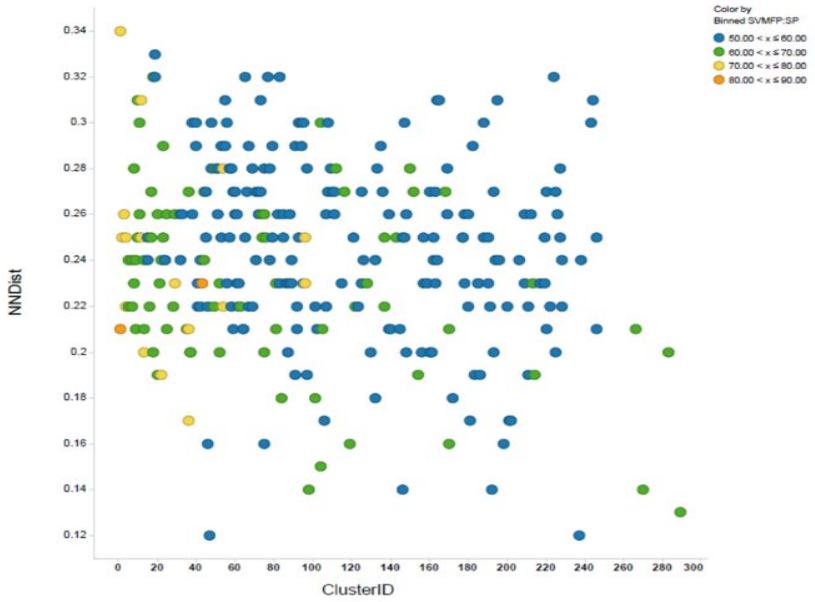
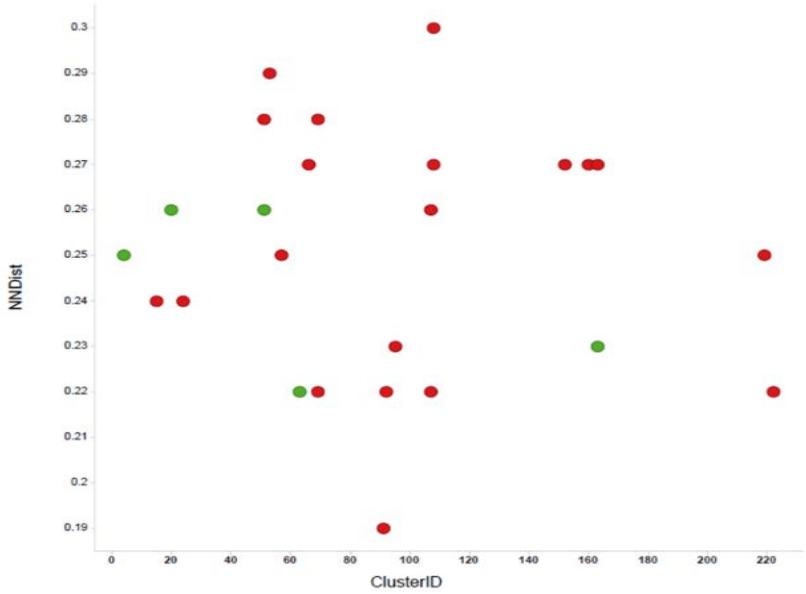
Supporting Information 1: Cluster assignment vs distance to Lilly collection plots



(a) Plot of cluster number vs NN distance to the Lilly collection of the selected PLC set of 285 compounds. Compounds are colored by their predicted ULK1 activity.



(b) Plot of cluster number vs NN distance of compounds prepared. ULK1 active compounds are in green, inactive in red.

Supporting Information 2: Methods

Computational

The computational tools used included structural fingerprint computation methods, distance calculation, substructure searching, clustering and predictive models. All code has been developed internally. For more information on the fingerprint computation methods and SVM predictive model implementations see [19]. Distance calculations were performed using the Tanimoto coefficient. For more information on substructure searching implementation see [4, 21]. Clustering was performed with an inhouse implementation of the sphere exclusion algorithm using 0.15 as the distance threshold (sphere radius) [MacCuish and MacCuish 2014]. An expanded human expert team which included both medicinal and organic chemists manually selected the compounds to synthesize from each cluster. PLC search for near neighbors of the hits identified in round 1 was performed using method ExpandSearch as described in [4]. Parts of the above code, namely substructure search and clustering, has been released to the public domain at [https://github.com/EliLillyCo/LillyMol]

Synthesis

Synthesis was performed on the ASL with a scale ranging from 0.3-0.5 mmol of the rate limiting agent. As the ASL integrates the automated synthesis, LCMS analysis and visualization, solid phase extraction work-up, and evaporation in one system, a chemist was able to check the LCMS results to determine how the reaction proceeded and the relative percentage of the desired product formation versus reagents and by-products. A crude reaction mixture containing 25% or higher product was subsequently sent to APL for reverse phase purification.

Purification

Samples were received by the APL team predissolved in 1.5 mL DMSO. Aliquots (8 µL) were dispensed to 96 well microtiter plates and dissolved with 0.5 mL MeOH using liquid handling robotics. Those samples were analyzed by LCMS using both high and low pH solvent systems.

Preparative chromatography was performed on each sample using the solvent system selected by the analyst. The high pH solvent system was selected for all compounds except one. Each preparative column measuring 30 X 75 mm was run at 85 mL/min assisted by a pre-column heater set at 50°C. The gradients varied and were selected automatically using software analysis of the analytical data. Each method employed a gradient from 0 to 8 min, followed by a column wash for a total cycle time of 10 min. All run parameters, including custom gradient and UV/MS thresholds, were computed using A-to-Prep software (On-the-Mark Solutions). Preparative chromatography fractions were dried under a heated stream of nitrogen gas. The dried samples were then transferred to a Hamilton liquid handler for dissolution, aliquot apportioning, and transfer. During apportioning, a sample aliquot sufficient to generate 1.5 mL of a 10 mM solution was transferred to a 3.5 mL vial and re-dried under nitrogen. Each sample was then reconstituted with 1.5 mL d6-DMSO. Aliquots were taken for final analytical LCMS purity assessment and NMR analysis. The remainder of the sample was sent for plating in preparation of biological testing.

Analytical chromatography was performed on Agilent LCMS 1100/MSD instruments running Chemstation software vB.04.03. Phenomenex Gemini-NX (high pH) and Luna (low pH) columns (2.1 X 50 mm) were used at a flow rate of 1.0 mL/min with a gradient of 5-100% ACN from 0 to 3 min. The high pH system employed 10 mM ammonium bicarbonate buffer, pH 10; and the low pH system employed 0.1% (v/v) trifluoroacetic acid as the aqueous components of the solvent system.

NMR

NMR samples were transferred to 4" 5.0 mm dia. Bruker NMR tubes held in a 96 sample SampleJet rack. Each tube is pre-equipped with a barcoded cap with an inlet hole. After sample is added to each tube, small Teflon balls are added to the cap to seal the samples. Data was acquired on a Bruker AS400 NMR.

The ^{1}H-CPMG NMR method, utilizes relaxation-edited one dimensional ^{1}H NMR spectra [Fesik 1997] that exploit differences in the magnetic relaxation properties of a ligand between its free and protein bound states. To detect ligand binding with this approach, several relaxation-edited ^{1}H NMR spectra were acquired with a transverse relaxation filter of 400 ms in duration. First, a relaxation-edited spectrum of the test compound in the absence of ULK1 was obtained. Next, a small amount of a concentrated stock solution of ULK1 was added to the test sample to reach a predetermined protein concentration, and the corresponding relaxation-edited spectrum was recorded. Signals from the test compound were then compared to those in the absence of ULK1, and a significant reduction above a threshold value (an empirical value of 25% was used in this study) in signal intensities indicated binding to the protein. In a final step, a competitor compound, namely a known ligand of ULK1 with high affinity and X-ray structure available, was added to the test sample and the signals of the test compound were again monitored by a relaxatoni-edited ^{1}H NMR spectrum. Recovery of the signals from the test compound above a predetermined threshold level (an empirical value of 50% was used in this study) indicates the test compound and the competitor compound bind to similar sites on the receptor protein.

Protein Crystallography

BTC was obtained as neat stock (dry powder) and dissolved in DMSO to make a 100mM stock solution. 14 mg/mL ULK1 protein in 50mM Tris pH 8, 150mM NaCl, 10% glycerol, 2.5mM TCEP was pre-incubated at 4°C in a 1:5 molar ratio with BTC diluted from 100mM DMSO stock for 1 hr. The protein-ligand mixture was filtered by centrifugal filtration device to remove any formed precipitate and subsequently set up in sitting drop crystallization trays using a Phoenix liquid handling robot mixing 0.3 µL of protein with 0.3 µL of well solution.

The protein-ligand complex crystallized by vapor diffusion at 8°C with a well solution of 31% PEG 4K, 200mM calcium chloride and 100mM bis tris propane pH 8.5. Crystals were transferred into a drop containing 22% glycerol in well solution for several seconds and then flash frozen in liquid nitrogen.

Diffraction data were collected at LRL-CAT (Lilly Research Laboratories Collaborative Access Team), sector 31ID of the Advanced Photon Source at Argonne National Laboratory, Chicago, Illinois. Crystals stored in liquid nitrogen were mounted on a goniometer equipped with an Oxford Cryosystems cryostream maintained at a temperature of 100 Kelvin. The wavelength used was 0.9793 Å collecting 180 diffraction images at a 1 degree oscillation angle and 0.2 seconds exposure time on a Rayonix 225-

HE CCD detector at a distiance of 119 mm. The images were indexed with MOSFLM and further processed with Scala and Truncate from CCP4 [36].

The diffraction data for ULK1 were isomorphous to previously obtained protein structures of ULK1 from the Lilly Biotechnology Center, San Diego, California (not published). The initial structure coordinates were further refined using Refmac5 (CCP4) applying isotropic temperature factors. Model building including placement of BTC was performed with Coot (CCP4) and final structure validation with MolProbity [37] and CCP4 validation tools.

The crystal structure obtained is supplied as SI3 and SI4 to this manuscript in pdb and pdf file formats respectively.

Supporting Information 3: pdb file containing the crystal structure of the complex of ULK1 and BTC submitted to the public PDB database (https://www.rcsb.org/) under the access code 6MNH

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HEADER    ULK1 - 3207658                  25-NOV-13   F6802
TITLE     CLONE 8253a25SPt1p1 D068926 8253F3R6  SP  + S195A/S224A
AUTHOR    J.Hendle, Eli Lilly & Company
KEYWDS    ULK1, GENE ID: 8408, 8253a25SPt1p1,
KEYWDS   2 8253F3R6  SP  + S195A/S224A, 3207658,
KEYWDS   3 ULK1_8253a25SPt1p1_3207658_T01_D068926_P01,
KEYWDS   4 Crystal ID: 188732
HETNAM     SX1 3207658
SMILES    N(C(=O)C1=CC2=C(C=C1)NN=N2)C(C)C(C)C
HETNAM      CL CHLORIDE ION
HETNAM     DMS DIMETHYL SULFOXIDE
REMARK   2 RESOLUTION. 1.73 ANGSTROMS.
REMARK   3
REMARK   3 REFINEMENT.
REMARK   3   PROGRAM     : REFMAC 5.8.0103
REMARK   3   AUTHORS     : MURSHUDOV,SKUBAK,LEBEDEV,PANNU,
REMARK   3               STEINER,NICHOLLS,WINN,LONG,VAGIN
REMARK   3
REMARK   3    REFINEMENT TARGET : MAXIMUM LIKELIHOOD
REMARK   3
REMARK   3  DATA USED IN REFINEMENT.
REMARK   3   RESOLUTION RANGE HIGH (ANGSTROMS) :   1.73
REMARK   3   RESOLUTION RANGE LOW  (ANGSTROMS) :  29.14
REMARK   3   DATA CUTOFF           (SIGMA(F)) : NONE
REMARK   3   COMPLETENESS FOR RANGE       (%) :  98.55
REMARK   3   NUMBER OF REFLECTIONS          :   26741
REMARK   3
REMARK   3  FIT TO DATA USED IN REFINEMENT.
REMARK   3   CROSS-VALIDATION METHOD        : THROUGHOUT
REMARK   3   FREE R VALUE TEST SET SELECTION  : RANDOM
REMARK   3   R VALUE     (WORKING + TEST SET) : 0.19290
REMARK   3   R VALUE          (WORKING SET) :  0.19102
REMARK   3   FREE R VALUE                   :  0.22853
REMARK   3   FREE R VALUE TEST SET SIZE   (%) :  5.0
REMARK   3   FREE R VALUE TEST SET COUNT      :  1407
REMARK   3
REMARK   3  FIT IN THE HIGHEST RESOLUTION BIN.
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REMARK 3 TOTAL NUMBER OF BINS USED : 20
REMARK 3 BIN RESOLUTION RANGE HIGH : 1.730
REMARK 3 BIN RESOLUTION RANGE LOW : 1.775
REMARK 3 REFLECTION IN BIN (WORKING SET) : 1953
REMARK 3 BIN COMPLETENESS (WORKING+TEST) (%) : 99.85
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REMARK 3 BIN FREE R VALUE SET COUNT : 102
REMARK 3 BIN FREE R VALUE : 0.271
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REMARK 3 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK 3 ALL ATOMS : 2400
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REMARK 3 B VALUES.
REMARK 3 FROM WILSON PLOT (A**2) : NULL
REMARK 3 MEAN B VALUE (OVERALL, A**2) : 22.069
REMARK 3 OVERALL ANISOTROPIC B VALUE.
REMARK 3 B11 (A**2) : 0.40
REMARK 3 B22 (A**2) : -0.79
REMARK 3 B33 (A**2) : 0.39
REMARK 3 B12 (A**2) : 0.00
REMARK 3 B13 (A**2) : -0.00
REMARK 3 B23 (A**2) : 0.00
REMARK 3
REMARK 3 ESTIMATED OVERALL COORDINATE ERROR.
REMARK 3 ESU BASED ON R VALUE (A): 0.126
REMARK 3 ESU BASED ON FREE R VALUE (A): 0.121
REMARK 3 ESU BASED ON MAXIMUM LIKELIHOOD (A): 0.082
REMARK 3 ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2): 2.519
REMARK 3
REMARK 3 CORRELATION COEFFICIENTS.
REMARK 3 CORRELATION COEFFICIENT FO-FC : 0.951
REMARK 3 CORRELATION COEFFICIENT FO-FC FREE : 0.925
REMARK 3
REMARK 3 RMS DEVIATIONS FROM IDEAL VALUES COUNT RMS WEIGHT
REMARK 3 BOND LENGTHS REFINED ATOMS (A): 2214 ; 0.009 ; 0.019
REMARK 3 BOND ANGLES REFINED ATOMS (DEGREES): 2993 ; 1.287 ; 1.982
REMARK 3 TORSION ANGLES, PERIOD 1 (DEGREES): 273 ; 5.362 ; 5.000
REMARK 3 TORSION ANGLES, PERIOD 2 (DEGREES): 99 ;35.842 ;23.030
REMARK 3 TORSION ANGLES, PERIOD 3 (DEGREES): 396 ;13.752 ;15.000
REMARK 3 TORSION ANGLES, PERIOD 4 (DEGREES): 17 ;18.747 ;15.000
REMARK 3 CHIRAL-CENTER RESTRAINTS (A**3): 335 ; 0.082 ; 0.200
REMARK 3 GENERAL PLANES REFINED ATOMS (A): 1646 ; 0.005 ; 0.021

REMARK 3
REMARK 3 ISOTROPIC THERMAL FACTOR RESTRAINTS. COUNT RMS WEIGHT
REMARK 3 MAIN-CHAIN BOND REFINED ATOMS (A**2): 1068 ; 2.721 ; 5.724
REMARK 3 MAIN-CHAIN ANGLE REFINED ATOMS (A**2): 1331 ; 3.692 ; 8.496
REMARK 3 SIDE-CHAIN BOND REFINED ATOMS (A**2): 1146 ; 4.375 ; 6.777
REMARK 3 LONG RANGE B REFINED ATOMS (A**2) : 3528 ; 7.501 ;28.191
REMARK 3
REMARK 3 NCS RESTRAINTS STATISTICS
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REMARK 3 TWIN DETAILS
REMARK 3 NUMBER OF TWIN DOMAINS : NULL
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REMARK 3
REMARK 3 TLS DETAILS
REMARK 3 NUMBER OF TLS GROUPS : NULL
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REMARK 3
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REMARK 3 METHOD USED : MASK
REMARK 3 PARAMETERS FOR MASK CALCULATION
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REMARK 3 ION PROBE RADIUS : 0.80
REMARK 3 SHRINKAGE RADIUS : 0.80
REMARK 3
REMARK 3 OTHER REFINEMENT REMARKS:
REMARK 3 HYDROGENS HAVE BEEN USED IF PRESENT IN THE INPUT
REMARK 3 U VALUES : REFINED INDIVIDUALLY
REMARK 3
REMARK 6
REMARK 6 LIGAND OMIT DENSITY CC, MEAN B-FACTOR, MEAN OCCUPANCY
REMARK 6 I 1 SX1 0.9374 24.645 1.00
REMARK 6 K 1 DMS 0.5958 51.470 1.00
REMARK 6 K 2 CL 0.8570 33.000 1.00
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SEQRES 3 A 287 VAL PHE LYS GLY ARG HIS ARG GLU LYS HIS ASP LEU GLU
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SEQRES 8 A 287 CYS ASN GLY GLY ASP LEU ALA ASP TYR LEU HIS ALA MET

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SEQRES   9 A  287  ARG THR LEU SER GLU ASP THR ILE ARG LEU PHE LEU GLN
SEQRES  10 A  287  GLN ILE ALA GLY ALA MET ARG LEU LEU HIS SER LYS GLY
SEQRES  11 A  287  ILE ILE HIS ARG ASP LEU LYS PRO GLN ASN ILE LEU LEU
SEQRES  12 A  287  SER ASN PRO ALA GLY ARG ARG ALA ASN PRO ASN SER ILE
SEQRES  13 A  287  ARG VAL LYS ILE ALA ASP PHE GLY PHE ALA ARG TYR LEU
SEQRES  14 A  287  GLN SER ASN MET MET ALA ALA THR LEU CYS GLY SER PRO
SEQRES  15 A  287  MET TYR MET ALA PRO GLU VAL ILE MET ALA GLN HIS TYR
SEQRES  16 A  287  ASP GLY LYS ALA ASP LEU TRP SER ILE GLY THR ILE VAL
SEQRES  17 A  287  TYR GLN CYS LEU THR GLY LYS ALA PRO PHE GLN ALA ALA
SEQRES  18 A  287  SER PRO GLN ASP LEU ARG LEU PHE TYR GLU LYS ASN LYS
SEQRES  19 A  287  THR LEU VAL PRO THR ILE PRO ARG GLU THR SER ALA PRO
SEQRES  20 A  287  LEU ARG GLN LEU LEU LEU ALA LEU LEU GLN ARG ASN HIS
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SEQRES  23 A  287  VAL
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ATOM    27  CG1 VAL A  11      14.542   3.038  39.617  1.00 25.36           C
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ATOM    41  NZ  LYS A  13      19.061  10.862  47.663  1.00 32.52           N
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ATOM    58  CG  GLU A  15       6.963   8.756  43.662  1.00 26.96           C
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ATOM    61  OE2 GLU A  15       5.967  10.285  45.183  1.00 42.37           O
ATOM    62  C   GLU A  15       7.405   7.240  41.113  1.00 21.08           C
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ATOM    65  CA  PHE A  16       5.534   6.330  39.818  1.00 23.54           C
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ATOM     66  CB  PHE A  16       6.158   5.968  38.449  1.00 21.56           C
ATOM     67  CG  PHE A  16       6.645   4.542  38.343  1.00 21.28           C
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ATOM     69  CE1 PHE A  16       6.306   2.247  37.605  1.00 16.83           C
ATOM     70  CZ  PHE A  16       7.554   1.896  38.118  1.00 21.90           C
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ATOM     72  CD2 PHE A  16       7.899   4.173  38.846  1.00 19.58           C
ATOM     73  C   PHE A  16       4.328   5.452  40.105  1.00 21.82           C
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ATOM     75  N   SER A  17       3.180   5.861  39.565  1.00 23.81           N
ATOM     76  CA  SER A  17       1.984   5.033  39.519  1.00 24.29           C
ATOM     77  CB  SER A  17       0.759   5.816  39.982  1.00 24.61           C
ATOM     78  OG  SER A  17      -0.439   5.098  39.714  1.00 28.43           O
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ATOM     87  CZ  ARG A  18       5.303  -1.724  36.258  1.00 23.42           C
ATOM     88  NH1 ARG A  18       5.094  -2.005  34.972  1.00 22.93           N
ATOM     89  NH2 ARG A  18       6.474  -2.004  36.810  1.00 21.44           N
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ATOM     92  N   LYS A  19      -0.917   3.893  36.794  1.00 26.12           N
ATOM     93  CA  LYS A  19      -2.068   4.637  36.268  1.00 26.57           C
ATOM     94  CB  LYS A  19      -2.838   5.342  37.389  1.00 30.95           C
ATOM     95  CG  LYS A  19      -3.642   4.421  38.288  1.00 29.67           C
ATOM     96  CD  LYS A  19      -4.628   5.230  39.116  1.00 42.35           C
ATOM     97  CE  LYS A  19      -5.309   4.372  40.168  1.00 49.28           C
ATOM     98  NZ  LYS A  19      -6.391   5.123  40.864  1.00 43.31           N
ATOM     99  C   LYS A  19      -1.622   5.676  35.240  1.00 24.30           C
ATOM    100  O   LYS A  19      -2.334   5.947  34.285  1.00 24.57           O
ATOM    101  N   ASP A  20      -0.423   6.225  35.430  1.00 22.27           N
ATOM    102  CA  ASP A  20       0.098   7.293  34.575  1.00 22.14           C
ATOM    103  CB  ASP A  20       0.856   8.318  35.429  1.00 22.19           C
ATOM    104  CG  ASP A  20      -0.029   8.962  36.483  1.00 29.94           C
ATOM    105  OD1 ASP A  20      -1.211   9.230  36.197  1.00 32.53           O
ATOM    106  OD2 ASP A  20       0.456   9.191  37.606  1.00 30.98           O
ATOM    107  C   ASP A  20       0.950   6.762  33.413  1.00 20.67           C
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ATOM    108  O   ASP A  20       2.103   7.133  33.249  1.00 21.66           O
ATOM    109  N   LEU A  21       0.334   5.898  32.611  1.00 22.72           N
ATOM    110  CA  LEU A  21       0.950   5.287  31.435  1.00 26.03           C
ATOM    111  CB  LEU A  21       0.083   4.092  31.010  1.00 24.74           C
ATOM    112  CG  LEU A  21       0.318   3.259  29.752  1.00 26.31           C
ATOM    113  CD1 LEU A  21       1.675   2.599  29.785  1.00 23.19           C
ATOM    114  CD2 LEU A  21      -0.772   2.202  29.627  1.00 26.69           C
ATOM    115  C   LEU A  21       1.110   6.307  30.298  1.00 23.76           C
ATOM    116  O   LEU A  21       0.120   6.885  29.838  1.00 25.99           O
ATOM    117  N   ILE A  22       2.354   6.532  29.867  1.00 18.48           N
ATOM    118  CA  ILE A  22       2.672   7.552  28.833  1.00 19.64           C
ATOM    119  CB  ILE A  22       3.463   8.766  29.409  1.00 22.95           C
ATOM    120  CG1 ILE A  22       4.846   8.344  29.952  1.00 21.74           C
ATOM    121  CD1 ILE A  22       5.799   9.488  30.265  1.00 18.06           C
ATOM    122  CG2 ILE A  22       2.617   9.499  30.461  1.00 22.76           C
ATOM    123  C   ILE A  22       3.354   7.017  27.553  1.00 19.26           C
ATOM    124  O   ILE A  22       3.500   7.748  26.569  1.00 20.54           O
ATOM    125  N   GLY A  23       3.782   5.759  27.575  1.00 19.66           N
ATOM    126  CA  GLY A  23       4.410   5.127  26.403  1.00 18.02           C
ATOM    127  C   GLY A  23       4.344   3.625  26.486  1.00 20.10           C
ATOM    128  O   GLY A  23       4.429   3.047  27.569  1.00 19.02           O
ATOM    129  N   HIS A  24       4.199   2.977  25.332  1.00 16.84           N
ATOM    130  CA  HIS A  24       4.034   1.538  25.306  1.00 15.32           C
ATOM    131  CB  HIS A  24       2.567   1.173  25.602  1.00 14.89           C
ATOM    132  CG  HIS A  24       2.321  -0.285  25.823  1.00 14.65           C
ATOM    133  ND1 HIS A  24       1.048  -0.808  25.911  1.00 19.50           N
ATOM    134  CE1 HIS A  24       1.123  -2.113  26.094  1.00 20.53           C
ATOM    135  NE2 HIS A  24       2.399  -2.456  26.136  1.00 22.47           N
ATOM    136  CD2 HIS A  24       3.169  -1.331  25.963  1.00 15.53           C
ATOM    137  C   HIS A  24       4.499   1.027  23.957  1.00 17.47           C
ATOM    138  O   HIS A  24       3.967   1.405  22.918  1.00 16.30           O
ATOM    139  N   GLY A  25       5.549   0.222  23.992  1.00 15.13           N
ATOM    140  CA  GLY A  25       6.087  -0.401  22.792  1.00 16.82           C
ATOM    141  C   GLY A  25       6.182  -1.880  23.072  1.00 18.77           C
ATOM    142  O   GLY A  25       5.860  -2.327  24.188  1.00 21.81           O
ATOM    143  N   ALA A  26       6.633  -2.642  22.073  1.00 18.11           N
ATOM    144  CA  ALA A  26       6.828  -4.082  22.227  1.00 18.47           C
ATOM    145  CB  ALA A  26       7.277  -4.693  20.905  1.00 20.29           C
ATOM    146  C   ALA A  26       7.844  -4.399  23.324  1.00 18.11           C
ATOM    147  O   ALA A  26       7.750  -5.446  23.981  1.00 18.99           O
ATOM    148  N   PHE A  27       8.805  -3.492  23.528  1.00 16.52           N
ATOM    149  CA  PHE A  27       9.937  -3.768  24.423  1.00 18.04           C
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ATOM    150  CB  PHE A  27      11.237  -3.860  23.622  1.00 18.32           C
ATOM    151  CG  PHE A  27      11.118  -4.748  22.408  1.00 20.51           C
ATOM    152  CD1 PHE A  27      10.876  -6.119  22.553  1.00 22.49           C
ATOM    153  CE1 PHE A  27      10.731  -6.941  21.436  1.00 23.80           C
ATOM    154  CZ  PHE A  27      10.825  -6.393  20.161  1.00 19.69           C
ATOM    155  CE2 PHE A  27      11.059  -5.032  20.003  1.00 20.59           C
ATOM    156  CD2 PHE A  27      11.191  -4.210  21.122  1.00 22.25           C
ATOM    157  C   PHE A  27      10.089  -2.860  25.644  1.00 18.51           C
ATOM    158  O   PHE A  27      11.087  -2.946  26.366  1.00 16.97           O
ATOM    159  N   ALA A  28       9.093  -2.008  25.879  1.00 17.99           N
ATOM    160  CA  ALA A  28       9.095  -1.140  27.055  1.00 17.97           C
ATOM    161  CB  ALA A  28      10.106  -0.007  26.899  1.00 16.20           C
ATOM    162  C   ALA A  28       7.723  -0.573  27.351  1.00 18.95           C
ATOM    163  O   ALA A  28       6.909  -0.363  26.455  1.00 18.71           O
ATOM    164  N   VAL A  29       7.468  -0.344  28.632  1.00 17.53           N
ATOM    165  CA  VAL A  29       6.292   0.403  29.062  1.00 17.91           C
ATOM    166  CB  VAL A  29       5.310  -0.465  29.900  1.00 21.76           C
ATOM    167  CG1 VAL A  29       3.967   0.212  30.007  1.00 26.51           C
ATOM    168  CG2 VAL A  29       5.073  -1.827  29.263  1.00 23.30           C
ATOM    169  C   VAL A  29       6.811   1.613  29.849  1.00 18.34           C
ATOM    170  O   VAL A  29       7.735   1.476  30.649  1.00 17.39           O
ATOM    171  N   VAL A  30       6.247   2.794  29.590  1.00 16.18           N
ATOM    172  CA  VAL A  30       6.758   4.046  30.168  1.00 15.86           C
ATOM    173  CB  VAL A  30       7.336   5.023  29.103  1.00 15.79           C
ATOM    174  CG1 VAL A  30       8.149   6.131  29.764  1.00 15.60           C
ATOM    175  CG2 VAL A  30       8.219   4.297  28.099  1.00 14.66           C
ATOM    176  C   VAL A  30       5.685   4.760  30.979  1.00 17.23           C
ATOM    177  O   VAL A  30       4.564   4.965  30.507  1.00 17.79           O
ATOM    178  N   PHE A  31       6.063   5.174  32.190  1.00 15.93           N
ATOM    179  CA  PHE A  31       5.136   5.842  33.104  1.00 19.07           C
ATOM    180  CB  PHE A  31       4.899   4.970  34.340  1.00 18.99           C
ATOM    181  CG  PHE A  31       4.451   3.575  34.017  1.00 17.74           C
ATOM    182  CD1 PHE A  31       5.363   2.511  34.046  1.00 18.65           C
ATOM    183  CE1 PHE A  31       4.952   1.221  33.738  1.00 23.33           C
ATOM    184  CZ  PHE A  31       3.623   0.981  33.397  1.00 22.00           C
ATOM    185  CE2 PHE A  31       2.709   2.029  33.351  1.00 21.42           C
ATOM    186  CD2 PHE A  31       3.122   3.318  33.667  1.00 20.50           C
ATOM    187  C   PHE A  31       5.646   7.209  33.529  1.00 18.19           C
ATOM    188  O   PHE A  31       6.850   7.397  33.678  1.00 21.39           O
ATOM    189  N   LYS A  32       4.725   8.157  33.723  1.00 18.88           N
ATOM    190  CA  LYS A  32       5.090   9.439  34.319  1.00 16.66           C
ATOM    191  CB  LYS A  32       3.974  10.466  34.169  1.00 18.71           C
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ATOM    192  CG  LYS A  32       4.421  11.908  34.386  1.00 19.81           C
ATOM    193  CD  LYS A  32       3.234  12.842  34.195  1.00 24.56           C
ATOM    194  CE  LYS A  32       3.509  14.221  34.756  1.00 36.51           C
ATOM    195  NZ  LYS A  32       2.326  15.112  34.606  1.00 40.87           N
ATOM    196  C   LYS A  32       5.354   9.185  35.796  1.00 18.57           C
ATOM    197  O   LYS A  32       4.653   8.392  36.424  1.00 18.89           O
ATOM    198  N   GLY A  33       6.374   9.851  36.323  1.00 20.04           N
ATOM    199  CA  GLY A  33       6.727   9.729  37.730  1.00 23.92           C
ATOM    200  C   GLY A  33       7.258  11.028  38.284  1.00 26.37           C
ATOM    201  O   GLY A  33       7.260  12.054  37.599  1.00 23.41           O
ATOM    202  N   ARG A  34       7.719  10.979  39.531  1.00 23.85           N
ATOM    203  CA  ARG A  34       8.221  12.172  40.215  1.00 24.53           C
ATOM    204  CB  ARG A  34       7.083  12.915  40.948  1.00 24.81           C
ATOM    205  CG  ARG A  34       6.385  12.130  42.052  1.00 28.35           C
ATOM    206  CD  ARG A  34       5.171  12.858  42.623  1.00 37.29           C
ATOM    207  NE  ARG A  34       4.446  12.007  43.574  1.00 49.27           N
ATOM    208  CZ  ARG A  34       3.228  12.239  44.070  1.00 52.06           C
ATOM    209  NH1 ARG A  34       2.535  13.325  43.743  1.00 48.69           N
ATOM    210  NH2 ARG A  34       2.700  11.373  44.925  1.00 61.87           N
ATOM    211  C   ARG A  34       9.368  11.822  41.156  1.00 24.23           C
ATOM    212  O   ARG A  34       9.509  10.663  41.561  1.00 21.13           O
ATOM    213  N   HIS A  35      10.210  12.815  41.458  1.00 23.07           N
ATOM    214  CA  HIS A  35      11.215  12.690  42.513  1.00 20.32           C
ATOM    215  CB  HIS A  35      12.191  13.875  42.485  1.00 20.85           C
ATOM    216  CG  HIS A  35      13.463  13.623  43.229  1.00 23.90           C
ATOM    217  ND1 HIS A  35      13.528  13.612  44.607  1.00 22.67           N
ATOM    218  CE1 HIS A  35      14.769  13.362  44.985  1.00 21.21           C
ATOM    219  NE2 HIS A  35      15.510  13.203  43.903  1.00 24.22           N
ATOM    220  CD2 HIS A  35      14.718  13.363  42.792  1.00 23.48           C
ATOM    221  C   HIS A  35      10.502  12.607  43.867  1.00 20.71           C
ATOM    222  O   HIS A  35       9.567  13.371  44.135  1.00 25.30           O
ATOM    223  N   ARG A  36      10.945  11.678  44.715  1.00 21.26           N
ATOM    224  CA  ARG A  36      10.241  11.392  45.975  1.00 21.31           C
ATOM    225  CB  ARG A  36      10.668  10.042  46.549  1.00 20.45           C
ATOM    226  CG  ARG A  36      10.234   8.858  45.704  1.00 21.04           C
ATOM    227  CD  ARG A  36      11.017   7.612  46.088  1.00 22.81           C
ATOM    228  NE  ARG A  36      10.517   7.022  47.331  1.00 18.22           N
ATOM    229  CZ  ARG A  36      11.079   5.992  47.951  1.00 16.74           C
ATOM    230  NH1 ARG A  36      12.170   5.421  47.460  1.00 17.56           N
ATOM    231  NH2 ARG A  36      10.535   5.528  49.068  1.00 20.17           N
ATOM    232  C   ARG A  36      10.422  12.489  47.025  1.00 19.45           C
ATOM    233  O   ARG A  36       9.587  12.640  47.915  1.00 19.43           O
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ATOM    234  N   GLU A  37      11.488  13.269  46.878  1.00 21.15           N
ATOM    235  CA  GLU A  37      11.801  14.362  47.805  1.00 22.42           C
ATOM    236  CB  GLU A  37      13.299  14.423  48.081  1.00 17.62           C
ATOM    237  CG  GLU A  37      13.928  13.093  48.461  1.00 18.89           C
ATOM    238  CD  GLU A  37      15.415  13.200  48.696  1.00 20.17           C
ATOM    239  OE1 GLU A  37      16.079  14.072  48.095  1.00 24.57           O
ATOM    240  OE2 GLU A  37      15.931  12.414  49.498  1.00 22.22           O
ATOM    241  C   GLU A  37      11.330  15.707  47.256  1.00 28.27           C
ATOM    242  O   GLU A  37      10.922  16.584  48.024  1.00 20.79           O
ATOM    243  N   LYS A  38      11.415  15.856  45.930  1.00 29.44           N
ATOM    244  CA  LYS A  38      11.042  17.084  45.218  1.00 32.76           C
ATOM    245  CB  LYS A  38      12.245  17.654  44.446  1.00 40.02           C
ATOM    246  CG  LYS A  38      13.528  17.837  45.250  1.00 44.55           C
ATOM    247  CD  LYS A  38      14.755  17.663  44.365  1.00 46.17           C
ATOM    248  CE  LYS A  38      16.033  17.635  45.189  1.00 56.91           C
ATOM    249  NZ  LYS A  38      17.177  17.023  44.453  1.00 51.56           N
ATOM    250  C   LYS A  38       9.906  16.727  44.260  1.00 32.80           C
ATOM    251  O   LYS A  38      10.143  16.408  43.091  1.00 34.27           O
ATOM    252  N   HIS A  39       8.677  16.779  44.773  1.00 32.92           N
ATOM    253  CA  HIS A  39       7.483  16.281  44.077  1.00 40.60           C
ATOM    254  CB  HIS A  39       6.285  16.254  45.030  1.00 46.33           C
ATOM    255  CG  HIS A  39       6.152  14.973  45.793  1.00 51.19           C
ATOM    256  ND1 HIS A  39       4.973  14.262  45.851  1.00 53.07           N
ATOM    257  CE1 HIS A  39       5.149  13.179  46.588  1.00 51.93           C
ATOM    258  NE2 HIS A  39       6.403  13.158  47.002  1.00 64.57           N
ATOM    259  CD2 HIS A  39       7.052  14.268  46.520  1.00 53.28           C
ATOM    260  C   HIS A  39       7.115  16.987  42.768  1.00 41.55           C
ATOM    261  O   HIS A  39       6.371  16.430  41.951  1.00 41.57           O
ATOM    262  N   ASP A  40       7.647  18.193  42.576  1.00 38.83           N
ATOM    263  CA  ASP A  40       7.425  18.972  41.355  1.00 39.21           C
ATOM    264  CB  ASP A  40       7.402  20.472  41.672  1.00 36.34           C
ATOM    265  CG  ASP A  40       6.164  20.885  42.472  1.00 43.88           C
ATOM    266  OD1 ASP A  40       5.090  20.258  42.310  1.00 46.60           O
ATOM    267  OD2 ASP A  40       6.263  21.845  43.264  1.00 57.79           O
ATOM    268  C   ASP A  40       8.414  18.645  40.230  1.00 35.95           C
ATOM    269  O   ASP A  40       8.263  19.137  39.109  1.00 33.75           O
ATOM    270  N   LEU A  41       9.418  17.822  40.531  1.00 31.31           N
ATOM    271  CA  LEU A  41      10.330  17.302  39.511  1.00 32.08           C
ATOM    272  CB  LEU A  41      11.739  17.041  40.079  1.00 34.31           C
ATOM    273  CG  LEU A  41      12.810  16.240  39.302  1.00 46.77           C
ATOM    274  CD1 LEU A  41      13.091  16.758  37.891  1.00 47.55           C
ATOM    275  CD2 LEU A  41      14.102  16.180  40.106  1.00 49.78           C
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ATOM    276  C   LEU A  41      9.722  16.059  38.858  1.00 35.04           C
ATOM    277  O   LEU A  41      9.652  14.985  39.469  1.00 27.07           O
ATOM    278  N   GLU A  42      9.266  16.229  37.616  1.00 27.11           N
ATOM    279  CA  GLU A  42      8.649  15.155  36.846  1.00 29.19           C
ATOM    280  CB  GLU A  42      7.672  15.732  35.815  1.00 29.52           C
ATOM    281  CG  GLU A  42      6.449  16.416  36.419  1.00 31.58           C
ATOM    282  CD  GLU A  42      5.702  17.276  35.413  1.00 41.91           C
ATOM    283  OE1 GLU A  42      6.357  17.995  34.620  1.00 39.95           O
ATOM    284  OE2 GLU A  42      4.456  17.236  35.419  1.00 41.67           O
ATOM    285  C   GLU A  42      9.711  14.310  36.148  1.00 20.05           C
ATOM    286  O   GLU A  42     10.753  14.828  35.739  1.00 23.94           O
ATOM    287  N   VAL A  43      9.456  13.005  36.044  1.00 19.20           N
ATOM    288  CA  VAL A  43     10.311  12.094  35.258  1.00 17.75           C
ATOM    289  CB  VAL A  43     11.345  11.296  36.123  1.00 16.38           C
ATOM    290  CG1 VAL A  43     12.390  12.205  36.768  1.00 20.48           C
ATOM    291  CG2 VAL A  43     10.647  10.414  37.155  1.00 21.08           C
ATOM    292  C   VAL A  43      9.448  11.101  34.468  1.00 16.58           C
ATOM    293  O   VAL A  43      8.231  11.024  34.664  1.00 16.92           O
ATOM    294  N   ALA A  44     10.102  10.365  33.571  1.00 17.99           N
ATOM    295  CA  ALA A  44      9.520   9.204  32.902  1.00 17.39           C
ATOM    296  CB  ALA A  44      9.619   9.339  31.386  1.00 19.96           C
ATOM    297  C   ALA A  44     10.280   7.977  33.378  1.00 16.90           C
ATOM    298  O   ALA A  44     11.505   7.991  33.444  1.00 21.63           O
ATOM    299  N   VAL A  45      9.548   6.930  33.744  1.00 17.88           N
ATOM    300  CA  VAL A  45     10.180   5.679  34.151  1.00 17.13           C
ATOM    301  CB  VAL A  45      9.742   5.204  35.558  1.00 17.16           C
ATOM    302  CG1 VAL A  45     10.566   3.994  35.990  1.00 20.19           C
ATOM    303  CG2 VAL A  45      9.887   6.328  36.577  1.00 19.76           C
ATOM    304  C   VAL A  45      9.878   4.621  33.097  1.00 14.02           C
ATOM    305  O   VAL A  45      8.725   4.216  32.917  1.00 15.54           O
ATOM    306  N   LYS A  46     10.937   4.204  32.411  1.00 15.06           N
ATOM    307  CA  LYS A  46     10.868   3.162  31.376  1.00 16.44           C
ATOM    308  CB  LYS A  46     11.886   3.482  30.269  1.00 17.06           C
ATOM    309  CG  LYS A  46     11.706   2.694  28.979  1.00 20.35           C
ATOM    310  CD  LYS A  46     12.594   3.290  27.898  1.00 17.59           C
ATOM    311  CE  LYS A  46     12.359   2.646  26.534  1.00 18.12           C
ATOM    312  NZ  LYS A  46     13.199   3.314  25.506  1.00 18.34           N
ATOM    313  C   LYS A  46     11.116   1.778  31.978  1.00 19.23           C
ATOM    314  O   LYS A  46     12.164   1.533  32.589  1.00 18.59           O
ATOM    315  N   CYS A  47     10.139   0.885  31.805  1.00 16.70           N
ATOM    316  CA  CYS A  47     10.172  -0.448  32.412  1.00 18.46           C
ATOM    317  CB  CYS A  47      8.964  -0.641  33.325  1.00 20.56           C
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ATOM    318  SG  CYS A  47       8.648   0.732  34.449  1.00 22.42           S
ATOM    319  C   CYS A  47      10.172  -1.527  31.345  1.00 21.28           C
ATOM    320  O   CYS A  47       9.891  -1.248  30.177  1.00 19.34           O
ATOM    321  N   ILE A  48      10.485  -2.754  31.763  1.00 20.91           N
ATOM    322  CA  ILE A  48      10.367  -3.951  30.927  1.00 22.90           C
ATOM    323  CB  ILE A  48      10.931  -5.209  31.663  1.00 29.86           C
ATOM    324  CG1 ILE A  48      12.456  -5.078  31.810  1.00 30.78           C
ATOM    325  CD1 ILE A  48      13.188  -6.320  32.270  1.00 45.25           C
ATOM    326  CG2 ILE A  48      10.553  -6.517  30.961  1.00 36.45           C
ATOM    327  C   ILE A  48       8.921  -4.150  30.463  1.00 22.99           C
ATOM    328  O   ILE A  48       7.977  -3.836  31.192  1.00 22.29           O
ATOM    329  N   ASN A  49       8.763  -4.602  29.220  1.00 20.28           N
ATOM    330  CA  ASN A  49       7.497  -5.151  28.772  1.00 20.64           C
ATOM    331  CB  ASN A  49       7.164  -4.734  27.334  1.00 22.71           C
ATOM    332  CG  ASN A  49       5.750  -5.127  26.923  1.00 25.76           C
ATOM    333  OD1 ASN A  49       5.144  -6.039  27.499  1.00 31.96           O
ATOM    334  ND2 ASN A  49       5.218  -4.444  25.914  1.00 24.31           N
ATOM    335  C   ASN A  49       7.585  -6.666  28.892  1.00 27.16           C
ATOM    336  O   ASN A  49       8.314  -7.317  28.128  1.00 21.43           O
ATOM    337  N   LYS A  50       6.838  -7.206  29.859  1.00 28.19           N
ATOM    338  CA  LYS A  50       6.845  -8.642  30.188  1.00 30.04           C
ATOM    339  CB  LYS A  50       6.071  -8.900  31.482  1.00 35.21           C
ATOM    340  CG  LYS A  50       6.735  -8.362  32.744  1.00 36.87           C
ATOM    341  CD  LYS A  50       6.021  -8.860  33.993  1.00 43.54           C
ATOM    342  CE  LYS A  50       4.699  -8.144  34.221  1.00 45.81           C
ATOM    343  NZ  LYS A  50       3.790  -8.909  35.119  1.00 59.03           N
ATOM    344  C   LYS A  50       6.316  -9.567  29.088  1.00 30.55           C
ATOM    345  O   LYS A  50       6.601 -10.772  29.103  1.00 23.34           O
ATOM    346  N   LYS A  51       5.550  -9.012  28.146  1.00 29.29           N
ATOM    347  CA  LYS A  51       5.104  -9.746  26.954  1.00 28.14           C
ATOM    348  CB  LYS A  51       4.158  -8.886  26.114  1.00 28.95           C
ATOM    349  CG  LYS A  51       3.270  -9.651  25.138  1.00 32.50           C
ATOM    350  CD  LYS A  51       2.296  -8.704  24.453  1.00 34.49           C
ATOM    351  CE  LYS A  51       1.582  -9.357  23.276  1.00 29.80           C
ATOM    352  NZ  LYS A  51       0.641  -8.404  22.613  1.00 26.32           N
ATOM    353  C   LYS A  51       6.295 -10.198  26.104  1.00 28.01           C
ATOM    354  O   LYS A  51       6.219 -11.222  25.419  1.00 33.12           O
ATOM    355  N   ASN A  52       7.381  -9.425  26.158  1.00 24.32           N
ATOM    356  CA  ASN A  52       8.613  -9.716  25.433  1.00 25.42           C
ATOM    357  CB  ASN A  52       8.755  -8.773  24.228  1.00 24.29           C
ATOM    358  CG  ASN A  52       7.653  -8.973  23.208  1.00 24.48           C
ATOM    359  OD1 ASN A  52       7.567 -10.030  22.583  1.00 29.22           O
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ATOM    360  ND2 ASN A  52       6.797  -7.967  23.043  1.00 21.64           N
ATOM    361  C   ASN A  52       9.807  -9.596  26.365  1.00 25.47           C
ATOM    362  O   ASN A  52      10.779  -8.901  26.056  1.00 24.17           O
ATOM    363  N   LEU A  53       9.723 -10.299  27.497  1.00 24.91           N
ATOM    364  CA  LEU A  53      10.647 -10.119  28.631  1.00 28.67           C
ATOM    365  CB  LEU A  53      10.345 -11.124  29.763  1.00 28.64           C
ATOM    366  CG  LEU A  53      10.943 -10.844  31.157  1.00 34.53           C
ATOM    367  CD1 LEU A  53       9.958 -11.212  32.259  1.00 47.99           C
ATOM    368  CD2 LEU A  53      12.275 -11.549  31.385  1.00 46.23           C
ATOM    369  C   LEU A  53      12.121 -10.160  28.256  1.00 27.96           C
ATOM    370  O   LEU A  53      12.841  -9.188  28.493  1.00 24.97           O
ATOM    371  N   ALA A  54      12.562 -11.280  27.682  1.00 34.18           N
ATOM    372  CA  ALA A  54      13.979 -11.492  27.376  1.00 33.95           C
ATOM    373  CB  ALA A  54      14.197 -12.853  26.721  1.00 32.31           C
ATOM    374  C   ALA A  54      14.543 -10.368  26.508  1.00 28.98           C
ATOM    375  O   ALA A  54      15.564  -9.753  26.859  1.00 25.26           O
ATOM    376  N   LYS A  55      13.855 -10.084  25.401  1.00 26.46           N
ATOM    377  CA  LYS A  55      14.288  -9.047  24.462  1.00 23.25           C
ATOM    378  CB  LYS A  55      13.484  -9.120  23.155  1.00 22.73           C
ATOM    379  CG  LYS A  55      13.994  -8.220  22.037  1.00 25.09           C
ATOM    380  CD  LYS A  55      15.368  -8.620  21.522  1.00 31.31           C
ATOM    381  CE  LYS A  55      15.746  -7.790  20.307  1.00 41.64           C
ATOM    382  NZ  LYS A  55      17.074  -8.178  19.757  1.00 52.37           N
ATOM    383  C   LYS A  55      14.238  -7.647  25.087  1.00 21.37           C
ATOM    384  O   LYS A  55      15.185  -6.876  24.938  1.00 20.76           O
ATOM    385  N   SER A  56      13.152  -7.357  25.804  1.00 22.87           N
ATOM    386  CA  SER A  56      12.968  -6.092  26.530  1.00 21.61           C
ATOM    387  CB  SER A  56      11.624  -6.105  27.270  1.00 21.29           C
ATOM    388  OG  SER A  56      11.454  -4.954  28.071  1.00 22.73           O
ATOM    389  C   SER A  56      14.132  -5.843  27.503  1.00 22.18           C
ATOM    390  O   SER A  56      14.733  -4.767  27.499  1.00 18.06           O
ATOM    391  N   GLN A  57      14.462  -6.863  28.299  1.00 22.28           N
ATOM    392  CA  GLN A  57      15.563  -6.795  29.259  1.00 24.32           C
ATOM    393  CB  GLN A  57      15.642  -8.093  30.077  1.00 26.92           C
ATOM    394  CG  GLN A  57      16.437  -7.983  31.371  1.00 47.37           C
ATOM    395  CD  GLN A  57      15.907  -8.879  32.485  1.00 54.92           C
ATOM    396  OE1 GLN A  57      15.088  -9.778  32.257  1.00 47.60           O
ATOM    397  NE2 GLN A  57      16.375  -8.631  33.706  1.00 51.99           N
ATOM    398  C   GLN A  57      16.885  -6.498  28.563  1.00 20.07           C
ATOM    399  O   GLN A  57      17.624  -5.618  29.012  1.00 20.46           O
ATOM    400  N   THR A  58      17.162  -7.221  27.470  1.00 21.62           N
ATOM    401  CA  THR A  58      18.365  -7.017  26.650  1.00 24.18           C
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ATOM    402  CB  THR A  58      18.458  -8.042  25.480  1.00 29.27           C
ATOM    403  OG1 THR A  58      18.272  -9.372  25.980  1.00 33.83           O
ATOM    404  CG2 THR A  58      19.816  -7.970  24.774  1.00 31.13           C
ATOM    405  C   THR A  58      18.417  -5.594  26.095  1.00 22.42           C
ATOM    406  O   THR A  58      19.459  -4.943  26.154  1.00 19.70           O
ATOM    407  N   LEU A  59      17.289  -5.112  25.571  1.00 19.71           N
ATOM    408  CA  LEU A  59      17.255  -3.790  24.943  1.00 19.18           C
ATOM    409  CB  LEU A  59      15.981  -3.616  24.106  1.00 16.27           C
ATOM    410  CG  LEU A  59      15.936  -4.441  22.804  1.00 19.15           C
ATOM    411  CD1 LEU A  59      14.536  -4.431  22.225  1.00 18.55           C
ATOM    412  CD2 LEU A  59      16.950  -3.968  21.765  1.00 18.44           C
ATOM    413  C   LEU A  59      17.423  -2.643  25.942  1.00 18.40           C
ATOM    414  O   LEU A  59      18.103  -1.661  25.653  1.00 20.62           O
ATOM    415  N   LEU A  60      16.812  -2.778  27.115  1.00 18.37           N
ATOM    416  CA  LEU A  60      16.906  -1.738  28.138  1.00 19.65           C
ATOM    417  CB  LEU A  60      15.825  -1.908  29.213  1.00 19.04           C
ATOM    418  CG  LEU A  60      14.378  -1.658  28.756  1.00 21.27           C
ATOM    419  CD1 LEU A  60      13.408  -2.094  29.834  1.00 20.71           C
ATOM    420  CD2 LEU A  60      14.119  -0.210  28.364  1.00 22.50           C
ATOM    421  C   LEU A  60      18.310  -1.672  28.731  1.00 21.30           C
ATOM    422  O   LEU A  60      18.823  -0.582  28.988  1.00 20.77           O
ATOM    423  N   GLY A  61      18.935  -2.839  28.897  1.00 23.78           N
ATOM    424  CA  GLY A  61      20.350  -2.925  29.281  1.00 23.49           C
ATOM    425  C   GLY A  61      21.254  -2.186  28.309  1.00 25.87           C
ATOM    426  O   GLY A  61      22.089  -1.380  28.727  1.00 23.77           O
ATOM    427  N   LYS A  62      21.065  -2.442  27.011  1.00 26.58           N
ATOM    428  CA  LYS A  62      21.835  -1.787  25.942  1.00 24.83           C
ATOM    429  CB  LYS A  62      21.493  -2.391  24.574  1.00 32.32           C
ATOM    430  CG  LYS A  62      22.064  -3.784  24.352  1.00 41.32           C
ATOM    431  CD  LYS A  62      21.548  -4.418  23.070  1.00 45.55           C
ATOM    432  CE  LYS A  62      22.219  -5.759  22.805  1.00 46.64           C
ATOM    433  NZ  LYS A  62      23.668  -5.618  22.478  1.00 46.07           N
ATOM    434  C   LYS A  62      21.626  -0.278  25.924  1.00 22.65           C
ATOM    435  O   LYS A  62      22.584   0.486  25.758  1.00 25.98           O
ATOM    436  N   GLU A  63      20.372   0.137  26.119  1.00 22.82           N
ATOM    437  CA  GLU A  63      20.002   1.552  26.185  1.00 21.36           C
ATOM    438  CB  GLU A  63      18.480   1.731  26.241  1.00 17.99           C
ATOM    439  CG  GLU A  63      18.042   3.189  26.166  1.00 18.63           C
ATOM    440  CD  GLU A  63      16.578   3.386  25.811  1.00 19.09           C
ATOM    441  OE1 GLU A  63      15.719   2.561  26.184  1.00 20.91           O
ATOM    442  OE2 GLU A  63      16.284   4.408  25.163  1.00 22.17           O
ATOM    443  C   GLU A  63      20.681   2.275  27.354  1.00 17.92           C
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ATOM    444  O   GLU A  63      21.158   3.397  27.179  1.00 20.28           O
ATOM    445  N   ILE A  64      20.728   1.636  28.527  1.00 21.14           N
ATOM    446  CA  ILE A  64      21.490   2.181  29.672  1.00 21.17           C
ATOM    447  CB  ILE A  64      21.456   1.251  30.919  1.00 20.74           C
ATOM    448  CG1 ILE A  64      20.055   1.259  31.540  1.00 19.55           C
ATOM    449  CD1 ILE A  64      19.770   0.136  32.517  1.00 21.24           C
ATOM    450  CG2 ILE A  64      22.482   1.689  31.968  1.00 22.66           C
ATOM    451  C   ILE A  64      22.920   2.504  29.221  1.00 22.38           C
ATOM    452  O   ILE A  64      23.363   3.647  29.346  1.00 24.45           O
ATOM    453  N   LYS A  65      23.602   1.510  28.650  1.00 22.23           N
ATOM    454  CA  LYS A  65      25.009   1.646  28.241  1.00 27.25           C
ATOM    455  CB  LYS A  65      25.563   0.301  27.755  1.00 28.98           C
ATOM    456  C   LYS A  65      25.254   2.735  27.190  1.00 30.45           C
ATOM    457  O   LYS A  65      26.265   3.429  27.252  1.00 28.21           O
ATOM    458  N   ILE A  66      24.325   2.886  26.242  1.00 30.66           N
ATOM    459  CA  ILE A  66      24.430   3.897  25.175  1.00 30.12           C
ATOM    460  CB  ILE A  66      23.461   3.585  23.988  1.00 33.04           C
ATOM    461  CG1 ILE A  66      23.922   2.340  23.204  1.00 32.45           C
ATOM    462  CD1 ILE A  66      25.121   2.535  22.288  1.00 38.12           C
ATOM    463  CG2 ILE A  66      23.281   4.782  23.050  1.00 32.47           C
ATOM    464  C   ILE A  66      24.214   5.313  25.724  1.00 29.94           C
ATOM    465  O   ILE A  66      25.020   6.210  25.468  1.00 33.86           O
ATOM    466  N   LEU A  67      23.133   5.498  26.482  1.00 28.18           N
ATOM    467  CA  LEU A  67      22.751   6.820  26.995  1.00 31.19           C
ATOM    468  CB  LEU A  67      21.311   6.819  27.515  1.00 24.77           C
ATOM    469  CG  LEU A  67      20.219   6.750  26.443  1.00 28.61           C
ATOM    470  CD1 LEU A  67      18.888   6.642  27.147  1.00 21.97           C
ATOM    471  CD2 LEU A  67      20.225   7.953  25.504  1.00 25.63           C
ATOM    472  C   LEU A  67      23.690   7.421  28.041  1.00 30.59           C
ATOM    473  O   LEU A  67      23.738   8.643  28.190  1.00 33.93           O
ATOM    474  N   LYS A  68      24.419   6.563  28.755  1.00 37.71           N
ATOM    475  CA  LYS A  68      25.485   6.994  29.672  1.00 44.59           C
ATOM    476  CB  LYS A  68      26.123   5.788  30.369  1.00 44.77           C
ATOM    477  CG  LYS A  68      25.302   5.245  31.529  1.00 49.96           C
ATOM    478  CD  LYS A  68      25.677   3.813  31.880  1.00 56.47           C
ATOM    479  CE  LYS A  68      26.601   3.739  33.085  1.00 63.32           C
ATOM    480  NZ  LYS A  68      26.588   2.375  33.684  1.00 58.96           N
ATOM    481  C   LYS A  68      26.549   7.817  28.945  1.00 47.34           C
ATOM    482  O   LYS A  68      27.125   8.741  29.525  1.00 52.86           O
ATOM    483  N   GLU A  69      26.776   7.482  27.672  1.00 49.23           N
ATOM    484  CA  GLU A  69      27.753   8.157  26.815  1.00 45.86           C
ATOM    485  CB  GLU A  69      28.411   7.147  25.868  1.00 57.57           C
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ATOM    486  C   GLU A  69      27.173   9.330  26.016  1.00 47.61           C
ATOM    487  O   GLU A  69      27.923  10.198  25.564  1.00 54.59           O
ATOM    488  N   LEU A  70      25.850   9.355  25.844  1.00 42.51           N
ATOM    489  CA  LEU A  70      25.183  10.408  25.068  1.00 40.47           C
ATOM    490  CB  LEU A  70      24.189   9.815  24.062  1.00 42.11           C
ATOM    491  CG  LEU A  70      24.680   8.984  22.876  1.00 40.90           C
ATOM    492  CD1 LEU A  70      23.468   8.355  22.216  1.00 38.75           C
ATOM    493  CD2 LEU A  70      25.480   9.800  21.870  1.00 35.73           C
ATOM    494  C   LEU A  70      24.472  11.434  25.935  1.00 40.34           C
ATOM    495  O   LEU A  70      23.549  11.097  26.677  1.00 51.75           O
ATOM    496  N   LYS A  71      24.914  12.686  25.833  1.00 32.14           N
ATOM    497  CA  LYS A  71      24.278  13.816  26.517  1.00 33.10           C
ATOM    498  CB  LYS A  71      25.091  14.259  27.744  1.00 38.14           C
ATOM    499  CG  LYS A  71      25.128  13.254  28.886  1.00 44.00           C
ATOM    500  CD  LYS A  71      26.141  13.662  29.942  1.00 53.12           C
ATOM    501  CE  LYS A  71      26.417  12.525  30.913  1.00 60.89           C
ATOM    502  NZ  LYS A  71      27.605  12.812  31.765  1.00 68.29           N
ATOM    503  C   LYS A  71      24.124  14.966  25.526  1.00 36.43           C
ATOM    504  O   LYS A  71      25.117  15.491  25.013  1.00 31.87           O
ATOM    505  N   HIS A  72      22.870  15.326  25.247  1.00 29.30           N
ATOM    506  CA  HIS A  72      22.524  16.376  24.281  1.00 24.93           C
ATOM    507  CB  HIS A  72      22.605  15.829  22.845  1.00 22.84           C
ATOM    508  CG  HIS A  72      22.632  16.892  21.788  1.00 23.62           C
ATOM    509  ND1 HIS A  72      21.485  17.454  21.266  1.00 23.37           N
ATOM    510  CE1 HIS A  72      21.811  18.360  20.363  1.00 26.12           C
ATOM    511  NE2 HIS A  72      23.130  18.406  20.277  1.00 25.31           N
ATOM    512  CD2 HIS A  72      23.667  17.494  21.154  1.00 26.40           C
ATOM    513  C   HIS A  72      21.123  16.890  24.576  1.00 23.94           C
ATOM    514  O   HIS A  72      20.259  16.125  25.018  1.00 24.61           O
ATOM    515  N   GLU A  73      20.888  18.177  24.318  1.00 22.06           N
ATOM    516  CA  GLU A  73      19.585  18.807  24.590  1.00 25.53           C
ATOM    517  CB  GLU A  73      19.647  20.332  24.394  1.00 29.58           C
ATOM    518  CG  GLU A  73      19.960  20.812  22.983  1.00 37.45           C
ATOM    519  CD  GLU A  73      19.594  22.271  22.755  1.00 58.96           C
ATOM    520  OE1 GLU A  73      18.396  22.616  22.855  1.00 56.66           O
ATOM    521  OE2 GLU A  73      20.501  23.077  22.460  1.00 59.36           O
ATOM    522  C   GLU A  73      18.421  18.199  23.782  1.00 24.58           C
ATOM    523  O   GLU A  73      17.256  18.336  24.170  1.00 22.76           O
ATOM    524  N   ASN A  74      18.762  17.535  22.678  1.00 23.61           N
ATOM    525  CA  ASN A  74      17.783  16.867  21.802  1.00 21.46           C
ATOM    526  CB  ASN A  74      17.890  17.410  20.366  1.00 20.38           C
ATOM    527  CG  ASN A  74      17.629  18.895  20.286  1.00 19.94           C
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ATOM 528 OD1 ASN A 74 18.518 19.672 19.938 1.00 22.24 O
ATOM 529 ND2 ASN A 74 16.405 19.301 20.601 1.00 21.07 N
ATOM 530 C ASN A 74 17.855 15.332 21.830 1.00 20.72 C
ATOM 531 O ASN A 74 17.323 14.650 20.930 1.00 20.10 O
ATOM 532 N ILE A 75 18.524 14.797 22.853 1.00 18.38 N
ATOM 533 CA ILE A 75 18.465 13.372 23.188 1.00 20.18 C
ATOM 534 CB ILE A 75 19.846 12.676 23.076 1.00 19.81 C
ATOM 535 CG1 ILE A 75 20.381 12.766 21.630 1.00 19.47 C
ATOM 536 CD1 ILE A 75 21.816 12.304 21.421 1.00 19.88 C
ATOM 537 CG2 ILE A 75 19.771 11.222 23.550 1.00 16.13 C
ATOM 538 C ILE A 75 17.906 13.277 24.607 1.00 23.43 C
ATOM 539 O ILE A 75 18.418 13.933 25.519 1.00 21.61 O
ATOM 540 N VAL A 76 16.853 12.474 24.791 1.00 20.24 N
ATOM 541 CA VAL A 76 16.266 12.262 26.125 1.00 22.88 C
ATOM 542 CB VAL A 76 15.132 11.196 26.107 1.00 23.55 C
ATOM 543 CG1 VAL A 76 15.649 9.819 25.704 1.00 28.24 C
ATOM 544 CG2 VAL A 76 14.413 11.132 27.450 1.00 22.72 C
ATOM 545 C VAL A 76 17.369 11.916 27.146 1.00 23.11 C
ATOM 546 O VAL A 76 18.159 10.991 26.928 1.00 23.30 O
ATOM 547 N ALA A 77 17.420 12.686 28.231 1.00 26.42 N
ATOM 548 CA ALA A 77 18.416 12.486 29.294 1.00 31.73 C
ATOM 549 CB ALA A 77 18.506 13.727 30.165 1.00 27.80 C
ATOM 550 C ALA A 77 18.110 11.257 30.156 1.00 27.15 C
ATOM 551 O ALA A 77 16.946 10.933 30.386 1.00 25.50 O
ATOM 552 N LEU A 78 19.164 10.585 30.620 1.00 27.35 N
ATOM 553 CA LEU A 78 19.048 9.506 31.600 1.00 22.72 C
ATOM 554 CB LEU A 78 19.839 8.262 31.151 1.00 21.95 C
ATOM 555 CG LEU A 78 19.866 7.016 32.054 1.00 22.95 C
ATOM 556 CD1 LEU A 78 18.537 6.270 32.069 1.00 21.20 C
ATOM 557 CD2 LEU A 78 20.997 6.082 31.647 1.00 23.45 C
ATOM 558 C LEU A 78 19.516 10.016 32.969 1.00 25.32 C
ATOM 559 O LEU A 78 20.669 10.446 33.124 1.00 24.16 O
ATOM 560 N TYR A 79 18.611 9.967 33.947 1.00 22.53 N
ATOM 561 CA TYR A 79 18.877 10.476 35.289 1.00 26.79 C
ATOM 562 CB TYR A 79 17.611 11.093 35.894 1.00 28.34 C
ATOM 563 CG TYR A 79 17.035 12.297 35.168 1.00 27.13 C
ATOM 564 CD1 TYR A 79 17.854 13.190 34.457 1.00 33.35 C
ATOM 565 CE1 TYR A 79 17.314 14.297 33.808 1.00 28.07 C
ATOM 566 CZ TYR A 79 15.947 14.536 33.885 1.00 28.15 C
ATOM 567 OH TYR A 79 15.417 15.638 33.250 1.00 35.82 O
ATOM 568 CE2 TYR A 79 15.118 13.680 34.596 1.00 26.24 C
ATOM 569 CD2 TYR A 79 15.664 12.571 35.232 1.00 29.53 C

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ATOM    570  C   TYR A  79      19.410   9.396  36.233  1.00 33.16           C
ATOM    571  O   TYR A  79      20.306   9.657  37.048  1.00 30.61           O
ATOM    572  N   ASP A  80      18.831   8.199  36.125  1.00 27.77           N
ATOM    573  CA  ASP A  80      19.117   7.059  37.004  1.00 27.17           C
ATOM    574  CB  ASP A  80      18.420   7.250  38.364  1.00 28.62           C
ATOM    575  CG  ASP A  80      18.962   6.323  39.459  1.00 31.81           C
ATOM    576  OD1 ASP A  80      20.046   5.725  39.291  1.00 28.21           O
ATOM    577  OD2 ASP A  80      18.284   6.195  40.498  1.00 31.84           O
ATOM    578  C   ASP A  80      18.635   5.767  36.341  1.00 30.36           C
ATOM    579  O   ASP A  80      17.860   5.803  35.378  1.00 23.83           O
ATOM    580  N   PHE A  81      19.096   4.633  36.860  1.00 25.99           N
ATOM    581  CA  PHE A  81      18.731   3.307  36.353  1.00 29.17           C
ATOM    582  CB  PHE A  81      19.525   2.956  35.081  1.00 31.46           C
ATOM    583  CG  PHE A  81      21.017   3.080  35.230  1.00 35.54           C
ATOM    584  CD1 PHE A  81      21.789   1.978  35.612  1.00 40.74           C
ATOM    585  CE1 PHE A  81      23.170   2.090  35.741  1.00 43.98           C
ATOM    586  CZ  PHE A  81      23.794   3.307  35.481  1.00 52.70           C
ATOM    587  CE2 PHE A  81      23.041   4.409  35.093  1.00 49.61           C
ATOM    588  CD2 PHE A  81      21.661   4.292  34.964  1.00 40.90           C
ATOM    589  C   PHE A  81      18.941   2.233  37.415  1.00 32.69           C
ATOM    590  O   PHE A  81      19.810   2.385  38.279  1.00 29.79           O
ATOM    591  N   GLN A  82      18.145   1.164  37.330  1.00 29.25           N
ATOM    592  CA  GLN A  82      18.264  -0.024  38.187  1.00 31.50           C
ATOM    593  CB  GLN A  82      17.200   0.012  39.300  1.00 34.69           C
ATOM    594  CG  GLN A  82      17.253  -1.150  40.288  1.00 39.75           C
ATOM    595  CD  GLN A  82      15.904  -1.457  40.912  1.00 46.93           C
ATOM    596  OE1 GLN A  82      15.267  -2.457  40.574  1.00 62.21           O
ATOM    597  NE2 GLN A  82      15.458  -0.597  41.826  1.00 39.98           N
ATOM    598  C   GLN A  82      18.114  -1.308  37.351  1.00 39.33           C
ATOM    599  O   GLN A  82      17.119  -1.475  36.631  1.00 30.09           O
ATOM    600  N   GLU A  83      19.097  -2.205  37.464  1.00 43.74           N
ATOM    601  CA  GLU A  83      19.089  -3.500  36.766  1.00 45.19           C
ATOM    602  CB  GLU A  83      20.315  -3.639  35.855  1.00 44.70           C
ATOM    603  CG  GLU A  83      20.187  -2.882  34.547  1.00 47.44           C
ATOM    604  CD  GLU A  83      21.245  -3.249  33.522  1.00 47.20           C
ATOM    605  OE1 GLU A  83      22.334  -2.639  33.536  1.00 44.75           O
ATOM    606  OE2 GLU A  83      20.973  -4.130  32.679  1.00 48.18           O
ATOM    607  C   GLU A  83      18.982  -4.693  37.723  1.00 47.96           C
ATOM    608  O   GLU A  83      19.954  -5.063  38.385  1.00 69.32           O
ATOM    609  N   MET A  84      17.786  -5.275  37.787  1.00 58.17           N
ATOM    610  CA  MET A  84      17.503  -6.449  38.617  1.00 64.24           C
ATOM    611  CB  MET A  84      16.209  -6.235  39.413  1.00 61.72           C
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ATOM    612  C   MET A  84      17.421  -7.723  37.764  1.00 65.70           C
ATOM    613  O   MET A  84      17.613  -7.671  36.543  1.00 60.35           O
ATOM    614  N   ALA A  85      17.133  -8.853  38.414  1.00 64.70           N
ATOM    615  CA  ALA A  85      17.132 -10.177  37.780  1.00 59.51           C
ATOM    616  CB  ALA A  85      16.986 -11.265  38.832  1.00 50.56           C
ATOM    617  C   ALA A  85      16.067 -10.340  36.698  1.00 61.23           C
ATOM    618  O   ALA A  85      16.364 -10.822  35.602  1.00 68.36           O
ATOM    619  N   ASN A  86      14.838  -9.940  37.015  1.00 55.60           N
ATOM    620  CA  ASN A  86      13.710 -10.073  36.096  1.00 58.52           C
ATOM    621  CB  ASN A  86      12.578 -10.869  36.753  1.00 63.61           C
ATOM    622  C   ASN A  86      13.192  -8.737  35.558  1.00 57.29           C
ATOM    623  O   ASN A  86      12.400  -8.718  34.611  1.00 64.16           O
HETATM  624  N   SEP A  87      13.647  -7.634  36.156  1.00 52.41           N
HETATM  625  CA  SEP A  87      13.211  -6.282  35.772  1.00 54.79           C
HETATM  626  CB  SEP A  87      12.181  -5.770  36.773  1.00 61.23           C
HETATM  627  OG  SEP A  87      12.826  -5.399  37.987  1.00 75.80           O
HETATM  628  P   SEP A  87      12.323  -5.959  39.408  1.00 82.94           P
HETATM  629  O1P SEP A  87      12.684  -7.425  39.366  1.00 91.67           O
HETATM  630  O2P SEP A  87      13.136  -5.139  40.386  1.00 63.80           O
HETATM  631  O3P SEP A  87      10.833  -5.694  39.436  1.00 69.98           O
HETATM  632  C   SEP A  87      14.364  -5.316  35.616  1.00 47.32           C
HETATM  633  O   SEP A  87      15.439  -5.519  36.185  1.00 44.45           O
ATOM    634  N   VAL A  88      14.139  -4.269  34.817  1.00 29.97           N
ATOM    635  CA  VAL A  88      15.111  -3.197  34.559  1.00 25.53           C
ATOM    636  CB  VAL A  88      15.904  -3.419  33.234  1.00 31.18           C
ATOM    637  CG1 VAL A  88      16.873  -2.274  32.958  1.00 25.62           C
ATOM    638  CG2 VAL A  88      16.685  -4.729  33.243  1.00 41.02           C
ATOM    639  C   VAL A  88      14.327  -1.878  34.493  1.00 25.86           C
ATOM    640  O   VAL A  88      13.230  -1.840  33.933  1.00 26.63           O
ATOM    641  N   TYR A  89      14.892  -0.808  35.055  1.00 26.13           N
ATOM    642  CA  TYR A  89      14.230   0.506  35.082  1.00 24.07           C
ATOM    643  CB  TYR A  89      13.692   0.828  36.483  1.00 25.31           C
ATOM    644  CG  TYR A  89      12.694  -0.172  37.010  1.00 28.95           C
ATOM    645  CD1 TYR A  89      13.117  -1.267  37.775  1.00 29.59           C
ATOM    646  CE1 TYR A  89      12.208  -2.193  38.259  1.00 34.10           C
ATOM    647  CZ  TYR A  89      10.858  -2.040  37.976  1.00 37.78           C
ATOM    648  OH  TYR A  89       9.969  -2.968  38.460  1.00 38.33           O
ATOM    649  CE2 TYR A  89      10.407  -0.965  37.216  1.00 32.15           C
ATOM    650  CD2 TYR A  89      11.327  -0.036  36.740  1.00 29.22           C
ATOM    651  C   TYR A  89      15.163   1.618  34.644  1.00 24.78           C
ATOM    652  O   TYR A  89      16.314   1.670  35.077  1.00 23.35           O
ATOM    653  N   LEU A  90      14.660   2.506  33.781  1.00 20.26           N
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ATOM    654  CA  LEU A  90      15.388   3.704  33.382  1.00 19.81           C
ATOM    655  CB  LEU A  90      15.638   3.740  31.861  1.00 23.23           C
ATOM    656  CG  LEU A  90      16.737   2.851  31.256  1.00 22.12           C
ATOM    657  CD1 LEU A  90      16.351   1.380  31.230  1.00 25.05           C
ATOM    658  CD2 LEU A  90      17.099   3.314  29.847  1.00 24.75           C
ATOM    659  C   LEU A  90      14.583   4.918  33.811  1.00 23.49           C
ATOM    660  O   LEU A  90      13.401   5.037  33.466  1.00 21.62           O
ATOM    661  N   VAL A  91      15.220   5.800  34.584  1.00 21.37           N
ATOM    662  CA  VAL A  91      14.587   7.053  35.009  1.00 19.47           C
ATOM    663  CB  VAL A  91      14.855   7.397  36.497  1.00 18.22           C
ATOM    664  CG1 VAL A  91      14.141   8.695  36.871  1.00 16.29           C
ATOM    665  CG2 VAL A  91      14.388   6.250  37.392  1.00 17.47           C
ATOM    666  C   VAL A  91      15.082   8.158  34.095  1.00 18.40           C
ATOM    667  O   VAL A  91      16.276   8.464  34.056  1.00 23.05           O
ATOM    668  N   MET A  92      14.143   8.737  33.349  1.00 18.85           N
ATOM    669  CA  MET A  92      14.483   9.632  32.246  1.00 20.29           C
ATOM    670  CB  MET A  92      14.198   8.942  30.894  1.00 22.37           C
ATOM    671  CG  MET A  92      14.402   7.433  30.884  1.00 33.35           C
ATOM    672  SD  MET A  92      14.342   6.689  29.252  1.00 31.47           S
ATOM    673  CE  MET A  92      15.787   7.443  28.537  1.00 24.77           C
ATOM    674  C   MET A  92      13.739  10.954  32.299  1.00 17.34           C
ATOM    675  O   MET A  92      12.703  11.105  32.964  1.00 19.77           O
ATOM    676  N   GLU A  93      14.292  11.904  31.557  1.00 17.63           N
ATOM    677  CA  GLU A  93      13.674  13.177  31.259  1.00 21.25           C
ATOM    678  CB  GLU A  93      14.506  13.854  30.171  1.00 21.84           C
ATOM    679  CG  GLU A  93      13.940  15.150  29.616  1.00 23.26           C
ATOM    680  CD  GLU A  93      14.897  15.838  28.669  1.00 24.67           C
ATOM    681  OE1 GLU A  93      14.768  17.064  28.510  1.00 31.87           O
ATOM    682  OE2 GLU A  93      15.782  15.162  28.098  1.00 22.67           O
ATOM    683  C   GLU A  93      12.237  12.948  30.804  1.00 19.03           C
ATOM    684  O   GLU A  93      11.985  12.085  29.945  1.00 20.45           O
ATOM    685  N   TYR A  94      11.310  13.680  31.425  1.00 18.70           N
ATOM    686  CA  TYR A  94       9.901  13.675  31.030  1.00 20.67           C
ATOM    687  CB  TYR A  94       8.985  14.027  32.211  1.00 18.57           C
ATOM    688  CG  TYR A  94       7.502  14.170  31.875  1.00 18.17           C
ATOM    689  CD1 TYR A  94       6.782  13.121  31.282  1.00 19.94           C
ATOM    690  CE1 TYR A  94       5.434  13.255  30.977  1.00 21.59           C
ATOM    691  CZ  TYR A  94       4.776  14.449  31.279  1.00 20.70           C
ATOM    692  OH  TYR A  94       3.440  14.583  30.985  1.00 24.11           O
ATOM    693  CE2 TYR A  94       5.460  15.494  31.875  1.00 20.35           C
ATOM    694  CD2 TYR A  94       6.815  15.356  32.164  1.00 20.77           C
ATOM    695  C   TYR A  94       9.694  14.651  29.871  1.00 21.16           C
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ATOM    696  O   TYR A  94      10.127  15.803  29.931  1.00 19.98           O
ATOM    697  N   CYS A  95       9.063  14.151  28.808  1.00 20.88           N
ATOM    698  CA  CYS A  95       8.698  14.957  27.645  1.00 18.53           C
ATOM    699  CB  CYS A  95       9.251  14.314  26.359  1.00 18.47           C
ATOM    700  SG  CYS A  95      11.062  14.161  26.314  1.00 19.88           S
ATOM    701  C   CYS A  95       7.176  15.045  27.653  1.00 18.00           C
ATOM    702  O   CYS A  95       6.478  14.038  27.483  1.00 20.26           O
ATOM    703  N   ASN A  96       6.666  16.250  27.898  1.00 17.68           N
ATOM    704  CA  ASN A  96       5.235  16.454  28.193  1.00 17.12           C
ATOM    705  CB  ASN A  96       5.060  17.664  29.134  1.00 21.05           C
ATOM    706  CG  ASN A  96       5.560  18.969  28.527  1.00 26.75           C
ATOM    707  OD1 ASN A  96       5.709  19.100  27.315  1.00 28.08           O
ATOM    708  ND2 ASN A  96       5.825  19.945  29.380  1.00 30.98           N
ATOM    709  C   ASN A  96       4.318  16.630  26.976  1.00 17.95           C
ATOM    710  O   ASN A  96       3.114  16.854  27.132  1.00 20.31           O
ATOM    711  N   GLY A  97       4.888  16.555  25.776  1.00 19.65           N
ATOM    712  CA  GLY A  97       4.113  16.799  24.563  1.00 17.85           C
ATOM    713  C   GLY A  97       3.835  15.590  23.687  1.00 19.44           C
ATOM    714  O   GLY A  97       3.464  15.757  22.526  1.00 18.84           O
ATOM    715  N   GLY A  98       3.995  14.384  24.233  1.00 18.48           N
ATOM    716  CA  GLY A  98       3.720  13.156  23.484  1.00 16.70           C
ATOM    717  C   GLY A  98       4.814  12.907  22.464  1.00 15.26           C
ATOM    718  O   GLY A  98       5.955  13.337  22.639  1.00 16.87           O
ATOM    719  N   ASP A  99       4.478  12.216  21.383  1.00 13.87           N
ATOM    720  CA  ASP A  99       5.500  11.927  20.367  1.00 14.61           C
ATOM    721  CB  ASP A  99       5.825  10.431  20.316  1.00 15.67           C
ATOM    722  CG  ASP A  99       4.587   9.569  20.079  1.00 20.64           C
ATOM    723  OD1 ASP A  99       3.827   9.813  19.127  1.00 17.34           O
ATOM    724  OD2 ASP A  99       4.349   8.655  20.871  1.00 29.92           O
ATOM    725  C   ASP A  99       5.066  12.453  19.004  1.00 12.48           C
ATOM    726  O   ASP A  99       3.954  12.941  18.850  1.00 12.27           O
ATOM    727  N   LEU A 100       5.947  12.346  18.017  1.00 13.19           N
ATOM    728  CA  LEU A 100       5.615  12.808  16.661  1.00 11.89           C
ATOM    729  CB  LEU A 100       6.861  12.784  15.762  1.00 11.16           C
ATOM    730  CG  LEU A 100       6.777  13.393  14.354  1.00 11.14           C
ATOM    731  CD1 LEU A 100       6.312  14.848  14.407  1.00  9.63           C
ATOM    732  CD2 LEU A 100       8.140  13.304  13.671  1.00 11.20           C
ATOM    733  C   LEU A 100       4.449  12.041  16.016  1.00 10.72           C
ATOM    734  O   LEU A 100       3.668  12.631  15.252  1.00 12.40           O
ATOM    735  N   ALA A 101       4.312  10.751  16.331  1.00 10.97           N
ATOM    736  CA  ALA A 101       3.180   9.958  15.839  1.00 11.66           C
ATOM    737  CB  ALA A 101       3.300   8.497  16.273  1.00 14.73           C
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ATOM    738  C   ALA A 101      1.838  10.556  16.278  1.00 13.50           C
ATOM    739  O   ALA A 101      0.921  10.710  15.445  1.00 12.67           O
ATOM    740  N   ASP A 102      1.728  10.916  17.563  1.00 10.76           N
ATOM    741  CA  ASP A 102      0.501  11.572  18.078  1.00 13.58           C
ATOM    742  CB  ASP A 102      0.601  11.943  19.567  1.00 15.71           C
ATOM    743  CG  ASP A 102      0.931  10.782  20.463  1.00 20.62           C
ATOM    744  OD1 ASP A 102      0.304   9.710  20.327  1.00 20.38           O
ATOM    745  OD2 ASP A 102      1.813  10.982  21.342  1.00 22.02           O
ATOM    746  C   ASP A 102      0.271  12.892  17.364  1.00 11.65           C
ATOM    747  O   ASP A 102     -0.861  13.246  17.035  1.00 11.58           O
ATOM    748  N   TYR A 103      1.347  13.655  17.200  1.00 11.44           N
ATOM    749  CA  TYR A 103      1.267  14.998  16.648  1.00 11.71           C
ATOM    750  CB  TYR A 103      2.623  15.694  16.777  1.00 12.72           C
ATOM    751  CG  TYR A 103      2.587  17.197  16.607  1.00 15.23           C
ATOM    752  CD1 TYR A 103      1.822  18.005  17.466  1.00 19.84           C
ATOM    753  CE1 TYR A 103      1.792  19.388  17.307  1.00 20.49           C
ATOM    754  CZ  TYR A 103      2.541  19.977  16.299  1.00 19.69           C
ATOM    755  OH  TYR A 103      2.525  21.351  16.149  1.00 26.71           O
ATOM    756  CE2 TYR A 103      3.311  19.200  15.442  1.00 16.61           C
ATOM    757  CD2 TYR A 103      3.329  17.815  15.600  1.00 13.74           C
ATOM    758  C   TYR A 103      0.795  14.951  15.196  1.00 11.54           C
ATOM    759  O   TYR A 103     -0.078  15.721  14.798  1.00 10.82           O
ATOM    760  N   LEU A 104      1.359  14.034  14.409  1.00 10.99           N
ATOM    761  CA  LEU A 104      0.945  13.888  13.012  1.00  9.49           C
ATOM    762  CB  LEU A 104      1.920  12.982  12.247  1.00 11.31           C
ATOM    763  CG  LEU A 104      3.323  13.547  12.060  1.00 13.09           C
ATOM    764  CD1 LEU A 104      4.194  12.549  11.303  1.00 13.17           C
ATOM    765  CD2 LEU A 104      3.292  14.880  11.325  1.00 16.05           C
ATOM    766  C   LEU A 104     -0.472  13.367  12.879  1.00 10.94           C
ATOM    767  O   LEU A 104     -1.214  13.804  11.989  1.00 12.50           O
ATOM    768  N   HIS A 105     -0.864  12.439  13.746  1.00 10.20           N
ATOM    769  CA  HIS A 105     -2.267  12.000  13.737  1.00 11.92           C
ATOM    770  CB  HIS A 105     -2.537  10.886  14.752  1.00 11.14           C
ATOM    771  CG  HIS A 105     -3.938  10.356  14.694  1.00 12.06           C
ATOM    772  ND1 HIS A 105     -4.944  10.822  15.515  1.00 14.87           N
ATOM    773  CE1 HIS A 105     -6.072  10.195  15.224  1.00 11.83           C
ATOM    774  NE2 HIS A 105     -5.830   9.338  14.246  1.00 15.34           N
ATOM    775  CD2 HIS A 105     -4.508   9.431  13.887  1.00 14.72           C
ATOM    776  C   HIS A 105     -3.218  13.180  13.958  1.00 14.32           C
ATOM    777  O   HIS A 105     -4.254  13.279  13.284  1.00 13.91           O
ATOM    778  N   ALA A 106     -2.844  14.076  14.874  1.00 12.14           N
ATOM    779  CA  ALA A 106     -3.683  15.228  15.243  1.00 13.15           C
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ATOM    780  CB  ALA A 106      -3.235  15.794  16.583  1.00 14.41           C
ATOM    781  C   ALA A 106      -3.697  16.322  14.176  1.00 14.90           C
ATOM    782  O   ALA A 106      -4.758  16.874  13.877  1.00 14.26           O
ATOM    783  N   MET A 107      -2.524  16.619  13.608  1.00 11.82           N
ATOM    784  CA  MET A 107      -2.343  17.748  12.679  1.00 10.94           C
ATOM    785  CB  MET A 107      -0.942  18.364  12.829  1.00 14.04           C
ATOM    786  CG  MET A 107      -0.534  18.864  14.208  1.00 18.66           C
ATOM    787  SD  MET A 107      -1.540  20.275  14.697  1.00 26.22           S
ATOM    788  CE  MET A 107      -2.775  19.483  15.713  1.00 30.14           C
ATOM    789  C   MET A 107      -2.533  17.387  11.201  1.00 10.13           C
ATOM    790  O   MET A 107      -2.760  18.281  10.370  1.00 10.92           O
ATOM    791  N   ARG A 108      -2.379  16.094  10.896  1.00 10.50           N
ATOM    792  CA  ARG A 108      -2.411  15.472   9.556  1.00 10.95           C
ATOM    793  CB  ARG A 108      -3.690  15.789   8.743  1.00 13.57           C
ATOM    794  CG  ARG A 108      -5.004  15.735   9.523  1.00 18.82           C
ATOM    795  CD  ARG A 108      -5.246  14.416  10.248  1.00 21.74           C
ATOM    796  NE  ARG A 108      -5.477  13.297   9.333  1.00 23.29           N
ATOM    797  CZ  ARG A 108      -5.493  12.012   9.698  1.00 33.37           C
ATOM    798  NH1 ARG A 108      -5.288  11.657  10.969  1.00 24.83           N
ATOM    799  NH2 ARG A 108      -5.714  11.072   8.788  1.00 29.40           N
ATOM    800  C   ARG A 108      -1.157  15.740   8.735  1.00 10.09           C
ATOM    801  O   ARG A 108      -0.512  14.798   8.271  1.00 11.46           O
ATOM    802  N   THR A 109      -0.823  17.018   8.561  1.00  9.12           N
ATOM    803  CA  THR A 109       0.423  17.430   7.901  1.00 10.24           C
ATOM    804  CB  THR A 109       0.236  17.817   6.412  1.00  9.43           C
ATOM    805  OG1 THR A 109      -0.817  18.791   6.294  1.00 12.35           O
ATOM    806  CG2 THR A 109      -0.056  16.611   5.551  1.00  9.55           C
ATOM    807  C   THR A 109       0.987  18.628   8.649  1.00 11.23           C
ATOM    808  O   THR A 109       0.252  19.335   9.357  1.00 11.58           O
ATOM    809  N   LEU A 110       2.288  18.844   8.491  1.00  9.54           N
ATOM    810  CA  LEU A 110       2.977  19.981   9.109  1.00 11.07           C
ATOM    811  CB  LEU A 110       4.191  19.503   9.924  1.00 10.90           C
ATOM    812  CG  LEU A 110       3.966  18.392  10.941  1.00 13.00           C
ATOM    813  CD1 LEU A 110       5.226  18.162  11.755  1.00 12.45           C
ATOM    814  CD2 LEU A 110       2.798  18.699  11.873  1.00 16.16           C
ATOM    815  C   LEU A 110       3.449  20.968   8.067  1.00 10.45           C
ATOM    816  O   LEU A 110       3.790  20.564   6.946  1.00 10.19           O
ATOM    817  N   SER A 111       3.498  22.256   8.441  1.00  9.78           N
ATOM    818  CA  SER A 111       4.061  23.291   7.554  1.00  9.76           C
ATOM    819  CB  SER A 111       3.863  24.697   8.115  1.00 11.51           C
ATOM    820  OG  SER A 111       4.643  24.886   9.292  1.00 11.38           O
ATOM    821  C   SER A 111       5.551  23.027   7.359  1.00  9.62           C
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ATOM 822 O SER A 111 6.181 22.409 8.220 1.00 10.12 O
ATOM 823 N GLU A 112 6.101 23.497 6.242 1.00 10.30 N
ATOM 824 CA GLU A 112 7.559 23.360 6.016 1.00 10.42 C
ATOM 825 CB GLU A 112 7.973 23.901 4.647 1.00 11.27 C
ATOM 826 CG GLU A 112 7.359 23.154 3.473 1.00 10.23 C
ATOM 827 CD GLU A 112 8.127 23.343 2.175 1.00 12.17 C
ATOM 828 OE1 GLU A 112 9.261 23.861 2.204 1.00 13.65 O
ATOM 829 OE2 GLU A 112 7.596 22.961 1.120 1.00 11.07 O
ATOM 830 C GLU A 112 8.357 24.049 7.121 1.00 10.77 C
ATOM 831 O GLU A 112 9.398 23.554 7.508 1.00 10.26 O
ATOM 832 N ASP A 113 7.852 25.167 7.652 1.00 11.96 N
ATOM 833 CA ASP A 113 8.519 25.850 8.778 1.00 12.73 C
ATOM 834 CB ASP A 113 7.841 27.198 9.075 1.00 13.42 C
ATOM 835 CG ASP A 113 8.564 28.001 10.153 1.00 20.33 C
ATOM 836 OD1 ASP A 113 9.669 28.519 9.873 1.00 27.78 O
ATOM 837 OD2 ASP A 113 8.025 28.120 11.282 1.00 25.05 O
ATOM 838 C ASP A 113 8.594 24.982 10.045 1.00 11.73 C
ATOM 839 O ASP A 113 9.643 24.920 10.689 1.00 10.60 O
ATOM 840 N THR A 114 7.489 24.321 10.404 1.00 9.97 N
ATOM 841 CA THR A 114 7.479 23.371 11.534 1.00 10.51 C
ATOM 842 CB THR A 114 6.053 22.853 11.836 1.00 11.60 C
ATOM 843 OG1 THR A 114 5.256 23.939 12.329 1.00 14.71 O
ATOM 844 CG2 THR A 114 6.051 21.743 12.873 1.00 12.85 C
ATOM 845 C THR A 114 8.450 22.216 11.266 1.00 11.28 C
ATOM 846 O THR A 114 9.205 21.815 12.159 1.00 9.81 O
ATOM 847 N ILE A 115 8.439 21.701 10.031 1.00 8.82 N
ATOM 848 CA ILE A 115 9.347 20.601 9.665 1.00 9.26 C
ATOM 849 CB ILE A 115 9.090 20.076 8.231 1.00 9.36 C
ATOM 850 CG1 ILE A 115 7.680 19.457 8.147 1.00 11.37 C
ATOM 851 CD1 ILE A 115 7.230 19.078 6.743 1.00 9.96 C
ATOM 852 CG2 ILE A 115 10.171 19.075 7.802 1.00 10.09 C
ATOM 853 C ILE A 115 10.803 21.038 9.864 1.00 10.07 C
ATOM 854 O ILE A 115 11.596 20.282 10.444 1.00 11.75 O
ATOM 855 N ARG A 116 11.123 22.256 9.407 1.00 10.07 N
ATOM 856 CA AARG A 116 12.474 22.818 9.565 0.50 11.89 C
ATOM 857 CA BARG A 116 12.465 22.830 9.559 0.50 12.72 C
ATOM 858 CB AARG A 116 12.580 24.192 8.898 0.50 12.23 C
ATOM 859 CB BARG A 116 12.515 24.214 8.905 0.50 14.47 C
ATOM 860 CG AARG A 116 13.910 24.913 9.111 0.50 14.35 C
ATOM 861 CG BARG A 116 13.872 24.900 8.944 0.50 19.64 C
ATOM 862 CD AARG A 116 13.901 26.189 8.301 0.50 18.72 C
ATOM 863 CD BARG A 116 13.735 26.339 8.481 0.50 26.81 C

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ATOM    864  NE AARG A 116      13.037  26.020   7.144  0.50 20.46           N
ATOM    865  NE BARG A 116      12.665  26.511   7.501  0.50 32.43           N
ATOM    866  CZ AARG A 116      11.854  26.613   7.009  0.50 17.53           C
ATOM    867  CZ BARG A 116      12.813  26.378   6.185  0.50 29.41           C
ATOM    868  NH1AARG A 116      11.425  27.453   7.940  0.50 13.63           N
ATOM    869  NH1BARG A 116      13.992  26.067   5.667  0.50 20.17           N
ATOM    870  NH2AARG A 116      11.119  26.375   5.938  0.50 16.47           N
ATOM    871  NH2BARG A 116      11.773  26.550   5.385  0.50 30.55           N
ATOM    872  C   ARG A 116      12.870  22.904  11.036  1.00 12.30           C
ATOM    873  O   ARG A 116      13.977  22.521  11.394  1.00 14.39           O
ATOM    874  N   LEU A 117      11.953  23.401  11.871  1.00 12.06           N
ATOM    875  CA  LEU A 117      12.185  23.542  13.315  1.00 12.71           C
ATOM    876  CB  LEU A 117      10.990  24.227  14.007  1.00 16.67           C
ATOM    877  CG  LEU A 117      10.915  25.759  13.874  1.00 25.02           C
ATOM    878  CD1 LEU A 117       9.504  26.303  14.064  1.00 25.22           C
ATOM    879  CD2 LEU A 117      11.873  26.426  14.862  1.00 30.48           C
ATOM    880  C   LEU A 117      12.524  22.206  13.971  1.00 14.23           C
ATOM    881  O   LEU A 117      13.496  22.114  14.717  1.00 15.36           O
ATOM    882  N   PHE A 118      11.756  21.165  13.645  1.00 12.90           N
ATOM    883  CA  PHE A 118      11.965  19.833  14.233  1.00 13.17           C
ATOM    884  CB  PHE A 118      10.766  18.919  13.912  1.00 11.95           C
ATOM    885  CG  PHE A 118       9.495  19.232  14.678  1.00 13.39           C
ATOM    886  CD1 PHE A 118       9.395  20.317  15.559  1.00 14.24           C
ATOM    887  CE1 PHE A 118       8.206  20.576  16.248  1.00 14.19           C
ATOM    888  CZ  PHE A 118       7.100  19.758  16.059  1.00 12.92           C
ATOM    889  CE2 PHE A 118       7.172  18.680  15.174  1.00 14.20           C
ATOM    890  CD2 PHE A 118       8.364  18.417  14.494  1.00 13.22           C
ATOM    891  C   PHE A 118      13.242  19.201  13.680  1.00 13.69           C
ATOM    892  O   PHE A 118      13.997  18.544  14.406  1.00 13.92           O
ATOM    893  N   LEU A 119      13.474  19.399  12.386  1.00 11.82           N
ATOM    894  CA  LEU A 119      14.587  18.756  11.703  1.00 11.53           C
ATOM    895  CB  LEU A 119      14.388  18.795  10.183  1.00 11.56           C
ATOM    896  CG  LEU A 119      15.361  18.013   9.298  1.00 12.48           C
ATOM    897  CD1 LEU A 119      15.377  16.541   9.696  1.00 10.09           C
ATOM    898  CD2 LEU A 119      14.952  18.181   7.833  1.00 11.29           C
ATOM    899  C   LEU A 119      15.936  19.352  12.117  1.00 11.66           C
ATOM    900  O   LEU A 119      16.928  18.617  12.231  1.00 13.29           O
ATOM    901  N   GLN A 120      15.971  20.664  12.366  1.00 12.88           N
ATOM    902  CA  GLN A 120      17.191  21.306  12.929  1.00 14.29           C
ATOM    903  CB  GLN A 120      16.957  22.795  13.217  1.00 19.42           C
ATOM    904  CG  GLN A 120      16.831  23.675  11.982  1.00 24.38           C
ATOM    905  CD  GLN A 120      16.472  25.127  12.300  1.00 29.68           C
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ATOM 906 OE1 GLN A 120 15.654 25.410 13.180 1.00 30.92 O
ATOM 907 NE2 GLN A 120 17.073 26.052 11.565 1.00 32.91 N
ATOM 908 C GLN A 120 17.610 20.626 14.232 1.00 14.31 C
ATOM 909 O GLN A 120 18.801 20.343 14.452 1.00 14.20 O
ATOM 910 N GLN A 121 16.616 20.360 15.081 1.00 15.40 N
ATOM 911 CA GLN A 121 16.830 19.729 16.385 1.00 16.35 C
ATOM 912 CB GLN A 121 15.569 19.847 17.248 1.00 18.55 C
ATOM 913 CG GLN A 121 15.198 21.281 17.615 1.00 18.52 C
ATOM 914 CD GLN A 121 13.973 21.356 18.498 1.00 18.73 C
ATOM 915 OE1 GLN A 121 14.008 20.951 19.652 1.00 25.77 O
ATOM 916 NE2 GLN A 121 12.876 21.872 17.952 1.00 19.74 N
ATOM 917 C GLN A 121 17.291 18.277 16.232 1.00 18.17 C
ATOM 918 O GLN A 121 18.292 17.866 16.845 1.00 19.63 O
ATOM 919 N ILE A 122 16.581 17.504 15.406 1.00 15.15 N
ATOM 920 CA ILE A 122 17.030 16.155 15.026 1.00 14.82 C
ATOM 921 CB ILE A 122 16.080 15.514 13.977 1.00 14.11 C
ATOM 922 CG1 ILE A 122 14.714 15.222 14.606 1.00 16.00 C
ATOM 923 CD1 ILE A 122 13.584 14.991 13.604 1.00 17.09 C
ATOM 924 CG2 ILE A 122 16.698 14.241 13.401 1.00 13.39 C
ATOM 925 C ILE A 122 18.487 16.166 14.526 1.00 15.00 C
ATOM 926 O ILE A 122 19.302 15.336 14.963 1.00 17.68 O
ATOM 927 N ALA A 123 18.814 17.117 13.648 1.00 14.68 N
ATOM 928 CA ALA A 123 20.156 17.226 13.055 1.00 14.71 C
ATOM 929 CB ALA A 123 20.188 18.327 12.010 1.00 16.01 C
ATOM 930 C ALA A 123 21.265 17.447 14.097 1.00 15.27 C
ATOM 931 O ALA A 123 22.355 16.893 13.960 1.00 16.90 O
ATOM 932 N GLY A 124 20.968 18.254 15.116 1.00 16.90 N
ATOM 933 CA GLY A 124 21.879 18.471 16.256 1.00 18.07 C
ATOM 934 C GLY A 124 22.182 17.198 17.036 1.00 21.24 C
ATOM 935 O GLY A 124 23.345 16.897 17.306 1.00 19.44 O
ATOM 936 N ALA A 125 21.132 16.450 17.385 1.00 18.55 N
ATOM 937 CA ALA A 125 21.275 15.138 18.019 1.00 18.17 C
ATOM 938 CB ALA A 125 19.904 14.557 18.337 1.00 18.65 C
ATOM 939 C ALA A 125 22.090 14.170 17.149 1.00 18.28 C
ATOM 940 O ALA A 125 23.017 13.509 17.638 1.00 16.27 O
ATOM 941 N MET A 126 21.765 14.125 15.855 1.00 14.82 N
ATOM 942 CA AMET A 126 22.424 13.224 14.904 0.50 14.62 C
ATOM 943 CA BMET A 126 22.430 13.209 14.929 0.50 15.69 C
ATOM 944 CB AMET A 126 21.699 13.241 13.553 0.50 15.60 C
ATOM 945 CB BMET A 126 21.661 13.117 13.604 0.50 19.78 C
ATOM 946 CG AMET A 126 20.322 12.591 13.569 0.50 14.86 C
ATOM 947 CG BMET A 126 20.309 12.428 13.754 0.50 20.52 C

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ATOM    948  SD AMET A 126      20.314  10.872  14.119  0.50 14.67           S
ATOM    949  SD BMET A 126      19.437  12.161  12.201  0.50 26.10           S
ATOM    950  CE AMET A 126      19.905  11.024  15.838  0.50 18.48           C
ATOM    951  CE BMET A 126      20.559  11.016  11.412  0.50 26.17           C
ATOM    952  C   MET A 126      23.903  13.570  14.717  1.00 16.53           C
ATOM    953  O   MET A 126      24.732  12.678  14.484  1.00 17.11           O
ATOM    954  N   ARG A 127      24.232  14.864  14.831  1.00 18.82           N
ATOM    955  CA  ARG A 127      25.634  15.293  14.736  1.00 20.38           C
ATOM    956  CB  ARG A 127      25.807  16.820  14.754  1.00 25.12           C
ATOM    957  CG  ARG A 127      27.242  17.237  14.408  1.00 30.23           C
ATOM    958  CD  ARG A 127      27.444  18.743  14.299  1.00 37.45           C
ATOM    959  NE  ARG A 127      27.001  19.467  15.493  1.00 44.13           N
ATOM    960  CZ  ARG A 127      27.199  20.764  15.723  1.00 47.14           C
ATOM    961  NH1 ARG A 127      27.850  21.523  14.849  1.00 49.34           N
ATOM    962  NH2 ARG A 127      26.738  21.309  16.840  1.00 49.27           N
ATOM    963  C   ARG A 127      26.484  14.617  15.818  1.00 21.06           C
ATOM    964  O   ARG A 127      27.571  14.120  15.517  1.00 21.58           O
ATOM    965  N   LEU A 128      25.964  14.575  17.046  1.00 20.30           N
ATOM    966  CA  LEU A 128      26.619  13.855  18.150  1.00 21.57           C
ATOM    967  CB  LEU A 128      25.947  14.158  19.492  1.00 22.63           C
ATOM    968  CG  LEU A 128      26.546  13.539  20.769  1.00 24.68           C
ATOM    969  CD1 LEU A 128      27.930  14.098  21.088  1.00 30.71           C
ATOM    970  CD2 LEU A 128      25.604  13.768  21.940  1.00 25.91           C
ATOM    971  C   LEU A 128      26.744  12.347  17.925  1.00 25.54           C
ATOM    972  O   LEU A 128      27.810  11.780  18.189  1.00 24.64           O
ATOM    973  N   LEU A 129      25.673  11.700  17.442  1.00 19.41           N
ATOM    974  CA  LEU A 129      25.730  10.272  17.110  1.00 20.44           C
ATOM    975  CB  LEU A 129      24.376   9.734  16.598  1.00 19.97           C
ATOM    976  CG  LEU A 129      23.055   9.751  17.385  1.00 28.42           C
ATOM    977  CD1 LEU A 129      22.240   8.519  17.005  1.00 30.87           C
ATOM    978  CD2 LEU A 129      23.202   9.808  18.891  1.00 30.57           C
ATOM    979  C   LEU A 129      26.820   9.992  16.076  1.00 19.34           C
ATOM    980  O   LEU A 129      27.607   9.059  16.239  1.00 21.54           O
ATOM    981  N   HIS A 130      26.845  10.811  15.025  1.00 18.09           N
ATOM    982  CA  HIS A 130      27.829  10.710  13.950  1.00 19.78           C
ATOM    983  CB  HIS A 130      27.570  11.753  12.861  1.00 17.88           C
ATOM    984  CG  HIS A 130      28.472  11.622  11.671  1.00 21.70           C
ATOM    985  ND1 HIS A 130      29.487  12.517  11.405  1.00 25.49           N
ATOM    986  CE1 HIS A 130      30.116  12.152  10.303  1.00 23.84           C
ATOM    987  NE2 HIS A 130      29.550  11.052   9.847  1.00 24.33           N
ATOM    988  CD2 HIS A 130      28.523  10.696  10.687  1.00 17.75           C
ATOM    989  C   HIS A 130      29.261  10.821  14.471  1.00 19.47           C
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ATOM    990  O   HIS A 130      30.116  10.024  14.088  1.00 22.97           O
ATOM    991  N   SER A 131      29.506  11.793  15.347  1.00 19.76           N
ATOM    992  CA  SER A 131      30.850  11.984  15.914  1.00 26.23           C
ATOM    993  CB  SER A 131      30.935  13.283  16.719  1.00 29.65           C
ATOM    994  OG  SER A 131      30.141  13.226  17.886  1.00 40.72           O
ATOM    995  C   SER A 131      31.296  10.783  16.754  1.00 27.74           C
ATOM    996  O   SER A 131      32.462  10.391  16.695  1.00 27.11           O
ATOM    997  N   LYS A 132      30.359  10.192  17.497  1.00 24.55           N
ATOM    998  CA  LYS A 132      30.626   9.015  18.348  1.00 25.47           C
ATOM    999  CB  LYS A 132      29.635   8.961  19.514  1.00 28.34           C
ATOM   1000  CG  LYS A 132      29.888   9.997  20.598  1.00 36.58           C
ATOM   1001  CD  LYS A 132      29.386   9.514  21.948  1.00 42.11           C
ATOM   1002  CE  LYS A 132      30.203  10.102  23.090  1.00 55.60           C
ATOM   1003  NZ  LYS A 132      29.887  11.533  23.372  1.00 52.50           N
ATOM   1004  C   LYS A 132      30.643   7.673  17.598  1.00 30.64           C
ATOM   1005  O   LYS A 132      31.002   6.634  18.182  1.00 32.89           O
ATOM   1006  N   GLY A 133      30.265   7.702  16.314  1.00 25.14           N
ATOM   1007  CA  GLY A 133      30.126   6.505  15.479  1.00 26.20           C
ATOM   1008  C   GLY A 133      28.965   5.606  15.876  1.00 26.29           C
ATOM   1009  O   GLY A 133      29.096   4.380  15.838  1.00 26.82           O
ATOM   1010  N   ILE A 134      27.832   6.214  16.242  1.00 21.38           N
ATOM   1011  CA  ILE A 134      26.628   5.483  16.675  1.00 20.75           C
ATOM   1012  CB  ILE A 134      26.111   5.983  18.059  1.00 21.63           C
ATOM   1013  CG1 ILE A 134      27.139   5.697  19.167  1.00 23.69           C
ATOM   1014  CD1 ILE A 134      26.908   6.503  20.435  1.00 25.83           C
ATOM   1015  CG2 ILE A 134      24.763   5.362  18.430  1.00 20.01           C
ATOM   1016  C   ILE A 134      25.513   5.604  15.634  1.00 21.27           C
ATOM   1017  O   ILE A 134      25.227   6.710  15.173  1.00 24.16           O
ATOM   1018  N   ILE A 135      24.912   4.461  15.280  1.00 19.31           N
ATOM   1019  CA AILE A 135      23.722   4.431  14.424  0.70 21.89           C
ATOM   1020  CA BILE A 135      23.726   4.405  14.407  0.30 18.25           C
ATOM   1021  CB AILE A 135      23.908   3.563  13.146  0.70 22.57           C
ATOM   1022  CB BILE A 135      23.895   3.420  13.214  0.30 16.61           C
ATOM   1023  CG1AILE A 135      22.632   3.582  12.286  0.70 23.48           C
ATOM   1024  CG1BILE A 135      25.226   3.629  12.477  0.30 14.88           C
ATOM   1025  CD1AILE A 135      22.625   2.656  11.096  0.70 26.14           C
ATOM   1026  CD1BILE A 135      26.230   2.522  12.700  0.30 17.06           C
ATOM   1027  CG2AILE A 135      24.389   2.155  13.478  0.70 27.49           C
ATOM   1028  CG2BILE A 135      22.755   3.555  12.211  0.30 16.10           C
ATOM   1029  C   ILE A 135      22.523   4.005  15.270  1.00 18.44           C
ATOM   1030  O   ILE A 135      22.587   3.022  16.014  1.00 19.01           O
ATOM   1031  N   HIS A 136      21.443   4.779  15.187  1.00 16.08           N
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ATOM 1032 CA HIS A 136 20.265 4.541 16.015 1.00 15.06 C
ATOM 1033 CB HIS A 136 19.356 5.790 16.002 1.00 14.40 C
ATOM 1034 CG HIS A 136 18.153 5.695 16.893 1.00 13.76 C
ATOM 1035 ND1 HIS A 136 17.090 4.854 16.625 1.00 13.10 N
ATOM 1036 CE1 HIS A 136 16.169 5.000 17.560 1.00 13.79 C
ATOM 1037 NE2 HIS A 136 16.591 5.908 18.421 1.00 12.25 N
ATOM 1038 CD2 HIS A 136 17.830 6.357 18.031 1.00 12.62 C
ATOM 1039 C HIS A 136 19.527 3.279 15.565 1.00 14.85 C
ATOM 1040 O HIS A 136 19.184 2.444 16.399 1.00 15.51 O
ATOM 1041 N ARG A 137 19.278 3.176 14.251 1.00 14.20 N
ATOM 1042 CA ARG A 137 18.700 1.990 13.558 1.00 15.59 C
ATOM 1043 CB ARG A 137 19.401 0.664 13.952 1.00 15.49 C
ATOM 1044 CG ARG A 137 20.904 0.623 13.728 1.00 20.54 C
ATOM 1045 CD ARG A 137 21.411 -0.807 13.672 1.00 19.82 C
ATOM 1046 NE ARG A 137 21.191 -1.535 14.927 1.00 23.94 N
ATOM 1047 CZ ARG A 137 21.051 -2.858 15.026 1.00 25.52 C
ATOM 1048 NH1 ARG A 137 20.854 -3.411 16.216 1.00 22.05 N
ATOM 1049 NH2 ARG A 137 21.105 -3.631 13.943 1.00 23.87 N
ATOM 1050 C ARG A 137 17.184 1.817 13.668 1.00 16.52 C
ATOM 1051 O ARG A 137 16.610 0.986 12.955 1.00 17.31 O
ATOM 1052 N ASP A 138 16.537 2.596 14.536 1.00 13.10 N
ATOM 1053 CA ASP A 138 15.105 2.438 14.790 1.00 14.10 C
ATOM 1054 CB ASP A 138 14.911 1.598 16.075 1.00 15.79 C
ATOM 1055 CG ASP A 138 13.461 1.137 16.302 1.00 20.83 C
ATOM 1056 OD1 ASP A 138 12.723 0.822 15.348 1.00 16.76 O
ATOM 1057 OD2 ASP A 138 13.055 1.080 17.474 1.00 23.07 O
ATOM 1058 C ASP A 138 14.397 3.802 14.869 1.00 11.86 C
ATOM 1059 O ASP A 138 13.475 3.991 15.663 1.00 13.88 O
ATOM 1060 N LEU A 139 14.824 4.765 14.045 1.00 11.14 N
ATOM 1061 CA LEU A 139 14.156 6.081 14.041 1.00 11.58 C
ATOM 1062 CB LEU A 139 15.019 7.150 13.369 1.00 11.01 C
ATOM 1063 CG LEU A 139 16.341 7.535 14.041 1.00 12.62 C
ATOM 1064 CD1 LEU A 139 17.153 8.400 13.079 1.00 11.16 C
ATOM 1065 CD2 LEU A 139 16.083 8.254 15.360 1.00 11.91 C
ATOM 1066 C LEU A 139 12.788 5.994 13.372 1.00 12.85 C
ATOM 1067 O LEU A 139 12.667 5.445 12.295 1.00 12.33 O
ATOM 1068 N LYS A 140 11.769 6.527 14.046 1.00 11.09 N
ATOM 1069 CA LYS A 140 10.373 6.493 13.593 1.00 10.31 C
ATOM 1070 CB LYS A 140 9.769 5.089 13.773 1.00 11.07 C
ATOM 1071 CG LYS A 140 9.740 4.593 15.211 1.00 12.06 C
ATOM 1072 CD LYS A 140 9.596 3.090 15.269 1.00 17.59 C
ATOM 1073 CE LYS A 140 9.636 2.624 16.708 1.00 20.54 C

ATOM 1074 NZ LYS A 140 10.073 1.202 16.814 1.00 21.74 N
ATOM 1075 C LYS A 140 9.606 7.549 14.405 1.00 10.43 C
ATOM 1076 O LYS A 140 10.115 8.008 15.425 1.00 12.96 O
ATOM 1077 N PRO A 141 8.385 7.940 13.971 1.00 10.52 N
ATOM 1078 CA PRO A 141 7.696 9.019 14.703 1.00 10.69 C
ATOM 1079 CB PRO A 141 6.386 9.196 13.909 1.00 11.98 C
ATOM 1080 CG PRO A 141 6.759 8.774 12.510 1.00 10.88 C
ATOM 1081 CD PRO A 141 7.681 7.591 12.720 1.00 10.89 C
ATOM 1082 C PRO A 141 7.420 8.719 16.182 1.00 11.33 C
ATOM 1083 O PRO A 141 7.407 9.648 16.994 1.00 11.76 O
ATOM 1084 N GLN A 142 7.271 7.439 16.526 1.00 13.18 N
ATOM 1085 CA GLN A 142 7.041 6.988 17.911 1.00 16.28 C
ATOM 1086 CB GLN A 142 6.710 5.490 17.960 1.00 17.67 C
ATOM 1087 CG GLN A 142 5.367 5.094 17.356 1.00 16.38 C
ATOM 1088 CD GLN A 142 5.338 5.110 15.832 1.00 21.47 C
ATOM 1089 OE1 GLN A 142 6.376 5.081 15.169 1.00 16.83 O
ATOM 1090 NE2 GLN A 142 4.129 5.164 15.267 1.00 23.75 N
ATOM 1091 C GLN A 142 8.199 7.263 18.858 1.00 17.35 C
ATOM 1092 O GLN A 142 7.986 7.362 20.070 1.00 17.57 O
ATOM 1093 N ASN A 143 9.423 7.364 18.339 1.00 13.60 N
ATOM 1094 CA ASN A 143 10.533 7.711 19.228 1.00 16.73 C
ATOM 1095 CB ASN A 143 11.549 6.560 19.382 1.00 20.10 C
ATOM 1096 CG ASN A 143 12.072 6.040 18.072 1.00 21.21 C
ATOM 1097 OD1 ASN A 143 12.276 6.801 17.120 1.00 20.84 O
ATOM 1098 ND2 ASN A 143 12.342 4.725 18.026 1.00 15.25 N
ATOM 1099 C ASN A 143 11.174 9.080 18.993 1.00 15.87 C
ATOM 1100 O ASN A 143 12.296 9.348 19.431 1.00 15.92 O
ATOM 1101 N ILE A 144 10.416 9.957 18.334 1.00 15.15 N
ATOM 1102 CA ILE A 144 10.732 11.373 18.270 1.00 13.73 C
ATOM 1103 CB ILE A 144 10.558 11.963 16.840 1.00 15.22 C
ATOM 1104 CG1 ILE A 144 11.431 11.220 15.791 1.00 14.19 C
ATOM 1105 CD1 ILE A 144 12.935 11.259 16.015 1.00 20.91 C
ATOM 1106 CG2 ILE A 144 10.813 13.469 16.835 1.00 15.42 C
ATOM 1107 C ILE A 144 9.777 12.028 19.278 1.00 14.22 C
ATOM 1108 O ILE A 144 8.587 12.167 19.018 1.00 13.85 O
ATOM 1109 N LEU A 145 10.304 12.378 20.445 1.00 12.95 N
ATOM 1110 CA LEU A 145 9.468 12.898 21.535 1.00 14.74 C
ATOM 1111 CB LEU A 145 10.014 12.432 22.892 1.00 16.54 C
ATOM 1112 CG LEU A 145 10.240 10.935 23.113 1.00 20.56 C
ATOM 1113 CD1 LEU A 145 10.654 10.715 24.561 1.00 23.45 C
ATOM 1114 CD2 LEU A 145 9.015 10.092 22.771 1.00 18.07 C
ATOM 1115 C LEU A 145 9.394 14.414 21.524 1.00 13.89 C

ATOM 1116 O LEU A 145 10.371 15.073 21.177 1.00 17.80 O
ATOM 1117 N LEU A 146 8.240 14.950 21.936 1.00 14.58 N
ATOM 1118 CA LEU A 146 7.995 16.395 21.957 1.00 16.94 C
ATOM 1119 CB LEU A 146 6.780 16.773 21.094 1.00 18.77 C
ATOM 1120 CG LEU A 146 6.774 16.307 19.621 1.00 18.87 C
ATOM 1121 CD1 LEU A 146 5.490 16.747 18.935 1.00 20.54 C
ATOM 1122 CD2 LEU A 146 7.988 16.801 18.843 1.00 19.00 C
ATOM 1123 C LEU A 146 7.807 16.895 23.392 1.00 17.78 C
ATOM 1124 O LEU A 146 7.276 16.186 24.236 1.00 18.61 O
ATOM 1125 N SER A 147 8.248 18.123 23.639 1.00 22.58 N
ATOM 1126 CA SER A 147 8.206 18.725 24.971 1.00 27.75 C
ATOM 1127 CB SER A 147 9.493 18.388 25.725 1.00 26.52 C
ATOM 1128 OG SER A 147 9.523 19.001 26.998 1.00 55.83 O
ATOM 1129 C SER A 147 8.034 20.238 24.851 1.00 32.95 C
ATOM 1130 O SER A 147 8.739 20.886 24.069 1.00 31.56 O
ATOM 1131 N ASN A 148 7.086 20.786 25.613 1.00 35.46 N
ATOM 1132 CA ASN A 148 6.831 22.234 25.630 1.00 42.46 C
ATOM 1133 CB ASN A 148 5.347 22.526 25.869 1.00 43.63 C
ATOM 1134 C ASN A 148 7.689 22.959 26.666 1.00 43.62 C
ATOM 1135 O ASN A 148 7.778 22.535 27.822 1.00 34.13 O
ATOM 1136 N SER A 158 8.076 26.830 20.486 1.00 33.35 N
ATOM 1137 CA SER A 158 8.918 26.417 21.606 1.00 41.28 C
ATOM 1138 CB SER A 158 8.494 27.145 22.886 1.00 29.61 C
ATOM 1139 OG SER A 158 7.165 26.814 23.241 1.00 43.12 O
ATOM 1140 C SER A 158 8.943 24.895 21.839 1.00 39.59 C
ATOM 1141 O SER A 158 9.577 24.427 22.801 1.00 43.28 O
ATOM 1142 N ILE A 159 8.266 24.136 20.965 1.00 38.89 N
ATOM 1143 CA ILE A 159 8.274 22.666 21.026 1.00 31.85 C
ATOM 1144 CB ILE A 159 7.327 21.995 19.987 1.00 29.86 C
ATOM 1145 CG1 ILE A 159 5.859 22.285 20.326 1.00 35.64 C
ATOM 1146 CD1 ILE A 159 4.864 21.916 19.243 1.00 38.01 C
ATOM 1147 CG2 ILE A 159 7.554 20.477 19.934 1.00 30.36 C
ATOM 1148 C ILE A 159 9.707 22.187 20.845 1.00 27.27 C
ATOM 1149 O ILE A 159 10.359 22.491 19.835 1.00 31.19 O
ATOM 1150 N ARG A 160 10.198 21.480 21.858 1.00 27.74 N
ATOM 1151 CA ARG A 160 11.497 20.829 21.799 1.00 25.69 C
ATOM 1152 CB ARG A 160 12.232 20.895 23.148 1.00 34.93 C
ATOM 1153 CG ARG A 160 12.413 22.292 23.755 1.00 39.54 C
ATOM 1154 CD ARG A 160 13.088 23.295 22.823 1.00 33.52 C
ATOM 1155 NE ARG A 160 14.454 22.909 22.465 1.00 35.10 N
ATOM 1156 CZ ARG A 160 15.104 23.326 21.377 1.00 42.46 C
ATOM 1157 NH1 ARG A 160 16.339 22.898 21.145 1.00 33.44 N

ATOM 1158 NH2 ARG A 160 14.526 24.154 20.508 1.00 37.73 N
ATOM 1159 C ARG A 160 11.328 19.376 21.348 1.00 26.10 C
ATOM 1160 O ARG A 160 10.362 18.701 21.735 1.00 23.12 O
ATOM 1161 N VAL A 161 12.259 18.932 20.506 1.00 21.27 N
ATOM 1162 CA VAL A 161 12.318 17.561 19.985 1.00 21.18 C
ATOM 1163 CB VAL A 161 12.607 17.548 18.455 1.00 21.45 C
ATOM 1164 CG1 VAL A 161 13.020 16.158 17.961 1.00 22.92 C
ATOM 1165 CG2 VAL A 161 11.412 18.063 17.678 1.00 29.16 C
ATOM 1166 C VAL A 161 13.432 16.829 20.719 1.00 22.68 C
ATOM 1167 O VAL A 161 14.542 17.357 20.876 1.00 23.88 O
ATOM 1168 N LYS A 162 13.136 15.611 21.157 1.00 20.68 N
ATOM 1169 CA LYS A 162 14.132 14.750 21.779 1.00 22.61 C
ATOM 1170 CB LYS A 162 13.980 14.747 23.301 1.00 22.21 C
ATOM 1171 CG LYS A 162 14.657 15.942 23.972 1.00 28.80 C
ATOM 1172 CD LYS A 162 13.791 16.541 25.058 1.00 33.73 C
ATOM 1173 CE LYS A 162 14.125 18.009 25.295 1.00 32.82 C
ATOM 1174 NZ LYS A 162 15.341 18.187 26.135 1.00 32.21 N
ATOM 1175 C LYS A 162 14.037 13.337 21.226 1.00 21.05 C
ATOM 1176 O LYS A 162 12.960 12.724 21.238 1.00 19.91 O
ATOM 1177 N ILE A 163 15.170 12.833 20.747 1.00 14.87 N
ATOM 1178 CA ILE A 163 15.247 11.463 20.230 1.00 16.59 C
ATOM 1179 CB ILE A 163 16.411 11.290 19.224 1.00 17.82 C
ATOM 1180 CG1 ILE A 163 16.200 12.258 18.046 1.00 18.18 C
ATOM 1181 CD1 ILE A 163 17.320 12.313 17.037 1.00 25.12 C
ATOM 1182 CG2 ILE A 163 16.510 9.840 18.746 1.00 17.88 C
ATOM 1183 C ILE A 163 15.331 10.491 21.417 1.00 18.56 C
ATOM 1184 O ILE A 163 16.123 10.691 22.353 1.00 18.90 O
ATOM 1185 N ALA A 164 14.476 9.471 21.383 1.00 16.50 N
ATOM 1186 CA ALA A 164 14.434 8.452 22.417 1.00 21.23 C
ATOM 1187 CB ALA A 164 13.075 8.468 23.099 1.00 17.00 C
ATOM 1188 C ALA A 164 14.716 7.070 21.843 1.00 18.93 C
ATOM 1189 O ALA A 164 14.938 6.923 20.629 1.00 19.41 O
ATOM 1190 N ASP A 165 14.730 6.075 22.738 1.00 17.02 N
ATOM 1191 CA ASP A 165 14.591 4.652 22.391 1.00 15.02 C
ATOM 1192 CB ASP A 165 13.343 4.458 21.516 1.00 21.24 C
ATOM 1193 CG ASP A 165 12.687 3.117 21.690 1.00 23.40 C
ATOM 1194 OD1 ASP A 165 12.849 2.478 22.750 1.00 21.20 O
ATOM 1195 OD2 ASP A 165 11.966 2.721 20.745 1.00 27.85 O
ATOM 1196 C ASP A 165 15.859 4.140 21.720 1.00 20.03 C
ATOM 1197 O ASP A 165 15.865 3.808 20.523 1.00 14.62 O
ATOM 1198 N PHE A 166 16.937 4.091 22.502 1.00 15.34 N
ATOM 1199 CA PHE A 166 18.268 3.775 21.987 1.00 16.88 C

ATOM 1200 CB PHE A 166 19.305 4.741 22.602 1.00 16.39 C
ATOM 1201 CG PHE A 166 19.370 6.080 21.913 1.00 15.29 C
ATOM 1202 CD1 PHE A 166 20.368 6.344 20.970 1.00 17.60 C
ATOM 1203 CE1 PHE A 166 20.430 7.584 20.332 1.00 20.05 C
ATOM 1204 CZ PHE A 166 19.495 8.576 20.639 1.00 16.27 C
ATOM 1205 CE2 PHE A 166 18.499 8.325 21.574 1.00 16.20 C
ATOM 1206 CD2 PHE A 166 18.443 7.085 22.211 1.00 18.63 C
ATOM 1207 C PHE A 166 18.715 2.318 22.157 1.00 17.76 C
ATOM 1208 O PHE A 166 19.893 2.014 21.969 1.00 19.64 O
ATOM 1209 N GLY A 167 17.781 1.420 22.477 1.00 19.05 N
ATOM 1210 CA GLY A 167 18.092 -0.005 22.688 1.00 20.47 C
ATOM 1211 C GLY A 167 18.668 -0.745 21.490 1.00 21.42 C
ATOM 1212 O GLY A 167 19.443 -1.694 21.658 1.00 19.65 O
ATOM 1213 N PHE A 168 18.287 -0.320 20.283 1.00 16.84 N
ATOM 1214 CA PHE A 168 18.785 -0.944 19.052 1.00 18.06 C
ATOM 1215 CB PHE A 168 17.693 -0.987 17.970 1.00 17.01 C
ATOM 1216 CG PHE A 168 16.670 -2.074 18.174 1.00 20.29 C
ATOM 1217 CD1 PHE A 168 17.006 -3.425 17.982 1.00 20.73 C
ATOM 1218 CE1 PHE A 168 16.053 -4.428 18.160 1.00 23.86 C
ATOM 1219 CZ PHE A 168 14.754 -4.092 18.536 1.00 25.23 C
ATOM 1220 CE2 PHE A 168 14.407 -2.757 18.723 1.00 26.36 C
ATOM 1221 CD2 PHE A 168 15.364 -1.756 18.541 1.00 22.06 C
ATOM 1222 C PHE A 168 20.049 -0.290 18.502 1.00 18.45 C
ATOM 1223 O PHE A 168 20.588 -0.752 17.488 1.00 19.30 O
ATOM 1224 N ALA A 169 20.522 0.771 19.164 1.00 17.88 N
ATOM 1225 CA ALA A 169 21.685 1.529 18.692 1.00 17.69 C
ATOM 1226 CB ALA A 169 21.883 2.799 19.499 1.00 19.65 C
ATOM 1227 C ALA A 169 22.949 0.681 18.705 1.00 27.06 C
ATOM 1228 O ALA A 169 23.120 -0.173 19.581 1.00 24.55 O
ATOM 1229 N ARG A 170 23.812 0.896 17.716 1.00 23.69 N
ATOM 1230 CA ARG A 170 25.103 0.206 17.683 1.00 31.70 C
ATOM 1231 CB ARG A 170 25.050 -1.070 16.822 1.00 34.41 C
ATOM 1232 CG ARG A 170 24.871 -0.859 15.331 1.00 38.87 C
ATOM 1233 CD ARG A 170 25.554 -1.945 14.511 1.00 54.55 C
ATOM 1234 NE ARG A 170 25.653 -1.556 13.100 1.00 68.55 N
ATOM 1235 CZ ARG A 170 26.257 -2.264 12.144 1.00 72.65 C
ATOM 1236 NH1 ARG A 170 26.841 -3.431 12.414 1.00 92.29 N
ATOM 1237 NH2 ARG A 170 26.277 -1.798 10.901 1.00 53.80 N
ATOM 1238 C ARG A 170 26.242 1.126 17.271 1.00 32.16 C
ATOM 1239 O ARG A 170 26.025 2.131 16.589 1.00 23.31 O
ATOM 1240 N TYR A 171 27.446 0.793 17.732 1.00 32.92 N
ATOM 1241 CA TYR A 171 28.666 1.440 17.267 1.00 32.02 C

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ATOM   1242  CB  TYR A 171      29.784   1.304  18.306  1.00 34.01          C
ATOM   1243  CG  TYR A 171      29.586   2.145  19.551  1.00 36.98          C
ATOM   1244  CD1 TYR A 171      30.176   3.412  19.666  1.00 35.28          C
ATOM   1245  CE1 TYR A 171      30.003   4.185  20.811  1.00 37.94          C
ATOM   1246  CZ  TYR A 171      29.226   3.690  21.858  1.00 38.81          C
ATOM   1247  OH  TYR A 171      29.042   4.438  22.998  1.00 46.39          O
ATOM   1248  CE2 TYR A 171      28.634   2.441  21.769  1.00 39.26          C
ATOM   1249  CD2 TYR A 171      28.812   1.676  20.622  1.00 39.57          C
ATOM   1250  C   TYR A 171      29.081   0.825  15.929  1.00 30.71          C
ATOM   1251  O   TYR A 171      28.981  -0.392  15.741  1.00 33.51          O
ATOM   1252  N   LEU A 172      29.543   1.676  15.013  1.00 29.24          N
ATOM   1253  CA  LEU A 172      29.865   1.291  13.628  1.00 33.38          C
ATOM   1254  CB  LEU A 172      30.272   2.526  12.819  1.00 36.90          C
ATOM   1255  C   LEU A 172      30.933   0.195  13.494  1.00 44.48          C
ATOM   1256  O   LEU A 172      31.732  -0.038  14.405  1.00 51.01          O
ATOM   1257  N   THR A 180      19.864  -8.311  16.597  1.00 43.75          N
ATOM   1258  CA  THR A 180      18.645  -8.627  15.863  1.00 44.11          C
ATOM   1259  CB  THR A 180      17.930  -9.879  16.441  1.00 54.06          C
ATOM   1260  OG1 THR A 180      18.893 -10.875  16.821  1.00 57.22          O
ATOM   1261  CG2 THR A 180      16.956 -10.477  15.421  1.00 52.76          C
ATOM   1262  C   THR A 180      17.702  -7.417  15.878  1.00 35.29          C
ATOM   1263  O   THR A 180      17.105  -7.099  16.913  1.00 37.12          O
ATOM   1264  N   LEU A 181      17.579  -6.753  14.729  1.00 29.50          N
ATOM   1265  CA  LEU A 181      16.720  -5.570  14.588  1.00 23.94          C
ATOM   1266  CB  LEU A 181      17.321  -4.572  13.581  1.00 28.75          C
ATOM   1267  CG  LEU A 181      16.604  -3.246  13.275  1.00 26.85          C
ATOM   1268  CD1 LEU A 181      16.614  -2.300  14.470  1.00 27.73          C
ATOM   1269  CD2 LEU A 181      17.265  -2.587  12.075  1.00 27.56          C
ATOM   1270  C   LEU A 181      15.291  -5.925  14.190  1.00 25.48          C
ATOM   1271  O   LEU A 181      15.074  -6.705  13.259  1.00 27.45          O
HETATM 1272  N   CSO A 182      14.327  -5.362  14.918  1.00 20.20          N
HETATM 1273  CA  CSO A 182      12.930  -5.306  14.465  1.00 25.14          C
HETATM 1274  CB  CSO A 182      12.039  -6.468  14.935  1.00 23.17          C
HETATM 1275  SG  CSO A 182      11.954  -6.596  16.698  1.00 27.59          S
HETATM 1276  OD  CSO A 182      13.218  -7.772  16.977  1.00 31.77          O
HETATM 1277  C   CSO A 182      12.373  -3.963  14.856  1.00 22.32          C
HETATM 1278  O   CSO A 182      12.799  -3.356  15.846  1.00 28.32          O
ATOM   1279  N   GLY A 183      11.447  -3.471  14.048  1.00 20.98          N
ATOM   1280  CA  GLY A 183      10.759  -2.226  14.342  1.00 17.89          C
ATOM   1281  C   GLY A 183       9.685  -1.977  13.313  1.00 16.49          C
ATOM   1282  O   GLY A 183       8.717  -2.736  13.215  1.00 17.36          O
ATOM   1283  N   SER A 184       9.855  -0.907  12.542  1.00 16.25          N
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ATOM   1284  CA  SER A 184      8.870  -0.551  11.510  1.00 14.38         C
ATOM   1285  CB  SER A 184      8.118   0.732  11.871  1.00 16.61         C
ATOM   1286  OG  SER A 184      7.423   0.553  13.098  1.00 19.65         O
ATOM   1287  C   SER A 184      9.550  -0.440  10.160  1.00 16.51         C
ATOM   1288  O   SER A 184     10.147   0.595   9.848  1.00 13.01         O
ATOM   1289  N   PRO A 185      9.475  -1.520   9.353  1.00 15.19         N
ATOM   1290  CA  PRO A 185     10.201  -1.573   8.078  1.00 12.71         C
ATOM   1291  CB  PRO A 185      9.702  -2.884   7.460  1.00 13.25         C
ATOM   1292  CG  PRO A 185      9.451  -3.755   8.655  1.00 14.82         C
ATOM   1293  CD  PRO A 185      8.844  -2.821   9.672  1.00 15.76         C
ATOM   1294  C   PRO A 185      9.950  -0.376   7.144  1.00 12.33         C
ATOM   1295  O   PRO A 185     10.851  -0.010   6.376  1.00 12.44         O
ATOM   1296  N   MET A 186      8.775   0.266   7.226  1.00 11.54         N
ATOM   1297  CA  MET A 186      8.506   1.421   6.348  1.00 11.15         C
ATOM   1298  CB  MET A 186      7.047   1.902   6.418  1.00 16.10         C
ATOM   1299  CG  MET A 186      6.617   2.530   7.729  1.00 21.70         C
ATOM   1300  SD  MET A 186      5.009   3.361   7.607  1.00 28.92         S
ATOM   1301  CE  MET A 186      4.005   2.164   6.728  1.00 30.43         C
ATOM   1302  C   MET A 186      9.495   2.580   6.560  1.00  9.99         C
ATOM   1303  O   MET A 186      9.698   3.370   5.643  1.00 10.22         O
ATOM   1304  N   TYR A 187     10.114   2.647   7.752  1.00  8.10         N
ATOM   1305  CA  TYR A 187     11.142   3.666   8.061  1.00  8.73         C
ATOM   1306  CB  TYR A 187     10.942   4.258   9.460  1.00  8.41         C
ATOM   1307  CG  TYR A 187      9.551   4.810   9.651  1.00  8.64         C
ATOM   1308  CD1 TYR A 187      8.619   4.107  10.413  1.00  9.71         C
ATOM   1309  CE1 TYR A 187      7.330   4.587  10.582  1.00 11.17         C
ATOM   1310  CZ  TYR A 187      6.946   5.776   9.971  1.00 13.11         C
ATOM   1311  OH  TYR A 187      5.653   6.208  10.161  1.00 12.36         O
ATOM   1312  CE2 TYR A 187      7.846   6.500   9.194  1.00 11.62         C
ATOM   1313  CD2 TYR A 187      9.144   6.007   9.030  1.00 10.63         C
ATOM   1314  C   TYR A 187     12.596   3.190   7.893  1.00  8.62         C
ATOM   1315  O   TYR A 187     13.524   3.982   8.045  1.00 11.14         O
ATOM   1316  N   MET A 188     12.786   1.934   7.514  1.00  9.27         N
ATOM   1317  CA  MET A 188     14.127   1.353   7.417  1.00  9.63         C
ATOM   1318  CB  MET A 188     14.075  -0.113   7.826  1.00 11.65         C
ATOM   1319  CG  MET A 188     13.775  -0.292   9.303  1.00 16.05         C
ATOM   1320  SD  MET A 188     13.722  -2.044   9.665  1.00 20.68         S
ATOM   1321  CE  MET A 188     13.465  -1.943  11.441  1.00 24.87         C
ATOM   1322  C   MET A 188     14.725   1.475   6.022  1.00  8.93         C
ATOM   1323  O   MET A 188     14.023   1.328   5.020  1.00  9.35         O
ATOM   1324  N   ALA A 189     16.027   1.759   5.964  1.00  8.86         N
ATOM   1325  CA  ALA A 189     16.720   1.948   4.689  1.00  9.34         C
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ATOM   1326  CB  ALA A 189      18.168   2.381   4.935  1.00  9.48           C
ATOM   1327  C   ALA A 189      16.680   0.673   3.839  1.00  9.03           C
ATOM   1328  O   ALA A 189      16.691  -0.435   4.396  1.00  9.80           O
ATOM   1329  N   PRO A 190      16.659   0.820   2.493  1.00  9.00           N
ATOM   1330  CA  PRO A 190      16.656  -0.351   1.618  1.00  8.60           C
ATOM   1331  CB  PRO A 190      16.789   0.257   0.223  1.00  8.56           C
ATOM   1332  CG  PRO A 190      16.064   1.585   0.366  1.00  8.66           C
ATOM   1333  CD  PRO A 190      16.524   2.073   1.710  1.00  8.62           C
ATOM   1334  C   PRO A 190      17.785  -1.343   1.917  1.00  8.26           C
ATOM   1335  O   PRO A 190      17.528  -2.539   1.973  1.00  7.13           O
ATOM   1336  N   GLU A 191      18.994  -0.840   2.175  1.00  8.55           N
ATOM   1337  CA  GLU A 191      20.132  -1.731   2.515  1.00  9.25           C
ATOM   1338  CB  GLU A 191      21.467  -0.971   2.514  1.00 10.18           C
ATOM   1339  CG  GLU A 191      21.603   0.119   3.580  1.00  9.38           C
ATOM   1340  CD  GLU A 191      21.107   1.502   3.161  1.00  8.37           C
ATOM   1341  OE1 GLU A 191      20.275   1.643   2.242  1.00  8.53           O
ATOM   1342  OE2 GLU A 191      21.540   2.481   3.798  1.00  8.93           O
ATOM   1343  C   GLU A 191      19.931  -2.512   3.821  1.00 11.64           C
ATOM   1344  O   GLU A 191      20.433  -3.631   3.972  1.00 11.91           O
ATOM   1345  N   VAL A 192      19.182  -1.932   4.755  1.00 10.37           N
ATOM   1346  CA  VAL A 192      18.874  -2.611   6.004  1.00  9.97           C
ATOM   1347  CB  VAL A 192      18.348  -1.646   7.081  1.00  9.28           C
ATOM   1348  CG1 VAL A 192      17.839  -2.401   8.306  1.00  8.93           C
ATOM   1349  CG2 VAL A 192      19.406  -0.619   7.456  1.00 10.71           C
ATOM   1350  C   VAL A 192      17.868  -3.720   5.720  1.00 11.10           C
ATOM   1351  O   VAL A 192      18.067  -4.869   6.125  1.00 13.23           O
ATOM   1352  N   ILE A 193      16.786  -3.372   5.033  1.00 10.35           N
ATOM   1353  CA  ILE A 193      15.756  -4.354   4.645  1.00 12.16           C
ATOM   1354  CB  ILE A 193      14.583  -3.629   3.958  1.00 15.45           C
ATOM   1355  CG1 ILE A 193      13.741  -2.941   5.041  1.00 20.64           C
ATOM   1356  CD1 ILE A 193      13.004  -1.730   4.543  1.00 30.99           C
ATOM   1357  CG2 ILE A 193      13.704  -4.579   3.152  1.00 17.46           C
ATOM   1358  C   ILE A 193      16.313  -5.518   3.799  1.00 13.09           C
ATOM   1359  O   ILE A 193      15.900  -6.684   3.962  1.00 14.68           O
ATOM   1360  N   MET A 194      17.267  -5.199   2.936  1.00 12.28           N
ATOM   1361  CA  MET A 194      17.851  -6.173   2.013  1.00 12.33           C
ATOM   1362  CB  MET A 194      18.220  -5.509   0.681  1.00 12.32           C
ATOM   1363  CG  MET A 194      17.019  -5.017  -0.130  1.00 12.89           C
ATOM   1364  SD  MET A 194      17.408  -4.352  -1.761  1.00 15.67           S
ATOM   1365  CE  MET A 194      18.449  -2.922  -1.431  1.00  9.92           C
ATOM   1366  C   MET A 194      19.043  -6.925   2.611  1.00 13.92           C
ATOM   1367  O   MET A 194      19.711  -7.681   1.896  1.00 15.36           O
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ATOM   1368  N   ALA A 195      19.289  -6.716   3.906  1.00 13.39           N
ATOM   1369  CA  ALA A 195      20.310  -7.440   4.683  1.00 16.18           C
ATOM   1370  CB  ALA A 195      19.951  -8.936   4.789  1.00 18.84           C
ATOM   1371  C   ALA A 195      21.723  -7.227   4.121  1.00 18.67           C
ATOM   1372  O   ALA A 195      22.548  -8.158   4.059  1.00 15.88           O
ATOM   1373  N   GLN A 196      21.984  -5.991   3.707  1.00 14.01           N
ATOM   1374  CA  GLN A 196      23.280  -5.579   3.144  1.00 14.62           C
ATOM   1375  CB  GLN A 196      23.044  -4.704   1.911  1.00 13.01           C
ATOM   1376  CG  GLN A 196      22.336  -5.442   0.777  1.00 13.15           C
ATOM   1377  CD  GLN A 196      22.064  -4.565  -0.420  1.00 15.39           C
ATOM   1378  OE1 GLN A 196      22.453  -3.398  -0.453  1.00 22.68           O
ATOM   1379  NE2 GLN A 196      21.417  -5.130  -1.427  1.00 17.06           N
ATOM   1380  C   GLN A 196      24.093  -4.814   4.183  1.00 15.02           C
ATOM   1381  O   GLN A 196      23.624  -4.609   5.310  1.00 14.93           O
ATOM   1382  N   HIS A 197      25.315  -4.403   3.817  1.00 15.23           N
ATOM   1383  CA  HIS A 197      26.093  -3.461   4.636  1.00 16.61           C
ATOM   1384  CB  HIS A 197      27.448  -3.171   3.997  1.00 21.44           C
ATOM   1385  CG  HIS A 197      28.442  -4.271   4.174  1.00 28.97           C
ATOM   1386  ND1 HIS A 197      28.507  -5.356   3.326  1.00 33.80           N
ATOM   1387  CE1 HIS A 197      29.472  -6.165   3.727  1.00 39.47           C
ATOM   1388  NE2 HIS A 197      30.038  -5.641   4.799  1.00 26.44           N
ATOM   1389  CD2 HIS A 197      29.409  -4.458   5.104  1.00 32.44           C
ATOM   1390  C   HIS A 197      25.358  -2.129   4.801  1.00 16.57           C
ATOM   1391  O   HIS A 197      24.723  -1.649   3.868  1.00 18.72           O
ATOM   1392  N   TYR A 198      25.430  -1.546   5.993  1.00 13.42           N
ATOM   1393  CA  TYR A 198      24.920  -0.188   6.200  1.00 14.18           C
ATOM   1394  CB  TYR A 198      23.437  -0.184   6.596  1.00 14.48           C
ATOM   1395  CG  TYR A 198      23.103  -0.947   7.858  1.00 16.99           C
ATOM   1396  CD1 TYR A 198      23.030  -0.296   9.091  1.00 19.00           C
ATOM   1397  CE1 TYR A 198      22.702  -0.994  10.252  1.00 22.20           C
ATOM   1398  CZ  TYR A 198      22.432  -2.359  10.175  1.00 26.85           C
ATOM   1399  OH  TYR A 198      22.098  -3.064  11.307  1.00 27.91           O
ATOM   1400  CE2 TYR A 198      22.487  -3.023   8.961  1.00 22.52           C
ATOM   1401  CD2 TYR A 198      22.815  -2.315   7.811  1.00 20.00           C
ATOM   1402  C   TYR A 198      25.756   0.554   7.222  1.00 17.73           C
ATOM   1403  O   TYR A 198      26.511  -0.069   7.989  1.00 16.79           O
ATOM   1404  N   ASP A 199      25.655   1.879   7.197  1.00 15.23           N
ATOM   1405  CA  ASP A 199      26.236   2.720   8.243  1.00 16.10           C
ATOM   1406  CB  ASP A 199      27.605   3.282   7.814  1.00 18.94           C
ATOM   1407  CG  ASP A 199      27.542   4.164   6.553  1.00 24.62           C
ATOM   1408  OD1 ASP A 199      26.455   4.629   6.139  1.00 19.27           O
ATOM   1409  OD2 ASP A 199      28.621   4.414   5.979  1.00 29.26           O
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ATOM   1410  C   ASP A 199      25.237   3.801   8.639  1.00 16.27         C
ATOM   1411  O   ASP A 199      24.018   3.579   8.521  1.00 14.45         O
ATOM   1412  N   GLY A 200      25.739   4.959   9.083  1.00 14.80         N
ATOM   1413  CA  GLY A 200      24.901   6.050   9.562  1.00 16.54         C
ATOM   1414  C   GLY A 200      23.942   6.576   8.515  1.00 13.85         C
ATOM   1415  O   GLY A 200      22.933   7.189   8.855  1.00 13.75         O
ATOM   1416  N   LYS A 201      24.246   6.323   7.237  1.00 11.60         N
ATOM   1417  CA  LYS A 201      23.383   6.776   6.151  1.00 11.78         C
ATOM   1418  CB  LYS A 201      24.026   6.552   4.796  1.00 12.05         C
ATOM   1419  CG  LYS A 201      25.051   7.613   4.435  1.00 17.76         C
ATOM   1420  CD  LYS A 201      25.257   7.551   2.942  1.00 15.42         C
ATOM   1421  CE  LYS A 201      26.364   8.460   2.480  1.00 16.48         C
ATOM   1422  NZ  LYS A 201      26.572   8.231   1.034  1.00 14.61         N
ATOM   1423  C   LYS A 201      22.031   6.070   6.217  1.00 10.94         C
ATOM   1424  O   LYS A 201      21.051   6.595   5.688  1.00 10.13         O
ATOM   1425  N   ALA A 202      21.978   4.914   6.888  1.00 10.45         N
ATOM   1426  CA  ALA A 202      20.684   4.249   7.112  1.00 10.06         C
ATOM   1427  CB  ALA A 202      20.864   2.861   7.713  1.00 10.79         C
ATOM   1428  C   ALA A 202      19.733   5.116   7.966  1.00 10.70         C
ATOM   1429  O   ALA A 202      18.535   5.198   7.655  1.00  9.53         O
ATOM   1430  N   ASP A 203      20.261   5.795   8.994  1.00  8.55         N
ATOM   1431  CA  ASP A 203      19.455   6.763   9.770  1.00  9.80         C
ATOM   1432  CB  ASP A 203      20.222   7.279  10.992  1.00 10.51         C
ATOM   1433  CG  ASP A 203      20.304   6.267  12.135  1.00 14.63         C
ATOM   1434  OD1 ASP A 203      19.529   5.282  12.193  1.00 11.63         O
ATOM   1435  OD2 ASP A 203      21.175   6.477  13.014  1.00 14.87         O
ATOM   1436  C   ASP A 203      18.984   7.960   8.925  1.00  9.61         C
ATOM   1437  O   ASP A 203      17.879   8.488   9.139  1.00 10.60         O
ATOM   1438  N   LEU A 204      19.812   8.396   7.977  1.00  9.67         N
ATOM   1439  CA  LEU A 204      19.439   9.506   7.083  1.00 10.05         C
ATOM   1440  CB  LEU A 204      20.637   9.959   6.241  1.00 12.18         C
ATOM   1441  CG  LEU A 204      21.765  10.612   7.067  1.00 12.87         C
ATOM   1442  CD1 LEU A 204      22.923  11.015   6.167  1.00 10.20         C
ATOM   1443  CD2 LEU A 204      21.263  11.814   7.864  1.00 12.89         C
ATOM   1444  C   LEU A 204      18.196   9.190   6.211  1.00  9.72         C
ATOM   1445  O   LEU A 204      17.311  10.052   6.045  1.00  9.52         O
ATOM   1446  N   TRP A 205      18.136   7.959   5.697  1.00 10.06         N
ATOM   1447  CA  TRP A 205      16.955   7.442   5.003  1.00  9.09         C
ATOM   1448  CB  TRP A 205      17.156   5.994   4.552  1.00  9.01         C
ATOM   1449  CG  TRP A 205      15.879   5.388   3.982  1.00  7.60         C
ATOM   1450  CD1 TRP A 205      14.857   4.793   4.681  1.00  8.45         C
ATOM   1451  NE1 TRP A 205      13.887   4.363   3.813  1.00  8.23         N
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ATOM   1452  CE2 TRP A 205     14.255   4.681   2.533  1.00  8.32           C
ATOM   1453  CD2 TRP A 205     15.509   5.330   2.602  1.00  7.87           C
ATOM   1454  CE3 TRP A 205     16.121   5.754   1.409  1.00  8.45           C
ATOM   1455  CZ3 TRP A 205     15.476   5.517   0.197  1.00  8.05           C
ATOM   1456  CH2 TRP A 205     14.209   4.881   0.164  1.00 10.63           C
ATOM   1457  CZ2 TRP A 205     13.594   4.454   1.319  1.00  8.99           C
ATOM   1458  C   TRP A 205     15.735   7.512   5.928  1.00  8.05           C
ATOM   1459  O   TRP A 205     14.679   8.039   5.532  1.00  7.72           O
ATOM   1460  N   SER A 206     15.883   7.004   7.154  1.00  7.72           N
ATOM   1461  CA  SER A 206     14.768   7.011   8.117  1.00  8.00           C
ATOM   1462  CB  SER A 206     15.168   6.407   9.454  1.00  9.04           C
ATOM   1463  OG  SER A 206     15.652   5.095   9.281  1.00  8.43           O
ATOM   1464  C   SER A 206     14.264   8.428   8.323  1.00  7.86           C
ATOM   1465  O   SER A 206     13.060   8.674   8.303  1.00  7.98           O
ATOM   1466  N   ILE A 207     15.205   9.361   8.490  1.00  8.32           N
ATOM   1467  CA AILE A 207     14.876  10.776   8.662  0.50  8.15           C
ATOM   1468  CA BILE A 207     14.863  10.771   8.665  0.50  8.81           C
ATOM   1469  CB AILE A 207     16.149  11.602   8.993  0.50  8.49           C
ATOM   1470  CB BILE A 207     16.112  11.609   9.038  0.50 10.15           C
ATOM   1471  CG1AILE A 207     16.620  11.283  10.417  0.50  8.48           C
ATOM   1472  CG1BILE A 207     16.576  11.234  10.446  0.50 11.02           C
ATOM   1473  CD1AILE A 207     18.012  11.802  10.731  0.50  8.52           C
ATOM   1474  CD1BILE A 207     15.476  11.302  11.480  0.50 15.11           C
ATOM   1475  CG2AILE A 207     15.877  13.092   8.884  0.50  9.13           C
ATOM   1476  CG2BILE A 207     15.799  13.093   9.020  0.50 10.53           C
ATOM   1477  C   ILE A 207     14.116  11.295   7.430  1.00  9.13           C
ATOM   1478  O   ILE A 207     13.066  11.962   7.559  1.00  8.49           O
ATOM   1479  N   GLY A 208     14.619  10.968   6.241  1.00  8.77           N
ATOM   1480  CA  GLY A 208     13.936  11.330   4.988  1.00  8.09           C
ATOM   1481  C   GLY A 208     12.499  10.822   4.958  1.00  8.68           C
ATOM   1482  O   GLY A 208     11.584  11.551   4.540  1.00  7.53           O
ATOM   1483  N   THR A 209     12.290   9.591   5.421  1.00  6.90           N
ATOM   1484  CA  THR A 209     10.923   9.023   5.395  1.00  7.30           C
ATOM   1485  CB  THR A 209     10.863   7.490   5.649  1.00  7.91           C
ATOM   1486  OG1 THR A 209     11.290   7.167   6.973  1.00 10.16           O
ATOM   1487  CG2 THR A 209     11.724   6.746   4.645  1.00  6.23           C
ATOM   1488  C   THR A 209     10.004   9.760   6.367  1.00  8.00           C
ATOM   1489  O   THR A 209      8.840  10.002   6.056  1.00  7.27           O
ATOM   1490  N   ILE A 210     10.554  10.115   7.528  1.00  7.10           N
ATOM   1491  CA  ILE A 210      9.829  10.835   8.566  1.00  7.94           C
ATOM   1492  CB  ILE A 210     10.643  10.868   9.887  1.00  8.25           C
ATOM   1493  CG1 ILE A 210     10.719   9.448  10.480  1.00 11.25           C
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ATOM 1494 CD1 ILE A 210 11.816 9.285 11.516 1.00 10.81 C
ATOM 1495 CG2 ILE A 210 9.973 11.821 10.881 1.00 10.08 C
ATOM 1496 C ILE A 210 9.458 12.243 8.083 1.00 7.01 C
ATOM 1497 O ILE A 210 8.291 12.689 8.227 1.00 7.17 O
ATOM 1498 N VAL A 211 10.439 12.937 7.496 1.00 8.01 N
ATOM 1499 CA VAL A 211 10.214 14.265 6.900 1.00 7.18 C
ATOM 1500 CB VAL A 211 11.533 14.900 6.386 1.00 7.94 C
ATOM 1501 CG1 VAL A 211 11.277 16.205 5.638 1.00 8.47 C
ATOM 1502 CG2 VAL A 211 12.456 15.176 7.577 1.00 7.14 C
ATOM 1503 C VAL A 211 9.125 14.210 5.819 1.00 8.00 C
ATOM 1504 O VAL A 211 8.215 15.055 5.802 1.00 6.87 O
ATOM 1505 N TYR A 212 9.195 13.192 4.961 1.00 7.26 N
ATOM 1506 CA TYR A 212 8.198 12.978 3.903 1.00 7.90 C
ATOM 1507 CB TYR A 212 8.580 11.782 3.024 1.00 7.48 C
ATOM 1508 CG TYR A 212 7.632 11.604 1.855 1.00 8.08 C
ATOM 1509 CD1 TYR A 212 7.916 12.162 0.615 1.00 8.05 C
ATOM 1510 CE1 TYR A 212 7.036 12.012 -0.459 1.00 9.99 C
ATOM 1511 CZ TYR A 212 5.846 11.308 -0.275 1.00 8.75 C
ATOM 1512 OH TYR A 212 4.980 11.157 -1.358 1.00 11.84 O
ATOM 1513 CE2 TYR A 212 5.543 10.753 0.944 1.00 8.71 C
ATOM 1514 CD2 TYR A 212 6.434 10.895 2.009 1.00 8.01 C
ATOM 1515 C TYR A 212 6.794 12.804 4.489 1.00 7.89 C
ATOM 1516 O TYR A 212 5.825 13.396 3.984 1.00 8.87 O
ATOM 1517 N GLN A 213 6.709 12.018 5.560 1.00 7.79 N
ATOM 1518 CA GLN A 213 5.444 11.797 6.266 1.00 8.48 C
ATOM 1519 CB GLN A 213 5.567 10.676 7.288 1.00 8.60 C
ATOM 1520 CG GLN A 213 4.210 10.258 7.870 1.00 10.03 C
ATOM 1521 CD GLN A 213 4.359 9.231 8.970 1.00 11.52 C
ATOM 1522 OE1 GLN A 213 5.326 8.473 8.997 1.00 13.14 O
ATOM 1523 NE2 GLN A 213 3.408 9.210 9.893 1.00 14.85 N
ATOM 1524 C GLN A 213 4.908 13.069 6.917 1.00 8.52 C
ATOM 1525 O GLN A 213 3.698 13.322 6.877 1.00 7.57 O
ATOM 1526 N CYS A 214 5.794 13.890 7.476 1.00 7.33 N
ATOM 1527 CA CYS A 214 5.350 15.172 8.051 1.00 8.63 C
ATOM 1528 CB CYS A 214 6.511 15.922 8.698 1.00 8.75 C
ATOM 1529 SG CYS A 214 7.105 15.177 10.217 1.00 10.60 S
ATOM 1530 C CYS A 214 4.752 16.049 6.967 1.00 8.86 C
ATOM 1531 O CYS A 214 3.749 16.740 7.205 1.00 9.93 O
ATOM 1532 N LEU A 215 5.373 16.010 5.779 1.00 7.39 N
ATOM 1533 CA LEU A 215 4.983 16.868 4.652 1.00 8.40 C
ATOM 1534 CB LEU A 215 6.091 16.898 3.573 1.00 7.56 C
ATOM 1535 CG LEU A 215 5.852 17.794 2.335 1.00 9.17 C

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ATOM   1536  CD1 LEU A 215      6.940  17.529   1.299  1.00  8.96         C
ATOM   1537  CD2 LEU A 215      5.798  19.285   2.658  1.00 10.27         C
ATOM   1538  C   LEU A 215      3.653  16.445   4.020  1.00  8.86         C
ATOM   1539  O   LEU A 215      2.791  17.297   3.718  1.00  9.44         O
ATOM   1540  N   THR A 216      3.473  15.142   3.851  1.00  8.33         N
ATOM   1541  CA  THR A 216      2.365  14.625   3.037  1.00  9.72         C
ATOM   1542  CB  THR A 216      2.867  13.646   1.955  1.00 10.01         C
ATOM   1543  OG1 THR A 216      3.378  12.480   2.601  1.00 10.68         O
ATOM   1544  CG2 THR A 216      3.950  14.279   1.087  1.00 10.76         C
ATOM   1545  C   THR A 216      1.309  13.865   3.818  1.00 10.67         C
ATOM   1546  O   THR A 216      0.219  13.630   3.285  1.00 11.83         O
ATOM   1547  N   GLY A 217      1.637  13.449   5.043  1.00 10.88         N
ATOM   1548  CA  GLY A 217      0.742  12.592   5.845  1.00 12.15         C
ATOM   1549  C   GLY A 217      0.935  11.088   5.662  1.00 13.39         C
ATOM   1550  O   GLY A 217      0.299  10.290   6.351  1.00 16.31         O
ATOM   1551  N   LYS A 218      1.811  10.689   4.744  1.00 12.23         N
ATOM   1552  CA  LYS A 218      2.011   9.265   4.447  1.00 13.74         C
ATOM   1553  CB  LYS A 218      1.218   8.853   3.191  1.00 18.23         C
ATOM   1554  CG  LYS A 218      1.521   9.648   1.932  1.00 24.14         C
ATOM   1555  CD  LYS A 218      0.415   9.529   0.880  1.00 35.83         C
ATOM   1556  CE  LYS A 218     -0.741  10.484   1.138  1.00 42.39         C
ATOM   1557  NZ  LYS A 218     -1.649  10.619  -0.037  1.00 48.34         N
ATOM   1558  C   LYS A 218      3.488   8.944   4.277  1.00 13.02         C
ATOM   1559  O   LYS A 218      4.272   9.827   3.969  1.00  9.64         O
ATOM   1560  N   ALA A 219      3.851   7.682   4.461  1.00 16.70         N
ATOM   1561  CA  ALA A 219      5.232   7.246   4.171  1.00 14.87         C
ATOM   1562  CB  ALA A 219      5.525   5.885   4.788  1.00 16.62         C
ATOM   1563  C   ALA A 219      5.435   7.234   2.654  1.00 12.94         C
ATOM   1564  O   ALA A 219      4.483   7.028   1.902  1.00 14.34         O
ATOM   1565  N   PRO A 220      6.673   7.484   2.181  1.00 11.50         N
ATOM   1566  CA  PRO A 220      6.879   7.560   0.731  1.00 11.13         C
ATOM   1567  CB  PRO A 220      8.320   8.099   0.603  1.00 11.28         C
ATOM   1568  CG  PRO A 220      8.986   7.704   1.887  1.00 10.68         C
ATOM   1569  CD  PRO A 220      7.897   7.846   2.929  1.00 11.81         C
ATOM   1570  C   PRO A 220      6.741   6.250  -0.038  1.00 12.34         C
ATOM   1571  O   PRO A 220      6.375   6.285  -1.207  1.00 12.32         O
ATOM   1572  N   PHE A 221      7.073   5.132   0.606  1.00 13.67         N
ATOM   1573  CA  PHE A 221      7.031   3.812  -0.026  1.00 14.62         C
ATOM   1574  CB  PHE A 221      8.454   3.295  -0.335  1.00 12.76         C
ATOM   1575  CG  PHE A 221      9.311   4.302  -1.038  1.00 12.41         C
ATOM   1576  CD1 PHE A 221      9.147   4.552  -2.400  1.00 11.86         C
ATOM   1577  CE1 PHE A 221      9.923   5.503  -3.046  1.00 12.99         C
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ATOM 1578 CZ PHE A 221 10.871 6.226 -2.328 1.00 11.45 C
ATOM 1579 CE2 PHE A 221 11.047 5.989 -0.977 1.00 11.62 C
ATOM 1580 CD2 PHE A 221 10.271 5.034 -0.325 1.00 11.17 C
ATOM 1581 C PHE A 221 6.309 2.868 0.917 1.00 18.72 C
ATOM 1582 O PHE A 221 6.692 2.705 2.081 1.00 21.93 O
ATOM 1583 N GLN A 222 5.228 2.285 0.427 1.00 23.95 N
ATOM 1584 CA GLN A 222 4.478 1.347 1.244 1.00 28.67 C
ATOM 1585 CB GLN A 222 3.181 1.976 1.790 1.00 28.49 C
ATOM 1586 CG GLN A 222 3.431 3.077 2.821 1.00 35.91 C
ATOM 1587 CD GLN A 222 2.167 3.619 3.458 1.00 34.24 C
ATOM 1588 OE1 GLN A 222 1.374 2.870 4.029 1.00 35.64 O
ATOM 1589 NE2 GLN A 222 1.987 4.937 3.388 1.00 34.65 N
ATOM 1590 C GLN A 222 4.219 0.084 0.454 1.00 19.40 C
ATOM 1591 O GLN A 222 4.256 0.081 -0.776 1.00 19.57 O
ATOM 1592 N ALA A 223 4.024 -0.995 1.192 1.00 21.40 N
ATOM 1593 CA ALA A 223 3.729 -2.287 0.615 1.00 18.86 C
ATOM 1594 CB ALA A 223 5.014 -3.072 0.408 1.00 19.92 C
ATOM 1595 C ALA A 223 2.789 -3.008 1.562 1.00 20.31 C
ATOM 1596 O ALA A 223 2.568 -2.566 2.701 1.00 20.93 O
ATOM 1597 N ALA A 224 2.250 -4.126 1.084 1.00 19.50 N
ATOM 1598 CA ALA A 224 1.233 -4.882 1.796 1.00 21.86 C
ATOM 1599 CB ALA A 224 0.553 -5.832 0.822 1.00 19.91 C
ATOM 1600 C ALA A 224 1.776 -5.644 3.017 1.00 23.06 C
ATOM 1601 O ALA A 224 1.001 -6.074 3.869 1.00 22.03 O
ATOM 1602 N SER A 225 3.105 -5.794 3.088 1.00 17.46 N
ATOM 1603 CA SER A 225 3.798 -6.580 4.113 1.00 18.02 C
ATOM 1604 CB SER A 225 3.631 -8.093 3.852 1.00 17.08 C
ATOM 1605 OG SER A 225 4.380 -8.548 2.728 1.00 16.34 O
ATOM 1606 C SER A 225 5.288 -6.224 4.096 1.00 18.79 C
ATOM 1607 O SER A 225 5.771 -5.726 3.072 1.00 15.52 O
ATOM 1608 N PRO A 226 6.025 -6.500 5.205 1.00 20.48 N
ATOM 1609 CA PRO A 226 7.498 -6.363 5.212 1.00 20.30 C
ATOM 1610 CB PRO A 226 7.887 -6.938 6.574 1.00 18.37 C
ATOM 1611 CG PRO A 226 6.727 -6.592 7.436 1.00 20.53 C
ATOM 1612 CD PRO A 226 5.525 -6.828 6.556 1.00 19.18 C
ATOM 1613 C PRO A 226 8.190 -7.154 4.095 1.00 18.54 C
ATOM 1614 O PRO A 226 9.156 -6.667 3.495 1.00 16.32 O
ATOM 1615 N GLN A 227 7.683 -8.349 3.809 1.00 17.04 N
ATOM 1616 CA GLN A 227 8.206 -9.176 2.722 1.00 19.81 C
ATOM 1617 CB GLN A 227 7.597 -10.589 2.774 1.00 23.78 C
ATOM 1618 CG GLN A 227 7.809 -11.327 4.101 1.00 36.34 C
ATOM 1619 CD GLN A 227 6.552 -11.400 4.975 1.00 44.02 C

ATOM 1620 OE1 GLN A 227 6.099 -10.403 5.557 1.00 21.15 O
ATOM 1621 NE2 GLN A 227 5.993 -12.603 5.085 1.00 64.02 N
ATOM 1622 C GLN A 227 7.995 -8.510 1.345 1.00 17.40 C
ATOM 1623 O GLN A 227 8.907 -8.507 0.493 1.00 15.40 O
ATOM 1624 N ASP A 228 6.809 -7.932 1.136 1.00 17.04 N
ATOM 1625 CA ASP A 228 6.526 -7.214 -0.111 1.00 15.54 C
ATOM 1626 CB ASP A 228 5.040 -6.904 -0.267 1.00 17.96 C
ATOM 1627 CG ASP A 228 4.206 -8.156 -0.527 1.00 26.70 C
ATOM 1628 OD1 ASP A 228 4.645 -9.041 -1.290 1.00 26.00 O
ATOM 1629 OD2 ASP A 228 3.116 -8.254 0.051 1.00 29.18 O
ATOM 1630 C ASP A 228 7.345 -5.933 -0.246 1.00 13.24 C
ATOM 1631 O ASP A 228 7.684 -5.545 -1.359 1.00 12.18 O
ATOM 1632 N LEU A 229 7.636 -5.272 0.876 1.00 13.98 N
ATOM 1633 CA LEU A 229 8.502 -4.074 0.830 1.00 12.14 C
ATOM 1634 CB LEU A 229 8.526 -3.310 2.168 1.00 12.91 C
ATOM 1635 CG LEU A 229 9.277 -1.963 2.159 1.00 14.59 C
ATOM 1636 CD1 LEU A 229 8.538 -0.915 1.345 1.00 14.98 C
ATOM 1637 CD2 LEU A 229 9.503 -1.462 3.578 1.00 17.38 C
ATOM 1638 C LEU A 229 9.909 -4.482 0.400 1.00 13.20 C
ATOM 1639 O LEU A 229 10.510 -3.810 -0.449 1.00 13.23 O
ATOM 1640 N ARG A 230 10.421 -5.586 0.962 1.00 12.27 N
ATOM 1641 CA ARG A 230 11.735 -6.090 0.545 1.00 13.77 C
ATOM 1642 CB ARG A 230 12.175 -7.318 1.351 1.00 13.70 C
ATOM 1643 CG ARG A 230 13.514 -7.871 0.868 1.00 18.61 C
ATOM 1644 CD ARG A 230 14.184 -8.783 1.874 1.00 27.60 C
ATOM 1645 NE ARG A 230 15.448 -9.285 1.331 1.00 26.96 N
ATOM 1646 CZ ARG A 230 16.409 -9.873 2.045 1.00 31.24 C
ATOM 1647 NH1 ARG A 230 16.284 -10.028 3.355 1.00 31.44 N
ATOM 1648 NH2 ARG A 230 17.511 -10.299 1.436 1.00 27.46 N
ATOM 1649 C ARG A 230 11.753 -6.375 -0.963 1.00 15.79 C
ATOM 1650 O ARG A 230 12.659 -5.930 -1.681 1.00 13.44 O
ATOM 1651 N LEU A 231 10.740 -7.097 -1.450 1.00 13.71 N
ATOM 1652 CA LEU A 231 10.634 -7.366 -2.885 1.00 13.35 C
ATOM 1653 CB LEU A 231 9.418 -8.242 -3.186 1.00 15.24 C
ATOM 1654 CG LEU A 231 9.484 -9.674 -2.657 1.00 22.49 C
ATOM 1655 CD1 LEU A 231 8.100 -10.306 -2.728 1.00 25.83 C
ATOM 1656 CD2 LEU A 231 10.504 -10.500 -3.435 1.00 25.33 C
ATOM 1657 C LEU A 231 10.599 -6.101 -3.735 1.00 14.18 C
ATOM 1658 O LEU A 231 11.220 -6.054 -4.796 1.00 14.77 O
ATOM 1659 N PHE A 232 9.880 -5.083 -3.252 1.00 12.59 N
ATOM 1660 CA PHE A 232 9.796 -3.798 -3.928 1.00 11.76 C
ATOM 1661 CB PHE A 232 8.772 -2.889 -3.229 1.00 12.31 C

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ATOM   1662  CG  PHE A 232       8.663  -1.520  -3.848  1.00 17.06          C
ATOM   1663  CD1 PHE A 232       8.092  -1.348  -5.114  1.00 18.67          C
ATOM   1664  CE1 PHE A 232       8.024  -0.079  -5.697  1.00 17.95          C
ATOM   1665  CZ  PHE A 232       8.521   1.025  -5.009  1.00 18.94          C
ATOM   1666  CE2 PHE A 232       9.076   0.870  -3.743  1.00 16.05          C
ATOM   1667  CD2 PHE A 232       9.158  -0.399  -3.174  1.00 19.76          C
ATOM   1668  C   PHE A 232      11.163  -3.114  -4.028  1.00 11.56          C
ATOM   1669  O   PHE A 232      11.529  -2.630  -5.097  1.00 12.23          O
ATOM   1670  N   TYR A 233      11.910  -3.108  -2.917  1.00 11.04          N
ATOM   1671  CA  TYR A 233      13.241  -2.484  -2.877  1.00 10.06          C
ATOM   1672  CB  TYR A 233      13.726  -2.303  -1.435  1.00 10.48          C
ATOM   1673  CG  TYR A 233      13.030  -1.199  -0.653  1.00  9.46          C
ATOM   1674  CD1 TYR A 233      12.247  -0.234  -1.300  1.00 10.62          C
ATOM   1675  CE1 TYR A 233      11.615   0.782  -0.580  1.00 11.66          C
ATOM   1676  CZ  TYR A 233      11.786   0.855   0.806  1.00 10.69          C
ATOM   1677  OH  TYR A 233      11.168   1.867   1.520  1.00  9.62          O
ATOM   1678  CE2 TYR A 233      12.563  -0.086   1.470  1.00 10.22          C
ATOM   1679  CD2 TYR A 233      13.178  -1.108   0.741  1.00 10.13          C
ATOM   1680  C   TYR A 233      14.252  -3.272  -3.715  1.00 10.52          C
ATOM   1681  O   TYR A 233      15.095  -2.676  -4.380  1.00 12.19          O
ATOM   1682  N   GLU A 234      14.123  -4.600  -3.718  1.00 10.93          N
ATOM   1683  CA  GLU A 234      14.978  -5.462  -4.554  1.00 13.91          C
ATOM   1684  CB  GLU A 234      14.777  -6.944  -4.192  1.00 16.09          C
ATOM   1685  CG  GLU A 234      15.377  -7.336  -2.847  1.00 17.97          C
ATOM   1686  CD  GLU A 234      15.054  -8.764  -2.425  1.00 26.79          C
ATOM   1687  OE1 GLU A 234      14.107  -9.363  -2.970  1.00 28.17          O
ATOM   1688  OE2 GLU A 234      15.737  -9.280  -1.519  1.00 31.15          O
ATOM   1689  C   GLU A 234      14.763  -5.232  -6.055  1.00 13.77          C
ATOM   1690  O   GLU A 234      15.724  -5.194  -6.830  1.00 16.39          O
ATOM   1691  N   LYS A 235      13.507  -5.074  -6.463  1.00 15.03          N
ATOM   1692  CA  LYS A 235      13.159  -4.956  -7.875  1.00 14.90          C
ATOM   1693  CB  LYS A 235      11.686  -5.331  -8.089  1.00 15.47          C
ATOM   1694  C   LYS A 235      13.460  -3.577  -8.479  1.00 18.77          C
ATOM   1695  O   LYS A 235      13.807  -3.471  -9.663  1.00 24.21          O
ATOM   1696  N   ASN A 236      13.346  -2.532  -7.663  1.00 15.74          N
ATOM   1697  CA  ASN A 236      13.404  -1.155  -8.143  1.00 15.13          C
ATOM   1698  CB  ASN A 236      12.203  -0.366  -7.599  1.00 16.23          C
ATOM   1699  CG  ASN A 236      10.886  -0.881  -8.133  1.00 20.94          C
ATOM   1700  OD1 ASN A 236      10.424  -0.432  -9.180  1.00 32.50          O
ATOM   1701  ND2 ASN A 236      10.288  -1.847  -7.441  1.00 19.90          N
ATOM   1702  C   ASN A 236      14.712  -0.505  -7.739  1.00 16.18          C
ATOM   1703  O   ASN A 236      14.875  -0.100  -6.592  1.00 15.89          O
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ATOM   1704  N   LYS A 237      15.661  -0.445  -8.680  1.00 15.09           N
ATOM   1705  CA  LYS A 237      17.013   0.050  -8.380  1.00 17.57           C
ATOM   1706  CB  LYS A 237      18.043  -0.460  -9.404  1.00 19.71           C
ATOM   1707  CG  LYS A 237      17.987  -1.960  -9.680  1.00 26.62           C
ATOM   1708  CD  LYS A 237      18.581  -2.780  -8.551  1.00 31.17           C
ATOM   1709  CE  LYS A 237      18.777  -4.232  -8.968  1.00 37.28           C
ATOM   1710  NZ  LYS A 237      17.498  -4.995  -8.923  1.00 34.31           N
ATOM   1711  C   LYS A 237      17.059   1.582  -8.266  1.00 16.03           C
ATOM   1712  O   LYS A 237      18.034   2.136  -7.759  1.00 15.65           O
ATOM   1713  N   THR A 238      15.992   2.249  -8.712  1.00 15.84           N
ATOM   1714  CA  THR A 238      15.851   3.697  -8.585  1.00 17.14           C
ATOM   1715  CB  THR A 238      15.897   4.403  -9.963  1.00 17.43           C
ATOM   1716  OG1 THR A 238      17.133   4.094 -10.619  1.00 20.13           O
ATOM   1717  CG2 THR A 238      15.777   5.930  -9.816  1.00 19.61           C
ATOM   1718  C   THR A 238      14.526   3.976  -7.881  1.00 16.71           C
ATOM   1719  O   THR A 238      13.453   3.671  -8.416  1.00 17.56           O
ATOM   1720  N   LEU A 239      14.607   4.540  -6.678  1.00 12.67           N
ATOM   1721  CA  LEU A 239      13.406   4.953  -5.932  1.00 12.48           C
ATOM   1722  CB  LEU A 239      13.459   4.442  -4.483  1.00 12.21           C
ATOM   1723  CG  LEU A 239      13.532   2.926  -4.266  1.00 13.43           C
ATOM   1724  CD1 LEU A 239      13.771   2.636  -2.793  1.00 13.52           C
ATOM   1725  CD2 LEU A 239      12.302   2.189  -4.776  1.00 15.80           C
ATOM   1726  C   LEU A 239      13.280   6.471  -5.951  1.00 13.16           C
ATOM   1727  O   LEU A 239      14.235   7.186  -5.627  1.00 14.51           O
ATOM   1728  N   VAL A 240      12.112   6.968  -6.351  1.00 12.93           N
ATOM   1729  CA  VAL A 240      11.868   8.406  -6.359  1.00 13.19           C
ATOM   1730  CB  VAL A 240      11.775   9.029  -7.785  1.00 13.73           C
ATOM   1731  CG1 VAL A 240      11.676  10.552  -7.696  1.00 12.59           C
ATOM   1732  CG2 VAL A 240      12.974   8.661  -8.648  1.00 16.46           C
ATOM   1733  C   VAL A 240      10.568   8.647  -5.590  1.00 13.50           C
ATOM   1734  O   VAL A 240       9.508   8.157  -5.999  1.00 15.68           O
ATOM   1735  N   PRO A 241      10.644   9.382  -4.465  1.00 12.31           N
ATOM   1736  CA  PRO A 241       9.405   9.675  -3.753  1.00 12.48           C
ATOM   1737  CB  PRO A 241       9.901  10.268  -2.425  1.00 11.54           C
ATOM   1738  CG  PRO A 241      11.215  10.905  -2.766  1.00 11.73           C
ATOM   1739  CD  PRO A 241      11.816  10.052  -3.855  1.00 10.47           C
ATOM   1740  C   PRO A 241       8.570  10.675  -4.569  1.00 13.26           C
ATOM   1741  O   PRO A 241       9.145  11.491  -5.289  1.00 12.67           O
ATOM   1742  N   THR A 242       7.243  10.575  -4.483  1.00 12.16           N
ATOM   1743  CA  THR A 242       6.346  11.509  -5.177  1.00 14.21           C
ATOM   1744  CB  THR A 242       4.940  10.901  -5.358  1.00 15.20           C
ATOM   1745  OG1 THR A 242       5.052   9.643  -6.027  1.00 20.24           O
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ATOM 1746 CG2 THR A 242 4.061 11.825 -6.195 1.00 19.46 C
ATOM 1747 C THR A 242 6.225 12.785 -4.335 1.00 12.78 C
ATOM 1748 O THR A 242 5.535 12.791 -3.327 1.00 15.70 O
ATOM 1749 N ILE A 243 6.902 13.850 -4.747 1.00 12.65 N
ATOM 1750 CA ILE A 243 6.915 15.081 -3.946 1.00 11.20 C
ATOM 1751 CB ILE A 243 8.341 15.678 -3.879 1.00 10.81 C
ATOM 1752 CG1 ILE A 243 9.280 14.655 -3.222 1.00 12.64 C
ATOM 1753 CD1 ILE A 243 10.747 14.992 -3.350 1.00 15.58 C
ATOM 1754 CG2 ILE A 243 8.348 17.003 -3.119 1.00 11.89 C
ATOM 1755 C ILE A 243 5.929 16.064 -4.571 1.00 11.50 C
ATOM 1756 O ILE A 243 6.049 16.363 -5.757 1.00 13.24 O
ATOM 1757 N PRO A 244 4.963 16.578 -3.778 1.00 10.99 N
ATOM 1758 CA PRO A 244 3.954 17.485 -4.335 1.00 13.87 C
ATOM 1759 CB PRO A 244 3.196 17.959 -3.094 1.00 12.11 C
ATOM 1760 CG PRO A 244 3.321 16.834 -2.130 1.00 12.88 C
ATOM 1761 CD PRO A 244 4.718 16.298 -2.348 1.00 11.58 C
ATOM 1762 C PRO A 244 4.558 18.687 -5.070 1.00 14.28 C
ATOM 1763 O PRO A 244 5.633 19.170 -4.694 1.00 12.77 O
ATOM 1764 N ARG A 245 3.860 19.166 -6.101 1.00 15.80 N
ATOM 1765 CA ARG A 245 4.317 20.310 -6.907 1.00 15.27 C
ATOM 1766 CB ARG A 245 3.290 20.609 -8.022 1.00 23.02 C
ATOM 1767 CG ARG A 245 3.657 21.774 -8.945 1.00 29.79 C
ATOM 1768 CD ARG A 245 2.641 22.013 -10.062 1.00 34.54 C
ATOM 1769 NE ARG A 245 2.635 20.938 -11.056 1.00 46.17 N
ATOM 1770 CZ ARG A 245 3.458 20.849 -12.103 1.00 42.95 C
ATOM 1771 NH1 ARG A 245 4.386 21.774 -12.331 1.00 47.84 N
ATOM 1772 NH2 ARG A 245 3.351 19.817 -12.930 1.00 46.31 N
ATOM 1773 C ARG A 245 4.585 21.561 -6.051 1.00 15.03 C
ATOM 1774 O ARG A 245 5.525 22.310 -6.306 1.00 16.39 O
ATOM 1775 N GLU A 246 3.763 21.754 -5.018 1.00 15.36 N
ATOM 1776 CA GLU A 246 3.842 22.937 -4.155 1.00 14.44 C
ATOM 1777 CB GLU A 246 2.509 23.169 -3.414 1.00 13.80 C
ATOM 1778 CG GLU A 246 2.122 22.105 -2.384 1.00 17.37 C
ATOM 1779 CD GLU A 246 1.271 20.984 -2.953 1.00 17.52 C
ATOM 1780 OE1 GLU A 246 1.277 20.757 -4.189 1.00 16.08 O
ATOM 1781 OE2 GLU A 246 0.590 20.313 -2.153 1.00 17.43 O
ATOM 1782 C GLU A 246 5.008 22.960 -3.167 1.00 13.39 C
ATOM 1783 O GLU A 246 5.275 23.989 -2.558 1.00 14.09 O
ATOM 1784 N THR A 247 5.714 21.838 -3.021 1.00 10.83 N
ATOM 1785 CA THR A 247 6.862 21.764 -2.110 1.00 10.79 C
ATOM 1786 CB THR A 247 7.420 20.324 -2.055 1.00 9.30 C
ATOM 1787 OG1 THR A 247 6.343 19.398 -1.868 1.00 10.07 O

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ATOM   1788  CG2 THR A 247       8.480  20.137  -0.939  1.00  9.89           C
ATOM   1789  C   THR A 247       7.957  22.715  -2.571  1.00 11.14           C
ATOM   1790  O   THR A 247       8.199  22.865  -3.776  1.00 13.19           O
ATOM   1791  N   SER A 248       8.593  23.376  -1.607  1.00  9.79           N
ATOM   1792  CA  SER A 248       9.661  24.337  -1.902  1.00 10.58           C
ATOM   1793  CB  SER A 248      10.091  25.069  -0.633  1.00 10.90           C
ATOM   1794  OG  SER A 248      10.870  24.256   0.232  1.00 11.16           O
ATOM   1795  C   SER A 248      10.855  23.619  -2.530  1.00 11.29           C
ATOM   1796  O   SER A 248      11.073  22.425  -2.273  1.00 11.56           O
ATOM   1797  N   ALA A 249      11.593  24.331  -3.376  1.00 11.57           N
ATOM   1798  CA  ALA A 249      12.788  23.744  -4.016  1.00 11.48           C
ATOM   1799  CB  ALA A 249      13.440  24.731  -4.996  1.00 13.01           C
ATOM   1800  C   ALA A 249      13.815  23.147  -3.026  1.00 13.29           C
ATOM   1801  O   ALA A 249      14.269  22.030  -3.259  1.00 12.51           O
ATOM   1802  N   PRO A 250      14.177  23.861  -1.925  1.00 11.45           N
ATOM   1803  CA  PRO A 250      15.152  23.255  -0.989  1.00 11.93           C
ATOM   1804  CB  PRO A 250      15.360  24.358   0.073  1.00 12.58           C
ATOM   1805  CG  PRO A 250      15.033  25.619  -0.663  1.00 13.56           C
ATOM   1806  CD  PRO A 250      13.847  25.241  -1.500  1.00 12.90           C
ATOM   1807  C   PRO A 250      14.655  21.964  -0.333  1.00  9.83           C
ATOM   1808  O   PRO A 250      15.426  21.012  -0.196  1.00  9.71           O
ATOM   1809  N   LEU A 251      13.373  21.911   0.027  1.00  8.46           N
ATOM   1810  CA  LEU A 251      12.821  20.695   0.650  1.00  8.54           C
ATOM   1811  CB  LEU A 251      11.467  20.949   1.336  1.00  8.64           C
ATOM   1812  CG  LEU A 251      10.865  19.752   2.120  1.00  8.19           C
ATOM   1813  CD1 LEU A 251      11.853  19.148   3.115  1.00  9.45           C
ATOM   1814  CD2 LEU A 251       9.584  20.170   2.836  1.00  9.86           C
ATOM   1815  C   LEU A 251      12.748  19.543  -0.342  1.00  7.66           C
ATOM   1816  O   LEU A 251      13.098  18.409   0.027  1.00  7.93           O
ATOM   1817  N   ARG A 252      12.335  19.843  -1.583  1.00  8.17           N
ATOM   1818  CA AARG A 252      12.315  18.854  -2.661  0.50  7.65           C
ATOM   1819  CA BARG A 252      12.312  18.854  -2.660  0.50  8.00           C
ATOM   1820  CB AARG A 252      11.823  19.479  -3.976  0.50  8.44           C
ATOM   1821  CB BARG A 252      11.805  19.474  -3.975  0.50  9.59           C
ATOM   1822  CG AARG A 252      11.778  18.505  -5.153  0.50  8.84           C
ATOM   1823  CG BARG A 252      11.770  18.501  -5.155  0.50 10.93           C
ATOM   1824  CD AARG A 252      11.345  19.208  -6.430  0.50  8.92           C
ATOM   1825  CD BARG A 252      11.198  19.143  -6.411  0.50 12.09           C
ATOM   1826  NE AARG A 252      10.146  20.013  -6.190  0.50  9.93           N
ATOM   1827  NE BARG A 252       9.785  19.483  -6.238  0.50 14.50           N
ATOM   1828  CZ AARG A 252       8.914  19.515  -6.157  0.50 10.24           C
ATOM   1829  CZ BARG A 252       9.326  20.701  -5.958  0.50 14.86           C
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ATOM 1830 NH1AARG A 252 7.877 20.306 -5.922 0.50 10.15 N
ATOM 1831 NH1BARG A 252 8.024 20.892 -5.809 0.50 15.43 N
ATOM 1832 NH2AARG A 252 8.718 18.222 -6.370 0.50 10.22 N
ATOM 1833 NH2BARG A 252 10.158 21.731 -5.832 0.50 17.77 N
ATOM 1834 C ARG A 252 13.701 18.251 -2.849 1.00 7.88 C
ATOM 1835 O ARG A 252 13.849 17.034 -2.939 1.00 7.73 O
ATOM 1836 N GLN A 253 14.714 19.118 -2.916 1.00 7.76 N
ATOM 1837 CA GLN A 253 16.081 18.653 -3.126 1.00 8.81 C
ATOM 1838 CB GLN A 253 16.998 19.848 -3.358 1.00 10.72 C
ATOM 1839 CG GLN A 253 18.400 19.452 -3.770 1.00 14.10 C
ATOM 1840 CD GLN A 253 19.332 20.614 -3.657 1.00 20.86 C
ATOM 1841 OE1 GLN A 253 19.632 21.073 -2.556 1.00 20.79 O
ATOM 1842 NE2 GLN A 253 19.781 21.117 -4.796 1.00 20.14 N
ATOM 1843 C GLN A 253 16.569 17.782 -1.975 1.00 9.12 C
ATOM 1844 O GLN A 253 17.169 16.722 -2.213 1.00 8.39 O
ATOM 1845 N LEU A 254 16.279 18.213 -0.746 1.00 7.32 N
ATOM 1846 CA LEU A 254 16.660 17.468 0.453 1.00 8.23 C
ATOM 1847 CB LEU A 254 16.293 18.241 1.725 1.00 8.39 C
ATOM 1848 CG LEU A 254 16.591 17.576 3.084 1.00 10.50 C
ATOM 1849 CD1 LEU A 254 18.066 17.221 3.266 1.00 13.93 C
ATOM 1850 CD2 LEU A 254 16.146 18.481 4.226 1.00 14.86 C
ATOM 1851 C LEU A 254 16.023 16.086 0.474 1.00 8.21 C
ATOM 1852 O LEU A 254 16.705 15.094 0.730 1.00 7.93 O
ATOM 1853 N LEU A 255 14.721 16.029 0.194 1.00 7.61 N
ATOM 1854 CA LEU A 255 13.991 14.765 0.202 1.00 6.72 C
ATOM 1855 CB LEU A 255 12.488 15.024 0.061 1.00 7.37 C
ATOM 1856 CG LEU A 255 11.847 15.468 1.370 1.00 8.09 C
ATOM 1857 CD1 LEU A 255 11.893 14.334 2.393 1.00 7.20 C
ATOM 1858 CD2 LEU A 255 10.414 15.885 1.088 1.00 9.68 C
ATOM 1859 C LEU A 255 14.495 13.802 -0.874 1.00 7.17 C
ATOM 1860 O LEU A 255 14.708 12.637 -0.582 1.00 7.95 O
ATOM 1861 N LEU A 256 14.745 14.308 -2.086 1.00 7.34 N
ATOM 1862 CA LEU A 256 15.312 13.471 -3.151 1.00 8.29 C
ATOM 1863 CB LEU A 256 15.392 14.239 -4.479 1.00 9.01 C
ATOM 1864 CG LEU A 256 14.019 14.512 -5.135 1.00 8.79 C
ATOM 1865 CD1 LEU A 256 14.178 15.448 -6.336 1.00 10.66 C
ATOM 1866 CD2 LEU A 256 13.276 13.222 -5.498 1.00 11.95 C
ATOM 1867 C LEU A 256 16.678 12.878 -2.777 1.00 8.73 C
ATOM 1868 O LEU A 256 16.971 11.735 -3.112 1.00 9.80 O
ATOM 1869 N ALA A 257 17.488 13.661 -2.060 1.00 9.29 N
ATOM 1870 CA ALA A 257 18.852 13.256 -1.676 1.00 8.59 C
ATOM 1871 CB ALA A 257 19.697 14.495 -1.407 1.00 8.02 C

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ATOM   1872  C   ALA A 257     18.891  12.304  -0.480  1.00 10.28         C
ATOM   1873  O   ALA A 257     19.786  11.428  -0.380  1.00  6.39         O
ATOM   1874  N   LEU A 258     17.923  12.467   0.433  1.00  7.79         N
ATOM   1875  CA  LEU A 258     17.811  11.560   1.578  1.00  7.68         C
ATOM   1876  CB  LEU A 258     16.960  12.187   2.667  1.00  7.63         C
ATOM   1877  CG  LEU A 258     17.593  13.337   3.450  1.00  8.79         C
ATOM   1878  CD1 LEU A 258     16.551  13.934   4.389  1.00  8.62         C
ATOM   1879  CD2 LEU A 258     18.848  12.924   4.232  1.00  8.60         C
ATOM   1880  C   LEU A 258     17.215  10.233   1.137  1.00  8.51         C
ATOM   1881  O   LEU A 258     17.613   9.169   1.626  1.00  9.92         O
ATOM   1882  N   LEU A 259     16.278  10.301   0.198  1.00  8.33         N
ATOM   1883  CA  LEU A 259     15.560   9.098  -0.246  1.00  8.46         C
ATOM   1884  CB  LEU A 259     14.049   9.369  -0.373  1.00  8.68         C
ATOM   1885  CG  LEU A 259     13.418   9.719   0.983  1.00  8.04         C
ATOM   1886  CD1 LEU A 259     11.977  10.180   0.789  1.00  8.95         C
ATOM   1887  CD2 LEU A 259     13.482   8.584   1.997  1.00  9.33         C
ATOM   1888  C   LEU A 259     16.157   8.465  -1.508  1.00 10.23         C
ATOM   1889  O   LEU A 259     15.446   8.101  -2.463  1.00 11.05         O
ATOM   1890  N   GLN A 260     17.480   8.327  -1.487  1.00  8.51         N
ATOM   1891  CA  GLN A 260     18.208   7.574  -2.513  1.00  9.39         C
ATOM   1892  CB  GLN A 260     19.628   8.112  -2.678  1.00  9.49         C
ATOM   1893  CG  GLN A 260     19.699   9.495  -3.321  1.00 11.27         C
ATOM   1894  CD  GLN A 260     19.326   9.487  -4.792  1.00 12.57         C
ATOM   1895  OE1 GLN A 260     19.698   8.574  -5.542  1.00 12.28         O
ATOM   1896  NE2 GLN A 260     18.594  10.513  -5.220  1.00 13.14         N
ATOM   1897  C   GLN A 260     18.294   6.120  -2.103  1.00  8.44         C
ATOM   1898  O   GLN A 260     18.752   5.803  -0.989  1.00  7.80         O
ATOM   1899  N   ARG A 261     17.859   5.240  -3.000  1.00  8.86         N
ATOM   1900  CA  ARG A 261     17.818   3.789  -2.724  1.00 10.29         C
ATOM   1901  CB  ARG A 261     17.270   3.043  -3.937  1.00 13.15         C
ATOM   1902  CG  ARG A 261     17.029   1.575  -3.658  1.00 16.72         C
ATOM   1903  CD  ARG A 261     17.743   0.767  -4.699  1.00 19.05         C
ATOM   1904  NE  ARG A 261     17.370  -0.643  -4.705  1.00 13.77         N
ATOM   1905  CZ  ARG A 261     18.201  -1.603  -5.100  1.00 17.98         C
ATOM   1906  NH1 ARG A 261     17.811  -2.874  -5.115  1.00 12.74         N
ATOM   1907  NH2 ARG A 261     19.433  -1.281  -5.486  1.00 14.88         N
ATOM   1908  C   ARG A 261     19.213   3.231  -2.391  1.00  9.76         C
ATOM   1909  O   ARG A 261     19.377   2.462  -1.437  1.00  9.02         O
ATOM   1910  N   ASN A 262     20.193   3.649  -3.183  1.00  9.61         N
ATOM   1911  CA  ASN A 262     21.582   3.170  -3.058  1.00 11.09         C
ATOM   1912  CB  ASN A 262     22.204   3.031  -4.459  1.00 10.87         C
ATOM   1913  CG  ASN A 262     21.401   2.101  -5.345  1.00 13.16         C
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ATOM 1914 OD1 ASN A 262 21.135 0.961 -4.970 1.00 14.67 O
ATOM 1915 ND2 ASN A 262 20.980 2.591 -6.505 1.00 15.03 N
ATOM 1916 C ASN A 262 22.359 4.127 -2.192 1.00 9.12 C
ATOM 1917 O ASN A 262 22.460 5.307 -2.537 1.00 9.46 O
ATOM 1918 N HIS A 263 22.881 3.640 -1.053 1.00 9.53 N
ATOM 1919 CA HIS A 263 23.489 4.533 -0.059 1.00 9.92 C
ATOM 1920 CB HIS A 263 23.848 3.787 1.228 1.00 12.22 C
ATOM 1921 CG HIS A 263 24.848 2.687 1.028 1.00 12.86 C
ATOM 1922 ND1 HIS A 263 26.196 2.928 0.877 1.00 15.09 N
ATOM 1923 CE1 HIS A 263 26.830 1.777 0.721 1.00 13.42 C
ATOM 1924 NE2 HIS A 263 25.946 0.799 0.781 1.00 14.20 N
ATOM 1925 CD2 HIS A 263 24.695 1.344 0.968 1.00 15.86 C
ATOM 1926 C HIS A 263 24.701 5.306 -0.614 1.00 10.20 C
ATOM 1927 O HIS A 263 24.967 6.403 -0.160 1.00 11.89 O
ATOM 1928 N LYS A 264 25.392 4.755 -1.620 1.00 12.01 N
ATOM 1929 CA LYS A 264 26.498 5.493 -2.275 1.00 12.29 C
ATOM 1930 CB LYS A 264 27.184 4.663 -3.377 1.00 13.43 C
ATOM 1931 CG LYS A 264 26.409 4.517 -4.681 1.00 13.23 C
ATOM 1932 CD LYS A 264 27.317 4.014 -5.799 1.00 15.92 C
ATOM 1933 CE LYS A 264 26.560 3.802 -7.099 1.00 20.32 C
ATOM 1934 NZ LYS A 264 27.559 3.533 -8.178 1.00 23.58 N
ATOM 1935 C LYS A 264 26.045 6.848 -2.839 1.00 11.83 C
ATOM 1936 O LYS A 264 26.828 7.790 -2.861 1.00 12.98 O
ATOM 1937 N ASP A 265 24.786 6.918 -3.271 1.00 9.92 N
ATOM 1938 CA ASP A 265 24.185 8.116 -3.873 1.00 12.18 C
ATOM 1939 CB ASP A 265 23.157 7.705 -4.929 1.00 13.10 C
ATOM 1940 CG ASP A 265 23.745 6.866 -6.041 1.00 19.96 C
ATOM 1941 OD1 ASP A 265 24.857 7.171 -6.496 1.00 18.80 O
ATOM 1942 OD2 ASP A 265 23.074 5.902 -6.461 1.00 21.83 O
ATOM 1943 C ASP A 265 23.483 9.008 -2.855 1.00 10.99 C
ATOM 1944 O ASP A 265 23.148 10.162 -3.157 1.00 11.38 O
ATOM 1945 N ARG A 266 23.227 8.464 -1.672 1.00 9.12 N
ATOM 1946 CA ARG A 266 22.496 9.192 -0.624 1.00 8.12 C
ATOM 1947 CB ARG A 266 22.001 8.238 0.469 1.00 9.08 C
ATOM 1948 CG ARG A 266 20.882 8.800 1.352 1.00 7.79 C
ATOM 1949 CD ARG A 266 20.346 7.746 2.321 1.00 8.73 C
ATOM 1950 NE ARG A 266 19.934 6.527 1.603 1.00 7.65 N
ATOM 1951 CZ ARG A 266 20.141 5.272 2.026 1.00 7.05 C
ATOM 1952 NH1 ARG A 266 19.775 4.257 1.245 1.00 8.38 N
ATOM 1953 NH2 ARG A 266 20.701 5.013 3.215 1.00 6.90 N
ATOM 1954 C ARG A 266 23.383 10.276 -0.029 1.00 10.54 C
ATOM 1955 O ARG A 266 24.585 10.077 0.154 1.00 11.54 O

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ATOM   1956  N   MET A 267      22.783  11.425   0.242  1.00  7.71           N
ATOM   1957  CA  MET A 267      23.439  12.515   0.988  1.00 11.08           C
ATOM   1958  CB  MET A 267      22.341  13.498   1.403  1.00 15.70           C
ATOM   1959  CG  MET A 267      22.782  14.719   2.177  1.00 18.79           C
ATOM   1960  SD  MET A 267      21.357  15.807   2.441  1.00 23.88           S
ATOM   1961  CE  MET A 267      21.345  16.715   0.896  1.00 22.85           C
ATOM   1962  C   MET A 267      24.158  11.978   2.231  1.00 12.15           C
ATOM   1963  O   MET A 267      23.592  11.141   2.956  1.00 13.35           O
ATOM   1964  N   ASP A 268      25.393  12.441   2.478  1.00 14.67           N
ATOM   1965  CA AASP A 268      26.115  12.081   3.696  0.50 14.53           C
ATOM   1966  CA BASP A 268      26.106  12.059   3.712  0.50 15.35           C
ATOM   1967  CB AASP A 268      27.632  11.893   3.442  0.50 16.92           C
ATOM   1968  CB BASP A 268      27.626  11.912   3.496  0.50 19.43           C
ATOM   1969  CG AASP A 268      28.414  13.203   3.364  0.50 18.96           C
ATOM   1970  CG BASP A 268      28.255  10.810   4.377  0.50 24.70           C
ATOM   1971  OD1AASP A 268      27.833  14.295   3.182  0.50 15.94           O
ATOM   1972  OD1BASP A 268      27.765  10.529   5.502  0.50 21.79           O
ATOM   1973  OD2AASP A 268      29.655  13.125   3.487  0.50 25.28           O
ATOM   1974  OD2BASP A 268      29.253  10.208   3.932  0.50 30.56           O
ATOM   1975  C   ASP A 268      25.785  13.046   4.831  1.00 14.34           C
ATOM   1976  O   ASP A 268      25.079  14.062   4.610  1.00 12.72           O
ATOM   1977  N   PHE A 269      26.266  12.742   6.037  1.00 13.43           N
ATOM   1978  CA  PHE A 269      25.919  13.579   7.179  1.00 14.78           C
ATOM   1979  CB  PHE A 269      26.323  13.014   8.539  1.00 18.74           C
ATOM   1980  CG  PHE A 269      25.689  13.783   9.652  1.00 23.29           C
ATOM   1981  CD1 PHE A 269      24.345  13.566   9.975  1.00 26.92           C
ATOM   1982  CE1 PHE A 269      23.718  14.337  10.946  1.00 25.75           C
ATOM   1983  CZ  PHE A 269      24.428  15.350  11.583  1.00 20.83           C
ATOM   1984  CE2 PHE A 269      25.757  15.589  11.252  1.00 19.94           C
ATOM   1985  CD2 PHE A 269      26.377  14.822  10.285  1.00 22.32           C
ATOM   1986  C   PHE A 269      26.348  15.045   7.069  1.00 13.90           C
ATOM   1987  O   PHE A 269      25.568  15.931   7.417  1.00 13.82           O
ATOM   1988  N   ASP A 270      27.569  15.293   6.595  1.00 15.01           N
ATOM   1989  CA  ASP A 270      28.043  16.676   6.373  1.00 13.86           C
ATOM   1990  CB  ASP A 270      29.431  16.714   5.731  1.00 17.92           C
ATOM   1991  CG  ASP A 270      29.870  18.159   5.402  1.00 19.82           C
ATOM   1992  OD1 ASP A 270      30.069  18.934   6.341  1.00 21.28           O
ATOM   1993  OD2 ASP A 270      29.948  18.538   4.216  1.00 29.78           O
ATOM   1994  C   ASP A 270      27.086  17.509   5.513  1.00 11.98           C
ATOM   1995  O   ASP A 270      26.708  18.627   5.890  1.00 12.78           O
ATOM   1996  N   GLU A 271      26.701  16.953   4.363  1.00 11.63           N
ATOM   1997  CA  GLU A 271      25.814  17.629   3.429  1.00 12.31           C
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ATOM 1998 CB GLU A 271 25.707 16.845 2.112 1.00 12.67 C
ATOM 1999 CG GLU A 271 24.902 17.577 1.035 1.00 15.59 C
ATOM 2000 CD GLU A 271 24.892 16.905 -0.329 1.00 15.06 C
ATOM 2001 OE1 GLU A 271 25.349 15.767 -0.461 1.00 17.69 O
ATOM 2002 OE2 GLU A 271 24.432 17.544 -1.299 1.00 19.96 O
ATOM 2003 C GLU A 271 24.431 17.856 4.055 1.00 13.08 C
ATOM 2004 O GLU A 271 23.832 18.935 3.889 1.00 11.69 O
ATOM 2005 N PHE A 272 23.945 16.851 4.789 1.00 11.94 N
ATOM 2006 CA PHE A 272 22.664 16.967 5.508 1.00 11.81 C
ATOM 2007 CB PHE A 272 22.293 15.619 6.167 1.00 10.64 C
ATOM 2008 CG PHE A 272 21.151 15.708 7.162 1.00 12.10 C
ATOM 2009 CD1 PHE A 272 19.839 15.978 6.735 1.00 12.13 C
ATOM 2010 CE1 PHE A 272 18.788 16.071 7.648 1.00 12.36 C
ATOM 2011 CZ PHE A 272 19.033 15.868 9.006 1.00 12.60 C
ATOM 2012 CE2 PHE A 272 20.336 15.604 9.447 1.00 13.80 C
ATOM 2013 CD2 PHE A 272 21.382 15.515 8.523 1.00 11.19 C
ATOM 2014 C PHE A 272 22.678 18.109 6.538 1.00 12.40 C
ATOM 2015 O PHE A 272 21.800 18.993 6.522 1.00 10.94 O
ATOM 2016 N PHE A 273 23.686 18.091 7.409 1.00 12.54 N
ATOM 2017 CA PHE A 273 23.814 19.068 8.493 1.00 14.10 C
ATOM 2018 CB PHE A 273 25.013 18.758 9.398 1.00 16.43 C
ATOM 2019 CG PHE A 273 25.053 19.601 10.647 1.00 20.80 C
ATOM 2020 CD1 PHE A 273 24.273 19.261 11.768 1.00 28.45 C
ATOM 2021 CE1 PHE A 273 24.302 20.044 12.923 1.00 24.88 C
ATOM 2022 CZ PHE A 273 25.111 21.180 12.968 1.00 24.82 C
ATOM 2023 CE2 PHE A 273 25.889 21.534 11.863 1.00 29.96 C
ATOM 2024 CD2 PHE A 273 25.861 20.747 10.711 1.00 27.03 C
ATOM 2025 C PHE A 273 23.889 20.505 7.974 1.00 13.05 C
ATOM 2026 O PHE A 273 23.312 21.413 8.584 1.00 15.19 O
ATOM 2027 N HIS A 274 24.561 20.690 6.833 1.00 12.46 N
ATOM 2028 CA HIS A 274 24.749 22.012 6.240 1.00 11.66 C
ATOM 2029 CB HIS A 274 26.192 22.170 5.720 1.00 11.45 C
ATOM 2030 CG HIS A 274 27.206 22.087 6.798 1.00 12.78 C
ATOM 2031 ND1 HIS A 274 27.935 20.948 7.043 1.00 13.25 N
ATOM 2032 CE1 HIS A 274 28.736 21.158 8.074 1.00 16.94 C
ATOM 2033 NE2 HIS A 274 28.547 22.391 8.505 1.00 17.43 N
ATOM 2034 CD2 HIS A 274 27.598 22.996 7.720 1.00 14.90 C
ATOM 2035 C HIS A 274 23.753 22.375 5.157 1.00 11.73 C
ATOM 2036 O HIS A 274 23.929 23.389 4.461 1.00 13.06 O
ATOM 2037 N HIS A 275 22.688 21.575 5.012 1.00 10.64 N
ATOM 2038 CA HIS A 275 21.743 21.807 3.932 1.00 10.38 C
ATOM 2039 CB HIS A 275 20.777 20.618 3.744 1.00 10.39 C

ATOM 2040 CG HIS A 275 20.023 20.677 2.449 1.00 10.78 C
ATOM 2041 ND1 HIS A 275 18.868 21.413 2.297 1.00 10.14 N
ATOM 2042 CE1 HIS A 275 18.441 21.313 1.052 1.00 11.73 C
ATOM 2043 NE2 HIS A 275 19.289 20.553 0.382 1.00 11.07 N
ATOM 2044 CD2 HIS A 275 20.297 20.159 1.228 1.00 11.30 C
ATOM 2045 C HIS A 275 20.974 23.122 4.137 1.00 10.53 C
ATOM 2046 O HIS A 275 20.564 23.424 5.260 1.00 13.02 O
ATOM 2047 N PRO A 276 20.767 23.892 3.050 1.00 12.42 N
ATOM 2048 CA PRO A 276 20.050 25.176 3.178 1.00 13.83 C
ATOM 2049 CB PRO A 276 19.952 25.664 1.738 1.00 17.99 C
ATOM 2050 CG PRO A 276 21.151 25.077 1.077 1.00 17.05 C
ATOM 2051 CD PRO A 276 21.309 23.712 1.686 1.00 12.95 C
ATOM 2052 C PRO A 276 18.654 25.056 3.781 1.00 14.25 C
ATOM 2053 O PRO A 276 18.181 26.014 4.402 1.00 14.80 O
ATOM 2054 N PHE A 277 17.995 23.904 3.626 1.00 12.17 N
ATOM 2055 CA PHE A 277 16.661 23.762 4.219 1.00 13.48 C
ATOM 2056 CB PHE A 277 15.940 22.473 3.799 1.00 14.51 C
ATOM 2057 CG PHE A 277 14.556 22.341 4.405 1.00 11.87 C
ATOM 2058 CD1 PHE A 277 13.484 23.079 3.895 1.00 13.96 C
ATOM 2059 CE1 PHE A 277 12.206 22.978 4.466 1.00 14.05 C
ATOM 2060 CZ PHE A 277 12.002 22.144 5.554 1.00 11.30 C
ATOM 2061 CE2 PHE A 277 13.067 21.398 6.074 1.00 11.64 C
ATOM 2062 CD2 PHE A 277 14.338 21.511 5.504 1.00 12.24 C
ATOM 2063 C PHE A 277 16.680 23.893 5.736 1.00 16.96 C
ATOM 2064 O PHE A 277 15.701 24.339 6.331 1.00 15.83 O
ATOM 2065 N LEU A 278 17.780 23.483 6.355 1.00 13.10 N
ATOM 2066 CA LEU A 278 17.929 23.577 7.800 1.00 18.07 C
ATOM 2067 CB LEU A 278 18.943 22.540 8.312 1.00 20.67 C
ATOM 2068 CG LEU A 278 18.465 21.085 8.302 1.00 23.11 C
ATOM 2069 CD1 LEU A 278 19.534 20.164 8.854 1.00 25.79 C
ATOM 2070 CD2 LEU A 278 17.201 20.960 9.121 1.00 31.92 C
ATOM 2071 C LEU A 278 18.238 24.988 8.321 1.00 29.69 C
ATOM 2072 O LEU A 278 18.469 25.164 9.518 1.00 33.88 O
ATOM 2073 N ASP A 279 18.233 25.978 7.424 1.00 30.25 N
ATOM 2074 CA ASP A 279 18.286 27.409 7.785 1.00 41.25 C
ATOM 2075 CB ASP A 279 19.247 28.161 6.855 1.00 45.46 C
ATOM 2076 CG ASP A 279 20.648 28.318 7.441 1.00 48.23 C
ATOM 2077 OD1 ASP A 279 20.978 27.666 8.456 1.00 59.85 O
ATOM 2078 OD2 ASP A 279 21.428 29.111 6.877 1.00 50.97 O
ATOM 2079 C ASP A 279 16.898 28.056 7.735 1.00 44.26 C
ATOM 2080 O ASP A 279 16.140 27.820 6.785 1.00 36.32 O
ATOM 2081 N ALA A 280 16.592 28.876 8.748 1.00 40.74 N

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ATOM   2082  CA  ALA A 280      15.266  29.507   8.957  1.00 43.93           C
ATOM   2083  CB  ALA A 280      15.341  30.551  10.069  1.00 55.60           C
ATOM   2084  C   ALA A 280      14.598  30.098   7.708  1.00 36.41           C
ATOM   2085  O   ALA A 280      15.199  30.890   6.980  1.00 34.24           O
ATOM   2086  N   SER A 283      14.129 -10.969   6.464  1.00 42.34           N
ATOM   2087  CA  SER A 283      15.205 -10.786   7.439  1.00 34.55           C
ATOM   2088  CB  SER A 283      16.517 -10.391   6.746  1.00 39.79           C
ATOM   2089  C   SER A 283      14.844  -9.768   8.515  1.00 34.53           C
ATOM   2090  O   SER A 283      15.239  -9.931   9.678  1.00 32.80           O
ATOM   2091  N   VAL A 284      14.121  -8.713   8.119  1.00 30.22           N
ATOM   2092  CA  VAL A 284      13.613  -7.702   9.059  1.00 33.82           C
ATOM   2093  CB  VAL A 284      14.249  -6.294   8.871  1.00 33.18           C
ATOM   2094  CG1 VAL A 284      15.736  -6.370   8.537  1.00 35.70           C
ATOM   2095  CG2 VAL A 284      14.058  -5.467  10.129  1.00 38.38           C
ATOM   2096  C   VAL A 284      12.087  -7.594   8.951  1.00 31.53           C
ATOM   2097  O   VAL A 284      11.543  -7.439   7.858  1.00 34.02           O
ATOM   2098  N   ARG A 285      11.409  -7.681  10.092  1.00 32.01           N
ATOM   2099  CA  ARG A 285       9.955  -7.551  10.132  1.00 25.90           C
ATOM   2100  CB  ARG A 285       9.288  -8.910  10.408  1.00 30.37           C
ATOM   2101  CG  ARG A 285       9.592  -9.509  11.783  1.00 33.32           C
ATOM   2102  CD  ARG A 285       9.207 -10.975  11.853  1.00 36.88           C
ATOM   2103  NE  ARG A 285      10.007 -11.787  10.930  1.00 36.65           N
ATOM   2104  CZ  ARG A 285       9.760 -13.059  10.620  1.00 39.71           C
ATOM   2105  NH1 ARG A 285       8.727 -13.705  11.158  1.00 30.04           N
ATOM   2106  NH2 ARG A 285      10.553 -13.691   9.765  1.00 33.30           N
ATOM   2107  C   ARG A 285       9.524  -6.499  11.150  1.00 24.70           C
ATOM   2108  O   ARG A 285      10.368  -5.788  11.722  1.00 23.69           O
ATOM   2109  N   LYS A 286       8.205  -6.384  11.335  1.00 23.34           N
ATOM   2110  CA  LYS A 286       7.649  -5.558  12.383  1.00 27.43           C
ATOM   2111  CB  LYS A 286       6.127  -5.451  12.264  1.00 32.65           C
ATOM   2112  CG  LYS A 286       5.632  -4.340  11.361  1.00 37.36           C
ATOM   2113  CD  LYS A 286       4.818  -4.868  10.197  1.00 47.12           C
ATOM   2114  CE  LYS A 286       4.044  -3.740   9.532  1.00 48.67           C
ATOM   2115  NZ  LYS A 286       3.155  -4.229   8.444  1.00 53.38           N
ATOM   2116  C   LYS A 286       8.008  -6.123  13.754  1.00 25.61           C
ATOM   2117  O   LYS A 286       8.023  -7.347  13.963  1.00 20.61           O
ATOM   2118  N   SER A 287       8.295  -5.217  14.684  1.00 21.01           N
ATOM   2119  CA  SER A 287       8.244  -5.537  16.110  1.00 20.28           C
ATOM   2120  CB  SER A 287       8.511  -4.273  16.934  1.00 18.27           C
ATOM   2121  OG  SER A 287       7.647  -3.217  16.538  1.00 24.95           O
ATOM   2122  C   SER A 287       6.842  -6.112  16.380  1.00 20.11           C
ATOM   2123  O   SER A 287       5.909  -5.774  15.640  1.00 18.72           O
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ATOM   2124  N   PRO A 288      6.685  -6.991  17.413  1.00 22.70           N
ATOM   2125  CA  PRO A 288      5.384  -7.636  17.687  1.00 24.42           C
ATOM   2126  CB  PRO A 288      5.684  -8.590  18.853  1.00 23.73           C
ATOM   2127  CG  PRO A 288      7.165  -8.697  18.930  1.00 24.04           C
ATOM   2128  CD  PRO A 288      7.714  -7.415  18.384  1.00 21.78           C
ATOM   2129  C   PRO A 288      4.287  -6.633  18.102  1.00 24.54           C
ATOM   2130  O   PRO A 288      4.615  -5.569  18.639  1.00 19.94           O
ATOM   2131  N   PRO A 289      2.999  -6.966  17.852  1.00 22.81           N
ATOM   2132  CA  PRO A 289      1.901  -6.053  18.198  1.00 25.11           C
ATOM   2133  CB  PRO A 289      0.643  -6.857  17.847  1.00 24.27           C
ATOM   2134  CG  PRO A 289      1.094  -7.850  16.837  1.00 27.72           C
ATOM   2135  CD  PRO A 289      2.488  -8.214  17.246  1.00 20.74           C
ATOM   2136  C   PRO A 289      1.902  -5.708  19.685  1.00 27.96           C
ATOM   2137  O   PRO A 289      2.130  -6.582  20.532  1.00 29.40           O
ATOM   2138  N   VAL A 290      1.664  -4.433  19.976  1.00 30.95           N
ATOM   2139  CA  VAL A 290      1.723  -3.899  21.334  1.00 31.46           C
ATOM   2140  CB  VAL A 290      1.964  -2.370  21.306  1.00 34.23           C
ATOM   2141  CG1 VAL A 290      1.826  -1.762  22.689  1.00 35.29           C
ATOM   2142  CG2 VAL A 290      3.340  -2.050  20.723  1.00 31.37           C
ATOM   2143  C   VAL A 290      0.445  -4.254  22.100  1.00 38.64           C
ATOM   2144  O   VAL A 290      0.502  -4.936  23.126  1.00 36.27           O
TER
HETATM 2145  C1  SX1 I   1     11.551   7.660  26.812  1.00 26.99           C
HETATM 2146  C2  SX1 I   1     11.622   8.787  27.643  1.00 24.10           C
HETATM 2147  C3  SX1 I   1      9.190   8.079  26.313  1.00 17.79           C
HETATM 2148  C4  SX1 I   1     10.358   7.308  26.160  1.00 22.88           C
HETATM 2149  C5  SX1 I   1      9.300   9.201  27.153  1.00 19.41           C
HETATM 2150  C6  SX1 I   1     10.471   9.573  27.808  1.00 17.63           C
HETATM 2151  C7  SX1 I   1     10.411   6.104  25.292  1.00 26.59           C
HETATM 2152  C8  SX1 I   1      7.100   3.683  24.444  1.00 34.20           C
HETATM 2153  C9  SX1 I   1      8.769   2.147  23.375  1.00 39.25           C
HETATM 2154  C10 SX1 I   1      9.079   4.977  22.267  1.00 26.73           C
HETATM 2155  C11 SX1 I   1      8.586   3.391  24.252  1.00 29.56           C
HETATM 2156  C12 SX1 I   1      9.403   4.593  23.708  1.00 29.18           C
HETATM 2157  N13 SX1 I   1      8.419  10.170  27.541  1.00 18.83           N
HETATM 2158  N14 SX1 I   1      8.987  11.068  28.378  1.00 18.72           N
HETATM 2159  N15 SX1 I   1     10.264  10.718  28.538  1.00 16.44           N
HETATM 2160  N16 SX1 I   1      9.293   5.769  24.564  1.00 27.16           N
HETATM 2161  O17 SX1 I   1     11.469   5.469  25.222  1.00 23.51           O
TER
HETATM 2162  O   DMS K   1      6.235  24.665  15.699  1.00 45.19           O
HETATM 2163  S   DMS K   1      6.577  24.556  17.138  1.00 60.63           S
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HETATM 2164  C2  DMS K   1      5.550  25.550  18.080  1.00 51.19          C
HETATM 2165  C1  DMS K   1      8.075  25.318  17.443  1.00 48.87          C
HETATM 2166 CL    CL K   2      5.607  -8.439  10.525  1.00 33.00         CL
TER
HETATM 2167  O   HOH W   1     15.153  10.082  -4.590  1.00 12.77          O
HETATM 2168  O   HOH W   2      6.167  -0.867   8.768  1.00 14.01          O
HETATM 2169  O   HOH W   3      2.706  19.952   4.647  1.00 10.44          O
HETATM 2170  O   HOH W   4     27.385   8.507  -6.573  1.00 37.26          O
HETATM 2171  O   HOH W   5      3.193   8.067  12.539  1.00 21.40          O
HETATM 2172  O   HOH W   6     11.710   2.252   4.022  1.00 13.22          O
HETATM 2173  O   HOH W   7     16.803   4.628  11.780  1.00 10.47          O
HETATM 2174  O   HOH W   8     17.649   7.761  42.817  1.00 27.17          O
HETATM 2175  O   HOH W   9     20.125   5.748  -5.355  1.00 12.98          O
HETATM 2176  O   HOH W  10     20.205  -5.540  41.310  1.00 29.81          O
HETATM 2177  O   HOH W  11      8.395   4.475   3.258  1.00 16.93          O
HETATM 2178  O   HOH W  12      4.269  24.571   4.269  1.00 12.22          O
HETATM 2179  O   HOH W  13     20.883  13.834  26.629  1.00 23.62          O
HETATM 2180  O  AHOH W  14     13.044  -0.924  25.037  0.50 12.49          O
HETATM 2181  O  BHOH W  14     15.337  -0.166  25.141  0.50 16.48          O
HETATM 2182  O   HOH W  15      0.034  21.228   4.543  1.00 47.54          O
HETATM 2183  O   HOH W  16      6.102   8.534  -2.848  1.00 29.21          O
HETATM 2184  O   HOH W  17     25.789  24.405   2.581  1.00 11.22          O
HETATM 2185  O   HOH W  18     16.775   6.064  -5.438  1.00 14.29          O
HETATM 2186  O   HOH W  19     15.990  10.063  50.842  1.00 16.81          O
HETATM 2187  O   HOH W  20      2.596  -4.688  -1.766  1.00 21.30          O
HETATM 2188  O   HOH W  21     14.669  21.462  -5.903  1.00 15.77          O
HETATM 2189  O   HOH W  22     17.293   2.533   8.428  1.00  9.08          O
HETATM 2190  O   HOH W  23     23.911   2.868   5.026  1.00 12.23          O
HETATM 2191  O   HOH W  24     24.706  -1.923   1.139  1.00 19.69          O
HETATM 2192  O   HOH W  25     22.075  23.793   7.483  1.00 18.86          O
HETATM 2193  O   HOH W  26      8.869  13.511  -7.088  1.00 15.25          O
HETATM 2194  O   HOH W  27      4.899  22.411   0.982  1.00 14.58          O
HETATM 2195  O   HOH W  28     29.610   0.541   5.800  1.00 38.28          O
HETATM 2196  O   HOH W  29     14.985  18.806  -6.669  1.00 19.09          O
HETATM 2197  O   HOH W  30     22.502  -6.089   7.296  1.00 21.81          O
HETATM 2198  O   HOH W  31     21.767   0.934  -0.371  1.00 17.21          O
HETATM 2199  O   HOH W  32     10.228  16.039  -7.366  1.00 17.39          O
HETATM 2200  O   HOH W  33     17.904   2.387  18.905  1.00 17.07          O
HETATM 2201  O   HOH W  34     15.082   0.827  22.344  1.00 24.72          O
HETATM 2202  O   HOH W  35     17.717   7.842  -7.456  1.00 24.56          O
HETATM 2203  O   HOH W  36     24.939  14.166  -2.693  1.00 28.99          O
HETATM 2204  O   HOH W  37     11.943   0.954  12.870  1.00 18.49          O
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HETATM 2205  O   HOH W  38      9.406  -1.073  22.295  1.00 18.53          O
HETATM 2206  O   HOH W  39      2.683  -2.314  33.282  1.00 20.01          O
HETATM 2207  O   HOH W  40      3.282   8.296  -3.327  1.00 35.74          O
HETATM 2208  O  AHOH W  41     12.679  26.127   1.848  0.50 14.50          O
HETATM 2209  O  BHOH W  41     14.529  26.393   2.850  0.50  9.32          O
HETATM 2210  O   HOH W  42     15.093  -0.996 -11.434  1.00 28.47          O
HETATM 2211  O   HOH W  43     18.708  19.885  -7.283  1.00 34.79          O
HETATM 2212  O   HOH W  44     24.357  20.938   2.113  1.00 14.61          O
HETATM 2213  O   HOH W  45     -3.263  17.844   5.285  1.00 19.13          O
HETATM 2214  O   HOH W  46     10.991  27.127  -3.707  1.00 17.80          O
HETATM 2215  O   HOH W  47      4.271  20.098  -0.358  1.00 13.58          O
HETATM 2216  O   HOH W  48     27.776   5.396   1.257  1.00 18.37          O
HETATM 2217  O   HOH W  49     29.698  13.255   6.480  1.00 18.04          O
HETATM 2218  O   HOH W  50      2.443  14.874  20.246  1.00 15.87          O
HETATM 2219  O   HOH W  51      6.677   7.141  24.591  1.00 23.57          O
HETATM 2220  O   HOH W  52      6.723  -1.521  19.509  1.00 23.60          O
HETATM 2221  O   HOH W  53      3.196  22.129   2.961  1.00 15.90          O
HETATM 2222  O   HOH W  54      0.661   9.115  13.290  1.00 19.03          O
HETATM 2223  O   HOH W  55     12.210  15.397  33.435  1.00 26.17          O
HETATM 2224  O   HOH W  56     11.699 -11.817  24.534  1.00 27.91          O
HETATM 2225  O   HOH W  57      5.801  26.320   2.335  1.00 33.75          O
HETATM 2226  O   HOH W  58     -3.140  12.274  18.354  1.00 26.58          O
HETATM 2227  O   HOH W  59      5.991  26.983   6.253  1.00 14.35          O
HETATM 2228  O   HOH W  60     27.500  -1.802  19.637  1.00 30.29          O
HETATM 2229  O   HOH W  61     13.465   2.926  11.446  1.00 14.65          O
HETATM 2230  O   HOH W  62      3.854  13.179  27.059  1.00 32.23          O
HETATM 2231  O   HOH W  63      7.091   1.387  19.136  1.00 30.71          O
HETATM 2232  O   HOH W  64     16.836   1.796 -12.060  1.00 26.62          O
HETATM 2233  O   HOH W  65      5.903  26.537  11.940  1.00 17.53          O
HETATM 2234  O   HOH W  66      9.426  -1.524  19.303  1.00 34.60          O
HETATM 2235  O   HOH W  67     11.067  -3.379  34.634  1.00 26.92          O
HETATM 2236  O   HOH W  68     32.611  -6.351   4.606  1.00 15.04          O
HETATM 2237  O   HOH W  69     21.813  -2.814  20.093  1.00 36.44          O
HETATM 2238  O   HOH W  70     11.607  -1.469  17.550  1.00 23.58          O
HETATM 2239  O   HOH W  71     18.776  13.431  -5.340  1.00 19.25          O
HETATM 2240  O   HOH W  72      3.029  27.306  23.902  1.00 48.91          O
HETATM 2241  O   HOH W  73      5.372  -3.108  17.795  1.00 20.68          O
HETATM 2242  O   HOH W  74     17.827  16.506  26.832  1.00 26.60          O
HETATM 2243  O   HOH W  75     -0.698   6.441  27.000  1.00 34.98          O
HETATM 2244  O   HOH W  76     19.695  -5.877   8.007  1.00 22.15          O
HETATM 2245  O   HOH W  77      8.485  18.069  29.143  1.00 29.26          O
HETATM 2246  O   HOH W  78      2.957   5.990  -0.261  1.00 44.62          O
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HETATM 2247  O   HOH W  79      5.977   6.852  21.748  1.00 20.76           O
HETATM 2248  O   HOH W  80      8.037  -0.443  15.710  1.00 23.38           O
HETATM 2249  O   HOH W  81      6.090  -3.038   6.333  1.00 30.84           O
HETATM 2250  O   HOH W  82      3.997   5.161  12.273  1.00 35.39           O
HETATM 2251  O   HOH W  83     14.648   6.605  25.508  1.00 28.76           O
HETATM 2252  O   HOH W  84     18.171  12.470  43.529  1.00 36.26           O
HETATM 2253  O   HOH W  85     26.683  -3.381   8.141  1.00 31.93           O
HETATM 2254  O   HOH W  86      2.319  18.549   1.076  1.00 20.76           O
HETATM 2255  O   HOH W  87      1.761  13.549   8.777  1.00 26.50           O
HETATM 2256  O   HOH W  88     22.327  12.872  -2.693  1.00 26.15           O
HETATM 2257  O   HOH W  89     28.226   6.420   9.066  1.00 26.09           O
HETATM 2258  O   HOH W  90     15.922   2.074  10.630  1.00 20.25           O
HETATM 2259  O   HOH W  91     23.797  -1.795  30.944  1.00 34.55           O
HETATM 2260  O   HOH W  92     23.390   7.884  12.353  1.00 34.21           O
HETATM 2261  O   HOH W  93     23.264  19.784  23.844  1.00 38.02           O
HETATM 2262  O   HOH W  94      6.329  -5.773  -3.812  1.00 20.66           O
HETATM 2263  O   HOH W  95     25.969  18.485  23.831  1.00 47.48           O
HETATM 2264  O   HOH W  96      9.801   1.333  19.676  1.00 29.25           O
HETATM 2265  O   HOH W  97     15.042  24.435  15.762  1.00 31.62           O
HETATM 2266  O   HOH W  98     13.658  -7.987   5.219  1.00 24.80           O
HETATM 2267  O   HOH W  99      5.225  -8.302  -4.051  1.00 35.25           O
HETATM 2268  O   HOH W 100      6.944  22.302  -8.872  1.00 37.57           O
HETATM 2269  O   HOH W 101      2.940   8.551  38.527  1.00 24.41           O
HETATM 2270  O   HOH W 102     10.056  26.280   3.320  1.00 22.10           O
HETATM 2271  O   HOH W 103     27.814  13.128  25.166  1.00 42.11           O
HETATM 2272  O   HOH W 104     17.049  22.920  -6.505  1.00 39.62           O
HETATM 2273  O   HOH W 105      8.842  27.992  -1.810  1.00 36.90           O
HETATM 2274  O   HOH W 106     21.234  -1.556  39.092  1.00 33.43           O
HETATM 2275  O   HOH W 107     23.268  20.816  18.698  1.00 36.70           O
HETATM 2276  O   HOH W 108     12.249  28.415  -0.745  1.00 35.39           O
HETATM 2277  O   HOH W 109      7.207  31.871  13.655  1.00 29.74           O
HETATM 2278  O   HOH W 110     13.565   1.538 -10.390  1.00 27.23           O
HETATM 2279  O   HOH W 111      4.893  13.618  38.098  1.00 29.27           O
HETATM 2280  O   HOH W 112     26.752  13.844   0.594  1.00 26.15           O
HETATM 2281  O   HOH W 113     10.924 -13.678  26.657  1.00 41.50           O
HETATM 2282  O   HOH W 114      3.914  -6.064  30.248  1.00 37.66           O
HETATM 2283  O   HOH W 115      6.662  12.007  25.202  1.00 31.17           O
HETATM 2284  O   HOH W 116      3.313   4.692  23.267  1.00 27.08           O
HETATM 2285  O   HOH W 117     16.040  21.005  23.638  1.00 40.05           O
HETATM 2286  O   HOH W 118     25.592  18.522  17.804  1.00 29.94           O
HETATM 2287  O   HOH W 119     30.665   2.000   9.228  1.00 41.96           O
HETATM 2288  O   HOH W 120     20.827  11.032  27.443  1.00 37.30           O
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HETATM 2289  O   HOH W 121      29.665  23.322  10.800  1.00 43.72           O
HETATM 2290  O   HOH W 122       2.097   7.379  19.769  1.00 33.25           O
HETATM 2291  O  AHOH W 123       6.470  25.574  -0.312  0.50 16.29           O
HETATM 2292  O  BHOH W 123       4.859  26.258  -1.502  0.50  8.70           O
HETATM 2293  O   HOH W 124      12.721  22.271  -7.705  1.00 24.95           O
HETATM 2294  O   HOH W 125      12.066  -0.503  46.259  1.00 45.91           O
HETATM 2295  O   HOH W 126       4.551 -13.677  24.999  1.00 42.75           O
HETATM 2296  O   HOH W 127      14.743   1.304  19.603  1.00 26.38           O
HETATM 2297  O   HOH W 128       1.523  17.585  -7.070  1.00 23.16           O
HETATM 2298  O  AHOH W 129      27.460   7.589  11.950  0.50 18.90           O
HETATM 2299  O  BHOH W 129      26.062   8.050  12.790  0.50 15.51           O
HETATM 2300  O   HOH W 130       7.096  -3.612  33.978  1.00 37.15           O
HETATM 2301  O   HOH W 131      30.463  10.443   7.065  1.00 40.07           O
HETATM 2302  O   HOH W 132       9.568  -9.560  15.323  1.00 37.50           O
HETATM 2303  O   HOH W 133      21.752  -6.429  27.178  1.00 35.06           O
HETATM 2304  O   HOH W 134      -0.486  18.691  -5.156  1.00 31.52           O
HETATM 2305  O   HOH W 135      11.186   0.583  23.708  1.00 28.35           O
HETATM 2306  O   HOH W 136       6.818   7.081  -5.457  1.00 38.28           O
HETATM 2307  O   HOH W 137       5.406  -1.269   3.964  1.00 43.93           O
HETATM 2308  O   HOH W 138      -2.651  10.849   6.429  1.00 38.74           O
HETATM 2309  O   HOH W 139      31.537  -4.913  29.184  1.00 40.68           O
HETATM 2310  O   HOH W 140      19.459  -7.355  12.580  1.00 43.94           O
HETATM 2311  O   HOH W 141       8.726  -3.870  36.345  1.00 40.18           O
HETATM 2312  O   HOH W 142      28.840   9.685   0.528  1.00 42.21           O
HETATM 2313  O   HOH W 143      11.255  -6.206   5.434  1.00 29.16           O
HETATM 2314  O   HOH W 144      23.506  21.653  15.925  1.00 30.83           O
HETATM 2315  O   HOH W 145      21.951  11.298  30.145  1.00 50.05           O
HETATM 2316  O   HOH W 146      30.192   8.037  12.354  1.00 26.85           O
HETATM 2317  O   HOH W 147       5.914   4.863  -3.596  1.00 42.93           O
HETATM 2318  O   HOH W 148       5.452  32.142  17.291  1.00 33.05           O
HETATM 2319  O   HOH W 149       1.093  23.054  17.657  1.00 44.28           O
HETATM 2320  O   HOH W 150      10.277 -10.994  22.152  1.00 45.22           O
HETATM 2321  O   HOH W 151      24.109  10.625  12.449  1.00 32.32           O
HETATM 2322  O   HOH W 152       1.557   1.595  40.260  1.00 37.06           O
HETATM 2323  O   HOH W 153      26.299   3.749   3.588  1.00 27.21           O
HETATM 2324  O  AHOH W 154       5.065   2.657  20.583  0.50 13.96           O
HETATM 2325  O  BHOH W 154       4.651   4.442  20.834  0.50 15.74           O
HETATM 2326  O   HOH W 155      -1.585  12.146   8.924  1.00 32.66           O
HETATM 2327  O   HOH W 156      16.933  -8.414  11.610  1.00 37.36           O
HETATM 2328  O   HOH W 157      30.026   6.247  -0.455  1.00 37.86           O
HETATM 2329  O   HOH W 158       3.147  -5.742  14.752  1.00 36.65           O
HETATM 2330  O   HOH W 159       6.153   2.821  13.555  1.00 23.38           O
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HETATM 2331  O   HOH W 160      1.421  10.545  -3.728  1.00 39.34           O
HETATM 2332  O   HOH W 161     11.335  17.700  31.847  1.00 39.70           O
HETATM 2333  O   HOH W 162     13.782 -10.110  -5.671  1.00 33.40           O
HETATM 2334  O   HOH W 163      2.160   8.489  22.575  1.00 42.32           O
HETATM 2335  O   HOH W 164     19.092   4.839  -7.937  1.00 32.82           O
HETATM 2336  O   HOH W 165     -1.312  11.780  -3.293  1.00 52.46           O
HETATM 2337  O   HOH W 166     11.625  -8.384  -6.218  1.00 29.05           O
HETATM 2338  O   HOH W 167     -2.404  12.883   4.335  1.00 41.35           O
HETATM 2339  O   HOH W 168     24.836  11.945  -4.917  1.00 42.53           O
HETATM 2340  O   HOH W 169     19.818   6.841  44.621  1.00 42.47           O
HETATM 2341  O   HOH W 170     21.444  21.631  13.536  1.00 37.60           O
HETATM 2342  O   HOH W 171     -1.889  -4.091  17.369  1.00 33.89           O
HETATM 2343  O   HOH W 172     26.552  10.580  -1.803  1.00 28.47           O
HETATM 2344  O   HOH W 173      7.724  27.929   3.918  1.00 36.10           O
HETATM 2345  O   HOH W 174      5.596  19.360  32.143  1.00 40.79           O
HETATM 2346  O   HOH W 175     22.861  21.649  21.527  1.00 45.92           O
HETATM 2347  O   HOH W 176     10.816 -10.941   0.530  1.00 46.46           O
HETATM 2348  O   HOH W 177      8.930 -13.105  -0.432  1.00 53.30           O
HETATM 2349  O   HOH W 178      8.901  -2.485  40.889  1.00 46.06           O
HETATM 2350  O   HOH W 179      2.816  24.781   0.121  1.00 47.10           O
HETATM 2351  O   HOH W 180     15.697  20.933  26.501  1.00 40.74           O
HETATM 2352  O   HOH W 181     10.702   2.804  -8.551  1.00 34.18           O
HETATM 2353  O   HOH W 182      2.587  13.221  -3.133  1.00 33.29           O
HETATM 2354  O   HOH W 183     20.436  -5.132  10.648  1.00 32.67           O
HETATM 2355  O   HOH W 184      6.827  26.597  -3.596  1.00 46.37           O
HETATM 2356  O   HOH W 185     29.575  14.545  13.344  1.00 40.39           O
HETATM 2357  O   HOH W 186      1.332  -7.743   6.313  1.00 38.91           O
HETATM 2358  O   HOH W 187      3.865 -11.222   2.514  1.00 34.07           O
HETATM 2359  O   HOH W 188      2.967  -2.487  16.260  1.00 47.86           O
HETATM 2360  O   HOH W 189     18.013  28.831   3.792  1.00 39.33           O
HETATM 2361  O   HOH W 190     -1.400  -5.470  14.804  1.00 38.65           O
HETATM 2362  O  AHOH W 191     -0.661  10.220  11.106  0.50 11.59           O
HETATM 2363  O  BHOH W 191      0.854  10.581   9.516  0.50 14.63           O
HETATM 2364  O   HOH W 192     24.154  -0.702  -1.759  1.00 22.41           O
HETATM 2365  O   HOH W 193     16.818  24.376  -3.955  1.00 34.13           O
HETATM 2366  O   HOH W 194     17.321  17.445  -6.804  1.00 18.50           O
HETATM 2367  O   HOH W 195     23.464  20.494  -0.390  1.00 18.27           O
HETATM 2368  O   HOH W 196      0.754  -2.694  18.083  1.00 32.86           O
HETATM 2369  O   HOH W 197      4.763   2.195  -3.253  1.00 51.07           O
HETATM 2370  O   HOH W 198      0.554  16.428  -0.095  1.00 27.16           O
HETATM 2371  O   HOH W 199     13.815  18.188  48.888  1.00 25.56           O
HETATM 2372  O   HOH W 200     16.807  -9.780  -5.855  1.00 45.45           O
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HETATM 2373  O   HOH W 201      9.859   4.658  -6.485  1.00 24.81           O
HETATM 2374  O   HOH W 202     12.096  29.900   3.665  1.00 30.56           O
HETATM 2375  O   HOH W 203      1.791  14.766  -5.406  1.00 31.88           O
HETATM 2376  O   HOH W 204      7.937  -5.740  -6.211  1.00 26.19           O
HETATM 2377  O   HOH W 205      7.745  -3.495  -8.166  1.00 43.88           O
HETATM 2378  O   HOH W 206     23.952  -4.705  27.550  1.00 37.02           O
HETATM 2379  O   HOH W 207     27.822  -1.317  31.536  1.00 44.32           O
HETATM 2380  O   HOH W 208     27.387   0.834   4.107  1.00 34.80           O
HETATM 2381  O   HOH W 209     16.520  27.925   1.426  1.00 39.18           O
HETATM 2382  O   HOH W 210      2.532  14.867  41.636  1.00 36.44           O
HETATM 2383  O   HOH W 211     29.104  -0.164   1.723  1.00 25.94           O
HETATM 2384  O   HOH W 212     23.760 -10.088   3.245  1.00 20.73           O
HETATM 2385  O  AHOH W 213      2.651  23.032  11.137  0.50  9.31           O
HETATM 2386  O  BHOH W 213      0.930  23.253  10.494  0.50 18.30           O
HETATM 2387  O   HOH W 214      6.545  17.484  -9.360  1.00 30.72           O
HETATM 2388  O   HOH W 215     24.262   9.750   9.744  1.00 25.92           O
HETATM 2389  O   HOH W 216     -0.004  22.448  -6.347  0.50 26.70           O
HETATM 2390  O   HOH W 217      2.132   6.355   6.914  1.00 31.90           O
HETATM 2391  O   HOH W 218      0.947  23.062   1.967  1.00 31.19           O
HETATM 2392  O   HOH W 219     -0.337  15.439  19.904  1.00 27.32           O
HETATM 2393  O   HOH W 220     31.340  14.740   8.471  1.00 31.26           O
HETATM 2394  O   HOH W 221     16.911 -11.180  23.407  1.00 38.71           O
HETATM 2395  O   HOH W 222      6.037   1.456  16.534  1.00 32.30           O
HETATM 2396  O   HOH W 223      7.322  29.046  14.049  1.00 39.88           O
HETATM 2397  O   HOH W 224     30.414  14.428   1.001  1.00 37.71           O
HETATM 2398  O   HOH W 225      1.389  10.725  24.247  1.00 44.67           O
HETATM 2399  O   HOH W 226      5.745  -5.190  31.965  1.00 39.61           O
HETATM 2400  O   HOH W 227     32.571  16.602   6.127  1.00 36.58           O
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