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HEADER    ISOMERASE                               02-JUL-92   1FKB
TITLE     ATOMIC STRUCTURE OF THE RAPAMYCIN HUMAN IMMUNOPHILIN FKBP-
TITLE    2 12 COMPLEX
COMPND    MOL_ID: 1;
COMPND   2 MOLECULE: FK506 BINDING PROTEIN;
COMPND   3 CHAIN: A;
COMPND   4 ENGINEERED: YES
SOURCE    MOL_ID: 1;
SOURCE   2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
SOURCE   3 ORGANISM_COMMON: HUMAN;
SOURCE   4 ORGANISM_TAXID: 9606
KEYWDS    ISOMERASE
EXPDTA    X-RAY DIFFRACTION
AUTHOR    G.D.VAN DUYNE,R.F.STANDAERT,S.L.SCHREIBER,J.C.CLARDY
REVDAT   2   24-FEB-09 1FKB    1       VERSN
REVDAT   1   31-OCT-93 1FKB    0
JRNL        AUTH   G.D.VAN DUYNE,R.F.STANDAERT,S.L.SCHREIBER,J.CLARDY
JRNL        TITL   ATOMIC STRUCTURE OF THE RAPAMYCIN HUMAN
JRNL        TITL 2 IMMUNOPHILIN FKBP-12 COMPLEX
JRNL        REF    J.AM.CHEM.SOC.                V. 113  7433 1991
JRNL        REFN                   ISSN 0002-7863
REMARK   1
REMARK   2
REMARK   2 RESOLUTION.    1.70 ANGSTROMS.
REMARK   3
REMARK   3 REFINEMENT.
REMARK   3   PROGRAM     : X-PLOR
REMARK   3   AUTHORS     : BRUNGER
REMARK   3
REMARK   3  DATA USED IN REFINEMENT.
REMARK   3   RESOLUTION RANGE HIGH (ANGSTROMS) : 1.70
REMARK   3   RESOLUTION RANGE LOW  (ANGSTROMS) : 10.00
REMARK   3   DATA CUTOFF            (SIGMA(F)) : NULL
REMARK   3   DATA CUTOFF HIGH         (ABS(F)) : NULL
REMARK   3   DATA CUTOFF LOW          (ABS(F)) : NULL
REMARK   3   COMPLETENESS (WORKING+TEST)   (%) : NULL
REMARK   3   NUMBER OF REFLECTIONS             : NULL
REMARK   3
REMARK   3  FIT TO DATA USED IN REFINEMENT.
REMARK   3   CROSS-VALIDATION METHOD          : NULL
REMARK   3   FREE R VALUE TEST SET SELECTION  : NULL
REMARK   3   R VALUE            (WORKING SET) : 0.165
REMARK   3   FREE R VALUE                     : NULL
REMARK   3   FREE R VALUE TEST SET SIZE   (%) : NULL
REMARK   3   FREE R VALUE TEST SET COUNT      : NULL
REMARK   3   ESTIMATED ERROR OF FREE R VALUE  : NULL
REMARK   3
REMARK   3  FIT IN THE HIGHEST RESOLUTION BIN.
REMARK   3   TOTAL NUMBER OF BINS USED           : NULL
REMARK   3   BIN RESOLUTION RANGE HIGH       (A) : NULL
REMARK   3   BIN RESOLUTION RANGE LOW        (A) : NULL
REMARK   3   BIN COMPLETENESS (WORKING+TEST) (%) : NULL
REMARK   3   REFLECTIONS IN BIN    (WORKING SET) : NULL
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REMARK   3   BIN R VALUE           (WORKING SET) : NULL
REMARK   3   BIN FREE R VALUE                    : NULL
REMARK   3   BIN FREE R VALUE TEST SET SIZE  (%) : NULL
REMARK   3   BIN FREE R VALUE TEST SET COUNT     : NULL
REMARK   3   ESTIMATED ERROR OF BIN FREE R VALUE : NULL
REMARK   3
REMARK   3  NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK   3   PROTEIN ATOMS            : 1028
REMARK   3   NUCLEIC ACID ATOMS       : 0
REMARK   3   HETEROGEN ATOMS          : 68
REMARK   3   SOLVENT ATOMS            : 133
REMARK   3
REMARK   3  B VALUES.
REMARK   3   FROM WILSON PLOT           (A**2) : NULL
REMARK   3   MEAN B VALUE      (OVERALL, A**2) : NULL
REMARK   3   OVERALL ANISOTROPIC B VALUE.
REMARK   3    B11 (A**2) : NULL
REMARK   3    B22 (A**2) : NULL
REMARK   3    B33 (A**2) : NULL
REMARK   3    B12 (A**2) : NULL
REMARK   3    B13 (A**2) : NULL
REMARK   3    B23 (A**2) : NULL
REMARK   3
REMARK   3  ESTIMATED COORDINATE ERROR.
REMARK   3   ESD FROM LUZZATI PLOT        (A) : NULL
REMARK   3   ESD FROM SIGMAA              (A) : NULL
REMARK   3   LOW RESOLUTION CUTOFF        (A) : NULL
REMARK   3
REMARK   3  CROSS-VALIDATED ESTIMATED COORDINATE ERROR.
REMARK   3   ESD FROM C-V LUZZATI PLOT    (A) : NULL
REMARK   3   ESD FROM C-V SIGMAA          (A) : NULL
REMARK   3
REMARK   3  RMS DEVIATIONS FROM IDEAL VALUES.
REMARK   3   BOND LENGTHS                 (A) : 0.010
REMARK   3   BOND ANGLES            (DEGREES) : 2.80
REMARK   3   DIHEDRAL ANGLES        (DEGREES) : NULL
REMARK   3   IMPROPER ANGLES        (DEGREES) : NULL
REMARK   3
REMARK   3  ISOTROPIC THERMAL MODEL : NULL
REMARK   3
REMARK   3  ISOTROPIC THERMAL FACTOR RESTRAINTS.    RMS    SIGMA
REMARK   3   MAIN-CHAIN BOND              (A**2) : NULL  ; NULL
REMARK   3   MAIN-CHAIN ANGLE             (A**2) : NULL  ; NULL
REMARK   3   SIDE-CHAIN BOND              (A**2) : NULL  ; NULL
REMARK   3   SIDE-CHAIN ANGLE             (A**2) : NULL  ; NULL
REMARK   3
REMARK   3  NCS MODEL : NULL
REMARK   3
REMARK   3  NCS RESTRAINTS.                         RMS   SIGMA/WEIGHT
REMARK   3   GROUP  1  POSITIONAL             (A) : NULL  ; NULL
REMARK   3   GROUP  1  B-FACTOR           (A**2) : NULL  ; NULL
REMARK   3
REMARK   3  PARAMETER FILE  1  : NULL
REMARK   3  TOPOLOGY FILE  1   : NULL
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REMARK   3
REMARK   3  OTHER REFINEMENT REMARKS: NULL
REMARK   4
REMARK   4 1FKB COMPLIES WITH FORMAT V. 3.15, 01-DEC-08
REMARK 100
REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY BNL.
REMARK 200
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200  EXPERIMENT TYPE                : X-RAY DIFFRACTION
REMARK 200  DATE OF DATA COLLECTION        : NULL
REMARK 200  TEMPERATURE           (KELVIN) : NULL
REMARK 200  PH                             : NULL
REMARK 200  NUMBER OF CRYSTALS USED        : NULL
REMARK 200
REMARK 200  SYNCHROTRON              (Y/N) : NULL
REMARK 200  RADIATION SOURCE               : NULL
REMARK 200  BEAMLINE                       : NULL
REMARK 200  X-RAY GENERATOR MODEL          : NULL
REMARK 200  MONOCHROMATIC OR LAUE    (M/L) : NULL
REMARK 200  WAVELENGTH OR RANGE        (A) : NULL
REMARK 200  MONOCHROMATOR                  : NULL
REMARK 200  OPTICS                         : NULL
REMARK 200
REMARK 200  DETECTOR TYPE                  : NULL
REMARK 200  DETECTOR MANUFACTURER          : NULL
REMARK 200  INTENSITY-INTEGRATION SOFTWARE : NULL
REMARK 200  DATA SCALING SOFTWARE          : NULL
REMARK 200
REMARK 200  NUMBER OF UNIQUE REFLECTIONS   : NULL
REMARK 200  RESOLUTION RANGE HIGH      (A) : NULL
REMARK 200  RESOLUTION RANGE LOW       (A) : NULL
REMARK 200  REJECTION CRITERIA  (SIGMA(I)) : NULL
REMARK 200
REMARK 200 OVERALL.
REMARK 200  COMPLETENESS FOR RANGE     (%) : NULL
REMARK 200  DATA REDUNDANCY                : NULL
REMARK 200  R MERGE                    (I) : NULL
REMARK 200  R SYM                      (I) : NULL
REMARK 200  <I/SIGMA(I)> FOR THE DATA SET  : NULL
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : NULL
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE LOW  (A) : NULL
REMARK 200  COMPLETENESS FOR SHELL     (%) : NULL
REMARK 200  DATA REDUNDANCY IN SHELL       : NULL
REMARK 200  R MERGE FOR SHELL          (I) : NULL
REMARK 200  R SYM FOR SHELL            (I) : NULL
REMARK 200  <I/SIGMA(I)> FOR SHELL         : NULL
REMARK 200
REMARK 200 DIFFRACTION PROTOCOL: NULL
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: NULL
REMARK 200 SOFTWARE USED: MERLOT, X-PLOR
REMARK 200 STARTING MODEL: NULL
REMARK 200
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REMARK 200 REMARK: NULL
REMARK 280
REMARK 280 CRYSTAL
REMARK 280 SOLVENT CONTENT, VS   (%): 52.33
REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): 2.58
REMARK 280
REMARK 280 CRYSTALLIZATION CONDITIONS: NULL
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 21 21 21
REMARK 290
REMARK 290      SYMOP   SYMMETRY
REMARK 290     NNNMMM   OPERATOR
REMARK 290       1555   X,Y,Z
REMARK 290       2555   -X+1/2,-Y,Z+1/2
REMARK 290       3555   -X,Y+1/2,-Z+1/2
REMARK 290       4555   X+1/2,-Y+1/2,-Z
REMARK 290
REMARK 290     WHERE NNN -> OPERATOR NUMBER
REMARK 290           MMM -> TRANSLATION VECTOR
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS
REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM
REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY
REMARK 290 RELATED MOLECULES.
REMARK 290   SMTRY1   1  1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY2   1  0.000000  1.000000  0.000000        0.00000
REMARK 290   SMTRY3   1  0.000000  0.000000  1.000000        0.00000
REMARK 290   SMTRY1   2 -1.000000  0.000000  0.000000       22.71000
REMARK 290   SMTRY2   2  0.000000 -1.000000  0.000000        0.00000
REMARK 290   SMTRY3   2  0.000000  0.000000  1.000000       27.37000
REMARK 290   SMTRY1   3 -1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY2   3  0.000000  1.000000  0.000000       24.58000
REMARK 290   SMTRY3   3  0.000000  0.000000 -1.000000       27.37000
REMARK 290   SMTRY1   4  1.000000  0.000000  0.000000       22.71000
REMARK 290   SMTRY2   4  0.000000 -1.000000  0.000000       24.58000
REMARK 290   SMTRY3   4  0.000000  0.000000 -1.000000        0.00000
REMARK 290
REMARK 290 REMARK: NULL
REMARK 300
REMARK 300 BIOMOLECULE: 1
REMARK 300 SEE REMARK 350 FOR THE AUTHOR PROVIDED AND/OR PROGRAM
REMARK 300 GENERATED ASSEMBLY INFORMATION FOR THE STRUCTURE IN
REMARK 300 THIS ENTRY. THE REMARK MAY ALSO PROVIDE INFORMATION ON
REMARK 300 BURIED SURFACE AREA.
REMARK 350
REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN
REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE
REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS
REMARK 350 GIVEN BELOW.  BOTH NON-CRYSTALLOGRAPHIC AND
REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.
REMARK 350
REMARK 350 BIOMOLECULE: 1
REMARK 350 AUTHOR DETERMINED BIOLOGICAL UNIT: MONOMERIC
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REMARK 350 APPLY THE FOLLOWING TO CHAINS: A
REMARK 350   BIOMT1   1  1.000000  0.000000  0.000000        0.00000
REMARK 350   BIOMT2   1  0.000000  1.000000  0.000000        0.00000
REMARK 350   BIOMT3   1  0.000000  0.000000  1.000000        0.00000
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND LENGTHS
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X,I3,1X,2(A3,1X,A1,I4,A1,1X,A4,3X),1X,F6.3)
REMARK 500
REMARK 500 EXPECTED VALUES PROTEIN: ENGH AND HUBER, 1999
REMARK 500 EXPECTED VALUES NUCLEIC ACID: CLOWNEY ET AL 1996
REMARK 500
REMARK 500  M RES CSSEQI ATM1   RES CSSEQI ATM2   DEVIATION
REMARK 500    HIS A  87   NE2   HIS A  87   CD2    -0.075
REMARK 500
REMARK 500 REMARK: NULL
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND ANGLES
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X,I3,1X,A3,1X,A1,I4,A1,3(1X,A4,2X),12X,F5.1)
REMARK 500
REMARK 500 EXPECTED VALUES PROTEIN: ENGH AND HUBER, 1999
REMARK 500 EXPECTED VALUES NUCLEIC ACID: CLOWNEY ET AL 1996
REMARK 500
REMARK 500  M RES CSSEQI ATM1   ATM2   ATM3
REMARK 500    TRP A  59   CD1 -  CG  -  CD2 ANGL. DEV. =   5.7 DEGREES
REMARK 500
REMARK 500 REMARK: NULL
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: TORSION ANGLES
REMARK 500
REMARK 500 TORSION ANGLES OUTSIDE THE EXPECTED RAMACHANDRAN REGIONS:
REMARK 500 (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER;
REMARK 500 SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT:(10X,I3,1X,A3,1X,A1,I4,A1,4X,F7.2,3X,F7.2)
REMARK 500
REMARK 500 EXPECTED VALUES: GJ KLEYWEGT AND TA JONES (1996). PHI/PSI-
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REMARK 500 CHOLOGY: RAMACHANDRAN REVISITED. STRUCTURE 4, 1395 - 1400
REMARK 500
REMARK 500  M RES CSSEQI        PSI       PHI
REMARK 500    ARG A  13      -42.57   -135.16
REMARK 500    ASN A  43       13.54     60.00
REMARK 500    ALA A  81     -117.61   -131.57
REMARK 500    ILE A  90      -56.84   -125.78
REMARK 500
REMARK 500 REMARK: NULL
REMARK 525
REMARK 525 SOLVENT
REMARK 525
REMARK 525 THE SOLVENT MOLECULES HAVE CHAIN IDENTIFIERS THAT
REMARK 525 INDICATE THE POLYMER CHAIN WITH WHICH THEY ARE MOST
REMARK 525 CLOSELY ASSOCIATED. THE REMARK LISTS ALL THE SOLVENT
REMARK 525 MOLECULES WHICH ARE MORE THAN 5A AWAY FROM THE
REMARK 525 NEAREST POLYMER CHAIN (M = MODEL NUMBER;
REMARK 525 RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE
REMARK 525 NUMBER; I=INSERTION CODE):
REMARK 525
REMARK 525  M RES CSSEQI
REMARK 525    HOH A 191        DISTANCE =  5.54 ANGSTROMS
REMARK 525    HOH A 219        DISTANCE =  6.83 ANGSTROMS
REMARK 525    HOH A 223        DISTANCE =  5.65 ANGSTROMS
REMARK 525    HOH A 233        DISTANCE =  5.82 ANGSTROMS
REMARK 800
REMARK 800 SITE
REMARK 800 SITE_IDENTIFIER: BP
REMARK 800 EVIDENCE_CODE: UNKNOWN
REMARK 800 SITE_DESCRIPTION: NULL
REMARK 800 SITE_IDENTIFIER: AC1
REMARK 800 EVIDENCE_CODE: SOFTWARE
REMARK 800 SITE_DESCRIPTION: BINDING SITE FOR RESIDUE RAP A 108
DBREF  1FKB A    1   107  UNP    P62942   FKB1A_HUMAN      1    107
SEQRES   1 A  107  GLY VAL GLN VAL GLU THR ILE SER PRO GLY ASP GLY ARG
SEQRES   2 A  107  THR PHE PRO LYS ARG GLY GLN THR CYS VAL VAL HIS TYR
SEQRES   3 A  107  THR GLY MET LEU GLU ASP GLY LYS LYS PHE ASP SER SER
SEQRES   4 A  107  ARG ASP ARG ASN LYS PRO PHE LYS PHE MET LEU GLY LYS
SEQRES   5 A  107  GLN GLU VAL ILE ARG GLY TRP GLU GLU GLY VAL ALA GLN
SEQRES   6 A  107  MET SER VAL GLY GLN ARG ALA LYS LEU THR ILE SER PRO
SEQRES   7 A  107  ASP TYR ALA TYR GLY ALA THR GLY HIS PRO GLY ILE ILE
SEQRES   8 A  107  PRO PRO HIS ALA THR LEU VAL PHE ASP VAL GLU LEU LEU
SEQRES   9 A  107  LYS LEU GLU
HET    RAP  A 108      68
HETNAM     RAP RAPAMYCIN IMMUNOSUPPRESSANT DRUG
FORMUL   2  RAP    C51 H79 N O13
FORMUL   3  HOH   *133(H2 O)
HELIX    1   A ARG A   57  VAL A   63  1                                   7
SHEET    1  A1 5 VAL A   2  SER A   8  0
SHEET    2  A1 5 ARG A  71  ILE A  76 -1  O  THR A  75   N  GLN A   3
SHEET    3  A1 5 LEU A  97  LEU A 106 -1  N  LEU A  97   O  ILE A  76
SHEET    4  A1 5 THR A  21  LEU A  30 -1  N  VAL A  23   O  LYS A 105
SHEET    5  A1 5 LYS A  35  SER A  38 -1  N  PHE A  36   O  GLY A  28
SHEET    1  A2 5 VAL A   2  SER A   8  0
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SHEET    2  A2 5 ARG A  71  ILE A  76 -1  N  THR A  75   O  GLN A   3
SHEET    3  A2 5 LEU A  97  LEU A 106 -1  N  LEU A  97   O  ILE A  76
SHEET    4  A2 5 THR A  21  LEU A  30 -1  N  VAL A  23   O  LYS A 105
SHEET    5  A2 5 PHE A  46  MET A  49 -1  N  PHE A  46   O  VAL A  24
SITE     1  BP  6 TYR A  26  PHE A  46  VAL A  55  ILE A  56
SITE     2  BP  6 TRP A  59  PHE A  99
SITE     1 AC1 20 THR A   6  TYR A  26  THR A  27  MET A  29
SITE     2 AC1 20 PHE A  36  ASP A  37  PHE A  46  GLN A  53
SITE     3 AC1 20 GLU A  54  VAL A  55  ILE A  56  TRP A  59
SITE     4 AC1 20 TYR A  82  PHE A  99  ASP A 100  HOH A 126
SITE     5 AC1 20 HOH A 127  HOH A 145  HOH A 189  HOH A 197
CRYST1   45.420   49.160   54.740  90.00  90.00  90.00 P 21 21 21    4
ORIGX1      1.000000  0.000000  0.000000        0.00000
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
SCALE1      0.022017  0.000000  0.000000        0.00000
SCALE2      0.000000  0.020342  0.000000        0.00000
SCALE3      0.000000  0.000000  0.018268        0.00000
ATOM      1  N   GLY A   1      15.915  -2.029   8.513  1.00 11.28           N
ATOM      2  CA  GLY A   1      14.978  -1.665   7.474  1.00 14.35           C
ATOM      3  C   GLY A   1      13.558  -1.877   7.981  1.00 15.91           C
ATOM      4  O   GLY A   1      13.306  -1.692   9.187  1.00 16.11           O
ATOM      5  H1  GLY A   1      15.621  -1.498   9.359  1.00 13.77           H
ATOM      6  H2  GLY A   1      15.806  -3.035   8.734  1.00 13.77           H
ATOM      7  H3  GLY A   1      16.887  -1.796   8.245  1.00 10.73           H
ATOM      8  N   VAL A   2      12.677  -2.258   7.058  1.00 11.40           N
ATOM      9  CA  VAL A   2      11.288  -2.572   7.337  1.00  7.65           C
ATOM     10  C   VAL A   2      10.997  -3.900   6.634  1.00 18.43           C
ATOM     11  O   VAL A   2      11.349  -4.131   5.471  1.00 15.55           O
ATOM     12  CB  VAL A   2      10.348  -1.404   6.904  1.00 14.21           C
ATOM     13  CG1 VAL A   2      10.467  -1.021   5.431  1.00 16.55           C
ATOM     14  CG2 VAL A   2       8.887  -1.700   7.235  1.00 15.47           C
ATOM     15  H   VAL A   2      12.943  -2.422   6.127  1.00  9.02           H
ATOM     16  N   GLN A   3      10.439  -4.825   7.387  1.00  9.33           N
ATOM     17  CA  GLN A   3      10.028  -6.109   6.837  1.00 10.30           C
ATOM     18  C   GLN A   3       8.506  -6.047   6.705  1.00 10.81           C
ATOM     19  O   GLN A   3       7.858  -5.607   7.648  1.00 11.33           O
ATOM     20  CB  GLN A   3      10.455  -7.166   7.821  1.00 13.36           C
ATOM     21  CG  GLN A   3      10.169  -8.570   7.309  1.00 55.99           C
ATOM     22  CD  GLN A   3      10.506  -9.683   8.292  1.00 68.84           C
ATOM     23  OE1 GLN A   3      11.212  -9.503   9.275  1.00 72.87           O
ATOM     24  NE2 GLN A   3      10.044 -10.909   8.101  1.00 57.49           N
ATOM     25  H   GLN A   3      10.217  -4.614   8.319  1.00  9.00           H
ATOM     26 HE21 GLN A   3      10.307 -11.549   8.795  1.00 36.45           H
ATOM     27 HE22 GLN A   3       9.485 -11.129   7.332  1.00 36.45           H
ATOM     28  N   VAL A   4       7.878  -6.429   5.593  1.00 14.73           N
ATOM     29  CA  VAL A   4       6.430  -6.364   5.422  1.00 15.13           C
ATOM     30  C   VAL A   4       5.972  -7.817   5.319  1.00 14.25           C
ATOM     31  O   VAL A   4       6.386  -8.538   4.411  1.00 16.89           O
ATOM     32  CB  VAL A   4       6.069  -5.557   4.135  1.00 11.91           C
ATOM     33  CG1 VAL A   4       4.574  -5.482   3.905  1.00 13.25           C
ATOM     34  CG2 VAL A   4       6.644  -4.148   4.195  1.00  9.78           C
ATOM     35  H   VAL A   4       8.374  -6.815   4.853  1.00 13.59           H
ATOM     36  N   GLU A   5       5.174  -8.303   6.249  1.00  8.60           N
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ATOM     37  CA  GLU A   5       4.637  -9.657   6.191  1.00  9.41           C
ATOM     38  C   GLU A   5       3.122  -9.577   6.038  1.00  7.91           C
ATOM     39  O   GLU A   5       2.492  -8.892   6.835  1.00 14.55           O
ATOM     40  CB  GLU A   5       4.958 -10.352   7.479  1.00  9.26           C
ATOM     41  CG  GLU A   5       6.429 -10.624   7.556  1.00  7.92           C
ATOM     42  CD  GLU A   5       6.796 -11.234   8.891  1.00 28.31           C
ATOM     43  OE1 GLU A   5       7.086 -10.482   9.814  1.00 26.39           O
ATOM     44  OE2 GLU A   5       6.797 -12.460   9.003  1.00 39.66           O
ATOM     45  H   GLU A   5       4.883  -7.720   6.981  1.00  5.83           H
ATOM     46  N   THR A   6       2.483 -10.198   5.049  1.00 11.40           N
ATOM     47  CA  THR A   6       1.050 -10.065   4.801  1.00  9.56           C
ATOM     48  C   THR A   6       0.135 -10.732   5.817  1.00 11.24           C
ATOM     49  O   THR A   6       0.355 -11.888   6.159  1.00 13.61           O
ATOM     50  CB  THR A   6       0.786 -10.568   3.404  1.00 14.22           C
ATOM     51  OG1 THR A   6       1.470  -9.646   2.578  1.00 18.55           O
ATOM     52  CG2 THR A   6      -0.674 -10.584   3.000  1.00 18.19           C
ATOM     53  H   THR A   6       2.987 -10.761   4.441  1.00  7.55           H
ATOM     54  HG1 THR A   6       1.637 -10.053   1.722  1.00 14.49           H
ATOM     55  N   ILE A   7      -0.850 -10.012   6.359  1.00 10.07           N
ATOM     56  CA  ILE A   7      -1.896 -10.635   7.149  1.00  9.55           C
ATOM     57  C   ILE A   7      -3.054 -10.999   6.213  1.00 14.31           C
ATOM     58  O   ILE A   7      -3.600 -12.093   6.327  1.00 15.11           O
ATOM     59  CB  ILE A   7      -2.288  -9.703   8.324  1.00 15.34           C
ATOM     60  CG1 ILE A   7      -1.088  -9.498   9.248  1.00  8.63           C
ATOM     61  CG2 ILE A   7      -3.508 -10.227   9.092  1.00  4.62           C
ATOM     62  CD1 ILE A   7      -1.211  -8.308  10.228  1.00 11.85           C
ATOM     63  H   ILE A   7      -0.835  -9.044   6.238  1.00  5.00           H
ATOM     64  N   SER A   8      -3.465 -10.137   5.280  1.00 16.77           N
ATOM     65  CA  SER A   8      -4.521 -10.403   4.303  1.00 22.81           C
ATOM     66  C   SER A   8      -4.096  -9.684   3.023  1.00 16.94           C
ATOM     67  O   SER A   8      -3.584  -8.557   3.080  1.00 11.53           O
ATOM     68  CB  SER A   8      -5.868  -9.853   4.740  1.00 16.46           C
ATOM     69  OG  SER A   8      -6.033  -9.995   6.140  1.00 42.67           O
ATOM     70  H   SER A   8      -3.009  -9.270   5.208  1.00 10.34           H
ATOM     71  HG  SER A   8      -5.936  -9.106   6.499  1.00 39.81           H
ATOM     72  N   PRO A   9      -4.201 -10.303   1.861  1.00 14.85           N
ATOM     73  CA  PRO A   9      -3.773  -9.717   0.615  1.00 16.28           C
ATOM     74  C   PRO A   9      -4.625  -8.548   0.137  1.00 15.80           C
ATOM     75  O   PRO A   9      -5.822  -8.466   0.374  1.00 16.79           O
ATOM     76  CB  PRO A   9      -3.781 -10.908  -0.331  1.00 17.69           C
ATOM     77  CG  PRO A   9      -4.908 -11.757   0.188  1.00 20.98           C
ATOM     78  CD  PRO A   9      -4.668 -11.683   1.687  1.00 13.76           C
ATOM     79  N   GLY A  10      -3.971  -7.584  -0.490  1.00 11.05           N
ATOM     80  CA  GLY A  10      -4.670  -6.518  -1.160  1.00 12.34           C
ATOM     81  C   GLY A  10      -4.996  -6.956  -2.571  1.00 16.73           C
ATOM     82  O   GLY A  10      -4.919  -8.134  -2.922  1.00 24.91           O
ATOM     83  H   GLY A  10      -3.004  -7.640  -0.556  1.00  8.18           H
ATOM     84  N   ASP A  11      -5.303  -6.001  -3.430  1.00 14.36           N
ATOM     85  CA  ASP A  11      -5.633  -6.357  -4.802  1.00 28.85           C
ATOM     86  C   ASP A  11      -4.434  -6.674  -5.692  1.00 27.10           C
ATOM     87  O   ASP A  11      -4.615  -7.013  -6.860  1.00 20.65           O
ATOM     88  CB  ASP A  11      -6.515  -5.278  -5.442  1.00 23.16           C
ATOM     89  CG  ASP A  11      -5.875  -3.943  -5.797  1.00 17.74           C
ATOM     90  OD1 ASP A  11      -4.693  -3.728  -5.552  1.00 15.46           O
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ATOM     91  OD2 ASP A  11      -6.586  -3.101  -6.329  1.00 19.20           O
ATOM     92  H   ASP A  11      -5.412  -5.082  -3.102  1.00 14.04           H
ATOM     93  N   GLY A  12      -3.211  -6.420  -5.217  1.00 15.02           N
ATOM     94  CA  GLY A  12      -1.994  -6.703  -5.971  1.00 19.67           C
ATOM     95  C   GLY A  12      -1.805  -5.836  -7.210  1.00 16.55           C
ATOM     96  O   GLY A  12      -0.980  -6.150  -8.056  1.00 15.65           O
ATOM     97  H   GLY A  12      -3.125  -6.046  -4.317  1.00 14.44           H
ATOM     98  N   ARG A  13      -2.527  -4.729  -7.349  1.00 11.39           N
ATOM     99  CA  ARG A  13      -2.502  -3.910  -8.541  1.00 11.95           C
ATOM    100  C   ARG A  13      -2.408  -2.438  -8.220  1.00 10.82           C
ATOM    101  O   ARG A  13      -1.685  -1.701  -8.893  1.00 19.47           O
ATOM    102  CB  ARG A  13      -3.768  -4.076  -9.383  1.00 25.46           C
ATOM    103  CG  ARG A  13      -3.946  -5.441 -10.001  1.00 42.88           C
ATOM    104  CD  ARG A  13      -4.558  -5.218 -11.364  1.00 67.90           C
ATOM    105  NE  ARG A  13      -4.520  -6.435 -12.166  1.00 80.80           N
ATOM    106  CZ  ARG A  13      -3.611  -6.646 -13.138  1.00 94.75           C
ATOM    107  NH1 ARG A  13      -2.600  -5.798 -13.398  1.00 98.27           N
ATOM    108  NH2 ARG A  13      -3.707  -7.756 -13.879  1.00 90.34           N
ATOM    109  H   ARG A  13      -3.092  -4.480  -6.604  1.00 10.19           H
ATOM    110  HE  ARG A  13      -5.181  -7.136 -11.990  1.00 50.00           H
ATOM    111 HH11 ARG A  13      -2.481  -4.953 -12.875  1.00 50.00           H
ATOM    112 HH12 ARG A  13      -1.963  -6.006 -14.144  1.00 50.00           H
ATOM    113 HH21 ARG A  13      -4.443  -8.411 -13.713  1.00 50.00           H
ATOM    114 HH22 ARG A  13      -3.044  -7.923 -14.613  1.00 50.00           H
ATOM    115  N   THR A  14      -3.160  -1.969  -7.223  1.00 16.37           N
ATOM    116  CA  THR A  14      -3.242  -0.567  -6.846  1.00 20.68           C
ATOM    117  C   THR A  14      -2.342  -0.232  -5.671  1.00 14.00           C
ATOM    118  O   THR A  14      -2.668  -0.503  -4.509  1.00 12.73           O
ATOM    119  CB  THR A  14      -4.728  -0.226  -6.500  1.00 17.19           C
ATOM    120  OG1 THR A  14      -5.539  -0.798  -7.518  1.00 20.12           O
ATOM    121  CG2 THR A  14      -4.956   1.250  -6.453  1.00 14.89           C
ATOM    122  H   THR A  14      -3.858  -2.541  -6.881  1.00  8.83           H
ATOM    123  HG1 THR A  14      -6.394  -0.358  -7.606  1.00 17.77           H
ATOM    124  N   PHE A  15      -1.234   0.407  -5.994  1.00 12.81           N
ATOM    125  CA  PHE A  15      -0.211   0.731  -5.024  1.00  7.88           C
ATOM    126  C   PHE A  15      -0.157   2.235  -4.870  1.00 18.25           C
ATOM    127  O   PHE A  15      -0.427   2.887  -5.885  1.00 22.03           O
ATOM    128  CB  PHE A  15       1.156   0.231  -5.529  1.00 11.94           C
ATOM    129  CG  PHE A  15       1.295  -1.284  -5.530  1.00 11.45           C
ATOM    130  CD1 PHE A  15       0.868  -2.038  -6.622  1.00  9.87           C
ATOM    131  CD2 PHE A  15       1.850  -1.917  -4.432  1.00 11.12           C
ATOM    132  CE1 PHE A  15       0.975  -3.411  -6.611  1.00  7.22           C
ATOM    133  CE2 PHE A  15       1.925  -3.302  -4.421  1.00 10.85           C
ATOM    134  CZ  PHE A  15       1.482  -4.046  -5.501  1.00 10.98           C
ATOM    135  H   PHE A  15      -1.154   0.805  -6.884  1.00 12.28           H
ATOM    136  N   PRO A  16       0.175   2.836  -3.714  1.00 13.24           N
ATOM    137  CA  PRO A  16       0.267   4.278  -3.551  1.00 16.94           C
ATOM    138  C   PRO A  16       1.341   4.869  -4.454  1.00 27.68           C
ATOM    139  O   PRO A  16       2.370   4.252  -4.765  1.00 18.36           O
ATOM    140  CB  PRO A  16       0.646   4.454  -2.094  1.00 11.36           C
ATOM    141  CG  PRO A  16       0.354   3.156  -1.405  1.00 13.31           C
ATOM    142  CD  PRO A  16       0.627   2.156  -2.501  1.00 17.07           C
ATOM    143  N   LYS A  17       1.062   6.076  -4.919  1.00 17.83           N
ATOM    144  CA  LYS A  17       2.014   6.903  -5.619  1.00 24.33           C
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ATOM    145  C   LYS A  17       2.442   7.991  -4.619  1.00 27.42           C
ATOM    146  O   LYS A  17       1.749   8.343  -3.654  1.00 25.81           O
ATOM    147  CB  LYS A  17       1.294   7.482  -6.842  1.00 20.44           C
ATOM    148  CG  LYS A  17       2.171   8.205  -7.839  1.00 73.40           C
ATOM    149  CD  LYS A  17       1.368   8.988  -8.878  1.00 83.60           C
ATOM    150  CE  LYS A  17       2.349   9.860  -9.675  1.00 79.68           C
ATOM    151  NZ  LYS A  17       1.746  10.467 -10.851  1.00 88.66           N
ATOM    152  H   LYS A  17       0.162   6.437  -4.763  1.00 17.77           H
ATOM    153  HZ1 LYS A  17       1.340   9.722 -11.454  1.00 50.00           H
ATOM    154  HZ2 LYS A  17       1.000  11.132 -10.568  1.00 50.00           H
ATOM    155  HZ3 LYS A  17       2.478  10.970 -11.394  1.00 50.00           H
ATOM    156  N   ARG A  18       3.659   8.501  -4.815  1.00 23.19           N
ATOM    157  CA  ARG A  18       4.168   9.657  -4.102  1.00 25.30           C
ATOM    158  C   ARG A  18       3.181  10.797  -4.283  1.00 20.31           C
ATOM    159  O   ARG A  18       2.682  11.050  -5.389  1.00 26.79           O
ATOM    160  CB  ARG A  18       5.484  10.053  -4.758  1.00 36.42           C
ATOM    161  CG  ARG A  18       6.671  10.236  -3.828  1.00 61.98           C
ATOM    162  CD  ARG A  18       7.174   8.920  -3.251  1.00 70.36           C
ATOM    163  NE  ARG A  18       7.663   7.999  -4.274  1.00 91.69           N
ATOM    164  CZ  ARG A  18       7.783   6.682  -4.033  1.00 99.06           C
ATOM    165  NH1 ARG A  18       7.391   6.136  -2.874  1.00 87.08           N
ATOM    166  NH2 ARG A  18       8.287   5.879  -4.974  1.00 91.74           N
ATOM    167  H   ARG A  18       4.208   8.111  -5.521  1.00 22.37           H
ATOM    168  HE  ARG A  18       7.895   8.344  -5.160  1.00 50.00           H
ATOM    169 HH11 ARG A  18       6.990   6.706  -2.155  1.00 45.39           H
ATOM    170 HH12 ARG A  18       7.505   5.155  -2.715  1.00 45.39           H
ATOM    171 HH21 ARG A  18       8.577   6.257  -5.851  1.00 50.00           H
ATOM    172 HH22 ARG A  18       8.390   4.902  -4.783  1.00 50.00           H
ATOM    173  N   GLY A  19       2.864  11.439  -3.175  1.00 28.49           N
ATOM    174  CA  GLY A  19       1.926  12.537  -3.206  1.00 22.19           C
ATOM    175  C   GLY A  19       0.489  12.085  -2.986  1.00 24.43           C
ATOM    176  O   GLY A  19      -0.358  12.934  -2.706  1.00 27.40           O
ATOM    177  H   GLY A  19       3.239  11.160  -2.322  1.00 29.31           H
ATOM    178  N   GLN A  20       0.150  10.799  -3.069  1.00 20.21           N
ATOM    179  CA  GLN A  20      -1.208  10.390  -2.756  1.00 22.26           C
ATOM    180  C   GLN A  20      -1.385  10.310  -1.259  1.00 19.19           C
ATOM    181  O   GLN A  20      -0.426  10.014  -0.529  1.00 24.35           O
ATOM    182  CB  GLN A  20      -1.546   9.019  -3.285  1.00 16.69           C
ATOM    183  CG  GLN A  20      -1.718   9.040  -4.765  1.00 32.77           C
ATOM    184  CD  GLN A  20      -2.345   7.753  -5.235  1.00 32.00           C
ATOM    185  OE1 GLN A  20      -1.695   6.716  -5.369  1.00 30.66           O
ATOM    186  NE2 GLN A  20      -3.645   7.793  -5.467  1.00 35.54           N
ATOM    187  H   GLN A  20       0.818  10.113  -3.267  1.00 25.04           H
ATOM    188 HE21 GLN A  20      -4.074   7.000  -5.838  1.00 33.30           H
ATOM    189 HE22 GLN A  20      -4.128   8.625  -5.251  1.00 33.30           H
ATOM    190  N   THR A  21      -2.626  10.531  -0.844  1.00 12.61           N
ATOM    191  CA  THR A  21      -3.061  10.316   0.523  1.00 14.09           C
ATOM    192  C   THR A  21      -3.416   8.850   0.708  1.00 12.40           C
ATOM    193  O   THR A  21      -4.296   8.296   0.039  1.00 17.06           O
ATOM    194  CB  THR A  21      -4.299  11.210   0.824  1.00 17.25           C
ATOM    195  OG1 THR A  21      -3.788  12.529   0.655  1.00 23.17           O
ATOM    196  CG2 THR A  21      -4.896  11.052   2.231  1.00 11.48           C
ATOM    197  H   THR A  21      -3.316  10.769  -1.506  1.00 10.21           H
ATOM    198  HG1 THR A  21      -3.998  12.779  -0.257  1.00 21.91           H
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ATOM    199  N   CYS A  22      -2.727   8.204   1.629  1.00 13.20           N
ATOM    200  CA  CYS A  22      -3.072   6.841   2.021  1.00 13.95           C
ATOM    201  C   CYS A  22      -3.990   6.926   3.232  1.00 13.08           C
ATOM    202  O   CYS A  22      -3.723   7.718   4.170  1.00 15.66           O
ATOM    203  CB  CYS A  22      -1.800   6.115   2.412  1.00 10.31           C
ATOM    204  SG  CYS A  22      -0.631   6.186   1.042  1.00 17.72           S
ATOM    205  H   CYS A  22      -1.985   8.661   2.079  1.00 13.00           H
ATOM    206  N   VAL A  23      -5.066   6.127   3.208  1.00 11.74           N
ATOM    207  CA  VAL A  23      -6.009   6.048   4.324  1.00  8.67           C
ATOM    208  C   VAL A  23      -5.829   4.665   4.944  1.00  9.34           C
ATOM    209  O   VAL A  23      -6.007   3.652   4.263  1.00 13.93           O
ATOM    210  CB  VAL A  23      -7.470   6.229   3.853  1.00 12.47           C
ATOM    211  CG1 VAL A  23      -8.395   6.418   5.051  1.00 14.36           C
ATOM    212  CG2 VAL A  23      -7.576   7.428   2.952  1.00 13.59           C
ATOM    213  H   VAL A  23      -5.224   5.548   2.433  1.00  9.07           H
ATOM    214  N   VAL A  24      -5.428   4.593   6.217  1.00  9.59           N
ATOM    215  CA  VAL A  24      -5.040   3.333   6.843  1.00  9.14           C
ATOM    216  C   VAL A  24      -5.674   3.153   8.211  1.00 10.95           C
ATOM    217  O   VAL A  24      -6.064   4.134   8.852  1.00 11.27           O
ATOM    218  CB  VAL A  24      -3.513   3.204   7.057  1.00  8.47           C
ATOM    219  CG1 VAL A  24      -2.770   3.323   5.732  1.00  9.52           C
ATOM    220  CG2 VAL A  24      -2.957   4.172   8.102  1.00  8.56           C
ATOM    221  H   VAL A  24      -5.407   5.406   6.771  1.00  8.97           H
ATOM    222  N   HIS A  25      -5.791   1.917   8.686  1.00  9.36           N
ATOM    223  CA  HIS A  25      -5.944   1.680  10.114  1.00  9.60           C
ATOM    224  C   HIS A  25      -4.667   1.066  10.631  1.00  5.10           C
ATOM    225  O   HIS A  25      -4.039   0.296   9.902  1.00  9.82           O
ATOM    226  CB  HIS A  25      -7.097   0.749  10.449  1.00 10.47           C
ATOM    227  CG  HIS A  25      -8.341   1.527  10.841  1.00 16.45           C
ATOM    228  ND1 HIS A  25      -8.305   2.502  11.741  1.00 14.62           N
ATOM    229  CD2 HIS A  25      -9.594   1.265  10.371  1.00 17.08           C
ATOM    230  CE1 HIS A  25      -9.570   2.856  11.861  1.00 20.93           C
ATOM    231  NE2 HIS A  25     -10.318   2.113  11.060  1.00 20.18           N
ATOM    232  H   HIS A  25      -5.652   1.157   8.076  1.00  6.37           H
ATOM    233  HE2 HIS A  25     -11.295   2.175  11.006  1.00 20.07           H
ATOM    234  N   TYR A  26      -4.255   1.400  11.855  1.00  8.15           N
ATOM    235  CA  TYR A  26      -3.055   0.828  12.426  1.00  5.33           C
ATOM    236  C   TYR A  26      -3.187   0.576  13.922  1.00 10.06           C
ATOM    237  O   TYR A  26      -4.009   1.188  14.609  1.00  9.71           O
ATOM    238  CB  TYR A  26      -1.812   1.698  12.127  1.00  6.71           C
ATOM    239  CG  TYR A  26      -1.729   2.985  12.947  1.00  6.72           C
ATOM    240  CD1 TYR A  26      -2.330   4.116  12.436  1.00 14.55           C
ATOM    241  CD2 TYR A  26      -1.089   3.009  14.183  1.00  5.79           C
ATOM    242  CE1 TYR A  26      -2.307   5.281  13.168  1.00  8.62           C
ATOM    243  CE2 TYR A  26      -1.064   4.170  14.924  1.00 13.96           C
ATOM    244  CZ  TYR A  26      -1.688   5.298  14.401  1.00 13.12           C
ATOM    245  OH  TYR A  26      -1.706   6.470  15.111  1.00 11.19           O
ATOM    246  H   TYR A  26      -4.791   2.005  12.411  1.00  7.26           H
ATOM    247  HH  TYR A  26      -2.285   7.105  14.682  1.00 10.85           H
ATOM    248  N   THR A  27      -2.375  -0.377  14.389  1.00 12.99           N
ATOM    249  CA  THR A  27      -2.069  -0.647  15.794  1.00  7.71           C
ATOM    250  C   THR A  27      -0.546  -0.688  15.842  1.00 11.95           C
ATOM    251  O   THR A  27       0.081  -1.324  14.988  1.00 11.60           O
ATOM    252  CB  THR A  27      -2.668  -2.003  16.259  1.00 11.34           C
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ATOM    253  OG1 THR A  27      -4.065  -1.808  16.133  1.00 14.19           O
ATOM    254  CG2 THR A  27      -2.234  -2.460  17.644  1.00 11.50           C
ATOM    255  H   THR A  27      -1.885  -0.911  13.721  1.00 10.32           H
ATOM    256  HG1 THR A  27      -4.242  -1.481  15.247  1.00  9.41           H
ATOM    257  N   GLY A  28       0.060   0.004  16.796  1.00  8.64           N
ATOM    258  CA  GLY A  28       1.493  -0.004  16.981  1.00  9.01           C
ATOM    259  C   GLY A  28       1.850  -0.583  18.345  1.00 15.91           C
ATOM    260  O   GLY A  28       1.187  -0.318  19.344  1.00 10.99           O
ATOM    261  H   GLY A  28      -0.476   0.470  17.464  1.00  7.88           H
ATOM    262  N   MET A  29       2.929  -1.348  18.403  1.00 12.93           N
ATOM    263  CA  MET A  29       3.462  -1.861  19.655  1.00 11.46           C
ATOM    264  C   MET A  29       4.979  -1.943  19.563  1.00  8.02           C
ATOM    265  O   MET A  29       5.574  -1.915  18.473  1.00 12.78           O
ATOM    266  CB  MET A  29       2.849  -3.235  20.000  1.00 12.38           C
ATOM    267  CG  MET A  29       3.291  -4.355  19.114  1.00 17.40           C
ATOM    268  SD  MET A  29       2.503  -5.953  19.399  1.00 21.98           S
ATOM    269  CE  MET A  29       3.979  -6.652  20.063  1.00 33.26           C
ATOM    270  H   MET A  29       3.419  -1.578  17.577  1.00 13.04           H
ATOM    271  N   LEU A  30       5.617  -1.935  20.729  1.00 16.97           N
ATOM    272  CA  LEU A  30       7.060  -2.152  20.818  1.00 14.92           C
ATOM    273  C   LEU A  30       7.310  -3.646  20.595  1.00 20.11           C
ATOM    274  O   LEU A  30       6.464  -4.433  21.034  1.00 15.50           O
ATOM    275  CB  LEU A  30       7.517  -1.726  22.205  1.00 16.10           C
ATOM    276  CG  LEU A  30       7.312  -0.272  22.669  1.00 20.40           C
ATOM    277  CD1 LEU A  30       7.744  -0.157  24.122  1.00 36.95           C
ATOM    278  CD2 LEU A  30       8.157   0.663  21.839  1.00 22.00           C
ATOM    279  H   LEU A  30       5.081  -1.867  21.547  1.00 16.28           H
ATOM    280  N   GLU A  31       8.384  -4.066  19.904  1.00 19.84           N
ATOM    281  CA  GLU A  31       8.657  -5.481  19.648  1.00 30.77           C
ATOM    282  C   GLU A  31       8.701  -6.234  20.964  1.00 23.77           C
ATOM    283  O   GLU A  31       9.466  -5.871  21.849  1.00 40.64           O
ATOM    284  CB  GLU A  31       9.986  -5.716  18.950  1.00 21.80           C
ATOM    285  CG  GLU A  31      10.127  -7.196  18.569  1.00 32.10           C
ATOM    286  CD  GLU A  31      11.094  -7.512  17.428  1.00 69.47           C
ATOM    287  OE1 GLU A  31      12.309  -7.462  17.595  1.00 72.56           O
ATOM    288  OE2 GLU A  31      10.619  -7.758  16.323  1.00 61.02           O
ATOM    289  H   GLU A  31       8.999  -3.375  19.585  1.00 18.53           H
ATOM    290  N   ASP A  32       7.800  -7.216  21.077  1.00 31.32           N
ATOM    291  CA  ASP A  32       7.557  -7.960  22.312  1.00 55.76           C
ATOM    292  C   ASP A  32       7.350  -7.114  23.565  1.00 36.62           C
ATOM    293  O   ASP A  32       7.855  -7.359  24.666  1.00 49.81           O
ATOM    294  CB  ASP A  32       8.596  -9.076  22.500  1.00 57.01           C
ATOM    295  CG  ASP A  32       8.544 -10.107  21.374  1.00 64.95           C
ATOM    296  OD1 ASP A  32       7.451 -10.455  20.913  1.00 71.74           O
ATOM    297  OD2 ASP A  32       9.608 -10.558  20.949  1.00 71.59           O
ATOM    298  H   ASP A  32       7.217  -7.390  20.317  1.00 29.65           H
ATOM    299  N   GLY A  33       6.522  -6.101  23.343  1.00 48.70           N
ATOM    300  CA  GLY A  33       6.247  -5.113  24.351  1.00 34.41           C
ATOM    301  C   GLY A  33       4.833  -4.565  24.207  1.00 34.23           C
ATOM    302  O   GLY A  33       3.914  -5.167  23.633  1.00 27.91           O
ATOM    303  H   GLY A  33       6.064  -6.003  22.481  1.00 38.22           H
ATOM    304  N   LYS A  34       4.738  -3.348  24.740  1.00 30.73           N
ATOM    305  CA  LYS A  34       3.482  -2.662  24.973  1.00 29.07           C
ATOM    306  C   LYS A  34       2.884  -2.167  23.656  1.00 15.38           C
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ATOM    307  O   LYS A  34       3.623  -1.666  22.797  1.00 17.31           O
ATOM    308  CB  LYS A  34       3.847  -1.499  25.893  1.00 28.79           C
ATOM    309  CG  LYS A  34       2.778  -0.999  26.841  1.00 59.76           C
ATOM    310  CD  LYS A  34       3.514  -0.163  27.871  1.00 72.83           C
ATOM    311  CE  LYS A  34       2.560   0.475  28.874  1.00 77.19           C
ATOM    312  NZ  LYS A  34       3.291   1.313  29.816  1.00 83.47           N
ATOM    313  H   LYS A  34       5.568  -2.875  24.936  1.00 25.42           H
ATOM    314  HZ1 LYS A  34       3.921   1.957  29.293  1.00 50.00           H
ATOM    315  HZ2 LYS A  34       2.625   1.880  30.379  1.00 50.00           H
ATOM    316  HZ3 LYS A  34       3.859   0.711  30.444  1.00 50.00           H
ATOM    317  N   LYS A  35       1.577  -2.352  23.450  1.00 19.66           N
ATOM    318  CA  LYS A  35       0.845  -1.563  22.462  1.00 18.14           C
ATOM    319  C   LYS A  35       0.808  -0.117  22.936  1.00 23.43           C
ATOM    320  O   LYS A  35       0.490   0.167  24.089  1.00 34.44           O
ATOM    321  CB  LYS A  35      -0.549  -2.100  22.290  1.00 14.74           C
ATOM    322  CG  LYS A  35      -1.477  -1.178  21.503  1.00 41.82           C
ATOM    323  CD  LYS A  35      -2.919  -1.567  21.823  1.00 73.09           C
ATOM    324  CE  LYS A  35      -3.964  -0.642  21.227  1.00 53.04           C
ATOM    325  NZ  LYS A  35      -4.072   0.542  22.051  1.00 53.35           N
ATOM    326  H   LYS A  35       1.096  -3.007  23.995  1.00 22.19           H
ATOM    327  HZ1 LYS A  35      -4.322   0.223  23.009  1.00 50.00           H
ATOM    328  HZ2 LYS A  35      -3.158   1.033  22.056  1.00 50.00           H
ATOM    329  HZ3 LYS A  35      -4.821   1.159  21.679  1.00 50.00           H
ATOM    330  N   PHE A  36       1.185   0.793  22.049  1.00 20.64           N
ATOM    331  CA  PHE A  36       1.237   2.187  22.414  1.00 13.73           C
ATOM    332  C   PHE A  36       0.196   2.995  21.645  1.00 20.97           C
ATOM    333  O   PHE A  36      -0.093   4.119  22.052  1.00 19.29           O
ATOM    334  CB  PHE A  36       2.670   2.766  22.244  1.00 11.07           C
ATOM    335  CG  PHE A  36       3.260   2.688  20.848  1.00 14.52           C
ATOM    336  CD1 PHE A  36       2.861   3.563  19.847  1.00 14.79           C
ATOM    337  CD2 PHE A  36       4.183   1.694  20.578  1.00 15.57           C
ATOM    338  CE1 PHE A  36       3.365   3.401  18.567  1.00  9.39           C
ATOM    339  CE2 PHE A  36       4.688   1.555  19.302  1.00 12.97           C
ATOM    340  CZ  PHE A  36       4.269   2.393  18.294  1.00  9.22           C
ATOM    341  H   PHE A  36       1.433   0.506  21.145  1.00 16.81           H
ATOM    342  N   ASP A  37      -0.377   2.524  20.520  1.00 16.37           N
ATOM    343  CA  ASP A  37      -1.368   3.313  19.782  1.00 22.26           C
ATOM    344  C   ASP A  37      -2.206   2.481  18.816  1.00 19.09           C
ATOM    345  O   ASP A  37      -1.748   1.434  18.362  1.00 11.13           O
ATOM    346  CB  ASP A  37      -0.679   4.456  19.026  1.00 10.58           C
ATOM    347  CG  ASP A  37      -1.605   5.543  18.500  1.00 13.87           C
ATOM    348  OD1 ASP A  37      -2.731   5.671  18.959  1.00 20.82           O
ATOM    349  OD2 ASP A  37      -1.200   6.279  17.616  1.00 16.84           O
ATOM    350  H   ASP A  37      -0.146   1.637  20.172  1.00 14.61           H
ATOM    351  N   SER A  38      -3.446   2.869  18.520  1.00 12.66           N
ATOM    352  CA  SER A  38      -4.246   2.209  17.530  1.00 17.76           C
ATOM    353  C   SER A  38      -5.268   3.214  17.063  1.00 19.03           C
ATOM    354  O   SER A  38      -5.996   3.775  17.879  1.00 23.31           O
ATOM    355  CB  SER A  38      -5.006   1.063  18.146  1.00 15.16           C
ATOM    356  OG  SER A  38      -5.843   0.424  17.203  1.00 19.65           O
ATOM    357  H   SER A  38      -3.850   3.629  18.992  1.00 16.25           H
ATOM    358  HG  SER A  38      -5.364  -0.372  16.920  1.00 20.60           H
ATOM    359  N   SER A  39      -5.378   3.398  15.757  1.00 12.37           N
ATOM    360  CA  SER A  39      -6.440   4.219  15.226  1.00 14.57           C
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ATOM    361  C   SER A  39      -7.785   3.510  15.317  1.00 15.72           C
ATOM    362  O   SER A  39      -8.837   4.139  15.252  1.00 19.07           O
ATOM    363  CB  SER A  39      -6.101   4.576  13.793  1.00 10.13           C
ATOM    364  OG  SER A  39      -5.997   3.425  12.980  1.00 13.17           O
ATOM    365  H   SER A  39      -4.798   2.915  15.128  1.00 19.30           H
ATOM    366  HG  SER A  39      -6.783   3.433  12.415  1.00 11.96           H
ATOM    367  N   ARG A  40      -7.792   2.183  15.454  1.00 18.89           N
ATOM    368  CA  ARG A  40      -9.025   1.414  15.499  1.00 15.31           C
ATOM    369  C   ARG A  40      -9.842   1.769  16.728  1.00 31.13           C
ATOM    370  O   ARG A  40     -11.041   1.982  16.606  1.00 36.87           O
ATOM    371  CB  ARG A  40      -8.735  -0.088  15.440  1.00 30.45           C
ATOM    372  CG  ARG A  40      -8.214  -0.516  14.075  1.00 26.49           C
ATOM    373  CD  ARG A  40      -7.845  -2.005  14.000  1.00 36.88           C
ATOM    374  NE  ARG A  40      -7.282  -2.329  12.691  1.00 30.75           N
ATOM    375  CZ  ARG A  40      -8.049  -2.663  11.642  1.00 50.14           C
ATOM    376  NH1 ARG A  40      -9.381  -2.694  11.718  1.00 35.76           N
ATOM    377  NH2 ARG A  40      -7.484  -2.936  10.466  1.00 25.34           N
ATOM    378  H   ARG A  40      -6.936   1.710  15.517  1.00 21.59           H
ATOM    379  HE  ARG A  40      -6.329  -2.206  12.530  1.00 33.35           H
ATOM    380 HH11 ARG A  40      -9.838  -2.457  12.574  1.00 17.34           H
ATOM    381 HH12 ARG A  40      -9.914  -2.949  10.915  1.00 17.34           H
ATOM    382 HH21 ARG A  40      -6.496  -2.877  10.346  1.00 16.23           H
ATOM    383 HH22 ARG A  40      -8.062  -3.199   9.701  1.00 16.23           H
ATOM    384  N   ASP A  41      -9.168   1.932  17.876  1.00 32.90           N
ATOM    385  CA  ASP A  41      -9.753   2.382  19.150  1.00 42.46           C
ATOM    386  C   ASP A  41     -10.553   3.670  18.998  1.00 49.35           C
ATOM    387  O   ASP A  41     -11.604   3.909  19.597  1.00 52.42           O
ATOM    388  CB  ASP A  41      -8.668   2.761  20.201  1.00 58.24           C
ATOM    389  CG  ASP A  41      -7.759   1.709  20.846  1.00 77.12           C
ATOM    390  OD1 ASP A  41      -8.072   0.513  20.824  1.00 72.34           O
ATOM    391  OD2 ASP A  41      -6.727   2.113  21.395  1.00 77.19           O
ATOM    392  H   ASP A  41      -8.212   1.717  17.853  1.00 30.00           H
ATOM    393  N   ARG A  42      -9.936   4.531  18.200  1.00 55.02           N
ATOM    394  CA  ARG A  42     -10.429   5.864  17.980  1.00 31.32           C
ATOM    395  C   ARG A  42     -11.542   5.911  16.952  1.00 32.97           C
ATOM    396  O   ARG A  42     -12.118   6.975  16.702  1.00 39.40           O
ATOM    397  CB  ARG A  42      -9.284   6.726  17.500  1.00 33.76           C
ATOM    398  CG  ARG A  42      -8.390   7.201  18.609  1.00 43.44           C
ATOM    399  CD  ARG A  42      -7.599   8.365  18.026  1.00 55.11           C
ATOM    400  NE  ARG A  42      -6.641   7.928  17.021  1.00 68.77           N
ATOM    401  CZ  ARG A  42      -5.501   7.312  17.363  1.00 34.61           C
ATOM    402  NH1 ARG A  42      -5.250   6.978  18.633  1.00 29.77           N
ATOM    403  NH2 ARG A  42      -4.604   7.027  16.419  1.00 50.73           N
ATOM    404  H   ARG A  42      -9.159   4.236  17.684  1.00 49.11           H
ATOM    405  HE  ARG A  42      -6.831   8.092  16.074  1.00 39.69           H
ATOM    406 HH11 ARG A  42      -5.907   7.195  19.355  1.00 24.47           H
ATOM    407 HH12 ARG A  42      -4.397   6.527  18.872  1.00 24.47           H
ATOM    408 HH21 ARG A  42      -4.790   7.268  15.467  1.00 44.70           H
ATOM    409 HH22 ARG A  42      -3.753   6.563  16.666  1.00 44.70           H
ATOM    410  N   ASN A  43     -11.797   4.777  16.288  1.00 23.56           N
ATOM    411  CA  ASN A  43     -12.825   4.649  15.268  1.00 42.03           C
ATOM    412  C   ASN A  43     -12.577   5.608  14.099  1.00 70.45           C
ATOM    413  O   ASN A  43     -13.453   5.786  13.246  1.00 92.53           O
ATOM    414  CB  ASN A  43     -14.251   4.842  15.863  1.00 61.12           C
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ATOM    415  CG  ASN A  43     -14.624   3.954  17.056  1.00 61.70           C
ATOM    416  OD1 ASN A  43     -14.630   2.729  16.997  1.00 55.55           O
ATOM    417  ND2 ASN A  43     -14.967   4.509  18.211  1.00 33.11           N
ATOM    418  H   ASN A  43     -11.275   3.973  16.489  1.00 22.60           H
ATOM    419 HD21 ASN A  43     -15.134   3.883  18.941  1.00 43.61           H
ATOM    420 HD22 ASN A  43     -14.998   5.483  18.285  1.00 43.61           H
ATOM    421  N   LYS A  44     -11.384   6.218  13.984  1.00 58.24           N
ATOM    422  CA  LYS A  44     -11.083   7.162  12.914  1.00 52.71           C
ATOM    423  C   LYS A  44      -9.813   6.678  12.190  1.00 19.74           C
ATOM    424  O   LYS A  44      -8.837   6.310  12.860  1.00 30.95           O
ATOM    425  CB  LYS A  44     -10.906   8.591  13.467  1.00 56.69           C
ATOM    426  CG  LYS A  44     -10.823   9.607  12.323  1.00 79.88           C
ATOM    427  CD  LYS A  44     -10.478  11.054  12.671  1.00 81.56           C
ATOM    428  CE  LYS A  44     -10.280  11.723  11.308  1.00 84.21           C
ATOM    429  NZ  LYS A  44      -9.964  13.136  11.408  1.00 86.18           N
ATOM    430  H   LYS A  44     -10.652   5.977  14.587  1.00 50.00           H
ATOM    431  HZ1 LYS A  44      -9.103  13.264  11.974  1.00 50.00           H
ATOM    432  HZ2 LYS A  44      -9.811  13.521  10.452  1.00 50.00           H
ATOM    433  HZ3 LYS A  44     -10.760  13.637  11.852  1.00 50.00           H
ATOM    434  N   PRO A  45      -9.793   6.558  10.845  1.00 32.57           N
ATOM    435  CA  PRO A  45      -8.622   6.152  10.091  1.00 16.22           C
ATOM    436  C   PRO A  45      -7.668   7.325  10.053  1.00 14.54           C
ATOM    437  O   PRO A  45      -8.069   8.500  10.083  1.00 16.32           O
ATOM    438  CB  PRO A  45      -9.166   5.844   8.692  1.00 14.02           C
ATOM    439  CG  PRO A  45     -10.632   5.615   8.923  1.00 31.07           C
ATOM    440  CD  PRO A  45     -10.924   6.706   9.937  1.00 32.99           C
ATOM    441  N   PHE A  46      -6.401   6.936   9.931  1.00 10.29           N
ATOM    442  CA  PHE A  46      -5.294   7.853   9.877  1.00  9.03           C
ATOM    443  C   PHE A  46      -5.006   8.087   8.408  1.00  8.52           C
ATOM    444  O   PHE A  46      -5.061   7.159   7.594  1.00 11.40           O
ATOM    445  CB  PHE A  46      -4.078   7.243  10.593  1.00  8.19           C
ATOM    446  CG  PHE A  46      -2.762   8.005  10.471  1.00  9.99           C
ATOM    447  CD1 PHE A  46      -2.512   9.093  11.283  1.00 20.12           C
ATOM    448  CD2 PHE A  46      -1.783   7.575   9.584  1.00 13.29           C
ATOM    449  CE1 PHE A  46      -1.286   9.739  11.208  1.00 21.39           C
ATOM    450  CE2 PHE A  46      -0.562   8.229   9.529  1.00 10.10           C
ATOM    451  CZ  PHE A  46      -0.317   9.312  10.328  1.00 10.55           C
ATOM    452  H   PHE A  46      -6.219   5.988   9.740  1.00 13.49           H
ATOM    453  N   LYS A  47      -4.686   9.329   8.045  1.00  9.33           N
ATOM    454  CA  LYS A  47      -4.357   9.639   6.671  1.00  7.21           C
ATOM    455  C   LYS A  47      -3.020  10.347   6.698  1.00 12.96           C
ATOM    456  O   LYS A  47      -2.716  11.128   7.616  1.00 14.92           O
ATOM    457  CB  LYS A  47      -5.375  10.584   6.066  1.00 12.42           C
ATOM    458  CG  LYS A  47      -6.777  10.063   6.134  1.00 15.45           C
ATOM    459  CD  LYS A  47      -7.658  10.992   5.357  1.00 22.52           C
ATOM    460  CE  LYS A  47      -9.069  10.523   5.624  1.00 20.02           C
ATOM    461  NZ  LYS A  47      -9.974  11.333   4.838  1.00 31.31           N
ATOM    462  H   LYS A  47      -4.545  10.027   8.710  1.00  8.09           H
ATOM    463  HZ1 LYS A  47      -9.871  12.333   5.099  1.00 37.20           H
ATOM    464  HZ2 LYS A  47      -9.750  11.212   3.829  1.00 37.20           H
ATOM    465  HZ3 LYS A  47     -10.949  11.022   5.014  1.00 37.20           H
ATOM    466  N   PHE A  48      -2.199  10.029   5.710  1.00 18.97           N
ATOM    467  CA  PHE A  48      -0.949  10.741   5.518  1.00 24.29           C
ATOM    468  C   PHE A  48      -0.628  10.760   4.031  1.00 15.17           C
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ATOM    469  O   PHE A  48      -1.079   9.910   3.248  1.00 14.27           O
ATOM    470  CB  PHE A  48       0.201  10.117   6.312  1.00  8.79           C
ATOM    471  CG  PHE A  48       0.690   8.803   5.717  1.00  8.83           C
ATOM    472  CD1 PHE A  48      -0.012   7.636   5.941  1.00 12.25           C
ATOM    473  CD2 PHE A  48       1.872   8.797   4.981  1.00 15.63           C
ATOM    474  CE1 PHE A  48       0.494   6.452   5.434  1.00 16.62           C
ATOM    475  CE2 PHE A  48       2.356   7.621   4.465  1.00 15.50           C
ATOM    476  CZ  PHE A  48       1.666   6.440   4.694  1.00 14.07           C
ATOM    477  H   PHE A  48      -2.457   9.335   5.059  1.00 14.35           H
ATOM    478  N   MET A  49       0.207  11.707   3.639  1.00 11.11           N
ATOM    479  CA  MET A  49       0.577  11.826   2.242  1.00 13.52           C
ATOM    480  C   MET A  49       1.934  11.179   2.050  1.00 17.48           C
ATOM    481  O   MET A  49       2.930  11.506   2.721  1.00 14.22           O
ATOM    482  CB  MET A  49       0.619  13.297   1.884  1.00 15.86           C
ATOM    483  CG  MET A  49       0.328  13.504   0.426  1.00 52.57           C
ATOM    484  SD  MET A  49       0.381  15.258   0.020  1.00 50.59           S
ATOM    485  CE  MET A  49      -1.045  15.719   0.957  1.00 35.23           C
ATOM    486  H   MET A  49       0.619  12.298   4.295  1.00 10.91           H
ATOM    487  N   LEU A  50       1.952  10.225   1.129  1.00 12.57           N
ATOM    488  CA  LEU A  50       3.136   9.450   0.882  1.00 14.16           C
ATOM    489  C   LEU A  50       4.170  10.346   0.236  1.00 18.48           C
ATOM    490  O   LEU A  50       3.852  11.195  -0.587  1.00 23.65           O
ATOM    491  CB  LEU A  50       2.839   8.264  -0.015  1.00 11.95           C
ATOM    492  CG  LEU A  50       3.980   7.264  -0.161  1.00 23.71           C
ATOM    493  CD1 LEU A  50       4.115   6.383   1.057  1.00 21.03           C
ATOM    494  CD2 LEU A  50       3.739   6.394  -1.348  1.00 23.88           C
ATOM    495  H   LEU A  50       1.148  10.074   0.584  1.00 14.70           H
ATOM    496  N   GLY A  51       5.409  10.218   0.693  1.00 16.43           N
ATOM    497  CA  GLY A  51       6.523  10.908   0.085  1.00 25.36           C
ATOM    498  C   GLY A  51       6.812  12.284   0.664  1.00 37.86           C
ATOM    499  O   GLY A  51       7.845  12.847   0.309  1.00 41.17           O
ATOM    500  H   GLY A  51       5.564   9.643   1.466  1.00 17.23           H
ATOM    501  N   LYS A  52       6.008  12.837   1.580  1.00 23.52           N
ATOM    502  CA  LYS A  52       6.246  14.174   2.133  1.00 16.40           C
ATOM    503  C   LYS A  52       7.053  14.205   3.423  1.00 17.66           C
ATOM    504  O   LYS A  52       7.093  15.225   4.100  1.00 25.35           O
ATOM    505  CB  LYS A  52       4.903  14.813   2.443  1.00 17.13           C
ATOM    506  CG  LYS A  52       3.982  14.851   1.242  1.00 34.16           C
ATOM    507  CD  LYS A  52       4.528  15.656   0.068  1.00 39.60           C
ATOM    508  CE  LYS A  52       3.987  17.087   0.051  1.00 79.21           C
ATOM    509  NZ  LYS A  52       4.352  17.800  -1.168  1.00 68.49           N
ATOM    510  H   LYS A  52       5.194  12.362   1.852  1.00 24.55           H
ATOM    511  HZ1 LYS A  52       4.033  17.261  -1.998  1.00 50.00           H
ATOM    512  HZ2 LYS A  52       3.899  18.736  -1.168  1.00 50.00           H
ATOM    513  HZ3 LYS A  52       5.385  17.914  -1.200  1.00 50.00           H
ATOM    514  N   GLN A  53       7.643  13.068   3.832  1.00 25.80           N
ATOM    515  CA  GLN A  53       8.286  12.911   5.139  1.00 26.19           C
ATOM    516  C   GLN A  53       7.455  13.308   6.375  1.00 17.56           C
ATOM    517  O   GLN A  53       7.939  13.755   7.411  1.00 17.09           O
ATOM    518  CB  GLN A  53       9.651  13.589   5.158  1.00 41.87           C
ATOM    519  CG  GLN A  53      10.720  12.906   4.332  1.00 26.68           C
ATOM    520  CD  GLN A  53      12.054  13.629   4.498  1.00 64.57           C
ATOM    521  OE1 GLN A  53      12.146  14.857   4.445  1.00 59.44           O
ATOM    522  NE2 GLN A  53      13.118  12.873   4.721  1.00 66.86           N
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ATOM    523  H   GLN A  53       7.733  12.356   3.172  1.00 20.07           H
ATOM    524 HE21 GLN A  53      14.011  13.287   4.763  1.00 48.95           H
ATOM    525 HE22 GLN A  53      12.985  11.913   4.790  1.00 48.95           H
ATOM    526  N   GLU A  54       6.150  13.067   6.283  1.00 12.54           N
ATOM    527  CA  GLU A  54       5.266  13.265   7.417  1.00 13.97           C
ATOM    528  C   GLU A  54       5.419  12.178   8.471  1.00 12.18           C
ATOM    529  O   GLU A  54       5.185  12.417   9.655  1.00 12.93           O
ATOM    530  CB  GLU A  54       3.843  13.293   6.925  1.00 13.36           C
ATOM    531  CG  GLU A  54       3.575  14.437   5.960  1.00 13.00           C
ATOM    532  CD  GLU A  54       2.128  14.544   5.492  1.00 21.07           C
ATOM    533  OE1 GLU A  54       1.303  13.667   5.760  1.00 22.75           O
ATOM    534  OE2 GLU A  54       1.803  15.524   4.844  1.00 26.18           O
ATOM    535  H   GLU A  54       5.783  12.846   5.410  1.00 11.96           H
ATOM    536  N   VAL A  55       5.792  10.964   8.039  1.00 11.28           N
ATOM    537  CA  VAL A  55       5.866   9.820   8.929  1.00  5.68           C
ATOM    538  C   VAL A  55       7.259   9.193   8.880  1.00  9.59           C
ATOM    539  O   VAL A  55       8.072   9.481   7.993  1.00 13.30           O
ATOM    540  CB  VAL A  55       4.749   8.801   8.577  1.00  8.42           C
ATOM    541  CG1 VAL A  55       3.370   9.373   8.930  1.00  5.29           C
ATOM    542  CG2 VAL A  55       4.865   8.327   7.100  1.00 10.91           C
ATOM    543  H   VAL A  55       6.195  10.871   7.157  1.00 10.12           H
ATOM    544  N   ILE A  56       7.539   8.306   9.827  1.00  6.13           N
ATOM    545  CA  ILE A  56       8.812   7.611   9.893  1.00 11.35           C
ATOM    546  C   ILE A  56       9.121   6.836   8.626  1.00 11.05           C
ATOM    547  O   ILE A  56       8.226   6.388   7.895  1.00 10.94           O
ATOM    548  CB  ILE A  56       8.912   6.698  11.145  1.00  9.45           C
ATOM    549  CG1 ILE A  56       7.807   5.617  11.167  1.00  5.31           C
ATOM    550  CG2 ILE A  56       8.933   7.580  12.397  1.00  8.84           C
ATOM    551  CD1 ILE A  56       7.892   4.605  12.297  1.00  7.74           C
ATOM    552  H   ILE A  56       6.858   8.156  10.512  1.00  6.00           H
ATOM    553  N   ARG A  57      10.413   6.641   8.372  1.00  8.31           N
ATOM    554  CA  ARG A  57      10.883   6.046   7.139  1.00  9.12           C
ATOM    555  C   ARG A  57      10.329   4.657   6.830  1.00  9.73           C
ATOM    556  O   ARG A  57      10.001   4.310   5.688  1.00 11.55           O
ATOM    557  CB  ARG A  57      12.390   6.009   7.226  1.00 13.65           C
ATOM    558  CG  ARG A  57      13.025   5.548   5.952  1.00 13.35           C
ATOM    559  CD  ARG A  57      14.540   5.650   6.054  1.00 27.70           C
ATOM    560  NE  ARG A  57      15.067   5.173   4.782  1.00 32.60           N
ATOM    561  CZ  ARG A  57      16.373   5.108   4.477  1.00 63.58           C
ATOM    562  NH1 ARG A  57      17.328   5.506   5.317  1.00 64.64           N
ATOM    563  NH2 ARG A  57      16.740   4.674   3.272  1.00 55.48           N
ATOM    564  H   ARG A  57      11.064   6.900   9.055  1.00 10.24           H
ATOM    565  HE  ARG A  57      14.430   4.872   4.100  1.00 33.42           H
ATOM    566 HH11 ARG A  57      17.095   5.933   6.185  1.00 48.07           H
ATOM    567 HH12 ARG A  57      18.290   5.387   5.086  1.00 48.07           H
ATOM    568 HH21 ARG A  57      16.057   4.414   2.590  1.00 40.69           H
ATOM    569 HH22 ARG A  57      17.712   4.620   3.037  1.00 40.69           H
ATOM    570  N   GLY A  58      10.196   3.847   7.877  1.00  9.85           N
ATOM    571  CA  GLY A  58       9.639   2.519   7.752  1.00 11.31           C
ATOM    572  C   GLY A  58       8.208   2.498   7.242  1.00 11.34           C
ATOM    573  O   GLY A  58       7.827   1.531   6.578  1.00 12.57           O
ATOM    574  H   GLY A  58      10.497   4.159   8.757  1.00  7.54           H
ATOM    575  N   TRP A  59       7.418   3.536   7.565  1.00  9.25           N
ATOM    576  CA  TRP A  59       6.084   3.662   7.036  1.00  5.89           C
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ATOM    577  C   TRP A  59       6.173   4.115   5.604  1.00 11.62           C
ATOM    578  O   TRP A  59       5.462   3.562   4.776  1.00 10.65           O
ATOM    579  CB  TRP A  59       5.212   4.650   7.798  1.00  2.00           C
ATOM    580  CG  TRP A  59       4.390   3.977   8.883  1.00  7.15           C
ATOM    581  CD1 TRP A  59       4.957   3.282   9.922  1.00  9.09           C
ATOM    582  CD2 TRP A  59       3.022   4.024   8.981  1.00 12.44           C
ATOM    583  NE1 TRP A  59       3.938   2.910  10.664  1.00 14.82           N
ATOM    584  CE2 TRP A  59       2.776   3.338  10.155  1.00  9.06           C
ATOM    585  CE3 TRP A  59       1.976   4.592   8.280  1.00 10.43           C
ATOM    586  CZ2 TRP A  59       1.492   3.225  10.673  1.00  6.28           C
ATOM    587  CZ3 TRP A  59       0.701   4.489   8.796  1.00 12.15           C
ATOM    588  CH2 TRP A  59       0.456   3.812   9.975  1.00  8.16           C
ATOM    589  H   TRP A  59       7.774   4.261   8.120  1.00  7.13           H
ATOM    590  HE1 TRP A  59       4.020   2.358  11.470  1.00 13.77           H
ATOM    591  N   GLU A  60       7.038   5.084   5.269  1.00 10.64           N
ATOM    592  CA  GLU A  60       7.183   5.548   3.898  1.00 10.98           C
ATOM    593  C   GLU A  60       7.543   4.411   2.943  1.00 15.13           C
ATOM    594  O   GLU A  60       6.959   4.255   1.870  1.00 18.15           O
ATOM    595  CB  GLU A  60       8.260   6.631   3.809  1.00 10.74           C
ATOM    596  CG  GLU A  60       8.012   7.965   4.510  1.00 19.92           C
ATOM    597  CD  GLU A  60       7.200   8.970   3.705  1.00 18.76           C
ATOM    598  OE1 GLU A  60       6.054   8.703   3.381  1.00 32.83           O
ATOM    599  OE2 GLU A  60       7.729  10.028   3.398  1.00 44.50           O
ATOM    600  H   GLU A  60       7.589   5.487   5.974  1.00  9.88           H
ATOM    601  N   GLU A  61       8.496   3.579   3.335  1.00  9.75           N
ATOM    602  CA  GLU A  61       8.879   2.443   2.520  1.00 11.54           C
ATOM    603  C   GLU A  61       7.951   1.256   2.638  1.00  8.40           C
ATOM    604  O   GLU A  61       7.754   0.522   1.668  1.00 11.35           O
ATOM    605  CB  GLU A  61      10.292   2.007   2.872  1.00 11.79           C
ATOM    606  CG  GLU A  61      11.215   3.062   2.265  1.00 44.46           C
ATOM    607  CD  GLU A  61      12.709   2.945   2.517  1.00 52.63           C
ATOM    608  OE1 GLU A  61      13.235   1.867   2.791  1.00 26.54           O
ATOM    609  OE2 GLU A  61      13.367   3.969   2.403  1.00 28.84           O
ATOM    610  H   GLU A  61       8.966   3.757   4.173  1.00  8.57           H
ATOM    611  N   GLY A  62       7.393   1.043   3.819  1.00  6.34           N
ATOM    612  CA  GLY A  62       6.525  -0.089   4.072  1.00 11.76           C
ATOM    613  C   GLY A  62       5.216   0.039   3.329  1.00 14.21           C
ATOM    614  O   GLY A  62       4.843  -0.847   2.556  1.00 11.00           O
ATOM    615  H   GLY A  62       7.581   1.656   4.558  1.00  5.00           H
ATOM    616  N   VAL A  63       4.532   1.176   3.508  1.00 12.36           N
ATOM    617  CA  VAL A  63       3.231   1.383   2.893  1.00  8.38           C
ATOM    618  C   VAL A  63       3.316   1.490   1.369  1.00 10.73           C
ATOM    619  O   VAL A  63       2.426   1.004   0.671  1.00 11.09           O
ATOM    620  CB  VAL A  63       2.477   2.554   3.586  1.00 10.46           C
ATOM    621  CG1 VAL A  63       1.152   2.864   2.892  1.00  7.10           C
ATOM    622  CG2 VAL A  63       2.236   2.219   5.070  1.00 13.30           C
ATOM    623  H   VAL A  63       4.916   1.884   4.063  1.00  9.81           H
ATOM    624  N   ALA A  64       4.406   2.049   0.822  1.00  8.64           N
ATOM    625  CA  ALA A  64       4.603   2.091  -0.611  1.00  5.07           C
ATOM    626  C   ALA A  64       4.567   0.745  -1.337  1.00 10.97           C
ATOM    627  O   ALA A  64       4.244   0.673  -2.531  1.00 11.35           O
ATOM    628  CB  ALA A  64       5.946   2.736  -0.902  1.00  9.58           C
ATOM    629  H   ALA A  64       5.071   2.477   1.402  1.00  7.42           H
ATOM    630  N   GLN A  65       4.866  -0.363  -0.648  1.00  8.60           N
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ATOM    631  CA  GLN A  65       4.817  -1.649  -1.328  1.00  3.86           C
ATOM    632  C   GLN A  65       3.521  -2.390  -1.037  1.00  7.84           C
ATOM    633  O   GLN A  65       3.405  -3.585  -1.318  1.00 13.14           O
ATOM    634  CB  GLN A  65       6.063  -2.460  -1.029  1.00 14.43           C
ATOM    635  CG  GLN A  65       6.304  -2.643   0.436  1.00  9.21           C
ATOM    636  CD  GLN A  65       7.655  -3.240   0.752  1.00 18.89           C
ATOM    637  OE1 GLN A  65       7.850  -4.456   0.694  1.00 16.81           O
ATOM    638  NE2 GLN A  65       8.622  -2.417   1.129  1.00 16.04           N
ATOM    639  H   GLN A  65       5.042  -0.323   0.315  1.00  6.02           H
ATOM    640 HE21 GLN A  65       9.494  -2.809   1.330  1.00 13.74           H
ATOM    641 HE22 GLN A  65       8.401  -1.460   1.188  1.00 13.74           H
ATOM    642  N   MET A  66       2.526  -1.708  -0.469  1.00 12.58           N
ATOM    643  CA  MET A  66       1.278  -2.360  -0.162  1.00  9.01           C
ATOM    644  C   MET A  66       0.279  -1.954  -1.229  1.00  5.22           C
ATOM    645  O   MET A  66       0.324  -0.856  -1.779  1.00 11.06           O
ATOM    646  CB  MET A  66       0.795  -1.977   1.233  1.00  8.72           C
ATOM    647  CG  MET A  66       1.586  -2.584   2.396  1.00 14.13           C
ATOM    648  SD  MET A  66       1.010  -1.927   3.979  1.00 13.76           S
ATOM    649  CE  MET A  66      -0.513  -2.835   4.016  1.00 11.06           C
ATOM    650  H   MET A  66       2.587  -0.736  -0.357  1.00  7.87           H
ATOM    651  N   SER A  67      -0.624  -2.870  -1.551  1.00  8.79           N
ATOM    652  CA  SER A  67      -1.719  -2.517  -2.428  1.00 11.09           C
ATOM    653  C   SER A  67      -3.022  -2.272  -1.664  1.00 15.47           C
ATOM    654  O   SER A  67      -3.145  -2.711  -0.508  1.00 12.61           O
ATOM    655  CB  SER A  67      -1.871  -3.548  -3.519  1.00  8.47           C
ATOM    656  OG  SER A  67      -2.072  -4.887  -3.109  1.00 11.08           O
ATOM    657  H   SER A  67      -0.598  -3.730  -1.081  1.00  5.60           H
ATOM    658  HG  SER A  67      -1.404  -5.088  -2.439  1.00 11.49           H
ATOM    659  N   VAL A  68      -4.015  -1.616  -2.286  1.00 13.66           N
ATOM    660  CA  VAL A  68      -5.265  -1.301  -1.624  1.00 10.45           C
ATOM    661  C   VAL A  68      -5.930  -2.574  -1.150  1.00  6.70           C
ATOM    662  O   VAL A  68      -5.995  -3.535  -1.918  1.00 10.56           O
ATOM    663  CB  VAL A  68      -6.183  -0.467  -2.550  1.00 22.97           C
ATOM    664  CG1 VAL A  68      -7.561  -0.162  -1.944  1.00 11.78           C
ATOM    665  CG2 VAL A  68      -5.511   0.851  -2.829  1.00 13.49           C
ATOM    666  H   VAL A  68      -3.845  -1.276  -3.185  1.00 10.34           H
ATOM    667  N   GLY A  69      -6.344  -2.591   0.112  1.00 12.27           N
ATOM    668  CA  GLY A  69      -7.019  -3.716   0.737  1.00 12.60           C
ATOM    669  C   GLY A  69      -6.084  -4.587   1.575  1.00 16.68           C
ATOM    670  O   GLY A  69      -6.540  -5.404   2.375  1.00 12.60           O
ATOM    671  H   GLY A  69      -6.171  -1.805   0.665  1.00  9.34           H
ATOM    672  N   GLN A  70      -4.767  -4.425   1.407  1.00  9.90           N
ATOM    673  CA  GLN A  70      -3.837  -5.290   2.065  1.00  5.02           C
ATOM    674  C   GLN A  70      -3.777  -4.939   3.543  1.00  8.32           C
ATOM    675  O   GLN A  70      -3.816  -3.767   3.911  1.00 13.62           O
ATOM    676  CB  GLN A  70      -2.479  -5.108   1.444  1.00  2.98           C
ATOM    677  CG  GLN A  70      -1.464  -6.150   1.926  1.00  6.45           C
ATOM    678  CD  GLN A  70      -0.145  -6.045   1.200  1.00 11.80           C
ATOM    679  OE1 GLN A  70      -0.071  -5.465   0.116  1.00 16.00           O
ATOM    680  NE2 GLN A  70       0.943  -6.614   1.680  1.00 12.64           N
ATOM    681  H   GLN A  70      -4.433  -3.674   0.873  1.00  8.31           H
ATOM    682 HE21 GLN A  70       1.766  -6.470   1.167  1.00 12.73           H
ATOM    683 HE22 GLN A  70       0.903  -7.147   2.502  1.00 12.73           H
ATOM    684  N   ARG A  71      -3.610  -5.952   4.386  1.00  8.72           N
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ATOM    685  CA  ARG A  71      -3.298  -5.763   5.789  1.00  6.13           C
ATOM    686  C   ARG A  71      -1.942  -6.416   6.008  1.00 11.97           C
ATOM    687  O   ARG A  71      -1.748  -7.566   5.592  1.00  9.70           O
ATOM    688  CB  ARG A  71      -4.398  -6.389   6.650  1.00  4.08           C
ATOM    689  CG  ARG A  71      -4.161  -6.112   8.095  1.00  5.95           C
ATOM    690  CD  ARG A  71      -5.408  -6.513   8.869  1.00 15.19           C
ATOM    691  NE  ARG A  71      -5.181  -6.428  10.310  1.00 14.21           N
ATOM    692  CZ  ARG A  71      -6.097  -6.771  11.224  1.00 19.71           C
ATOM    693 NH1 ARG A  71      -7.273  -7.277  10.883  1.00 19.34           N
ATOM    694 NH2 ARG A  71      -5.842  -6.612  12.514  1.00 14.73           N
ATOM    695  H   ARG A  71      -3.640  -6.864   4.024  1.00  9.72           H
ATOM    696  HE  ARG A  71      -4.288  -6.214  10.622  1.00 15.80           H
ATOM    697 HH11 ARG A  71      -7.504  -7.415   9.920  1.00 23.16           H
ATOM    698 HH12 ARG A  71      -7.931  -7.520  11.596  1.00 23.16           H
ATOM    699 HH21 ARG A  71      -4.980  -6.219  12.806  1.00 12.53           H
ATOM    700 HH22 ARG A  71      -6.520  -6.884  13.196  1.00 12.53           H
ATOM    701  N   ALA A  72      -0.987  -5.740   6.640  1.00  7.24           N
ATOM    702  CA  ALA A  72       0.354  -6.268   6.821  1.00 11.91           C
ATOM    703  C   ALA A  72       0.958  -5.948   8.187  1.00  8.84           C
ATOM    704  O   ALA A  72       0.586  -4.995   8.862  1.00  8.80           O
ATOM    705  CB  ALA A  72       1.255  -5.702   5.728  1.00 10.80           C
ATOM    706  H   ALA A  72      -1.181  -4.852   7.016  1.00  5.52           H
ATOM    707  N   LYS A  73       1.848  -6.815   8.647  1.00  7.18           N
ATOM    708  CA  LYS A  73       2.652  -6.581   9.821  1.00  6.47           C
ATOM    709  C   LYS A  73       3.945  -5.968   9.276  1.00  8.25           C
ATOM    710  O   LYS A  73       4.612  -6.541   8.407  1.00 10.41           O
ATOM    711  CB  LYS A  73       2.933  -7.910  10.482  1.00  7.24           C
ATOM    712  CG  LYS A  73       3.850  -7.802  11.652  1.00 10.08           C
ATOM    713  CD  LYS A  73       4.298  -9.215  11.830  1.00 20.02           C
ATOM    714  CE  LYS A  73       5.555  -9.246  12.640  1.00 40.73           C
ATOM    715  NZ  LYS A  73       5.263  -9.663  13.984  1.00 23.83           N
ATOM    716  H   LYS A  73       2.019  -7.630   8.133  1.00  5.00           H
ATOM    717  HZ1 LYS A  73       4.823 -10.604  13.963  1.00 22.87           H
ATOM    718  HZ2 LYS A  73       6.144  -9.695  14.535  1.00 22.87           H
ATOM    719  HZ3 LYS A  73       4.607  -8.980  14.414  1.00 22.87           H
ATOM    720  N   LEU A  74       4.261  -4.765   9.749  1.00  7.63           N
ATOM    721  CA  LEU A  74       5.503  -4.073   9.414  1.00  6.00           C
ATOM    722  C   LEU A  74       6.433  -4.158  10.600  1.00  8.48           C
ATOM    723  O   LEU A  74       6.048  -3.694  11.666  1.00 11.64           O
ATOM    724  CB  LEU A  74       5.252  -2.594   9.077  1.00  7.28           C
ATOM    725  CG  LEU A  74       4.823  -2.163   7.690  1.00 10.30           C
ATOM    726 CD1 LEU A  74       3.492  -2.735   7.286  1.00 26.74           C
ATOM    727 CD2 LEU A  74       4.673  -0.655   7.703  1.00 11.53           C
ATOM    728  H   LEU A  74       3.662  -4.334  10.384  1.00  6.31           H
ATOM    729  N   THR A  75       7.622  -4.744  10.507  1.00  8.68           N
ATOM    730  CA  THR A  75       8.595  -4.703  11.598  1.00 12.38           C
ATOM    731  C   THR A  75       9.671  -3.694  11.212  1.00 12.11           C
ATOM    732  O   THR A  75      10.273  -3.804  10.139  1.00 11.11           O
ATOM    733  CB  THR A  75       9.245  -6.062  11.812  1.00 10.07           C
ATOM    734  OG1 THR A  75       8.156  -6.961  11.983  1.00 11.55           O
ATOM    735 CG2 THR A  75      10.174  -6.048  13.032  1.00 13.86           C
ATOM    736  H   THR A  75       7.879  -5.144   9.646  1.00  7.78           H
ATOM    737  HG1 THR A  75       7.394  -6.668  11.476  1.00 10.83           H
ATOM    738  N   ILE A  76       9.916  -2.689  12.042  1.00  8.14           N
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ATOM    739  CA  ILE A  76      10.710  -1.548  11.658  1.00  7.06           C
ATOM    740  C   ILE A  76      11.859  -1.432  12.660  1.00  9.06           C
ATOM    741  O   ILE A  76      11.692  -1.294  13.880  1.00 11.09           O
ATOM    742  CB  ILE A  76       9.796  -0.291  11.673  1.00  8.36           C
ATOM    743  CG1 ILE A  76       8.618  -0.412  10.733  1.00 10.32           C
ATOM    744  CG2 ILE A  76      10.605   0.942  11.331  1.00  7.99           C
ATOM    745  CD1 ILE A  76       7.546   0.672  10.920  1.00 10.56           C
ATOM    746  H   ILE A  76       9.555  -2.717  12.954  1.00  6.76           H
ATOM    747  N   SER A  77      13.068  -1.411  12.113  1.00  8.81           N
ATOM    748  CA  SER A  77      14.250  -1.311  12.952  1.00  7.83           C
ATOM    749  C   SER A  77      14.345   0.106  13.479  1.00  7.30           C
ATOM    750  O   SER A  77      13.849   0.992  12.789  1.00 11.14           O
ATOM    751  CB  SER A  77      15.497  -1.685  12.137  1.00  8.20           C
ATOM    752  OG  SER A  77      15.654  -0.913  10.938  1.00 15.98           O
ATOM    753  H   SER A  77      13.138  -1.429  11.140  1.00  5.58           H
ATOM    754  HG  SER A  77      15.238  -0.057  11.127  1.00 16.20           H
ATOM    755  N   PRO A  78      15.036   0.422  14.569  1.00 11.54           N
ATOM    756  CA  PRO A  78      15.088   1.750  15.171  1.00  7.44           C
ATOM    757  C   PRO A  78      15.574   2.803  14.213  1.00  8.77           C
ATOM    758  O   PRO A  78      15.087   3.921  14.275  1.00 14.50           O
ATOM    759  CB  PRO A  78      16.115   1.632  16.249  1.00 14.11           C
ATOM    760  CG  PRO A  78      16.041   0.202  16.644  1.00 16.36           C
ATOM    761  CD  PRO A  78      15.821  -0.524  15.340  1.00 16.21           C
ATOM    762  N   ASP A  79      16.521   2.494  13.334  1.00 10.39           N
ATOM    763  CA  ASP A  79      16.994   3.458  12.367  1.00 11.10           C
ATOM    764  C   ASP A  79      15.969   3.832  11.306  1.00 20.89           C
ATOM    765  O   ASP A  79      16.142   4.825  10.614  1.00 18.96           O
ATOM    766  CB  ASP A  79      18.304   3.017  11.724  1.00 10.92           C
ATOM    767  CG  ASP A  79      18.248   1.750  10.895  1.00 22.06           C
ATOM    768  OD1 ASP A  79      17.790   0.743  11.413  1.00 22.96           O
ATOM    769  OD2 ASP A  79      18.672   1.770   9.743  1.00 25.87           O
ATOM    770  H   ASP A  79      16.933   1.613  13.373  1.00 13.50           H
ATOM    771  N   TYR A  80      14.892   3.062  11.156  1.00 15.31           N
ATOM    772  CA  TYR A  80      13.797   3.412  10.251  1.00 10.00           C
ATOM    773  C   TYR A  80      12.598   3.956  11.020  1.00 10.44           C
ATOM    774  O   TYR A  80      11.528   4.195  10.453  1.00  9.56           O
ATOM    775  CB  TYR A  80      13.396   2.189   9.444  1.00 12.34           C
ATOM    776  CG  TYR A  80      14.202   2.043   8.172  1.00 12.21           C
ATOM    777  CD1 TYR A  80      15.574   2.049   8.242  1.00 19.81           C
ATOM    778  CD2 TYR A  80      13.558   1.947   6.952  1.00  9.98           C
ATOM    779  CE1 TYR A  80      16.319   1.955   7.090  1.00 32.48           C
ATOM    780  CE2 TYR A  80      14.302   1.828   5.795  1.00 13.63           C
ATOM    781  CZ  TYR A  80      15.678   1.808   5.880  1.00 40.19           C
ATOM    782  OH  TYR A  80      16.439   1.587   4.751  1.00 35.14           O
ATOM    783  H   TYR A  80      14.747   2.327  11.773  1.00 11.31           H
ATOM    784  HH  TYR A  80      15.972   1.898   3.968  1.00 37.08           H
ATOM    785  N   ALA A  81      12.765   4.168  12.326  1.00  9.86           N
ATOM    786  CA  ALA A  81      11.712   4.569  13.230  1.00  6.99           C
ATOM    787  C   ALA A  81      12.286   5.753  14.032  1.00 13.78           C
ATOM    788  O   ALA A  81      12.649   6.757  13.432  1.00 14.63           O
ATOM    789  CB  ALA A  81      11.424   3.384  14.120  1.00  4.72           C
ATOM    790  H   ALA A  81      13.672   4.168  12.693  1.00  7.46           H
ATOM    791  N   TYR A  82      12.463   5.740  15.343  1.00 10.57           N
ATOM    792  CA  TYR A  82      12.896   6.895  16.115  1.00  7.88           C
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ATOM    793  C   TYR A  82      14.326   6.832  16.605  1.00  9.94           C
ATOM    794  O   TYR A  82      14.759   7.711  17.359  1.00 11.53           O
ATOM    795  CB  TYR A  82      11.927   7.081  17.303  1.00  8.60           C
ATOM    796  CG  TYR A  82      10.480   7.353  16.885  1.00 11.16           C
ATOM    797  CD1 TYR A  82      10.118   8.604  16.401  1.00 10.94           C
ATOM    798  CD2 TYR A  82       9.557   6.324  16.916  1.00  6.14           C
ATOM    799  CE1 TYR A  82       8.842   8.820  15.897  1.00 14.49           C
ATOM    800  CE2 TYR A  82       8.275   6.533  16.422  1.00 13.98           C
ATOM    801  CZ  TYR A  82       7.934   7.781  15.919  1.00 14.00           C
ATOM    802  OH  TYR A  82       6.668   7.997  15.452  1.00 10.90           O
ATOM    803  H   TYR A  82      12.259   4.924  15.823  1.00  7.19           H
ATOM    804  HH  TYR A  82       6.175   7.165  15.497  1.00  9.22           H
ATOM    805  N   GLY A  83      15.077   5.781  16.257  1.00  8.29           N
ATOM    806  CA  GLY A  83      16.521   5.780  16.424  1.00 13.72           C
ATOM    807  C   GLY A  83      17.007   5.856  17.852  1.00  9.49           C
ATOM    808  O   GLY A  83      16.369   5.371  18.777  1.00 10.37           O
ATOM    809  H   GLY A  83      14.644   5.029  15.809  1.00  8.74           H
ATOM    810  N   ALA A  84      18.142   6.510  18.054  1.00 11.50           N
ATOM    811  CA  ALA A  84      18.739   6.468  19.371  1.00 14.29           C
ATOM    812  C   ALA A  84      18.082   7.446  20.325  1.00 19.90           C
ATOM    813  O   ALA A  84      18.271   7.385  21.525  1.00 19.35           O
ATOM    814  CB  ALA A  84      20.213   6.768  19.254  1.00 13.93           C
ATOM    815  H   ALA A  84      18.565   7.022  17.334  1.00 11.82           H
ATOM    816  N   THR A  85      17.247   8.337  19.838  1.00 11.93           N
ATOM    817  CA  THR A  85      16.613   9.331  20.683  1.00 26.11           C
ATOM    818  C   THR A  85      15.247   8.879  21.166  1.00 19.04           C
ATOM    819  O   THR A  85      14.824   9.266  22.257  1.00 18.38           O
ATOM    820  CB  THR A  85      16.600  10.722  19.972  1.00 18.88           C
ATOM    821  OG1 THR A  85      15.321  11.318  20.063  1.00 46.16           O
ATOM    822  CG2 THR A  85      17.090  10.721  18.526  1.00 35.65           C
ATOM    823  H   THR A  85      16.961   8.277  18.907  1.00 11.01           H
ATOM    824  HG1 THR A  85      15.009  11.278  20.976  1.00 38.30           H
ATOM    825  N   GLY A  86      14.535   8.115  20.331  1.00 14.37           N
ATOM    826  CA  GLY A  86      13.198   7.678  20.663  1.00  8.67           C
ATOM    827  C   GLY A  86      12.228   8.842  20.429  1.00  8.93           C
ATOM    828  O   GLY A  86      12.537   9.865  19.804  1.00 15.03           O
ATOM    829  H   GLY A  86      14.855   7.964  19.418  1.00 13.44           H
ATOM    830  N   HIS A  87      11.001   8.657  20.894  1.00 11.92           N
ATOM    831  CA  HIS A  87       9.984   9.667  20.776  1.00 13.18           C
ATOM    832  C   HIS A  87       9.610   9.972  22.211  1.00  8.36           C
ATOM    833  O   HIS A  87       9.003   9.127  22.884  1.00 12.76           O
ATOM    834  CB  HIS A  87       8.783   9.118  20.021  1.00 12.71           C
ATOM    835  CG  HIS A  87       7.728  10.207  19.827  1.00 10.84           C
ATOM    836  ND1 HIS A  87       7.793  11.283  19.044  1.00 16.17           N
ATOM    837  CD2 HIS A  87       6.543  10.244  20.513  1.00 11.90           C
ATOM    838  CE1 HIS A  87       6.693  11.981  19.247  1.00 10.11           C
ATOM    839  NE2 HIS A  87       5.957  11.333  20.120  1.00 16.02           N
ATOM    840  H   HIS A  87      10.833   7.861  21.439  1.00  8.36           H
ATOM    841  HD1 HIS A  87       8.474  11.468  18.369  1.00 15.87           H
ATOM    842  HE2 HIS A  87       5.093  11.653  20.461  1.00 13.02           H
ATOM    843  N   PRO A  88       9.957  11.157  22.713  1.00 20.43           N
ATOM    844  CA  PRO A  88       9.857  11.525  24.124  1.00 40.00           C
ATOM    845  C   PRO A  88       8.530  11.195  24.776  1.00 16.70           C
ATOM    846  O   PRO A  88       7.461  11.464  24.228  1.00 31.15           O
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ATOM    847  CB  PRO A  88      10.101  13.013  24.098  1.00 47.23           C
ATOM    848  CG  PRO A  88       9.769  13.445  22.687  1.00 43.23           C
ATOM    849  CD  PRO A  88      10.394  12.300  21.918  1.00 45.60           C
ATOM    850  N   GLY A  89       8.635  10.487  25.885  1.00 17.71           N
ATOM    851  CA  GLY A  89       7.477  10.104  26.645  1.00 14.18           C
ATOM    852  C   GLY A  89       6.884   8.800  26.184  1.00 19.36           C
ATOM    853  O   GLY A  89       6.171   8.171  26.951  1.00 25.36           O
ATOM    854  H   GLY A  89       9.514  10.195  26.194  1.00 16.99           H
ATOM    855  N   ILE A  90       7.139   8.328  24.961  1.00 19.64           N
ATOM    856  CA  ILE A  90       6.369   7.223  24.404  1.00 16.74           C
ATOM    857  C   ILE A  90       7.332   6.117  23.957  1.00 14.30           C
ATOM    858  O   ILE A  90       7.232   4.980  24.409  1.00 16.09           O
ATOM    859  CB AILE A  90       5.468   7.723  23.227  0.50 18.90           C
ATOM    860  CB BILE A  90       5.525   7.697  23.180  0.50 22.58           C
ATOM    861  CG1AILE A  90       4.597   8.930  23.621  0.50 20.70           C
ATOM    862  CG1BILE A  90       4.731   8.994  23.409  0.50 26.06           C
ATOM    863  CG2AILE A  90       4.603   6.573  22.728  0.50 14.95           C
ATOM    864  CG2BILE A  90       4.617   6.567  22.707  0.50 14.82           C
ATOM    865  CD1AILE A  90       3.777   9.621  22.505  0.50 13.02           C
ATOM    866  CD1BILE A  90       3.699   8.977  24.553  0.50 27.61           C
ATOM    867  H   ILE A  90       7.858   8.722  24.434  1.00 14.01           H
ATOM    868  N   ILE A  91       8.302   6.386  23.074  1.00 20.63           N
ATOM    869  CA  ILE A  91       9.112   5.319  22.478  1.00  9.02           C
ATOM    870  C   ILE A  91      10.518   5.518  23.031  1.00 10.99           C
ATOM    871  O   ILE A  91      11.048   6.622  22.882  1.00  8.91           O
ATOM    872  CB  ILE A  91       9.112   5.420  20.926  1.00 13.49           C
ATOM    873  CG1 ILE A  91       7.726   5.403  20.279  1.00 15.53           C
ATOM    874  CG2 ILE A  91       9.999   4.380  20.291  1.00 11.43           C
ATOM    875  CD1 ILE A  91       6.855   4.203  20.549  1.00 11.48           C
ATOM    876  H   ILE A  91       8.573   7.308  22.924  1.00 15.61           H
ATOM    877  N   PRO A  92      11.137   4.511  23.669  1.00 14.31           N
ATOM    878  CA  PRO A  92      12.512   4.569  24.185  1.00  8.63           C
ATOM    879  C   PRO A  92      13.561   4.595  23.054  1.00 11.44           C
ATOM    880  O   PRO A  92      13.250   4.212  21.910  1.00  9.68           O
ATOM    881  CB  PRO A  92      12.640   3.226  24.953  1.00 13.25           C
ATOM    882  CG  PRO A  92      11.294   2.557  24.973  1.00 14.48           C
ATOM    883  CD  PRO A  92      10.605   3.142  23.767  1.00 23.63           C
ATOM    884  N   PRO A  93      14.827   4.991  23.322  1.00 17.49           N
ATOM    885  CA  PRO A  93      15.940   4.825  22.401  1.00 10.43           C
ATOM    886  C   PRO A  93      16.043   3.372  21.956  1.00  8.59           C
ATOM    887  O   PRO A  93      15.801   2.417  22.705  1.00  9.95           O
ATOM    888  CB  PRO A  93      17.138   5.192  23.264  1.00  9.89           C
ATOM    889  CG  PRO A  93      16.617   6.269  24.167  1.00 12.29           C
ATOM    890  CD  PRO A  93      15.290   5.628  24.560  1.00 16.81           C
ATOM    891  N   HIS A  94      16.398   3.247  20.674  1.00  7.49           N
ATOM    892  CA  HIS A  94      16.720   1.961  20.078  1.00 11.47           C
ATOM    893  C   HIS A  94      15.547   0.984  20.149  1.00 10.68           C
ATOM    894  O   HIS A  94      15.782  -0.213  20.308  1.00 12.00           O
ATOM    895  CB  HIS A  94      17.976   1.374  20.767  1.00 13.33           C
ATOM    896  CG  HIS A  94      18.600   0.239  19.990  1.00 12.75           C
ATOM    897  ND1 HIS A  94      18.608  -1.059  20.281  1.00 23.48           N
ATOM    898  CD2 HIS A  94      19.281   0.418  18.810  1.00 20.24           C
ATOM    899  CE1 HIS A  94      19.282  -1.681  19.339  1.00 16.30           C
ATOM    900  NE2 HIS A  94      19.679  -0.778  18.464  1.00 28.26           N
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ATOM    901  H   HIS A  94      16.375   4.054  20.124  1.00  6.99           H
ATOM    902  HD1 HIS A  94      18.062  -1.490  20.978  1.00 17.79           H
ATOM    903  HE2 HIS A  94      20.205  -0.979  17.659  1.00 17.68           H
ATOM    904  N   ALA A  95      14.295   1.424  19.985  1.00  5.88           N
ATOM    905  CA  ALA A  95      13.196   0.485  19.964  1.00  6.75           C
ATOM    906  C   ALA A  95      12.853   0.009  18.548  1.00 16.10           C
ATOM    907  O   ALA A  95      12.811   0.800  17.590  1.00 13.72           O
ATOM    908  CB  ALA A  95      11.935   1.098  20.567  1.00  7.08           C
ATOM    909  H   ALA A  95      14.102   2.382  19.903  1.00  5.00           H
ATOM    910  N   THR A  96      12.679  -1.316  18.404  1.00 11.69           N
ATOM    911  CA  THR A  96      12.098  -1.931  17.217  1.00 10.07           C
ATOM    912  C   THR A  96      10.557  -1.838  17.339  1.00  7.93           C
ATOM    913  O   THR A  96       9.998  -2.132  18.406  1.00 13.22           O
ATOM    914  CB  THR A  96      12.599  -3.419  17.057  1.00 15.74           C
ATOM    915  OG1 THR A  96      14.021  -3.381  16.899  1.00 14.12           O
ATOM    916  CG2 THR A  96      11.974  -4.155  15.861  1.00 11.48           C
ATOM    917  H   THR A  96      12.900  -1.900  19.149  1.00 13.93           H
ATOM    918  HG1 THR A  96      14.366  -4.209  17.248  1.00 13.94           H
ATOM    919  N   LEU A  97       9.866  -1.408  16.273  1.00 11.13           N
ATOM    920  CA  LEU A  97       8.430  -1.167  16.316  1.00 12.13           C
ATOM    921  C   LEU A  97       7.766  -2.178  15.408  1.00  8.98           C
ATOM    922  O   LEU A  97       8.268  -2.498  14.331  1.00  7.48           O
ATOM    923  CB  LEU A  97       8.035   0.267  15.842  1.00  5.98           C
ATOM    924  CG  LEU A  97       8.713   1.455  16.513  1.00 14.61           C
ATOM    925  CD1 LEU A  97       8.154   2.783  15.998  1.00 10.49           C
ATOM    926  CD2 LEU A  97       8.609   1.342  18.027  1.00 10.50           C
ATOM    927  H   LEU A  97      10.345  -1.277  15.423  1.00  9.23           H
ATOM    928  N   VAL A  98       6.635  -2.694  15.854  1.00  9.66           N
ATOM    929  CA  VAL A  98       5.812  -3.488  14.970  1.00  9.32           C
ATOM    930  C   VAL A  98       4.443  -2.824  14.832  1.00  8.48           C
ATOM    931  O   VAL A  98       3.830  -2.387  15.800  1.00  8.62           O
ATOM    932  CB AVAL A  98       5.780  -5.019  15.309  0.50  9.81           C
ATOM    933  CB BVAL A  98       5.766  -5.013  15.350  0.50  8.56           C
ATOM    934  CG1AVAL A  98       7.134  -5.518  15.794  0.50  2.00           C
ATOM    935  CG1BVAL A  98       5.842  -5.274  16.826  0.50 21.38           C
ATOM    936  CG2AVAL A  98       4.687  -5.488  16.208  0.50 14.46           C
ATOM    937  CG2BVAL A  98       4.578  -5.764  14.748  0.50  2.00           C
ATOM    938  H   VAL A  98       6.283  -2.461  16.742  1.00  7.57           H
ATOM    939  N   PHE A  99       4.039  -2.628  13.579  1.00 12.47           N
ATOM    940  CA  PHE A  99       2.739  -2.065  13.257  1.00 11.83           C
ATOM    941  C   PHE A  99       1.895  -3.058  12.471  1.00 11.96           C
ATOM    942  O   PHE A  99       2.383  -3.742  11.569  1.00 14.60           O
ATOM    943  CB  PHE A  99       2.843  -0.764  12.443  1.00  9.84           C
ATOM    944  CG  PHE A  99       3.321   0.444  13.238  1.00 12.64           C
ATOM    945  CD1 PHE A  99       4.687   0.685  13.377  1.00 11.18           C
ATOM    946  CD2 PHE A  99       2.387   1.353  13.754  1.00  9.23           C
ATOM    947  CE1 PHE A  99       5.118   1.852  13.988  1.00  9.63           C
ATOM    948  CE2 PHE A  99       2.841   2.499  14.372  1.00  8.47           C
ATOM    949  CZ  PHE A  99       4.197   2.754  14.488  1.00 10.83           C
ATOM    950  H   PHE A  99       4.615  -2.934  12.841  1.00  9.67           H
ATOM    951  N   ASP A 100       0.614  -3.105  12.792  1.00  6.70           N
ATOM    952  CA  ASP A 100      -0.379  -3.770  11.956  1.00  7.98           C
ATOM    953  C   ASP A 100      -1.039  -2.659  11.134  1.00  7.35           C
ATOM    954  O   ASP A 100      -1.632  -1.764  11.724  1.00 12.17           O
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ATOM    955  CB  ASP A 100      -1.324  -4.481  12.930  1.00 10.14           C
ATOM    956  CG  ASP A 100      -2.605  -5.090  12.425  1.00  9.95           C
ATOM    957  OD1 ASP A 100      -2.950  -4.951  11.258  1.00 11.11           O
ATOM    958  OD2 ASP A 100      -3.285  -5.677  13.249  1.00 15.34           O
ATOM    959  H   ASP A 100       0.312  -2.608  13.579  1.00  7.14           H
ATOM    960  N   VAL A 101      -0.931  -2.646   9.808  1.00  5.55           N
ATOM    961  CA  VAL A 101      -1.390  -1.566   8.975  1.00  7.61           C
ATOM    962  C   VAL A 101      -2.294  -2.156   7.914  1.00  8.52           C
ATOM    963  O   VAL A 101      -1.958  -3.138   7.247  1.00  9.25           O
ATOM    964  CB  VAL A 101      -0.219  -0.822   8.287  1.00  7.15           C
ATOM    965  CG1 VAL A 101      -0.756   0.324   7.443  1.00 15.13           C
ATOM    966  CG2 VAL A 101       0.747  -0.254   9.298  1.00  7.68           C
ATOM    967  H   VAL A 101      -0.521  -3.420   9.361  1.00  6.45           H
ATOM    968  N   GLU A 102      -3.461  -1.547   7.760  1.00  7.96           N
ATOM    969  CA  GLU A 102      -4.403  -1.955   6.737  1.00  9.92           C
ATOM    970  C   GLU A 102      -4.604  -0.785   5.781  1.00 13.06           C
ATOM    971  O   GLU A 102      -5.052   0.294   6.203  1.00 12.50           O
ATOM    972  CB  GLU A 102      -5.695  -2.390   7.379  1.00  5.36           C
ATOM    973  CG  GLU A 102      -6.606  -2.921   6.277  1.00 13.32           C
ATOM    974  CD  GLU A 102      -8.027  -3.374   6.662  1.00 26.98           C
ATOM    975  OE1 GLU A 102      -8.444  -3.183   7.801  1.00 18.82           O
ATOM    976  OE2 GLU A 102      -8.726  -3.911   5.797  1.00 35.49           O
ATOM    977  H   GLU A 102      -3.672  -0.769   8.321  1.00  7.09           H
ATOM    978  N   LEU A 103      -4.264  -0.934   4.499  1.00 10.24           N
ATOM    979  CA  LEU A 103      -4.412   0.162   3.545  1.00 17.35           C
ATOM    980  C   LEU A 103      -5.842   0.131   2.996  1.00 16.77           C
ATOM    981  O   LEU A 103      -6.218  -0.674   2.131  1.00 10.58           O
ATOM    982  CB  LEU A 103      -3.383   0.101   2.396  1.00  6.83           C
ATOM    983  CG  LEU A 103      -3.420   1.173   1.322  1.00  6.78           C
ATOM    984  CD1 LEU A 103      -3.355   2.593   1.903  1.00  9.81           C
ATOM    985  CD2 LEU A 103      -2.305   0.884   0.336  1.00  7.93           C
ATOM    986  H   LEU A 103      -3.985  -1.823   4.179  1.00  5.61           H
ATOM    987  N   LEU A 104      -6.632   1.054   3.534  1.00 12.27           N
ATOM    988  CA  LEU A 104      -8.049   1.135   3.206  1.00 19.13           C
ATOM    989  C   LEU A 104      -8.359   1.714   1.814  1.00 26.84           C
ATOM    990  O   LEU A 104      -9.183   1.175   1.064  1.00 20.98           O
ATOM    991  CB  LEU A 104      -8.760   1.959   4.286  1.00 11.01           C
ATOM    992  CG  LEU A 104      -8.697   1.550   5.741  1.00 13.52           C
ATOM    993  CD1 LEU A 104      -9.264   2.663   6.620  1.00 15.82           C
ATOM    994  CD2 LEU A 104      -9.395   0.223   5.923  1.00 17.08           C
ATOM    995  H   LEU A 104      -6.243   1.701   4.162  1.00  8.40           H
ATOM    996  N   LYS A 105      -7.714   2.825   1.437  1.00 17.27           N
ATOM    997  CA  LYS A 105      -8.164   3.660   0.330  1.00 22.31           C
ATOM    998  C   LYS A 105      -7.044   4.641   0.029  1.00 15.60           C
ATOM    999  O   LYS A 105      -6.223   4.973   0.895  1.00 15.20           O
ATOM   1000  CB  LYS A 105      -9.399   4.418   0.867  1.00 19.05           C
ATOM   1001  CG  LYS A 105     -10.040   5.538   0.110  1.00 31.96           C
ATOM   1002  CD  LYS A 105     -11.223   5.999   0.948  1.00 34.16           C
ATOM   1003  CE  LYS A 105     -12.030   7.009   0.125  1.00 71.57           C
ATOM   1004  NZ  LYS A 105     -13.268   7.398   0.781  1.00 74.94           N
ATOM   1005  H   LYS A 105      -6.934   3.132   1.952  1.00 14.54           H
ATOM   1006  HZ1 LYS A 105     -13.049   7.778   1.724  1.00 50.00           H
ATOM   1007  HZ2 LYS A 105     -13.743   8.131   0.215  1.00 50.00           H
ATOM   1008  HZ3 LYS A 105     -13.889   6.570   0.873  1.00 50.00           H
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ATOM   1009  N   LEU A 106      -7.008   5.096  -1.213  1.00 14.99           N
ATOM   1010  CA  LEU A 106      -6.121   6.152  -1.629  1.00 11.65           C
ATOM   1011  C   LEU A 106      -6.996   7.338  -2.035  1.00 14.03           C
ATOM   1012  O   LEU A 106      -8.065   7.137  -2.605  1.00 28.26           O
ATOM   1013  CB  LEU A 106      -5.295   5.656  -2.810  1.00 18.89           C
ATOM   1014  CG  LEU A 106      -4.296   4.535  -2.575  1.00 13.45           C
ATOM   1015  CD1 LEU A 106      -3.659   4.162  -3.895  1.00 18.28           C
ATOM   1016  CD2 LEU A 106      -3.206   4.994  -1.580  1.00 27.57           C
ATOM   1017  H   LEU A 106      -7.703   4.847  -1.855  1.00 13.04           H
ATOM   1018  N   GLU A 107      -6.585   8.553  -1.697  1.00 20.68           N
ATOM   1019  CA  GLU A 107      -7.208   9.779  -2.162  1.00 17.07           C
ATOM   1020  C   GLU A 107      -6.108  10.687  -2.745  1.00 21.33           C
ATOM   1021  O   GLU A 107      -4.930  10.316  -2.752  1.00 47.95           O
ATOM   1022  CB  GLU A 107      -7.864  10.477  -1.003  1.00 24.97           C
ATOM   1023  CG  GLU A 107      -8.835   9.575  -0.288  1.00 20.19           C
ATOM   1024  CD  GLU A 107      -9.421  10.133   0.990  1.00 30.01           C
ATOM   1025  OE1 GLU A 107      -8.949  11.142   1.525  1.00 31.02           O
ATOM   1026  OE2 GLU A 107     -10.372   9.522   1.466  1.00 46.48           O
ATOM   1027  OXT GLU A 107      -6.431  11.768  -3.232  1.00 62.18           O
ATOM   1028  H   GLU A 107      -5.744   8.663  -1.209  1.00 17.46           H
TER    1029      GLU A 107
HETATM 1030  C1  RAP A 108       4.633   8.500  12.847  1.00  5.98           C
HETATM 1031  O1  RAP A 108       4.264   9.593  13.679  1.00  9.08           O
HETATM 1032  O2  RAP A 108       5.367   8.726  11.888  1.00 14.08           O
HETATM 1033  C2  RAP A 108       4.177   7.070  13.135  1.00  6.42           C
HETATM 1034  C3  RAP A 108       3.720   6.374  11.862  1.00  5.50           C
HETATM 1035  C4  RAP A 108       2.354   6.832  11.372  1.00  4.49           C
HETATM 1036  C5  RAP A 108       1.360   6.653  12.505  1.00  4.19           C
HETATM 1037  C6  RAP A 108       1.783   7.430  13.713  1.00  3.25           C
HETATM 1038  N7  RAP A 108       3.105   6.934  14.127  1.00  8.46           N
HETATM 1039  C8  RAP A 108       3.385   6.549  15.382  1.00 10.06           C
HETATM 1040  O3  RAP A 108       4.552   6.237  15.654  1.00 10.38           O
HETATM 1041  C9  RAP A 108       2.397   6.409  16.381  1.00 11.13           C
HETATM 1042  O4  RAP A 108       1.783   5.339  16.474  1.00 10.60           O
HETATM 1043  C10 RAP A 108       2.056   7.541  17.368  1.00 16.59           C
HETATM 1044  O5  RAP A 108       1.280   8.457  16.631  1.00 10.76           O
HETATM 1045  O6  RAP A 108       1.310   6.992  18.458  1.00 14.16           O
HETATM 1046  C11 RAP A 108       3.332   8.282  17.940  1.00 10.40           C
HETATM 1047  C12 RAP A 108       2.942   9.591  18.664  1.00 12.17           C
HETATM 1048  C13 RAP A 108       2.010  10.423  17.795  1.00 12.80           C
HETATM 1049  C14 RAP A 108       0.842   9.628  17.221  1.00 10.37           C
HETATM 1050  C15 RAP A 108       0.193  10.413  16.094  1.00  5.94           C
HETATM 1051  C16 RAP A 108      -0.582  11.664  16.490  1.00  9.79           C
HETATM 1052  O7  RAP A 108      -1.627  11.272  17.324  1.00 20.17           O
HETATM 1053  C17 RAP A 108      -1.145  12.371  15.276  1.00 15.52           C
HETATM 1054  C18 RAP A 108      -0.672  13.571  14.967  1.00 14.38           C
HETATM 1055  C19 RAP A 108      -1.096  14.367  13.807  1.00  9.73           C
HETATM 1056  C20 RAP A 108      -0.586  15.578  13.634  1.00 10.26           C
HETATM 1057  C21 RAP A 108      -0.900  16.377  12.435  1.00 11.40           C
HETATM 1058  C22 RAP A 108      -0.248  17.488  12.149  1.00 17.77           C
HETATM 1059  C23 RAP A 108      -0.450  18.289  10.881  1.00 15.64           C
HETATM 1060  C24 RAP A 108       0.911  18.401  10.216  1.00 14.68           C
HETATM 1061  C25 RAP A 108       1.674  17.112   9.975  1.00 11.87           C
HETATM 1062  C26 RAP A 108       3.157  17.391   9.771  1.00 11.65           C
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HETATM 1063  O8  RAP A 108       3.611  17.669   8.663  1.00 18.31           O
HETATM 1064  C27 RAP A 108       4.048  17.297  11.005  1.00  8.13           C
HETATM 1065  O9  RAP A 108       5.210  18.050  10.778  1.00 23.09           O
HETATM 1066  C28 RAP A 108       4.513  15.841  11.329  1.00 10.80           C
HETATM 1067  O10 RAP A 108       4.824  15.200  10.084  1.00 12.16           O
HETATM 1068  C29 RAP A 108       3.462  15.014  12.094  1.00  9.60           C
HETATM 1069  C30 RAP A 108       2.808  13.989  11.549  1.00  8.55           C
HETATM 1070  C31 RAP A 108       1.773  13.042  12.175  1.00  8.43           C
HETATM 1071  C32 RAP A 108       2.433  11.701  12.495  1.00 10.69           C
HETATM 1072  O11 RAP A 108       2.264  10.701  11.791  1.00  9.49           O
HETATM 1073  C33 RAP A 108       3.358  11.693  13.707  1.00  6.51           C
HETATM 1074  C34 RAP A 108       4.630  10.909  13.455  1.00  9.62           C
HETATM 1075  C35 RAP A 108       5.846  11.169  14.367  1.00  9.58           C
HETATM 1076  C36 RAP A 108       6.551  12.480  14.027  1.00 10.31           C
HETATM 1077  C37 RAP A 108       7.210  12.586  12.650  1.00 22.90           C
HETATM 1078  C38 RAP A 108       7.812  13.983  12.461  1.00 14.17           C
HETATM 1079  C39 RAP A 108       8.386  14.202  11.059  1.00 34.20           C
HETATM 1080  O12 RAP A 108       9.041  15.444  11.086  1.00 30.82           O
HETATM 1081  C40 RAP A 108       9.399  13.057  10.711  1.00 38.24           C
HETATM 1082  O13 RAP A 108       9.803  13.189   9.349  1.00 28.84           O
HETATM 1083  C41 RAP A 108       8.819  11.645  10.930  1.00 16.32           C
HETATM 1084  C42 RAP A 108       8.243  11.505  12.332  1.00 14.05           C
HETATM 1085  C43 RAP A 108       4.258   7.412  18.840  1.00 11.25           C
HETATM 1086  C44 RAP A 108      -2.257  11.621  14.522  1.00 14.40           C
HETATM 1087  C45 RAP A 108      -1.014  19.668  11.190  1.00  9.23           C
HETATM 1088  C46 RAP A 108       1.099  16.327   8.793  1.00 15.99           C
HETATM 1089  C47 RAP A 108       3.222  15.475  13.519  1.00 14.60           C
HETATM 1090  C48 RAP A 108       0.625  12.830  11.175  1.00  9.37           C
HETATM 1091  C49 RAP A 108       5.482  11.130  15.824  1.00  8.29           C
HETATM 1092  C50 RAP A 108      -2.123  12.243  18.189  1.00 28.36           C
HETATM 1093  C51 RAP A 108       5.134  19.387  11.130  1.00 19.04           C
HETATM 1094  C52 RAP A 108       8.352  16.524  10.556  1.00 28.14           C
HETATM 1095  HO6 RAP A 108       1.193   6.051  18.296  1.00 13.32           H
HETATM 1096  HO1 RAP A 108       5.144  14.296  10.221  1.00 13.32           H
HETATM 1097  HO3 RAP A 108       9.118  13.653   8.851  1.00 13.32           H
HETATM 1098  O   HOH A 109      13.711   4.614  19.317  1.00 10.44           O
HETATM 1099  O   HOH A 110      12.370   3.552  17.185  1.00 10.27           O
HETATM 1100  O   HOH A 111      -1.241  -8.284  -1.434  1.00 12.23           O
HETATM 1101  O   HOH A 112       7.154  -7.826   9.801  1.00 13.23           O
HETATM 1102  O   HOH A 113      14.014  -2.120   4.238  1.00 21.56           O
HETATM 1103  O   HOH A 114      12.989  -4.988  10.267  0.88 14.72           O
HETATM 1104  O   HOH A 115      14.742   0.139  23.855  1.00 20.97           O
HETATM 1105  O   HOH A 116      -4.908  -2.760  13.811  1.00 20.45           O
HETATM 1106  O   HOH A 117       3.308  -6.273  -0.446  1.00 19.05           O
HETATM 1107  O   HOH A 118      15.723  -2.951  18.984  0.92 19.73           O
HETATM 1108  O   HOH A 119      -4.683  -2.710  10.979  1.00 21.45           O
HETATM 1109  O   HOH A 120       9.150   0.338  -0.871  1.00 21.75           O
HETATM 1110  O   HOH A 121      12.319   7.586  10.611  0.89 16.22           O
HETATM 1111  O   HOH A 122       4.956  11.211   4.410  1.00 20.92           O
HETATM 1112  O   HOH A 123       0.223  -6.141  -2.826  1.00 19.78           O
HETATM 1113  O   HOH A 124       4.496   2.494  -4.547  0.86 22.55           O
HETATM 1114  O   HOH A 125      -8.981  15.116  13.622  0.93 29.61           O
HETATM 1115  O   HOH A 126      -2.561   8.843  18.364  0.51  9.74           O
HETATM 1116  O   HOH A 127       0.579   7.596  21.102  0.83 21.64           O
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HETATM 1117  O   HOH A 128      -1.361  15.053   5.335  0.97 27.18           O
HETATM 1118  O   HOH A 129       9.868  12.384  17.361  0.99 26.41           O
HETATM 1119  O   HOH A 130      13.021  -3.084  20.746  0.84 25.47           O
HETATM 1120  O   HOH A 131      13.147  -6.244  19.809  1.00 33.69           O
HETATM 1121  O   HOH A 132      19.691   7.330  15.401  1.00 34.12           O
HETATM 1122  O   HOH A 133       4.131 -12.241   3.833  0.61 29.31           O
HETATM 1123  O   HOH A 134      10.563  10.031   7.095  1.00 34.36           O
HETATM 1124  O   HOH A 135      19.240   3.723  15.306  1.00 30.14           O
HETATM 1125  O   HOH A 136      -7.944  -8.631   7.452  0.76 26.11           O
HETATM 1126  O   HOH A 137       9.738  -7.426   3.673  0.77 29.04           O
HETATM 1127  O   HOH A 138      19.287   3.331  18.119  1.00 29.46           O
HETATM 1128  O   HOH A 139      15.311  -2.532  22.773  0.59 18.35           O
HETATM 1129  O   HOH A 140      12.602  -7.831  10.522  0.70 26.37           O
HETATM 1130  O   HOH A 141      20.311   7.632  23.452  0.88 32.87           O
HETATM 1131  O   HOH A 142      -8.290  -6.594  13.906  1.00 37.66           O
HETATM 1132  O   HOH A 143       6.000  -7.155   0.752  1.00 36.79           O
HETATM 1133  O   HOH A 144      11.712   8.562  25.025  1.00 37.93           O
HETATM 1134  O   HOH A 145       6.408  17.304   7.663  1.00 42.88           O
HETATM 1135  O   HOH A 146       8.316   5.712  -0.315  0.89 35.11           O
HETATM 1136  O   HOH A 147      -8.695   3.719  -3.268  0.41 27.28           O
HETATM 1137  O   HOH A 148      -6.139  -2.153  17.988  0.79 28.45           O
HETATM 1138  O   HOH A 149       0.610  -9.863  -0.440  0.99 38.91           O
HETATM 1139  O   HOH A 150      15.715   9.985  24.770  1.00 42.21           O
HETATM 1140  O   HOH A 151      -0.495   1.447  -8.979  0.64 30.72           O
HETATM 1141  O   HOH A 152       4.285  -9.238   1.709  1.00 37.55           O
HETATM 1142  O   HOH A 153     -11.723  -0.712  23.869  1.00 40.86           O
HETATM 1143  O   HOH A 154      11.488  -3.074   2.350  0.72 41.01           O
HETATM 1144  O   HOH A 155      15.120   7.199   9.581  0.59 20.76           O
HETATM 1145  O   HOH A 156       9.795  11.399  -2.302  0.98 37.75           O
HETATM 1146  O   HOH A 157      -8.735  -4.901  -2.370  0.50 33.79           O
HETATM 1147  O   HOH A 158      -0.568  -3.277  25.728  0.85 51.27           O
HETATM 1148  O   HOH A 159      19.373   8.856  25.776  1.00 38.05           O
HETATM 1149  O   HOH A 160      -2.602  -9.850  -3.927  1.00 43.85           O
HETATM 1150  O   HOH A 161       0.050 -14.393   2.288  1.00 40.23           O
HETATM 1151  O   HOH A 162       1.610 -14.281   5.871  0.76 37.91           O
HETATM 1152  O   HOH A 163       5.428 -14.217   6.653  0.80 37.24           O
HETATM 1153  O   HOH A 164      -9.314  -2.214  -5.662  1.00 34.97           O
HETATM 1154  O   HOH A 165      -2.162   4.552  -7.445  0.90 44.53           O
HETATM 1155  O   HOH A 166      -7.983  -6.626   5.079  1.00 38.42           O
HETATM 1156  O   HOH A 167      21.106  -2.754  16.088  0.82 44.40           O
HETATM 1157  O   HOH A 168       8.565 -10.372   3.861  1.00 49.24           O
HETATM 1158  O   HOH A 169      -8.100  -8.798   1.688  0.95 45.19           O
HETATM 1159  O   HOH A 170       9.799   3.505  -1.518  1.00 39.70           O
HETATM 1160  O   HOH A 171       0.503  -4.780 -10.227  0.92 41.96           O
HETATM 1161  O   HOH A 172      19.059  -0.774  13.939  0.40 46.58           O
HETATM 1162  O   HOH A 173       4.165 -11.485   2.776  0.68 46.57           O
HETATM 1163  O   HOH A 174       6.724  -9.652  16.834  0.75 43.11           O
HETATM 1164  O   HOH A 175       8.449  20.615  10.147  1.00 52.53           O
HETATM 1165  O   HOH A 176      -6.246   8.458  13.805  0.99 43.67           O
HETATM 1166  O   HOH A 177      18.565  -0.788   8.535  0.58 25.28           O
HETATM 1167  O   HOH A 178      12.524  14.156  15.048  0.75 50.62           O
HETATM 1168  O   HOH A 179      -7.361   4.286  -6.120  0.87 45.92           O
HETATM 1169  O   HOH A 180       9.084   8.193  30.107  0.73 50.62           O
HETATM 1170  O   HOH A 181       5.353   7.074  -7.617  1.00 45.14           O
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HETATM 1171  O   HOH A 182       7.071  14.671  -2.213  0.72 44.31           O
HETATM 1172  O   HOH A 183      11.390  -5.548   2.903  1.00 45.24           O
HETATM 1173  O   HOH A 184       3.705 -11.294  15.714  0.73 62.78           O
HETATM 1174  O   HOH A 185       6.290 -12.577  11.834  0.91 63.29           O
HETATM 1175  O   HOH A 186      15.724   7.740  12.569  0.84 43.78           O
HETATM 1176  O   HOH A 187      15.320   3.814  -0.109  1.00 46.69           O
HETATM 1177  O   HOH A 188      11.066  12.165  14.148  1.00 52.26           O
HETATM 1178  O   HOH A 189      -2.305  13.015  10.396  0.69 48.40           O
HETATM 1179  O   HOH A 190      10.289  15.215   2.271  1.00 49.99           O
HETATM 1180  O   HOH A 191     -14.194  -3.824   4.927  0.56 46.37           O
HETATM 1181  O   HOH A 192      15.576  -4.385  14.703  1.00 56.00           O
HETATM 1182  O   HOH A 193      -4.948  11.515   9.936  0.75 45.07           O
HETATM 1183  O   HOH A 194      11.767  -6.802  23.315  0.67 45.81           O
HETATM 1184  O   HOH A 195      19.013  11.621  24.860  1.00 66.21           O
HETATM 1185  O   HOH A 196      12.529  17.914  12.306  0.59 50.92           O
HETATM 1186  O   HOH A 197       4.616  20.134   7.429  1.00 56.06           O
HETATM 1187  O   HOH A 198      11.720  10.374  28.067  0.78 49.39           O
HETATM 1188  O   HOH A 199      21.956   9.297  22.399  0.92 61.45           O
HETATM 1189  O   HOH A 200       3.813 -10.487  21.876  1.00 60.11           O
HETATM 1190  O   HOH A 201     -10.177  -5.766   1.941  0.89 47.46           O
HETATM 1191  O   HOH A 202      12.912  11.341  17.471  0.72 29.24           O
HETATM 1192  O   HOH A 203     -13.247  13.956  10.938  0.58 53.33           O
HETATM 1193  O   HOH A 204       2.516 -14.263   2.186  0.72 45.69           O
HETATM 1194  O   HOH A 205      11.923  -9.286  21.896  0.98 45.91           O
HETATM 1195  O   HOH A 206      -5.617  14.450   1.733  1.00 50.10           O
HETATM 1196  O   HOH A 207      13.176  -7.604  14.206  0.50 41.46           O
HETATM 1197  O   HOH A 208      -5.817  10.729  11.860  1.00 44.20           O
HETATM 1198  O   HOH A 209       2.093 -13.180  -0.045  0.68 49.74           O
HETATM 1199  O   HOH A 210      11.679  -0.994  23.351  0.62 46.69           O
HETATM 1200  O   HOH A 211      12.019  19.146   9.856  0.62 48.55           O
HETATM 1201  O   HOH A 212       2.351  20.217   6.237  0.82 55.30           O
HETATM 1202  O   HOH A 213      -0.468  -8.897  -8.871  0.60 43.26           O
HETATM 1203  O   HOH A 214      12.074   6.391   1.989  0.68 42.25           O
HETATM 1204  O   HOH A 215     -10.022  -8.902  11.765  0.97 59.16           O
HETATM 1205  O   HOH A 216      17.246   5.567   7.897  0.96 72.72           O
HETATM 1206  O   HOH A 217      10.220  -8.740  26.275  0.53 48.13           O
HETATM 1207  O   HOH A 218       5.332   3.455  25.799  0.60 49.45           O
HETATM 1208  O   HOH A 219     -14.447  -4.763  15.812  0.67 49.47           O
HETATM 1209  O   HOH A 220     -11.952  -7.785   3.937  0.59 48.74           O
HETATM 1210  O   HOH A 221      11.239  -2.520  21.226  0.59 41.21           O
HETATM 1211  O   HOH A 222      19.871   7.101   2.737  0.70 54.57           O
HETATM 1212  O   HOH A 223      -9.253   8.067  22.611  0.88 71.92           O
HETATM 1213  O   HOH A 224      14.762  -9.286  11.495  0.43 54.93           O
HETATM 1214  O   HOH A 225       8.516  18.025   4.379  0.71 53.38           O
HETATM 1215  O   HOH A 226      13.793  -1.543   0.127  0.66 49.81           O
HETATM 1216  O   HOH A 227     -12.297   6.615   5.037  0.61 48.14           O
HETATM 1217  O   HOH A 228      11.923   8.740   4.379  0.71 46.89           O
HETATM 1218  O   HOH A 229      10.123  -6.243   0.055  0.54 49.94           O
HETATM 1219  O   HOH A 230     -10.759  -8.925   9.485  1.00 68.01           O
HETATM 1220  O   HOH A 231     -10.487  14.161  -0.107  0.80 46.65           O
HETATM 1221  O   HOH A 232       3.196  18.042   4.596  0.69 59.09           O
HETATM 1222  O   HOH A 233      11.610 -14.657   3.936  0.44 80.48           O
HETATM 1223  O   HOH A 234      12.491  -0.546   2.190  0.65 47.59           O
HETATM 1224  O   HOH A 235      10.787   7.101   0.000  0.52 49.42           O
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HETATM 1225  O   HOH A 236      -9.426  -6.421   8.886  0.34 47.03           O
HETATM 1226  O   HOH A 237      11.923   0.546  -0.547  0.89 45.99           O
HETATM 1227  O   HOH A 238      -2.327  14.131   7.962  0.56 52.95           O
HETATM 1228  O   HOH A 239      14.190   8.846   3.456  0.54 52.74           O
HETATM 1229  O   HOH A 240       1.142   1.871  26.400  0.44 45.02           O
HETATM 1230  O   HOH A 241     -10.179  -5.869  12.400  0.74 80.37           O
CONECT 1030 1031 1032 1033
CONECT 1031 1030 1074
CONECT 1032 1030
CONECT 1033 1030 1034 1038
CONECT 1034 1033 1035
CONECT 1035 1034 1036
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CONECT 1077 1076 1078 1084
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CONECT 1080 1079 1094
CONECT 1081 1079 1082 1083
CONECT 1082 1081 1097
CONECT 1083 1081 1084
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CONECT 1093 1065
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CONECT 1097 1082
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