  1.00  0.00
ATOM   3608  CG  ASN A 239      60.136  58.588  38.192  1.00  0.00
ATOM   3609  OD1 ASN A 239      60.951  58.608  39.119  1.00  0.00
ATOM   3610  ND2 ASN A 239      59.085  57.717  38.155  1.00  0.00
ATOM   3611 HD21 ASN A 239      58.953  57.079  38.914  1.00  0.00
ATOM   3612 HD22 ASN A 239      58.449  57.730  37.384  1.00  0.00
ATOM   3613  C   ASN A 239      61.371  61.566  36.082  1.00  0.00
ATOM   3614  O   ASN A 239      62.432  61.496  35.465  1.00  0.00
ATOM   3615  N   ALA A 240      60.356  62.339  35.690  1.00  0.00
ATOM   3616  HN  ALA A 240      59.512  62.376  36.222  1.00  0.00
ATOM   3617  CA  ALA A 240      60.350  63.136  34.488  1.00  0.00
ATOM   3618  HA  ALA A 240      60.605  62.481  33.666  1.00  0.00
ATOM   3619  CB  ALA A 240      58.940  63.708  34.235  1.00  0.00
ATOM   3620  HB1 ALA A 240      58.624  64.371  35.068  1.00  0.00
ATOM   3621  HB2 ALA A 240      58.207  62.876  34.163  1.00  0.00
ATOM   3622  HB3 ALA A 240      58.904  64.283  33.284  1.00  0.00
ATOM   3623  C   ALA A 240      61.330  64.291  34.474  1.00  0.00
ATOM   3624  O   ALA A 240      62.029  64.495  33.483  1.00  0.00
ATOM   3625  N   LEU A 241      61.387  65.063  35.565  1.00  0.00
ATOM   3626  HN  LEU A 241      60.837  64.862  36.373  1.00  0.00
ATOM   3627  CA  LEU A 241      62.063  66.347  35.554  1.00  0.00
ATOM   3628  HA  LEU A 241      62.403  66.596  34.558  1.00  0.00
ATOM   3629  CB  LEU A 241      61.099  67.457  36.048  1.00  0.00
ATOM   3630  HB1 LEU A 241      61.624  68.438  36.029  1.00  0.00
ATOM   3631  HB2 LEU A 241      60.810  67.240  37.101  1.00  0.00
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ATOM   3632  CG  LEU A 241      59.787  67.619  35.243  1.00  0.00
ATOM   3633  HG  LEU A 241      59.194  66.682  35.358  1.00  0.00
ATOM   3634  CD1 LEU A 241      58.945  68.765  35.835  1.00  0.00
ATOM   3635 HD11 LEU A 241      59.473  69.735  35.714  1.00  0.00
ATOM   3636 HD12 LEU A 241      58.775  68.594  36.919  1.00  0.00
ATOM   3637 HD13 LEU A 241      57.961  68.829  35.324  1.00  0.00
ATOM   3638  CD2 LEU A 241      60.025  67.841  33.737  1.00  0.00
ATOM   3639 HD21 LEU A 241      60.563  66.980  33.290  1.00  0.00
ATOM   3640 HD22 LEU A 241      60.625  68.760  33.574  1.00  0.00
ATOM   3641 HD23 LEU A 241      59.055  67.956  33.210  1.00  0.00
ATOM   3642  C   LEU A 241      63.267  66.382  36.461  1.00  0.00
ATOM   3643  O   LEU A 241      64.168  67.195  36.261  1.00  0.00
ATOM   3644  N   GLY A 242      63.315  65.494  37.455  1.00  0.00
ATOM   3645  HN  GLY A 242      62.578  64.838  37.598  1.00  0.00
ATOM   3646  CA  GLY A 242      64.421  65.404  38.389  1.00  0.00
ATOM   3647  HA1 GLY A 242      64.011  65.074  39.331  1.00  0.00
ATOM   3648  HA2 GLY A 242      64.937  66.353  38.461  1.00  0.00
ATOM   3649  C   GLY A 242      65.390  64.361  37.910  1.00  0.00
ATOM   3650  O   GLY A 242      66.599  64.487  38.102  1.00  0.00
ATOM   3651  N   GLY A 243      64.862  63.318  37.268  1.00  0.00
ATOM   3652  HN  GLY A 243      63.870  63.242  37.177  1.00  0.00
ATOM   3653  CA  GLY A 243      65.609  62.274  36.611  1.00  0.00
ATOM   3654  HA1 GLY A 243      66.602  62.632  36.375  1.00  0.00
ATOM   3655  HA2 GLY A 243      65.050  62.007  35.728  1.00  0.00
ATOM   3656  C   GLY A 243      65.747  61.037  37.453  1.00  0.00
ATOM   3657  O   GLY A 243      66.452  60.111  37.057  1.00  0.00
ATOM   3658  N   SER A 244      65.089  60.973  38.613  1.00  0.00
ATOM   3659  HN  SER A 244      64.501  61.717  38.926  1.00  0.00
ATOM   3660  CA  SER A 244      65.176  59.818  39.478  1.00  0.00
ATOM   3661  HA  SER A 244      65.110  58.920  38.878  1.00  0.00
ATOM   3662  CB  SER A 244      66.508  59.840  40.284  1.00  0.00
ATOM   3663  HB1 SER A 244      66.584  60.762  40.892  1.00  0.00
ATOM   3664  HB2 SER A 244      67.358  59.852  39.572  1.00  0.00
ATOM   3665  OG  SER A 244      66.655  58.701  41.129  1.00  0.00
ATOM   3666  HG  SER A 244      67.586  58.670  41.392  1.00  0.00
ATOM   3667  C   SER A 244      63.989  59.853  40.404  1.00  0.00
ATOM   3668  O   SER A 244      63.409  60.910  40.635  1.00  0.00
ATOM   3669  N   GLY A 245      63.611  58.690  40.943  1.00  0.00
ATOM   3670  HN  GLY A 245      64.107  57.853  40.726  1.00  0.00
ATOM   3671  CA  GLY A 245      62.477  58.528  41.833  1.00  0.00
ATOM   3672  HA1 GLY A 245      62.042  57.568  41.600  1.00  0.00
ATOM   3673  HA2 GLY A 245      61.779  59.344  41.703  1.00  0.00
ATOM   3674  C   GLY A 245      62.913  58.498  43.264  1.00  0.00
ATOM   3675  O   GLY A 245      62.100  58.702  44.162  1.00  0.00
ATOM   3676  N   ILE A 246      64.207  58.259  43.495  1.00  0.00
ATOM   3677  HN  ILE A 246      64.823  58.119  42.722  1.00  0.00
ATOM   3678  CA  ILE A 246      64.864  58.168  44.786  1.00  0.00
ATOM   3679  HA  ILE A 246      64.335  57.419  45.358  1.00  0.00
ATOM   3680  CB  ILE A 246      66.324  57.742  44.626  1.00  0.00
ATOM   3681  HB  ILE A 246      66.848  58.486  43.979  1.00  0.00
ATOM   3682  CG2 ILE A 246      66.355  56.387  43.882  1.00  0.00
ATOM   3683 HG21 ILE A 246      65.974  56.482  42.845  1.00  0.00
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ATOM   3684 HG22 ILE A 246      65.742  55.630  44.414  1.00  0.00
ATOM   3685 HG23 ILE A 246      67.399  56.013  43.824  1.00  0.00
ATOM   3686  CG1 ILE A 246      67.119  57.663  45.958  1.00  0.00
ATOM   3687 HG11 ILE A 246      67.167  58.668  46.428  1.00  0.00
ATOM   3688 HG12 ILE A 246      68.163  57.373  45.706  1.00  0.00
ATOM   3689  CD1 ILE A 246      66.575  56.661  46.979  1.00  0.00
ATOM   3690  HD1 ILE A 246      66.613  55.624  46.582  1.00  0.00
ATOM   3691  HD2 ILE A 246      65.523  56.904  47.234  1.00  0.00
ATOM   3692  HD3 ILE A 246      67.178  56.698  47.912  1.00  0.00
ATOM   3693  C   ILE A 246      64.759  59.482  45.532  1.00  0.00
ATOM   3694  O   ILE A 246      64.609  59.504  46.753  1.00  0.00
ATOM   3695  N   LEU A 247      64.807  60.591  44.786  1.00  0.00
ATOM   3696  HN  LEU A 247      64.907  60.507  43.799  1.00  0.00
ATOM   3697  CA  LEU A 247      64.752  61.958  45.259  1.00  0.00
ATOM   3698  HA  LEU A 247      65.617  62.130  45.880  1.00  0.00
ATOM   3699  CB  LEU A 247      64.729  62.941  44.051  1.00  0.00
ATOM   3700  HB1 LEU A 247      64.856  63.982  44.423  1.00  0.00
ATOM   3701  HB2 LEU A 247      63.741  62.885  43.547  1.00  0.00
ATOM   3702  CG  LEU A 247      65.777  62.685  42.944  1.00  0.00
ATOM   3703  HG  LEU A 247      65.677  61.629  42.608  1.00  0.00
ATOM   3704  CD1 LEU A 247      65.507  63.561  41.705  1.00  0.00
ATOM   3705 HD11 LEU A 247      65.532  64.634  41.984  1.00  0.00
ATOM   3706 HD12 LEU A 247      64.509  63.334  41.276  1.00  0.00
ATOM   3707 HD13 LEU A 247      66.275  63.376  40.924  1.00  0.00
ATOM   3708  CD2 LEU A 247      67.207  62.883  43.460  1.00  0.00
ATOM   3709 HD21 LEU A 247      67.405  62.204  44.316  1.00  0.00
ATOM   3710 HD22 LEU A 247      67.360  63.930  43.797  1.00  0.00
ATOM   3711 HD23 LEU A 247      67.941  62.660  42.657  1.00  0.00
ATOM   3712  C   LEU A 247      63.498  62.246  46.051  1.00  0.00
ATOM   3713  O   LEU A 247      63.542  62.919  47.079  1.00  0.00
ATOM   3714  N   SER A 248      62.359  61.745  45.572  1.00  0.00
ATOM   3715  HN  SER A 248      62.352  61.141  44.779  1.00  0.00
ATOM   3716  CA  SER A 248      61.072  62.142  46.084  1.00  0.00
ATOM   3717  HA  SER A 248      61.165  63.064  46.639  1.00  0.00
ATOM   3718  CB  SER A 248      60.081  62.393  44.912  1.00  0.00
ATOM   3719  HB1 SER A 248      60.443  63.267  44.329  1.00  0.00
ATOM   3720  HB2 SER A 248      59.067  62.640  45.295  1.00  0.00
ATOM   3721  OG  SER A 248      59.979  61.279  44.028  1.00  0.00
ATOM   3722  HG  SER A 248      60.771  61.295  43.483  1.00  0.00
ATOM   3723  C   SER A 248      60.465  61.127  47.003  1.00  0.00
ATOM   3724  O   SER A 248      59.803  61.505  47.961  1.00  0.00
ATOM   3725  N   ILE A 249      60.652  59.837  46.717  1.00  0.00
ATOM   3726  HN  ILE A 249      61.237  59.561  45.957  1.00  0.00
ATOM   3727  CA  ILE A 249      59.899  58.762  47.336  1.00  0.00
ATOM   3728  HA  ILE A 249      58.868  59.061  47.217  1.00  0.00
ATOM   3729  CB  ILE A 249      60.058  57.452  46.568  1.00  0.00
ATOM   3730  HB  ILE A 249      59.939  57.696  45.485  1.00  0.00
ATOM   3731  CG2 ILE A 249      61.481  56.881  46.738  1.00  0.00
ATOM   3732 HG21 ILE A 249      61.610  56.452  47.753  1.00  0.00
ATOM   3733 HG22 ILE A 249      62.251  57.664  46.581  1.00  0.00
ATOM   3734 HG23 ILE A 249      61.655  56.078  45.992  1.00  0.00
ATOM   3735  CG1 ILE A 249      58.955  56.413  46.902  1.00  0.00
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ATOM   3736 HG11 ILE A 249      58.997  56.158  47.981  1.00  0.00
ATOM   3737 HG12 ILE A 249      59.177  55.484  46.330  1.00  0.00
ATOM   3738  CD1 ILE A 249      57.535  56.863  46.537  1.00  0.00
ATOM   3739  HD1 ILE A 249      57.490  57.182  45.474  1.00  0.00
ATOM   3740  HD2 ILE A 249      57.209  57.709  47.177  1.00  0.00
ATOM   3741  HD3 ILE A 249      56.818  56.028  46.679  1.00  0.00
ATOM   3742  C   ILE A 249      60.111  58.614  48.833  1.00  0.00
ATOM   3743  O   ILE A 249      59.167  58.359  49.579  1.00  0.00
ATOM   3744  N   TYR A 250      61.348  58.802  49.303  1.00  0.00
ATOM   3745  HN  TYR A 250      62.106  58.975  48.679  1.00  0.00
ATOM   3746  CA  TYR A 250      61.681  58.846  50.714  1.00  0.00
ATOM   3747  HA  TYR A 250      61.282  57.947  51.162  1.00  0.00
ATOM   3748  CB  TYR A 250      63.219  58.863  50.911  1.00  0.00
ATOM   3749  HB1 TYR A 250      63.490  59.265  51.913  1.00  0.00
ATOM   3750  HB2 TYR A 250      63.703  59.504  50.143  1.00  0.00
ATOM   3751  CG  TYR A 250      63.789  57.469  50.813  1.00  0.00
ATOM   3752  CD1 TYR A 250      64.188  56.791  51.978  1.00  0.00
ATOM   3753  HD1 TYR A 250      64.093  57.272  52.939  1.00  0.00
ATOM   3754  CE1 TYR A 250      64.694  55.490  51.912  1.00  0.00
ATOM   3755  HE1 TYR A 250      64.978  54.990  52.826  1.00  0.00
ATOM   3756  CZ  TYR A 250      64.805  54.840  50.677  1.00  0.00
ATOM   3757  OH  TYR A 250      65.312  53.524  50.612  1.00  0.00
ATOM   3758  HH  TYR A 250      65.667  53.302  51.482  1.00  0.00
ATOM   3759  CD2 TYR A 250      63.930  56.818  49.575  1.00  0.00
ATOM   3760  HD2 TYR A 250      63.648  57.328  48.667  1.00  0.00
ATOM   3761  CE2 TYR A 250      64.416  55.505  49.507  1.00  0.00
ATOM   3762  HE2 TYR A 250      64.499  55.011  48.550  1.00  0.00
ATOM   3763  C   TYR A 250      61.042  59.996  51.449  1.00  0.00
ATOM   3764  O   TYR A 250      60.530  59.828  52.555  1.00  0.00
ATOM   3765  N   LEU A 251      61.036  61.175  50.825  1.00  0.00
ATOM   3766  HN  LEU A 251      61.452  61.279  49.925  1.00  0.00
ATOM   3767  CA  LEU A 251      60.417  62.368  51.357  1.00  0.00
ATOM   3768  HA  LEU A 251      60.718  62.468  52.389  1.00  0.00
ATOM   3769  CB  LEU A 251      60.886  63.614  50.567  1.00  0.00
ATOM   3770  HB1 LEU A 251      60.403  64.523  50.991  1.00  0.00
ATOM   3771  HB2 LEU A 251      60.567  63.523  49.505  1.00  0.00
ATOM   3772  CG  LEU A 251      62.420  63.840  50.592  1.00  0.00
ATOM   3773  HG  LEU A 251      62.916  62.948  50.143  1.00  0.00
ATOM   3774  CD1 LEU A 251      62.814  65.045  49.728  1.00  0.00
ATOM   3775 HD11 LEU A 251      62.359  65.974  50.130  1.00  0.00
ATOM   3776 HD12 LEU A 251      62.475  64.904  48.680  1.00  0.00
ATOM   3777 HD13 LEU A 251      63.918  65.165  49.732  1.00  0.00
ATOM   3778  CD2 LEU A 251      62.974  64.016  52.018  1.00  0.00
ATOM   3779 HD21 LEU A 251      62.871  63.074  52.591  1.00  0.00
ATOM   3780 HD22 LEU A 251      62.432  64.828  52.548  1.00  0.00
ATOM   3781 HD23 LEU A 251      64.053  64.279  51.981  1.00  0.00
ATOM   3782  C   LEU A 251      58.910  62.274  51.336  1.00  0.00
ATOM   3783  O   LEU A 251      58.249  62.804  52.219  1.00  0.00
ATOM   3784  N   THR A 252      58.348  61.560  50.357  1.00  0.00
ATOM   3785  HN  THR A 252      58.928  61.168  49.644  1.00  0.00
ATOM   3786  CA  THR A 252      56.931  61.254  50.235  1.00  0.00
ATOM   3787  HA  THR A 252      56.398  62.193  50.272  1.00  0.00
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ATOM   3788  CB  THR A 252      56.574  60.560  48.922  1.00  0.00
ATOM   3789  HB  THR A 252      57.099  59.585  48.837  1.00  0.00
ATOM   3790  OG1 THR A 252      56.983  61.367  47.826  1.00  0.00
ATOM   3791  HG1 THR A 252      57.939  61.458  47.898  1.00  0.00
ATOM   3792  CG2 THR A 252      55.054  60.313  48.797  1.00  0.00
ATOM   3793 HG21 THR A 252      54.494  61.264  48.924  1.00  0.00
ATOM   3794 HG22 THR A 252      54.701  59.586  49.557  1.00  0.00
ATOM   3795 HG23 THR A 252      54.816  59.894  47.795  1.00  0.00
ATOM   3796  C   THR A 252      56.463  60.427  51.409  1.00  0.00
ATOM   3797  O   THR A 252      55.385  60.660  51.953  1.00  0.00
ATOM   3798  N   GLY A 253      57.292  59.476  51.846  1.00  0.00
ATOM   3799  HN  GLY A 253      58.154  59.296  51.373  1.00  0.00
ATOM   3800  CA  GLY A 253      57.047  58.668  53.020  1.00  0.00
ATOM   3801  HA1 GLY A 253      57.862  57.966  53.092  1.00  0.00
ATOM   3802  HA2 GLY A 253      56.085  58.189  52.906  1.00  0.00
ATOM   3803  C   GLY A 253      57.018  59.486  54.284  1.00  0.00
ATOM   3804  O   GLY A 253      56.154  59.279  55.129  1.00  0.00
ATOM   3805  N   LEU A 254      57.942  60.440  54.426  1.00  0.00
ATOM   3806  HN  LEU A 254      58.651  60.558  53.734  1.00  0.00
ATOM   3807  CA  LEU A 254      57.989  61.394  55.519  1.00  0.00
ATOM   3808  HA  LEU A 254      57.969  60.827  56.439  1.00  0.00
ATOM   3809  CB  LEU A 254      59.299  62.215  55.454  1.00  0.00
ATOM   3810  HB1 LEU A 254      59.273  63.046  56.194  1.00  0.00
ATOM   3811  HB2 LEU A 254      59.400  62.668  54.446  1.00  0.00
ATOM   3812  CG  LEU A 254      60.568  61.390  55.759  1.00  0.00
ATOM   3813  HG  LEU A 254      60.555  60.462  55.142  1.00  0.00
ATOM   3814  CD1 LEU A 254      61.840  62.164  55.373  1.00  0.00
ATOM   3815 HD11 LEU A 254      61.881  63.133  55.912  1.00  0.00
ATOM   3816 HD12 LEU A 254      61.841  62.367  54.284  1.00  0.00
ATOM   3817 HD13 LEU A 254      62.747  61.574  55.622  1.00  0.00
ATOM   3818  CD2 LEU A 254      60.611  60.970  57.235  1.00  0.00
ATOM   3819 HD21 LEU A 254      59.786  60.268  57.474  1.00  0.00
ATOM   3820 HD22 LEU A 254      60.530  61.857  57.896  1.00  0.00
ATOM   3821 HD23 LEU A 254      61.572  60.460  57.448  1.00  0.00
ATOM   3822  C   LEU A 254      56.809  62.339  55.570  1.00  0.00
ATOM   3823  O   LEU A 254      56.301  62.648  56.646  1.00  0.00
ATOM   3824  N   LEU A 255      56.359  62.813  54.405  1.00  0.00
ATOM   3825  HN  LEU A 255      56.824  62.573  53.554  1.00  0.00
ATOM   3826  CA  LEU A 255      55.193  63.660  54.244  1.00  0.00
ATOM   3827  HA  LEU A 255      55.323  64.518  54.888  1.00  0.00
ATOM   3828  CB  LEU A 255      55.069  64.141  52.772  1.00  0.00
ATOM   3829  HB1 LEU A 255      54.071  64.601  52.598  1.00  0.00
ATOM   3830  HB2 LEU A 255      55.151  63.256  52.105  1.00  0.00
ATOM   3831  CG  LEU A 255      56.130  65.187  52.342  1.00  0.00
ATOM   3832  HG  LEU A 255      57.127  64.853  52.704  1.00  0.00
ATOM   3833  CD1 LEU A 255      56.217  65.315  50.809  1.00  0.00
ATOM   3834 HD11 LEU A 255      55.236  65.625  50.390  1.00  0.00
ATOM   3835 HD12 LEU A 255      56.510  64.348  50.351  1.00  0.00
ATOM   3836 HD13 LEU A 255      56.976  66.077  50.533  1.00  0.00
ATOM   3837  CD2 LEU A 255      55.886  66.565  52.973  1.00  0.00
ATOM   3838 HD21 LEU A 255      55.893  66.493  54.080  1.00  0.00
ATOM   3839 HD22 LEU A 255      54.909  66.974  52.642  1.00  0.00
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ATOM   3840 HD23 LEU A 255      56.686  67.270  52.662  1.00  0.00
ATOM   3841  C   LEU A 255      53.918  62.969  54.676  1.00  0.00
ATOM   3842  O   LEU A 255      53.044  63.588  55.282  1.00  0.00
ATOM   3843  N   LEU A 256      53.804  61.671  54.385  1.00  0.00
ATOM   3844  HN  LEU A 256      54.513  61.197  53.866  1.00  0.00
ATOM   3845  CA  LEU A 256      52.683  60.856  54.799  1.00  0.00
ATOM   3846  HA  LEU A 256      51.779  61.442  54.714  1.00  0.00
ATOM   3847  CB  LEU A 256      52.568  59.613  53.881  1.00  0.00
ATOM   3848  HB1 LEU A 256      51.831  58.890  54.297  1.00  0.00
ATOM   3849  HB2 LEU A 256      53.562  59.113  53.851  1.00  0.00
ATOM   3850  CG  LEU A 256      52.132  59.918  52.425  1.00  0.00
ATOM   3851  HG  LEU A 256      52.781  60.732  52.029  1.00  0.00
ATOM   3852  CD1 LEU A 256      52.347  58.689  51.520  1.00  0.00
ATOM   3853 HD11 LEU A 256      51.726  57.838  51.871  1.00  0.00
ATOM   3854 HD12 LEU A 256      53.413  58.382  51.536  1.00  0.00
ATOM   3855 HD13 LEU A 256      52.063  58.927  50.473  1.00  0.00
ATOM   3856  CD2 LEU A 256      50.672  60.408  52.337  1.00  0.00
ATOM   3857 HD21 LEU A 256      50.533  61.343  52.917  1.00  0.00
ATOM   3858 HD22 LEU A 256      49.981  59.635  52.735  1.00  0.00
ATOM   3859 HD23 LEU A 256      50.401  60.610  51.279  1.00  0.00
ATOM   3860  C   LEU A 256      52.792  60.409  56.243  1.00  0.00
ATOM   3861  O   LEU A 256      51.777  60.142  56.884  1.00  0.00
ATOM   3862  N   GLY A 257      54.009  60.363  56.790  1.00  0.00
ATOM   3863  HN  GLY A 257      54.832  60.547  56.255  1.00  0.00
ATOM   3864  CA  GLY A 257      54.203  60.041  58.183  1.00  0.00
ATOM   3865  HA1 GLY A 257      53.750  59.077  58.373  1.00  0.00
ATOM   3866  HA2 GLY A 257      53.777  60.842  58.772  1.00  0.00
ATOM   3867  C   GLY A 257      55.662  59.923  58.508  1.00  0.00
ATOM   3868  O   GLY A 257      56.321  58.961  58.122  1.00  0.00
ATOM   3869  N   ASN A 258      56.185  60.893  59.267  1.00  0.00
ATOM   3870  HN  ASN A 258      55.635  61.692  59.495  1.00  0.00
ATOM   3871  CA  ASN A 258      57.497  60.872  59.888  1.00  0.00
ATOM   3872  HA  ASN A 258      58.221  60.660  59.114  1.00  0.00
ATOM   3873  CB  ASN A 258      57.788  62.268  60.521  1.00  0.00
ATOM   3874  HB1 ASN A 258      57.024  62.493  61.294  1.00  0.00
ATOM   3875  HB2 ASN A 258      57.708  63.034  59.721  1.00  0.00
ATOM   3876  CG  ASN A 258      59.204  62.351  61.122  1.00  0.00
ATOM   3877  OD1 ASN A 258      60.144  61.710  60.645  1.00  0.00
ATOM   3878  ND2 ASN A 258      59.342  63.146  62.224  1.00  0.00
ATOM   3879 HD21 ASN A 258      60.240  63.237  62.653  1.00  0.00
ATOM   3880 HD22 ASN A 258      58.555  63.645  62.584  1.00  0.00
ATOM   3881  C   ASN A 258      57.578  59.777  60.934  1.00  0.00
ATOM   3882  O   ASN A 258      58.576  59.066  61.031  1.00  0.00
ATOM   3883  N   ARG A 259      56.503  59.623  61.711  1.00  0.00
ATOM   3884  HN  ARG A 259      55.713  60.219  61.596  1.00  0.00
ATOM   3885  CA  ARG A 259      56.355  58.611  62.730  1.00  0.00
ATOM   3886  HA  ARG A 259      57.192  57.928  62.718  1.00  0.00
ATOM   3887  CB  ARG A 259      56.254  59.267  64.131  1.00  0.00
ATOM   3888  HB1 ARG A 259      56.021  58.484  64.886  1.00  0.00
ATOM   3889  HB2 ARG A 259      55.423  60.007  64.133  1.00  0.00
ATOM   3890  CG  ARG A 259      57.535  59.989  64.592  1.00  0.00
ATOM   3891  HG1 ARG A 259      57.303  60.487  65.562  1.00  0.00
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ATOM   3892  HG2 ARG A 259      57.800  60.782  63.859  1.00  0.00
ATOM   3893  CD  ARG A 259      58.727  59.040  64.791  1.00  0.00
ATOM   3894  HD1 ARG A 259      59.061  58.607  63.824  1.00  0.00
ATOM   3895  HD2 ARG A 259      58.439  58.227  65.493  1.00  0.00
ATOM   3896  NE  ARG A 259      59.862  59.821  65.379  1.00  0.00
ATOM   3897  HE  ARG A 259      59.816  60.818  65.351  1.00  0.00
ATOM   3898  CZ  ARG A 259      60.945  59.245  65.951  1.00  0.00
ATOM   3899  NH1 ARG A 259      61.083  57.907  66.022  1.00  0.00
ATOM   3900 HH11 ARG A 259      60.376  57.316  65.639  1.00  0.00
ATOM   3901 HH12 ARG A 259      61.895  57.512  66.449  1.00  0.00
ATOM   3902  NH2 ARG A 259      61.916  60.032  66.463  1.00  0.00
ATOM   3903 HH21 ARG A 259      61.831  61.025  66.416  1.00  0.00
ATOM   3904 HH22 ARG A 259      62.721  59.618  66.885  1.00  0.00
ATOM   3905  C   ARG A 259      55.088  57.843  62.432  1.00  0.00
ATOM   3906  O   ARG A 259      54.080  58.058  63.107  1.00  0.00
ATOM   3907  N   PRO A 260      55.058  56.962  61.417  1.00  0.00
ATOM   3908  CD  PRO A 260      56.233  56.486  60.679  1.00  0.00
ATOM   3909  HD1 PRO A 260      57.007  56.099  61.376  1.00  0.00
ATOM   3910  HD2 PRO A 260      56.642  57.317  60.069  1.00  0.00
ATOM   3911  CA  PRO A 260      53.835  56.372  60.913  1.00  0.00
ATOM   3912  HA  PRO A 260      53.090  57.147  60.799  1.00  0.00
ATOM   3913  CB  PRO A 260      54.240  55.750  59.570  1.00  0.00
ATOM   3914  HB1 PRO A 260      54.165  56.533  58.782  1.00  0.00
ATOM   3915  HB2 PRO A 260      53.612  54.888  59.271  1.00  0.00
ATOM   3916  CG  PRO A 260      55.717  55.381  59.752  1.00  0.00
ATOM   3917  HG1 PRO A 260      55.799  54.396  60.260  1.00  0.00
ATOM   3918  HG2 PRO A 260      56.267  55.344  58.791  1.00  0.00
ATOM   3919  C   PRO A 260      53.290  55.343  61.866  1.00  0.00
ATOM   3920  O   PRO A 260      52.078  55.181  61.912  1.00  0.00
ATOM   3921  N   THR A 261      54.137  54.619  62.597  1.00  0.00
ATOM   3922  HN  THR A 261      55.121  54.760  62.515  1.00  0.00
ATOM   3923  CA  THR A 261      53.758  53.533  63.482  1.00  0.00
ATOM   3924  HA  THR A 261      53.248  52.795  62.879  1.00  0.00
ATOM   3925  CB  THR A 261      54.985  52.894  64.131  1.00  0.00
ATOM   3926  HB  THR A 261      55.399  53.551  64.928  1.00  0.00
ATOM   3927  OG1 THR A 261      56.017  52.724  63.166  1.00  0.00
ATOM   3928  HG1 THR A 261      56.781  52.397  63.648  1.00  0.00
ATOM   3929  CG2 THR A 261      54.629  51.519  64.727  1.00  0.00
ATOM   3930 HG21 THR A 261      54.250  50.840  63.934  1.00  0.00
ATOM   3931 HG22 THR A 261      53.851  51.614  65.513  1.00  0.00
ATOM   3932 HG23 THR A 261      55.525  51.051  65.187  1.00  0.00
ATOM   3933  C   THR A 261      52.805  54.014  64.559  1.00  0.00
ATOM   3934  O   THR A 261      51.843  53.330  64.901  1.00  0.00
ATOM   3935  N   ARG A 262      53.064  55.210  65.095  1.00  0.00
ATOM   3936  HN  ARG A 262      53.826  55.756  64.760  1.00  0.00
ATOM   3937  CA  ARG A 262      52.317  55.803  66.178  1.00  0.00
ATOM   3938  HA  ARG A 262      52.363  55.112  67.009  1.00  0.00
ATOM   3939  CB  ARG A 262      52.991  57.130  66.610  1.00  0.00
ATOM   3940  HB1 ARG A 262      52.412  57.580  67.449  1.00  0.00
ATOM   3941  HB2 ARG A 262      52.984  57.851  65.762  1.00  0.00
ATOM   3942  CG  ARG A 262      54.442  56.948  67.092  1.00  0.00
ATOM   3943  HG1 ARG A 262      55.064  56.597  66.238  1.00  0.00
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ATOM   3944  HG2 ARG A 262      54.458  56.159  67.878  1.00  0.00
ATOM   3945  CD  ARG A 262      55.047  58.240  67.662  1.00  0.00
ATOM   3946  HD1 ARG A 262      54.496  58.556  68.575  1.00  0.00
ATOM   3947  HD2 ARG A 262      55.011  59.051  66.902  1.00  0.00
ATOM   3948  NE  ARG A 262      56.476  57.974  68.026  1.00  0.00
ATOM   3949  HE  ARG A 262      56.813  57.035  67.971  1.00  0.00
ATOM   3950  CZ  ARG A 262      57.313  58.930  68.492  1.00  0.00
ATOM   3951  NH1 ARG A 262      58.573  58.591  68.838  1.00  0.00
ATOM   3952 HH11 ARG A 262      58.866  57.639  68.778  1.00  0.00
ATOM   3953 HH12 ARG A 262      59.188  59.283  69.213  1.00  0.00
ATOM   3954  NH2 ARG A 262      56.917  60.211  68.626  1.00  0.00
ATOM   3955 HH21 ARG A 262      55.979  60.465  68.398  1.00  0.00
ATOM   3956 HH22 ARG A 262      57.546  60.891  69.000  1.00  0.00
ATOM   3957  C   ARG A 262      50.852  56.079  65.901  1.00  0.00
ATOM   3958  O   ARG A 262      50.004  55.774  66.738  1.00  0.00
ATOM   3959  N   SER A 263      50.541  56.671  64.743  1.00  0.00
ATOM   3960  HN  SER A 263      51.237  56.893  64.065  1.00  0.00
ATOM   3961  CA  SER A 263      49.203  57.181  64.486  1.00  0.00
ATOM   3962  HA  SER A 263      48.509  56.772  65.207  1.00  0.00
ATOM   3963  CB  SER A 263      49.189  58.727  64.651  1.00  0.00
ATOM   3964  HB1 SER A 263      49.381  58.960  65.722  1.00  0.00
ATOM   3965  HB2 SER A 263      48.199  59.154  64.382  1.00  0.00
ATOM   3966  OG  SER A 263      50.208  59.364  63.884  1.00  0.00
ATOM   3967  HG  SER A 263      50.153  60.301  64.089  1.00  0.00
ATOM   3968  C   SER A 263      48.637  56.815  63.132  1.00  0.00
ATOM   3969  O   SER A 263      47.441  56.979  62.901  1.00  0.00
ATOM   3970  N   ARG A 264      49.477  56.328  62.218  1.00  0.00
ATOM   3971  HN  ARG A 264      50.432  56.135  62.433  1.00  0.00
ATOM   3972  CA  ARG A 264      49.110  56.133  60.831  1.00  0.00
ATOM   3973  HA  ARG A 264      48.035  56.168  60.713  1.00  0.00
ATOM   3974  CB  ARG A 264      49.768  57.228  59.945  1.00  0.00
ATOM   3975  HB1 ARG A 264      49.454  57.074  58.888  1.00  0.00
ATOM   3976  HB2 ARG A 264      50.876  57.148  59.993  1.00  0.00
ATOM   3977  CG  ARG A 264      49.375  58.659  60.357  1.00  0.00
ATOM   3978  HG1 ARG A 264      49.808  58.885  61.354  1.00  0.00
ATOM   3979  HG2 ARG A 264      48.267  58.693  60.451  1.00  0.00
ATOM   3980  CD  ARG A 264      49.841  59.731  59.362  1.00  0.00
ATOM   3981  HD1 ARG A 264      49.483  59.468  58.342  1.00  0.00
ATOM   3982  HD2 ARG A 264      50.948  59.818  59.366  1.00  0.00
ATOM   3983  NE  ARG A 264      49.252  61.044  59.783  1.00  0.00
ATOM   3984  HE  ARG A 264      48.873  61.114  60.704  1.00  0.00
ATOM   3985  CZ  ARG A 264      49.023  62.069  58.929  1.00  0.00
ATOM   3986  NH1 ARG A 264      49.472  62.060  57.659  1.00  0.00
ATOM   3987 HH11 ARG A 264      50.028  61.297  57.331  1.00  0.00
ATOM   3988 HH12 ARG A 264      49.203  62.807  57.043  1.00  0.00
ATOM   3989  NH2 ARG A 264      48.297  63.122  59.357  1.00  0.00
ATOM   3990 HH21 ARG A 264      47.908  63.115  60.280  1.00  0.00
ATOM   3991 HH22 ARG A 264      48.052  63.853  58.711  1.00  0.00
ATOM   3992  C   ARG A 264      49.581  54.773  60.387  1.00  0.00
ATOM   3993  O   ARG A 264      50.382  54.647  59.463  1.00  0.00
ATOM   3994  N   HIS A 265      49.103  53.719  61.051  1.00  0.00
ATOM   3995  HN  HIS A 265      48.439  53.826  61.787  1.00  0.00
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ATOM   3996  CA  HIS A 265      49.627  52.382  60.850  1.00  0.00
ATOM   3997  HA  HIS A 265      50.671  52.444  60.574  1.00  0.00
ATOM   3998  CB  HIS A 265      49.499  51.575  62.173  1.00  0.00
ATOM   3999  HB1 HIS A 265      48.463  51.206  62.331  1.00  0.00
ATOM   4000  HB2 HIS A 265      49.730  52.274  63.009  1.00  0.00
ATOM   4001  ND1 HIS A 265      50.498  49.297  61.535  1.00  0.00
ATOM   4002  HD1 HIS A 265      49.883  49.103  60.766  1.00  0.00
ATOM   4003  CG  HIS A 265      50.493  50.442  62.300  1.00  0.00
ATOM   4004  CE1 HIS A 265      51.504  48.511  61.984  1.00  0.00
ATOM   4005  HE1 HIS A 265      51.744  47.541  61.553  1.00  0.00
ATOM   4006  NE2 HIS A 265      52.132  49.081  62.994  1.00  0.00
ATOM   4007  CD2 HIS A 265      51.498  50.294  63.207  1.00  0.00
ATOM   4008  HD2 HIS A 265      51.814  50.942  64.011  1.00  0.00
ATOM   4009  C   HIS A 265      48.855  51.678  59.747  1.00  0.00
ATOM   4010  O   HIS A 265      49.227  50.596  59.301  1.00  0.00
ATOM   4011  N   ALA A 266      47.782  52.302  59.254  1.00  0.00
ATOM   4012  HN  ALA A 266      47.498  53.183  59.623  1.00  0.00
ATOM   4013  CA  ALA A 266      46.962  51.788  58.177  1.00  0.00
ATOM   4014  HA  ALA A 266      46.601  50.815  58.480  1.00  0.00
ATOM   4015  CB  ALA A 266      45.753  52.708  57.914  1.00  0.00
ATOM   4016  HB1 ALA A 266      46.083  53.721  57.601  1.00  0.00
ATOM   4017  HB2 ALA A 266      45.152  52.812  58.843  1.00  0.00
ATOM   4018  HB3 ALA A 266      45.097  52.286  57.124  1.00  0.00
ATOM   4019  C   ALA A 266      47.720  51.621  56.873  1.00  0.00
ATOM   4020  O   ALA A 266      47.588  50.602  56.200  1.00  0.00
ATOM   4021  N   ILE A 267      48.546  52.611  56.515  1.00  0.00
ATOM   4022  HN  ILE A 267      48.632  53.426  57.082  1.00  0.00
ATOM   4023  CA  ILE A 267      49.404  52.585  55.343  1.00  0.00
ATOM   4024  HA  ILE A 267      48.766  52.302  54.516  1.00  0.00
ATOM   4025  CB  ILE A 267      49.991  53.958  54.982  1.00  0.00
ATOM   4026  HB  ILE A 267      49.132  54.607  54.696  1.00  0.00
ATOM   4027  CG2 ILE A 267      50.656  54.618  56.211  1.00  0.00
ATOM   4028 HG21 ILE A 267      51.493  54.001  56.596  1.00  0.00
ATOM   4029 HG22 ILE A 267      49.917  54.779  57.021  1.00  0.00
ATOM   4030 HG23 ILE A 267      51.063  55.613  55.929  1.00  0.00
ATOM   4031  CG1 ILE A 267      50.951  53.956  53.760  1.00  0.00
ATOM   4032 HG11 ILE A 267      51.846  53.335  53.973  1.00  0.00
ATOM   4033 HG12 ILE A 267      51.308  55.001  53.616  1.00  0.00
ATOM   4034  CD1 ILE A 267      50.306  53.504  52.446  1.00  0.00
ATOM   4035  HD1 ILE A 267      49.447  54.162  52.200  1.00  0.00
ATOM   4036  HD2 ILE A 267      49.945  52.458  52.515  1.00  0.00
ATOM   4037  HD3 ILE A 267      51.042  53.565  51.616  1.00  0.00
ATOM   4038  C   ILE A 267      50.471  51.514  55.428  1.00  0.00
ATOM   4039  O   ILE A 267      50.796  50.873  54.432  1.00  0.00
ATOM   4040  N   LEU A 268      51.018  51.282  56.624  1.00  0.00
ATOM   4041  HN  LEU A 268      50.738  51.806  57.425  1.00  0.00
ATOM   4042  CA  LEU A 268      52.017  50.261  56.872  1.00  0.00
ATOM   4043  HA  LEU A 268      52.836  50.440  56.191  1.00  0.00
ATOM   4044  CB  LEU A 268      52.537  50.348  58.328  1.00  0.00
ATOM   4045  HB1 LEU A 268      53.334  49.583  58.470  1.00  0.00
ATOM   4046  HB2 LEU A 268      51.716  50.112  59.037  1.00  0.00
ATOM   4047  CG  LEU A 268      53.134  51.722  58.722  1.00  0.00
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ATOM   4048  HG  LEU A 268      52.321  52.484  58.678  1.00  0.00
ATOM   4049  CD1 LEU A 268      53.641  51.691  60.176  1.00  0.00
ATOM   4050 HD11 LEU A 268      54.459  50.949  60.285  1.00  0.00
ATOM   4051 HD12 LEU A 268      52.818  51.413  60.867  1.00  0.00
ATOM   4052 HD13 LEU A 268      54.029  52.688  60.471  1.00  0.00
ATOM   4053  CD2 LEU A 268      54.249  52.179  57.759  1.00  0.00
ATOM   4054 HD21 LEU A 268      53.851  52.327  56.734  1.00  0.00
ATOM   4055 HD22 LEU A 268      55.060  51.421  57.721  1.00  0.00
ATOM   4056 HD23 LEU A 268      54.684  53.140  58.098  1.00  0.00
ATOM   4057  C   LEU A 268      51.508  48.865  56.589  1.00  0.00
ATOM   4058  O   LEU A 268      52.223  48.041  56.023  1.00  0.00
ATOM   4059  N   ASN A 269      50.254  48.593  56.957  1.00  0.00
ATOM   4060  HN  ASN A 269      49.716  49.274  57.449  1.00  0.00
ATOM   4061  CA  ASN A 269      49.556  47.356  56.657  1.00  0.00
ATOM   4062  HA  ASN A 269      50.157  46.538  57.031  1.00  0.00
ATOM   4063  CB  ASN A 269      48.161  47.341  57.343  1.00  0.00
ATOM   4064  HB1 ASN A 269      47.640  46.386  57.112  1.00  0.00
ATOM   4065  HB2 ASN A 269      47.542  48.180  56.964  1.00  0.00
ATOM   4066  CG  ASN A 269      48.290  47.449  58.871  1.00  0.00
ATOM   4067  OD1 ASN A 269      49.355  47.230  59.458  1.00  0.00
ATOM   4068  ND2 ASN A 269      47.156  47.828  59.532  1.00  0.00
ATOM   4069 HD21 ASN A 269      47.175  47.919  60.527  1.00  0.00
ATOM   4070 HD22 ASN A 269      46.314  47.999  59.022  1.00  0.00
ATOM   4071  C   ASN A 269      49.365  47.146  55.167  1.00  0.00
ATOM   4072  O   ASN A 269      49.510  46.033  54.666  1.00  0.00
ATOM   4073  N   VAL A 270      49.036  48.218  54.438  1.00  0.00
ATOM   4074  HN  VAL A 270      48.901  49.103  54.878  1.00  0.00
ATOM   4075  CA  VAL A 270      48.892  48.221  52.992  1.00  0.00
ATOM   4076  HA  VAL A 270      48.208  47.420  52.747  1.00  0.00
ATOM   4077  CB  VAL A 270      48.264  49.517  52.476  1.00  0.00
ATOM   4078  HB  VAL A 270      48.803  50.391  52.903  1.00  0.00
ATOM   4079  CG1 VAL A 270      46.801  49.557  52.968  1.00  0.00
ATOM   4080 HG11 VAL A 270      46.745  49.522  54.074  1.00  0.00
ATOM   4081 HG12 VAL A 270      46.236  48.691  52.561  1.00  0.00
ATOM   4082 HG13 VAL A 270      46.305  50.487  52.625  1.00  0.00
ATOM   4083  CG2 VAL A 270      48.322  49.628  50.935  1.00  0.00
ATOM   4084 HG21 VAL A 270      47.869  48.730  50.464  1.00  0.00
ATOM   4085 HG22 VAL A 270      49.366  49.737  50.575  1.00  0.00
ATOM   4086 HG23 VAL A 270      47.754  50.523  50.600  1.00  0.00
ATOM   4087  C   VAL A 270      50.190  47.890  52.288  1.00  0.00
ATOM   4088  O   VAL A 270      50.205  47.094  51.351  1.00  0.00
ATOM   4089  N   LEU A 271      51.303  48.458  52.761  1.00  0.00
ATOM   4090  HN  LEU A 271      51.258  49.121  53.507  1.00  0.00
ATOM   4091  CA  LEU A 271      52.638  48.146  52.289  1.00  0.00
ATOM   4092  HA  LEU A 271      52.647  48.302  51.220  1.00  0.00
ATOM   4093  CB  LEU A 271      53.684  49.084  52.948  1.00  0.00
ATOM   4094  HB1 LEU A 271      53.535  49.067  54.048  1.00  0.00
ATOM   4095  HB2 LEU A 271      54.715  48.716  52.742  1.00  0.00
ATOM   4096  CG  LEU A 271      53.625  50.554  52.460  1.00  0.00
ATOM   4097  HG  LEU A 271      52.566  50.897  52.509  1.00  0.00
ATOM   4098  CD1 LEU A 271      54.440  51.478  53.386  1.00  0.00
ATOM   4099 HD11 LEU A 271      54.370  52.531  53.038  1.00  0.00
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ATOM   4100 HD12 LEU A 271      54.052  51.424  54.425  1.00  0.00
ATOM   4101 HD13 LEU A 271      55.508  51.176  53.389  1.00  0.00
ATOM   4102  CD2 LEU A 271      54.094  50.703  50.998  1.00  0.00
ATOM   4103 HD21 LEU A 271      54.051  51.768  50.689  1.00  0.00
ATOM   4104 HD22 LEU A 271      55.141  50.349  50.891  1.00  0.00
ATOM   4105 HD23 LEU A 271      53.448  50.116  50.314  1.00  0.00
ATOM   4106  C   LEU A 271      53.013  46.705  52.519  1.00  0.00
ATOM   4107  O   LEU A 271      53.578  46.076  51.636  1.00  0.00
ATOM   4108  N   ASP A 272      52.657  46.144  53.678  1.00  0.00
ATOM   4109  HN  ASP A 272      52.201  46.682  54.385  1.00  0.00
ATOM   4110  CA  ASP A 272      52.890  44.750  54.023  1.00  0.00
ATOM   4111  HA  ASP A 272      53.957  44.590  53.945  1.00  0.00
ATOM   4112  CB  ASP A 272      52.425  44.495  55.488  1.00  0.00
ATOM   4113  HB1 ASP A 272      52.817  45.307  56.137  1.00  0.00
ATOM   4114  HB2 ASP A 272      51.318  44.509  55.553  1.00  0.00
ATOM   4115  CG  ASP A 272      52.943  43.162  56.045  1.00  0.00
ATOM   4116  OD1 ASP A 272      53.907  42.590  55.474  1.00  0.00
ATOM   4117  OD2 ASP A 272      52.419  42.748  57.114  1.00  0.00
ATOM   4118  C   ASP A 272      52.196  43.814  53.043  1.00  0.00
ATOM   4119  O   ASP A 272      52.745  42.790  52.638  1.00  0.00
ATOM   4120  N   GLY A 273      50.993  44.196  52.610  1.00  0.00
ATOM   4121  HN  GLY A 273      50.585  45.038  52.958  1.00  0.00
ATOM   4122  CA  GLY A 273      50.181  43.466  51.663  1.00  0.00
ATOM   4123  HA1 GLY A 273      49.201  43.917  51.694  1.00  0.00
ATOM   4124  HA2 GLY A 273      50.170  42.425  51.959  1.00  0.00
ATOM   4125  C   GLY A 273      50.672  43.545  50.236  1.00  0.00
ATOM   4126  O   GLY A 273      50.201  42.772  49.403  1.00  0.00
ATOM   4127  N   MET A 274      51.584  44.469  49.906  1.00  0.00
ATOM   4128  HN  MET A 274      51.989  45.063  50.598  1.00  0.00
ATOM   4129  CA  MET A 274      51.909  44.769  48.524  1.00  0.00
ATOM   4130  HA  MET A 274      51.440  44.051  47.866  1.00  0.00
ATOM   4131  CB  MET A 274      51.383  46.184  48.157  1.00  0.00
ATOM   4132  HB1 MET A 274      51.747  46.485  47.149  1.00  0.00
ATOM   4133  HB2 MET A 274      51.779  46.918  48.894  1.00  0.00
ATOM   4134  CG  MET A 274      49.844  46.288  48.133  1.00  0.00
ATOM   4135  HG1 MET A 274      49.577  47.356  47.970  1.00  0.00
ATOM   4136  HG2 MET A 274      49.447  46.009  49.132  1.00  0.00
ATOM   4137  SD  MET A 274      49.050  45.265  46.853  1.00  0.00
ATOM   4138  CE  MET A 274      47.351  45.633  47.376  1.00  0.00
ATOM   4139  HE1 MET A 274      47.144  46.723  47.324  1.00  0.00
ATOM   4140  HE2 MET A 274      47.175  45.299  48.421  1.00  0.00
ATOM   4141  HE3 MET A 274      46.615  45.113  46.724  1.00  0.00
ATOM   4142  C   MET A 274      53.383  44.732  48.181  1.00  0.00
ATOM   4143  O   MET A 274      53.731  44.502  47.024  1.00  0.00
ATOM   4144  N   THR A 275      54.273  44.943  49.156  1.00  0.00
ATOM   4145  HN  THR A 275      53.985  45.134  50.095  1.00  0.00
ATOM   4146  CA  THR A 275      55.718  44.949  48.948  1.00  0.00
ATOM   4147  HA  THR A 275      55.906  45.634  48.133  1.00  0.00
ATOM   4148  CB  THR A 275      56.549  45.444  50.136  1.00  0.00
ATOM   4149  HB  THR A 275      57.634  45.242  49.981  1.00  0.00
ATOM   4150  OG1 THR A 275      56.153  44.818  51.351  1.00  0.00
ATOM   4151  HG1 THR A 275      56.769  45.122  52.022  1.00  0.00
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ATOM   4152  CG2 THR A 275      56.394  46.975  50.262  1.00  0.00
ATOM   4153 HG21 THR A 275      55.328  47.270  50.341  1.00  0.00
ATOM   4154 HG22 THR A 275      56.829  47.477  49.373  1.00  0.00
ATOM   4155 HG23 THR A 275      56.928  47.343  51.163  1.00  0.00
ATOM   4156  C   THR A 275      56.265  43.613  48.503  1.00  0.00
ATOM   4157  O   THR A 275      57.141  43.552  47.644  1.00  0.00
ATOM   4158  N   TRP A 276      55.758  42.528  49.093  1.00  0.00
ATOM   4159  HN  TRP A 276      55.065  42.623  49.804  1.00  0.00
ATOM   4160  CA  TRP A 276      56.151  41.169  48.789  1.00  0.00
ATOM   4161  HA  TRP A 276      57.222  41.104  48.928  1.00  0.00
ATOM   4162  CB  TRP A 276      55.458  40.200  49.788  1.00  0.00
ATOM   4163  HB1 TRP A 276      54.355  40.328  49.714  1.00  0.00
ATOM   4164  HB2 TRP A 276      55.746  40.524  50.813  1.00  0.00
ATOM   4165  CG  TRP A 276      55.782  38.742  49.646  1.00  0.00
ATOM   4166  CD1 TRP A 276      56.812  38.076  50.257  1.00  0.00
ATOM   4167  HD1 TRP A 276      57.539  38.533  50.913  1.00  0.00
ATOM   4168  NE1 TRP A 276      56.769  36.750  49.921  1.00  0.00
ATOM   4169  HE1 TRP A 276      57.377  36.060  50.250  1.00  0.00
ATOM   4170  CE2 TRP A 276      55.710  36.521  49.090  1.00  0.00
ATOM   4171  CD2 TRP A 276      55.060  37.760  48.884  1.00  0.00
ATOM   4172  CE3 TRP A 276      53.928  37.813  48.071  1.00  0.00
ATOM   4173  HE3 TRP A 276      53.405  38.741  47.893  1.00  0.00
ATOM   4174  CZ3 TRP A 276      53.457  36.632  47.495  1.00  0.00
ATOM   4175  HZ3 TRP A 276      52.575  36.659  46.870  1.00  0.00
ATOM   4176  CZ2 TRP A 276      55.244  35.346  48.517  1.00  0.00
ATOM   4177  HZ2 TRP A 276      55.730  34.397  48.684  1.00  0.00
ATOM   4178  CH2 TRP A 276      54.098  35.418  47.724  1.00  0.00
ATOM   4179  HH2 TRP A 276      53.701  34.516  47.281  1.00  0.00
ATOM   4180  C   TRP A 276      55.847  40.800  47.354  1.00  0.00
ATOM   4181  O   TRP A 276      56.689  40.231  46.663  1.00  0.00
ATOM   4182  N   LEU A 277      54.653  41.161  46.880  1.00  0.00
ATOM   4183  HN  LEU A 277      53.996  41.620  47.473  1.00  0.00
ATOM   4184  CA  LEU A 277      54.224  40.999  45.508  1.00  0.00
ATOM   4185  HA  LEU A 277      54.356  39.957  45.251  1.00  0.00
ATOM   4186  CB  LEU A 277      52.724  41.374  45.390  1.00  0.00
ATOM   4187  HB1 LEU A 277      52.151  40.712  46.076  1.00  0.00
ATOM   4188  HB2 LEU A 277      52.584  42.418  45.748  1.00  0.00
ATOM   4189  CG  LEU A 277      52.097  41.259  43.978  1.00  0.00
ATOM   4190  HG  LEU A 277      52.641  41.950  43.292  1.00  0.00
ATOM   4191  CD1 LEU A 277      52.214  39.837  43.394  1.00  0.00
ATOM   4192 HD11 LEU A 277      51.746  39.796  42.388  1.00  0.00
ATOM   4193 HD12 LEU A 277      53.278  39.537  43.294  1.00  0.00
ATOM   4194 HD13 LEU A 277      51.699  39.107  44.053  1.00  0.00
ATOM   4195  CD2 LEU A 277      50.629  41.728  43.999  1.00  0.00
ATOM   4196 HD21 LEU A 277      50.197  41.690  42.976  1.00  0.00
ATOM   4197 HD22 LEU A 277      50.025  41.075  44.664  1.00  0.00
ATOM   4198 HD23 LEU A 277      50.561  42.772  44.372  1.00  0.00
ATOM   4199  C   LEU A 277      55.046  41.830  44.546  1.00  0.00
ATOM   4200  O   LEU A 277      55.422  41.361  43.474  1.00  0.00
ATOM   4201  N   ALA A 278      55.344  43.075  44.933  1.00  0.00
ATOM   4202  HN  ALA A 278      55.011  43.417  45.811  1.00  0.00
ATOM   4203  CA  ALA A 278      56.105  44.039  44.167  1.00  0.00
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ATOM   4204  HA  ALA A 278      55.600  44.156  43.218  1.00  0.00
ATOM   4205  CB  ALA A 278      56.158  45.417  44.858  1.00  0.00
ATOM   4206  HB1 ALA A 278      55.127  45.790  45.038  1.00  0.00
ATOM   4207  HB2 ALA A 278      56.680  45.356  45.836  1.00  0.00
ATOM   4208  HB3 ALA A 278      56.685  46.159  44.221  1.00  0.00
ATOM   4209  C   ALA A 278      57.512  43.583  43.882  1.00  0.00
ATOM   4210  O   ALA A 278      58.019  43.783  42.781  1.00  0.00
ATOM   4211  N   GLN A 279      58.155  42.951  44.867  1.00  0.00
ATOM   4212  HN  GLN A 279      57.719  42.840  45.759  1.00  0.00
ATOM   4213  CA  GLN A 279      59.477  42.371  44.753  1.00  0.00
ATOM   4214  HA  GLN A 279      60.156  43.160  44.462  1.00  0.00
ATOM   4215  CB  GLN A 279      59.921  41.818  46.133  1.00  0.00
ATOM   4216  HB1 GLN A 279      59.105  41.171  46.526  1.00  0.00
ATOM   4217  HB2 GLN A 279      60.021  42.685  46.824  1.00  0.00
ATOM   4218  CG  GLN A 279      61.236  41.010  46.125  1.00  0.00
ATOM   4219  HG1 GLN A 279      62.048  41.623  45.679  1.00  0.00
ATOM   4220  HG2 GLN A 279      61.128  40.082  45.525  1.00  0.00
ATOM   4221  CD  GLN A 279      61.646  40.627  47.554  1.00  0.00
ATOM   4222  OE1 GLN A 279      62.688  41.065  48.050  1.00  0.00
ATOM   4223  NE2 GLN A 279      60.803  39.783  48.218  1.00  0.00
ATOM   4224 HE21 GLN A 279      61.027  39.501  49.150  1.00  0.00
ATOM   4225 HE22 GLN A 279      59.968  39.460  47.775  1.00  0.00
ATOM   4226  C   GLN A 279      59.559  41.289  43.703  1.00  0.00
ATOM   4227  O   GLN A 279      60.489  41.262  42.900  1.00  0.00
ATOM   4228  N   ILE A 280      58.565  40.396  43.675  1.00  0.00
ATOM   4229  HN  ILE A 280      57.822  40.438  44.339  1.00  0.00
ATOM   4230  CA  ILE A 280      58.451  39.343  42.683  1.00  0.00
ATOM   4231  HA  ILE A 280      59.386  38.801  42.683  1.00  0.00
ATOM   4232  CB  ILE A 280      57.327  38.348  43.005  1.00  0.00
ATOM   4233  HB  ILE A 280      56.349  38.882  42.983  1.00  0.00
ATOM   4234  CG2 ILE A 280      57.291  37.220  41.944  1.00  0.00
ATOM   4235 HG21 ILE A 280      58.251  36.663  41.948  1.00  0.00
ATOM   4236 HG22 ILE A 280      57.123  37.618  40.925  1.00  0.00
ATOM   4237 HG23 ILE A 280      56.469  36.506  42.160  1.00  0.00
ATOM   4238  CG1 ILE A 280      57.501  37.762  44.431  1.00  0.00
ATOM   4239 HG11 ILE A 280      57.651  38.575  45.168  1.00  0.00
ATOM   4240 HG12 ILE A 280      58.414  37.134  44.449  1.00  0.00
ATOM   4241  CD1 ILE A 280      56.312  36.925  44.913  1.00  0.00
ATOM   4242  HD1 ILE A 280      56.202  36.010  44.295  1.00  0.00
ATOM   4243  HD2 ILE A 280      55.371  37.512  44.855  1.00  0.00
ATOM   4244  HD3 ILE A 280      56.465  36.612  45.968  1.00  0.00
ATOM   4245  C   ILE A 280      58.259  39.927  41.302  1.00  0.00
ATOM   4246  O   ILE A 280      58.928  39.522  40.355  1.00  0.00
ATOM   4247  N   GLY A 281      57.367  40.915  41.183  1.00  0.00
ATOM   4248  HN  GLY A 281      56.879  41.253  41.987  1.00  0.00
ATOM   4249  CA  GLY A 281      56.945  41.473  39.918  1.00  0.00
ATOM   4250  HA1 GLY A 281      56.101  42.111  40.132  1.00  0.00
ATOM   4251  HA2 GLY A 281      56.694  40.657  39.256  1.00  0.00
ATOM   4252  C   GLY A 281      57.991  42.311  39.244  1.00  0.00
ATOM   4253  O   GLY A 281      58.193  42.186  38.038  1.00  0.00
ATOM   4254  N   MET A 282      58.671  43.178  39.998  1.00  0.00
ATOM   4255  HN  MET A 282      58.480  43.261  40.975  1.00  0.00
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ATOM   4256  CA  MET A 282      59.699  44.068  39.495  1.00  0.00
ATOM   4257  HA  MET A 282      59.256  44.653  38.702  1.00  0.00
ATOM   4258  CB  MET A 282      60.165  45.031  40.622  1.00  0.00
ATOM   4259  HB1 MET A 282      60.463  44.425  41.508  1.00  0.00
ATOM   4260  HB2 MET A 282      59.298  45.655  40.928  1.00  0.00
ATOM   4261  CG  MET A 282      61.347  45.956  40.260  1.00  0.00
ATOM   4262  HG1 MET A 282      62.247  45.335  40.065  1.00  0.00
ATOM   4263  HG2 MET A 282      61.583  46.577  41.153  1.00  0.00
ATOM   4264  SD  MET A 282      61.020  47.051  38.839  1.00  0.00
ATOM   4265  CE  MET A 282      62.765  47.359  38.440  1.00  0.00
ATOM   4266  HE1 MET A 282      63.267  46.423  38.110  1.00  0.00
ATOM   4267  HE2 MET A 282      63.317  47.748  39.322  1.00  0.00
ATOM   4268  HE3 MET A 282      62.859  48.103  37.620  1.00  0.00
ATOM   4269  C   MET A 282      60.889  43.342  38.917  1.00  0.00
ATOM   4270  O   MET A 282      61.380  43.689  37.844  1.00  0.00
ATOM   4271  N   PHE A 283      61.359  42.302  39.609  1.00  0.00
ATOM   4272  HN  PHE A 283      60.949  42.022  40.475  1.00  0.00
ATOM   4273  CA  PHE A 283      62.497  41.531  39.164  1.00  0.00
ATOM   4274  HA  PHE A 283      63.200  42.207  38.697  1.00  0.00
ATOM   4275  CB  PHE A 283      63.208  40.868  40.370  1.00  0.00
ATOM   4276  HB1 PHE A 283      63.876  40.042  40.040  1.00  0.00
ATOM   4277  HB2 PHE A 283      62.463  40.448  41.078  1.00  0.00
ATOM   4278  CG  PHE A 283      64.072  41.874  41.088  1.00  0.00
ATOM   4279  CD1 PHE A 283      65.394  42.083  40.655  1.00  0.00
ATOM   4280  HD1 PHE A 283      65.782  41.510  39.825  1.00  0.00
ATOM   4281  CE1 PHE A 283      66.206  43.042  41.271  1.00  0.00
ATOM   4282  HE1 PHE A 283      67.216  43.200  40.923  1.00  0.00
ATOM   4283  CZ  PHE A 283      65.707  43.794  42.341  1.00  0.00
ATOM   4284  HZ  PHE A 283      66.331  44.532  42.816  1.00  0.00
ATOM   4285  CD2 PHE A 283      63.590  42.626  42.174  1.00  0.00
ATOM   4286  HD2 PHE A 283      62.580  42.486  42.521  1.00  0.00
ATOM   4287  CE2 PHE A 283      64.401  43.583  42.797  1.00  0.00
ATOM   4288  HE2 PHE A 283      64.018  44.162  43.626  1.00  0.00
ATOM   4289  C   PHE A 283      62.147  40.511  38.112  1.00  0.00
ATOM   4290  O   PHE A 283      63.006  40.100  37.335  1.00  0.00
ATOM   4291  N   LEU A 284      60.876  40.112  38.035  1.00  0.00
ATOM   4292  HN  LEU A 284      60.192  40.418  38.695  1.00  0.00
ATOM   4293  CA  LEU A 284      60.383  39.272  36.964  1.00  0.00
ATOM   4294  HA  LEU A 284      61.044  38.419  36.909  1.00  0.00
ATOM   4295  CB  LEU A 284      58.957  38.767  37.297  1.00  0.00
ATOM   4296  HB1 LEU A 284      58.278  39.636  37.436  1.00  0.00
ATOM   4297  HB2 LEU A 284      59.013  38.222  38.264  1.00  0.00
ATOM   4298  CG  LEU A 284      58.322  37.796  36.274  1.00  0.00
ATOM   4299  HG  LEU A 284      58.212  38.328  35.301  1.00  0.00
ATOM   4300  CD1 LEU A 284      59.208  36.557  36.038  1.00  0.00
ATOM   4301 HD11 LEU A 284      59.359  36.002  36.988  1.00  0.00
ATOM   4302 HD12 LEU A 284      60.200  36.850  35.637  1.00  0.00
ATOM   4303 HD13 LEU A 284      58.733  35.878  35.304  1.00  0.00
ATOM   4304  CD2 LEU A 284      56.909  37.386  36.731  1.00  0.00
ATOM   4305 HD21 LEU A 284      56.278  38.287  36.886  1.00  0.00
ATOM   4306 HD22 LEU A 284      56.961  36.821  37.686  1.00  0.00
ATOM   4307 HD23 LEU A 284      56.422  36.745  35.969  1.00  0.00
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ATOM   4308  C   LEU A 284      60.413  39.960  35.617  1.00  0.00
ATOM   4309  O   LEU A 284      60.835  39.369  34.623  1.00  0.00
ATOM   4310  N   VAL A 285      60.003  41.234  35.573  1.00  0.00
ATOM   4311  HN  VAL A 285      59.669  41.700  36.390  1.00  0.00
ATOM   4312  CA  VAL A 285      59.960  42.006  34.344  1.00  0.00
ATOM   4313  HA  VAL A 285      59.662  41.333  33.554  1.00  0.00
ATOM   4314  CB  VAL A 285      58.928  43.135  34.339  1.00  0.00
ATOM   4315  HB  VAL A 285      58.931  43.624  33.338  1.00  0.00
ATOM   4316  CG1 VAL A 285      59.233  44.222  35.391  1.00  0.00
ATOM   4317 HG11 VAL A 285      60.217  44.699  35.206  1.00  0.00
ATOM   4318 HG12 VAL A 285      59.232  43.792  36.411  1.00  0.00
ATOM   4319 HG13 VAL A 285      58.454  45.013  35.351  1.00  0.00
ATOM   4320  CG2 VAL A 285      57.525  42.516  34.524  1.00  0.00
ATOM   4321 HG21 VAL A 285      57.431  42.028  35.516  1.00  0.00
ATOM   4322 HG22 VAL A 285      57.328  41.760  33.735  1.00  0.00
ATOM   4323 HG23 VAL A 285      56.749  43.308  34.454  1.00  0.00
ATOM   4324  C   VAL A 285      61.332  42.531  33.976  1.00  0.00
ATOM   4325  O   VAL A 285      61.590  42.854  32.819  1.00  0.00
ATOM   4326  N   LEU A 286      62.253  42.567  34.944  1.00  0.00
ATOM   4327  HN  LEU A 286      62.017  42.327  35.883  1.00  0.00
ATOM   4328  CA  LEU A 286      63.637  42.926  34.719  1.00  0.00
ATOM   4329  HA  LEU A 286      63.661  43.782  34.060  1.00  0.00
ATOM   4330  CB  LEU A 286      64.306  43.290  36.070  1.00  0.00
ATOM   4331  HB1 LEU A 286      64.245  42.415  36.752  1.00  0.00
ATOM   4332  HB2 LEU A 286      63.713  44.113  36.528  1.00  0.00
ATOM   4333  CG  LEU A 286      65.784  43.752  36.010  1.00  0.00
ATOM   4334  HG  LEU A 286      66.401  42.897  35.647  1.00  0.00
ATOM   4335  CD1 LEU A 286      66.000  44.925  35.036  1.00  0.00
ATOM   4336 HD11 LEU A 286      65.391  45.800  35.347  1.00  0.00
ATOM   4337 HD12 LEU A 286      65.714  44.642  34.002  1.00  0.00
ATOM   4338 HD13 LEU A 286      67.071  45.222  35.030  1.00  0.00
ATOM   4339  CD2 LEU A 286      66.301  44.112  37.416  1.00  0.00
ATOM   4340 HD21 LEU A 286      66.196  43.243  38.099  1.00  0.00
ATOM   4341 HD22 LEU A 286      65.723  44.963  37.835  1.00  0.00
ATOM   4342 HD23 LEU A 286      67.373  44.400  37.373  1.00  0.00
ATOM   4343  C   LEU A 286      64.381  41.782  34.062  1.00  0.00
ATOM   4344  O   LEU A 286      65.369  41.990  33.362  1.00  0.00
ATOM   4345  N   GLY A 287      63.873  40.558  34.232  1.00  0.00
ATOM   4346  HN  GLY A 287      63.056  40.427  34.791  1.00  0.00
ATOM   4347  CA  GLY A 287      64.437  39.344  33.679  1.00  0.00
ATOM   4348  HA1 GLY A 287      63.957  38.522  34.188  1.00  0.00
ATOM   4349  HA2 GLY A 287      65.509  39.360  33.824  1.00  0.00
ATOM   4350  C   GLY A 287      64.151  39.196  32.213  1.00  0.00
ATOM   4351  O   GLY A 287      64.793  38.400  31.532  1.00  0.00
ATOM   4352  N   LEU A 288      63.189  39.964  31.695  1.00  0.00
ATOM   4353  HN  LEU A 288      62.679  40.595  32.274  1.00  0.00
ATOM   4354  CA  LEU A 288      62.813  39.971  30.298  1.00  0.00
ATOM   4355  HA  LEU A 288      62.798  38.950  29.941  1.00  0.00
ATOM   4356  CB  LEU A 288      61.408  40.608  30.125  1.00  0.00
ATOM   4357  HB1 LEU A 288      61.118  40.570  29.051  1.00  0.00
ATOM   4358  HB2 LEU A 288      61.452  41.678  30.428  1.00  0.00
ATOM   4359  CG  LEU A 288      60.279  39.928  30.944  1.00  0.00
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ATOM   4360  HG  LEU A 288      60.545  40.005  32.022  1.00  0.00
ATOM   4361  CD1 LEU A 288      58.933  40.657  30.761  1.00  0.00
ATOM   4362 HD11 LEU A 288      58.617  40.629  29.697  1.00  0.00
ATOM   4363 HD12 LEU A 288      59.021  41.716  31.078  1.00  0.00
ATOM   4364 HD13 LEU A 288      58.146  40.172  31.378  1.00  0.00
ATOM   4365  CD2 LEU A 288      60.132  38.430  30.619  1.00  0.00
ATOM   4366 HD21 LEU A 288      61.075  37.892  30.844  1.00  0.00
ATOM   4367 HD22 LEU A 288      59.888  38.287  29.545  1.00  0.00
ATOM   4368 HD23 LEU A 288      59.322  37.979  31.230  1.00  0.00
ATOM   4369  C   LEU A 288      63.812  40.743  29.459  1.00  0.00
ATOM   4370  O   LEU A 288      63.864  40.581  28.242  1.00  0.00
ATOM   4371  N   LEU A 289      64.636  41.570  30.107  1.00  0.00
ATOM   4372  HN  LEU A 289      64.575  41.670  31.098  1.00  0.00
ATOM   4373  CA  LEU A 289      65.648  42.386  29.470  1.00  0.00
ATOM   4374  HA  LEU A 289      65.439  42.494  28.416  1.00  0.00
ATOM   4375  CB  LEU A 289      65.684  43.782  30.144  1.00  0.00
ATOM   4376  HB1 LEU A 289      66.556  44.376  29.794  1.00  0.00
ATOM   4377  HB2 LEU A 289      65.805  43.632  31.241  1.00  0.00
ATOM   4378  CG  LEU A 289      64.413  44.630  29.900  1.00  0.00
ATOM   4379  HG  LEU A 289      63.596  43.959  29.550  1.00  0.00
ATOM   4380  CD1 LEU A 289      63.920  45.285  31.203  1.00  0.00
ATOM   4381 HD11 LEU A 289      64.694  45.965  31.616  1.00  0.00
ATOM   4382 HD12 LEU A 289      63.689  44.507  31.960  1.00  0.00
ATOM   4383 HD13 LEU A 289      62.999  45.872  31.010  1.00  0.00
ATOM   4384  CD2 LEU A 289      64.648  45.681  28.798  1.00  0.00
ATOM   4385 HD21 LEU A 289      65.015  45.195  27.870  1.00  0.00
ATOM   4386 HD22 LEU A 289      65.408  46.422  29.128  1.00  0.00
ATOM   4387 HD23 LEU A 289      63.705  46.219  28.568  1.00  0.00
ATOM   4388  C   LEU A 289      67.018  41.766  29.628  1.00  0.00
ATOM   4389  O   LEU A 289      68.013  42.339  29.184  1.00  0.00
ATOM   4390  N   VAL A 290      67.089  40.587  30.249  1.00  0.00
ATOM   4391  HN  VAL A 290      66.263  40.116  30.552  1.00  0.00
ATOM   4392  CA  VAL A 290      68.333  39.939  30.599  1.00  0.00
ATOM   4393  HA  VAL A 290      69.168  40.576  30.343  1.00  0.00
ATOM   4394  CB  VAL A 290      68.424  39.634  32.093  1.00  0.00
ATOM   4395  HB  VAL A 290      67.478  39.152  32.429  1.00  0.00
ATOM   4396  CG1 VAL A 290      68.589  40.971  32.848  1.00  0.00
ATOM   4397 HG11 VAL A 290      67.758  41.669  32.618  1.00  0.00
ATOM   4398 HG12 VAL A 290      69.545  41.459  32.560  1.00  0.00
ATOM   4399 HG13 VAL A 290      68.602  40.793  33.944  1.00  0.00
ATOM   4400  CG2 VAL A 290      69.595  38.682  32.423  1.00  0.00
ATOM   4401 HG21 VAL A 290      70.553  39.104  32.054  1.00  0.00
ATOM   4402 HG22 VAL A 290      69.447  37.676  31.981  1.00  0.00
ATOM   4403 HG23 VAL A 290      69.663  38.556  33.524  1.00  0.00
ATOM   4404  C   VAL A 290      68.446  38.682  29.777  1.00  0.00
ATOM   4405  O   VAL A 290      67.654  37.751  29.921  1.00  0.00
ATOM   4406  N   THR A 291      69.443  38.645  28.893  1.00  0.00
ATOM   4407  HN  THR A 291      70.040  39.434  28.761  1.00  0.00
ATOM   4408  CA  THR A 291      69.820  37.486  28.120  1.00  0.00
ATOM   4409  HA  THR A 291      69.687  36.611  28.741  1.00  0.00
ATOM   4410  CB  THR A 291      68.997  37.383  26.830  1.00  0.00
ATOM   4411  HB  THR A 291      67.921  37.494  27.102  1.00  0.00
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ATOM   4412  OG1 THR A 291      69.115  36.101  26.231  1.00  0.00
ATOM   4413  HG1 THR A 291      68.668  35.488  26.820  1.00  0.00
ATOM   4414  CG2 THR A 291      69.336  38.484  25.800  1.00  0.00
ATOM   4415 HG21 THR A 291      70.380  38.394  25.440  1.00  0.00
ATOM   4416 HG22 THR A 291      69.201  39.491  26.249  1.00  0.00
ATOM   4417 HG23 THR A 291      68.660  38.404  24.922  1.00  0.00
ATOM   4418  C   THR A 291      71.300  37.731  27.893  1.00  0.00
ATOM   4419  O   THR A 291      71.665  38.895  27.744  1.00  0.00
ATOM   4420  N   PRO A 292      72.246  36.779  27.887  1.00  0.00
ATOM   4421  CD  PRO A 292      73.646  37.153  28.124  1.00  0.00
ATOM   4422  HD1 PRO A 292      73.716  37.731  29.073  1.00  0.00
ATOM   4423  HD2 PRO A 292      74.039  37.760  27.279  1.00  0.00
ATOM   4424  CA  PRO A 292      72.055  35.339  27.886  1.00  0.00
ATOM   4425  HA  PRO A 292      71.111  35.068  28.334  1.00  0.00
ATOM   4426  CB  PRO A 292      73.289  34.848  28.658  1.00  0.00
ATOM   4427  HB1 PRO A 292      73.555  33.793  28.453  1.00  0.00
ATOM   4428  HB2 PRO A 292      73.091  34.957  29.748  1.00  0.00
ATOM   4429  CG  PRO A 292      74.398  35.829  28.261  1.00  0.00
ATOM   4430  HG1 PRO A 292      75.212  35.877  29.012  1.00  0.00
ATOM   4431  HG2 PRO A 292      74.823  35.537  27.276  1.00  0.00
ATOM   4432  C   PRO A 292      72.101  34.852  26.453  1.00  0.00
ATOM   4433  O   PRO A 292      72.108  33.640  26.243  1.00  0.00
ATOM   4434  N   SER A 293      72.139  35.769  25.482  1.00  0.00
ATOM   4435  HN  SER A 293      72.123  36.735  25.730  1.00  0.00
ATOM   4436  CA  SER A 293      72.180  35.516  24.055  1.00  0.00
ATOM   4437  HA  SER A 293      71.332  34.891  23.812  1.00  0.00
ATOM   4438  CB  SER A 293      72.070  36.858  23.281  1.00  0.00
ATOM   4439  HB1 SER A 293      72.939  37.512  23.508  1.00  0.00
ATOM   4440  HB2 SER A 293      71.148  37.383  23.607  1.00  0.00
ATOM   4441  OG  SER A 293      71.980  36.672  21.871  1.00  0.00
ATOM   4442  HG  SER A 293      72.810  36.275  21.594  1.00  0.00
ATOM   4443  C   SER A 293      73.442  34.794  23.636  1.00  0.00
ATOM   4444  O   SER A 293      73.419  33.965  22.729  1.00  0.00
ATOM   4445  N   GLU A 294      74.562  35.107  24.290  1.00  0.00
ATOM   4446  HN  GLU A 294      74.551  35.765  25.039  1.00  0.00
ATOM   4447  CA  GLU A 294      75.869  34.602  23.935  1.00  0.00
ATOM   4448  HA  GLU A 294      75.992  34.707  22.868  1.00  0.00
ATOM   4449  CB  GLU A 294      76.968  35.444  24.629  1.00  0.00
ATOM   4450  HB1 GLU A 294      76.758  35.496  25.719  1.00  0.00
ATOM   4451  HB2 GLU A 294      77.958  34.950  24.493  1.00  0.00
ATOM   4452  CG  GLU A 294      77.082  36.864  24.041  1.00  0.00
ATOM   4453  HG1 GLU A 294      77.318  36.793  22.957  1.00  0.00
ATOM   4454  HG2 GLU A 294      76.125  37.414  24.154  1.00  0.00
ATOM   4455  CD  GLU A 294      78.192  37.640  24.751  1.00  0.00
ATOM   4456  OE1 GLU A 294      79.265  37.852  24.126  1.00  0.00
ATOM   4457  OE2 GLU A 294      77.976  38.025  25.932  1.00  0.00
ATOM   4458  C   GLU A 294      76.068  33.143  24.281  1.00  0.00
ATOM   4459  O   GLU A 294      76.939  32.483  23.721  1.00  0.00
ATOM   4460  N   LEU A 295      75.246  32.609  25.186  1.00  0.00
ATOM   4461  HN  LEU A 295      74.514  33.151  25.592  1.00  0.00
ATOM   4462  CA  LEU A 295      75.373  31.256  25.689  1.00  0.00
ATOM   4463  HA  LEU A 295      76.371  30.887  25.500  1.00  0.00
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ATOM   4464  CB  LEU A 295      75.111  31.232  27.222  1.00  0.00
ATOM   4465  HB1 LEU A 295      74.284  31.938  27.447  1.00  0.00
ATOM   4466  HB2 LEU A 295      74.778  30.224  27.557  1.00  0.00
ATOM   4467  CG  LEU A 295      76.338  31.570  28.116  1.00  0.00
ATOM   4468  HG  LEU A 295      75.949  31.640  29.161  1.00  0.00
ATOM   4469  CD1 LEU A 295      77.376  30.430  28.111  1.00  0.00
ATOM   4470 HD11 LEU A 295      78.190  30.647  28.835  1.00  0.00
ATOM   4471 HD12 LEU A 295      76.898  29.469  28.398  1.00  0.00
ATOM   4472 HD13 LEU A 295      77.825  30.314  27.103  1.00  0.00
ATOM   4473  CD2 LEU A 295      77.013  32.920  27.805  1.00  0.00
ATOM   4474 HD21 LEU A 295      77.778  33.154  28.575  1.00  0.00
ATOM   4475 HD22 LEU A 295      77.516  32.886  26.816  1.00  0.00
ATOM   4476 HD23 LEU A 295      76.262  33.735  27.796  1.00  0.00
ATOM   4477  C   LEU A 295      74.418  30.323  24.972  1.00  0.00
ATOM   4478  O   LEU A 295      74.194  29.194  25.407  1.00  0.00
ATOM   4479  N   MET A 296      73.870  30.760  23.834  1.00  0.00
ATOM   4480  HN  MET A 296      74.057  31.677  23.490  1.00  0.00
ATOM   4481  CA  MET A 296      72.952  29.965  23.044  1.00  0.00
ATOM   4482  HA  MET A 296      72.449  29.241  23.670  1.00  0.00
ATOM   4483  CB  MET A 296      71.902  30.889  22.371  1.00  0.00
ATOM   4484  HB1 MET A 296      72.428  31.612  21.706  1.00  0.00
ATOM   4485  HB2 MET A 296      71.217  30.284  21.735  1.00  0.00
ATOM   4486  CG  MET A 296      71.034  31.703  23.352  1.00  0.00
ATOM   4487  HG1 MET A 296      71.689  32.345  23.976  1.00  0.00
ATOM   4488  HG2 MET A 296      70.402  32.386  22.741  1.00  0.00
ATOM   4489  SD  MET A 296      69.962  30.698  24.423  1.00  0.00
ATOM   4490  CE  MET A 296      69.001  32.111  25.037  1.00  0.00
ATOM   4491  HE1 MET A 296      68.246  31.783  25.783  1.00  0.00
ATOM   4492  HE2 MET A 296      69.662  32.861  25.520  1.00  0.00
ATOM   4493  HE3 MET A 296      68.463  32.616  24.207  1.00  0.00
ATOM   4494  C   MET A 296      73.678  29.231  21.937  1.00  0.00
ATOM   4495  O   MET A 296      73.072  28.453  21.202  1.00  0.00
ATOM   4496  N   GLU A 297      74.989  29.447  21.818  1.00  0.00
ATOM   4497  HN  GLU A 297      75.468  30.068  22.434  1.00  0.00
ATOM   4498  CA  GLU A 297      75.813  28.797  20.830  1.00  0.00
ATOM   4499  HA  GLU A 297      75.439  27.797  20.654  1.00  0.00
ATOM   4500  CB  GLU A 297      75.796  29.599  19.501  1.00  0.00
ATOM   4501  HB1 GLU A 297      74.778  29.501  19.061  1.00  0.00
ATOM   4502  HB2 GLU A 297      75.927  30.672  19.750  1.00  0.00
ATOM   4503  CG  GLU A 297      76.840  29.213  18.429  1.00  0.00
ATOM   4504  HG1 GLU A 297      76.691  29.852  17.532  1.00  0.00
ATOM   4505  HG2 GLU A 297      77.867  29.396  18.809  1.00  0.00
ATOM   4506  CD  GLU A 297      76.691  27.749  18.012  1.00  0.00
ATOM   4507  OE1 GLU A 297      77.680  26.984  18.173  1.00  0.00
ATOM   4508  OE2 GLU A 297      75.589  27.379  17.529  1.00  0.00
ATOM   4509  C   GLU A 297      77.188  28.665  21.430  1.00  0.00
ATOM   4510  O   GLU A 297      77.603  29.491  22.242  1.00  0.00
ATOM   4511  N   ILE A 298      77.883  27.579  21.083  1.00  0.00
ATOM   4512  HN  ILE A 298      77.535  26.986  20.357  1.00  0.00
ATOM   4513  CA  ILE A 298      79.096  27.090  21.701  1.00  0.00
ATOM   4514  HA  ILE A 298      78.866  26.943  22.746  1.00  0.00
ATOM   4515  CB  ILE A 298      79.503  25.744  21.090  1.00  0.00
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ATOM   4516  HB  ILE A 298      79.698  25.888  20.000  1.00  0.00
ATOM   4517  CG2 ILE A 298      78.309  24.765  21.203  1.00  0.00
ATOM   4518 HG21 ILE A 298      77.455  25.093  20.575  1.00  0.00
ATOM   4519 HG22 ILE A 298      77.967  24.682  22.255  1.00  0.00
ATOM   4520 HG23 ILE A 298      78.614  23.756  20.851  1.00  0.00
ATOM   4521  CG1 ILE A 298      80.794  25.130  21.704  1.00  0.00
ATOM   4522 HG11 ILE A 298      81.664  25.784  21.484  1.00  0.00
ATOM   4523 HG12 ILE A 298      80.985  24.162  21.190  1.00  0.00
ATOM   4524  CD1 ILE A 298      80.731  24.872  23.215  1.00  0.00
ATOM   4525  HD1 ILE A 298      79.907  24.172  23.463  1.00  0.00
ATOM   4526  HD2 ILE A 298      80.572  25.819  23.772  1.00  0.00
ATOM   4527  HD3 ILE A 298      81.685  24.421  23.564  1.00  0.00
ATOM   4528  C   ILE A 298      80.264  28.054  21.625  1.00  0.00
ATOM   4529  O   ILE A 298      80.945  28.288  22.623  1.00  0.00
ATOM   4530  N   ALA A 299      80.500  28.636  20.447  1.00  0.00
ATOM   4531  HN  ALA A 299      79.906  28.465  19.664  1.00  0.00
ATOM   4532  CA  ALA A 299      81.694  29.413  20.180  1.00  0.00
ATOM   4533  HA  ALA A 299      82.382  29.355  21.014  1.00  0.00
ATOM   4534  CB  ALA A 299      82.403  28.891  18.914  1.00  0.00
ATOM   4535  HB1 ALA A 299      81.739  28.968  18.027  1.00  0.00
ATOM   4536  HB2 ALA A 299      82.674  27.822  19.052  1.00  0.00
ATOM   4537  HB3 ALA A 299      83.338  29.458  18.715  1.00  0.00
ATOM   4538  C   ALA A 299      81.345  30.863  19.963  1.00  0.00
ATOM   4539  O   ALA A 299      82.198  31.667  19.589  1.00  0.00
ATOM   4540  N   LEU A 300      80.086  31.221  20.211  1.00  0.00
ATOM   4541  HN  LEU A 300      79.428  30.541  20.525  1.00  0.00
ATOM   4542  CA  LEU A 300      79.563  32.564  20.096  1.00  0.00
ATOM   4543  HA  LEU A 300      79.775  32.869  19.081  1.00  0.00
ATOM   4544  CB  LEU A 300      78.019  32.521  20.228  1.00  0.00
ATOM   4545  HB1 LEU A 300      77.753  32.036  21.191  1.00  0.00
ATOM   4546  HB2 LEU A 300      77.654  31.864  19.409  1.00  0.00
ATOM   4547  CG  LEU A 300      77.240  33.857  20.131  1.00  0.00
ATOM   4548  HG  LEU A 300      77.574  34.519  20.962  1.00  0.00
ATOM   4549  CD1 LEU A 300      77.483  34.595  18.800  1.00  0.00
ATOM   4550 HD11 LEU A 300      77.156  33.964  17.947  1.00  0.00
ATOM   4551 HD12 LEU A 300      78.557  34.837  18.667  1.00  0.00
ATOM   4552 HD13 LEU A 300      76.907  35.544  18.779  1.00  0.00
ATOM   4553  CD2 LEU A 300      75.732  33.605  20.326  1.00  0.00
ATOM   4554 HD21 LEU A 300      75.551  33.057  21.275  1.00  0.00
ATOM   4555 HD22 LEU A 300      75.331  32.995  19.489  1.00  0.00
ATOM   4556 HD23 LEU A 300      75.179  34.567  20.361  1.00  0.00
ATOM   4557  C   LEU A 300      80.180  33.638  20.991  1.00  0.00
ATOM   4558  O   LEU A 300      80.383  34.722  20.447  1.00  0.00
ATOM   4559  N   PRO A 301      80.501  33.484  22.295  1.00  0.00
ATOM   4560  CD  PRO A 301      80.263  32.268  23.083  1.00  0.00
ATOM   4561  HD1 PRO A 301      81.074  31.543  22.855  1.00  0.00
ATOM   4562  HD2 PRO A 301      79.276  31.817  22.855  1.00  0.00
ATOM   4563  CA  PRO A 301      80.936  34.576  23.166  1.00  0.00
ATOM   4564  HA  PRO A 301      80.068  35.209  23.295  1.00  0.00
ATOM   4565  CB  PRO A 301      81.317  33.889  24.482  1.00  0.00
ATOM   4566  HB1 PRO A 301      81.210  34.568  25.353  1.00  0.00
ATOM   4567  HB2 PRO A 301      82.359  33.500  24.439  1.00  0.00
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ATOM   4568  CG  PRO A 301      80.352  32.704  24.547  1.00  0.00
ATOM   4569  HG1 PRO A 301      80.712  31.894  25.212  1.00  0.00
ATOM   4570  HG2 PRO A 301      79.355  33.054  24.894  1.00  0.00
ATOM   4571  C   PRO A 301      82.047  35.473  22.667  1.00  0.00
ATOM   4572  O   PRO A 301      83.065  34.966  22.197  1.00  0.00
ATOM   4573  N   GLY A 302      81.860  36.791  22.789  1.00  0.00
ATOM   4574  HN  GLY A 302      81.003  37.144  23.166  1.00  0.00
ATOM   4575  CA  GLY A 302      82.855  37.797  22.487  1.00  0.00
ATOM   4576  HA1 GLY A 302      82.317  38.694  22.216  1.00  0.00
ATOM   4577  HA2 GLY A 302      83.515  37.439  21.708  1.00  0.00
ATOM   4578  C   GLY A 302      83.665  38.079  23.722  1.00  0.00
ATOM   4579  O   GLY A 302      83.814  37.229  24.600  1.00  0.00
ATOM   4580  N   LEU A 303      84.208  39.295  23.818  1.00  0.00
ATOM   4581  HN  LEU A 303      84.095  39.967  23.091  1.00  0.00
ATOM   4582  CA  LEU A 303      84.919  39.764  24.989  1.00  0.00
ATOM   4583  HA  LEU A 303      85.612  38.989  25.287  1.00  0.00
ATOM   4584  CB  LEU A 303      85.710  41.056  24.652  1.00  0.00
ATOM   4585  HB1 LEU A 303      84.997  41.824  24.278  1.00  0.00
ATOM   4586  HB2 LEU A 303      86.413  40.824  23.822  1.00  0.00
ATOM   4587  CG  LEU A 303      86.526  41.676  25.816  1.00  0.00
ATOM   4588  HG  LEU A 303      85.817  41.915  26.637  1.00  0.00
ATOM   4589  CD1 LEU A 303      87.582  40.709  26.386  1.00  0.00
ATOM   4590 HD11 LEU A 303      88.307  40.423  25.596  1.00  0.00
ATOM   4591 HD12 LEU A 303      87.105  39.788  26.780  1.00  0.00
ATOM   4592 HD13 LEU A 303      88.138  41.194  27.216  1.00  0.00
ATOM   4593  CD2 LEU A 303      87.175  43.008  25.392  1.00  0.00
ATOM   4594 HD21 LEU A 303      86.401  43.719  25.032  1.00  0.00
ATOM   4595 HD22 LEU A 303      87.907  42.838  24.575  1.00  0.00
ATOM   4596 HD23 LEU A 303      87.706  43.471  26.251  1.00  0.00
ATOM   4597  C   LEU A 303      83.948  40.017  26.123  1.00  0.00
ATOM   4598  O   LEU A 303      82.952  40.719  25.954  1.00  0.00
ATOM   4599  N   ALA A 304      84.226  39.435  27.292  1.00  0.00
ATOM   4600  HN  ALA A 304      85.046  38.883  27.413  1.00  0.00
ATOM   4601  CA  ALA A 304      83.307  39.429  28.409  1.00  0.00
ATOM   4602  HA  ALA A 304      82.298  39.585  28.052  1.00  0.00
ATOM   4603  CB  ALA A 304      83.359  38.075  29.145  1.00  0.00
ATOM   4604  HB1 ALA A 304      84.373  37.884  29.556  1.00  0.00
ATOM   4605  HB2 ALA A 304      83.112  37.255  28.436  1.00  0.00
ATOM   4606  HB3 ALA A 304      82.623  38.041  29.976  1.00  0.00
ATOM   4607  C   ALA A 304      83.629  40.513  29.409  1.00  0.00
ATOM   4608  O   ALA A 304      82.911  40.687  30.393  1.00  0.00
ATOM   4609  N   LEU A 305      84.690  41.281  29.156  1.00  0.00
ATOM   4610  HN  LEU A 305      85.250  41.119  28.348  1.00  0.00
ATOM   4611  CA  LEU A 305      85.107  42.367  30.012  1.00  0.00
ATOM   4612  HA  LEU A 305      84.703  42.240  31.007  1.00  0.00
ATOM   4613  CB  LEU A 305      86.654  42.438  30.077  1.00  0.00
ATOM   4614  HB1 LEU A 305      86.946  43.287  30.731  1.00  0.00
ATOM   4615  HB2 LEU A 305      87.073  42.626  29.063  1.00  0.00
ATOM   4616  CG  LEU A 305      87.339  41.164  30.631  1.00  0.00
ATOM   4617  HG  LEU A 305      87.086  40.311  29.958  1.00  0.00
ATOM   4618  CD1 LEU A 305      88.871  41.318  30.605  1.00  0.00
ATOM   4619 HD11 LEU A 305      89.185  42.159  31.259  1.00  0.00
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ATOM   4620 HD12 LEU A 305      89.222  41.523  29.571  1.00  0.00
ATOM   4621 HD13 LEU A 305      89.360  40.388  30.965  1.00  0.00
ATOM   4622  CD2 LEU A 305      86.848  40.800  32.046  1.00  0.00
ATOM   4623 HD21 LEU A 305      85.760  40.581  32.043  1.00  0.00
ATOM   4624 HD22 LEU A 305      87.041  41.638  32.748  1.00  0.00
ATOM   4625 HD23 LEU A 305      87.381  39.899  32.416  1.00  0.00
ATOM   4626  C   LEU A 305      84.565  43.651  29.445  1.00  0.00
ATOM   4627  O   LEU A 305      83.833  44.357  30.134  1.00  0.00
ATOM   4628  N   ALA A 306      84.886  43.926  28.176  1.00  0.00
ATOM   4629  HN  ALA A 306      85.476  43.284  27.694  1.00  0.00
ATOM   4630  CA  ALA A 306      84.494  45.051  27.344  1.00  0.00
ATOM   4631  HA  ALA A 306      85.360  45.241  26.728  1.00  0.00
ATOM   4632  CB  ALA A 306      83.357  44.665  26.375  1.00  0.00
ATOM   4633  HB1 ALA A 306      82.433  44.410  26.932  1.00  0.00
ATOM   4634  HB2 ALA A 306      83.656  43.767  25.792  1.00  0.00
ATOM   4635  HB3 ALA A 306      83.140  45.482  25.655  1.00  0.00
ATOM   4636  C   ALA A 306      84.222  46.362  28.062  1.00  0.00
ATOM   4637  O   ALA A 306      85.122  46.960  28.647  1.00  0.00
ATOM   4638  N   VAL A 307      82.980  46.845  27.999  1.00  0.00
ATOM   4639  HN  VAL A 307      82.262  46.345  27.521  1.00  0.00
ATOM   4640  CA  VAL A 307      82.576  48.113  28.571  1.00  0.00
ATOM   4641  HA  VAL A 307      83.424  48.784  28.607  1.00  0.00
ATOM   4642  CB  VAL A 307      81.485  48.743  27.700  1.00  0.00
ATOM   4643  HB  VAL A 307      80.652  48.013  27.572  1.00  0.00
ATOM   4644  CG1 VAL A 307      82.089  49.034  26.307  1.00  0.00
ATOM   4645 HG11 VAL A 307      82.406  48.102  25.796  1.00  0.00
ATOM   4646 HG12 VAL A 307      82.970  49.705  26.402  1.00  0.00
ATOM   4647 HG13 VAL A 307      81.336  49.537  25.664  1.00  0.00
ATOM   4648  CG2 VAL A 307      80.897  50.036  28.306  1.00  0.00
ATOM   4649 HG21 VAL A 307      81.705  50.761  28.537  1.00  0.00
ATOM   4650 HG22 VAL A 307      80.321  49.827  29.231  1.00  0.00
ATOM   4651 HG23 VAL A 307      80.198  50.504  27.580  1.00  0.00
ATOM   4652  C   VAL A 307      82.095  47.888  29.993  1.00  0.00
ATOM   4653  O   VAL A 307      81.983  48.821  30.786  1.00  0.00
ATOM   4654  N   GLY A 308      81.873  46.625  30.369  1.00  0.00
ATOM   4655  HN  GLY A 308      82.004  45.876  29.723  1.00  0.00
ATOM   4656  CA  GLY A 308      81.443  46.229  31.694  1.00  0.00
ATOM   4657  HA1 GLY A 308      81.339  45.154  31.679  1.00  0.00
ATOM   4658  HA2 GLY A 308      80.514  46.738  31.910  1.00  0.00
ATOM   4659  C   GLY A 308      82.437  46.581  32.768  1.00  0.00
ATOM   4660  O   GLY A 308      82.046  47.067  33.823  1.00  0.00
ATOM   4661  N   MET A 309      83.734  46.373  32.519  1.00  0.00
ATOM   4662  HN  MET A 309      84.025  45.958  31.659  1.00  0.00
ATOM   4663  CA  MET A 309      84.800  46.725  33.441  1.00  0.00
ATOM   4664  HA  MET A 309      84.551  46.272  34.390  1.00  0.00
ATOM   4665  CB  MET A 309      86.155  46.114  32.993  1.00  0.00
ATOM   4666  HB1 MET A 309      86.065  45.007  33.084  1.00  0.00
ATOM   4667  HB2 MET A 309      86.952  46.435  33.701  1.00  0.00
ATOM   4668  CG  MET A 309      86.595  46.422  31.549  1.00  0.00
ATOM   4669  HG1 MET A 309      86.553  47.518  31.379  1.00  0.00
ATOM   4670  HG2 MET A 309      85.872  45.948  30.853  1.00  0.00
ATOM   4671  SD  MET A 309      88.277  45.836  31.170  1.00  0.00
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ATOM   4672  CE  MET A 309      88.258  46.304  29.416  1.00  0.00
ATOM   4673  HE1 MET A 309      88.031  47.385  29.294  1.00  0.00
ATOM   4674  HE2 MET A 309      87.489  45.727  28.860  1.00  0.00
ATOM   4675  HE3 MET A 309      89.243  46.106  28.941  1.00  0.00
ATOM   4676  C   MET A 309      84.941  48.209  33.691  1.00  0.00
ATOM   4677  O   MET A 309      85.270  48.630  34.799  1.00  0.00
ATOM   4678  N   ILE A 310      84.684  49.024  32.664  1.00  0.00
ATOM   4679  HN  ILE A 310      84.427  48.645  31.779  1.00  0.00
ATOM   4680  CA  ILE A 310      84.685  50.474  32.725  1.00  0.00
ATOM   4681  HA  ILE A 310      85.644  50.772  33.127  1.00  0.00
ATOM   4682  CB  ILE A 310      84.549  51.097  31.331  1.00  0.00
ATOM   4683  HB  ILE A 310      83.600  50.755  30.861  1.00  0.00
ATOM   4684  CG2 ILE A 310      84.482  52.635  31.442  1.00  0.00
ATOM   4685 HG21 ILE A 310      85.376  53.024  31.970  1.00  0.00
ATOM   4686 HG22 ILE A 310      83.573  52.952  31.993  1.00  0.00
ATOM   4687 HG23 ILE A 310      84.431  53.108  30.440  1.00  0.00
ATOM   4688  CG1 ILE A 310      85.717  50.621  30.421  1.00  0.00
ATOM   4689 HG11 ILE A 310      85.680  49.514  30.322  1.00  0.00
ATOM   4690 HG12 ILE A 310      86.679  50.885  30.913  1.00  0.00
ATOM   4691  CD1 ILE A 310      85.710  51.211  29.005  1.00  0.00
ATOM   4692  HD1 ILE A 310      85.869  52.309  29.026  1.00  0.00
ATOM   4693  HD2 ILE A 310      84.744  50.998  28.499  1.00  0.00
ATOM   4694  HD3 ILE A 310      86.530  50.763  28.404  1.00  0.00
ATOM   4695  C   ILE A 310      83.621  50.973  33.689  1.00  0.00
ATOM   4696  O   ILE A 310      83.868  51.869  34.496  1.00  0.00
ATOM   4697  N   LEU A 311      82.436  50.361  33.646  1.00  0.00
ATOM   4698  HN  LEU A 311      82.265  49.627  32.992  1.00  0.00
ATOM   4699  CA  LEU A 311      81.312  50.710  34.490  1.00  0.00
ATOM   4700  HA  LEU A 311      81.297  51.782  34.625  1.00  0.00
ATOM   4701  CB  LEU A 311      79.991  50.252  33.818  1.00  0.00
ATOM   4702  HB1 LEU A 311      79.130  50.475  34.487  1.00  0.00
ATOM   4703  HB2 LEU A 311      80.031  49.150  33.667  1.00  0.00
ATOM   4704  CG  LEU A 311      79.697  50.911  32.446  1.00  0.00
ATOM   4705  HG  LEU A 311      80.561  50.718  31.770  1.00  0.00
ATOM   4706  CD1 LEU A 311      78.463  50.268  31.784  1.00  0.00
ATOM   4707 HD11 LEU A 311      77.560  50.433  32.408  1.00  0.00
ATOM   4708 HD12 LEU A 311      78.617  49.174  31.663  1.00  0.00
ATOM   4709 HD13 LEU A 311      78.288  50.712  30.781  1.00  0.00
ATOM   4710  CD2 LEU A 311      79.531  52.440  32.543  1.00  0.00
ATOM   4711 HD21 LEU A 311      80.460  52.916  32.920  1.00  0.00
ATOM   4712 HD22 LEU A 311      78.694  52.696  33.226  1.00  0.00
ATOM   4713 HD23 LEU A 311      79.307  52.861  31.540  1.00  0.00
ATOM   4714  C   LEU A 311      81.400  50.072  35.865  1.00  0.00
ATOM   4715  O   LEU A 311      80.715  50.496  36.794  1.00  0.00
ATOM   4716  N   PHE A 312      82.263  49.063  36.022  1.00  0.00
ATOM   4717  HN  PHE A 312      82.802  48.738  35.247  1.00  0.00
ATOM   4718  CA  PHE A 312      82.468  48.334  37.261  1.00  0.00
ATOM   4719  HA  PHE A 312      81.503  48.181  37.726  1.00  0.00
ATOM   4720  CB  PHE A 312      83.120  46.952  36.946  1.00  0.00
ATOM   4721  HB1 PHE A 312      84.106  47.099  36.460  1.00  0.00
ATOM   4722  HB2 PHE A 312      82.472  46.391  36.243  1.00  0.00
ATOM   4723  CG  PHE A 312      83.302  46.092  38.176  1.00  0.00
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ATOM   4724  CD1 PHE A 312      84.589  45.771  38.646  1.00  0.00
ATOM   4725  HD1 PHE A 312      85.459  46.154  38.132  1.00  0.00
ATOM   4726  CE1 PHE A 312      84.754  44.966  39.779  1.00  0.00
ATOM   4727  HE1 PHE A 312      85.746  44.730  40.134  1.00  0.00
ATOM   4728  CZ  PHE A 312      83.632  44.466  40.451  1.00  0.00
ATOM   4729  HZ  PHE A 312      83.758  43.843  41.325  1.00  0.00
ATOM   4730  CD2 PHE A 312      82.184  45.580  38.856  1.00  0.00
ATOM   4731  HD2 PHE A 312      81.191  45.814  38.502  1.00  0.00
ATOM   4732  CE2 PHE A 312      82.346  44.772  39.989  1.00  0.00
ATOM   4733  HE2 PHE A 312      81.480  44.386  40.507  1.00  0.00
ATOM   4734  C   PHE A 312      83.338  49.129  38.215  1.00  0.00
ATOM   4735  O   PHE A 312      83.337  48.892  39.422  1.00  0.00
ATOM   4736  N   ALA A 313      84.066  50.115  37.688  1.00  0.00
ATOM   4737  HN  ALA A 313      84.027  50.317  36.712  1.00  0.00
ATOM   4738  CA  ALA A 313      85.030  50.877  38.444  1.00  0.00
ATOM   4739  HA  ALA A 313      85.478  50.243  39.197  1.00  0.00
ATOM   4740  CB  ALA A 313      86.136  51.414  37.514  1.00  0.00
ATOM   4741  HB1 ALA A 313      85.709  52.084  36.737  1.00  0.00
ATOM   4742  HB2 ALA A 313      86.637  50.566  36.999  1.00  0.00
ATOM   4743  HB3 ALA A 313      86.905  51.974  38.088  1.00  0.00
ATOM   4744  C   ALA A 313      84.384  52.058  39.128  1.00  0.00
ATOM   4745  O   ALA A 313      85.023  52.738  39.925  1.00  0.00
ATOM   4746  N   ARG A 314      83.103  52.303  38.847  1.00  0.00
ATOM   4747  HN  ARG A 314      82.602  51.703  38.227  1.00  0.00
ATOM   4748  CA  ARG A 314      82.367  53.454  39.322  1.00  0.00
ATOM   4749  HA  ARG A 314      82.903  54.317  38.951  1.00  0.00
ATOM   4750  CB  ARG A 314      80.974  53.492  38.633  1.00  0.00
ATOM   4751  HB1 ARG A 314      80.586  52.450  38.579  1.00  0.00
ATOM   4752  HB2 ARG A 314      81.116  53.844  37.588  1.00  0.00
ATOM   4753  CG  ARG A 314      79.887  54.340  39.318  1.00  0.00
ATOM   4754  HG1 ARG A 314      80.288  55.357  39.518  1.00  0.00
ATOM   4755  HG2 ARG A 314      79.638  53.868  40.295  1.00  0.00
ATOM   4756  CD  ARG A 314      78.605  54.449  38.477  1.00  0.00
ATOM   4757  HD1 ARG A 314      78.343  53.454  38.056  1.00  0.00
ATOM   4758  HD2 ARG A 314      78.723  55.172  37.642  1.00  0.00
ATOM   4759  NE  ARG A 314      77.466  54.860  39.358  1.00  0.00
ATOM   4760  HE  ARG A 314      76.836  54.143  39.658  1.00  0.00
ATOM   4761  CZ  ARG A 314      77.360  56.074  39.945  1.00  0.00
ATOM   4762  NH1 ARG A 314      78.153  57.109  39.612  1.00  0.00
ATOM   4763 HH11 ARG A 314      78.850  56.991  38.907  1.00  0.00
ATOM   4764 HH12 ARG A 314      78.043  57.985  40.079  1.00  0.00
ATOM   4765  NH2 ARG A 314      76.435  56.245  40.910  1.00  0.00
ATOM   4766 HH21 ARG A 314      75.853  55.484  41.193  1.00  0.00
ATOM   4767 HH22 ARG A 314      76.345  57.131  41.375  1.00  0.00
ATOM   4768  C   ARG A 314      82.263  53.668  40.826  1.00  0.00
ATOM   4769  O   ARG A 314      82.562  54.790  41.236  1.00  0.00
ATOM   4770  N   PRO A 315      81.910  52.725  41.720  1.00  0.00
ATOM   4771  CD  PRO A 315      81.238  51.463  41.395  1.00  0.00
ATOM   4772  HD1 PRO A 315      81.834  50.862  40.677  1.00  0.00
ATOM   4773  HD2 PRO A 315      80.237  51.689  40.968  1.00  0.00
ATOM   4774  CA  PRO A 315      81.883  53.002  43.149  1.00  0.00
ATOM   4775  HA  PRO A 315      81.421  53.965  43.325  1.00  0.00
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ATOM   4776  CB  PRO A 315      81.063  51.858  43.771  1.00  0.00
ATOM   4777  HB1 PRO A 315      80.015  52.202  43.903  1.00  0.00
ATOM   4778  HB2 PRO A 315      81.439  51.521  44.759  1.00  0.00
ATOM   4779  CG  PRO A 315      81.090  50.728  42.731  1.00  0.00
ATOM   4780  HG1 PRO A 315      81.984  50.091  42.903  1.00  0.00
ATOM   4781  HG2 PRO A 315      80.179  50.098  42.771  1.00  0.00
ATOM   4782  C   PRO A 315      83.281  53.043  43.702  1.00  0.00
ATOM   4783  O   PRO A 315      83.565  53.911  44.523  1.00  0.00
ATOM   4784  N   ILE A 316      84.128  52.098  43.289  1.00  0.00
ATOM   4785  HN  ILE A 316      83.836  51.449  42.591  1.00  0.00
ATOM   4786  CA  ILE A 316      85.447  51.844  43.827  1.00  0.00
ATOM   4787  HA  ILE A 316      85.329  51.688  44.889  1.00  0.00
ATOM   4788  CB  ILE A 316      86.065  50.584  43.215  1.00  0.00
ATOM   4789  HB  ILE A 316      86.277  50.765  42.134  1.00  0.00
ATOM   4790  CG2 ILE A 316      87.408  50.256  43.909  1.00  0.00
ATOM   4791 HG21 ILE A 316      87.267  50.161  45.006  1.00  0.00
ATOM   4792 HG22 ILE A 316      88.165  51.044  43.716  1.00  0.00
ATOM   4793 HG23 ILE A 316      87.811  49.297  43.521  1.00  0.00
ATOM   4794  CG1 ILE A 316      85.089  49.374  43.269  1.00  0.00
ATOM   4795 HG11 ILE A 316      85.631  48.482  42.882  1.00  0.00
ATOM   4796 HG12 ILE A 316      84.240  49.553  42.574  1.00  0.00
ATOM   4797  CD1 ILE A 316      84.533  49.043  44.661  1.00  0.00
ATOM   4798  HD1 ILE A 316      83.925  49.883  45.058  1.00  0.00
ATOM   4799  HD2 ILE A 316      85.357  48.834  45.375  1.00  0.00
ATOM   4800  HD3 ILE A 316      83.883  48.144  44.607  1.00  0.00
ATOM   4801  C   ILE A 316      86.367  53.030  43.646  1.00  0.00
ATOM   4802  O   ILE A 316      87.097  53.405  44.563  1.00  0.00
ATOM   4803  N   ALA A 317      86.328  53.640  42.458  1.00  0.00
ATOM   4804  HN  ALA A 317      85.700  53.324  41.748  1.00  0.00
ATOM   4805  CA  ALA A 317      87.205  54.710  42.049  1.00  0.00
ATOM   4806  HA  ALA A 317      88.216  54.337  42.135  1.00  0.00
ATOM   4807  CB  ALA A 317      86.964  55.111  40.579  1.00  0.00
ATOM   4808  HB1 ALA A 317      85.921  55.463  40.429  1.00  0.00
ATOM   4809  HB2 ALA A 317      87.133  54.235  39.918  1.00  0.00
ATOM   4810  HB3 ALA A 317      87.663  55.915  40.262  1.00  0.00
ATOM   4811  C   ALA A 317      87.113  55.968  42.881  1.00  0.00
ATOM   4812  O   ALA A 317      88.142  56.563  43.195  1.00  0.00
ATOM   4813  N   VAL A 318      85.894  56.399  43.230  1.00  0.00
ATOM   4814  HN  VAL A 318      85.072  55.879  43.011  1.00  0.00
ATOM   4815  CA  VAL A 318      85.701  57.741  43.752  1.00  0.00
ATOM   4816  HA  VAL A 318      86.659  58.179  43.996  1.00  0.00
ATOM   4817  CB  VAL A 318      85.036  58.678  42.730  1.00  0.00
ATOM   4818  HB  VAL A 318      84.841  59.672  43.199  1.00  0.00
ATOM   4819  CG1 VAL A 318      83.688  58.115  42.225  1.00  0.00
ATOM   4820 HG11 VAL A 318      82.972  57.972  43.060  1.00  0.00
ATOM   4821 HG12 VAL A 318      83.832  57.145  41.706  1.00  0.00
ATOM   4822 HG13 VAL A 318      83.233  58.825  41.501  1.00  0.00
ATOM   4823  CG2 VAL A 318      86.016  58.942  41.566  1.00  0.00
ATOM   4824 HG21 VAL A 318      86.193  58.016  40.981  1.00  0.00
ATOM   4825 HG22 VAL A 318      86.988  59.312  41.954  1.00  0.00
ATOM   4826 HG23 VAL A 318      85.596  59.711  40.883  1.00  0.00
ATOM   4827  C   VAL A 318      84.903  57.820  45.035  1.00  0.00
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ATOM   4828  O   VAL A 318      84.972  58.834  45.729  1.00  0.00
ATOM   4829  N   TRP A 319      84.142  56.779  45.385  1.00  0.00
ATOM   4830  HN  TRP A 319      84.132  55.918  44.879  1.00  0.00
ATOM   4831  CA  TRP A 319      83.121  56.939  46.408  1.00  0.00
ATOM   4832  HA  TRP A 319      82.927  57.991  46.574  1.00  0.00
ATOM   4833  CB  TRP A 319      81.793  56.281  45.920  1.00  0.00
ATOM   4834  HB1 TRP A 319      81.832  55.178  46.056  1.00  0.00
ATOM   4835  HB2 TRP A 319      81.712  56.461  44.826  1.00  0.00
ATOM   4836  CG  TRP A 319      80.548  56.825  46.557  1.00  0.00
ATOM   4837  CD1 TRP A 319      79.809  56.290  47.580  1.00  0.00
ATOM   4838  HD1 TRP A 319      80.035  55.363  48.084  1.00  0.00
ATOM   4839  NE1 TRP A 319      78.779  57.136  47.901  1.00  0.00
ATOM   4840  HE1 TRP A 319      78.174  57.033  48.666  1.00  0.00
ATOM   4841  CE2 TRP A 319      78.819  58.234  47.089  1.00  0.00
ATOM   4842  CD2 TRP A 319      79.927  58.078  46.225  1.00  0.00
ATOM   4843  CE3 TRP A 319      80.213  59.072  45.291  1.00  0.00
ATOM   4844  HE3 TRP A 319      81.058  58.991  44.623  1.00  0.00
ATOM   4845  CZ3 TRP A 319      79.390  60.199  45.234  1.00  0.00
ATOM   4846  HZ3 TRP A 319      79.621  60.989  44.536  1.00  0.00
ATOM   4847  CZ2 TRP A 319      78.001  59.356  47.032  1.00  0.00
ATOM   4848  HZ2 TRP A 319      77.161  59.484  47.695  1.00  0.00
ATOM   4849  CH2 TRP A 319      78.303  60.340  46.091  1.00  0.00
ATOM   4850  HH2 TRP A 319      77.692  61.230  46.034  1.00  0.00
ATOM   4851  C   TRP A 319      83.518  56.322  47.735  1.00  0.00
ATOM   4852  O   TRP A 319      82.792  56.451  48.720  1.00  0.00
ATOM   4853  N   ILE A 320      84.679  55.662  47.801  1.00  0.00
ATOM   4854  HN  ILE A 320      85.290  55.605  47.016  1.00  0.00
ATOM   4855  CA  ILE A 320      85.041  54.861  48.961  1.00  0.00
ATOM   4856  HA  ILE A 320      84.154  54.673  49.551  1.00  0.00
ATOM   4857  CB  ILE A 320      85.622  53.488  48.602  1.00  0.00
ATOM   4858  HB  ILE A 320      86.670  53.602  48.238  1.00  0.00
ATOM   4859  CG2 ILE A 320      85.635  52.589  49.862  1.00  0.00
ATOM   4860 HG21 ILE A 320      84.610  52.463  50.268  1.00  0.00
ATOM   4861 HG22 ILE A 320      86.274  53.015  50.660  1.00  0.00
ATOM   4862 HG23 ILE A 320      86.036  51.589  49.601  1.00  0.00
ATOM   4863  CG1 ILE A 320      84.851  52.797  47.445  1.00  0.00
ATOM   4864 HG11 ILE A 320      85.319  51.802  47.273  1.00  0.00
ATOM   4865 HG12 ILE A 320      85.000  53.385  46.516  1.00  0.00
ATOM   4866  CD1 ILE A 320      83.349  52.591  47.677  1.00  0.00
ATOM   4867  HD1 ILE A 320      82.825  53.560  47.802  1.00  0.00
ATOM   4868  HD2 ILE A 320      83.168  51.973  48.582  1.00  0.00
ATOM   4869  HD3 ILE A 320      82.899  52.069  46.806  1.00  0.00
ATOM   4870  C   ILE A 320      86.000  55.662  49.826  1.00  0.00
ATOM   4871  O   ILE A 320      87.136  55.263  50.083  1.00  0.00
ATOM   4872  N   GLY A 321      85.542  56.821  50.306  1.00  0.00
ATOM   4873  HN  GLY A 321      84.629  57.134  50.054  1.00  0.00
ATOM   4874  CA  GLY A 321      86.241  57.656  51.266  1.00  0.00
ATOM   4875  HA1 GLY A 321      86.476  57.048  52.128  1.00  0.00
ATOM   4876  HA2 GLY A 321      85.574  58.470  51.506  1.00  0.00
ATOM   4877  C   GLY A 321      87.520  58.257  50.751  1.00  0.00
ATOM   4878  O   GLY A 321      88.452  58.481  51.522  1.00  0.00
ATOM   4879  N   LEU A 322      87.592  58.524  49.445  1.00  0.00
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ATOM   4880  HN  LEU A 322      86.832  58.303  48.839  1.00  0.00
ATOM   4881  CA  LEU A 322      88.743  59.128  48.807  1.00  0.00
ATOM   4882  HA  LEU A 322      89.641  58.712  49.241  1.00  0.00
ATOM   4883  CB  LEU A 322      88.697  58.821  47.285  1.00  0.00
ATOM   4884  HB1 LEU A 322      87.726  59.179  46.875  1.00  0.00
ATOM   4885  HB2 LEU A 322      88.716  57.715  47.162  1.00  0.00
ATOM   4886  CG  LEU A 322      89.835  59.418  46.420  1.00  0.00
ATOM   4887  HG  LEU A 322      89.795  60.528  46.500  1.00  0.00
ATOM   4888  CD1 LEU A 322      91.231  58.965  46.889  1.00  0.00
ATOM   4889 HD11 LEU A 322      91.315  57.859  46.839  1.00  0.00
ATOM   4890 HD12 LEU A 322      91.420  59.289  47.934  1.00  0.00
ATOM   4891 HD13 LEU A 322      92.017  59.409  46.241  1.00  0.00
ATOM   4892  CD2 LEU A 322      89.624  59.078  44.932  1.00  0.00
ATOM   4893 HD21 LEU A 322      88.631  59.437  44.589  1.00  0.00
ATOM   4894 HD22 LEU A 322      89.677  57.980  44.779  1.00  0.00
ATOM   4895 HD23 LEU A 322      90.408  59.560  44.310  1.00  0.00
ATOM   4896  C   LEU A 322      88.744  60.626  49.022  1.00  0.00
ATOM   4897  O   LEU A 322      89.798  61.258  49.089  1.00  0.00
ATOM   4898  N   ALA A 323      87.553  61.209  49.168  1.00  0.00
ATOM   4899  HN  ALA A 323      86.722  60.662  49.124  1.00  0.00
ATOM   4900  CA  ALA A 323      87.338  62.614  49.423  1.00  0.00
ATOM   4901  HA  ALA A 323      88.011  63.170  48.785  1.00  0.00
ATOM   4902  CB  ALA A 323      85.877  62.995  49.108  1.00  0.00
ATOM   4903  HB1 ALA A 323      85.176  62.407  49.739  1.00  0.00
ATOM   4904  HB2 ALA A 323      85.655  62.770  48.043  1.00  0.00
ATOM   4905  HB3 ALA A 323      85.683  64.073  49.277  1.00  0.00
ATOM   4906  C   ALA A 323      87.622  62.921  50.882  1.00  0.00
ATOM   4907  O   ALA A 323      87.543  62.007  51.703  1.00  0.00
ATOM   4908  N   PRO A 324      87.964  64.162  51.275  1.00  0.00
ATOM   4909  CD  PRO A 324      88.184  65.289  50.365  1.00  0.00
ATOM   4910  HD1 PRO A 324      87.324  65.438  49.678  1.00  0.00
ATOM   4911  HD2 PRO A 324      89.113  65.099  49.783  1.00  0.00
ATOM   4912  CA  PRO A 324      88.314  64.497  52.653  1.00  0.00
ATOM   4913  HA  PRO A 324      88.972  63.736  53.046  1.00  0.00
ATOM   4914  CB  PRO A 324      88.999  65.870  52.526  1.00  0.00
ATOM   4915  HB1 PRO A 324      90.082  65.707  52.327  1.00  0.00
ATOM   4916  HB2 PRO A 324      88.900  66.512  53.424  1.00  0.00
ATOM   4917  CG  PRO A 324      88.365  66.498  51.282  1.00  0.00
ATOM   4918  HG1 PRO A 324      87.370  66.921  51.543  1.00  0.00
ATOM   4919  HG2 PRO A 324      88.999  67.287  50.831  1.00  0.00
ATOM   4920  C   PRO A 324      87.099  64.582  53.561  1.00  0.00
ATOM   4921  O   PRO A 324      87.270  64.914  54.734  1.00  0.00
ATOM   4922  N   PHE A 325      85.897  64.271  53.069  1.00  0.00
ATOM   4923  HN  PHE A 325      85.795  64.047  52.104  1.00  0.00
ATOM   4924  CA  PHE A 325      84.703  64.089  53.867  1.00  0.00
ATOM   4925  HA  PHE A 325      84.613  64.950  54.515  1.00  0.00
ATOM   4926  CB  PHE A 325      83.447  63.978  52.962  1.00  0.00
ATOM   4927  HB1 PHE A 325      82.537  63.783  53.570  1.00  0.00
ATOM   4928  HB2 PHE A 325      83.573  63.142  52.240  1.00  0.00
ATOM   4929  CG  PHE A 325      83.202  65.258  52.204  1.00  0.00
ATOM   4930  CD1 PHE A 325      83.147  65.280  50.798  1.00  0.00
ATOM   4931  HD1 PHE A 325      83.285  64.365  50.241  1.00  0.00
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ATOM   4932  CE1 PHE A 325      82.918  66.479  50.111  1.00  0.00
ATOM   4933  HE1 PHE A 325      82.882  66.487  49.032  1.00  0.00
ATOM   4934  CZ  PHE A 325      82.738  67.669  50.827  1.00  0.00
ATOM   4935  HZ  PHE A 325      82.571  68.599  50.304  1.00  0.00
ATOM   4936  CD2 PHE A 325      82.998  66.459  52.908  1.00  0.00
ATOM   4937  HD2 PHE A 325      83.017  66.461  53.988  1.00  0.00
ATOM   4938  CE2 PHE A 325      82.772  67.659  52.225  1.00  0.00
ATOM   4939  HE2 PHE A 325      82.625  68.575  52.777  1.00  0.00
ATOM   4940  C   PHE A 325      84.801  62.870  54.753  1.00  0.00
ATOM   4941  O   PHE A 325      85.495  61.907  54.429  1.00  0.00
ATOM   4942  N   LYS A 326      84.118  62.909  55.902  1.00  0.00
ATOM   4943  HN  LYS A 326      83.565  63.704  56.136  1.00  0.00
ATOM   4944  CA  LYS A 326      84.089  61.840  56.881  1.00  0.00
ATOM   4945  HA  LYS A 326      85.110  61.648  57.177  1.00  0.00
ATOM   4946  CB  LYS A 326      83.264  62.265  58.122  1.00  0.00
ATOM   4947  HB1 LYS A 326      83.228  61.425  58.851  1.00  0.00
ATOM   4948  HB2 LYS A 326      82.219  62.486  57.806  1.00  0.00
ATOM   4949  CG  LYS A 326      83.821  63.501  58.856  1.00  0.00
ATOM   4950  HG1 LYS A 326      83.132  63.744  59.697  1.00  0.00
ATOM   4951  HG2 LYS A 326      83.817  64.369  58.163  1.00  0.00
ATOM   4952  CD  LYS A 326      85.235  63.300  59.431  1.00  0.00
ATOM   4953  HD1 LYS A 326      85.945  63.052  58.613  1.00  0.00
ATOM   4954  HD2 LYS A 326      85.205  62.427  60.123  1.00  0.00
ATOM   4955  CE  LYS A 326      85.775  64.509  60.212  1.00  0.00
ATOM   4956  HE1 LYS A 326      86.754  64.261  60.674  1.00  0.00
ATOM   4957  HE2 LYS A 326      85.062  64.810  61.008  1.00  0.00
ATOM   4958  NZ  LYS A 326      85.985  65.677  59.323  1.00  0.00
ATOM   4959  HZ1 LYS A 326      85.080  65.952  58.892  1.00  0.00
ATOM   4960  HZ2 LYS A 326      86.661  65.423  58.573  1.00  0.00
ATOM   4961  HZ3 LYS A 326      86.363  66.472  59.875  1.00  0.00
ATOM   4962  C   LYS A 326      83.533  60.554  56.308  1.00  0.00
ATOM   4963  O   LYS A 326      82.600  60.569  55.507  1.00  0.00
ATOM   4964  N   SER A 327      84.129  59.425  56.693  1.00  0.00
ATOM   4965  HN  SER A 327      84.854  59.419  57.378  1.00  0.00
ATOM   4966  CA  SER A 327      83.830  58.146  56.100  1.00  0.00
ATOM   4967  HA  SER A 327      82.780  58.104  55.841  1.00  0.00
ATOM   4968  CB  SER A 327      84.736  57.910  54.855  1.00  0.00
ATOM   4969  HB1 SER A 327      85.804  57.856  55.160  1.00  0.00
ATOM   4970  HB2 SER A 327      84.631  58.779  54.171  1.00  0.00
ATOM   4971  OG  SER A 327      84.384  56.735  54.125  1.00  0.00
ATOM   4972  HG  SER A 327      83.546  56.925  53.694  1.00  0.00
ATOM   4973  C   SER A 327      84.112  57.106  57.150  1.00  0.00
ATOM   4974  O   SER A 327      84.869  57.348  58.089  1.00  0.00
ATOM   4975  N   PHE A 328      83.481  55.937  57.010  1.00  0.00
ATOM   4976  HN  PHE A 328      82.864  55.796  56.241  1.00  0.00
ATOM   4977  CA  PHE A 328      83.624  54.785  57.874  1.00  0.00
ATOM   4978  HA  PHE A 328      83.373  55.112  58.875  1.00  0.00
ATOM   4979  CB  PHE A 328      82.636  53.673  57.448  1.00  0.00
ATOM   4980  HB1 PHE A 328      82.813  52.748  58.033  1.00  0.00
ATOM   4981  HB2 PHE A 328      82.771  53.444  56.373  1.00  0.00
ATOM   4982  CG  PHE A 328      81.205  54.092  57.666  1.00  0.00
ATOM   4983  CD1 PHE A 328      80.640  54.038  58.953  1.00  0.00
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ATOM   4984  HD1 PHE A 328      81.236  53.694  59.785  1.00  0.00
ATOM   4985  CE1 PHE A 328      79.312  54.428  59.167  1.00  0.00
ATOM   4986  HE1 PHE A 328      78.889  54.385  60.160  1.00  0.00
ATOM   4987  CZ  PHE A 328      78.535  54.878  58.094  1.00  0.00
ATOM   4988  HZ  PHE A 328      77.514  55.188  58.260  1.00  0.00
ATOM   4989  CD2 PHE A 328      80.402  54.518  56.590  1.00  0.00
ATOM   4990  HD2 PHE A 328      80.813  54.548  55.592  1.00  0.00
ATOM   4991  CE2 PHE A 328      79.077  54.916  56.803  1.00  0.00
ATOM   4992  HE2 PHE A 328      78.472  55.251  55.973  1.00  0.00
ATOM   4993  C   PHE A 328      85.030  54.227  57.929  1.00  0.00
ATOM   4994  O   PHE A 328      85.775  54.297  56.952  1.00  0.00
ATOM   4995  N   THR A 329      85.408  53.701  59.099  1.00  0.00
ATOM   4996  HN  THR A 329      84.758  53.647  59.853  1.00  0.00
ATOM   4997  CA  THR A 329      86.762  53.326  59.466  1.00  0.00
ATOM   4998  HA  THR A 329      87.368  54.208  59.308  1.00  0.00
ATOM   4999  CB  THR A 329      86.870  52.958  60.947  1.00  0.00
ATOM   5000  HB  THR A 329      86.279  52.044  61.171  1.00  0.00
ATOM   5001  OG1 THR A 329      86.327  54.006  61.741  1.00  0.00
ATOM   5002  HG1 THR A 329      86.266  53.661  62.635  1.00  0.00
ATOM   5003  CG2 THR A 329      88.342  52.738  61.364  1.00  0.00
ATOM   5004 HG21 THR A 329      88.950  53.638  61.132  1.00  0.00
ATOM   5005 HG22 THR A 329      88.785  51.867  60.839  1.00  0.00
ATOM   5006 HG23 THR A 329      88.407  52.543  62.455  1.00  0.00
ATOM   5007  C   THR A 329      87.349  52.232  58.598  1.00  0.00
ATOM   5008  O   THR A 329      88.216  52.498  57.767  1.00  0.00
ATOM   5009  N   ALA A 330      86.900  50.990  58.792  1.00  0.00
ATOM   5010  HN  ALA A 330      86.176  50.796  59.447  1.00  0.00
ATOM   5011  CA  ALA A 330      87.492  49.848  58.136  1.00  0.00
ATOM   5012  HA  ALA A 330      88.003  50.161  57.235  1.00  0.00
ATOM   5013  CB  ALA A 330      88.488  49.107  59.053  1.00  0.00
ATOM   5014  HB1 ALA A 330      88.015  48.804  60.011  1.00  0.00
ATOM   5015  HB2 ALA A 330      89.339  49.780  59.294  1.00  0.00
ATOM   5016  HB3 ALA A 330      88.896  48.204  58.550  1.00  0.00
ATOM   5017  C   ALA A 330      86.400  48.911  57.714  1.00  0.00
ATOM   5018  O   ALA A 330      86.126  48.761  56.528  1.00  0.00
ATOM   5019  N   ARG A 331      85.759  48.250  58.681  1.00  0.00
ATOM   5020  HN  ARG A 331      85.989  48.404  59.638  1.00  0.00
ATOM   5021  CA  ARG A 331      84.777  47.211  58.447  1.00  0.00
ATOM   5022  HA  ARG A 331      85.264  46.456  57.846  1.00  0.00
ATOM   5023  CB  ARG A 331      84.346  46.581  59.796  1.00  0.00
ATOM   5024  HB1 ARG A 331      83.880  47.363  60.436  1.00  0.00
ATOM   5025  HB2 ARG A 331      85.268  46.241  60.319  1.00  0.00
ATOM   5026  CG  ARG A 331      83.372  45.387  59.689  1.00  0.00
ATOM   5027  HG1 ARG A 331      82.379  45.760  59.352  1.00  0.00
ATOM   5028  HG2 ARG A 331      83.230  44.959  60.707  1.00  0.00
ATOM   5029  CD  ARG A 331      83.811  44.266  58.728  1.00  0.00
ATOM   5030  HD1 ARG A 331      83.854  44.651  57.686  1.00  0.00
ATOM   5031  HD2 ARG A 331      83.100  43.414  58.776  1.00  0.00
ATOM   5032  NE  ARG A 331      85.167  43.774  59.136  1.00  0.00
ATOM   5033  HE  ARG A 331      85.490  43.992  60.055  1.00  0.00
ATOM   5034  CZ  ARG A 331      85.986  43.069  58.320  1.00  0.00
ATOM   5035  NH1 ARG A 331      85.621  42.729  57.068  1.00  0.00
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ATOM   5036 HH11 ARG A 331      84.723  42.996  56.725  1.00  0.00
ATOM   5037 HH12 ARG A 331      86.247  42.210  56.490  1.00  0.00
ATOM   5038  NH2 ARG A 331      87.203  42.699  58.771  1.00  0.00
ATOM   5039 HH21 ARG A 331      87.487  42.942  59.696  1.00  0.00
ATOM   5040 HH22 ARG A 331      87.816  42.179  58.178  1.00  0.00
ATOM   5041  C   ARG A 331      83.563  47.694  57.682  1.00  0.00
ATOM   5042  O   ARG A 331      83.062  47.002  56.798  1.00  0.00
ATOM   5043  N   GLU A 332      83.100  48.906  57.990  1.00  0.00
ATOM   5044  HN  GLU A 332      83.540  49.459  58.693  1.00  0.00
ATOM   5045  CA  GLU A 332      81.908  49.478  57.408  1.00  0.00
ATOM   5046  HA  GLU A 332      81.235  48.692  57.098  1.00  0.00
ATOM   5047  CB  GLU A 332      81.185  50.351  58.467  1.00  0.00
ATOM   5048  HB1 GLU A 332      80.378  50.949  57.988  1.00  0.00
ATOM   5049  HB2 GLU A 332      81.924  51.056  58.904  1.00  0.00
ATOM   5050  CG  GLU A 332      80.548  49.537  59.612  1.00  0.00
ATOM   5051  HG1 GLU A 332      81.318  48.921  60.123  1.00  0.00
ATOM   5052  HG2 GLU A 332      79.771  48.860  59.199  1.00  0.00
ATOM   5053  CD  GLU A 332      79.921  50.484  60.636  1.00  0.00
ATOM   5054  OE1 GLU A 332      78.680  50.414  60.843  1.00  0.00
ATOM   5055  OE2 GLU A 332      80.679  51.296  61.232  1.00  0.00
ATOM   5056  C   GLU A 332      82.229  50.339  56.198  1.00  0.00
ATOM   5057  O   GLU A 332      81.329  50.906  55.580  1.00  0.00
ATOM   5058  N   LYS A 333      83.513  50.437  55.837  1.00  0.00
ATOM   5059  HN  LYS A 333      84.214  49.925  56.330  1.00  0.00
ATOM   5060  CA  LYS A 333      84.018  51.287  54.775  1.00  0.00
ATOM   5061  HA  LYS A 333      83.707  52.294  54.996  1.00  0.00
ATOM   5062  CB  LYS A 333      85.565  51.276  54.774  1.00  0.00
ATOM   5063  HB1 LYS A 333      85.938  50.255  54.545  1.00  0.00
ATOM   5064  HB2 LYS A 333      85.908  51.543  55.799  1.00  0.00
ATOM   5065  CG  LYS A 333      86.205  52.260  53.779  1.00  0.00
ATOM   5066  HG1 LYS A 333      85.728  53.254  53.923  1.00  0.00
ATOM   5067  HG2 LYS A 333      86.001  51.922  52.740  1.00  0.00
ATOM   5068  CD  LYS A 333      87.725  52.392  53.967  1.00  0.00
ATOM   5069  HD1 LYS A 333      88.183  51.386  53.828  1.00  0.00
ATOM   5070  HD2 LYS A 333      87.935  52.713  55.012  1.00  0.00
ATOM   5071  CE  LYS A 333      88.393  53.368  52.986  1.00  0.00
ATOM   5072  HE1 LYS A 333      88.199  53.060  51.938  1.00  0.00
ATOM   5073  HE2 LYS A 333      89.490  53.397  53.158  1.00  0.00
ATOM   5074  NZ  LYS A 333      87.875  54.747  53.159  1.00  0.00
ATOM   5075  HZ1 LYS A 333      88.091  55.083  54.119  1.00  0.00
ATOM   5076  HZ2 LYS A 333      86.845  54.748  53.017  1.00  0.00
ATOM   5077  HZ3 LYS A 333      88.318  55.377  52.459  1.00  0.00
ATOM   5078  C   LYS A 333      83.500  50.965  53.393  1.00  0.00
ATOM   5079  O   LYS A 333      83.191  51.870  52.621  1.00  0.00
ATOM   5080  N   TRP A 334      83.397  49.676  53.061  1.00  0.00
ATOM   5081  HN  TRP A 334      83.612  48.958  53.717  1.00  0.00
ATOM   5082  CA  TRP A 334      83.105  49.232  51.711  1.00  0.00
ATOM   5083  HA  TRP A 334      83.343  50.025  51.014  1.00  0.00
ATOM   5084  CB  TRP A 334      83.985  48.005  51.349  1.00  0.00
ATOM   5085  HB1 TRP A 334      83.667  47.584  50.369  1.00  0.00
ATOM   5086  HB2 TRP A 334      83.845  47.208  52.111  1.00  0.00
ATOM   5087  CG  TRP A 334      85.441  48.333  51.236  1.00  0.00
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ATOM   5088  CD1 TRP A 334      86.041  48.889  50.137  1.00  0.00
ATOM   5089  HD1 TRP A 334      85.528  49.154  49.223  1.00  0.00
ATOM   5090  NE1 TRP A 334      87.375  49.070  50.378  1.00  0.00
ATOM   5091  HE1 TRP A 334      88.024  49.433  49.745  1.00  0.00
ATOM   5092  CE2 TRP A 334      87.679  48.621  51.631  1.00  0.00
ATOM   5093  CD2 TRP A 334      86.481  48.140  52.209  1.00  0.00
ATOM   5094  CE3 TRP A 334      86.511  47.597  53.492  1.00  0.00
ATOM   5095  HE3 TRP A 334      85.617  47.217  53.965  1.00  0.00
ATOM   5096  CZ3 TRP A 334      87.731  47.541  54.170  1.00  0.00
ATOM   5097  HZ3 TRP A 334      87.768  47.114  55.163  1.00  0.00
ATOM   5098  CZ2 TRP A 334      88.888  48.582  52.312  1.00  0.00
ATOM   5099  HZ2 TRP A 334      89.802  48.950  51.871  1.00  0.00
ATOM   5100  CH2 TRP A 334      88.898  48.031  53.593  1.00  0.00
ATOM   5101  HH2 TRP A 334      89.828  47.979  54.143  1.00  0.00
ATOM   5102  C   TRP A 334      81.649  48.891  51.496  1.00  0.00
ATOM   5103  O   TRP A 334      81.281  48.340  50.460  1.00  0.00
ATOM   5104  N   PHE A 335      80.783  49.258  52.441  1.00  0.00
ATOM   5105  HN  PHE A 335      81.087  49.716  53.274  1.00  0.00
ATOM   5106  CA  PHE A 335      79.356  49.024  52.329  1.00  0.00
ATOM   5107  HA  PHE A 335      79.170  48.205  51.646  1.00  0.00
ATOM   5108  CB  PHE A 335      78.765  48.649  53.712  1.00  0.00
ATOM   5109  HB1 PHE A 335      77.657  48.741  53.720  1.00  0.00
ATOM   5110  HB2 PHE A 335      79.172  49.318  54.501  1.00  0.00
ATOM   5111  CG  PHE A 335      79.085  47.219  54.064  1.00  0.00
ATOM   5112  CD1 PHE A 335      80.208  46.885  54.840  1.00  0.00
ATOM   5113  HD1 PHE A 335      80.876  47.663  55.175  1.00  0.00
ATOM   5114  CE1 PHE A 335      80.472  45.550  55.174  1.00  0.00
ATOM   5115  HE1 PHE A 335      81.336  45.301  55.772  1.00  0.00
ATOM   5116  CZ  PHE A 335      79.612  44.535  54.736  1.00  0.00
ATOM   5117  HZ  PHE A 335      79.814  43.506  54.995  1.00  0.00
ATOM   5118  CD2 PHE A 335      78.232  46.189  53.628  1.00  0.00
ATOM   5119  HD2 PHE A 335      77.364  46.434  53.035  1.00  0.00
ATOM   5120  CE2 PHE A 335      78.491  44.855  53.961  1.00  0.00
ATOM   5121  HE2 PHE A 335      77.826  44.074  53.622  1.00  0.00
ATOM   5122  C   PHE A 335      78.640  50.224  51.758  1.00  0.00
ATOM   5123  O   PHE A 335      77.416  50.226  51.648  1.00  0.00
ATOM   5124  N   VAL A 336      79.397  51.234  51.321  1.00  0.00
ATOM   5125  HN  VAL A 336      80.388  51.209  51.429  1.00  0.00
ATOM   5126  CA  VAL A 336      78.878  52.423  50.676  1.00  0.00
ATOM   5127  HA  VAL A 336      77.841  52.555  50.956  1.00  0.00
ATOM   5128  CB  VAL A 336      79.639  53.693  51.067  1.00  0.00
ATOM   5129  HB  VAL A 336      79.150  54.578  50.593  1.00  0.00
ATOM   5130  CG1 VAL A 336      79.527  53.891  52.594  1.00  0.00
ATOM   5131 HG11 VAL A 336      80.026  53.067  53.146  1.00  0.00
ATOM   5132 HG12 VAL A 336      78.460  53.933  52.896  1.00  0.00
ATOM   5133 HG13 VAL A 336      80.009  54.847  52.889  1.00  0.00
ATOM   5134  CG2 VAL A 336      81.110  53.654  50.591  1.00  0.00
ATOM   5135 HG21 VAL A 336      81.175  53.682  49.484  1.00  0.00
ATOM   5136 HG22 VAL A 336      81.619  52.739  50.950  1.00  0.00
ATOM   5137 HG23 VAL A 336      81.658  54.537  50.983  1.00  0.00
ATOM   5138  C   VAL A 336      78.935  52.243  49.169  1.00  0.00
ATOM   5139  O   VAL A 336      78.708  53.181  48.406  1.00  0.00
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ATOM   5140  N   SER A 337      79.215  51.020  48.708  1.00  0.00
ATOM   5141  HN  SER A 337      79.326  50.254  49.336  1.00  0.00
ATOM   5142  CA  SER A 337      79.523  50.749  47.319  1.00  0.00
ATOM   5143  HA  SER A 337      79.993  51.617  46.876  1.00  0.00
ATOM   5144  CB  SER A 337      80.480  49.531  47.208  1.00  0.00
ATOM   5145  HB1 SER A 337      80.753  49.348  46.146  1.00  0.00
ATOM   5146  HB2 SER A 337      80.000  48.615  47.614  1.00  0.00
ATOM   5147  OG  SER A 337      81.687  49.752  47.926  1.00  0.00
ATOM   5148  HG  SER A 337      81.491  49.562  48.849  1.00  0.00
ATOM   5149  C   SER A 337      78.284  50.403  46.525  1.00  0.00
ATOM   5150  O   SER A 337      78.369  50.106  45.334  1.00  0.00
ATOM   5151  N   TRP A 338      77.108  50.474  47.154  1.00  0.00
ATOM   5152  HN  TRP A 338      77.051  50.729  48.117  1.00  0.00
ATOM   5153  CA  TRP A 338      75.852  50.146  46.507  1.00  0.00
ATOM   5154  HA  TRP A 338      76.025  49.468  45.682  1.00  0.00
ATOM   5155  CB  TRP A 338      74.876  49.477  47.519  1.00  0.00
ATOM   5156  HB1 TRP A 338      73.944  49.184  46.987  1.00  0.00
ATOM   5157  HB2 TRP A 338      74.598  50.232  48.286  1.00  0.00
ATOM   5158  CG  TRP A 338      75.391  48.268  48.240  1.00  0.00
ATOM   5159  CD1 TRP A 338      76.399  47.413  47.869  1.00  0.00
ATOM   5160  HD1 TRP A 338      76.981  47.496  46.963  1.00  0.00
ATOM   5161  NE1 TRP A 338      76.559  46.444  48.824  1.00  0.00
ATOM   5162  HE1 TRP A 338      77.213  45.720  48.797  1.00  0.00
ATOM   5163  CE2 TRP A 338      75.652  46.633  49.827  1.00  0.00
ATOM   5164  CD2 TRP A 338      74.883  47.771  49.490  1.00  0.00
ATOM   5165  CE3 TRP A 338      73.854  48.177  50.339  1.00  0.00
ATOM   5166  HE3 TRP A 338      73.234  49.029  50.104  1.00  0.00
ATOM   5167  CZ3 TRP A 338      73.628  47.460  51.516  1.00  0.00
ATOM   5168  HZ3 TRP A 338      72.830  47.763  52.178  1.00  0.00
ATOM   5169  CZ2 TRP A 338      75.427  45.918  50.996  1.00  0.00
ATOM   5170  HZ2 TRP A 338      76.015  45.051  51.255  1.00  0.00
ATOM   5171  CH2 TRP A 338      74.407  46.354  51.844  1.00  0.00
ATOM   5172  HH2 TRP A 338      74.207  45.816  52.759  1.00  0.00
ATOM   5173  C   TRP A 338      75.203  51.403  45.974  1.00  0.00
ATOM   5174  O   TRP A 338      74.149  51.348  45.346  1.00  0.00
ATOM   5175  N   VAL A 339      75.858  52.553  46.168  1.00  0.00
ATOM   5176  HN  VAL A 339      76.695  52.571  46.710  1.00  0.00
ATOM   5177  CA  VAL A 339      75.471  53.828  45.601  1.00  0.00
ATOM   5178  HA  VAL A 339      74.395  53.922  45.663  1.00  0.00
ATOM   5179  CB  VAL A 339      76.119  54.986  46.364  1.00  0.00
ATOM   5180  HB  VAL A 339      77.228  54.885  46.338  1.00  0.00
ATOM   5181  CG1 VAL A 339      75.668  54.916  47.838  1.00  0.00
ATOM   5182 HG11 VAL A 339      76.022  53.985  48.327  1.00  0.00
ATOM   5183 HG12 VAL A 339      74.561  54.963  47.908  1.00  0.00
ATOM   5184 HG13 VAL A 339      76.088  55.774  48.403  1.00  0.00
ATOM   5185  CG2 VAL A 339      75.739  56.356  45.759  1.00  0.00
ATOM   5186 HG21 VAL A 339      74.636  56.451  45.689  1.00  0.00
ATOM   5187 HG22 VAL A 339      76.180  56.491  44.750  1.00  0.00
ATOM   5188 HG23 VAL A 339      76.118  57.174  46.406  1.00  0.00
ATOM   5189  C   VAL A 339      75.870  53.856  44.135  1.00  0.00
ATOM   5190  O   VAL A 339      75.262  54.548  43.319  1.00  0.00
ATOM   5191  N   GLY A 340      76.873  53.050  43.770  1.00  0.00
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ATOM   5192  HN  GLY A 340      77.329  52.478  44.448  1.00  0.00
ATOM   5193  CA  GLY A 340      77.383  52.945  42.422  1.00  0.00
ATOM   5194  HA1 GLY A 340      78.378  52.541  42.498  1.00  0.00
ATOM   5195  HA2 GLY A 340      77.372  53.922  41.966  1.00  0.00
ATOM   5196  C   GLY A 340      76.582  51.998  41.571  1.00  0.00
ATOM   5197  O   GLY A 340      76.647  52.072  40.346  1.00  0.00
ATOM   5198  N   LEU A 341      75.853  51.074  42.200  1.00  0.00
ATOM   5199  HN  LEU A 341      75.813  51.068  43.196  1.00  0.00
ATOM   5200  CA  LEU A 341      75.093  50.018  41.561  1.00  0.00
ATOM   5201  HA  LEU A 341      75.771  49.513  40.888  1.00  0.00
ATOM   5202  CB  LEU A 341      74.610  49.010  42.641  1.00  0.00
ATOM   5203  HB1 LEU A 341      73.915  49.537  43.332  1.00  0.00
ATOM   5204  HB2 LEU A 341      75.497  48.705  43.240  1.00  0.00
ATOM   5205  CG  LEU A 341      73.914  47.717  42.144  1.00  0.00
ATOM   5206  HG  LEU A 341      73.018  48.004  41.548  1.00  0.00
ATOM   5207  CD1 LEU A 341      74.828  46.865  41.240  1.00  0.00
ATOM   5208 HD11 LEU A 341      75.744  46.564  41.791  1.00  0.00
ATOM   5209 HD12 LEU A 341      75.129  47.430  40.334  1.00  0.00
ATOM   5210 HD13 LEU A 341      74.297  45.946  40.915  1.00  0.00
ATOM   5211  CD2 LEU A 341      73.402  46.883  43.336  1.00  0.00
ATOM   5212 HD21 LEU A 341      72.691  47.477  43.947  1.00  0.00
ATOM   5213 HD22 LEU A 341      74.251  46.572  43.982  1.00  0.00
ATOM   5214 HD23 LEU A 341      72.881  45.971  42.975  1.00  0.00
ATOM   5215  C   LEU A 341      73.909  50.518  40.754  1.00  0.00
ATOM   5216  O   LEU A 341      73.207  51.439  41.170  1.00  0.00
ATOM   5217  N   ARG A 342      73.665  49.892  39.599  1.00  0.00
ATOM   5218  HN  ARG A 342      74.280  49.183  39.261  1.00  0.00
ATOM   5219  CA  ARG A 342      72.453  50.044  38.825  1.00  0.00
ATOM   5220  HA  ARG A 342      71.635  50.324  39.476  1.00  0.00
ATOM   5221  CB  ARG A 342      72.607  51.067  37.664  1.00  0.00
ATOM   5222  HB1 ARG A 342      71.686  50.982  37.041  1.00  0.00
ATOM   5223  HB2 ARG A 342      73.475  50.807  37.022  1.00  0.00
ATOM   5224  CG  ARG A 342      72.673  52.554  38.054  1.00  0.00
ATOM   5225  HG1 ARG A 342      72.014  52.725  38.932  1.00  0.00
ATOM   5226  HG2 ARG A 342      72.244  53.129  37.198  1.00  0.00
ATOM   5227  CD  ARG A 342      74.084  53.103  38.311  1.00  0.00
ATOM   5228  HD1 ARG A 342      74.723  52.944  37.415  1.00  0.00
ATOM   5229  HD2 ARG A 342      74.568  52.625  39.180  1.00  0.00
ATOM   5230  NE  ARG A 342      73.986  54.580  38.536  1.00  0.00
ATOM   5231  HE  ARG A 342      74.014  55.170  37.727  1.00  0.00
ATOM   5232  CZ  ARG A 342      73.597  55.137  39.705  1.00  0.00
ATOM   5233  NH1 ARG A 342      73.442  54.405  40.823  1.00  0.00
ATOM   5234 HH11 ARG A 342      73.560  53.411  40.793  1.00  0.00
ATOM   5235 HH12 ARG A 342      73.074  54.837  41.649  1.00  0.00
ATOM   5236  NH2 ARG A 342      73.353  56.464  39.744  1.00  0.00
ATOM   5237 HH21 ARG A 342      73.390  56.995  38.895  1.00  0.00
ATOM   5238 HH22 ARG A 342      72.974  56.887  40.569  1.00  0.00
ATOM   5239  C   ARG A 342      72.138  48.706  38.211  1.00  0.00
ATOM   5240  O   ARG A 342      73.046  47.941  37.885  1.00  0.00
ATOM   5241  N   GLY A 343      70.845  48.409  38.055  1.00  0.00
ATOM   5242  HN  GLY A 343      70.136  49.034  38.378  1.00  0.00
ATOM   5243  CA  GLY A 343      70.359  47.186  37.451  1.00  0.00
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ATOM   5244  HA1 GLY A 343      69.766  46.680  38.199  1.00  0.00
ATOM   5245  HA2 GLY A 343      71.179  46.586  37.080  1.00  0.00
ATOM   5246  C   GLY A 343      69.474  47.523  36.292  1.00  0.00
ATOM   5247  O   GLY A 343      69.833  47.296  35.138  1.00  0.00
ATOM   5248  N   ALA A 344      68.281  48.045  36.586  1.00  0.00
ATOM   5249  HN  ALA A 344      68.027  48.209  37.540  1.00  0.00
ATOM   5250  CA  ALA A 344      67.265  48.407  35.620  1.00  0.00
ATOM   5251  HA  ALA A 344      67.063  47.528  35.027  1.00  0.00
ATOM   5252  CB  ALA A 344      65.959  48.834  36.317  1.00  0.00
ATOM   5253  HB1 ALA A 344      66.114  49.746  36.931  1.00  0.00
ATOM   5254  HB2 ALA A 344      65.611  48.021  36.990  1.00  0.00
ATOM   5255  HB3 ALA A 344      65.158  49.036  35.574  1.00  0.00
ATOM   5256  C   ALA A 344      67.681  49.506  34.669  1.00  0.00
ATOM   5257  O   ALA A 344      67.395  49.435  33.478  1.00  0.00
ATOM   5258  N   VAL A 345      68.364  50.532  35.184  1.00  0.00
ATOM   5259  HN  VAL A 345      68.602  50.540  36.151  1.00  0.00
ATOM   5260  CA  VAL A 345      68.750  51.723  34.446  1.00  0.00
ATOM   5261  HA  VAL A 345      67.828  52.132  34.055  1.00  0.00
ATOM   5262  CB  VAL A 345      69.320  52.798  35.376  1.00  0.00
ATOM   5263  HB  VAL A 345      70.031  52.326  36.091  1.00  0.00
ATOM   5264  CG1 VAL A 345      68.137  53.384  36.176  1.00  0.00
ATOM   5265 HG11 VAL A 345      67.600  52.593  36.734  1.00  0.00
ATOM   5266 HG12 VAL A 345      67.417  53.878  35.489  1.00  0.00
ATOM   5267 HG13 VAL A 345      68.493  54.142  36.902  1.00  0.00
ATOM   5268  CG2 VAL A 345      70.080  53.920  34.630  1.00  0.00
ATOM   5269 HG21 VAL A 345      69.430  54.387  33.860  1.00  0.00
ATOM   5270 HG22 VAL A 345      71.003  53.538  34.145  1.00  0.00
ATOM   5271 HG23 VAL A 345      70.385  54.704  35.355  1.00  0.00
ATOM   5272  C   VAL A 345      69.619  51.480  33.218  1.00  0.00
ATOM   5273  O   VAL A 345      69.284  52.060  32.187  1.00  0.00
ATOM   5274  N   PRO A 346      70.676  50.650  33.169  1.00  0.00
ATOM   5275  CD  PRO A 346      71.457  50.229  34.329  1.00  0.00
ATOM   5276  HD1 PRO A 346      70.827  49.777  35.119  1.00  0.00
ATOM   5277  HD2 PRO A 346      71.995  51.117  34.726  1.00  0.00
ATOM   5278  CA  PRO A 346      71.435  50.461  31.944  1.00  0.00
ATOM   5279  HA  PRO A 346      71.629  51.429  31.501  1.00  0.00
ATOM   5280  CB  PRO A 346      72.744  49.770  32.372  1.00  0.00
ATOM   5281  HB1 PRO A 346      73.540  50.545  32.457  1.00  0.00
ATOM   5282  HB2 PRO A 346      73.091  48.985  31.670  1.00  0.00
ATOM   5283  CG  PRO A 346      72.451  49.214  33.768  1.00  0.00
ATOM   5284  HG1 PRO A 346      71.956  48.223  33.675  1.00  0.00
ATOM   5285  HG2 PRO A 346      73.361  49.116  34.392  1.00  0.00
ATOM   5286  C   PRO A 346      70.665  49.643  30.938  1.00  0.00
ATOM   5287  O   PRO A 346      70.844  49.897  29.751  1.00  0.00
ATOM   5288  N   ILE A 347      69.867  48.655  31.358  1.00  0.00
ATOM   5289  HN  ILE A 347      69.724  48.475  32.328  1.00  0.00
ATOM   5290  CA  ILE A 347      69.229  47.733  30.435  1.00  0.00
ATOM   5291  HA  ILE A 347      69.942  47.535  29.647  1.00  0.00
ATOM   5292  CB  ILE A 347      68.883  46.372  31.049  1.00  0.00
ATOM   5293  HB  ILE A 347      68.548  45.692  30.230  1.00  0.00
ATOM   5294  CG2 ILE A 347      67.734  46.468  32.075  1.00  0.00
ATOM   5295 HG21 ILE A 347      66.815  46.900  31.631  1.00  0.00
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ATOM   5296 HG22 ILE A 347      68.044  47.084  32.942  1.00  0.00
ATOM   5297 HG23 ILE A 347      67.484  45.452  32.450  1.00  0.00
ATOM   5298  CG1 ILE A 347      70.122  45.712  31.706  1.00  0.00
ATOM   5299 HG11 ILE A 347      69.823  44.701  32.061  1.00  0.00
ATOM   5300 HG12 ILE A 347      70.419  46.300  32.601  1.00  0.00
ATOM   5301  CD1 ILE A 347      71.334  45.567  30.784  1.00  0.00
ATOM   5302  HD1 ILE A 347      71.720  46.559  30.467  1.00  0.00
ATOM   5303  HD2 ILE A 347      71.071  44.979  29.879  1.00  0.00
ATOM   5304  HD3 ILE A 347      72.148  45.042  31.326  1.00  0.00
ATOM   5305  C   ILE A 347      68.023  48.328  29.738  1.00  0.00
ATOM   5306  O   ILE A 347      67.683  47.903  28.635  1.00  0.00
ATOM   5307  N   ILE A 348      67.395  49.350  30.334  1.00  0.00
ATOM   5308  HN  ILE A 348      67.663  49.670  31.241  1.00  0.00
ATOM   5309  CA  ILE A 348      66.297  50.065  29.702  1.00  0.00
ATOM   5310  HA  ILE A 348      65.731  49.353  29.117  1.00  0.00
ATOM   5311  CB  ILE A 348      65.310  50.730  30.669  1.00  0.00
ATOM   5312  HB  ILE A 348      64.511  51.240  30.078  1.00  0.00
ATOM   5313  CG2 ILE A 348      65.998  51.823  31.517  1.00  0.00
ATOM   5314 HG21 ILE A 348      66.382  52.645  30.881  1.00  0.00
ATOM   5315 HG22 ILE A 348      66.839  51.399  32.097  1.00  0.00
ATOM   5316 HG23 ILE A 348      65.272  52.262  32.233  1.00  0.00
ATOM   5317  CG1 ILE A 348      64.586  49.686  31.558  1.00  0.00
ATOM   5318 HG11 ILE A 348      64.059  50.234  32.371  1.00  0.00
ATOM   5319 HG12 ILE A 348      65.323  49.011  32.039  1.00  0.00
ATOM   5320  CD1 ILE A 348      63.547  48.854  30.801  1.00  0.00
ATOM   5321  HD1 ILE A 348      64.031  48.240  30.014  1.00  0.00
ATOM   5322  HD2 ILE A 348      62.795  49.515  30.319  1.00  0.00
ATOM   5323  HD3 ILE A 348      63.015  48.175  31.501  1.00  0.00
ATOM   5324  C   ILE A 348      66.831  51.095  28.728  1.00  0.00
ATOM   5325  O   ILE A 348      66.111  51.537  27.836  1.00  0.00
ATOM   5326  N   LEU A 349      68.111  51.457  28.861  1.00  0.00
ATOM   5327  HN  LEU A 349      68.675  51.084  29.594  1.00  0.00
ATOM   5328  CA  LEU A 349      68.773  52.400  27.988  1.00  0.00
ATOM   5329  HA  LEU A 349      68.046  52.998  27.460  1.00  0.00
ATOM   5330  CB  LEU A 349      69.711  53.325  28.811  1.00  0.00
ATOM   5331  HB1 LEU A 349      70.329  53.949  28.127  1.00  0.00
ATOM   5332  HB2 LEU A 349      70.401  52.689  29.409  1.00  0.00
ATOM   5333  CG  LEU A 349      68.993  54.301  29.776  1.00  0.00
ATOM   5334  HG  LEU A 349      68.358  53.701  30.465  1.00  0.00
ATOM   5335  CD1 LEU A 349      70.018  55.058  30.645  1.00  0.00
ATOM   5336 HD11 LEU A 349      70.678  55.685  30.008  1.00  0.00
ATOM   5337 HD12 LEU A 349      70.650  54.341  31.211  1.00  0.00
ATOM   5338 HD13 LEU A 349      69.497  55.717  31.371  1.00  0.00
ATOM   5339  CD2 LEU A 349      68.064  55.285  29.038  1.00  0.00
ATOM   5340 HD21 LEU A 349      67.260  54.741  28.500  1.00  0.00
ATOM   5341 HD22 LEU A 349      68.641  55.886  28.304  1.00  0.00
ATOM   5342 HD23 LEU A 349      67.586  55.977  29.764  1.00  0.00
ATOM   5343  C   LEU A 349      69.612  51.679  26.960  1.00  0.00
ATOM   5344  O   LEU A 349      70.227  52.312  26.105  1.00  0.00
ATOM   5345  N   ALA A 350      69.625  50.344  27.005  1.00  0.00
ATOM   5346  HN  ALA A 350      69.116  49.847  27.703  1.00  0.00
ATOM   5347  CA  ALA A 350      70.419  49.533  26.110  1.00  0.00
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ATOM   5348  HA  ALA A 350      71.205  50.124  25.673  1.00  0.00
ATOM   5349  CB  ALA A 350      71.069  48.348  26.847  1.00  0.00
ATOM   5350  HB1 ALA A 350      70.297  47.680  27.285  1.00  0.00
ATOM   5351  HB2 ALA A 350      71.713  48.723  27.669  1.00  0.00
ATOM   5352  HB3 ALA A 350      71.711  47.760  26.158  1.00  0.00
ATOM   5353  C   ALA A 350      69.562  48.985  24.998  1.00  0.00
ATOM   5354  O   ALA A 350      70.062  48.319  24.093  1.00  0.00
ATOM   5355  N   VAL A 351      68.262  49.283  25.039  1.00  0.00
ATOM   5356  HN  VAL A 351      67.895  49.823  25.792  1.00  0.00
ATOM   5357  CA  VAL A 351      67.289  48.854  24.059  1.00  0.00
ATOM   5358  HA  VAL A 351      67.791  48.395  23.219  1.00  0.00
ATOM   5359  CB  VAL A 351      66.280  47.859  24.642  1.00  0.00
ATOM   5360  HB  VAL A 351      65.549  47.564  23.853  1.00  0.00
ATOM   5361  CG1 VAL A 351      67.032  46.576  25.060  1.00  0.00
ATOM   5362 HG11 VAL A 351      67.739  46.783  25.890  1.00  0.00
ATOM   5363 HG12 VAL A 351      67.602  46.162  24.202  1.00  0.00
ATOM   5364 HG13 VAL A 351      66.312  45.807  25.409  1.00  0.00
ATOM   5365  CG2 VAL A 351      65.491  48.465  25.827  1.00  0.00
ATOM   5366 HG21 VAL A 351      64.896  49.346  25.511  1.00  0.00
ATOM   5367 HG22 VAL A 351      66.174  48.771  26.645  1.00  0.00
ATOM   5368 HG23 VAL A 351      64.787  47.707  26.233  1.00  0.00
ATOM   5369  C   VAL A 351      66.573  50.080  23.538  1.00  0.00
ATOM   5370  O   VAL A 351      65.531  49.970  22.896  1.00  0.00
ATOM   5371  N   PHE A 352      67.125  51.265  23.805  1.00  0.00
ATOM   5372  HN  PHE A 352      68.016  51.328  24.247  1.00  0.00
ATOM   5373  CA  PHE A 352      66.456  52.527  23.604  1.00  0.00
ATOM   5374  HA  PHE A 352      65.621  52.395  22.936  1.00  0.00
ATOM   5375  CB  PHE A 352      65.929  53.047  24.973  1.00  0.00
ATOM   5376  HB1 PHE A 352      65.178  52.331  25.371  1.00  0.00
ATOM   5377  HB2 PHE A 352      66.767  53.103  25.700  1.00  0.00
ATOM   5378  CG  PHE A 352      65.272  54.403  24.874  1.00  0.00
ATOM   5379  CD1 PHE A 352      65.912  55.548  25.383  1.00  0.00
ATOM   5380  HD1 PHE A 352      66.888  55.458  25.839  1.00  0.00
ATOM   5381  CE1 PHE A 352      65.300  56.803  25.296  1.00  0.00
ATOM   5382  HE1 PHE A 352      65.800  57.675  25.692  1.00  0.00
ATOM   5383  CZ  PHE A 352      64.038  56.927  24.703  1.00  0.00
ATOM   5384  HZ  PHE A 352      63.566  57.897  24.636  1.00  0.00
ATOM   5385  CD2 PHE A 352      63.998  54.537  24.295  1.00  0.00
ATOM   5386  HD2 PHE A 352      63.492  53.665  23.909  1.00  0.00
ATOM   5387  CE2 PHE A 352      63.386  55.793  24.202  1.00  0.00
ATOM   5388  HE2 PHE A 352      62.411  55.887  23.748  1.00  0.00
ATOM   5389  C   PHE A 352      67.481  53.479  23.018  1.00  0.00
ATOM   5390  O   PHE A 352      68.625  53.450  23.470  1.00  0.00
ATOM   5391  N   PRO A 353      67.158  54.359  22.050  1.00  0.00
ATOM   5392  CD  PRO A 353      68.077  55.438  21.698  1.00  0.00
ATOM   5393  HD1 PRO A 353      68.881  55.019  21.054  1.00  0.00
ATOM   5394  HD2 PRO A 353      68.516  55.915  22.602  1.00  0.00
ATOM   5395  CA  PRO A 353      65.984  54.358  21.179  1.00  0.00
ATOM   5396  HA  PRO A 353      65.130  54.539  21.813  1.00  0.00
ATOM   5397  CB  PRO A 353      66.219  55.510  20.192  1.00  0.00
ATOM   5398  HB1 PRO A 353      65.276  56.037  19.940  1.00  0.00
ATOM   5399  HB2 PRO A 353      66.689  55.143  19.257  1.00  0.00
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ATOM   5400  CG  PRO A 353      67.213  56.426  20.915  1.00  0.00
ATOM   5401  HG1 PRO A 353      67.803  57.053  20.217  1.00  0.00
ATOM   5402  HG2 PRO A 353      66.663  57.079  21.628  1.00  0.00
ATOM   5403  C   PRO A 353      65.757  53.036  20.484  1.00  0.00
ATOM   5404  O   PRO A 353      66.728  52.372  20.123  1.00  0.00
ATOM   5405  N   MET A 354      64.490  52.644  20.338  1.00  0.00
ATOM   5406  HN  MET A 354      63.745  53.248  20.609  1.00  0.00
ATOM   5407  CA  MET A 354      64.063  51.316  19.952  1.00  0.00
ATOM   5408  HA  MET A 354      64.463  50.627  20.682  1.00  0.00
ATOM   5409  CB  MET A 354      62.513  51.233  19.974  1.00  0.00
ATOM   5410  HB1 MET A 354      62.200  50.181  19.797  1.00  0.00
ATOM   5411  HB2 MET A 354      62.098  51.848  19.144  1.00  0.00
ATOM   5412  CG  MET A 354      61.852  51.740  21.278  1.00  0.00
ATOM   5413  HG1 MET A 354      60.758  51.563  21.186  1.00  0.00
ATOM   5414  HG2 MET A 354      61.984  52.843  21.331  1.00  0.00
ATOM   5415  SD  MET A 354      62.448  51.001  22.837  1.00  0.00
ATOM   5416  CE  MET A 354      62.015  49.267  22.519  1.00  0.00
ATOM   5417  HE1 MET A 354      62.607  48.853  21.675  1.00  0.00
ATOM   5418  HE2 MET A 354      60.937  49.162  22.274  1.00  0.00
ATOM   5419  HE3 MET A 354      62.225  48.643  23.415  1.00  0.00
ATOM   5420  C   MET A 354      64.551  50.875  18.588  1.00  0.00
ATOM   5421  O   MET A 354      64.966  49.730  18.418  1.00  0.00
ATOM   5422  N   MET A 355      64.501  51.775  17.603  1.00  0.00
ATOM   5423  HN  MET A 355      64.200  52.709  17.775  1.00  0.00
ATOM   5424  CA  MET A 355      64.740  51.437  16.214  1.00  0.00
ATOM   5425  HA  MET A 355      64.851  50.368  16.100  1.00  0.00
ATOM   5426  CB  MET A 355      63.543  51.913  15.347  1.00  0.00
ATOM   5427  HB1 MET A 355      63.732  51.685  14.276  1.00  0.00
ATOM   5428  HB2 MET A 355      63.445  53.018  15.441  1.00  0.00
ATOM   5429  CG  MET A 355      62.190  51.284  15.748  1.00  0.00
ATOM   5430  HG1 MET A 355      61.410  51.697  15.070  1.00  0.00
ATOM   5431  HG2 MET A 355      61.930  51.630  16.772  1.00  0.00
ATOM   5432  SD  MET A 355      62.125  49.461  15.699  1.00  0.00
ATOM   5433  CE  MET A 355      62.324  49.241  13.905  1.00  0.00
ATOM   5434  HE1 MET A 355      63.325  49.581  13.565  1.00  0.00
ATOM   5435  HE2 MET A 355      61.555  49.817  13.346  1.00  0.00
ATOM   5436  HE3 MET A 355      62.219  48.171  13.626  1.00  0.00
ATOM   5437  C   MET A 355      66.000  52.078  15.685  1.00  0.00
ATOM   5438  O   MET A 355      66.300  51.968  14.497  1.00  0.00
ATOM   5439  N   ALA A 356      66.769  52.743  16.553  1.00  0.00
ATOM   5440  HN  ALA A 356      66.512  52.813  17.514  1.00  0.00
ATOM   5441  CA  ALA A 356      68.032  53.365  16.198  1.00  0.00
ATOM   5442  HA  ALA A 356      67.843  54.030  15.366  1.00  0.00
ATOM   5443  CB  ALA A 356      68.618  54.193  17.357  1.00  0.00
ATOM   5444  HB1 ALA A 356      68.729  53.577  18.275  1.00  0.00
ATOM   5445  HB2 ALA A 356      67.942  55.044  17.580  1.00  0.00
ATOM   5446  HB3 ALA A 356      69.609  54.619  17.089  1.00  0.00
ATOM   5447  C   ALA A 356      69.088  52.378  15.761  1.00  0.00
ATOM   5448  O   ALA A 356      69.843  52.641  14.826  1.00  0.00
ATOM   5449  N   GLY A 357      69.166  51.236  16.449  1.00  0.00
ATOM   5450  HN  GLY A 357      68.501  51.028  17.163  1.00  0.00
ATOM   5451  CA  GLY A 357      70.235  50.272  16.285  1.00  0.00
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ATOM   5452  HA1 GLY A 357      70.547  50.239  15.250  1.00  0.00
ATOM   5453  HA2 GLY A 357      69.864  49.326  16.649  1.00  0.00
ATOM   5454  C   GLY A 357      71.410  50.672  17.137  1.00  0.00
ATOM   5455  O   GLY A 357      72.545  50.283  16.870  1.00  0.00
ATOM   5456  N   LEU A 358      71.143  51.464  18.176  1.00  0.00
ATOM   5457  HN  LEU A 358      70.208  51.744  18.375  1.00  0.00
ATOM   5458  CA  LEU A 358      72.134  52.009  19.062  1.00  0.00
ATOM   5459  HA  LEU A 358      73.026  51.409  19.032  1.00  0.00
ATOM   5460  CB  LEU A 358      72.452  53.477  18.666  1.00  0.00
ATOM   5461  HB1 LEU A 358      71.515  54.076  18.705  1.00  0.00
ATOM   5462  HB2 LEU A 358      72.798  53.483  17.609  1.00  0.00
ATOM   5463  CG  LEU A 358      73.530  54.185  19.526  1.00  0.00
ATOM   5464  HG  LEU A 358      73.244  54.085  20.599  1.00  0.00
ATOM   5465  CD1 LEU A 358      74.922  53.551  19.350  1.00  0.00
ATOM   5466 HD11 LEU A 358      75.280  53.690  18.308  1.00  0.00
ATOM   5467 HD12 LEU A 358      74.900  52.465  19.567  1.00  0.00
ATOM   5468 HD13 LEU A 358      75.646  54.029  20.043  1.00  0.00
ATOM   5469  CD2 LEU A 358      73.579  55.696  19.223  1.00  0.00
ATOM   5470 HD21 LEU A 358      72.587  56.160  19.409  1.00  0.00
ATOM   5471 HD22 LEU A 358      73.857  55.869  18.162  1.00  0.00
ATOM   5472 HD23 LEU A 358      74.328  56.197  19.872  1.00  0.00
ATOM   5473  C   LEU A 358      71.483  51.994  20.426  1.00  0.00
ATOM   5474  O   LEU A 358      70.330  52.417  20.516  1.00  0.00
ATOM   5475  N   PRO A 359      72.124  51.561  21.525  1.00  0.00
ATOM   5476  CD  PRO A 359      71.616  51.902  22.852  1.00  0.00
ATOM   5477  HD1 PRO A 359      70.762  51.232  23.093  1.00  0.00
ATOM   5478  HD2 PRO A 359      71.301  52.967  22.911  1.00  0.00
ATOM   5479  CA  PRO A 359      73.351  50.772  21.617  1.00  0.00
ATOM   5480  HA  PRO A 359      74.155  51.423  21.309  1.00  0.00
ATOM   5481  CB  PRO A 359      73.442  50.408  23.103  1.00  0.00
ATOM   5482  HB1 PRO A 359      74.486  50.242  23.433  1.00  0.00
ATOM   5483  HB2 PRO A 359      72.831  49.507  23.334  1.00  0.00
ATOM   5484  CG  PRO A 359      72.803  51.624  23.772  1.00  0.00
ATOM   5485  HG1 PRO A 359      72.523  51.455  24.826  1.00  0.00
ATOM   5486  HG2 PRO A 359      73.505  52.484  23.714  1.00  0.00
ATOM   5487  C   PRO A 359      73.395  49.554  20.728  1.00  0.00
ATOM   5488  O   PRO A 359      72.361  48.926  20.510  1.00  0.00
ATOM   5489  N   ASN A 360      74.581  49.239  20.201  1.00  0.00
ATOM   5490  HN  ASN A 360      75.388  49.787  20.413  1.00  0.00
ATOM   5491  CA  ASN A 360      74.851  48.100  19.348  1.00  0.00
ATOM   5492  HA  ASN A 360      74.149  48.162  18.527  1.00  0.00
ATOM   5493  CB  ASN A 360      76.284  48.191  18.743  1.00  0.00
ATOM   5494  HB1 ASN A 360      76.364  49.145  18.179  1.00  0.00
ATOM   5495  HB2 ASN A 360      76.446  47.360  18.024  1.00  0.00
ATOM   5496  CG  ASN A 360      77.372  48.194  19.830  1.00  0.00
ATOM   5497  OD1 ASN A 360      77.548  49.186  20.545  1.00  0.00
ATOM   5498  ND2 ASN A 360      78.141  47.070  19.920  1.00  0.00
ATOM   5499 HD21 ASN A 360      78.884  47.039  20.588  1.00  0.00
ATOM   5500 HD22 ASN A 360      77.991  46.310  19.290  1.00  0.00
ATOM   5501  C   ASN A 360      74.594  46.787  20.062  1.00  0.00
ATOM   5502  O   ASN A 360      74.659  46.709  21.287  1.00  0.00
ATOM   5503  N   ALA A 361      74.248  45.747  19.298  1.00  0.00
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ATOM   5504  HN  ALA A 361      74.220  45.838  18.306  1.00  0.00
ATOM   5505  CA  ALA A 361      73.775  44.472  19.797  1.00  0.00
ATOM   5506  HA  ALA A 361      72.874  44.668  20.363  1.00  0.00
ATOM   5507  CB  ALA A 361      73.428  43.517  18.638  1.00  0.00
ATOM   5508  HB1 ALA A 361      74.326  43.290  18.025  1.00  0.00
ATOM   5509  HB2 ALA A 361      72.669  43.988  17.978  1.00  0.00
ATOM   5510  HB3 ALA A 361      73.006  42.563  19.021  1.00  0.00
ATOM   5511  C   ALA A 361      74.746  43.761  20.713  1.00  0.00
ATOM   5512  O   ALA A 361      74.351  43.237  21.750  1.00  0.00
ATOM   5513  N   GLN A 362      76.034  43.759  20.354  1.00  0.00
ATOM   5514  HN  GLN A 362      76.322  44.186  19.503  1.00  0.00
ATOM   5515  CA  GLN A 362      77.099  43.176  21.148  1.00  0.00
ATOM   5516  HA  GLN A 362      76.833  42.145  21.335  1.00  0.00
ATOM   5517  CB  GLN A 362      78.438  43.233  20.370  1.00  0.00
ATOM   5518  HB1 GLN A 362      79.246  42.820  21.019  1.00  0.00
ATOM   5519  HB2 GLN A 362      78.700  44.288  20.142  1.00  0.00
ATOM   5520  CG  GLN A 362      78.448  42.427  19.052  1.00  0.00
ATOM   5521  HG1 GLN A 362      79.481  42.402  18.643  1.00  0.00
ATOM   5522  HG2 GLN A 362      77.797  42.928  18.305  1.00  0.00
ATOM   5523  CD  GLN A 362      77.982  40.983  19.293  1.00  0.00
ATOM   5524  OE1 GLN A 362      78.644  40.227  20.012  1.00  0.00
ATOM   5525  NE2 GLN A 362      76.821  40.601  18.686  1.00  0.00
ATOM   5526 HE21 GLN A 362      76.488  39.668  18.816  1.00  0.00
ATOM   5527 HE22 GLN A 362      76.317  41.247  18.115  1.00  0.00
ATOM   5528  C   GLN A 362      77.261  43.834  22.500  1.00  0.00
ATOM   5529  O   GLN A 362      77.449  43.155  23.508  1.00  0.00
ATOM   5530  N   LEU A 363      77.167  45.165  22.539  1.00  0.00
ATOM   5531  HN  LEU A 363      77.014  45.689  21.705  1.00  0.00
ATOM   5532  CA  LEU A 363      77.188  45.949  23.755  1.00  0.00
ATOM   5533  HA  LEU A 363      78.080  45.663  24.294  1.00  0.00
ATOM   5534  CB  LEU A 363      77.286  47.458  23.415  1.00  0.00
ATOM   5535  HB1 LEU A 363      76.435  47.745  22.762  1.00  0.00
ATOM   5536  HB2 LEU A 363      78.220  47.609  22.829  1.00  0.00
ATOM   5537  CG  LEU A 363      77.318  48.441  24.613  1.00  0.00
ATOM   5538  HG  LEU A 363      76.333  48.385  25.130  1.00  0.00
ATOM   5539  CD1 LEU A 363      78.411  48.099  25.645  1.00  0.00
ATOM   5540 HD11 LEU A 363      79.411  48.118  25.164  1.00  0.00
ATOM   5541 HD12 LEU A 363      78.249  47.094  26.084  1.00  0.00
ATOM   5542 HD13 LEU A 363      78.402  48.841  26.472  1.00  0.00
ATOM   5543  CD2 LEU A 363      77.490  49.889  24.116  1.00  0.00
ATOM   5544 HD21 LEU A 363      76.710  50.138  23.367  1.00  0.00
ATOM   5545 HD22 LEU A 363      78.485  50.015  23.637  1.00  0.00
ATOM   5546 HD23 LEU A 363      77.412  50.602  24.964  1.00  0.00
ATOM   5547  C   LEU A 363      76.006  45.662  24.656  1.00  0.00
ATOM   5548  O   LEU A 363      76.165  45.546  25.866  1.00  0.00
ATOM   5549  N   TYR A 364      74.809  45.504  24.078  1.00  0.00
ATOM   5550  HN  TYR A 364      74.695  45.623  23.094  1.00  0.00
ATOM   5551  CA  TYR A 364      73.611  45.128  24.810  1.00  0.00
ATOM   5552  HA  TYR A 364      73.486  45.860  25.596  1.00  0.00
ATOM   5553  CB  TYR A 364      72.355  45.225  23.877  1.00  0.00
ATOM   5554  HB1 TYR A 364      72.578  44.701  22.924  1.00  0.00
ATOM   5555  HB2 TYR A 364      72.144  46.291  23.647  1.00  0.00
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ATOM   5556  CG  TYR A 364      71.097  44.612  24.480  1.00  0.00
ATOM   5557  CD1 TYR A 364      70.701  44.901  25.801  1.00  0.00
ATOM   5558  HD1 TYR A 364      71.295  45.567  26.406  1.00  0.00
ATOM   5559  CE1 TYR A 364      69.577  44.289  26.368  1.00  0.00
ATOM   5560  HE1 TYR A 364      69.306  44.509  27.390  1.00  0.00
ATOM   5561  CZ  TYR A 364      68.812  43.394  25.609  1.00  0.00
ATOM   5562  OH  TYR A 364      67.688  42.763  26.184  1.00  0.00
ATOM   5563  HH  TYR A 364      67.690  42.960  27.125  1.00  0.00
ATOM   5564  CD2 TYR A 364      70.306  43.726  23.725  1.00  0.00
ATOM   5565  HD2 TYR A 364      70.587  43.492  22.709  1.00  0.00
ATOM   5566  CE2 TYR A 364      69.173  43.120  24.283  1.00  0.00
ATOM   5567  HE2 TYR A 364      68.586  42.432  23.692  1.00  0.00
ATOM   5568  C   TYR A 364      73.744  43.777  25.495  1.00  0.00
ATOM   5569  O   TYR A 364      73.389  43.636  26.664  1.00  0.00
ATOM   5570  N   PHE A 365      74.292  42.783  24.793  1.00  0.00
ATOM   5571  HN  PHE A 365      74.558  42.913  23.838  1.00  0.00
ATOM   5572  CA  PHE A 365      74.548  41.463  25.340  1.00  0.00
ATOM   5573  HA  PHE A 365      73.620  41.093  25.755  1.00  0.00
ATOM   5574  CB  PHE A 365      75.058  40.493  24.237  1.00  0.00
ATOM   5575  HB1 PHE A 365      75.219  39.480  24.665  1.00  0.00
ATOM   5576  HB2 PHE A 365      76.023  40.865  23.827  1.00  0.00
ATOM   5577  CG  PHE A 365      74.078  40.338  23.092  1.00  0.00
ATOM   5578  CD1 PHE A 365      74.579  40.035  21.812  1.00  0.00
ATOM   5579  HD1 PHE A 365      75.644  39.921  21.669  1.00  0.00
ATOM   5580  CE1 PHE A 365      73.719  39.893  20.717  1.00  0.00
ATOM   5581  HE1 PHE A 365      74.120  39.667  19.740  1.00  0.00
ATOM   5582  CZ  PHE A 365      72.339  40.045  20.888  1.00  0.00
ATOM   5583  HZ  PHE A 365      71.674  39.935  20.044  1.00  0.00
ATOM   5584  CD2 PHE A 365      72.681  40.467  23.250  1.00  0.00
ATOM   5585  HD2 PHE A 365      72.250  40.679  24.217  1.00  0.00
ATOM   5586  CE2 PHE A 365      71.820  40.330  22.155  1.00  0.00
ATOM   5587  HE2 PHE A 365      70.754  40.439  22.291  1.00  0.00
ATOM   5588  C   PHE A 365      75.543  41.492  26.477  1.00  0.00
ATOM   5589  O   PHE A 365      75.348  40.822  27.488  1.00  0.00
ATOM   5590  N   ASN A 366      76.605  42.294  26.332  1.00  0.00
ATOM   5591  HN  ASN A 366      76.741  42.804  25.484  1.00  0.00
ATOM   5592  CA  ASN A 366      77.611  42.512  27.351  1.00  0.00
ATOM   5593  HA  ASN A 366      77.996  41.539  27.622  1.00  0.00
ATOM   5594  CB  ASN A 366      78.779  43.367  26.763  1.00  0.00
ATOM   5595  HB1 ASN A 366      78.390  44.341  26.402  1.00  0.00
ATOM   5596  HB2 ASN A 366      79.221  42.833  25.896  1.00  0.00
ATOM   5597  CG  ASN A 366      79.885  43.646  27.799  1.00  0.00
ATOM   5598  OD1 ASN A 366      80.167  44.808  28.117  1.00  0.00
ATOM   5599  ND2 ASN A 366      80.511  42.556  28.331  1.00  0.00
ATOM   5600 HD21 ASN A 366      81.227  42.683  29.016  1.00  0.00
ATOM   5601 HD22 ASN A 366      80.254  41.637  28.032  1.00  0.00
ATOM   5602  C   ASN A 366      77.036  43.142  28.608  1.00  0.00
ATOM   5603  O   ASN A 366      77.337  42.695  29.709  1.00  0.00
ATOM   5604  N   LEU A 367      76.192  44.167  28.454  1.00  0.00
ATOM   5605  HN  LEU A 367      75.988  44.522  27.542  1.00  0.00
ATOM   5606  CA  LEU A 367      75.506  44.837  29.543  1.00  0.00
ATOM   5607  HA  LEU A 367      76.256  45.155  30.251  1.00  0.00
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ATOM   5608  CB  LEU A 367      74.750  46.086  29.017  1.00  0.00
ATOM   5609  HB1 LEU A 367      74.058  46.478  29.795  1.00  0.00
ATOM   5610  HB2 LEU A 367      74.138  45.784  28.139  1.00  0.00
ATOM   5611  CG  LEU A 367      75.665  47.266  28.605  1.00  0.00
ATOM   5612  HG  LEU A 367      76.484  46.871  27.963  1.00  0.00
ATOM   5613  CD1 LEU A 367      74.883  48.293  27.764  1.00  0.00
ATOM   5614 HD11 LEU A 367      74.051  48.725  28.361  1.00  0.00
ATOM   5615 HD12 LEU A 367      74.457  47.809  26.860  1.00  0.00
ATOM   5616 HD13 LEU A 367      75.552  49.118  27.440  1.00  0.00
ATOM   5617  CD2 LEU A 367      76.328  47.945  29.820  1.00  0.00
ATOM   5618 HD21 LEU A 367      76.956  47.223  30.382  1.00  0.00
ATOM   5619 HD22 LEU A 367      75.555  48.352  30.504  1.00  0.00
ATOM   5620 HD23 LEU A 367      76.976  48.781  29.482  1.00  0.00
ATOM   5621  C   LEU A 367      74.535  43.954  30.286  1.00  0.00
ATOM   5622  O   LEU A 367      74.492  43.966  31.513  1.00  0.00
ATOM   5623  N   ALA A 368      73.743  43.173  29.549  1.00  0.00
ATOM   5624  HN  ALA A 368      73.793  43.206  28.551  1.00  0.00
ATOM   5625  CA  ALA A 368      72.765  42.244  30.071  1.00  0.00
ATOM   5626  HA  ALA A 368      72.120  42.790  30.743  1.00  0.00
ATOM   5627  CB  ALA A 368      71.904  41.678  28.936  1.00  0.00
ATOM   5628  HB1 ALA A 368      72.543  41.172  28.181  1.00  0.00
ATOM   5629  HB2 ALA A 368      71.361  42.502  28.425  1.00  0.00
ATOM   5630  HB3 ALA A 368      71.153  40.959  29.324  1.00  0.00
ATOM   5631  C   ALA A 368      73.401  41.124  30.863  1.00  0.00
ATOM   5632  O   ALA A 368      72.898  40.729  31.912  1.00  0.00
ATOM   5633  N   PHE A 369      74.538  40.619  30.381  1.00  0.00
ATOM   5634  HN  PHE A 369      74.882  40.915  29.491  1.00  0.00
ATOM   5635  CA  PHE A 369      75.413  39.714  31.095  1.00  0.00
ATOM   5636  HA  PHE A 369      74.824  38.859  31.400  1.00  0.00
ATOM   5637  CB  PHE A 369      76.534  39.232  30.118  1.00  0.00
ATOM   5638  HB1 PHE A 369      76.982  40.113  29.611  1.00  0.00
ATOM   5639  HB2 PHE A 369      76.089  38.586  29.332  1.00  0.00
ATOM   5640  CG  PHE A 369      77.642  38.460  30.797  1.00  0.00
ATOM   5641  CD1 PHE A 369      78.913  39.041  30.971  1.00  0.00
ATOM   5642  HD1 PHE A 369      79.090  40.053  30.639  1.00  0.00
ATOM   5643  CE1 PHE A 369      79.952  38.317  31.568  1.00  0.00
ATOM   5644  HE1 PHE A 369      80.922  38.774  31.698  1.00  0.00
ATOM   5645  CZ  PHE A 369      79.732  37.002  31.993  1.00  0.00
ATOM   5646  HZ  PHE A 369      80.532  36.443  32.455  1.00  0.00
ATOM   5647  CD2 PHE A 369      77.432  37.140  31.230  1.00  0.00
ATOM   5648  HD2 PHE A 369      76.465  36.679  31.096  1.00  0.00
ATOM   5649  CE2 PHE A 369      78.472  36.413  31.824  1.00  0.00
ATOM   5650  HE2 PHE A 369      78.302  35.399  32.155  1.00  0.00
ATOM   5651  C   PHE A 369      75.977  40.356  32.356  1.00  0.00
ATOM   5652  O   PHE A 369      75.958  39.755  33.428  1.00  0.00
ATOM   5653  N   PHE A 370      76.454  41.597  32.235  1.00  0.00
ATOM   5654  HN  PHE A 370      76.419  42.053  31.346  1.00  0.00
ATOM   5655  CA  PHE A 370      77.131  42.363  33.260  1.00  0.00
ATOM   5656  HA  PHE A 370      77.959  41.750  33.590  1.00  0.00
ATOM   5657  CB  PHE A 370      77.744  43.658  32.630  1.00  0.00
ATOM   5658  HB1 PHE A 370      76.954  44.195  32.068  1.00  0.00
ATOM   5659  HB2 PHE A 370      78.549  43.379  31.918  1.00  0.00
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ATOM   5660  CG  PHE A 370      78.334  44.611  33.647  1.00  0.00
ATOM   5661  CD1 PHE A 370      79.416  44.213  34.451  1.00  0.00
ATOM   5662  HD1 PHE A 370      79.824  43.218  34.347  1.00  0.00
ATOM   5663  CE1 PHE A 370      79.961  45.090  35.396  1.00  0.00
ATOM   5664  HE1 PHE A 370      80.786  44.769  36.015  1.00  0.00
ATOM   5665  CZ  PHE A 370      79.436  46.380  35.540  1.00  0.00
ATOM   5666  HZ  PHE A 370      79.859  47.058  36.267  1.00  0.00
ATOM   5667  CD2 PHE A 370      77.824  45.916  33.791  1.00  0.00
ATOM   5668  HD2 PHE A 370      76.999  46.241  33.173  1.00  0.00
ATOM   5669  CE2 PHE A 370      78.371  46.796  34.733  1.00  0.00
ATOM   5670  HE2 PHE A 370      77.970  47.793  34.837  1.00  0.00
ATOM   5671  C   PHE A 370      76.298  42.637  34.495  1.00  0.00
ATOM   5672  O   PHE A 370      76.801  42.537  35.612  1.00  0.00
ATOM   5673  N   VAL A 371      75.016  42.976  34.318  1.00  0.00
ATOM   5674  HN  VAL A 371      74.631  43.075  33.402  1.00  0.00
ATOM   5675  CA  VAL A 371      74.105  43.237  35.421  1.00  0.00
ATOM   5676  HA  VAL A 371      74.599  43.973  36.038  1.00  0.00
ATOM   5677  CB  VAL A 371      72.771  43.879  35.036  1.00  0.00
ATOM   5678  HB  VAL A 371      72.126  43.968  35.942  1.00  0.00
ATOM   5679  CG1 VAL A 371      73.045  45.318  34.545  1.00  0.00
ATOM   5680 HG11 VAL A 371      73.677  45.313  33.634  1.00  0.00
ATOM   5681 HG12 VAL A 371      73.561  45.906  35.333  1.00  0.00
ATOM   5682 HG13 VAL A 371      72.087  45.825  34.303  1.00  0.00
ATOM   5683  CG2 VAL A 371      72.006  43.052  33.984  1.00  0.00
ATOM   5684 HG21 VAL A 371      71.801  42.025  34.347  1.00  0.00
ATOM   5685 HG22 VAL A 371      72.584  42.995  33.041  1.00  0.00
ATOM   5686 HG23 VAL A 371      71.032  43.537  33.760  1.00  0.00
ATOM   5687  C   VAL A 371      73.907  42.025  36.310  1.00  0.00
ATOM   5688  O   VAL A 371      73.858  42.157  37.530  1.00  0.00
ATOM   5689  N   VAL A 372      73.831  40.831  35.713  1.00  0.00
ATOM   5690  HN  VAL A 372      73.863  40.761  34.718  1.00  0.00
ATOM   5691  CA  VAL A 372      73.776  39.560  36.414  1.00  0.00
ATOM   5692  HA  VAL A 372      72.954  39.624  37.115  1.00  0.00
ATOM   5693  CB  VAL A 372      73.507  38.381  35.482  1.00  0.00
ATOM   5694  HB  VAL A 372      74.317  38.293  34.724  1.00  0.00
ATOM   5695  CG1 VAL A 372      72.182  38.641  34.740  1.00  0.00
ATOM   5696 HG11 VAL A 372      72.242  39.544  34.101  1.00  0.00
ATOM   5697 HG12 VAL A 372      71.351  38.773  35.465  1.00  0.00
ATOM   5698 HG13 VAL A 372      71.941  37.776  34.086  1.00  0.00
ATOM   5699  CG2 VAL A 372      73.430  37.050  36.267  1.00  0.00
ATOM   5700 HG21 VAL A 372      72.676  37.125  37.079  1.00  0.00
ATOM   5701 HG22 VAL A 372      74.409  36.780  36.711  1.00  0.00
ATOM   5702 HG23 VAL A 372      73.129  36.227  35.585  1.00  0.00
ATOM   5703  C   VAL A 372      75.035  39.313  37.215  1.00  0.00
ATOM   5704  O   VAL A 372      74.967  38.877  38.362  1.00  0.00
ATOM   5705  N   MET A 373      76.200  39.619  36.635  1.00  0.00
ATOM   5706  HN  MET A 373      76.230  39.977  35.704  1.00  0.00
ATOM   5707  CA  MET A 373      77.486  39.459  37.285  1.00  0.00
ATOM   5708  HA  MET A 373      77.554  38.426  37.593  1.00  0.00
ATOM   5709  CB  MET A 373      78.653  39.746  36.304  1.00  0.00
ATOM   5710  HB1 MET A 373      79.616  39.721  36.865  1.00  0.00
ATOM   5711  HB2 MET A 373      78.544  40.766  35.881  1.00  0.00
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ATOM   5712  CG  MET A 373      78.791  38.739  35.142  1.00  0.00
ATOM   5713  HG1 MET A 373      79.641  39.086  34.514  1.00  0.00
ATOM   5714  HG2 MET A 373      77.890  38.787  34.501  1.00  0.00
ATOM   5715  SD  MET A 373      79.100  37.013  35.641  1.00  0.00
ATOM   5716  CE  MET A 373      77.407  36.394  35.400  1.00  0.00
ATOM   5717  HE1 MET A 373      77.073  36.537  34.350  1.00  0.00
ATOM   5718  HE2 MET A 373      76.686  36.921  36.057  1.00  0.00
ATOM   5719  HE3 MET A 373      77.346  35.309  35.632  1.00  0.00
ATOM   5720  C   MET A 373      77.651  40.282  38.538  1.00  0.00
ATOM   5721  O   MET A 373      78.199  39.798  39.524  1.00  0.00
ATOM   5722  N   VAL A 374      77.139  41.517  38.541  1.00  0.00
ATOM   5723  HN  VAL A 374      76.688  41.897  37.735  1.00  0.00
ATOM   5724  CA  VAL A 374      77.266  42.403  39.683  1.00  0.00
ATOM   5725  HA  VAL A 374      78.157  42.131  40.231  1.00  0.00
ATOM   5726  CB  VAL A 374      77.424  43.875  39.309  1.00  0.00
ATOM   5727  HB  VAL A 374      77.557  44.482  40.236  1.00  0.00
ATOM   5728  CG1 VAL A 374      78.718  44.026  38.483  1.00  0.00
ATOM   5729 HG11 VAL A 374      78.637  43.488  37.516  1.00  0.00
ATOM   5730 HG12 VAL A 374      79.586  43.620  39.044  1.00  0.00
ATOM   5731 HG13 VAL A 374      78.906  45.099  38.268  1.00  0.00
ATOM   5732  CG2 VAL A 374      76.191  44.419  38.557  1.00  0.00
ATOM   5733 HG21 VAL A 374      75.273  44.351  39.177  1.00  0.00
ATOM   5734 HG22 VAL A 374      76.030  43.854  37.620  1.00  0.00
ATOM   5735 HG23 VAL A 374      76.349  45.486  38.294  1.00  0.00
ATOM   5736  C   VAL A 374      76.092  42.232  40.622  1.00  0.00
ATOM   5737  O   VAL A 374      76.046  42.851  41.683  1.00  0.00
ATOM   5738  N   SER A 375      75.166  41.330  40.282  1.00  0.00
ATOM   5739  HN  SER A 375      75.204  40.863  39.400  1.00  0.00
ATOM   5740  CA  SER A 375      74.118  40.893  41.178  1.00  0.00
ATOM   5741  HA  SER A 375      73.948  41.633  41.946  1.00  0.00
ATOM   5742  CB  SER A 375      72.791  40.671  40.410  1.00  0.00
ATOM   5743  HB1 SER A 375      72.008  40.280  41.096  1.00  0.00
ATOM   5744  HB2 SER A 375      72.926  39.947  39.579  1.00  0.00
ATOM   5745  OG  SER A 375      72.308  41.896  39.875  1.00  0.00
ATOM   5746  HG  SER A 375      72.905  42.128  39.155  1.00  0.00
ATOM   5747  C   SER A 375      74.519  39.590  41.829  1.00  0.00
ATOM   5748  O   SER A 375      73.805  39.090  42.694  1.00  0.00
ATOM   5749  N   LEU A 376      75.685  39.053  41.454  1.00  0.00
ATOM   5750  HN  LEU A 376      76.214  39.454  40.709  1.00  0.00
ATOM   5751  CA  LEU A 376      76.293  37.907  42.094  1.00  0.00
ATOM   5752  HA  LEU A 376      75.579  37.400  42.723  1.00  0.00
ATOM   5753  CB  LEU A 376      76.826  36.918  41.027  1.00  0.00
ATOM   5754  HB1 LEU A 376      77.477  36.148  41.499  1.00  0.00
ATOM   5755  HB2 LEU A 376      77.446  37.481  40.297  1.00  0.00
ATOM   5756  CG  LEU A 376      75.715  36.167  40.254  1.00  0.00
ATOM   5757  HG  LEU A 376      74.940  36.904  39.946  1.00  0.00
ATOM   5758  CD1 LEU A 376      76.272  35.534  38.964  1.00  0.00
ATOM   5759 HD11 LEU A 376      77.046  34.777  39.208  1.00  0.00
ATOM   5760 HD12 LEU A 376      76.729  36.315  38.322  1.00  0.00
ATOM   5761 HD13 LEU A 376      75.457  35.040  38.393  1.00  0.00
ATOM   5762  CD2 LEU A 376      75.018  35.110  41.131  1.00  0.00
ATOM   5763 HD21 LEU A 376      74.557  35.582  42.023  1.00  0.00
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ATOM   5764 HD22 LEU A 376      75.752  34.348  41.472  1.00  0.00
ATOM   5765 HD23 LEU A 376      74.221  34.597  40.553  1.00  0.00
ATOM   5766  C   LEU A 376      77.444  38.360  42.964  1.00  0.00
ATOM   5767  O   LEU A 376      77.842  37.654  43.888  1.00  0.00
ATOM   5768  N   VAL A 377      77.960  39.570  42.716  1.00  0.00
ATOM   5769  HN  VAL A 377      77.637  40.104  41.940  1.00  0.00
ATOM   5770  CA  VAL A 377      78.964  40.229  43.535  1.00  0.00
ATOM   5771  HA  VAL A 377      79.748  39.509  43.732  1.00  0.00
ATOM   5772  CB  VAL A 377      79.596  41.427  42.818  1.00  0.00
ATOM   5773  HB  VAL A 377      78.791  42.028  42.341  1.00  0.00
ATOM   5774  CG1 VAL A 377      80.536  40.883  41.721  1.00  0.00
ATOM   5775 HG11 VAL A 377      80.013  40.176  41.051  1.00  0.00
ATOM   5776 HG12 VAL A 377      81.393  40.348  42.184  1.00  0.00
ATOM   5777 HG13 VAL A 377      80.936  41.719  41.108  1.00  0.00
ATOM   5778  CG2 VAL A 377      80.384  42.363  43.763  1.00  0.00
ATOM   5779 HG21 VAL A 377      81.143  41.787  44.335  1.00  0.00
ATOM   5780 HG22 VAL A 377      79.711  42.883  44.476  1.00  0.00
ATOM   5781 HG23 VAL A 377      80.911  43.140  43.169  1.00  0.00
ATOM   5782  C   VAL A 377      78.389  40.620  44.879  1.00  0.00
ATOM   5783  O   VAL A 377      79.066  40.546  45.904  1.00  0.00
ATOM   5784  N   VAL A 378      77.111  41.006  44.898  1.00  0.00
ATOM   5785  HN  VAL A 378      76.565  41.012  44.064  1.00  0.00
ATOM   5786  CA  VAL A 378      76.462  41.556  46.069  1.00  0.00
ATOM   5787  HA  VAL A 378      77.215  41.999  46.707  1.00  0.00
ATOM   5788  CB  VAL A 378      75.462  42.656  45.725  1.00  0.00
ATOM   5789  HB  VAL A 378      74.995  43.039  46.660  1.00  0.00
ATOM   5790  CG1 VAL A 378      76.227  43.842  45.096  1.00  0.00
ATOM   5791 HG11 VAL A 378      76.708  43.546  44.141  1.00  0.00
ATOM   5792 HG12 VAL A 378      77.012  44.208  45.791  1.00  0.00
ATOM   5793 HG13 VAL A 378      75.526  44.678  44.888  1.00  0.00
ATOM   5794  CG2 VAL A 378      74.345  42.124  44.802  1.00  0.00
ATOM   5795 HG21 VAL A 378      73.760  41.321  45.295  1.00  0.00
ATOM   5796 HG22 VAL A 378      74.778  41.724  43.864  1.00  0.00
ATOM   5797 HG23 VAL A 378      73.647  42.947  44.538  1.00  0.00
ATOM   5798  C   VAL A 378      75.782  40.468  46.875  1.00  0.00
ATOM   5799  O   VAL A 378      75.141  40.745  47.887  1.00  0.00
ATOM   5800  N   GLN A 379      75.973  39.206  46.479  1.00  0.00
ATOM   5801  HN  GLN A 379      76.461  39.000  45.635  1.00  0.00
ATOM   5802  CA  GLN A 379      75.614  38.061  47.291  1.00  0.00
ATOM   5803  HA  GLN A 379      74.727  38.283  47.869  1.00  0.00
ATOM   5804  CB  GLN A 379      75.381  36.814  46.397  1.00  0.00
ATOM   5805  HB1 GLN A 379      75.119  35.950  47.051  1.00  0.00
ATOM   5806  HB2 GLN A 379      76.322  36.555  45.861  1.00  0.00
ATOM   5807  CG  GLN A 379      74.264  36.963  45.344  1.00  0.00
ATOM   5808  HG1 GLN A 379      74.085  35.989  44.843  1.00  0.00
ATOM   5809  HG2 GLN A 379      74.613  37.687  44.581  1.00  0.00
ATOM   5810  CD  GLN A 379      72.950  37.454  45.970  1.00  0.00
ATOM   5811  OE1 GLN A 379      72.508  36.937  47.002  1.00  0.00
ATOM   5812  NE2 GLN A 379      72.307  38.464  45.315  1.00  0.00
ATOM   5813 HE21 GLN A 379      71.448  38.819  45.681  1.00  0.00
ATOM   5814 HE22 GLN A 379      72.695  38.834  44.470  1.00  0.00
ATOM   5815  C   GLN A 379      76.751  37.754  48.242  1.00  0.00
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ATOM   5816  O   GLN A 379      76.584  36.986  49.188  1.00  0.00
ATOM   5817  N   GLY A 380      77.915  38.375  48.011  1.00  0.00
ATOM   5818  HN  GLY A 380      78.004  38.970  47.215  1.00  0.00
ATOM   5819  CA  GLY A 380      79.082  38.350  48.867  1.00  0.00
ATOM   5820  HA1 GLY A 380      79.818  38.989  48.402  1.00  0.00
ATOM   5821  HA2 GLY A 380      79.403  37.320  48.946  1.00  0.00
ATOM   5822  C   GLY A 380      78.824  38.876  50.256  1.00  0.00
ATOM   5823  O   GLY A 380      77.804  39.509  50.530  1.00  0.00
ATOM   5824  N   GLY A 381      79.777  38.628  51.155  1.00  0.00
ATOM   5825  HN  GLY A 381      80.600  38.127  50.898  1.00  0.00
ATOM   5826  CA  GLY A 381      79.674  38.952  52.559  1.00  0.00
ATOM   5827  HA1 GLY A 381      78.778  39.520  52.767  1.00  0.00
ATOM   5828  HA2 GLY A 381      80.582  39.470  52.831  1.00  0.00
ATOM   5829  C   GLY A 381      79.621  37.667  53.320  1.00  0.00
ATOM   5830  O   GLY A 381      79.853  36.593  52.767  1.00  0.00
ATOM   5831  N   THR A 382      79.331  37.763  54.616  1.00  0.00
ATOM   5832  HN  THR A 382      79.134  38.641  55.045  1.00  0.00
ATOM   5833  CA  THR A 382      79.256  36.629  55.509  1.00  0.00
ATOM   5834  HA  THR A 382      80.032  35.927  55.232  1.00  0.00
ATOM   5835  CB  THR A 382      79.507  37.028  56.963  1.00  0.00
ATOM   5836  HB  THR A 382      80.551  37.410  57.036  1.00  0.00
ATOM   5837  OG1 THR A 382      78.646  38.080  57.391  1.00  0.00
ATOM   5838  HG1 THR A 382      78.974  38.356  58.250  1.00  0.00
ATOM   5839  CG2 THR A 382      79.371  35.812  57.903  1.00  0.00
ATOM   5840 HG21 THR A 382      80.030  34.987  57.559  1.00  0.00
ATOM   5841 HG22 THR A 382      78.325  35.441  57.929  1.00  0.00
ATOM   5842 HG23 THR A 382      79.668  36.088  58.937  1.00  0.00
ATOM   5843  C   THR A 382      77.891  35.931  55.327  1.00  0.00
ATOM   5844  O   THR A 382      76.839  36.614  55.442  1.00  0.00
ATOM   5845  OXT THR A 382      77.897  34.700  55.059  1.00  0.00
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