Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# Supporting Information

## Interactions of a multifunctional di–triazole derivative with Alzheimer's $A\beta_{42}$ monomer and $A\beta_{42}$ protofibril: A systematic molecular dynamics study

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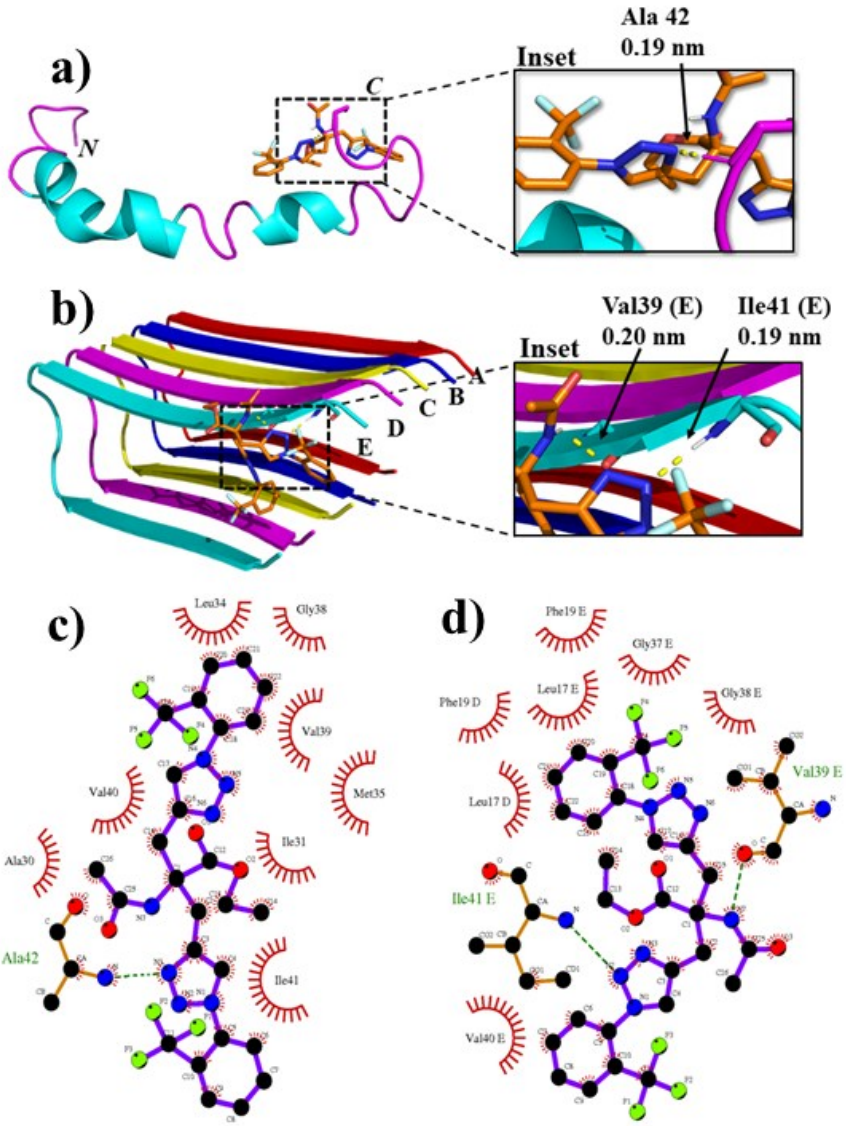


**Fig. S1**: The docked complex of **6n** with $A\beta_{42}$ monomer (PDB: 1Z0Q) highlighting the best–docked conformation is shown in panel a. The $A\beta_{42}$ structure is shown in the cartoon representation and **6n** is shown in the stick representation. The docked complex of **6n** with $A\beta_{42}$ fibril (PDB: 2BEG) is shown in panel b. The hydrogen bonds are represented as yellow dashed lines. The 2D interaction maps displaying the hydrophobic contacts of **6n** with $A\beta_{42}$ monomer and $A\beta_{42}$ protofibril are shown in panel c, and d, respectively. The maps were generated using LigPlot+ software. The green dashed lines depict the hydrogen bonds between $A\beta_{42}$ monomer–**6n**, and $A\beta_{42}$ protofibril–**6n.**[1]

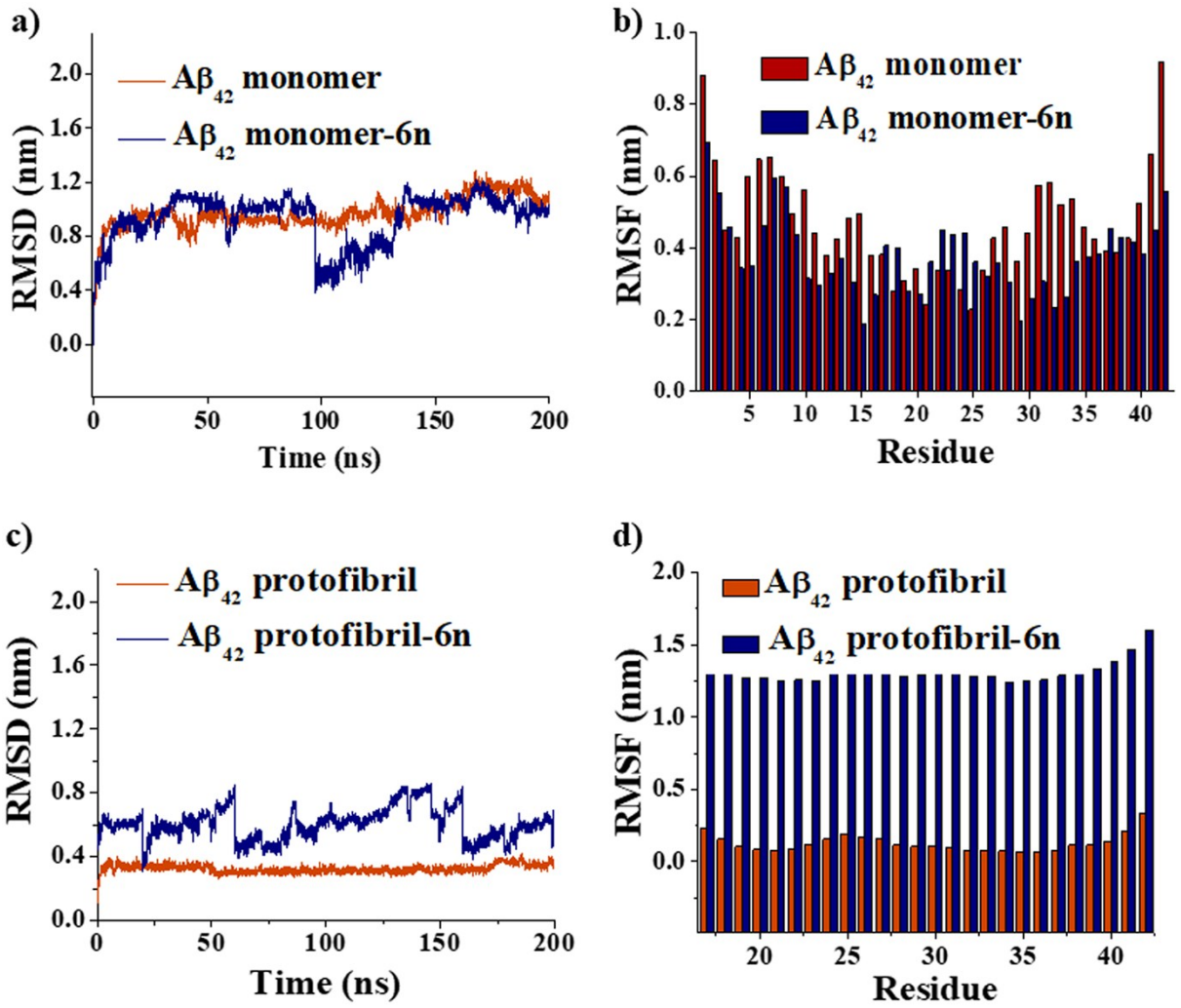


**Fig. S2**: The root–mean–square deviation (RMSD) and root–mean–square fluctuation (RMSF) for $A\beta_{42}$ monomer and $A\beta_{42}$ monomer–**6n** complex are shown in panel a, and b, respectively. The RMSD and RMSF for $A\beta_{42}$ protofibril and $A\beta_{42}$ protofibril–**6n** complex are shown in panel c, and d, respectively.

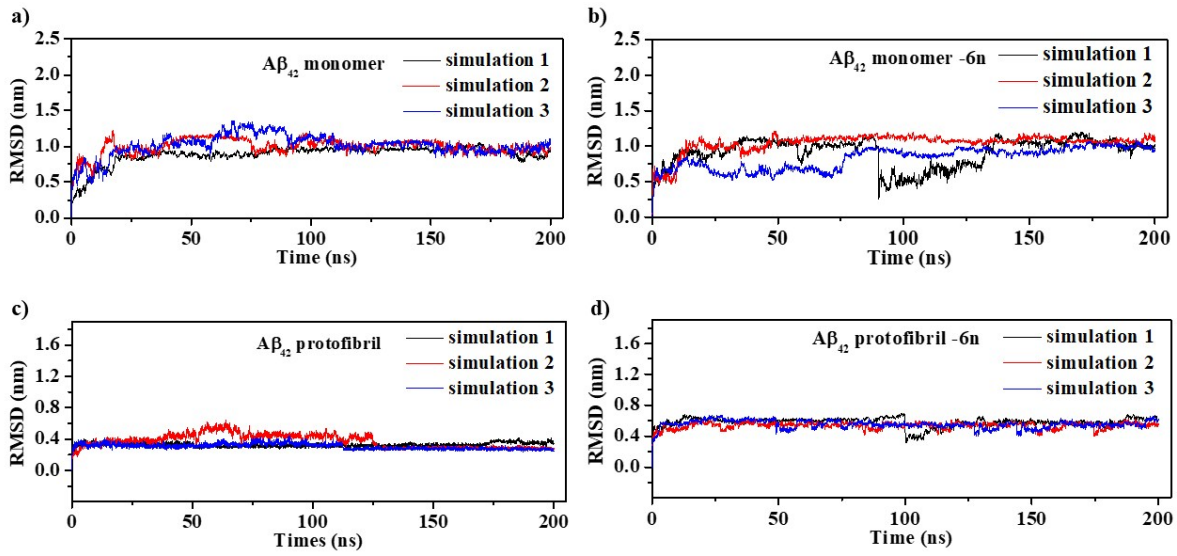


**Fig. S3**: The RMSD of triplicate simulations for $A\beta_{42}$ monomer, $A\beta_{42}$ monomer–**6n** complex, $A\beta_{42}$ protofibril, $A\beta_{42}$ protofibril–**6n** complex are shown in panel (a–d), respectively.

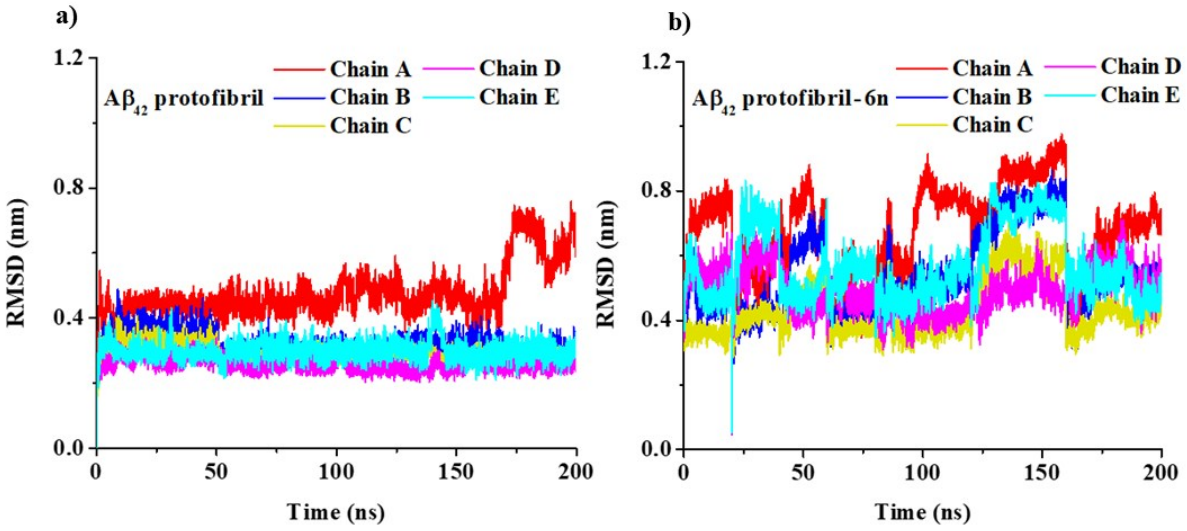


**Fig. S4**: The RMSD of the five chains, A–E, of $A\beta_{42}$ protofibril and $A\beta_{42}$ protofibril–**6n** complex is shown in panel a, and b, respectively.

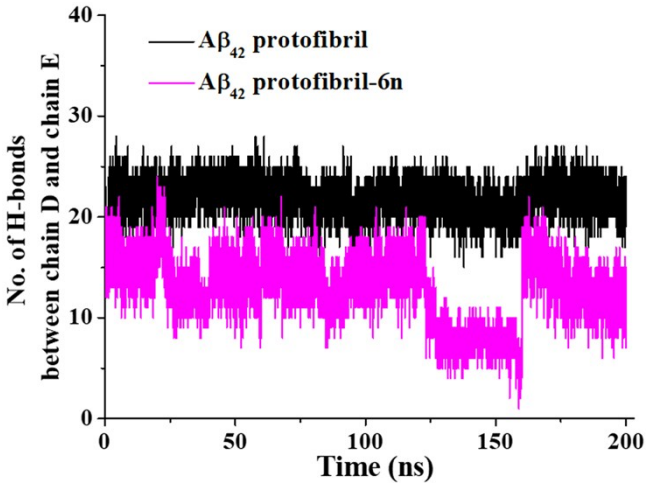


**Fig. S5**: The number of hydrogen bonds between $A\beta_{42}$ protofibril chains D–E for $A\beta_{42}$ protofibril (black) and $A\beta_{42}$ protofibril−**6n** complex (magenta) is shown during simulation.

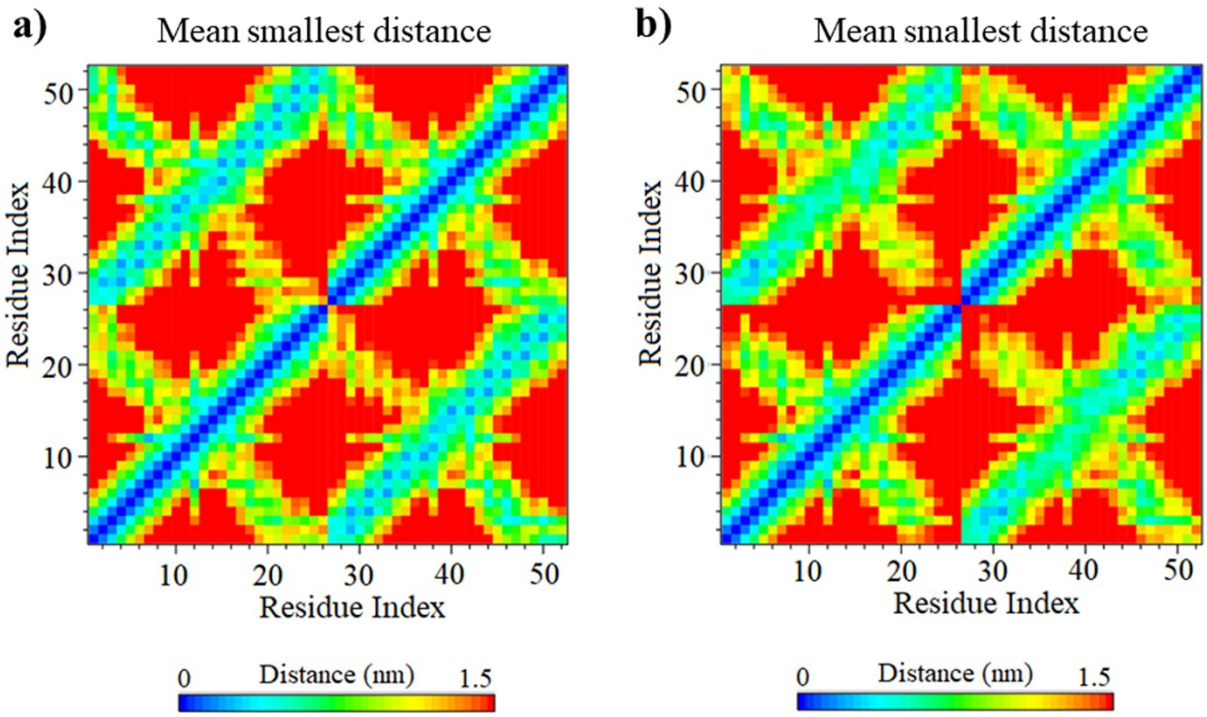


**Fig. S6**: The residue–residue contact maps between $A\beta_{42}$ protofibril chains D–E for $A\beta_{42}$ protofibril and $A\beta_{42}$ protofibril−**6n** complex are shown in panel a, and b, respectively. The cut–off distance between atoms used to define contact is 1.5 nm.

**Table S1**: The secondary structure component statistics of $A\beta_{42}$ monomer, $A\beta_{42}$ monomer–**6n** complex, $A\beta_{42}$ protofibril, and $A\beta_{42}$ protofibril–**6n** complex for triplicate simulations.

| Model system | Simulation | Secondary structure component (%) | | | | | |
|---|---|---|---|---|---|---|---|
| | | Helix[a] | β–sheet[b] | Coil | Bend | Turn | Chain–separator |
| $A\beta_{42}$ monomer | 1 | 46 | 4 | 29 | 13 | 8 | 0 |
| | 2 | 40 | 4 | 32 | 17 | 6 | 0 |
| | 3 | 38 | 4 | 33 | 17 | 7 | 0 |
| $A\beta_{42}$ monomer–**6n** | 1 | 53 | 0 | 25 | 11 | 11 | 0 |
| | 2 | 42 | 0 | 28 | 14 | 16 | 0 |
| | 3 | 45 | 0 | 23 | 8 | 24 | 0 |
| $A\beta_{42}$ protofibril | 1 | 0 | 69 | 20 | 8 | 0 | 3 |
| | 2 | 0 | 69 | 22 | 6 | 0 | 3 |
| | 3 | 0 | 74 | 18 | 5 | 0 | 3 |
| $A\beta_{42}$ protofibril–**6n** | 1 | 0 | 46 | 38 | 10 | 3 | 3 |
| | 2 | 0 | 42 | 38 | 12 | 5 | 3 |
| | 3 | 0 | 44 | 37 | 12 | 4 | 3 |

[a]Helix = α–helix+ π–helix+ $3_{10}$–helix; [b]β–sheet = β–strand + β–bridge

Coordinates of the representative structures from cluster analysis for $A\beta_{42}$ monomer, $A\beta_{42}$ monomer–**6n** complex, $A\beta_{42}$ protofibril, and $A\beta_{42}$ protofibril–**6n** complex.

1. $A\beta_{42}$ monomer

```
ATOM      1  N   ASP     1     -12.530  -7.438   8.267  1.00  0.00           N
ATOM      2  CA  ASP     1     -11.340  -6.944   7.555  1.00  0.00           C
ATOM      3  C   ASP     1     -11.510  -6.506   6.104  1.00  0.00           C
ATOM      4  O   ASP     1     -12.251  -7.139   5.347  1.00  0.00           O
ATOM      5  CB  ASP     1     -10.207  -7.976   7.649  1.00  0.00           C
ATOM      6  CG  ASP     1      -8.807  -7.385   7.503  1.00  0.00           C
ATOM      7  OD1 ASP     1      -8.096  -7.688   6.512  1.00  0.00           O
ATOM      8  OD2 ASP     1      -8.617  -6.389   8.221  1.00  0.00           O1-
ATOM      9  H1  ASP     1     -13.159  -6.668   8.350  1.00  0.00           H
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ATOM     12  N   ALA     2     -10.709  -5.547   5.636  1.00  0.00           N
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ATOM     14  C   ALA     2      -9.383  -4.990   3.517  1.00  0.00           C
ATOM     15  O   ALA     2      -8.303  -4.991   4.101  1.00  0.00           O
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ATOM    123  OE1 GLU    11     -10.612   5.643   5.565  1.00  0.00           O
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ATOM    160  HE1 HIS    14      -9.183   9.351   0.549  1.00  0.00           H
ATOM    161  HE2 HIS    14     -10.417   9.605  -1.604  1.00  0.00           H
ATOM    162  N   GLN    15      -5.015   7.573  -0.124  1.00  0.00           N
ATOM    163  CA  GLN    15      -4.137   7.670   1.052  1.00  0.00           C
ATOM    164  C   GLN    15      -3.494   6.359   1.493  1.00  0.00           C
ATOM    165  O   GLN    15      -2.264   6.307   1.489  1.00  0.00           O
ATOM    166  CB  GLN    15      -4.895   8.302   2.219  1.00  0.00           C
ATOM    167  CG  GLN    15      -5.263   9.756   1.928  1.00  0.00           C
ATOM    168  CD  GLN    15      -4.064  10.662   1.668  1.00  0.00           C
ATOM    169  NE2 GLN    15      -4.179  11.629   0.763  1.00  0.00           N
ATOM    170  OE1 GLN    15      -3.046  10.547   2.361  1.00  0.00           O
ATOM    171  H   GLN    15      -5.882   8.059  -0.035  1.00  0.00           H
ATOM    172 1HE2 GLN    15      -5.057  11.714   0.297  1.00  0.00           H
ATOM    173 2HE2 GLN    15      -3.367  12.121   0.436  1.00  0.00           H
ATOM    174  N   LYS    16      -4.233   5.253   1.494  1.00  0.00           N
ATOM    175  CA  LYS    16      -3.580   3.948   1.697  1.00  0.00           C
ATOM    176  C   LYS    16      -2.723   3.382   0.560  1.00  0.00           C
ATOM    177  O   LYS    16      -1.742   2.699   0.835  1.00  0.00           O
ATOM    178  CB  LYS    16      -4.513   2.855   2.215  1.00  0.00           C
ATOM    179  CG  LYS    16      -5.324   3.217   3.470  1.00  0.00           C
ATOM    180  CD  LYS    16      -4.529   2.692   4.663  1.00  0.00           C
ATOM    181  CE  LYS    16      -5.168   3.197   5.956  1.00  0.00           C
ATOM    182  NZ  LYS    16      -4.391   2.946   7.179  1.00  0.00          N1+
ATOM    183  H   LYS    16      -5.106   5.307   1.014  1.00  0.00           H
ATOM    184  HZ1 LYS    16      -3.429   3.198   7.090  1.00  0.00           H
ATOM    185  HZ2 LYS    16      -4.751   3.498   7.925  1.00  0.00           H
ATOM    186  HZ3 LYS    16      -4.401   1.979   7.441  1.00  0.00           H
ATOM    187  N   LEU    17      -2.995   3.781  -0.680  1.00  0.00           N
ATOM    188  CA  LEU    17      -2.037   3.548  -1.779  1.00  0.00           C
ATOM    189  C   LEU    17      -0.698   4.275  -1.732  1.00  0.00           C
ATOM    190  O   LEU    17       0.358   3.658  -1.865  1.00  0.00           O
ATOM    191  CB  LEU    17      -2.776   3.761  -3.102  1.00  0.00           C
ATOM    192  CG  LEU    17      -3.852   2.723  -3.431  1.00  0.00           C
ATOM    193  CD1 LEU    17      -4.551   3.058  -4.750  1.00  0.00           C
ATOM    194  CD2 LEU    17      -3.147   1.372  -3.612  1.00  0.00           C
ATOM    195  H   LEU    17      -3.925   3.997  -0.951  1.00  0.00           H
ATOM    196  N   VAL    18      -0.802   5.508  -1.237  1.00  0.00           N
ATOM    197  CA  VAL    18       0.430   6.265  -0.959  1.00  0.00           C
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ATOM    198  C   VAL    18       1.252   5.590   0.138  1.00  0.00           C
ATOM    199  O   VAL    18       2.430   5.332  -0.087  1.00  0.00           O
ATOM    200  CB  VAL    18       0.406   7.783  -0.763  1.00  0.00           C
ATOM    201  CG1 VAL    18       1.745   8.446  -0.447  1.00  0.00           C
ATOM    202  CG2 VAL    18      -0.229   8.468  -1.973  1.00  0.00           C
ATOM    203  H   VAL    18      -1.597   6.079  -1.395  1.00  0.00           H
ATOM    204  N   PHE    19       0.609   5.175   1.232  1.00  0.00           N
ATOM    205  CA  PHE    19       1.195   4.483   2.387  1.00  0.00           C
ATOM    206  C   PHE    19       1.793   3.138   1.969  1.00  0.00           C
ATOM    207  O   PHE    19       2.954   2.817   2.208  1.00  0.00           O
ATOM    208  CB  PHE    19       0.141   4.202   3.463  1.00  0.00           C
ATOM    209  CG  PHE    19       0.353   2.977   4.358  1.00  0.00           C
ATOM    210  CD1 PHE    19       1.129   3.211   5.487  1.00  0.00           C
ATOM    211  CD2 PHE    19      -0.520   1.898   4.274  1.00  0.00           C
ATOM    212  CE1 PHE    19       1.058   2.332   6.556  1.00  0.00           C
ATOM    213  CE2 PHE    19      -0.591   1.020   5.353  1.00  0.00           C
ATOM    214  CZ  PHE    19       0.218   1.229   6.463  1.00  0.00           C
ATOM    215  H   PHE    19      -0.387   5.204   1.250  1.00  0.00           H
ATOM    216  HD1 PHE    19       2.019   3.838   5.402  1.00  0.00           H
ATOM    217  HD2 PHE    19      -1.152   1.736   3.403  1.00  0.00           H
ATOM    218  HE1 PHE    19       1.650   2.526   7.454  1.00  0.00           H
ATOM    219  HE2 PHE    19      -1.299   0.196   5.489  1.00  0.00           H
ATOM    220  HZ  PHE    19       0.254   0.492   7.269  1.00  0.00           H
ATOM    221  N   PHE    20       1.112   2.371   1.119  1.00  0.00           N
ATOM    222  CA  PHE    20       1.596   1.153   0.442  1.00  0.00           C
ATOM    223  C   PHE    20       2.756   1.267  -0.551  1.00  0.00           C
ATOM    224  O   PHE    20       3.696   0.472  -0.485  1.00  0.00           O
ATOM    225  CB  PHE    20       0.639   0.339  -0.423  1.00  0.00           C
ATOM    226  CG  PHE    20      -0.599  -0.331   0.194  1.00  0.00           C
ATOM    227  CD1 PHE    20      -0.412  -1.250   1.226  1.00  0.00           C
ATOM    228  CD2 PHE    20      -1.777  -0.340  -0.531  1.00  0.00           C
ATOM    229  CE1 PHE    20      -1.377  -2.173   1.621  1.00  0.00           C
ATOM    230  CE2 PHE    20      -2.768  -1.228  -0.110  1.00  0.00           C
ATOM    231  CZ  PHE    20      -2.575  -2.139   0.920  1.00  0.00           C
ATOM    232  H   PHE    20       0.264   2.578   0.637  1.00  0.00           H
ATOM    233  HD1 PHE    20       0.549  -1.277   1.744  1.00  0.00           H
ATOM    234  HD2 PHE    20      -1.968   0.356  -1.356  1.00  0.00           H
ATOM    235  HE1 PHE    20      -1.410  -2.597   2.628  1.00  0.00           H
ATOM    236  HE2 PHE    20      -3.766  -1.278  -0.548  1.00  0.00           H
ATOM    237  HZ  PHE    20      -3.334  -2.911   1.092  1.00  0.00           H
ATOM    238  N   ALA    21       2.749   2.255  -1.439  1.00  0.00           N
ATOM    239  CA  ALA    21       3.891   2.764  -2.210  1.00  0.00           C
ATOM    240  C   ALA    21       5.037   3.333  -1.366  1.00  0.00           C
ATOM    241  O   ALA    21       6.183   3.203  -1.788  1.00  0.00           O
ATOM    242  CB  ALA    21       3.301   3.798  -3.175  1.00  0.00           C
ATOM    243  H   ALA    21       1.896   2.751  -1.609  1.00  0.00           H
ATOM    244  N   GLU    22       4.830   4.068  -0.283  1.00  0.00           N
ATOM    245  CA  GLU    22       5.919   4.359   0.662  1.00  0.00           C
ATOM    246  C   GLU    22       6.570   3.307   1.563  1.00  0.00           C
ATOM    247  O   GLU    22       7.569   2.664   1.236  1.00  0.00           O
ATOM    248  CB  GLU    22       5.411   5.492   1.563  1.00  0.00           C
ATOM    249  CG  GLU    22       5.229   6.850   0.885  1.00  0.00           C
ATOM    250  CD  GLU    22       5.313   7.864   2.029  1.00  0.00           C
ATOM    251  OE1 GLU    22       4.282   8.578   2.131  1.00  0.00           O
ATOM    252  OE2 GLU    22       6.275   7.966   2.818  1.00  0.00           O1-
ATOM    253  H   GLU    22       3.935   4.492  -0.127  1.00  0.00           H
ATOM    254  N   ASP    23       5.713   2.748   2.419  1.00  0.00           N
ATOM    255  CA  ASP    23       6.147   1.945   3.569  1.00  0.00           C
ATOM    256  C   ASP    23       6.846   0.633   3.196  1.00  0.00           C
ATOM    257  O   ASP    23       8.025   0.474   3.504  1.00  0.00           O
ATOM    258  CB  ASP    23       5.015   1.744   4.575  1.00  0.00           C
ATOM    259  CG  ASP    23       5.347   0.740   5.682  1.00  0.00           C
ATOM    260  OD1 ASP    23       4.757  -0.355   5.717  1.00  0.00           O
ATOM    261  OD2 ASP    23       6.175   1.138   6.538  1.00  0.00           O1-
ATOM    262  H   ASP    23       4.730   2.932   2.456  1.00  0.00           H
ATOM    263  N   VAL    24       6.086  -0.376   2.770  1.00  0.00           N
ATOM    264  CA  VAL    24       6.625  -1.614   2.193  1.00  0.00           C
ATOM    265  C   VAL    24       7.219  -1.404   0.796  1.00  0.00           C
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ATOM    266  O   VAL    24       8.208  -1.993   0.367  1.00  0.00           O
ATOM    267  CB  VAL    24       5.647  -2.786   2.106  1.00  0.00           C
ATOM    268  CG1 VAL    24       5.208  -3.200   3.519  1.00  0.00           C
ATOM    269  CG2 VAL    24       4.381  -2.373   1.348  1.00  0.00           C
ATOM    270  H   VAL    24       5.123  -0.528   3.014  1.00  0.00           H
ATOM    271  N   GLY    25       6.684  -0.484  -0.009  1.00  0.00           N
ATOM    272  CA  GLY    25       7.184  -0.004  -1.296  1.00  0.00           C
ATOM    273  C   GLY    25       8.580   0.623  -1.357  1.00  0.00           C
ATOM    274  O   GLY    25       9.578  -0.082  -1.314  1.00  0.00           O
ATOM    275  H   GLY    25       5.706  -0.268   0.124  1.00  0.00           H
ATOM    276  N   SER    26       8.630   1.948  -1.355  1.00  0.00           N
ATOM    277  CA  SER    26       9.903   2.681  -1.354  1.00  0.00           C
ATOM    278  C   SER    26      10.858   2.563  -0.163  1.00  0.00           C
ATOM    279  O   SER    26      12.077   2.600  -0.317  1.00  0.00           O
ATOM    280  CB  SER    26       9.768   4.190  -1.606  1.00  0.00           C
ATOM    281  OG  SER    26       8.847   4.776  -0.691  1.00  0.00           O
ATOM    282  H   SER    26       7.822   2.528  -1.228  1.00  0.00           H
ATOM    283  HG  SER    26       9.283   5.533  -0.205  1.00  0.00           H
ATOM    284  N   ASN    27      10.398   2.409   1.078  1.00  0.00           N
ATOM    285  CA  ASN    27      11.255   2.074   2.218  1.00  0.00           C
ATOM    286  C   ASN    27      11.830   0.657   2.267  1.00  0.00           C
ATOM    287  O   ASN    27      12.818   0.433   1.562  1.00  0.00           O
ATOM    288  CB  ASN    27      10.714   2.588   3.551  1.00  0.00           C
ATOM    289  CG  ASN    27      10.601   4.112   3.693  1.00  0.00           C
ATOM    290  ND2 ASN    27       9.796   4.564   4.654  1.00  0.00           N
ATOM    291  OD1 ASN    27      11.605   4.783   3.456  1.00  0.00           O
ATOM    292  H   ASN    27       9.441   2.457   1.364  1.00  0.00           H
ATOM    293 1HD2 ASN    27       9.264   3.966   5.261  1.00  0.00           H
ATOM    294 2HD2 ASN    27       9.683   5.541   4.790  1.00  0.00           H
ATOM    295  N   LYS    28      11.008  -0.239   2.787  1.00  0.00           N
ATOM    296  CA  LYS    28      11.278  -1.664   3.040  1.00  0.00           C
ATOM    297  C   LYS    28      11.700  -2.476   1.808  1.00  0.00           C
ATOM    298  O   LYS    28      12.340  -3.523   1.900  1.00  0.00           O
ATOM    299  CB  LYS    28      10.055  -2.171   3.808  1.00  0.00           C
ATOM    300  CG  LYS    28       9.933  -1.533   5.199  1.00  0.00           C
ATOM    301  CD  LYS    28       8.639  -2.086   5.799  1.00  0.00           C
ATOM    302  CE  LYS    28       8.402  -1.684   7.257  1.00  0.00           C
ATOM    303  NZ  LYS    28       6.982  -1.543   7.611  1.00  0.00           N1+
ATOM    304  H   LYS    28      10.189   0.076   3.273  1.00  0.00           H
ATOM    305  HZ1 LYS    28       6.547  -2.385   7.315  1.00  0.00           H
ATOM    306  HZ2 LYS    28       6.847  -1.284   8.576  1.00  0.00           H
ATOM    307  HZ3 LYS    28       6.523  -0.869   7.031  1.00  0.00           H
ATOM    308  N   GLY    29      11.123  -2.167   0.646  1.00  0.00           N
ATOM    309  CA  GLY    29      11.652  -2.603  -0.650  1.00  0.00           C
ATOM    310  C   GLY    29      12.969  -1.931  -1.060  1.00  0.00           C
ATOM    311  O   GLY    29      14.094  -2.410  -0.961  1.00  0.00           O
ATOM    312  H   GLY    29      10.192  -1.806   0.653  1.00  0.00           H
ATOM    313  N   ALA    30      12.644  -0.840  -1.765  1.00  0.00           N
ATOM    314  CA  ALA    30      13.587  -0.026  -2.546  1.00  0.00           C
ATOM    315  C   ALA    30      14.829   0.683  -2.005  1.00  0.00           C
ATOM    316  O   ALA    30      15.887   0.351  -2.532  1.00  0.00           O
ATOM    317  CB  ALA    30      12.721   0.912  -3.384  1.00  0.00           C
ATOM    318  H   ALA    30      11.700  -0.498  -1.721  1.00  0.00           H
ATOM    319  N   ILE    31      14.784   1.560  -1.005  1.00  0.00           N
ATOM    320  CA  ILE    31      16.018   2.124  -0.435  1.00  0.00           C
ATOM    321  C   ILE    31      17.064   1.161   0.135  1.00  0.00           C
ATOM    322  O   ILE    31      18.223   1.340  -0.225  1.00  0.00           O
ATOM    323  CB  ILE    31      15.742   3.218   0.605  1.00  0.00           C
ATOM    324  CG1 ILE    31      14.937   2.796   1.839  1.00  0.00           C
ATOM    325  CG2 ILE    31      15.182   4.444  -0.103  1.00  0.00           C
ATOM    326  CD  ILE    31      14.920   3.891   2.906  1.00  0.00           C
ATOM    327  H   ILE    31      13.910   1.766  -0.563  1.00  0.00           H
ATOM    328  N   ILE    32      16.625  -0.012   0.570  1.00  0.00           N
ATOM    329  CA  ILE    32      17.570  -1.068   0.953  1.00  0.00           C
ATOM    330  C   ILE    32      18.003  -2.047  -0.145  1.00  0.00           C
ATOM    331  O   ILE    32      19.102  -2.590  -0.123  1.00  0.00           O
ATOM    332  CB  ILE    32      17.250  -1.846   2.231  1.00  0.00           C
ATOM    333  CG1 ILE    32      15.854  -2.494   2.214  1.00  0.00           C
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ATOM    334  CG2 ILE    32      17.508  -0.928   3.429  1.00  0.00           C
ATOM    335  CD  ILE    32      16.034  -3.878   2.826  1.00  0.00           C
ATOM    336  H   ILE    32      15.685  -0.299   0.767  1.00  0.00           H
ATOM    337  N   GLY    33      17.111  -2.364  -1.083  1.00  0.00           N
ATOM    338  CA  GLY    33      17.340  -3.399  -2.100  1.00  0.00           C
ATOM    339  C   GLY    33      16.209  -3.723  -3.085  1.00  0.00           C
ATOM    340  O   GLY    33      15.482  -2.850  -3.555  1.00  0.00           O
ATOM    341  H   GLY    33      16.211  -1.933  -1.051  1.00  0.00           H
ATOM    342  N   LEU    34      15.791  -4.980  -3.168  1.00  0.00           N
ATOM    343  CA  LEU    34      14.698  -5.389  -4.058  1.00  0.00           C
ATOM    344  C   LEU    34      13.305  -5.458  -3.421  1.00  0.00           C
ATOM    345  O   LEU    34      13.098  -5.321  -2.210  1.00  0.00           O
ATOM    346  CB  LEU    34      15.102  -6.733  -4.673  1.00  0.00           C
ATOM    347  CG  LEU    34      16.425  -6.858  -5.439  1.00  0.00           C
ATOM    348  CD1 LEU    34      16.484  -8.313  -5.918  1.00  0.00           C
ATOM    349  CD2 LEU    34      16.666  -5.920  -6.618  1.00  0.00           C
ATOM    350  H   LEU    34      16.090  -5.681  -2.517  1.00  0.00           H
ATOM    351  N   MET    35      12.334  -5.427  -4.327  1.00  0.00           N
ATOM    352  CA  MET    35      10.987  -5.035  -3.897  1.00  0.00           C
ATOM    353  C   MET    35      10.166  -6.149  -3.233  1.00  0.00           C
ATOM    354  O   MET    35      10.298  -7.344  -3.462  1.00  0.00           O
ATOM    355  CB  MET    35      10.261  -4.380  -5.072  1.00  0.00           C
ATOM    356  CG  MET    35      10.822  -2.985  -5.378  1.00  0.00           C
ATOM    357  SD  MET    35       9.887  -1.796  -4.365  1.00  0.00           S
ATOM    358  CE  MET    35       9.843  -0.424  -5.499  1.00  0.00           C
ATOM    359  H   MET    35      12.434  -5.854  -5.226  1.00  0.00           H
ATOM    360  N   VAL    36       9.290  -5.682  -2.340  1.00  0.00           N
ATOM    361  CA  VAL    36       8.489  -6.567  -1.487  1.00  0.00           C
ATOM    362  C   VAL    36       6.987  -6.251  -1.457  1.00  0.00           C
ATOM    363  O   VAL    36       6.264  -7.227  -1.238  1.00  0.00           O
ATOM    364  CB  VAL    36       9.014  -6.702  -0.057  1.00  0.00           C
ATOM    365  CG1 VAL    36      10.390  -7.365   0.044  1.00  0.00           C
ATOM    366  CG2 VAL    36       9.048  -5.370   0.692  1.00  0.00           C
ATOM    367  H   VAL    36       9.340  -4.705  -2.137  1.00  0.00           H
ATOM    368  N   GLY    37       6.628  -4.984  -1.650  1.00  0.00           N
ATOM    369  CA  GLY    37       5.215  -4.609  -1.784  1.00  0.00           C
ATOM    370  C   GLY    37       4.828  -3.167  -2.121  1.00  0.00           C
ATOM    371  O   GLY    37       5.714  -2.367  -2.434  1.00  0.00           O
ATOM    372  H   GLY    37       7.245  -4.204  -1.616  1.00  0.00           H
ATOM    373  N   GLY    38       3.544  -2.988  -2.413  1.00  0.00           N
ATOM    374  CA  GLY    38       3.075  -1.619  -2.718  1.00  0.00           C
ATOM    375  C   GLY    38       1.657  -1.477  -3.256  1.00  0.00           C
ATOM    376  O   GLY    38       0.766  -2.183  -2.777  1.00  0.00           O
ATOM    377  H   GLY    38       2.898  -3.733  -2.287  1.00  0.00           H
ATOM    378  N   VAL    39       1.501  -0.755  -4.365  1.00  0.00           N
ATOM    379  CA  VAL    39       0.192  -0.498  -4.986  1.00  0.00           C
ATOM    380  C   VAL    39      -0.471  -1.737  -5.602  1.00  0.00           C
ATOM    381  O   VAL    39      -1.693  -1.838  -5.517  1.00  0.00           O
ATOM    382  CB  VAL    39       0.138   0.734  -5.887  1.00  0.00           C
ATOM    383  CG1 VAL    39       0.255   2.101  -5.224  1.00  0.00           C
ATOM    384  CG2 VAL    39       1.004   0.555  -7.142  1.00  0.00           C
ATOM    385  H   VAL    39       2.329  -0.274  -4.650  1.00  0.00           H
ATOM    386  N   VAL    40       0.223  -2.531  -6.423  1.00  0.00           N
ATOM    387  CA  VAL    40      -0.386  -3.790  -6.886  1.00  0.00           C
ATOM    388  C   VAL    40       0.242  -4.998  -6.178  1.00  0.00           C
ATOM    389  O   VAL    40      -0.464  -5.901  -5.729  1.00  0.00           O
ATOM    390  CB  VAL    40      -0.479  -3.984  -8.395  1.00  0.00           C
ATOM    391  CG1 VAL    40      -1.434  -2.953  -8.997  1.00  0.00           C
ATOM    392  CG2 VAL    40       0.859  -4.065  -9.141  1.00  0.00           C
ATOM    393  H   VAL    40       1.186  -2.434  -6.646  1.00  0.00           H
ATOM    394  N   ILE    41       1.559  -4.962  -6.044  1.00  0.00           N
ATOM    395  CA  ILE    41       2.370  -5.974  -5.350  1.00  0.00           C
ATOM    396  C   ILE    41       2.149  -6.054  -3.840  1.00  0.00           C
ATOM    397  O   ILE    41       1.951  -5.058  -3.135  1.00  0.00           O
ATOM    398  CB  ILE    41       3.832  -6.032  -5.795  1.00  0.00           C
ATOM    399  CG1 ILE    41       4.651  -4.767  -5.496  1.00  0.00           C
ATOM    400  CG2 ILE    41       3.919  -6.373  -7.292  1.00  0.00           C
ATOM    401  CD  ILE    41       6.183  -4.848  -5.575  1.00  0.00           C
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ATOM    402  H   ILE    41       2.049  -4.114  -6.297  1.00  0.00           H
ATOM    403  N   ALA    42       1.747  -7.289  -3.559  1.00  0.00           N
ATOM    404  CA  ALA    42       1.710  -7.931  -2.233  1.00  0.00           C
ATOM    405  C   ALA    42       1.716  -9.454  -2.304  1.00  0.00           C
ATOM    406  CB  ALA    42       0.349  -7.444  -1.707  1.00  0.00           C
ATOM    407  O1  ALA    42       0.842 -10.032  -2.988  1.00  0.00           O
ATOM    408  O2  ALA    42       2.502 -10.089  -1.569  1.00  0.00           O
ATOM    409  H   ALA    42       1.424  -7.839  -4.332  1.00  0.00           H
END
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2. $A\beta_{42}$ monomer-6n complex

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ATOM      1  N   ASP A   1     -18.802   6.079   5.843  1.00  0.00           N
ATOM      2  CA  ASP A   1     -19.155   5.368   4.610  1.00  0.00           C
ATOM      3  C   ASP A   1     -17.933   4.642   4.038  1.00  0.00           C
ATOM      4  O   ASP A   1     -16.885   5.269   3.878  1.00  0.00           O
ATOM      5  CB  ASP A   1     -19.795   6.385   3.660  1.00  0.00           C
ATOM      6  CG  ASP A   1     -20.731   5.806   2.594  1.00  0.00           C
ATOM      7  OD1 ASP A   1     -21.746   6.450   2.273  1.00  0.00           O
ATOM      8  OD2 ASP A   1     -20.306   4.809   1.968  1.00  0.00           O1-
ATOM      9  H1  ASP A   1     -18.334   5.464   6.477  1.00  0.00           H
ATOM     10  H2  ASP A   1     -18.306   6.953   5.800  1.00  0.00           H
ATOM     11  H3  ASP A   1     -19.659   6.251   6.343  1.00  0.00           H
ATOM     12  N   ALA A   2     -18.209   3.549   3.323  1.00  0.00           N
ATOM     13  CA  ALA A   2     -17.202   2.645   2.766  1.00  0.00           C
ATOM     14  C   ALA A   2     -16.139   2.012   3.665  1.00  0.00           C
ATOM     15  O   ALA A   2     -15.527   2.692   4.488  1.00  0.00           O
ATOM     16  CB  ALA A   2     -16.520   3.257   1.544  1.00  0.00           C
ATOM     17  H   ALA A   2     -19.140   3.464   2.960  1.00  0.00           H
ATOM     18  N   GLU A   3     -15.579   0.832   3.404  1.00  0.00           N
ATOM     19  CA  GLU A   3     -14.658   0.140   4.321  1.00  0.00           C
ATOM     20  C   GLU A   3     -13.546  -0.422   3.433  1.00  0.00           C
ATOM     21  O   GLU A   3     -13.909  -0.999   2.402  1.00  0.00           O
ATOM     22  CB  GLU A   3     -15.424  -0.999   4.983  1.00  0.00           C
ATOM     23  CG  GLU A   3     -14.890  -1.422   6.355  1.00  0.00           C
ATOM     24  CD  GLU A   3     -13.655  -2.323   6.216  1.00  0.00           C
ATOM     25  OE1 GLU A   3     -12.596  -1.964   6.769  1.00  0.00           O
ATOM     26  OE2 GLU A   3     -13.767  -3.417   5.624  1.00  0.00           O1-
ATOM     27  H   GLU A   3     -15.716   0.283   2.577  1.00  0.00           H
ATOM     28  N   PHE A   4     -12.388  -0.549   4.070  1.00  0.00           N
ATOM     29  CA  PHE A   4     -11.096  -0.918   3.461  1.00  0.00           C
ATOM     30  C   PHE A   4     -10.956  -2.386   3.031  1.00  0.00           C
ATOM     31  O   PHE A   4     -10.031  -2.639   2.262  1.00  0.00           O
ATOM     32  CB  PHE A   4      -9.789  -0.673   4.205  1.00  0.00           C
ATOM     33  CG  PHE A   4      -9.443   0.815   4.114  1.00  0.00           C
ATOM     34  CD1 PHE A   4      -9.930   1.738   5.033  1.00  0.00           C
ATOM     35  CD2 PHE A   4      -8.983   1.324   2.899  1.00  0.00           C
ATOM     36  CE1 PHE A   4      -9.791   3.088   4.731  1.00  0.00           C
ATOM     37  CE2 PHE A   4      -8.871   2.678   2.606  1.00  0.00           C
ATOM     38  CZ  PHE A   4      -9.202   3.606   3.595  1.00  0.00           C
ATOM     39  H   PHE A   4     -12.462  -0.396   5.051  1.00  0.00           H
ATOM     40  HD1 PHE A   4     -10.520   1.380   5.878  1.00  0.00           H
ATOM     41  HD2 PHE A   4      -8.757   0.501   2.220  1.00  0.00           H
ATOM     42  HE1 PHE A   4     -10.354   3.795   5.339  1.00  0.00           H
ATOM     43  HE2 PHE A   4      -8.619   3.074   1.621  1.00  0.00           H
ATOM     44  HZ  PHE A   4      -8.945   4.665   3.590  1.00  0.00           H
ATOM     45  N   ARG A   5     -11.613  -3.356   3.659  1.00  0.00           N
ATOM     46  CA  ARG A   5     -11.473  -4.749   3.198  1.00  0.00           C
ATOM     47  C   ARG A   5     -12.465  -5.332   2.180  1.00  0.00           C
ATOM     48  O   ARG A   5     -12.153  -6.338   1.556  1.00  0.00           O
ATOM     49  CB  ARG A   5     -11.339  -5.570   4.484  1.00  0.00           C
ATOM     50  CG  ARG A   5     -10.057  -6.397   4.535  1.00  0.00           C
ATOM     51  CD  ARG A   5      -9.798  -7.049   5.900  1.00  0.00           C
ATOM     52  NE  ARG A   5      -9.874  -6.089   7.008  1.00  0.00           N
ATOM     53  CZ  ARG A   5      -9.778  -6.299   8.327  1.00  0.00           C
ATOM     54  NH1 ARG A   5      -9.752  -7.546   8.806  1.00  0.00           N1+
ATOM     55  NH2 ARG A   5      -9.406  -5.283   9.129  1.00  0.00           N
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ATOM     56  H   ARG A   5     -12.177  -3.205   4.459  1.00  0.00           H
ATOM     57  HE  ARG A   5      -9.864  -5.150   6.660  1.00  0.00           H
ATOM     58 1HH1 ARG A   5      -9.717  -8.370   8.235  1.00  0.00           H
ATOM     59 2HH1 ARG A   5      -9.536  -7.706   9.770  1.00  0.00           H
ATOM     60 1HH2 ARG A   5      -9.238  -4.378   8.740  1.00  0.00           H
ATOM     61 2HH2 ARG A   5      -9.191  -5.569  10.064  1.00  0.00           H
ATOM     62  N   HIS A   6     -13.568  -4.637   1.906  1.00  0.00           N
ATOM     63  CA  HIS A   6     -14.630  -5.257   1.108  1.00  0.00           C
ATOM     64  C   HIS A   6     -14.501  -5.373  -0.413  1.00  0.00           C
ATOM     65  O   HIS A   6     -15.290  -6.088  -1.030  1.00  0.00           O
ATOM     66  CB  HIS A   6     -15.944  -4.689   1.655  1.00  0.00           C
ATOM     67  CG  HIS A   6     -17.242  -5.359   1.194  1.00  0.00           C
ATOM     68  CD2 HIS A   6     -18.170  -4.896   0.364  1.00  0.00           C
ATOM     69  ND1 HIS A   6     -17.765  -6.536   1.532  1.00  0.00           N
ATOM     70  CE1 HIS A   6     -18.924  -6.833   0.951  1.00  0.00           C
ATOM     71  NE2 HIS A   6     -19.196  -5.732   0.252  1.00  0.00           N
ATOM     72  H   HIS A   6     -13.705  -3.700   2.237  1.00  0.00           H
ATOM     73  HD2 HIS A   6     -18.271  -3.901  -0.072  1.00  0.00           H
ATOM     74  HE1 HIS A   6     -19.411  -7.801   0.993  1.00  0.00           H
ATOM     75  HE2 HIS A   6     -20.032  -5.593  -0.267  1.00  0.00           H
ATOM     76  N   ASP A   7     -13.271  -5.103  -0.852  1.00  0.00           N
ATOM     77  CA  ASP A   7     -12.959  -4.883  -2.279  1.00  0.00           C
ATOM     78  C   ASP A   7     -11.461  -4.747  -2.569  1.00  0.00           C
ATOM     79  O   ASP A   7     -10.802  -3.922  -1.959  1.00  0.00           O
ATOM     80  CB  ASP A   7     -13.598  -3.589  -2.762  1.00  0.00           C
ATOM     81  CG  ASP A   7     -13.381  -3.213  -4.224  1.00  0.00           C
ATOM     82  OD1 ASP A   7     -13.603  -4.132  -5.036  1.00  0.00           O
ATOM     83  OD2 ASP A   7     -12.911  -2.094  -4.531  1.00  0.00           O1-
ATOM     84  H   ASP A   7     -12.494  -5.124  -0.225  1.00  0.00           H
ATOM     85  N   SER A   8     -11.096  -5.199  -3.775  1.00  0.00           N
ATOM     86  CA  SER A   8      -9.774  -5.070  -4.397  1.00  0.00           C
ATOM     87  C   SER A   8      -9.281  -3.650  -4.673  1.00  0.00           C
ATOM     88  O   SER A   8      -8.205  -3.305  -4.181  1.00  0.00           O
ATOM     89  CB  SER A   8      -9.572  -5.996  -5.606  1.00  0.00           C
ATOM     90  OG  SER A   8      -8.172  -6.191  -5.818  1.00  0.00           O
ATOM     91  H   SER A   8     -11.841  -5.469  -4.375  1.00  0.00           H
ATOM     92  HG  SER A   8      -7.985  -5.603  -6.613  1.00  0.00           H
ATOM     93  N   GLY A   9     -10.145  -2.716  -5.075  1.00  0.00           N
ATOM     94  CA  GLY A   9      -9.850  -1.278  -5.120  1.00  0.00           C
ATOM     95  C   GLY A   9      -9.738  -0.616  -3.742  1.00  0.00           C
ATOM     96  O   GLY A   9      -8.882   0.242  -3.574  1.00  0.00           O
ATOM     97  H   GLY A   9     -10.833  -3.016  -5.728  1.00  0.00           H
ATOM     98  N   TYR A  10     -10.451  -1.076  -2.718  1.00  0.00           N
ATOM     99  CA  TYR A  10     -10.266  -0.639  -1.319  1.00  0.00           C
ATOM    100  C   TYR A  10      -9.042  -1.340  -0.705  1.00  0.00           C
ATOM    101  O   TYR A  10      -8.219  -0.605  -0.174  1.00  0.00           O
ATOM    102  CB  TYR A  10     -11.532  -0.766  -0.473  1.00  0.00           C
ATOM    103  CG  TYR A  10     -12.337   0.523  -0.564  1.00  0.00           C
ATOM    104  CD1 TYR A  10     -13.182   0.756  -1.646  1.00  0.00           C
ATOM    105  CD2 TYR A  10     -12.153   1.545   0.362  1.00  0.00           C
ATOM    106  CE1 TYR A  10     -13.958   1.896  -1.695  1.00  0.00           C
ATOM    107  CE2 TYR A  10     -12.721   2.795   0.149  1.00  0.00           C
ATOM    108  CZ  TYR A  10     -13.632   2.976  -0.878  1.00  0.00           C
ATOM    109  OH  TYR A  10     -14.231   4.175  -1.132  1.00  0.00           O
ATOM    110  H   TYR A  10     -11.251  -1.647  -2.891  1.00  0.00           H
ATOM    111  HD1 TYR A  10     -13.173   0.109  -2.526  1.00  0.00           H
ATOM    112  HD2 TYR A  10     -11.399   1.541   1.153  1.00  0.00           H
ATOM    113  HE1 TYR A  10     -14.870   1.834  -2.292  1.00  0.00           H
ATOM    114  HE2 TYR A  10     -12.745   3.518   0.975  1.00  0.00           H
ATOM    115  HH  TYR A  10     -13.923   4.883  -0.495  1.00  0.00           H
ATOM    116  N   GLU A  11      -8.751  -2.606  -0.978  1.00  0.00           N
ATOM    117  CA  GLU A  11      -7.481  -3.190  -0.545  1.00  0.00           C
ATOM    118  C   GLU A  11      -6.291  -2.463  -1.177  1.00  0.00           C
ATOM    119  O   GLU A  11      -5.311  -2.325  -0.453  1.00  0.00           O
ATOM    120  CB  GLU A  11      -7.417  -4.556  -1.239  1.00  0.00           C
ATOM    121  CG  GLU A  11      -8.158  -5.620  -0.423  1.00  0.00           C
ATOM    122  CD  GLU A  11      -7.951  -7.057  -0.918  1.00  0.00           C
ATOM    123  OE1 GLU A  11      -8.900  -7.696  -1.417  1.00  0.00           O
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ATOM    124  OE2 GLU A  11      -6.788  -7.491  -0.820  1.00  0.00           O1-
ATOM    125  H   GLU A  11      -9.402  -3.183  -1.483  1.00  0.00           H
ATOM    126  N   VAL A  12      -6.383  -2.020  -2.422  1.00  0.00           N
ATOM    127  CA  VAL A  12      -5.295  -1.237  -3.040  1.00  0.00           C
ATOM    128  C   VAL A  12      -5.222   0.226  -2.583  1.00  0.00           C
ATOM    129  O   VAL A  12      -4.143   0.606  -2.141  1.00  0.00           O
ATOM    130  CB  VAL A  12      -5.345  -1.313  -4.564  1.00  0.00           C
ATOM    131  CG1 VAL A  12      -3.989  -0.895  -5.138  1.00  0.00           C
ATOM    132  CG2 VAL A  12      -5.632  -2.699  -5.135  1.00  0.00           C
ATOM    133  H   VAL A  12      -6.973  -2.462  -3.100  1.00  0.00           H
ATOM    134  N   HIS A  13      -6.377   0.819  -2.306  1.00  0.00           N
ATOM    135  CA  HIS A  13      -6.329   1.981  -1.406  1.00  0.00           C
ATOM    136  C   HIS A  13      -5.566   1.904  -0.076  1.00  0.00           C
ATOM    137  O   HIS A  13      -4.635   2.669   0.157  1.00  0.00           O
ATOM    138  CB  HIS A  13      -7.641   2.717  -1.135  1.00  0.00           C
ATOM    139  CG  HIS A  13      -8.204   3.455  -2.352  1.00  0.00           C
ATOM    140  CD2 HIS A  13      -9.391   3.185  -2.888  1.00  0.00           C
ATOM    141  ND1 HIS A  13      -7.562   4.309  -3.141  1.00  0.00           N
ATOM    142  CE1 HIS A  13      -8.359   4.654  -4.149  1.00  0.00           C
ATOM    143  NE2 HIS A  13      -9.493   3.984  -3.955  1.00  0.00           N
ATOM    144  H   HIS A  13      -7.268   0.438  -2.531  1.00  0.00           H
ATOM    145  HD2 HIS A  13     -10.215   2.559  -2.551  1.00  0.00           H
ATOM    146  HE1 HIS A  13      -8.283   5.532  -4.789  1.00  0.00           H
ATOM    147  HE2 HIS A  13     -10.345   4.093  -4.457  1.00  0.00           H
ATOM    148  N   HIS A  14      -5.927   0.856   0.666  1.00  0.00           N
ATOM    149  CA  HIS A  14      -5.194   0.563   1.905  1.00  0.00           C
ATOM    150  C   HIS A  14      -3.696   0.323   1.707  1.00  0.00           C
ATOM    151  O   HIS A  14      -2.805   0.911   2.330  1.00  0.00           O
ATOM    152  CB  HIS A  14      -5.665  -0.704   2.622  1.00  0.00           C
ATOM    153  CG  HIS A  14      -5.108  -0.855   4.033  1.00  0.00           C
ATOM    154  CD2 HIS A  14      -4.101  -1.653   4.411  1.00  0.00           C
ATOM    155  ND1 HIS A  14      -5.543  -0.234   5.123  1.00  0.00           N
ATOM    156  CE1 HIS A  14      -4.811  -0.597   6.169  1.00  0.00           C
ATOM    157  NE2 HIS A  14      -3.964  -1.523   5.727  1.00  0.00           N
ATOM    158  H   HIS A  14      -6.764   0.415   0.338  1.00  0.00           H
ATOM    159  HD2 HIS A  14      -3.673  -2.390   3.736  1.00  0.00           H
ATOM    160  HE1 HIS A  14      -4.841  -0.251   7.199  1.00  0.00           H
ATOM    161  HE2 HIS A  14      -3.230  -1.980   6.229  1.00  0.00           H
ATOM    162  N   GLN A  15      -3.412  -0.562   0.756  1.00  0.00           N
ATOM    163  CA  GLN A  15      -2.062  -0.862   0.248  1.00  0.00           C
ATOM    164  C   GLN A  15      -1.315   0.423  -0.106  1.00  0.00           C
ATOM    165  O   GLN A  15      -0.204   0.714   0.329  1.00  0.00           O
ATOM    166  CB  GLN A  15      -1.968  -1.704  -1.024  1.00  0.00           C
ATOM    167  CG  GLN A  15      -1.752  -3.212  -0.922  1.00  0.00           C
ATOM    168  CD  GLN A  15      -1.905  -3.913  -2.269  1.00  0.00           C
ATOM    169  NE2 GLN A  15      -2.998  -4.686  -2.245  1.00  0.00           N
ATOM    170  OE1 GLN A  15      -1.043  -4.052  -3.135  1.00  0.00           O
ATOM    171  H   GLN A  15      -4.099  -1.221   0.453  1.00  0.00           H
ATOM    172 1HE2 GLN A  15      -3.579  -4.890  -1.457  1.00  0.00           H
ATOM    173 2HE2 GLN A  15      -3.167  -5.167  -3.099  1.00  0.00           H
ATOM    174  N   LYS A  16      -1.879   1.315  -0.918  1.00  0.00           N
ATOM    175  CA  LYS A  16      -1.359   2.655  -1.230  1.00  0.00           C
ATOM    176  C   LYS A  16      -1.119   3.554  -0.019  1.00  0.00           C
ATOM    177  O   LYS A  16      -0.017   4.108   0.017  1.00  0.00           O
ATOM    178  CB  LYS A  16      -2.275   3.438  -2.179  1.00  0.00           C
ATOM    179  CG  LYS A  16      -2.153   2.946  -3.619  1.00  0.00           C
ATOM    180  CD  LYS A  16      -3.024   3.805  -4.534  1.00  0.00           C
ATOM    181  CE  LYS A  16      -4.487   3.875  -4.090  1.00  0.00           C
ATOM    182  NZ  LYS A  16      -5.480   4.082  -5.149  1.00  0.00           N1+
ATOM    183  H   LYS A  16      -2.538   1.042  -1.621  1.00  0.00           H
ATOM    184  HZ1 LYS A  16      -5.311   4.945  -5.615  1.00  0.00           H
ATOM    185  HZ2 LYS A  16      -5.413   3.348  -5.828  1.00  0.00           H
ATOM    186  HZ3 LYS A  16      -6.411   4.136  -4.776  1.00  0.00           H
ATOM    187  N   LEU A  17      -1.964   3.547   1.013  1.00  0.00           N
ATOM    188  CA  LEU A  17      -1.722   4.201   2.304  1.00  0.00           C
ATOM    189  C   LEU A  17      -0.536   3.639   3.096  1.00  0.00           C
ATOM    190  O   LEU A  17       0.194   4.402   3.719  1.00  0.00           O
ATOM    191  CB  LEU A  17      -3.011   4.247   3.121  1.00  0.00           C
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ATOM    192  CG  LEU A  17      -4.054   5.159   2.479  1.00  0.00           C
ATOM    193  CD1 LEU A  17      -5.354   4.775   3.202  1.00  0.00           C
ATOM    194  CD2 LEU A  17      -3.819   6.660   2.639  1.00  0.00           C
ATOM    195  H   LEU A  17      -2.862   3.190   0.777  1.00  0.00           H
ATOM    196  N   VAL A  18      -0.361   2.322   3.041  1.00  0.00           N
ATOM    197  CA  VAL A  18       0.780   1.569   3.596  1.00  0.00           C
ATOM    198  C   VAL A  18       2.169   1.921   3.050  1.00  0.00           C
ATOM    199  O   VAL A  18       3.159   2.217   3.709  1.00  0.00           O
ATOM    200  CB  VAL A  18       0.618   0.052   3.698  1.00  0.00           C
ATOM    201  CG1 VAL A  18       1.678  -0.588   4.581  1.00  0.00           C
ATOM    202  CG2 VAL A  18      -0.576  -0.132   4.638  1.00  0.00           C
ATOM    203  H   VAL A  18      -1.116   1.758   2.708  1.00  0.00           H
ATOM    204  N   PHE A  19       2.126   2.134   1.741  1.00  0.00           N
ATOM    205  CA  PHE A  19       3.252   2.725   1.009  1.00  0.00           C
ATOM    206  C   PHE A  19       3.536   4.125   1.542  1.00  0.00           C
ATOM    207  O   PHE A  19       4.679   4.381   1.930  1.00  0.00           O
ATOM    208  CB  PHE A  19       2.908   2.705  -0.483  1.00  0.00           C
ATOM    209  CG  PHE A  19       4.127   3.189  -1.267  1.00  0.00           C
ATOM    210  CD1 PHE A  19       5.134   2.300  -1.624  1.00  0.00           C
ATOM    211  CD2 PHE A  19       4.190   4.533  -1.640  1.00  0.00           C
ATOM    212  CE1 PHE A  19       6.159   2.732  -2.450  1.00  0.00           C
ATOM    213  CE2 PHE A  19       5.219   4.953  -2.460  1.00  0.00           C
ATOM    214  CZ  PHE A  19       6.237   4.076  -2.798  1.00  0.00           C
ATOM    215  H   PHE A  19       1.276   2.052   1.221  1.00  0.00           H
ATOM    216  HD1 PHE A  19       4.964   1.229  -1.523  1.00  0.00           H
ATOM    217  HD2 PHE A  19       3.435   5.226  -1.280  1.00  0.00           H
ATOM    218  HE1 PHE A  19       6.980   2.019  -2.427  1.00  0.00           H
ATOM    219  HE2 PHE A  19       5.259   6.015  -2.730  1.00  0.00           H
ATOM    220  HZ  PHE A  19       7.167   4.465  -3.219  1.00  0.00           H
ATOM    221  N   PHE A  20       2.565   5.035   1.395  1.00  0.00           N
ATOM    222  CA  PHE A  20       2.613   6.411   1.906  1.00  0.00           C
ATOM    223  C   PHE A  20       2.870   6.763   3.373  1.00  0.00           C
ATOM    224  O   PHE A  20       3.296   7.915   3.517  1.00  0.00           O
ATOM    225  CB  PHE A  20       1.431   7.200   1.352  1.00  0.00           C
ATOM    226  CG  PHE A  20       1.426   7.769  -0.065  1.00  0.00           C
ATOM    227  CD1 PHE A  20       2.390   8.737  -0.358  1.00  0.00           C
ATOM    228  CD2 PHE A  20       0.639   7.151  -1.028  1.00  0.00           C
ATOM    229  CE1 PHE A  20       2.565   9.014  -1.707  1.00  0.00           C
ATOM    230  CE2 PHE A  20       0.829   7.380  -2.388  1.00  0.00           C
ATOM    231  CZ  PHE A  20       1.780   8.355  -2.656  1.00  0.00           C
ATOM    232  H   PHE A  20       1.717   4.784   0.925  1.00  0.00           H
ATOM    233  HD1 PHE A  20       3.059   9.068   0.432  1.00  0.00           H
ATOM    234  HD2 PHE A  20      -0.184   6.552  -0.665  1.00  0.00           H
ATOM    235  HE1 PHE A  20       3.001   9.973  -2.008  1.00  0.00           H
ATOM    236  HE2 PHE A  20       0.344   6.800  -3.177  1.00  0.00           H
ATOM    237  HZ  PHE A  20       2.016   8.723  -3.657  1.00  0.00           H
ATOM    238  N   ALA A  21       2.695   5.741   4.209  1.00  0.00           N
ATOM    239  CA  ALA A  21       2.993   5.936   5.636  1.00  0.00           C
ATOM    240  C   ALA A  21       4.441   5.625   6.038  1.00  0.00           C
ATOM    241  O   ALA A  21       4.943   6.408   6.842  1.00  0.00           O
ATOM    242  CB  ALA A  21       1.973   5.220   6.522  1.00  0.00           C
ATOM    243  H   ALA A  21       2.055   5.013   3.990  1.00  0.00           H
ATOM    244  N   GLU A  22       4.980   4.451   5.733  1.00  0.00           N
ATOM    245  CA  GLU A  22       6.350   4.126   6.141  1.00  0.00           C
ATOM    246  C   GLU A  22       7.355   4.985   5.370  1.00  0.00           C
ATOM    247  O   GLU A  22       7.259   5.504   4.264  1.00  0.00           O
ATOM    248  CB  GLU A  22       6.604   2.622   6.261  1.00  0.00           C
ATOM    249  CG  GLU A  22       5.456   1.881   6.959  1.00  0.00           C
ATOM    250  CD  GLU A  22       5.329   1.931   8.491  1.00  0.00           C
ATOM    251  OE1 GLU A  22       5.649   3.034   8.981  1.00  0.00           O
ATOM    252  OE2 GLU A  22       4.815   0.994   9.132  1.00  0.00           O1-
ATOM    253  H   GLU A  22       4.547   3.820   5.083  1.00  0.00           H
ATOM    254  N   ASP A  23       8.384   5.359   6.140  1.00  0.00           N
ATOM    255  CA  ASP A  23       9.400   6.358   5.792  1.00  0.00           C
ATOM    256  C   ASP A  23      10.176   6.099   4.492  1.00  0.00           C
ATOM    257  O   ASP A  23      10.435   4.952   4.127  1.00  0.00           O
ATOM    258  CB  ASP A  23      10.311   6.561   7.002  1.00  0.00           C
ATOM    259  CG  ASP A  23      10.865   5.273   7.612  1.00  0.00           C
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ATOM    260  OD1 ASP A  23      10.311   4.902   8.658  1.00  0.00           O
ATOM    261  OD2 ASP A  23      11.888   4.742   7.111  1.00  0.00           O1-
ATOM    262  H   ASP A  23       8.477   4.959   7.046  1.00  0.00           H
ATOM    263  N   VAL A  24      10.829   7.171   4.062  1.00  0.00           N
ATOM    264  CA  VAL A  24      11.580   7.148   2.787  1.00  0.00           C
ATOM    265  C   VAL A  24      12.593   6.022   2.617  1.00  0.00           C
ATOM    266  O   VAL A  24      12.252   5.214   1.754  1.00  0.00           O
ATOM    267  CB  VAL A  24      12.290   8.457   2.441  1.00  0.00           C
ATOM    268  CG1 VAL A  24      11.182   9.461   2.108  1.00  0.00           C
ATOM    269  CG2 VAL A  24      13.314   8.975   3.453  1.00  0.00           C
ATOM    270  H   VAL A  24      10.842   7.926   4.717  1.00  0.00           H
ATOM    271  N   GLY A  25      13.324   5.655   3.672  1.00  0.00           N
ATOM    272  CA  GLY A  25      14.270   4.541   3.791  1.00  0.00           C
ATOM    273  C   GLY A  25      13.474   3.229   3.842  1.00  0.00           C
ATOM    274  O   GLY A  25      13.841   2.418   2.985  1.00  0.00           O
ATOM    275  H   GLY A  25      13.199   6.190   4.501  1.00  0.00           H
ATOM    276  N   SER A  26      12.489   3.077   4.714  1.00  0.00           N
ATOM    277  CA  SER A  26      11.710   1.824   4.707  1.00  0.00           C
ATOM    278  C   SER A  26      10.954   1.598   3.393  1.00  0.00           C
ATOM    279  O   SER A  26      11.283   0.628   2.710  1.00  0.00           O
ATOM    280  CB  SER A  26      10.824   1.669   5.940  1.00  0.00           C
ATOM    281  OG  SER A  26      11.544   1.998   7.132  1.00  0.00           O
ATOM    282  H   SER A  26      12.334   3.713   5.466  1.00  0.00           H
ATOM    283  HG  SER A  26      11.340   2.910   7.486  1.00  0.00           H
ATOM    284  N   ASN A  27      10.395   2.671   2.843  1.00  0.00           N
ATOM    285  CA  ASN A  27       9.744   2.723   1.527  1.00  0.00           C
ATOM    286  C   ASN A  27      10.681   2.381   0.364  1.00  0.00           C
ATOM    287  O   ASN A  27      10.644   1.291  -0.215  1.00  0.00           O
ATOM    288  CB  ASN A  27       9.227   4.145   1.306  1.00  0.00           C
ATOM    289  CG  ASN A  27       8.365   4.280   0.047  1.00  0.00           C
ATOM    290  ND2 ASN A  27       7.054   4.304   0.230  1.00  0.00           N
ATOM    291  OD1 ASN A  27       8.852   4.453  -1.074  1.00  0.00           O
ATOM    292  H   ASN A  27      10.290   3.510   3.366  1.00  0.00           H
ATOM    293 1HD2 ASN A  27       6.579   4.305   1.102  1.00  0.00           H
ATOM    294 2HD2 ASN A  27       6.544   4.190  -0.632  1.00  0.00           H
ATOM    295  N   LYS A  28      11.744   3.156   0.202  1.00  0.00           N
ATOM    296  CA  LYS A  28      12.832   2.965  -0.772  1.00  0.00           C
ATOM    297  C   LYS A  28      13.929   1.971  -0.391  1.00  0.00           C
ATOM    298  O   LYS A  28      15.126   2.158  -0.561  1.00  0.00           O
ATOM    299  CB  LYS A  28      13.439   4.301  -1.187  1.00  0.00           C
ATOM    300  CG  LYS A  28      12.430   5.410  -1.476  1.00  0.00           C
ATOM    301  CD  LYS A  28      13.018   6.819  -1.495  1.00  0.00           C
ATOM    302  CE  LYS A  28      13.776   7.265  -2.746  1.00  0.00           C
ATOM    303  NZ  LYS A  28      14.125   8.686  -2.792  1.00  0.00           N1+
ATOM    304  H   LYS A  28      11.930   3.978   0.746  1.00  0.00           H
ATOM    305  HZ1 LYS A  28      13.470   9.211  -2.243  1.00  0.00           H
ATOM    306  HZ2 LYS A  28      15.053   8.812  -2.443  1.00  0.00           H
ATOM    307  HZ3 LYS A  28      14.054   9.058  -3.720  1.00  0.00           H
ATOM    308  N   GLY A  29      13.522   0.944   0.355  1.00  0.00           N
ATOM    309  CA  GLY A  29      14.365  -0.162   0.837  1.00  0.00           C
ATOM    310  C   GLY A  29      13.587  -1.428   1.218  1.00  0.00           C
ATOM    311  O   GLY A  29      13.449  -2.457   0.554  1.00  0.00           O
ATOM    312  H   GLY A  29      12.617   0.984   0.770  1.00  0.00           H
ATOM    313  N   ALA A  30      13.233  -1.510   2.494  1.00  0.00           N
ATOM    314  CA  ALA A  30      12.275  -2.519   2.981  1.00  0.00           C
ATOM    315  C   ALA A  30      11.003  -2.790   2.173  1.00  0.00           C
ATOM    316  O   ALA A  30      10.892  -3.855   1.573  1.00  0.00           O
ATOM    317  CB  ALA A  30      11.923  -2.307   4.451  1.00  0.00           C
ATOM    318  H   ALA A  30      13.775  -1.112   3.233  1.00  0.00           H
ATOM    319  N   ILE A  31      10.285  -1.719   1.837  1.00  0.00           N
ATOM    320  CA  ILE A  31       9.071  -1.867   1.031  1.00  0.00           C
ATOM    321  C   ILE A  31       9.312  -2.459  -0.353  1.00  0.00           C
ATOM    322  O   ILE A  31       8.738  -3.449  -0.832  1.00  0.00           O
ATOM    323  CB  ILE A  31       8.125  -0.659   1.015  1.00  0.00           C
ATOM    324  CG1 ILE A  31       7.618  -0.541   2.451  1.00  0.00           C
ATOM    325  CG2 ILE A  31       6.915  -0.741   0.085  1.00  0.00           C
ATOM    326  CD  ILE A  31       6.812   0.699   2.832  1.00  0.00           C
ATOM    327  H   ILE A  31      10.460  -0.826   2.257  1.00  0.00           H
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ATOM    328  N   ILE A  32      10.173  -1.813  -1.128  1.00  0.00           N
ATOM    329  CA  ILE A  32      10.560  -2.363  -2.426  1.00  0.00           C
ATOM    330  C   ILE A  32      11.516  -3.557  -2.515  1.00  0.00           C
ATOM    331  O   ILE A  32      11.635  -4.177  -3.569  1.00  0.00           O
ATOM    332  CB  ILE A  32      10.935  -1.279  -3.440  1.00  0.00           C
ATOM    333  CG1 ILE A  32      11.967  -0.264  -2.943  1.00  0.00           C
ATOM    334  CG2 ILE A  32       9.691  -0.576  -4.001  1.00  0.00           C
ATOM    335  CD  ILE A  32      13.407  -0.778  -3.051  1.00  0.00           C
ATOM    336  H   ILE A  32      10.298  -0.828  -1.030  1.00  0.00           H
ATOM    337  N   GLY A  33      12.042  -3.902  -1.341  1.00  0.00           N
ATOM    338  CA  GLY A  33      12.886  -5.088  -1.171  1.00  0.00           C
ATOM    339  C   GLY A  33      12.098  -6.401  -1.108  1.00  0.00           C
ATOM    340  O   GLY A  33      12.400  -7.387  -1.791  1.00  0.00           O
ATOM    341  H   GLY A  33      12.107  -3.245  -0.582  1.00  0.00           H
ATOM    342  N   LEU A  34      10.973  -6.268  -0.405  1.00  0.00           N
ATOM    343  CA  LEU A  34       9.989  -7.328  -0.162  1.00  0.00           C
ATOM    344  C   LEU A  34       8.786  -7.315  -1.099  1.00  0.00           C
ATOM    345  O   LEU A  34       8.484  -8.268  -1.827  1.00  0.00           O
ATOM    346  CB  LEU A  34       9.508  -7.226   1.292  1.00  0.00           C
ATOM    347  CG  LEU A  34      10.535  -7.690   2.327  1.00  0.00           C
ATOM    348  CD1 LEU A  34       9.997  -7.427   3.730  1.00  0.00           C
ATOM    349  CD2 LEU A  34      10.618  -9.211   2.178  1.00  0.00           C
ATOM    350  H   LEU A  34      10.723  -5.391  -0.007  1.00  0.00           H
ATOM    351  N   MET A  35       8.291  -6.115  -1.384  1.00  0.00           N
ATOM    352  CA  MET A  35       7.047  -5.945  -2.158  1.00  0.00           C
ATOM    353  C   MET A  35       7.239  -5.902  -3.668  1.00  0.00           C
ATOM    354  O   MET A  35       8.045  -5.105  -4.170  1.00  0.00           O
ATOM    355  CB  MET A  35       6.123  -4.862  -1.579  1.00  0.00           C
ATOM    356  CG  MET A  35       4.886  -4.567  -2.435  1.00  0.00           C
ATOM    357  SD  MET A  35       3.863  -6.058  -2.709  1.00  0.00           S
ATOM    358  CE  MET A  35       2.594  -5.390  -3.753  1.00  0.00           C
ATOM    359  H   MET A  35       8.836  -5.278  -1.326  1.00  0.00           H
ATOM    360  N   VAL A  36       6.536  -6.793  -4.363  1.00  0.00           N
ATOM    361  CA  VAL A  36       6.493  -7.019  -5.815  1.00  0.00           C
ATOM    362  C   VAL A  36       5.823  -5.938  -6.670  1.00  0.00           C
ATOM    363  O   VAL A  36       4.818  -5.418  -6.206  1.00  0.00           O
ATOM    364  CB  VAL A  36       5.840  -8.354  -6.185  1.00  0.00           C
ATOM    365  CG1 VAL A  36       6.800  -9.526  -5.935  1.00  0.00           C
ATOM    366  CG2 VAL A  36       4.493  -8.645  -5.512  1.00  0.00           C
ATOM    367  H   VAL A  36       6.300  -7.656  -3.906  1.00  0.00           H
ATOM    368  N   GLY A  37       6.289  -5.804  -7.904  1.00  0.00           N
ATOM    369  CA  GLY A  37       5.816  -4.916  -8.987  1.00  0.00           C
ATOM    370  C   GLY A  37       6.205  -3.474  -8.667  1.00  0.00           C
ATOM    371  O   GLY A  37       6.733  -3.135  -7.599  1.00  0.00           O
ATOM    372  H   GLY A  37       6.999  -6.484  -8.094  1.00  0.00           H
ATOM    373  N   GLY A  38       6.166  -2.667  -9.721  1.00  0.00           N
ATOM    374  CA  GLY A  38       6.284  -1.209  -9.599  1.00  0.00           C
ATOM    375  C   GLY A  38       5.064  -0.556  -8.939  1.00  0.00           C
ATOM    376  O   GLY A  38       3.951  -1.066  -9.034  1.00  0.00           O
ATOM    377  H   GLY A  38       6.318  -3.006 -10.651  1.00  0.00           H
ATOM    378  N   VAL A  39       5.315   0.528  -8.209  1.00  0.00           N
ATOM    379  CA  VAL A  39       4.283   1.112  -7.344  1.00  0.00           C
ATOM    380  C   VAL A  39       3.237   1.873  -8.164  1.00  0.00           C
ATOM    381  O   VAL A  39       3.662   2.811  -8.850  1.00  0.00           O
ATOM    382  CB  VAL A  39       4.869   1.938  -6.191  1.00  0.00           C
ATOM    383  CG1 VAL A  39       4.959   1.045  -4.948  1.00  0.00           C
ATOM    384  CG2 VAL A  39       6.004   2.893  -6.557  1.00  0.00           C
ATOM    385  H   VAL A  39       6.203   0.792  -7.830  1.00  0.00           H
ATOM    386  N   VAL A  40       1.986   1.440  -8.171  1.00  0.00           N
ATOM    387  CA  VAL A  40       0.964   2.205  -8.907  1.00  0.00           C
ATOM    388  C   VAL A  40       0.388   3.462  -8.260  1.00  0.00           C
ATOM    389  O   VAL A  40      -0.821   3.709  -8.221  1.00  0.00           O
ATOM    390  CB  VAL A  40      -0.096   1.297  -9.523  1.00  0.00           C
ATOM    391  CG1 VAL A  40       0.425   0.677 -10.815  1.00  0.00           C
ATOM    392  CG2 VAL A  40      -0.621   0.282  -8.506  1.00  0.00           C
ATOM    393  H   VAL A  40       1.765   0.533  -7.825  1.00  0.00           H
ATOM    394  N   ILE A  41       1.318   4.229  -7.710  1.00  0.00           N
ATOM    395  CA  ILE A  41       0.911   5.406  -6.921  1.00  0.00           C
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ATOM    396  C   ILE A  41       0.198   6.513  -7.690  1.00  0.00           C
ATOM    397  O   ILE A  41       0.731   6.839  -8.750  1.00  0.00           O
ATOM    398  CB  ILE A  41       1.994   5.902  -5.946  1.00  0.00           C
ATOM    399  CG1 ILE A  41       3.345   6.132  -6.615  1.00  0.00           C
ATOM    400  CG2 ILE A  41       1.997   4.990  -4.725  1.00  0.00           C
ATOM    401  CD  ILE A  41       4.265   6.771  -5.567  1.00  0.00           C
ATOM    402  H   ILE A  41       2.300   4.193  -7.932  1.00  0.00           H
ATOM    403  N   ALA A  42      -1.091   6.629  -7.368  1.00  0.00           N
ATOM    404  CA  ALA A  42      -2.046   7.587  -7.929  1.00  0.00           C
ATOM    405  C   ALA A  42      -3.423   7.347  -7.302  1.00  0.00           C
ATOM    406  CB  ALA A  42      -2.309   7.366  -9.420  1.00  0.00           C
ATOM    407  O1  ALA A  42      -4.395   8.104  -7.504  1.00  0.00           O
ATOM    408  O2  ALA A  42      -3.562   6.540  -6.363  1.00  0.00           O
ATOM    409  H   ALA A  42      -1.538   5.898  -6.851  1.00  0.00           H
ATOM    410  C1  6n  B  43       2.829  -3.620   1.431  1.00  0.00           C
ATOM    411  N1  6n  B  43       2.703  -1.456  -2.617  1.00  0.00           N
ATOM    412  O1  6n  B  43       2.451  -4.153   3.832  1.00  0.00           O
ATOM    413  C2  6n  B  43       2.194  -2.285   0.947  1.00  0.00           C
ATOM    414  N2  6n  B  43       3.822  -0.997  -2.005  1.00  0.00           N
ATOM    415  O2  6n  B  43       0.684  -4.081   2.462  1.00  0.00           O
ATOM    416  C3  6n  B  43       2.547  -1.832  -0.412  1.00  0.00           C
ATOM    417  N3  6n  B  43       3.785  -1.227  -0.772  1.00  0.00           N
ATOM    418  O3  6n  B  43       2.052  -6.657  -0.088  1.00  0.00           O
ATOM    419  C4  6n  B  43       1.846  -1.952  -1.630  1.00  0.00           C
ATOM    420  N4  6n  B  43       6.557  -5.134   3.854  1.00  0.00           N
ATOM    421  C5  6n  B  43       2.455  -1.607  -4.014  1.00  0.00           C
ATOM    422  N5  6n  B  43       7.119  -5.175   2.611  1.00  0.00           N
ATOM    423  C6  6n  B  43       3.379  -2.334  -4.786  1.00  0.00           C
ATOM    424  N6  6n  B  43       6.365  -4.646   1.760  1.00  0.00           N
ATOM    425  C7  6n  B  43       3.055  -2.798  -6.059  1.00  0.00           C
ATOM    426  N7  6n  B  43       2.688  -4.721   0.517  1.00  0.00           N
ATOM    427  C8  6n  B  43       1.802  -2.449  -6.563  1.00  0.00           C
ATOM    428  C9  6n  B  43       0.866  -1.757  -5.811  1.00  0.00           C
ATOM    429  C10 6n  B  43       1.197  -1.273  -4.549  1.00  0.00           C
ATOM    430  C11 6n  B  43       0.557   0.051  -4.125  1.00  0.00           C
ATOM    431  C12 6n  B  43       2.015  -3.932   2.698  1.00  0.00           C
ATOM    432  C13 6n  B  43      -0.171  -4.495   3.524  1.00  0.00           C
ATOM    433  C14 6n  B  43      -1.609  -4.041   3.421  1.00  0.00           C
ATOM    434  C15 6n  B  43       4.279  -3.180   1.831  1.00  0.00           C
ATOM    435  C16 6n  B  43       5.240  -4.092   2.472  1.00  0.00           C
ATOM    436  C17 6n  B  43       5.369  -4.389   3.842  1.00  0.00           C
ATOM    437  C18 6n  B  43       7.117  -5.759   5.003  1.00  0.00           C
ATOM    438  C19 6n  B  43       7.789  -4.931   5.921  1.00  0.00           C
ATOM    439  C20 6n  B  43       8.241  -5.425   7.133  1.00  0.00           C
ATOM    440  C21 6n  B  43       8.068  -6.785   7.381  1.00  0.00           C
ATOM    441  C22 6n  B  43       7.461  -7.642   6.480  1.00  0.00           C
ATOM    442  C23 6n  B  43       6.961  -7.137   5.289  1.00  0.00           C
ATOM    443  C24 6n  B  43       8.370  -3.578   5.488  1.00  0.00           C
ATOM    444  C25 6n  B  43       2.787  -6.083   0.755  1.00  0.00           C
ATOM    445  C26 6n  B  43       3.337  -6.769   1.974  1.00  0.00           C
ATOM    446  F1  6n  B  43       0.492   0.442  -2.807  1.00  0.00           F
ATOM    447  F2  6n  B  43       1.128   1.221  -4.583  1.00  0.00           F
ATOM    448  F3  6n  B  43      -0.762   0.271  -4.477  1.00  0.00           F
ATOM    449  F4  6n  B  43       9.045  -3.588   4.278  1.00  0.00           F
ATOM    450  F5  6n  B  43       7.482  -2.539   5.305  1.00  0.00           F
ATOM    451  F6  6n  B  43       9.229  -2.837   6.263  1.00  0.00           F
ATOM    452  H1  6n  B  43       2.353  -4.493  -0.397  1.00  0.00           H
ATOM    453  H03 6n  B  43       0.906  -2.473  -1.831  1.00  0.00           H
ATOM    454  H04 6n  B  43       4.384  -2.496  -4.380  1.00  0.00           H
ATOM    455  H05 6n  B  43       3.703  -3.470  -6.626  1.00  0.00           H
ATOM    456  H06 6n  B  43       1.642  -2.540  -7.647  1.00  0.00           H
ATOM    457  H07 6n  B  43      -0.134  -1.555  -6.218  1.00  0.00           H
ATOM    458  H11 6n  B  43       4.962  -3.965   4.757  1.00  0.00           H
ATOM    459  H12 6n  B  43       8.646  -4.665   7.822  1.00  0.00           H
ATOM    460  H13 6n  B  43       8.586  -7.191   8.274  1.00  0.00           H
ATOM    461  H14 6n  B  43       7.489  -8.740   6.549  1.00  0.00           H
ATOM    462  H15 6n  B  43       6.263  -7.747   4.704  1.00  0.00           H
END
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3. $A\beta_{42}$ protofibril

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ATOM      1  N   LEU A  17     -15.562  -0.631   7.381  1.00  0.00           N
ATOM      2  CA  LEU A  17     -14.456  -0.708   6.409  1.00  0.00           C
ATOM      3  C   LEU A  17     -13.193  -1.132   7.159  1.00  0.00           C
ATOM      4  O   LEU A  17     -12.999  -0.561   8.231  1.00  0.00           O
ATOM      5  CB  LEU A  17     -14.306   0.630   5.671  1.00  0.00           C
ATOM      6  CG  LEU A  17     -14.255   0.463   4.145  1.00  0.00           C
ATOM      7  CD1 LEU A  17     -14.645   1.753   3.432  1.00  0.00           C
ATOM      8  CD2 LEU A  17     -12.866   0.015   3.708  1.00  0.00           C
ATOM      9  H1  LEU A  17     -16.353  -1.028   6.914  1.00  0.00           H
ATOM     10  H2  LEU A  17     -15.357  -1.223   8.160  1.00  0.00           H
ATOM     11  H3  LEU A  17     -15.747   0.311   7.667  1.00  0.00           H
ATOM     12  N   VAL A  18     -12.197  -1.810   6.600  1.00  0.00           N
ATOM     13  CA  VAL A  18     -11.005  -2.392   7.228  1.00  0.00           C
ATOM     14  C   VAL A  18      -9.785  -2.044   6.381  1.00  0.00           C
ATOM     15  O   VAL A  18      -9.914  -2.184   5.159  1.00  0.00           O
ATOM     16  CB  VAL A  18     -11.045  -3.919   7.345  1.00  0.00           C
ATOM     17  CG1 VAL A  18     -10.021  -4.460   8.346  1.00  0.00           C
ATOM     18  CG2 VAL A  18     -12.470  -4.375   7.668  1.00  0.00           C
ATOM     19  H   VAL A  18     -12.055  -1.959   5.627  1.00  0.00           H
ATOM     20  N   PHE A  19      -8.837  -1.343   7.003  1.00  0.00           N
ATOM     21  CA  PHE A  19      -7.595  -0.953   6.310  1.00  0.00           C
ATOM     22  C   PHE A  19      -6.342  -1.603   6.897  1.00  0.00           C
ATOM     23  O   PHE A  19      -6.138  -1.481   8.109  1.00  0.00           O
ATOM     24  CB  PHE A  19      -7.346   0.549   6.364  1.00  0.00           C
ATOM     25  CG  PHE A  19      -8.341   1.480   5.680  1.00  0.00           C
ATOM     26  CD1 PHE A  19      -9.377   1.909   6.517  1.00  0.00           C
ATOM     27  CD2 PHE A  19      -8.559   1.556   4.312  1.00  0.00           C
ATOM     28  CE1 PHE A  19     -10.511   2.472   5.952  1.00  0.00           C
ATOM     29  CE2 PHE A  19      -9.730   2.130   3.848  1.00  0.00           C
ATOM     30  CZ  PHE A  19     -10.793   2.622   4.603  1.00  0.00           C
ATOM     31  H   PHE A  19      -8.965  -0.859   7.866  1.00  0.00           H
ATOM     32  HD1 PHE A  19      -9.479   1.514   7.524  1.00  0.00           H
ATOM     33  HD2 PHE A  19      -7.781   1.293   3.585  1.00  0.00           H
ATOM     34  HE1 PHE A  19     -11.203   2.878   6.693  1.00  0.00           H
ATOM     35  HE2 PHE A  19      -9.912   1.995   2.779  1.00  0.00           H
ATOM     36  HZ  PHE A  19     -11.544   3.320   4.217  1.00  0.00           H
ATOM     37  N   PHE A  20      -5.555  -2.453   6.232  1.00  0.00           N
ATOM     38  CA  PHE A  20      -4.323  -2.981   6.829  1.00  0.00           C
ATOM     39  C   PHE A  20      -3.000  -2.768   6.105  1.00  0.00           C
ATOM     40  O   PHE A  20      -2.812  -2.689   4.897  1.00  0.00           O
ATOM     41  CB  PHE A  20      -4.490  -4.479   7.138  1.00  0.00           C
ATOM     42  CG  PHE A  20      -4.935  -4.689   8.589  1.00  0.00           C
ATOM     43  CD1 PHE A  20      -4.035  -4.928   9.621  1.00  0.00           C
ATOM     44  CD2 PHE A  20      -6.297  -4.785   8.837  1.00  0.00           C
ATOM     45  CE1 PHE A  20      -4.509  -5.206  10.892  1.00  0.00           C
ATOM     46  CE2 PHE A  20      -6.760  -4.890  10.138  1.00  0.00           C
ATOM     47  CZ  PHE A  20      -5.865  -5.097  11.185  1.00  0.00           C
ATOM     48  H   PHE A  20      -5.634  -2.772   5.295  1.00  0.00           H
ATOM     49  HD1 PHE A  20      -2.975  -4.897   9.393  1.00  0.00           H
ATOM     50  HD2 PHE A  20      -6.966  -4.700   7.967  1.00  0.00           H
ATOM     51  HE1 PHE A  20      -3.784  -5.064  11.690  1.00  0.00           H
ATOM     52  HE2 PHE A  20      -7.811  -4.693  10.356  1.00  0.00           H
ATOM     53  HZ  PHE A  20      -6.139  -5.443  12.188  1.00  0.00           H
ATOM     54  N   ALA A  21      -2.036  -2.513   6.998  1.00  0.00           N
ATOM     55  CA  ALA A  21      -0.706  -2.157   6.492  1.00  0.00           C
ATOM     56  C   ALA A  21       0.376  -3.012   7.160  1.00  0.00           C
ATOM     57  O   ALA A  21       0.725  -2.758   8.314  1.00  0.00           O
ATOM     58  CB  ALA A  21      -0.341  -0.702   6.804  1.00  0.00           C
ATOM     59  H   ALA A  21      -2.213  -2.292   7.949  1.00  0.00           H
ATOM     60  N   GLU A  22       0.598  -4.162   6.523  1.00  0.00           N
ATOM     61  CA  GLU A  22       1.544  -5.167   7.008  1.00  0.00           C
ATOM     62  C   GLU A  22       2.958  -4.945   6.473  1.00  0.00           C
ATOM     63  O   GLU A  22       3.306  -5.168   5.314  1.00  0.00           O
ATOM     64  CB  GLU A  22       1.060  -6.584   6.692  1.00  0.00           C
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ATOM     65  CG  GLU A  22      -0.135  -6.759   7.620  1.00  0.00           C
ATOM     66  CD  GLU A  22       0.224  -7.456   8.941  1.00  0.00           C
ATOM     67  OE1 GLU A  22       0.362  -8.695   8.850  1.00  0.00           O
ATOM     68  OE2 GLU A  22       0.358  -6.883  10.035  1.00  0.00           O1-
ATOM     69  H   GLU A  22       0.233  -4.356   5.613  1.00  0.00           H
ATOM     70  N   ASP A  23       3.815  -4.684   7.459  1.00  0.00           N
ATOM     71  CA  ASP A  23       5.260  -4.503   7.316  1.00  0.00           C
ATOM     72  C   ASP A  23       6.014  -5.777   7.712  1.00  0.00           C
ATOM     73  O   ASP A  23       6.058  -6.258   8.841  1.00  0.00           O
ATOM     74  CB  ASP A  23       5.743  -3.168   7.880  1.00  0.00           C
ATOM     75  CG  ASP A  23       6.963  -3.188   8.804  1.00  0.00           C
ATOM     76  OD1 ASP A  23       6.790  -3.063  10.037  1.00  0.00           O
ATOM     77  OD2 ASP A  23       8.051  -3.522   8.284  1.00  0.00           O1-
ATOM     78  H   ASP A  23       3.532  -4.720   8.418  1.00  0.00           H
ATOM     79  N   VAL A  24       6.526  -6.460   6.700  1.00  0.00           N
ATOM     80  CA  VAL A  24       7.422  -7.627   6.718  1.00  0.00           C
ATOM     81  C   VAL A  24       8.846  -7.155   6.422  1.00  0.00           C
ATOM     82  O   VAL A  24       9.245  -6.985   5.274  1.00  0.00           O
ATOM     83  CB  VAL A  24       6.933  -8.643   5.671  1.00  0.00           C
ATOM     84  CG1 VAL A  24       7.929  -9.750   5.319  1.00  0.00           C
ATOM     85  CG2 VAL A  24       5.618  -9.260   6.141  1.00  0.00           C
ATOM     86  H   VAL A  24       6.134  -6.456   5.776  1.00  0.00           H
ATOM     87  N   GLY A  25       9.640  -6.868   7.457  1.00  0.00           N
ATOM     88  CA  GLY A  25      10.943  -6.204   7.273  1.00  0.00           C
ATOM     89  C   GLY A  25      12.055  -7.245   7.364  1.00  0.00           C
ATOM     90  O   GLY A  25      12.872  -7.292   8.284  1.00  0.00           O
ATOM     91  H   GLY A  25       9.341  -6.654   8.382  1.00  0.00           H
ATOM     92  N   SER A  26      12.142  -8.112   6.356  1.00  0.00           N
ATOM     93  CA  SER A  26      13.188  -9.143   6.396  1.00  0.00           C
ATOM     94  C   SER A  26      14.602  -8.563   6.447  1.00  0.00           C
ATOM     95  O   SER A  26      14.843  -7.497   5.888  1.00  0.00           O
ATOM     96  CB  SER A  26      13.163  -9.891   5.066  1.00  0.00           C
ATOM     97  OG  SER A  26      11.930 -10.584   4.816  1.00  0.00           O
ATOM     98  H   SER A  26      11.874  -7.901   5.412  1.00  0.00           H
ATOM     99  HG  SER A  26      11.344 -10.737   5.611  1.00  0.00           H
ATOM    100  N   ASN A  27      15.316  -9.220   7.356  1.00  0.00           N
ATOM    101  CA  ASN A  27      16.708  -8.955   7.768  1.00  0.00           C
ATOM    102  C   ASN A  27      17.139  -7.581   8.256  1.00  0.00           C
ATOM    103  O   ASN A  27      17.784  -7.536   9.306  1.00  0.00           O
ATOM    104  CB  ASN A  27      17.730  -9.431   6.726  1.00  0.00           C
ATOM    105  CG  ASN A  27      17.590 -10.929   6.455  1.00  0.00           C
ATOM    106  ND2 ASN A  27      17.736 -11.313   5.188  1.00  0.00           N
ATOM    107  OD1 ASN A  27      17.417 -11.747   7.365  1.00  0.00           O
ATOM    108  H   ASN A  27      15.021 -10.098   7.752  1.00  0.00           H
ATOM    109 1HD2 ASN A  27      18.034 -10.661   4.496  1.00  0.00           H
ATOM    110 2HD2 ASN A  27      17.456 -12.225   4.878  1.00  0.00           H
ATOM    111  N   LYS A  28      16.676  -6.449   7.724  1.00  0.00           N
ATOM    112  CA  LYS A  28      16.841  -5.133   8.352  1.00  0.00           C
ATOM    113  C   LYS A  28      15.577  -4.314   8.101  1.00  0.00           C
ATOM    114  O   LYS A  28      15.032  -4.256   6.999  1.00  0.00           O
ATOM    115  CB  LYS A  28      18.126  -4.567   7.739  1.00  0.00           C
ATOM    116  CG  LYS A  28      18.464  -3.201   8.343  1.00  0.00           C
ATOM    117  CD  LYS A  28      19.113  -2.309   7.274  1.00  0.00           C
ATOM    118  CE  LYS A  28      19.506  -0.905   7.737  1.00  0.00           C
ATOM    119  NZ  LYS A  28      18.296  -0.102   7.996  1.00  0.00           N1+
ATOM    120  H   LYS A  28      16.129  -6.459   6.888  1.00  0.00           H
ATOM    121  HZ1 LYS A  28      17.623  -0.664   8.489  1.00  0.00           H
ATOM    122  HZ2 LYS A  28      18.606   0.671   8.552  1.00  0.00           H
ATOM    123  HZ3 LYS A  28      17.871   0.219   7.149  1.00  0.00           H
ATOM    124  N   GLY A  29      14.985  -4.034   9.267  1.00  0.00           N
ATOM    125  CA  GLY A  29      13.878  -3.074   9.180  1.00  0.00           C
ATOM    126  C   GLY A  29      14.357  -1.630   8.994  1.00  0.00           C
ATOM    127  O   GLY A  29      15.462  -1.362   8.530  1.00  0.00           O
ATOM    128  H   GLY A  29      15.104  -4.583  10.091  1.00  0.00           H
ATOM    129  N   ALA A  30      13.537  -0.741   9.561  1.00  0.00           N
ATOM    130  CA  ALA A  30      13.526   0.714   9.387  1.00  0.00           C
ATOM    131  C   ALA A  30      12.651   1.349  10.468  1.00  0.00           C
ATOM    132  O   ALA A  30      11.661   0.780  10.911  1.00  0.00           O
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ATOM    133  CB  ALA A  30      13.036   1.039   7.973  1.00  0.00           C
ATOM    134  H   ALA A  30      12.972  -1.019  10.327  1.00  0.00           H
ATOM    135  N   ILE A  31      12.826   2.666  10.608  1.00  0.00           N
ATOM    136  CA  ILE A  31      12.254   3.390  11.746  1.00  0.00           C
ATOM    137  C   ILE A  31      10.738   3.542  11.558  1.00  0.00           C
ATOM    138  O   ILE A  31      10.317   4.196  10.602  1.00  0.00           O
ATOM    139  CB  ILE A  31      12.913   4.769  11.820  1.00  0.00           C
ATOM    140  CG1 ILE A  31      14.416   4.553  11.948  1.00  0.00           C
ATOM    141  CG2 ILE A  31      12.426   5.460  13.094  1.00  0.00           C
ATOM    142  CD  ILE A  31      15.230   5.850  11.972  1.00  0.00           C
ATOM    143  H   ILE A  31      13.314   3.166   9.897  1.00  0.00           H
ATOM    144  N   ILE A  32      10.006   2.951  12.495  1.00  0.00           N
ATOM    145  CA  ILE A  32       8.545   2.825  12.375  1.00  0.00           C
ATOM    146  C   ILE A  32       7.924   4.118  12.907  1.00  0.00           C
ATOM    147  O   ILE A  32       8.453   4.801  13.778  1.00  0.00           O
ATOM    148  CB  ILE A  32       8.124   1.618  13.219  1.00  0.00           C
ATOM    149  CG1 ILE A  32       8.498   0.297  12.557  1.00  0.00           C
ATOM    150  CG2 ILE A  32       6.627   1.613  13.546  1.00  0.00           C
ATOM    151  CD  ILE A  32       9.148  -0.730  13.491  1.00  0.00           C
ATOM    152  H   ILE A  32      10.365   2.795  13.417  1.00  0.00           H
ATOM    153  N   GLY A  33       6.973   4.674  12.155  1.00  0.00           N
ATOM    154  CA  GLY A  33       5.998   5.693  12.572  1.00  0.00           C
ATOM    155  C   GLY A  33       4.553   5.434  12.140  1.00  0.00           C
ATOM    156  O   GLY A  33       4.260   5.589  10.953  1.00  0.00           O
ATOM    157  H   GLY A  33       6.999   4.541  11.162  1.00  0.00           H
ATOM    158  N   LEU A  34       3.762   4.948  13.091  1.00  0.00           N
ATOM    159  CA  LEU A  34       2.312   4.806  12.923  1.00  0.00           C
ATOM    160  C   LEU A  34       1.529   6.119  13.029  1.00  0.00           C
ATOM    161  O   LEU A  34       1.633   6.826  14.029  1.00  0.00           O
ATOM    162  CB  LEU A  34       1.787   3.844  13.990  1.00  0.00           C
ATOM    163  CG  LEU A  34       0.413   3.312  13.574  1.00  0.00           C
ATOM    164  CD1 LEU A  34       0.520   2.428  12.325  1.00  0.00           C
ATOM    165  CD2 LEU A  34      -0.342   2.710  14.767  1.00  0.00           C
ATOM    166  H   LEU A  34       4.243   4.644  13.913  1.00  0.00           H
ATOM    167  N   MET A  35       1.018   6.404  11.825  1.00  0.00           N
ATOM    168  CA  MET A  35       0.123   7.519  11.502  1.00  0.00           C
ATOM    169  C   MET A  35      -1.320   7.082  11.233  1.00  0.00           C
ATOM    170  O   MET A  35      -1.622   6.494  10.187  1.00  0.00           O
ATOM    171  CB  MET A  35       0.671   8.311  10.321  1.00  0.00           C
ATOM    172  CG  MET A  35       2.101   8.738  10.663  1.00  0.00           C
ATOM    173  SD  MET A  35       2.935   9.637   9.304  1.00  0.00           S
ATOM    174  CE  MET A  35       4.436  10.110  10.143  1.00  0.00           C
ATOM    175  H   MET A  35       1.111   5.757  11.073  1.00  0.00           H
ATOM    176  N   VAL A  36      -2.115   7.262  12.280  1.00  0.00           N
ATOM    177  CA  VAL A  36      -3.539   6.896  12.222  1.00  0.00           C
ATOM    178  C   VAL A  36      -4.514   7.808  11.469  1.00  0.00           C
ATOM    179  O   VAL A  36      -4.609   9.013  11.676  1.00  0.00           O
ATOM    180  CB  VAL A  36      -4.103   6.537  13.601  1.00  0.00           C
ATOM    181  CG1 VAL A  36      -3.537   5.213  14.102  1.00  0.00           C
ATOM    182  CG2 VAL A  36      -3.937   7.764  14.498  1.00  0.00           C
ATOM    183  H   VAL A  36      -1.873   7.908  13.013  1.00  0.00           H
ATOM    184  N   GLY A  37      -5.258   7.274  10.507  1.00  0.00           N
ATOM    185  CA  GLY A  37      -6.266   8.113   9.839  1.00  0.00           C
ATOM    186  C   GLY A  37      -7.650   7.555  10.190  1.00  0.00           C
ATOM    187  O   GLY A  37      -8.085   6.467   9.814  1.00  0.00           O
ATOM    188  H   GLY A  37      -5.156   6.360  10.116  1.00  0.00           H
ATOM    189  N   GLY A  38      -8.459   8.362  10.873  1.00  0.00           N
ATOM    190  CA  GLY A  38      -9.872   8.245  11.238  1.00  0.00           C
ATOM    191  C   GLY A  38     -10.279   6.826  11.671  1.00  0.00           C
ATOM    192  O   GLY A  38      -9.611   6.299  12.547  1.00  0.00           O
ATOM    193  H   GLY A  38      -7.890   8.951  11.444  1.00  0.00           H
ATOM    194  N   VAL A  39     -10.931   6.083  10.774  1.00  0.00           N
ATOM    195  CA  VAL A  39     -11.216   4.656  11.022  1.00  0.00           C
ATOM    196  C   VAL A  39     -10.180   3.735  10.383  1.00  0.00           C
ATOM    197  O   VAL A  39      -9.913   3.831   9.191  1.00  0.00           O
ATOM    198  CB  VAL A  39     -12.629   4.236  10.638  1.00  0.00           C
ATOM    199  CG1 VAL A  39     -13.541   4.746  11.752  1.00  0.00           C
ATOM    200  CG2 VAL A  39     -13.113   4.904   9.346  1.00  0.00           C
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ATOM    201  H   VAL A  39     -11.041   6.376   9.831  1.00  0.00           H
ATOM    202  N   VAL A  40      -9.551   2.903  11.213  1.00  0.00           N
ATOM    203  CA  VAL A  40      -8.535   1.930  10.776  1.00  0.00           C
ATOM    204  C   VAL A  40      -9.240   0.566  10.660  1.00  0.00           C
ATOM    205  O   VAL A  40      -9.407   0.103   9.527  1.00  0.00           O
ATOM    206  CB  VAL A  40      -7.388   1.837  11.787  1.00  0.00           C
ATOM    207  CG1 VAL A  40      -6.163   1.249  11.073  1.00  0.00           C
ATOM    208  CG2 VAL A  40      -6.962   3.170  12.404  1.00  0.00           C
ATOM    209  H   VAL A  40      -9.651   2.939  12.205  1.00  0.00           H
ATOM    210  N   ILE A  41      -9.903   0.078  11.699  1.00  0.00           N
ATOM    211  CA  ILE A  41     -10.593  -1.220  11.703  1.00  0.00           C
ATOM    212  C   ILE A  41     -12.029  -0.952  12.173  1.00  0.00           C
ATOM    213  O   ILE A  41     -12.298  -0.873  13.365  1.00  0.00           O
ATOM    214  CB  ILE A  41      -9.856  -2.242  12.573  1.00  0.00           C
ATOM    215  CG1 ILE A  41      -8.373  -2.431  12.270  1.00  0.00           C
ATOM    216  CG2 ILE A  41     -10.571  -3.590  12.677  1.00  0.00           C
ATOM    217  CD  ILE A  41      -7.628  -3.195  13.368  1.00  0.00           C
ATOM    218  H   ILE A  41     -10.109   0.722  12.435  1.00  0.00           H
ATOM    219  N   ALA A  42     -12.943  -1.004  11.202  1.00  0.00           N
ATOM    220  CA  ALA A  42     -14.368  -0.901  11.539  1.00  0.00           C
ATOM    221  C   ALA A  42     -15.159  -2.187  11.249  1.00  0.00           C
ATOM    222  CB  ALA A  42     -14.933   0.252  10.702  1.00  0.00           C
ATOM    223  O1  ALA A  42     -15.254  -2.611  10.077  1.00  0.00           O
ATOM    224  O2  ALA A  42     -15.990  -2.474  12.135  1.00  0.00           O
ATOM    225  H   ALA A  42     -12.690  -1.250  10.263  1.00  0.00           H
ATOM    226  N   LEU B  17     -15.951  -4.016   1.649  1.00  0.00           N
ATOM    227  CA  LEU B  17     -14.695  -4.005   0.901  1.00  0.00           C
ATOM    228  C   LEU B  17     -13.554  -3.741   1.889  1.00  0.00           C
ATOM    229  O   LEU B  17     -13.545  -2.651   2.459  1.00  0.00           O
ATOM    230  CB  LEU B  17     -14.813  -2.933  -0.189  1.00  0.00           C
ATOM    231  CG  LEU B  17     -13.678  -3.125  -1.202  1.00  0.00           C
ATOM    232  CD1 LEU B  17     -13.817  -4.456  -1.950  1.00  0.00           C
ATOM    233  CD2 LEU B  17     -13.795  -1.978  -2.213  1.00  0.00           C
ATOM    234  H1  LEU B  17     -15.870  -4.514   2.516  1.00  0.00           H
ATOM    235  H2  LEU B  17     -16.253  -3.108   1.924  1.00  0.00           H
ATOM    236  H3  LEU B  17     -16.718  -4.397   1.128  1.00  0.00           H
ATOM    237  N   VAL B  18     -12.631  -4.691   1.999  1.00  0.00           N
ATOM    238  CA  VAL B  18     -11.448  -4.748   2.870  1.00  0.00           C
ATOM    239  C   VAL B  18     -10.196  -4.192   2.179  1.00  0.00           C
ATOM    240  O   VAL B  18      -9.907  -4.683   1.089  1.00  0.00           O
ATOM    241  CB  VAL B  18     -11.178  -6.208   3.271  1.00  0.00           C
ATOM    242  CG1 VAL B  18      -9.888  -6.253   4.096  1.00  0.00           C
ATOM    243  CG2 VAL B  18     -12.248  -6.795   4.187  1.00  0.00           C
ATOM    244  H   VAL B  18     -12.702  -5.420   1.317  1.00  0.00           H
ATOM    245  N   PHE B  19      -9.436  -3.259   2.735  1.00  0.00           N
ATOM    246  CA  PHE B  19      -8.212  -2.834   2.027  1.00  0.00           C
ATOM    247  C   PHE B  19      -6.925  -3.381   2.635  1.00  0.00           C
ATOM    248  O   PHE B  19      -6.938  -3.528   3.850  1.00  0.00           O
ATOM    249  CB  PHE B  19      -8.183  -1.320   1.851  1.00  0.00           C
ATOM    250  CG  PHE B  19      -9.177  -0.789   0.821  1.00  0.00           C
ATOM    251  CD1 PHE B  19      -8.691   0.008  -0.207  1.00  0.00           C
ATOM    252  CD2 PHE B  19     -10.549  -0.930   0.935  1.00  0.00           C
ATOM    253  CE1 PHE B  19      -9.485   0.644  -1.149  1.00  0.00           C
ATOM    254  CE2 PHE B  19     -11.380  -0.307   0.015  1.00  0.00           C
ATOM    255  CZ  PHE B  19     -10.855   0.513  -0.976  1.00  0.00           C
ATOM    256  H   PHE B  19      -9.633  -2.789   3.592  1.00  0.00           H
ATOM    257  HD1 PHE B  19      -7.627   0.226  -0.305  1.00  0.00           H
ATOM    258  HD2 PHE B  19     -10.954  -1.663   1.633  1.00  0.00           H
ATOM    259  HE1 PHE B  19      -9.083   1.037  -2.083  1.00  0.00           H
ATOM    260  HE2 PHE B  19     -12.455  -0.266   0.201  1.00  0.00           H
ATOM    261  HZ  PHE B  19     -11.580   1.042  -1.597  1.00  0.00           H
ATOM    262  N   PHE B  20      -6.016  -3.895   1.806  1.00  0.00           N
ATOM    263  CA  PHE B  20      -4.837  -4.510   2.440  1.00  0.00           C
ATOM    264  C   PHE B  20      -3.604  -4.177   1.605  1.00  0.00           C
ATOM    265  O   PHE B  20      -3.554  -4.243   0.376  1.00  0.00           O
ATOM    266  CB  PHE B  20      -5.103  -6.017   2.438  1.00  0.00           C
ATOM    267  CG  PHE B  20      -4.707  -6.563   3.813  1.00  0.00           C
ATOM    268  CD1 PHE B  20      -3.359  -6.707   4.115  1.00  0.00           C
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ATOM    269  CD2 PHE B  20      -5.666  -7.179   4.618  1.00  0.00           C
ATOM    270  CE1 PHE B  20      -2.937  -7.361   5.254  1.00  0.00           C
ATOM    271  CE2 PHE B  20      -5.238  -7.947   5.686  1.00  0.00           C
ATOM    272  CZ  PHE B  20      -3.889  -8.033   6.019  1.00  0.00           C
ATOM    273  H   PHE B  20      -6.284  -4.330   0.946  1.00  0.00           H
ATOM    274  HD1 PHE B  20      -2.571  -6.642   3.361  1.00  0.00           H
ATOM    275  HD2 PHE B  20      -6.680  -7.225   4.218  1.00  0.00           H
ATOM    276  HE1 PHE B  20      -2.029  -6.944   5.704  1.00  0.00           H
ATOM    277  HE2 PHE B  20      -5.977  -8.596   6.166  1.00  0.00           H
ATOM    278  HZ  PHE B  20      -3.563  -8.655   6.850  1.00  0.00           H
ATOM    279  N   ALA B  21      -2.616  -3.702   2.368  1.00  0.00           N
ATOM    280  CA  ALA B  21      -1.250  -3.410   1.933  1.00  0.00           C
ATOM    281  C   ALA B  21      -0.194  -4.288   2.616  1.00  0.00           C
ATOM    282  O   ALA B  21      -0.117  -4.301   3.846  1.00  0.00           O
ATOM    283  CB  ALA B  21      -0.879  -1.952   2.194  1.00  0.00           C
ATOM    284  H   ALA B  21      -2.769  -3.397   3.304  1.00  0.00           H
ATOM    285  N   GLU B  22       0.309  -5.275   1.892  1.00  0.00           N
ATOM    286  CA  GLU B  22       1.460  -6.067   2.365  1.00  0.00           C
ATOM    287  C   GLU B  22       2.813  -5.773   1.716  1.00  0.00           C
ATOM    288  O   GLU B  22       3.081  -6.115   0.560  1.00  0.00           O
ATOM    289  CB  GLU B  22       1.236  -7.572   2.209  1.00  0.00           C
ATOM    290  CG  GLU B  22       0.160  -7.923   3.245  1.00  0.00           C
ATOM    291  CD  GLU B  22      -0.090  -9.402   3.573  1.00  0.00           C
ATOM    292  OE1 GLU B  22      -1.164  -9.860   3.125  1.00  0.00           O
ATOM    293  OE2 GLU B  22       0.456  -9.888   4.588  1.00  0.00           O1-
ATOM    294  H   GLU B  22      -0.075  -5.677   1.059  1.00  0.00           H
ATOM    295  N   ASP B  23       3.641  -5.088   2.497  1.00  0.00           N
ATOM    296  CA  ASP B  23       5.001  -4.685   2.114  1.00  0.00           C
ATOM    297  C   ASP B  23       6.014  -5.795   2.393  1.00  0.00           C
ATOM    298  O   ASP B  23       6.691  -5.820   3.424  1.00  0.00           O
ATOM    299  CB  ASP B  23       5.357  -3.420   2.897  1.00  0.00           C
ATOM    300  CG  ASP B  23       6.724  -2.803   2.609  1.00  0.00           C
ATOM    301  OD1 ASP B  23       6.733  -1.588   2.882  1.00  0.00           O
ATOM    302  OD2 ASP B  23       7.678  -3.517   2.250  1.00  0.00           O1-
ATOM    303  H   ASP B  23       3.388  -4.893   3.445  1.00  0.00           H
ATOM    304  N   VAL B  24       6.129  -6.771   1.505  1.00  0.00           N
ATOM    305  CA  VAL B  24       7.101  -7.871   1.650  1.00  0.00           C
ATOM    306  C   VAL B  24       8.523  -7.388   1.363  1.00  0.00           C
ATOM    307  O   VAL B  24       8.971  -7.586   0.238  1.00  0.00           O
ATOM    308  CB  VAL B  24       6.542  -9.036   0.835  1.00  0.00           C
ATOM    309  CG1 VAL B  24       7.282 -10.363   0.996  1.00  0.00           C
ATOM    310  CG2 VAL B  24       5.068  -9.361   1.075  1.00  0.00           C
ATOM    311  H   VAL B  24       5.554  -6.795   0.682  1.00  0.00           H
ATOM    312  N   GLY B  25       9.235  -6.883   2.372  1.00  0.00           N
ATOM    313  CA  GLY B  25      10.396  -6.050   2.010  1.00  0.00           C
ATOM    314  C   GLY B  25      11.677  -6.723   2.488  1.00  0.00           C
ATOM    315  O   GLY B  25      11.903  -6.952   3.680  1.00  0.00           O
ATOM    316  H   GLY B  25       9.036  -7.100   3.319  1.00  0.00           H
ATOM    317  N   SER B  26      12.589  -7.006   1.558  1.00  0.00           N
ATOM    318  CA  SER B  26      13.952  -7.456   1.863  1.00  0.00           C
ATOM    319  C   SER B  26      14.989  -6.327   1.859  1.00  0.00           C
ATOM    320  O   SER B  26      15.459  -5.965   0.787  1.00  0.00           O
ATOM    321  CB  SER B  26      14.295  -8.747   1.105  1.00  0.00           C
ATOM    322  OG  SER B  26      15.379  -9.487   1.662  1.00  0.00           O
ATOM    323  H   SER B  26      12.608  -6.430   0.735  1.00  0.00           H
ATOM    324  HG  SER B  26      15.365 -10.389   1.232  1.00  0.00           H
ATOM    325  N   ASN B  27      15.444  -6.023   3.072  1.00  0.00           N
ATOM    326  CA  ASN B  27      16.265  -4.893   3.562  1.00  0.00           C
ATOM    327  C   ASN B  27      15.692  -3.513   3.285  1.00  0.00           C
ATOM    328  O   ASN B  27      15.824  -2.915   2.221  1.00  0.00           O
ATOM    329  CB  ASN B  27      17.710  -5.052   3.062  1.00  0.00           C
ATOM    330  CG  ASN B  27      18.537  -6.264   3.495  1.00  0.00           C
ATOM    331  ND2 ASN B  27      19.298  -6.740   2.512  1.00  0.00           N
ATOM    332  OD1 ASN B  27      18.284  -6.949   4.486  1.00  0.00           O
ATOM    333  H   ASN B  27      15.234  -6.637   3.826  1.00  0.00           H
ATOM    334 1HD2 ASN B  27      19.347  -6.292   1.629  1.00  0.00           H
ATOM    335 2HD2 ASN B  27      20.137  -7.258   2.701  1.00  0.00           H
ATOM    336  N   LYS B  28      15.206  -2.943   4.386  1.00  0.00           N
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ATOM    337  CA  LYS B  28      14.637  -1.585   4.458  1.00  0.00           C
ATOM    338  C   LYS B  28      15.725  -0.631   4.951  1.00  0.00           C
ATOM    339  O   LYS B  28      16.318  -0.799   6.020  1.00  0.00           O
ATOM    340  CB  LYS B  28      13.478  -1.660   5.448  1.00  0.00           C
ATOM    341  CG  LYS B  28      12.387  -2.568   4.867  1.00  0.00           C
ATOM    342  CD  LYS B  28      11.042  -2.384   5.583  1.00  0.00           C
ATOM    343  CE  LYS B  28      10.006  -3.209   4.823  1.00  0.00           C
ATOM    344  NZ  LYS B  28       8.671  -3.163   5.451  1.00  0.00           N1+
ATOM    345  H   LYS B  28      15.131  -3.419   5.254  1.00  0.00           H
ATOM    346  HZ1 LYS B  28       8.472  -3.566   6.340  1.00  0.00           H
ATOM    347  HZ2 LYS B  28       8.262  -2.261   5.446  1.00  0.00           H
ATOM    348  HZ3 LYS B  28       8.052  -3.654   4.844  1.00  0.00           H
ATOM    349  N   GLY B  29      15.884   0.521   4.317  1.00  0.00           N
ATOM    350  CA  GLY B  29      16.954   1.466   4.659  1.00  0.00           C
ATOM    351  C   GLY B  29      16.456   2.433   5.743  1.00  0.00           C
ATOM    352  O   GLY B  29      16.590   2.025   6.897  1.00  0.00           O
ATOM    353  H   GLY B  29      15.267   0.880   3.611  1.00  0.00           H
ATOM    354  N   ALA B  30      15.743   3.519   5.470  1.00  0.00           N
ATOM    355  CA  ALA B  30      15.545   4.553   6.492  1.00  0.00           C
ATOM    356  C   ALA B  30      14.219   4.645   7.255  1.00  0.00           C
ATOM    357  O   ALA B  30      14.194   3.944   8.262  1.00  0.00           O
ATOM    358  CB  ALA B  30      15.881   5.902   5.850  1.00  0.00           C
ATOM    359  H   ALA B  30      15.335   3.733   4.581  1.00  0.00           H
ATOM    360  N   ILE B  31      13.208   5.316   6.698  1.00  0.00           N
ATOM    361  CA  ILE B  31      11.965   5.565   7.441  1.00  0.00           C
ATOM    362  C   ILE B  31      10.615   5.042   6.930  1.00  0.00           C
ATOM    363  O   ILE B  31      10.386   5.175   5.725  1.00  0.00           O
ATOM    364  CB  ILE B  31      11.812   7.059   7.721  1.00  0.00           C
ATOM    365  CG1 ILE B  31      12.048   7.925   6.475  1.00  0.00           C
ATOM    366  CG2 ILE B  31      12.775   7.553   8.805  1.00  0.00           C
ATOM    367  CD  ILE B  31      12.046   9.437   6.626  1.00  0.00           C
ATOM    368  H   ILE B  31      13.316   5.774   5.812  1.00  0.00           H
ATOM    369  N   ILE B  32       9.906   4.438   7.879  1.00  0.00           N
ATOM    370  CA  ILE B  32       8.621   3.829   7.514  1.00  0.00           C
ATOM    371  C   ILE B  32       7.477   4.692   8.055  1.00  0.00           C
ATOM    372  O   ILE B  32       7.084   4.723   9.229  1.00  0.00           O
ATOM    373  CB  ILE B  32       8.349   2.377   7.909  1.00  0.00           C
ATOM    374  CG1 ILE B  32       9.555   1.576   7.417  1.00  0.00           C
ATOM    375  CG2 ILE B  32       7.088   1.863   7.222  1.00  0.00           C
ATOM    376  CD  ILE B  32       9.387   0.070   7.676  1.00  0.00           C
ATOM    377  H   ILE B  32      10.120   4.366   8.851  1.00  0.00           H
ATOM    378  N   GLY B  33       6.729   5.243   7.105  1.00  0.00           N
ATOM    379  CA  GLY B  33       5.487   6.021   7.257  1.00  0.00           C
ATOM    380  C   GLY B  33       4.275   5.135   6.939  1.00  0.00           C
ATOM    381  O   GLY B  33       3.955   4.997   5.764  1.00  0.00           O
ATOM    382  H   GLY B  33       7.032   5.170   6.155  1.00  0.00           H
ATOM    383  N   LEU B  34       3.767   4.525   7.995  1.00  0.00           N
ATOM    384  CA  LEU B  34       2.544   3.707   8.031  1.00  0.00           C
ATOM    385  C   LEU B  34       1.321   4.606   8.202  1.00  0.00           C
ATOM    386  O   LEU B  34       0.925   5.014   9.289  1.00  0.00           O
ATOM    387  CB  LEU B  34       2.659   2.815   9.271  1.00  0.00           C
ATOM    388  CG  LEU B  34       3.803   1.806   9.325  1.00  0.00           C
ATOM    389  CD1 LEU B  34       3.990   1.245  10.729  1.00  0.00           C
ATOM    390  CD2 LEU B  34       3.664   0.710   8.262  1.00  0.00           C
ATOM    391  H   LEU B  34       3.999   4.792   8.937  1.00  0.00           H
ATOM    392  N   MET B  35       0.740   5.025   7.078  1.00  0.00           N
ATOM    393  CA  MET B  35      -0.464   5.880   7.093  1.00  0.00           C
ATOM    394  C   MET B  35      -1.716   5.025   6.883  1.00  0.00           C
ATOM    395  O   MET B  35      -2.249   4.850   5.791  1.00  0.00           O
ATOM    396  CB  MET B  35      -0.513   6.968   6.020  1.00  0.00           C
ATOM    397  CG  MET B  35      -1.277   8.195   6.506  1.00  0.00           C
ATOM    398  SD  MET B  35      -3.040   8.018   6.973  1.00  0.00           S
ATOM    399  CE  MET B  35      -3.262   9.384   8.090  1.00  0.00           C
ATOM    400  H   MET B  35       1.163   4.764   6.218  1.00  0.00           H
ATOM    401  N   VAL B  36      -2.142   4.431   7.994  1.00  0.00           N
ATOM    402  CA  VAL B  36      -3.175   3.393   7.982  1.00  0.00           C
ATOM    403  C   VAL B  36      -4.541   3.940   8.432  1.00  0.00           C
ATOM    404  O   VAL B  36      -4.846   4.456   9.498  1.00  0.00           O
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ATOM    405  CB  VAL B  36      -2.633   2.275   8.864  1.00  0.00           C
ATOM    406  CG1 VAL B  36      -2.460   2.702  10.328  1.00  0.00           C
ATOM    407  CG2 VAL B  36      -3.520   1.029   8.976  1.00  0.00           C
ATOM    408  H   VAL B  36      -1.733   4.710   8.868  1.00  0.00           H
ATOM    409  N   GLY B  37      -5.320   4.061   7.356  1.00  0.00           N
ATOM    410  CA  GLY B  37      -6.757   4.308   7.576  1.00  0.00           C
ATOM    411  C   GLY B  37      -7.423   5.402   6.753  1.00  0.00           C
ATOM    412  O   GLY B  37      -6.863   6.063   5.879  1.00  0.00           O
ATOM    413  H   GLY B  37      -5.104   3.898   6.393  1.00  0.00           H
ATOM    414  N   GLY B  38      -8.725   5.374   7.028  1.00  0.00           N
ATOM    415  CA  GLY B  38      -9.819   6.055   6.319  1.00  0.00           C
ATOM    416  C   GLY B  38     -10.603   7.102   7.112  1.00  0.00           C
ATOM    417  O   GLY B  38     -11.089   6.953   8.238  1.00  0.00           O
ATOM    418  H   GLY B  38      -9.139   4.876   7.787  1.00  0.00           H
ATOM    419  N   VAL B  39     -10.870   8.132   6.308  1.00  0.00           N
ATOM    420  CA  VAL B  39     -11.390   9.417   6.798  1.00  0.00           C
ATOM    421  C   VAL B  39     -12.877   9.476   6.464  1.00  0.00           C
ATOM    422  O   VAL B  39     -13.157   9.559   5.268  1.00  0.00           O
ATOM    423  CB  VAL B  39     -10.626  10.641   6.277  1.00  0.00           C
ATOM    424  CG1 VAL B  39     -11.293  11.906   6.815  1.00  0.00           C
ATOM    425  CG2 VAL B  39      -9.169  10.552   6.709  1.00  0.00           C
ATOM    426  H   VAL B  39     -10.739   8.042   5.325  1.00  0.00           H
ATOM    427  N   VAL B  40     -13.753   9.529   7.464  1.00  0.00           N
ATOM    428  CA  VAL B  40     -15.217   9.610   7.409  1.00  0.00           C
ATOM    429  C   VAL B  40     -15.795  10.945   6.927  1.00  0.00           C
ATOM    430  O   VAL B  40     -15.640  11.908   7.678  1.00  0.00           O
ATOM    431  CB  VAL B  40     -15.816   9.009   8.680  1.00  0.00           C
ATOM    432  CG1 VAL B  40     -17.322   9.096   8.950  1.00  0.00           C
ATOM    433  CG2 VAL B  40     -15.561   7.498   8.674  1.00  0.00           C
ATOM    434  H   VAL B  40     -13.464   9.705   8.410  1.00  0.00           H
ATOM    435  N   ILE B  41     -16.436  10.954   5.765  1.00  0.00           N
ATOM    436  CA  ILE B  41     -17.234  12.086   5.253  1.00  0.00           C
ATOM    437  C   ILE B  41     -18.660  11.541   5.115  1.00  0.00           C
ATOM    438  O   ILE B  41     -18.950  10.899   4.098  1.00  0.00           O
ATOM    439  CB  ILE B  41     -16.578  12.592   3.968  1.00  0.00           C
ATOM    440  CG1 ILE B  41     -15.143  12.988   4.305  1.00  0.00           C
ATOM    441  CG2 ILE B  41     -17.504  13.583   3.251  1.00  0.00           C
ATOM    442  CD  ILE B  41     -14.820  14.421   4.714  1.00  0.00           C
ATOM    443  H   ILE B  41     -16.410  10.241   5.067  1.00  0.00           H
ATOM    444  N   ALA B  42     -19.443  11.969   6.087  1.00  0.00           N
ATOM    445  CA  ALA B  42     -20.823  11.513   6.308  1.00  0.00           C
ATOM    446  C   ALA B  42     -21.958  12.506   6.023  1.00  0.00           C
ATOM    447  CB  ALA B  42     -20.994  11.089   7.768  1.00  0.00           C
ATOM    448  O1  ALA B  42     -21.715  13.522   5.350  1.00  0.00           O
ATOM    449  O2  ALA B  42     -23.120  12.082   6.241  1.00  0.00           O
ATOM    450  H   ALA B  42     -19.202  12.777   6.619  1.00  0.00           H
ATOM    451  N   LEU C  17     -14.882  -8.766  -0.045  1.00  0.00           N
ATOM    452  CA  LEU C  17     -13.855  -8.881  -1.090  1.00  0.00           C
ATOM    453  C   LEU C  17     -12.664  -8.055  -0.618  1.00  0.00           C
ATOM    454  O   LEU C  17     -12.900  -7.008  -0.024  1.00  0.00           O
ATOM    455  CB  LEU C  17     -14.420  -8.335  -2.399  1.00  0.00           C
ATOM    456  CG  LEU C  17     -14.441  -9.149  -3.698  1.00  0.00           C
ATOM    457  CD1 LEU C  17     -15.343  -8.440  -4.701  1.00  0.00           C
ATOM    458  CD2 LEU C  17     -13.038  -9.376  -4.255  1.00  0.00           C
ATOM    459  H1  LEU C  17     -14.603  -8.385   0.845  1.00  0.00           H
ATOM    460  H2  LEU C  17     -15.697  -8.323  -0.405  1.00  0.00           H
ATOM    461  H3  LEU C  17     -15.201  -9.695   0.137  1.00  0.00           H
ATOM    462  N   VAL C  18     -11.419  -8.521  -0.642  1.00  0.00           N
ATOM    463  CA  VAL C  18     -10.175  -7.771  -0.372  1.00  0.00           C
ATOM    464  C   VAL C  18      -9.820  -6.942  -1.604  1.00  0.00           C
ATOM    465  O   VAL C  18      -9.920  -7.383  -2.743  1.00  0.00           O
ATOM    466  CB  VAL C  18      -9.088  -8.702   0.147  1.00  0.00           C
ATOM    467  CG1 VAL C  18      -8.875  -9.861  -0.833  1.00  0.00           C
ATOM    468  CG2 VAL C  18      -7.809  -7.979   0.584  1.00  0.00           C
ATOM    469  H   VAL C  18     -11.187  -9.472  -0.847  1.00  0.00           H
ATOM    470  N   PHE C  19      -9.337  -5.743  -1.290  1.00  0.00           N
ATOM    471  CA  PHE C  19      -8.576  -4.850  -2.180  1.00  0.00           C
ATOM    472  C   PHE C  19      -7.090  -4.944  -1.808  1.00  0.00           C
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ATOM    473  O   PHE C  19      -6.728  -4.455  -0.737  1.00  0.00           O
ATOM    474  CB  PHE C  19      -9.230  -3.488  -1.994  1.00  0.00           C
ATOM    475  CG  PHE C  19      -8.602  -2.516  -2.995  1.00  0.00           C
ATOM    476  CD1 PHE C  19      -7.458  -1.772  -2.711  1.00  0.00           C
ATOM    477  CD2 PHE C  19      -9.542  -2.148  -3.958  1.00  0.00           C
ATOM    478  CE1 PHE C  19      -7.147  -0.655  -3.475  1.00  0.00           C
ATOM    479  CE2 PHE C  19      -9.201  -1.022  -4.704  1.00  0.00           C
ATOM    480  CZ  PHE C  19      -8.084  -0.242  -4.415  1.00  0.00           C
ATOM    481  H   PHE C  19      -9.410  -5.371  -0.358  1.00  0.00           H
ATOM    482  HD1 PHE C  19      -6.857  -2.046  -1.847  1.00  0.00           H
ATOM    483  HD2 PHE C  19     -10.255  -2.913  -4.251  1.00  0.00           H
ATOM    484  HE1 PHE C  19      -6.281  -0.029  -3.264  1.00  0.00           H
ATOM    485  HE2 PHE C  19      -9.881  -0.676  -5.477  1.00  0.00           H
ATOM    486  HZ  PHE C  19      -7.953   0.719  -4.923  1.00  0.00           H
ATOM    487  N   PHE C  20      -6.361  -5.816  -2.478  1.00  0.00           N
ATOM    488  CA  PHE C  20      -5.001  -6.220  -2.080  1.00  0.00           C
ATOM    489  C   PHE C  20      -3.790  -5.614  -2.799  1.00  0.00           C
ATOM    490  O   PHE C  20      -3.823  -5.382  -4.007  1.00  0.00           O
ATOM    491  CB  PHE C  20      -4.978  -7.748  -2.106  1.00  0.00           C
ATOM    492  CG  PHE C  20      -3.735  -8.308  -1.403  1.00  0.00           C
ATOM    493  CD1 PHE C  20      -2.728  -8.931  -2.134  1.00  0.00           C
ATOM    494  CD2 PHE C  20      -3.632  -8.249  -0.024  1.00  0.00           C
ATOM    495  CE1 PHE C  20      -1.634  -9.462  -1.462  1.00  0.00           C
ATOM    496  CE2 PHE C  20      -2.490  -8.714   0.625  1.00  0.00           C
ATOM    497  CZ  PHE C  20      -1.501  -9.397  -0.075  1.00  0.00           C
ATOM    498  H   PHE C  20      -6.751  -6.284  -3.269  1.00  0.00           H
ATOM    499  HD1 PHE C  20      -2.747  -8.850  -3.214  1.00  0.00           H
ATOM    500  HD2 PHE C  20      -4.516  -8.009   0.568  1.00  0.00           H
ATOM    501  HE1 PHE C  20      -0.821  -9.871  -2.052  1.00  0.00           H
ATOM    502  HE2 PHE C  20      -2.291  -8.458   1.661  1.00  0.00           H
ATOM    503  HZ  PHE C  20      -0.839 -10.051   0.488  1.00  0.00           H
ATOM    504  N   ALA C  21      -2.744  -5.198  -2.089  1.00  0.00           N
ATOM    505  CA  ALA C  21      -1.427  -4.964  -2.685  1.00  0.00           C
ATOM    506  C   ALA C  21      -0.341  -5.859  -2.070  1.00  0.00           C
ATOM    507  O   ALA C  21      -0.350  -6.141  -0.873  1.00  0.00           O
ATOM    508  CB  ALA C  21      -1.082  -3.482  -2.620  1.00  0.00           C
ATOM    509  H   ALA C  21      -2.874  -4.897  -1.143  1.00  0.00           H
ATOM    510  N   GLU C  22       0.540  -6.344  -2.944  1.00  0.00           N
ATOM    511  CA  GLU C  22       1.853  -6.878  -2.532  1.00  0.00           C
ATOM    512  C   GLU C  22       2.996  -6.184  -3.265  1.00  0.00           C
ATOM    513  O   GLU C  22       3.146  -6.340  -4.470  1.00  0.00           O
ATOM    514  CB  GLU C  22       1.811  -8.351  -2.952  1.00  0.00           C
ATOM    515  CG  GLU C  22       2.161  -9.274  -1.794  1.00  0.00           C
ATOM    516  CD  GLU C  22       1.926 -10.759  -2.065  1.00  0.00           C
ATOM    517  OE1 GLU C  22       0.960 -11.060  -2.797  1.00  0.00           O
ATOM    518  OE2 GLU C  22       2.626 -11.607  -1.468  1.00  0.00          O1-
ATOM    519  H   GLU C  22       0.335  -6.486  -3.909  1.00  0.00           H
ATOM    520  N   ASP C  23       3.664  -5.298  -2.515  1.00  0.00           N
ATOM    521  CA  ASP C  23       4.923  -4.582  -2.767  1.00  0.00           C
ATOM    522  C   ASP C  23       6.058  -5.555  -2.425  1.00  0.00           C
ATOM    523  O   ASP C  23       6.414  -5.785  -1.267  1.00  0.00           O
ATOM    524  CB  ASP C  23       4.923  -3.263  -1.994  1.00  0.00           C
ATOM    525  CG  ASP C  23       6.167  -2.406  -2.250  1.00  0.00           C
ATOM    526  OD1 ASP C  23       7.247  -3.025  -2.253  1.00  0.00           O
ATOM    527  OD2 ASP C  23       6.061  -1.218  -2.608  1.00  0.00          O1-
ATOM    528  H   ASP C  23       3.220  -5.090  -1.645  1.00  0.00           H
ATOM    529  N   VAL C  24       6.439  -6.397  -3.374  1.00  0.00           N
ATOM    530  CA  VAL C  24       7.641  -7.205  -3.114  1.00  0.00           C
ATOM    531  C   VAL C  24       8.955  -6.595  -3.623  1.00  0.00           C
ATOM    532  O   VAL C  24       9.246  -6.628  -4.814  1.00  0.00           O
ATOM    533  CB  VAL C  24       7.579  -8.586  -3.753  1.00  0.00           C
ATOM    534  CG1 VAL C  24       8.729  -9.499  -3.320  1.00  0.00           C
ATOM    535  CG2 VAL C  24       6.220  -9.298  -3.793  1.00  0.00           C
ATOM    536  H   VAL C  24       6.230  -6.177  -4.331  1.00  0.00           H
ATOM    537  N   GLY C  25       9.644  -6.121  -2.588  1.00  0.00           N
ATOM    538  CA  GLY C  25      10.821  -5.262  -2.752  1.00  0.00           C
ATOM    539  C   GLY C  25      12.155  -5.815  -2.235  1.00  0.00           C
ATOM    540  O   GLY C  25      12.312  -6.120  -1.048  1.00  0.00           O
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ATOM    541  H   GLY C  25       9.382  -6.099  -1.620  1.00  0.00           H
ATOM    542  N   SER C  26      13.134  -5.728  -3.131  1.00  0.00           N
ATOM    543  CA  SER C  26      14.525  -6.044  -2.799  1.00  0.00           C
ATOM    544  C   SER C  26      15.357  -4.759  -2.683  1.00  0.00           C
ATOM    545  O   SER C  26      15.597  -4.123  -3.705  1.00  0.00           O
ATOM    546  CB  SER C  26      15.222  -7.004  -3.767  1.00  0.00           C
ATOM    547  OG  SER C  26      16.536  -7.442  -3.402  1.00  0.00           O
ATOM    548  H   SER C  26      12.876  -5.515  -4.075  1.00  0.00           H
ATOM    549  HG  SER C  26      17.017  -7.356  -4.284  1.00  0.00           H
ATOM    550  N   ASN C  27      15.774  -4.361  -1.485  1.00  0.00           N
ATOM    551  CA  ASN C  27      16.431  -3.098  -1.116  1.00  0.00           C
ATOM    552  C   ASN C  27      15.684  -1.777  -1.246  1.00  0.00           C
ATOM    553  O   ASN C  27      15.377  -1.152  -2.261  1.00  0.00           O
ATOM    554  CB  ASN C  27      17.756  -2.961  -1.868  1.00  0.00           C
ATOM    555  CG  ASN C  27      18.708  -2.053  -1.069  1.00  0.00           C
ATOM    556  ND2 ASN C  27      18.863  -0.797  -1.446  1.00  0.00           N
ATOM    557  OD1 ASN C  27      19.435  -2.518  -0.195  1.00  0.00           O
ATOM    558  H   ASN C  27      15.693  -5.012  -0.728  1.00  0.00           H
ATOM    559 1HD2 ASN C  27      18.437  -0.466  -2.295  1.00  0.00           H
ATOM    560 2HD2 ASN C  27      19.480  -0.251  -0.879  1.00  0.00           H
ATOM    561  N   LYS C  28      15.033  -1.318  -0.181  1.00  0.00           N
ATOM    562  CA  LYS C  28      14.136  -0.163  -0.084  1.00  0.00           C
ATOM    563  C   LYS C  28      14.793   0.925   0.772  1.00  0.00           C
ATOM    564  O   LYS C  28      14.837   0.864   2.001  1.00  0.00           O
ATOM    565  CB  LYS C  28      12.852  -0.671   0.569  1.00  0.00           C
ATOM    566  CG  LYS C  28      12.146  -1.761  -0.246  1.00  0.00           C
ATOM    567  CD  LYS C  28      10.758  -2.055   0.322  1.00  0.00           C
ATOM    568  CE  LYS C  28       9.826  -0.867   0.109  1.00  0.00           C
ATOM    569  NZ  LYS C  28       8.442  -1.344   0.201  1.00  0.00           N1+
ATOM    570  H   LYS C  28      15.159  -1.772   0.708  1.00  0.00           H
ATOM    571  HZ1 LYS C  28       8.226  -1.911   0.998  1.00  0.00           H
ATOM    572  HZ2 LYS C  28       7.803  -0.580   0.197  1.00  0.00           H
ATOM    573  HZ3 LYS C  28       8.200  -1.899  -0.598  1.00  0.00           H
ATOM    574  N   GLY C  29      15.133   2.017   0.073  1.00  0.00           N
ATOM    575  CA  GLY C  29      15.914   3.111   0.641  1.00  0.00           C
ATOM    576  C   GLY C  29      15.168   3.924   1.708  1.00  0.00           C
ATOM    577  O   GLY C  29      14.943   3.461   2.821  1.00  0.00           O
ATOM    578  H   GLY C  29      15.049   1.924  -0.924  1.00  0.00           H
ATOM    579  N   ALA C  30      15.355   5.216   1.445  1.00  0.00           N
ATOM    580  CA  ALA C  30      15.046   6.400   2.261  1.00  0.00           C
ATOM    581  C   ALA C  30      13.659   6.511   2.900  1.00  0.00           C
ATOM    582  O   ALA C  30      13.412   5.987   3.984  1.00  0.00           O
ATOM    583  CB  ALA C  30      15.534   7.581   1.430  1.00  0.00           C
ATOM    584  H   ALA C  30      15.991   5.333   0.685  1.00  0.00           H
ATOM    585  N   ILE C  31      12.664   6.840   2.078  1.00  0.00           N
ATOM    586  CA  ILE C  31      11.289   7.046   2.537  1.00  0.00           C
ATOM    587  C   ILE C  31      10.341   5.943   2.046  1.00  0.00           C
ATOM    588  O   ILE C  31      10.123   5.791   0.850  1.00  0.00           O
ATOM    589  CB  ILE C  31      10.712   8.382   2.064  1.00  0.00           C
ATOM    590  CG1 ILE C  31      11.688   9.505   2.398  1.00  0.00           C
ATOM    591  CG2 ILE C  31       9.409   8.682   2.810  1.00  0.00           C
ATOM    592  CD  ILE C  31      11.138  10.856   1.922  1.00  0.00           C
ATOM    593  H   ILE C  31      12.770   7.057   1.112  1.00  0.00           H
ATOM    594  N   ILE C  32       9.767   5.138   2.935  1.00  0.00           N
ATOM    595  CA  ILE C  32       8.962   3.938   2.681  1.00  0.00           C
ATOM    596  C   ILE C  32       7.538   4.245   3.124  1.00  0.00           C
ATOM    597  O   ILE C  32       7.264   4.566   4.284  1.00  0.00           O
ATOM    598  CB  ILE C  32       9.524   2.713   3.399  1.00  0.00           C
ATOM    599  CG1 ILE C  32      11.019   2.520   3.127  1.00  0.00           C
ATOM    600  CG2 ILE C  32       8.745   1.446   3.024  1.00  0.00           C
ATOM    601  CD  ILE C  32      11.653   1.465   4.036  1.00  0.00           C
ATOM    602  H   ILE C  32       9.999   5.245   3.906  1.00  0.00           H
ATOM    603  N   GLY C  33       6.687   4.447   2.117  1.00  0.00           N
ATOM    604  CA  GLY C  33       5.315   4.832   2.474  1.00  0.00           C
ATOM    605  C   GLY C  33       4.303   3.733   2.137  1.00  0.00           C
ATOM    606  O   GLY C  33       4.179   3.210   1.024  1.00  0.00           O
ATOM    607  H   GLY C  33       6.920   4.522   1.143  1.00  0.00           H
ATOM    608  N   LEU C  34       3.416   3.616   3.117  1.00  0.00           N
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ATOM    609  CA  LEU C  34       2.227   2.746   3.049  1.00  0.00           C
ATOM    610  C   LEU C  34       1.017   3.592   3.442  1.00  0.00           C
ATOM    611  O   LEU C  34       0.783   4.018   4.572  1.00  0.00           O
ATOM    612  CB  LEU C  34       2.297   1.453   3.863  1.00  0.00           C
ATOM    613  CG  LEU C  34       3.382   0.485   3.384  1.00  0.00           C
ATOM    614  CD1 LEU C  34       4.791   0.741   3.898  1.00  0.00           C
ATOM    615  CD2 LEU C  34       2.992  -0.939   3.767  1.00  0.00           C
ATOM    616  H   LEU C  34       3.469   4.114   3.982  1.00  0.00           H
ATOM    617  N   MET C  35       0.483   4.221   2.402  1.00  0.00           N
ATOM    618  CA  MET C  35      -0.719   5.063   2.399  1.00  0.00           C
ATOM    619  C   MET C  35      -1.960   4.223   2.084  1.00  0.00           C
ATOM    620  O   MET C  35      -2.360   4.033   0.940  1.00  0.00           O
ATOM    621  CB  MET C  35      -0.605   6.242   1.437  1.00  0.00           C
ATOM    622  CG  MET C  35       0.414   7.252   1.972  1.00  0.00           C
ATOM    623  SD  MET C  35       2.130   6.884   1.451  1.00  0.00           S
ATOM    624  CE  MET C  35       3.008   8.305   2.070  1.00  0.00           C
ATOM    625  H   MET C  35       0.814   4.054   1.477  1.00  0.00           H
ATOM    626  N   VAL C  36      -2.618   3.773   3.156  1.00  0.00           N
ATOM    627  CA  VAL C  36      -3.672   2.754   3.030  1.00  0.00           C
ATOM    628  C   VAL C  36      -4.973   3.469   3.367  1.00  0.00           C
ATOM    629  O   VAL C  36      -5.004   4.098   4.426  1.00  0.00           O
ATOM    630  CB  VAL C  36      -3.448   1.438   3.783  1.00  0.00           C
ATOM    631  CG1 VAL C  36      -4.211   0.274   3.146  1.00  0.00           C
ATOM    632  CG2 VAL C  36      -1.972   1.032   3.732  1.00  0.00           C
ATOM    633  H   VAL C  36      -2.501   4.158   4.071  1.00  0.00           H
ATOM    634  N   GLY C  37      -5.856   3.757   2.417  1.00  0.00           N
ATOM    635  CA  GLY C  37      -7.153   4.441   2.567  1.00  0.00           C
ATOM    636  C   GLY C  37      -7.399   5.781   1.861  1.00  0.00           C
ATOM    637  O   GLY C  37      -7.653   5.664   0.670  1.00  0.00           O
ATOM    638  H   GLY C  37      -5.574   3.421   1.524  1.00  0.00           H
ATOM    639  N   GLY C  38      -7.677   6.797   2.685  1.00  0.00           N
ATOM    640  CA  GLY C  38      -8.031   8.155   2.264  1.00  0.00           C
ATOM    641  C   GLY C  38      -9.481   8.512   2.607  1.00  0.00           C
ATOM    642  O   GLY C  38      -9.903   8.109   3.685  1.00  0.00           O
ATOM    643  H   GLY C  38      -7.434   6.729   3.645  1.00  0.00           H
ATOM    644  N   VAL C  39     -10.309   9.014   1.699  1.00  0.00           N
ATOM    645  CA  VAL C  39     -11.692   9.392   2.027  1.00  0.00           C
ATOM    646  C   VAL C  39     -12.849   8.439   1.739  1.00  0.00           C
ATOM    647  O   VAL C  39     -13.041   8.050   0.584  1.00  0.00           O
ATOM    648  CB  VAL C  39     -12.041  10.794   1.496  1.00  0.00           C
ATOM    649  CG1 VAL C  39     -11.520  11.837   2.486  1.00  0.00           C
ATOM    650  CG2 VAL C  39     -11.509  10.986   0.086  1.00  0.00           C
ATOM    651  H   VAL C  39     -10.176   8.964   0.709  1.00  0.00           H
ATOM    652  N   VAL C  40     -13.597   8.198   2.808  1.00  0.00           N
ATOM    653  CA  VAL C  40     -14.753   7.291   2.847  1.00  0.00           C
ATOM    654  C   VAL C  40     -16.007   8.152   2.711  1.00  0.00           C
ATOM    655  O   VAL C  40     -16.500   8.765   3.653  1.00  0.00           O
ATOM    656  CB  VAL C  40     -14.610   6.416   4.094  1.00  0.00           C
ATOM    657  CG1 VAL C  40     -15.825   5.501   3.974  1.00  0.00           C
ATOM    658  CG2 VAL C  40     -13.274   5.702   4.335  1.00  0.00           C
ATOM    659  H   VAL C  40     -13.507   8.712   3.660  1.00  0.00           H
ATOM    660  N   ILE C  41     -16.645   8.028   1.552  1.00  0.00           N
ATOM    661  CA  ILE C  41     -17.857   8.717   1.089  1.00  0.00           C
ATOM    662  C   ILE C  41     -18.924   7.618   1.180  1.00  0.00           C
ATOM    663  O   ILE C  41     -18.802   6.606   0.491  1.00  0.00           O
ATOM    664  CB  ILE C  41     -17.690   9.227  -0.346  1.00  0.00           C
ATOM    665  CG1 ILE C  41     -16.569  10.274  -0.379  1.00  0.00           C
ATOM    666  CG2 ILE C  41     -19.012   9.862  -0.766  1.00  0.00           C
ATOM    667  CD  ILE C  41     -16.269  10.986  -1.690  1.00  0.00           C
ATOM    668  H   ILE C  41     -16.288   7.444   0.812  1.00  0.00           H
ATOM    669  N   ALA C  42     -19.903   7.907   2.040  1.00  0.00           N
ATOM    670  CA  ALA C  42     -20.848   6.877   2.512  1.00  0.00           C
ATOM    671  C   ALA C  42     -22.020   7.429   3.321  1.00  0.00           C
ATOM    672  CB  ALA C  42     -20.068   5.816   3.286  1.00  0.00           C
ATOM    673  O1  ALA C  42     -21.904   8.507   3.941  1.00  0.00           O
ATOM    674  O2  ALA C  42     -23.122   6.870   3.105  1.00  0.00           O
ATOM    675  H   ALA C  42     -19.956   8.760   2.562  1.00  0.00           H
ATOM    676  N   LEU D  17     -14.317  -0.840  -8.645  1.00  0.00           N
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ATOM    677  CA  LEU D  17     -13.156  -1.573  -9.169  1.00  0.00           C
ATOM    678  C   LEU D  17     -12.389  -2.153  -7.981  1.00  0.00           C
ATOM    679  O   LEU D  17     -12.326  -1.537  -6.923  1.00  0.00           O
ATOM    680  CB  LEU D  17     -12.367  -0.525  -9.964  1.00  0.00           C
ATOM    681  CG  LEU D  17     -11.024  -1.072 -10.454  1.00  0.00           C
ATOM    682  CD1 LEU D  17     -11.110  -2.088 -11.593  1.00  0.00           C
ATOM    683  CD2 LEU D  17      -9.945   0.013 -10.573  1.00  0.00           C
ATOM    684  H1  LEU D  17     -14.404  -0.710  -7.660  1.00  0.00           H
ATOM    685  H2  LEU D  17     -14.353   0.047  -9.095  1.00  0.00           H
ATOM    686  H3  LEU D  17     -15.146  -1.311  -8.956  1.00  0.00           H
ATOM    687  N   VAL D  18     -11.985  -3.413  -8.137  1.00  0.00           N
ATOM    688  CA  VAL D  18     -11.211  -4.145  -7.126  1.00  0.00           C
ATOM    689  C   VAL D  18      -9.776  -4.303  -7.615  1.00  0.00           C
ATOM    690  O   VAL D  18      -9.548  -4.941  -8.647  1.00  0.00           O
ATOM    691  CB  VAL D  18     -11.862  -5.498  -6.819  1.00  0.00           C
ATOM    692  CG1 VAL D  18     -11.130  -6.309  -5.742  1.00  0.00           C
ATOM    693  CG2 VAL D  18     -13.303  -5.361  -6.325  1.00  0.00           C
ATOM    694  H   VAL D  18     -12.344  -3.980  -8.880  1.00  0.00           H
ATOM    695  N   PHE D  19      -8.830  -3.764  -6.853  1.00  0.00           N
ATOM    696  CA  PHE D  19      -7.443  -3.827  -7.338  1.00  0.00           C
ATOM    697  C   PHE D  19      -6.653  -4.886  -6.564  1.00  0.00           C
ATOM    698  O   PHE D  19      -6.627  -4.910  -5.342  1.00  0.00           O
ATOM    699  CB  PHE D  19      -6.732  -2.501  -7.083  1.00  0.00           C
ATOM    700  CG  PHE D  19      -6.006  -2.039  -8.342  1.00  0.00           C
ATOM    701  CD1 PHE D  19      -4.690  -2.416  -8.587  1.00  0.00           C
ATOM    702  CD2 PHE D  19      -6.443  -0.817  -8.860  1.00  0.00           C
ATOM    703  CE1 PHE D  19      -3.883  -1.635  -9.397  1.00  0.00           C
ATOM    704  CE2 PHE D  19      -5.621   0.007  -9.617  1.00  0.00           C
ATOM    705  CZ  PHE D  19      -4.346  -0.443  -9.939  1.00  0.00           C
ATOM    706  H   PHE D  19      -9.099  -3.115  -6.137  1.00  0.00           H
ATOM    707  HD1 PHE D  19      -4.226  -3.305  -8.149  1.00  0.00           H
ATOM    708  HD2 PHE D  19      -7.470  -0.440  -8.877  1.00  0.00           H
ATOM    709  HE1 PHE D  19      -2.826  -1.529  -9.120  1.00  0.00           H
ATOM    710  HE2 PHE D  19      -5.999   0.995  -9.871  1.00  0.00           H
ATOM    711  HZ  PHE D  19      -3.662   0.117 -10.575  1.00  0.00           H
ATOM    712  N   PHE D  20      -6.039  -5.777  -7.339  1.00  0.00           N
ATOM    713  CA  PHE D  20      -5.107  -6.817  -6.857  1.00  0.00           C
ATOM    714  C   PHE D  20      -3.761  -6.550  -7.541  1.00  0.00           C
ATOM    715  O   PHE D  20      -3.509  -6.913  -8.683  1.00  0.00           O
ATOM    716  CB  PHE D  20      -5.745  -8.118  -7.352  1.00  0.00           C
ATOM    717  CG  PHE D  20      -7.085  -8.364  -6.672  1.00  0.00           C
ATOM    718  CD1 PHE D  20      -8.264  -8.606  -7.369  1.00  0.00           C
ATOM    719  CD2 PHE D  20      -7.143  -8.543  -5.298  1.00  0.00           C
ATOM    720  CE1 PHE D  20      -9.400  -9.087  -6.724  1.00  0.00           C
ATOM    721  CE2 PHE D  20      -8.253  -9.043  -4.611  1.00  0.00           C
ATOM    722  CZ  PHE D  20      -9.390  -9.304  -5.345  1.00  0.00           C
ATOM    723  H   PHE D  20      -6.060  -5.765  -8.336  1.00  0.00           H
ATOM    724  HD1 PHE D  20      -8.291  -8.358  -8.427  1.00  0.00           H
ATOM    725  HD2 PHE D  20      -6.202  -8.610  -4.754  1.00  0.00           H
ATOM    726  HE1 PHE D  20     -10.322  -9.295  -7.271  1.00  0.00           H
ATOM    727  HE2 PHE D  20      -8.228  -9.216  -3.535  1.00  0.00           H
ATOM    728  HZ  PHE D  20     -10.350  -9.522  -4.874  1.00  0.00           H
ATOM    729  N   ALA D  21      -2.955  -5.938  -6.676  1.00  0.00           N
ATOM    730  CA  ALA D  21      -1.638  -5.404  -7.030  1.00  0.00           C
ATOM    731  C   ALA D  21      -0.565  -6.472  -6.811  1.00  0.00           C
ATOM    732  O   ALA D  21      -0.414  -7.000  -5.717  1.00  0.00           O
ATOM    733  CB  ALA D  21      -1.277  -4.053  -6.414  1.00  0.00           C
ATOM    734  H   ALA D  21      -3.283  -5.790  -5.738  1.00  0.00           H
ATOM    735  N   GLU D  22       0.306  -6.610  -7.817  1.00  0.00           N
ATOM    736  CA  GLU D  22       1.546  -7.371  -7.627  1.00  0.00           C
ATOM    737  C   GLU D  22       2.672  -6.547  -8.240  1.00  0.00           C
ATOM    738  O   GLU D  22       2.761  -6.259  -9.441  1.00  0.00           O
ATOM    739  CB  GLU D  22       1.407  -8.702  -8.374  1.00  0.00           C
ATOM    740  CG  GLU D  22       2.497  -9.655  -7.861  1.00  0.00           C
ATOM    741  CD  GLU D  22       2.542 -10.981  -8.605  1.00  0.00           C
ATOM    742  OE1 GLU D  22       3.677 -11.496  -8.729  1.00  0.00           O
ATOM    743  OE2 GLU D  22       1.552 -11.616  -9.034  1.00  0.00           O1-
ATOM    744  H   GLU D  22       0.052  -6.363  -8.747  1.00  0.00           H
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ATOM    745  N   ASP D  23       3.411  -5.983  -7.283  1.00  0.00           N
ATOM    746  CA  ASP D  23       4.614  -5.209  -7.615  1.00  0.00           C
ATOM    747  C   ASP D  23       5.893  -5.949  -7.216  1.00  0.00           C
ATOM    748  O   ASP D  23       6.442  -5.652  -6.156  1.00  0.00           O
ATOM    749  CB  ASP D  23       4.548  -3.877  -6.872  1.00  0.00           C
ATOM    750  CG  ASP D  23       5.598  -2.874  -7.383  1.00  0.00           C
ATOM    751  OD1 ASP D  23       6.714  -3.219  -7.821  1.00  0.00           O
ATOM    752  OD2 ASP D  23       5.302  -1.663  -7.273  1.00  0.00           O1-
ATOM    753  H   ASP D  23       3.177  -6.175  -6.328  1.00  0.00           H
ATOM    754  N   VAL D  24       6.448  -6.594  -8.236  1.00  0.00           N
ATOM    755  CA  VAL D  24       7.690  -7.366  -8.053  1.00  0.00           C
ATOM    756  C   VAL D  24       8.935  -6.543  -8.385  1.00  0.00           C
ATOM    757  O   VAL D  24       9.233  -6.503  -9.579  1.00  0.00           O
ATOM    758  CB  VAL D  24       7.742  -8.755  -8.684  1.00  0.00           C
ATOM    759  CG1 VAL D  24       8.661  -9.679  -7.877  1.00  0.00           C
ATOM    760  CG2 VAL D  24       6.394  -9.477  -8.733  1.00  0.00           C
ATOM    761  H   VAL D  24       6.082  -6.564  -9.165  1.00  0.00           H
ATOM    762  N   GLY D  25       9.548  -5.942  -7.370  1.00  0.00           N
ATOM    763  CA  GLY D  25      10.696  -5.087  -7.705  1.00  0.00           C
ATOM    764  C   GLY D  25      12.064  -5.049  -7.029  1.00  0.00           C
ATOM    765  O   GLY D  25      12.139  -5.232  -5.821  1.00  0.00           O
ATOM    766  H   GLY D  25       9.312  -6.060  -6.399  1.00  0.00           H
ATOM    767  N   SER D  26      13.153  -4.906  -7.786  1.00  0.00           N
ATOM    768  CA  SER D  26      14.536  -4.895  -7.278  1.00  0.00           C
ATOM    769  C   SER D  26      15.225  -3.544  -7.463  1.00  0.00           C
ATOM    770  O   SER D  26      15.075  -2.891  -8.488  1.00  0.00           O
ATOM    771  CB  SER D  26      15.364  -5.904  -8.078  1.00  0.00           C
ATOM    772  OG  SER D  26      16.765  -5.795  -7.812  1.00  0.00           O
ATOM    773  H   SER D  26      13.071  -4.896  -8.781  1.00  0.00           H
ATOM    774  HG  SER D  26      16.927  -6.223  -6.928  1.00  0.00           H
ATOM    775  N   ASN D  27      15.678  -2.931  -6.375  1.00  0.00           N
ATOM    776  CA  ASN D  27      16.374  -1.636  -6.287  1.00  0.00           C
ATOM    777  C   ASN D  27      15.426  -0.428  -6.189  1.00  0.00           C
ATOM    778  O   ASN D  27      15.380   0.351  -7.137  1.00  0.00           O
ATOM    779  CB  ASN D  27      17.462  -1.420  -7.341  1.00  0.00           C
ATOM    780  CG  ASN D  27      18.645  -0.708  -6.676  1.00  0.00           C
ATOM    781  ND2 ASN D  27      19.863  -1.224  -6.782  1.00  0.00           N
ATOM    782  OD1 ASN D  27      18.416   0.349  -6.094  1.00  0.00           O
ATOM    783  H   ASN D  27      15.723  -3.460  -5.532  1.00  0.00           H
ATOM    784 1HD2 ASN D  27      20.043  -2.013  -7.370  1.00  0.00           H
ATOM    785 2HD2 ASN D  27      20.577  -0.691  -6.337  1.00  0.00           H
ATOM    786  N   LYS D  28      14.688  -0.373  -5.091  1.00  0.00           N
ATOM    787  CA  LYS D  28      13.711   0.706  -4.867  1.00  0.00           C
ATOM    788  C   LYS D  28      14.220   1.877  -4.021  1.00  0.00           C
ATOM    789  O   LYS D  28      14.607   1.640  -2.883  1.00  0.00           O
ATOM    790  CB  LYS D  28      12.437   0.135  -4.233  1.00  0.00           C
ATOM    791  CG  LYS D  28      11.717  -0.971  -5.004  1.00  0.00           C
ATOM    792  CD  LYS D  28      10.205  -1.041  -4.797  1.00  0.00           C
ATOM    793  CE  LYS D  28       9.692  -2.407  -5.264  1.00  0.00           C
ATOM    794  NZ  LYS D  28       8.224  -2.359  -5.323  1.00  0.00           N1+
ATOM    795  H   LYS D  28      14.723  -1.044  -4.344  1.00  0.00           H
ATOM    796  HZ1 LYS D  28       7.967  -1.475  -5.725  1.00  0.00           H
ATOM    797  HZ2 LYS D  28       7.876  -3.014  -5.990  1.00  0.00           H
ATOM    798  HZ3 LYS D  28       7.716  -2.594  -4.495  1.00  0.00           H
ATOM    799  N   GLY D  29      14.770   2.787  -4.816  1.00  0.00           N
ATOM    800  CA  GLY D  29      15.411   3.946  -4.194  1.00  0.00           C
ATOM    801  C   GLY D  29      14.428   4.954  -3.592  1.00  0.00           C
ATOM    802  O   GLY D  29      13.233   5.063  -3.842  1.00  0.00           O
ATOM    803  H   GLY D  29      14.770   2.741  -5.813  1.00  0.00           H
ATOM    804  N   ALA D  30      15.153   5.914  -3.019  1.00  0.00           N
ATOM    805  CA  ALA D  30      14.744   7.116  -2.285  1.00  0.00           C
ATOM    806  C   ALA D  30      13.315   7.249  -1.771  1.00  0.00           C
ATOM    807  O   ALA D  30      13.067   6.924  -0.610  1.00  0.00           O
ATOM    808  CB  ALA D  30      15.184   8.361  -3.054  1.00  0.00           C
ATOM    809  H   ALA D  30      16.143   5.962  -3.188  1.00  0.00           H
ATOM    810  N   ILE D  31      12.374   7.535  -2.668  1.00  0.00           N
ATOM    811  CA  ILE D  31      10.946   7.702  -2.373  1.00  0.00           C
ATOM    812  C   ILE D  31      10.024   6.606  -2.916  1.00  0.00           C
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ATOM    813  O   ILE D  31       9.430   6.659  -3.996  1.00  0.00           O
ATOM    814  CB  ILE D  31      10.436   9.106  -2.707  1.00  0.00           C
ATOM    815  CG1 ILE D  31      11.020  10.004  -1.612  1.00  0.00           C
ATOM    816  CG2 ILE D  31       8.934   9.349  -2.738  1.00  0.00           C
ATOM    817  CD  ILE D  31      10.836  11.512  -1.465  1.00  0.00           C
ATOM    818  H   ILE D  31      12.425   7.376  -3.657  1.00  0.00           H
ATOM    819  N   ILE D  32       9.830   5.686  -1.977  1.00  0.00           N
ATOM    820  CA  ILE D  32       9.084   4.474  -2.312  1.00  0.00           C
ATOM    821  C   ILE D  32       7.695   4.479  -1.685  1.00  0.00           C
ATOM    822  O   ILE D  32       7.527   4.173  -0.499  1.00  0.00           O
ATOM    823  CB  ILE D  32       9.820   3.179  -1.953  1.00  0.00           C
ATOM    824  CG1 ILE D  32      11.332   3.266  -2.122  1.00  0.00           C
ATOM    825  CG2 ILE D  32       9.348   1.976  -2.784  1.00  0.00           C
ATOM    826  CD  ILE D  32      12.147   3.615  -0.876  1.00  0.00           C
ATOM    827  H   ILE D  32      10.166   5.877  -1.055  1.00  0.00           H
ATOM    828  N   GLY D  33       6.647   4.721  -2.470  1.00  0.00           N
ATOM    829  CA  GLY D  33       5.259   4.783  -1.995  1.00  0.00           C
ATOM    830  C   GLY D  33       4.272   3.723  -2.492  1.00  0.00           C
ATOM    831  O   GLY D  33       4.055   3.619  -3.707  1.00  0.00           O
ATOM    832  H   GLY D  33       6.686   4.797  -3.460  1.00  0.00           H
ATOM    833  N   LEU D  34       3.429   3.146  -1.656  1.00  0.00           N
ATOM    834  CA  LEU D  34       2.269   2.283  -1.899  1.00  0.00           C
ATOM    835  C   LEU D  34       1.060   3.017  -1.313  1.00  0.00           C
ATOM    836  O   LEU D  34       1.030   3.298  -0.113  1.00  0.00           O
ATOM    837  CB  LEU D  34       2.473   0.947  -1.182  1.00  0.00           C
ATOM    838  CG  LEU D  34       1.859  -0.229  -1.933  1.00  0.00           C
ATOM    839  CD1 LEU D  34       2.509  -0.611  -3.276  1.00  0.00           C
ATOM    840  CD2 LEU D  34       1.794  -1.484  -1.050  1.00  0.00           C
ATOM    841  H   LEU D  34       3.595   3.283  -0.679  1.00  0.00           H
ATOM    842  N   MET D  35       0.329   3.511  -2.314  1.00  0.00           N
ATOM    843  CA  MET D  35      -0.857   4.345  -2.082  1.00  0.00           C
ATOM    844  C   MET D  35      -2.113   3.506  -2.316  1.00  0.00           C
ATOM    845  O   MET D  35      -2.720   3.578  -3.388  1.00  0.00           O
ATOM    846  CB  MET D  35      -0.857   5.641  -2.899  1.00  0.00           C
ATOM    847  CG  MET D  35       0.275   6.621  -2.605  1.00  0.00           C
ATOM    848  SD  MET D  35       0.308   8.097  -3.678  1.00  0.00           S
ATOM    849  CE  MET D  35       1.452   9.025  -2.675  1.00  0.00           C
ATOM    850  H   MET D  35       0.678   3.472  -3.241  1.00  0.00           H
ATOM    851  N   VAL D  36      -2.577   2.820  -1.268  1.00  0.00           N
ATOM    852  CA  VAL D  36      -3.640   1.829  -1.460  1.00  0.00           C
ATOM    853  C   VAL D  36      -5.032   2.328  -1.082  1.00  0.00           C
ATOM    854  O   VAL D  36      -5.397   2.426   0.089  1.00  0.00           O
ATOM    855  CB  VAL D  36      -3.208   0.632  -0.612  1.00  0.00           C
ATOM    856  CG1 VAL D  36      -4.132  -0.574  -0.831  1.00  0.00           C
ATOM    857  CG2 VAL D  36      -1.876   0.122  -1.169  1.00  0.00           C
ATOM    858  H   VAL D  36      -2.298   2.992  -0.331  1.00  0.00           H
ATOM    859  N   GLY D  37      -5.814   2.708  -2.092  1.00  0.00           N
ATOM    860  CA  GLY D  37      -7.134   3.316  -1.878  1.00  0.00           C
ATOM    861  C   GLY D  37      -7.394   4.596  -2.675  1.00  0.00           C
ATOM    862  O   GLY D  37      -7.096   4.688  -3.867  1.00  0.00           O
ATOM    863  H   GLY D  37      -5.576   2.488  -3.046  1.00  0.00           H
ATOM    864  N   GLY D  38      -7.916   5.536  -1.901  1.00  0.00           N
ATOM    865  CA  GLY D  38      -8.123   6.919  -2.341  1.00  0.00           C
ATOM    866  C   GLY D  38      -9.480   7.509  -1.950  1.00  0.00           C
ATOM    867  O   GLY D  38      -9.594   7.902  -0.787  1.00  0.00           O
ATOM    868  H   GLY D  38      -7.897   5.421  -0.906  1.00  0.00           H
ATOM    869  N   VAL D  39     -10.404   7.458  -2.900  1.00  0.00           N
ATOM    870  CA  VAL D  39     -11.773   7.912  -2.627  1.00  0.00           C
ATOM    871  C   VAL D  39     -12.631   6.645  -2.614  1.00  0.00           C
ATOM    872  O   VAL D  39     -12.706   5.988  -3.654  1.00  0.00           O
ATOM    873  CB  VAL D  39     -12.126   8.930  -3.710  1.00  0.00           C
ATOM    874  CG1 VAL D  39     -13.480   9.614  -3.498  1.00  0.00           C
ATOM    875  CG2 VAL D  39     -11.082  10.024  -3.861  1.00  0.00           C
ATOM    876  H   VAL D  39     -10.220   7.357  -3.883  1.00  0.00           H
ATOM    877  N   VAL D  40     -13.246   6.370  -1.472  1.00  0.00           N
ATOM    878  CA  VAL D  40     -13.945   5.110  -1.170  1.00  0.00           C
ATOM    879  C   VAL D  40     -15.462   5.338  -1.147  1.00  0.00           C
ATOM    880  O   VAL D  40     -16.030   6.006  -0.283  1.00  0.00           O
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ATOM    881  CB  VAL D  40     -13.383   4.383   0.050  1.00  0.00           C
ATOM    882  CG1 VAL D  40     -14.026   3.003   0.249  1.00  0.00           C
ATOM    883  CG2 VAL D  40     -11.875   4.116  -0.068  1.00  0.00           C
ATOM    884  H   VAL D  40     -13.231   7.037  -0.726  1.00  0.00           H
ATOM    885  N   ILE D  41     -16.053   4.969  -2.284  1.00  0.00           N
ATOM    886  CA  ILE D  41     -17.492   5.189  -2.516  1.00  0.00           C
ATOM    887  C   ILE D  41     -18.290   3.951  -2.094  1.00  0.00           C
ATOM    888  O   ILE D  41     -18.574   3.113  -2.934  1.00  0.00           O
ATOM    889  CB  ILE D  41     -17.739   5.682  -3.947  1.00  0.00           C
ATOM    890  CG1 ILE D  41     -16.971   6.979  -4.176  1.00  0.00           C
ATOM    891  CG2 ILE D  41     -19.214   5.965  -4.260  1.00  0.00           C
ATOM    892  CD  ILE D  41     -16.537   7.133  -5.637  1.00  0.00           C
ATOM    893  H   ILE D  41     -15.524   4.610  -3.049  1.00  0.00           H
ATOM    894  N   ALA D  42     -18.712   4.002  -0.831  1.00  0.00           N
ATOM    895  CA  ALA D  42     -19.182   2.888   0.007  1.00  0.00           C
ATOM    896  C   ALA D  42     -20.671   2.726   0.311  1.00  0.00           C
ATOM    897  CB  ALA D  42     -18.373   2.789   1.302  1.00  0.00           C
ATOM    898  O1  ALA D  42     -21.445   3.694   0.203  1.00  0.00           O
ATOM    899  O2  ALA D  42     -21.047   1.785   1.036  1.00  0.00           O
ATOM    900  H   ALA D  42     -18.679   4.906  -0.412  1.00  0.00           H
ATOM    901  N   LEU E  17     -16.118  -6.141 -11.299  1.00  0.00           N
ATOM    902  CA  LEU E  17     -14.948  -5.402 -11.797  1.00  0.00           C
ATOM    903  C   LEU E  17     -13.641  -5.621 -11.044  1.00  0.00           C
ATOM    904  O   LEU E  17     -13.229  -4.856 -10.174  1.00  0.00           O
ATOM    905  CB  LEU E  17     -15.390  -3.969 -12.098  1.00  0.00           C
ATOM    906  CG  LEU E  17     -14.486  -3.289 -13.126  1.00  0.00           C
ATOM    907  CD1 LEU E  17     -14.673  -3.795 -14.556  1.00  0.00           C
ATOM    908  CD2 LEU E  17     -14.876  -1.807 -13.081  1.00  0.00           C
ATOM    909  H1  LEU E  17     -16.905  -5.703 -11.720  1.00  0.00           H
ATOM    910  H2  LEU E  17     -16.155  -7.097 -11.598  1.00  0.00           H
ATOM    911  H3  LEU E  17     -16.169  -6.146 -10.302  1.00  0.00           H
ATOM    912  N   VAL E  18     -12.780  -6.494 -11.565  1.00  0.00           N
ATOM    913  CA  VAL E  18     -11.441  -6.727 -10.992  1.00  0.00           C
ATOM    914  C   VAL E  18     -10.230  -6.327 -11.828  1.00  0.00           C
ATOM    915  O   VAL E  18     -10.249  -6.177 -13.052  1.00  0.00           O
ATOM    916  CB  VAL E  18     -11.292  -8.140 -10.423  1.00  0.00           C
ATOM    917  CG1 VAL E  18     -12.259  -8.495  -9.297  1.00  0.00           C
ATOM    918  CG2 VAL E  18     -11.467  -9.124 -11.576  1.00  0.00           C
ATOM    919  H   VAL E  18     -13.016  -7.074 -12.340  1.00  0.00           H
ATOM    920  N   PHE E  19      -9.157  -5.903 -11.160  1.00  0.00           N
ATOM    921  CA  PHE E  19      -7.899  -5.534 -11.809  1.00  0.00           C
ATOM    922  C   PHE E  19      -6.648  -6.248 -11.292  1.00  0.00           C
ATOM    923  O   PHE E  19      -6.168  -6.221 -10.162  1.00  0.00           O
ATOM    924  CB  PHE E  19      -7.590  -4.034 -11.777  1.00  0.00           C
ATOM    925  CG  PHE E  19      -6.624  -3.479 -12.825  1.00  0.00           C
ATOM    926  CD1 PHE E  19      -6.691  -3.934 -14.145  1.00  0.00           C
ATOM    927  CD2 PHE E  19      -5.632  -2.591 -12.430  1.00  0.00           C
ATOM    928  CE1 PHE E  19      -5.733  -3.513 -15.059  1.00  0.00           C
ATOM    929  CE2 PHE E  19      -4.675  -2.226 -13.364  1.00  0.00           C
ATOM    930  CZ  PHE E  19      -4.676  -2.707 -14.671  1.00  0.00           C
ATOM    931  H   PHE E  19      -9.154  -5.606 -10.207  1.00  0.00           H
ATOM    932  HD1 PHE E  19      -7.589  -4.466 -14.433  1.00  0.00           H
ATOM    933  HD2 PHE E  19      -5.540  -2.253 -11.395  1.00  0.00           H
ATOM    934  HE1 PHE E  19      -5.800  -3.778 -16.117  1.00  0.00           H
ATOM    935  HE2 PHE E  19      -3.835  -1.631 -13.005  1.00  0.00           H
ATOM    936  HZ  PHE E  19      -3.892  -2.372 -15.351  1.00  0.00           H
ATOM    937  N   PHE E  20      -6.121  -7.127 -12.137  1.00  0.00           N
ATOM    938  CA  PHE E  20      -4.827  -7.792 -11.925  1.00  0.00           C
ATOM    939  C   PHE E  20      -3.647  -7.042 -12.557  1.00  0.00           C
ATOM    940  O   PHE E  20      -3.179  -7.394 -13.635  1.00  0.00           O
ATOM    941  CB  PHE E  20      -5.028  -9.262 -12.270  1.00  0.00           C
ATOM    942  CG  PHE E  20      -5.659  -9.984 -11.069  1.00  0.00           C
ATOM    943  CD1 PHE E  20      -7.039 -10.131 -11.096  1.00  0.00           C
ATOM    944  CD2 PHE E  20      -4.823 -10.642 -10.174  1.00  0.00           C
ATOM    945  CE1 PHE E  20      -7.633 -10.763 -10.014  1.00  0.00           C
ATOM    946  CE2 PHE E  20      -5.429 -11.405  -9.180  1.00  0.00           C
ATOM    947  CZ  PHE E  20      -6.822 -11.458  -9.132  1.00  0.00           C
ATOM    948  H   PHE E  20      -6.627  -7.367 -12.975  1.00  0.00           H
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ATOM    949  HD1 PHE E  20      -7.676  -9.527 -11.743  1.00  0.00           H
ATOM    950  HD2 PHE E  20      -3.747 -10.630 -10.349  1.00  0.00           H
ATOM    951  HE1 PHE E  20      -8.710 -10.912  -9.917  1.00  0.00           H
ATOM    952  HE2 PHE E  20      -4.753 -11.866  -8.468  1.00  0.00           H
ATOM    953  HZ  PHE E  20      -7.233 -12.144  -8.391  1.00  0.00           H
ATOM    954  N   ALA E  21      -3.044  -6.303 -11.627  1.00  0.00           N
ATOM    955  CA  ALA E  21      -1.975  -5.347 -11.947  1.00  0.00           C
ATOM    956  C   ALA E  21      -0.635  -5.969 -11.540  1.00  0.00           C
ATOM    957  O   ALA E  21      -0.319  -6.206 -10.379  1.00  0.00           O
ATOM    958  CB  ALA E  21      -2.298  -4.126 -11.086  1.00  0.00           C
ATOM    959  H   ALA E  21      -3.432  -6.273 -10.707  1.00  0.00           H
ATOM    960  N   GLU E  22       0.125  -6.191 -12.609  1.00  0.00           N
ATOM    961  CA  GLU E  22       1.379  -6.942 -12.492  1.00  0.00           C
ATOM    962  C   GLU E  22       2.574  -6.220 -13.119  1.00  0.00           C
ATOM    963  O   GLU E  22       2.689  -6.302 -14.337  1.00  0.00           O
ATOM    964  CB  GLU E  22       1.160  -8.202 -13.341  1.00  0.00           C
ATOM    965  CG  GLU E  22       2.271  -9.246 -13.269  1.00  0.00           C
ATOM    966  CD  GLU E  22       1.990 -10.498 -14.118  1.00  0.00           C
ATOM    967  OE1 GLU E  22       2.054 -11.624 -13.587  1.00  0.00           O
ATOM    968  OE2 GLU E  22       1.850 -10.416 -15.358  1.00  0.00           O1-
ATOM    969  H   GLU E  22      -0.262  -6.217 -13.538  1.00  0.00           H
ATOM    970  N   ASP E  23       3.464  -5.736 -12.254  1.00  0.00           N
ATOM    971  CA  ASP E  23       4.682  -4.978 -12.574  1.00  0.00           C
ATOM    972  C   ASP E  23       5.904  -5.799 -12.169  1.00  0.00           C
ATOM    973  O   ASP E  23       6.034  -6.120 -10.989  1.00  0.00           O
ATOM    974  CB  ASP E  23       4.676  -3.575 -11.967  1.00  0.00           C
ATOM    975  CG  ASP E  23       5.776  -2.599 -12.393  1.00  0.00           C
ATOM    976  OD1 ASP E  23       6.824  -3.042 -12.903  1.00  0.00           O
ATOM    977  OD2 ASP E  23       5.621  -1.364 -12.240  1.00  0.00           O1-
ATOM    978  H   ASP E  23       3.458  -6.062 -11.313  1.00  0.00           H
ATOM    979  N   VAL E  24       6.839  -5.708 -13.115  1.00  0.00           N
ATOM    980  CA  VAL E  24       8.169  -6.345 -13.081  1.00  0.00           C
ATOM    981  C   VAL E  24       9.360  -5.429 -13.357  1.00  0.00           C
ATOM    982  O   VAL E  24       9.770  -5.202 -14.485  1.00  0.00           O
ATOM    983  CB  VAL E  24       8.265  -7.640 -13.882  1.00  0.00           C
ATOM    984  CG1 VAL E  24       7.524  -8.732 -13.091  1.00  0.00           C
ATOM    985  CG2 VAL E  24       7.718  -7.450 -15.302  1.00  0.00           C
ATOM    986  H   VAL E  24       6.837  -4.855 -13.621  1.00  0.00           H
ATOM    987  N   GLY E  25      10.139  -5.066 -12.345  1.00  0.00           N
ATOM    988  CA  GLY E  25      11.227  -4.092 -12.466  1.00  0.00           C
ATOM    989  C   GLY E  25      12.507  -4.505 -11.728  1.00  0.00           C
ATOM    990  O   GLY E  25      12.500  -4.799 -10.539  1.00  0.00           O
ATOM    991  H   GLY E  25       9.834  -5.147 -11.388  1.00  0.00           H
ATOM    992  N   SER E  26      13.659  -4.397 -12.399  1.00  0.00           N
ATOM    993  CA  SER E  26      15.038  -4.366 -11.895  1.00  0.00           C
ATOM    994  C   SER E  26      15.569  -2.961 -12.187  1.00  0.00           C
ATOM    995  O   SER E  26      15.461  -2.527 -13.337  1.00  0.00           O
ATOM    996  CB  SER E  26      16.025  -5.193 -12.711  1.00  0.00           C
ATOM    997  OG  SER E  26      15.976  -6.621 -12.611  1.00  0.00           O
ATOM    998  H   SER E  26      13.555  -4.380 -13.394  1.00  0.00           H
ATOM    999  HG  SER E  26      15.960  -7.055 -13.510  1.00  0.00           H
ATOM   1000  N   ASN E  27      15.582  -2.176 -11.106  1.00  0.00           N
ATOM   1001  CA  ASN E  27      15.890  -0.729 -11.085  1.00  0.00           C
ATOM   1002  C   ASN E  27      14.678   0.206 -11.134  1.00  0.00           C
ATOM   1003  O   ASN E  27      14.220   0.575 -12.212  1.00  0.00           O
ATOM   1004  CB  ASN E  27      17.011  -0.258 -12.012  1.00  0.00           C
ATOM   1005  CG  ASN E  27      18.376  -0.494 -11.358  1.00  0.00           C
ATOM   1006  ND2 ASN E  27      18.931   0.529 -10.711  1.00  0.00           N
ATOM   1007  OD1 ASN E  27      18.822  -1.641 -11.322  1.00  0.00           O
ATOM   1008  H   ASN E  27      15.272  -2.410 -10.193  1.00  0.00           H
ATOM   1009 1HD2 ASN E  27      18.590   1.459 -10.682  1.00  0.00           H
ATOM   1010 2HD2 ASN E  27      19.734   0.268 -10.179  1.00  0.00           H
ATOM   1011  N   LYS E  28      14.165   0.456  -9.935  1.00  0.00           N
ATOM   1012  CA  LYS E  28      13.177   1.503  -9.644  1.00  0.00           C
ATOM   1013  C   LYS E  28      13.889   2.741  -9.120  1.00  0.00           C
ATOM   1014  O   LYS E  28      14.401   2.926  -8.009  1.00  0.00           O
ATOM   1015  CB  LYS E  28      12.170   0.934  -8.632  1.00  0.00           C
ATOM   1016  CG  LYS E  28      11.334  -0.234  -9.155  1.00  0.00           C
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ATOM   1017  CD  LYS E  28      10.265   0.352 -10.081  1.00  0.00           C
ATOM   1018  CE  LYS E  28       9.188  -0.640 -10.507  1.00  0.00           C
ATOM   1019  NZ  LYS E  28       8.416  -0.139 -11.660  1.00  0.00           N1+
ATOM   1020  H   LYS E  28      14.528   0.015  -9.116  1.00  0.00           H
ATOM   1021  HZ1 LYS E  28       7.756   0.529 -11.302  1.00  0.00           H
ATOM   1022  HZ2 LYS E  28       9.056   0.141 -12.377  1.00  0.00           H
ATOM   1023  HZ3 LYS E  28       7.880  -0.922 -11.954  1.00  0.00           H
ATOM   1024  N   GLY E  29      14.128   3.625 -10.084  1.00  0.00           N
ATOM   1025  CA  GLY E  29      14.752   4.923  -9.832  1.00  0.00           C
ATOM   1026  C   GLY E  29      13.971   5.955  -9.017  1.00  0.00           C
ATOM   1027  O   GLY E  29      12.775   6.198  -9.209  1.00  0.00           O
ATOM   1028  H   GLY E  29      13.674   3.479 -10.970  1.00  0.00           H
ATOM   1029  N   ALA E  30      14.737   6.620  -8.160  1.00  0.00           N
ATOM   1030  CA  ALA E  30      14.407   7.725  -7.238  1.00  0.00           C
ATOM   1031  C   ALA E  30      13.029   7.851  -6.581  1.00  0.00           C
ATOM   1032  O   ALA E  30      12.831   7.772  -5.363  1.00  0.00           O
ATOM   1033  CB  ALA E  30      14.782   9.005  -7.971  1.00  0.00           C
ATOM   1034  H   ALA E  30      15.628   6.201  -7.989  1.00  0.00           H
ATOM   1035  N   ILE E  31      12.052   8.061  -7.454  1.00  0.00           N
ATOM   1036  CA  ILE E  31      10.678   8.485  -7.175  1.00  0.00           C
ATOM   1037  C   ILE E  31       9.768   7.411  -7.784  1.00  0.00           C
ATOM   1038  O   ILE E  31       9.337   7.328  -8.935  1.00  0.00           O
ATOM   1039  CB  ILE E  31      10.365   9.800  -7.885  1.00  0.00           C
ATOM   1040  CG1 ILE E  31      11.372  10.887  -7.495  1.00  0.00           C
ATOM   1041  CG2 ILE E  31       8.957  10.273  -7.523  1.00  0.00           C
ATOM   1042  CD  ILE E  31      11.312  12.185  -8.290  1.00  0.00           C
ATOM   1043  H   ILE E  31      12.227   7.548  -8.303  1.00  0.00           H
ATOM   1044  N   ILE E  32       9.258   6.531  -6.914  1.00  0.00           N
ATOM   1045  CA  ILE E  32       8.365   5.409  -7.220  1.00  0.00           C
ATOM   1046  C   ILE E  32       7.129   5.335  -6.319  1.00  0.00           C
ATOM   1047  O   ILE E  32       7.163   4.786  -5.218  1.00  0.00           O
ATOM   1048  CB  ILE E  32       9.132   4.080  -7.282  1.00  0.00           C
ATOM   1049  CG1 ILE E  32      10.135   3.749  -6.175  1.00  0.00           C
ATOM   1050  CG2 ILE E  32       9.728   3.875  -8.675  1.00  0.00           C
ATOM   1051  CD  ILE E  32      11.532   4.348  -6.360  1.00  0.00           C
ATOM   1052  H   ILE E  32       9.597   6.487  -5.981  1.00  0.00           H
ATOM   1053  N   GLY E  33       6.119   6.011  -6.846  1.00  0.00           N
ATOM   1054  CA  GLY E  33       4.802   6.078  -6.181  1.00  0.00           C
ATOM   1055  C   GLY E  33       3.686   5.272  -6.862  1.00  0.00           C
ATOM   1056  O   GLY E  33       3.273   5.680  -7.938  1.00  0.00           O
ATOM   1057  H   GLY E  33       6.323   6.744  -7.499  1.00  0.00           H
ATOM   1058  N   LEU E  34       3.309   4.118  -6.303  1.00  0.00           N
ATOM   1059  CA  LEU E  34       2.285   3.233  -6.881  1.00  0.00           C
ATOM   1060  C   LEU E  34       0.874   3.448  -6.330  1.00  0.00           C
ATOM   1061  O   LEU E  34       0.701   3.458  -5.108  1.00  0.00           O
ATOM   1062  CB  LEU E  34       2.705   1.766  -6.878  1.00  0.00           C
ATOM   1063  CG  LEU E  34       1.765   0.773  -7.581  1.00  0.00           C
ATOM   1064  CD1 LEU E  34       1.954   0.800  -9.095  1.00  0.00           C
ATOM   1065  CD2 LEU E  34       1.893  -0.646  -7.031  1.00  0.00           C
ATOM   1066  H   LEU E  34       3.696   3.846  -5.423  1.00  0.00           H
ATOM   1067  N   MET E  35      -0.007   3.913  -7.210  1.00  0.00           N
ATOM   1068  CA  MET E  35      -1.406   4.173  -6.831  1.00  0.00           C
ATOM   1069  C   MET E  35      -2.325   3.031  -7.285  1.00  0.00           C
ATOM   1070  O   MET E  35      -2.392   2.625  -8.441  1.00  0.00           O
ATOM   1071  CB  MET E  35      -1.852   5.544  -7.374  1.00  0.00           C
ATOM   1072  CG  MET E  35      -2.434   6.286  -6.178  1.00  0.00           C
ATOM   1073  SD  MET E  35      -4.004   5.532  -5.615  1.00  0.00           S
ATOM   1074  CE  MET E  35      -4.696   6.856  -4.640  1.00  0.00           C
ATOM   1075  H   MET E  35       0.253   4.070  -8.159  1.00  0.00           H
ATOM   1076  N   VAL E  36      -2.869   2.458  -6.214  1.00  0.00           N
ATOM   1077  CA  VAL E  36      -3.723   1.265  -6.255  1.00  0.00           C
ATOM   1078  C   VAL E  36      -5.142   1.730  -5.921  1.00  0.00           C
ATOM   1079  O   VAL E  36      -5.443   2.181  -4.813  1.00  0.00           O
ATOM   1080  CB  VAL E  36      -3.327   0.290  -5.150  1.00  0.00           C
ATOM   1081  CG1 VAL E  36      -3.837  -1.108  -5.509  1.00  0.00           C
ATOM   1082  CG2 VAL E  36      -1.811   0.189  -4.971  1.00  0.00           C
ATOM   1083  H   VAL E  36      -2.734   2.903  -5.331  1.00  0.00           H
ATOM   1084  N   GLY E  37      -5.803   2.088  -7.012  1.00  0.00           N
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ATOM   1085  CA  GLY E  37      -7.260   2.333  -6.963  1.00  0.00           C
ATOM   1086  C   GLY E  37      -7.558   3.726  -7.535  1.00  0.00           C
ATOM   1087  O   GLY E  37      -7.583   3.906  -8.754  1.00  0.00           O
ATOM   1088  H   GLY E  37      -5.225   2.480  -7.726  1.00  0.00           H
ATOM   1089  N   GLY E  38      -7.611   4.705  -6.639  1.00  0.00           N
ATOM   1090  CA  GLY E  38      -8.042   6.062  -6.977  1.00  0.00           C
ATOM   1091  C   GLY E  38      -9.509   6.293  -6.631  1.00  0.00           C
ATOM   1092  O   GLY E  38      -9.801   6.548  -5.469  1.00  0.00           O
ATOM   1093  H   GLY E  38      -7.244   4.614  -5.709  1.00  0.00           H
ATOM   1094  N   VAL E  39     -10.341   6.442  -7.660  1.00  0.00           N
ATOM   1095  CA  VAL E  39     -11.787   6.368  -7.373  1.00  0.00           C
ATOM   1096  C   VAL E  39     -12.338   4.939  -7.320  1.00  0.00           C
ATOM   1097  O   VAL E  39     -12.425   4.291  -8.361  1.00  0.00           O
ATOM   1098  CB  VAL E  39     -12.464   7.210  -8.457  1.00  0.00           C
ATOM   1099  CG1 VAL E  39     -13.984   7.290  -8.266  1.00  0.00           C
ATOM   1100  CG2 VAL E  39     -11.843   8.591  -8.686  1.00  0.00           C
ATOM   1101  H   VAL E  39     -10.076   6.191  -8.588  1.00  0.00           H
ATOM   1102  N   VAL E  40     -12.618   4.538  -6.083  1.00  0.00           N
ATOM   1103  CA  VAL E  40     -13.084   3.189  -5.721  1.00  0.00           C
ATOM   1104  C   VAL E  40     -14.531   3.074  -5.244  1.00  0.00           C
ATOM   1105  O   VAL E  40     -15.009   3.845  -4.422  1.00  0.00           O
ATOM   1106  CB  VAL E  40     -12.027   2.543  -4.825  1.00  0.00           C
ATOM   1107  CG1 VAL E  40     -12.383   1.149  -4.306  1.00  0.00           C
ATOM   1108  CG2 VAL E  40     -10.612   2.520  -5.409  1.00  0.00           C
ATOM   1109  H   VAL E  40     -12.377   5.138  -5.322  1.00  0.00           H
ATOM   1110  N   ILE E  41     -15.270   2.372  -6.106  1.00  0.00           N
ATOM   1111  CA  ILE E  41     -16.678   1.990  -5.969  1.00  0.00           C
ATOM   1112  C   ILE E  41     -16.710   0.541  -5.469  1.00  0.00           C
ATOM   1113  O   ILE E  41     -15.954  -0.304  -5.951  1.00  0.00           O
ATOM   1114  CB  ILE E  41     -17.490   2.227  -7.237  1.00  0.00           C
ATOM   1115  CG1 ILE E  41     -17.977   3.676  -7.214  1.00  0.00           C
ATOM   1116  CG2 ILE E  41     -18.640   1.230  -7.365  1.00  0.00           C
ATOM   1117  CD  ILE E  41     -17.285   4.349  -8.408  1.00  0.00           C
ATOM   1118  H   ILE E  41     -14.946   2.243  -7.047  1.00  0.00           H
ATOM   1119  N   ALA E  42     -17.340   0.411  -4.311  1.00  0.00           N
ATOM   1120  CA  ALA E  42     -17.511  -0.893  -3.651  1.00  0.00           C
ATOM   1121  C   ALA E  42     -18.471  -1.916  -4.267  1.00  0.00           C
ATOM   1122  CB  ALA E  42     -17.825  -0.642  -2.183  1.00  0.00           C
ATOM   1123  O1  ALA E  42     -18.196  -3.077  -3.878  1.00  0.00           O
ATOM   1124  O2  ALA E  42     -19.333  -1.661  -5.131  1.00  0.00           O
ATOM   1125  H   ALA E  42     -17.867   1.114  -3.831  1.00  0.00           H
END
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4. $A\beta_{42}$ protofibril-6n complex

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ATOM      1  N   LEU A  17     -13.204  -1.422   8.141  1.00  0.00           N
ATOM      2  CA  LEU A  17     -12.511  -2.613   7.643  1.00  0.00           C
ATOM      3  C   LEU A  17     -11.377  -2.873   8.637  1.00  0.00           C
ATOM      4  O   LEU A  17     -10.707  -2.002   9.189  1.00  0.00           O
ATOM      5  CB  LEU A  17     -11.945  -2.529   6.215  1.00  0.00           C
ATOM      6  CG  LEU A  17     -13.006  -2.216   5.160  1.00  0.00           C
ATOM      7  CD1 LEU A  17     -12.257  -1.332   4.161  1.00  0.00           C
ATOM      8  CD2 LEU A  17     -13.490  -3.531   4.547  1.00  0.00           C
ATOM      9  H1  LEU A  17     -14.151  -1.635   8.375  1.00  0.00           H
ATOM     10  H2  LEU A  17     -12.788  -1.106   8.995  1.00  0.00           H
ATOM     11  H3  LEU A  17     -13.142  -0.686   7.471  1.00  0.00           H
ATOM     12  N   VAL A  18     -11.030  -4.156   8.662  1.00  0.00           N
ATOM     13  CA  VAL A  18      -9.890  -4.505   9.527  1.00  0.00           C
ATOM     14  C   VAL A  18      -8.644  -4.376   8.645  1.00  0.00           C
ATOM     15  O   VAL A  18      -8.417  -5.222   7.786  1.00  0.00           O
ATOM     16  CB  VAL A  18      -9.950  -5.927  10.082  1.00  0.00           C
ATOM     17  CG1 VAL A  18      -8.783  -6.197  11.045  1.00  0.00           C
ATOM     18  CG2 VAL A  18     -11.282  -6.207  10.778  1.00  0.00           C
ATOM     19  H   VAL A  18     -11.509  -4.813   8.080  1.00  0.00           H
ATOM     20  N   PHE A  19      -8.049  -3.197   8.725  1.00  0.00           N
ATOM     21  CA  PHE A  19      -6.735  -2.893   8.127  1.00  0.00           C
ATOM     22  C   PHE A  19      -5.566  -3.607   8.812  1.00  0.00           C
ATOM     23  O   PHE A  19      -5.242  -3.460   9.981  1.00  0.00           O
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ATOM     24  CB  PHE A  19      -6.434  -1.396   7.994  1.00  0.00           C
ATOM     25  CG  PHE A  19      -7.439  -0.432   7.361  1.00  0.00           C
ATOM     26  CD1 PHE A  19      -8.375   0.222   8.158  1.00  0.00           C
ATOM     27  CD2 PHE A  19      -7.413  -0.308   5.972  1.00  0.00           C
ATOM     28  CE1 PHE A  19      -9.313   1.008   7.502  1.00  0.00           C
ATOM     29  CE2 PHE A  19      -8.393   0.462   5.370  1.00  0.00           C
ATOM     30  CZ  PHE A  19      -9.335   1.171   6.118  1.00  0.00           C
ATOM     31  H   PHE A  19      -8.370  -2.542   9.409  1.00  0.00           H
ATOM     32  HD1 PHE A  19      -8.493   0.045   9.218  1.00  0.00           H
ATOM     33  HD2 PHE A  19      -6.655  -0.760   5.344  1.00  0.00           H
ATOM     34  HE1 PHE A  19      -9.848   1.666   8.185  1.00  0.00           H
ATOM     35  HE2 PHE A  19      -8.503   0.303   4.296  1.00  0.00           H
ATOM     36  HZ  PHE A  19     -10.198   1.629   5.643  1.00  0.00           H
ATOM     37  N   PHE A  20      -4.911  -4.509   8.090  1.00  0.00           N
ATOM     38  CA  PHE A  20      -3.753  -5.280   8.569  1.00  0.00           C
ATOM     39  C   PHE A  20      -2.487  -5.027   7.746  1.00  0.00           C
ATOM     40  O   PHE A  20      -2.503  -4.820   6.537  1.00  0.00           O
ATOM     41  CB  PHE A  20      -4.083  -6.766   8.420  1.00  0.00           C
ATOM     42  CG  PHE A  20      -5.011  -7.344   9.495  1.00  0.00           C
ATOM     43  CD1 PHE A  20      -5.761  -8.420   9.046  1.00  0.00           C
ATOM     44  CD2 PHE A  20      -4.970  -6.993  10.841  1.00  0.00           C
ATOM     45  CE1 PHE A  20      -6.401  -9.225   9.973  1.00  0.00           C
ATOM     46  CE2 PHE A  20      -5.637  -7.783  11.766  1.00  0.00           C
ATOM     47  CZ  PHE A  20      -6.392  -8.868  11.318  1.00  0.00           C
ATOM     48  H   PHE A  20      -5.186  -4.730   7.156  1.00  0.00           H
ATOM     49  HD1 PHE A  20      -5.962  -8.596   7.987  1.00  0.00           H
ATOM     50  HD2 PHE A  20      -4.815  -5.958  11.106  1.00  0.00           H
ATOM     51  HE1 PHE A  20      -6.827 -10.190   9.703  1.00  0.00           H
ATOM     52  HE2 PHE A  20      -5.649  -7.545  12.834  1.00  0.00           H
ATOM     53  HZ  PHE A  20      -6.850  -9.589  11.997  1.00  0.00           H
ATOM     54  N   ALA A  21      -1.326  -5.131   8.391  1.00  0.00           N
ATOM     55  CA  ALA A  21       0.031  -4.946   7.853  1.00  0.00           C
ATOM     56  C   ALA A  21       1.056  -5.902   8.460  1.00  0.00           C
ATOM     57  O   ALA A  21       1.275  -5.830   9.667  1.00  0.00           O
ATOM     58  CB  ALA A  21       0.480  -3.489   8.020  1.00  0.00           C
ATOM     59  H   ALA A  21      -1.316  -5.490   9.318  1.00  0.00           H
ATOM     60  N   GLU A  22       1.769  -6.584   7.570  1.00  0.00           N
ATOM     61  CA  GLU A  22       2.877  -7.514   7.873  1.00  0.00           C
ATOM     62  C   GLU A  22       4.177  -7.074   7.199  1.00  0.00           C
ATOM     63  O   GLU A  22       4.124  -6.506   6.111  1.00  0.00           O
ATOM     64  CB  GLU A  22       2.618  -8.981   7.558  1.00  0.00           C
ATOM     65  CG  GLU A  22       1.579  -9.660   8.465  1.00  0.00           C
ATOM     66  CD  GLU A  22       2.086  -9.726   9.911  1.00  0.00           C
ATOM     67  OE1 GLU A  22       1.231  -9.564  10.801  1.00  0.00           O
ATOM     68  OE2 GLU A  22       3.236 -10.174  10.117  1.00  0.00           O1-
ATOM     69  H   GLU A  22       1.736  -6.309   6.616  1.00  0.00           H
ATOM     70  N   ASP A  23       5.254  -7.146   7.983  1.00  0.00           N
ATOM     71  CA  ASP A  23       6.620  -6.890   7.495  1.00  0.00           C
ATOM     72  C   ASP A  23       7.499  -8.142   7.629  1.00  0.00           C
ATOM     73  O   ASP A  23       7.571  -8.899   8.594  1.00  0.00           O
ATOM     74  CB  ASP A  23       7.299  -5.716   8.195  1.00  0.00           C
ATOM     75  CG  ASP A  23       7.714  -6.032   9.632  1.00  0.00           C
ATOM     76  OD1 ASP A  23       6.835  -6.089  10.515  1.00  0.00           O
ATOM     77  OD2 ASP A  23       8.923  -5.960   9.923  1.00  0.00           O1-
ATOM     78  H   ASP A  23       5.205  -7.220   8.983  1.00  0.00           H
ATOM     79  N   VAL A  24       8.192  -8.317   6.504  1.00  0.00           N
ATOM     80  CA  VAL A  24       9.177  -9.378   6.289  1.00  0.00           C
ATOM     81  C   VAL A  24      10.508  -8.761   5.848  1.00  0.00           C
ATOM     82  O   VAL A  24      10.701  -8.324   4.719  1.00  0.00           O
ATOM     83  CB  VAL A  24       8.738 -10.449   5.293  1.00  0.00           C
ATOM     84  CG1 VAL A  24       9.863 -11.447   5.018  1.00  0.00           C
ATOM     85  CG2 VAL A  24       7.498 -11.250   5.684  1.00  0.00           C
ATOM     86  H   VAL A  24       8.022  -7.849   5.634  1.00  0.00           H
ATOM     87  N   GLY A  25      11.362  -8.462   6.837  1.00  0.00           N
ATOM     88  CA  GLY A  25      12.672  -7.840   6.600  1.00  0.00           C
ATOM     89  C   GLY A  25      13.695  -8.513   5.684  1.00  0.00           C
ATOM     90  O   GLY A  25      14.635  -9.177   6.144  1.00  0.00           O
ATOM     91  H   GLY A  25      10.995  -8.382   7.754  1.00  0.00           H
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ATOM     92  N   SER A  26      13.309  -8.660   4.429  1.00  0.00           N
ATOM     93  CA  SER A  26      14.187  -9.127   3.340  1.00  0.00           C
ATOM     94  C   SER A  26      15.393  -8.203   3.116  1.00  0.00           C
ATOM     95  O   SER A  26      15.404  -7.079   2.633  1.00  0.00           O
ATOM     96  CB  SER A  26      13.558  -9.238   1.957  1.00  0.00           C
ATOM     97  OG  SER A  26      14.453  -9.769   0.976  1.00  0.00           O
ATOM     98  H   SER A  26      12.357  -8.577   4.129  1.00  0.00           H
ATOM     99  HG  SER A  26      14.098 -10.447   0.327  1.00  0.00           H
ATOM    100  N   ASN A  27      16.510  -8.650   3.696  1.00  0.00           N
ATOM    101  CA  ASN A  27      17.866  -8.120   3.881  1.00  0.00           C
ATOM    102  C   ASN A  27      17.923  -6.972   4.892  1.00  0.00           C
ATOM    103  O   ASN A  27      17.152  -6.027   4.722  1.00  0.00           O
ATOM    104  CB  ASN A  27      18.545  -7.689   2.582  1.00  0.00           C
ATOM    105  CG  ASN A  27      19.105  -8.814   1.707  1.00  0.00           C
ATOM    106  ND2 ASN A  27      20.193  -8.528   0.987  1.00  0.00           N
ATOM    107  OD1 ASN A  27      18.732  -9.979   1.617  1.00  0.00           O
ATOM    108  H   ASN A  27      16.441  -9.493   4.231  1.00  0.00           H
ATOM    109 1HD2 ASN A  27      20.675  -7.660   1.114  1.00  0.00           H
ATOM    110 2HD2 ASN A  27      20.498  -9.236   0.357  1.00  0.00           H
ATOM    111  N   LYS A  28      18.762  -7.040   5.921  1.00  0.00           N
ATOM    112  CA  LYS A  28      19.006  -6.078   7.002  1.00  0.00           C
ATOM    113  C   LYS A  28      17.811  -5.995   7.956  1.00  0.00           C
ATOM    114  O   LYS A  28      17.892  -6.394   9.122  1.00  0.00           O
ATOM    115  CB  LYS A  28      19.482  -4.721   6.484  1.00  0.00           C
ATOM    116  CG  LYS A  28      20.251  -4.023   7.598  1.00  0.00           C
ATOM    117  CD  LYS A  28      20.117  -2.501   7.651  1.00  0.00           C
ATOM    118  CE  LYS A  28      18.758  -2.041   8.181  1.00  0.00           C
ATOM    119  NZ  LYS A  28      18.735  -0.583   8.046  1.00  0.00           N1+
ATOM    120  H   LYS A  28      19.281  -7.881   6.082  1.00  0.00           H
ATOM    121  HZ1 LYS A  28      19.024  -0.224   7.158  1.00  0.00           H
ATOM    122  HZ2 LYS A  28      17.766  -0.401   8.220  1.00  0.00           H
ATOM    123  HZ3 LYS A  28      19.289  -0.307   8.839  1.00  0.00           H
ATOM    124  N   GLY A  29      16.651  -5.770   7.354  1.00  0.00           N
ATOM    125  CA  GLY A  29      15.340  -5.595   8.011  1.00  0.00           C
ATOM    126  C   GLY A  29      15.192  -4.198   8.596  1.00  0.00           C
ATOM    127  O   GLY A  29      16.108  -3.373   8.568  1.00  0.00           O
ATOM    128  H   GLY A  29      16.684  -5.650   6.369  1.00  0.00           H
ATOM    129  N   ALA A  30      14.004  -3.945   9.147  1.00  0.00           N
ATOM    130  CA  ALA A  30      13.657  -2.585   9.580  1.00  0.00           C
ATOM    131  C   ALA A  30      12.926  -2.601  10.921  1.00  0.00           C
ATOM    132  O   ALA A  30      12.404  -3.615  11.406  1.00  0.00           O
ATOM    133  CB  ALA A  30      12.839  -1.905   8.483  1.00  0.00           C
ATOM    134  H   ALA A  30      13.243  -4.586   9.290  1.00  0.00           H
ATOM    135  N   ILE A  31      12.916  -1.472  11.619  1.00  0.00           N
ATOM    136  CA  ILE A  31      12.419  -1.372  12.989  1.00  0.00           C
ATOM    137  C   ILE A  31      10.943  -0.976  12.927  1.00  0.00           C
ATOM    138  O   ILE A  31      10.542  -0.088  12.173  1.00  0.00           O
ATOM    139  CB  ILE A  31      13.264  -0.230  13.548  1.00  0.00           C
ATOM    140  CG1 ILE A  31      14.760  -0.111  13.249  1.00  0.00           C
ATOM    141  CG2 ILE A  31      13.017  -0.225  15.064  1.00  0.00           C
ATOM    142  CD  ILE A  31      15.139   1.331  13.613  1.00  0.00           C
ATOM    143  H   ILE A  31      13.131  -0.557  11.272  1.00  0.00           H
ATOM    144  N   ILE A  32      10.333  -1.107  14.097  1.00  0.00           N
ATOM    145  CA  ILE A  32       8.860  -1.142  14.182  1.00  0.00           C
ATOM    146  C   ILE A  32       8.338   0.268  14.448  1.00  0.00           C
ATOM    147  O   ILE A  32       8.381   0.749  15.578  1.00  0.00           O
ATOM    148  CB  ILE A  32       8.309  -2.118  15.227  1.00  0.00           C
ATOM    149  CG1 ILE A  32       8.761  -3.537  14.866  1.00  0.00           C
ATOM    150  CG2 ILE A  32       6.797  -2.110  14.971  1.00  0.00           C
ATOM    151  CD  ILE A  32       8.785  -4.386  16.134  1.00  0.00           C
ATOM    152  H   ILE A  32      10.797  -1.582  14.840  1.00  0.00           H
ATOM    153  N   GLY A  33       7.787   0.915  13.430  1.00  0.00           N
ATOM    154  CA  GLY A  33       7.057   2.180  13.566  1.00  0.00           C
ATOM    155  C   GLY A  33       5.549   2.036  13.306  1.00  0.00           C
ATOM    156  O   GLY A  33       5.219   1.527  12.237  1.00  0.00           O
ATOM    157  H   GLY A  33       7.932   0.665  12.470  1.00  0.00           H
ATOM    158  N   LEU A  34       4.673   2.454  14.217  1.00  0.00           N
ATOM    159  CA  LEU A  34       3.235   2.189  14.112  1.00  0.00           C
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ATOM    160  C   LEU A  34       2.507   3.539  14.124  1.00  0.00           C
ATOM    161  O   LEU A  34       2.606   4.268  15.107  1.00  0.00           O
ATOM    162  CB  LEU A  34       2.824   1.303  15.285  1.00  0.00           C
ATOM    163  CG  LEU A  34       1.353   0.892  15.322  1.00  0.00           C
ATOM    164  CD1 LEU A  34       0.877  -0.079  14.245  1.00  0.00           C
ATOM    165  CD2 LEU A  34       0.941   0.418  16.721  1.00  0.00           C
ATOM    166  H   LEU A  34       4.970   2.956  15.025  1.00  0.00           H
ATOM    167  N   MET A  35       1.835   3.969  13.054  1.00  0.00           N
ATOM    168  CA  MET A  35       1.106   5.239  12.981  1.00  0.00           C
ATOM    169  C   MET A  35      -0.381   5.012  12.714  1.00  0.00           C
ATOM    170  O   MET A  35      -0.805   4.061  12.059  1.00  0.00           O
ATOM    171  CB  MET A  35       1.661   6.134  11.872  1.00  0.00           C
ATOM    172  CG  MET A  35       3.158   6.441  11.846  1.00  0.00           C
ATOM    173  SD  MET A  35       4.115   5.180  10.919  1.00  0.00           S
ATOM    174  CE  MET A  35       5.788   5.759  11.066  1.00  0.00           C
ATOM    175  H   MET A  35       1.742   3.325  12.290  1.00  0.00           H
ATOM    176  N   VAL A  36      -1.197   5.884  13.315  1.00  0.00           N
ATOM    177  CA  VAL A  36      -2.610   5.837  12.894  1.00  0.00           C
ATOM    178  C   VAL A  36      -2.802   6.637  11.600  1.00  0.00           C
ATOM    179  O   VAL A  36      -1.960   7.408  11.145  1.00  0.00           O
ATOM    180  CB  VAL A  36      -3.479   6.430  14.004  1.00  0.00           C
ATOM    181  CG1 VAL A  36      -3.374   5.733  15.366  1.00  0.00           C
ATOM    182  CG2 VAL A  36      -3.014   7.858  14.281  1.00  0.00           C
ATOM    183  H   VAL A  36      -0.823   6.704  13.742  1.00  0.00           H
ATOM    184  N   GLY A  37      -3.711   6.064  10.820  1.00  0.00           N
ATOM    185  CA  GLY A  37      -4.200   6.827   9.651  1.00  0.00           C
ATOM    186  C   GLY A  37      -5.511   7.531   9.974  1.00  0.00           C
ATOM    187  O   GLY A  37      -5.557   8.272  10.966  1.00  0.00           O
ATOM    188  H   GLY A  37      -4.008   5.113  10.919  1.00  0.00           H
ATOM    189  N   GLY A  38      -6.585   7.263   9.235  1.00  0.00           N
ATOM    190  CA  GLY A  38      -7.990   7.192   9.664  1.00  0.00           C
ATOM    191  C   GLY A  38      -8.773   8.488   9.888  1.00  0.00           C
ATOM    192  O   GLY A  38      -9.975   8.585  10.096  1.00  0.00           O
ATOM    193  H   GLY A  38      -6.477   7.033   8.275  1.00  0.00           H
ATOM    194  N   VAL A  39      -8.010   9.577   9.742  1.00  0.00           N
ATOM    195  CA  VAL A  39      -8.403  10.984   9.597  1.00  0.00           C
ATOM    196  C   VAL A  39      -9.343  11.380   8.457  1.00  0.00           C
ATOM    197  O   VAL A  39      -9.212  10.777   7.390  1.00  0.00           O
ATOM    198  CB  VAL A  39      -7.177  11.902   9.575  1.00  0.00           C
ATOM    199  CG1 VAL A  39      -6.721  12.229  10.990  1.00  0.00           C
ATOM    200  CG2 VAL A  39      -5.888  11.406   8.920  1.00  0.00           C
ATOM    201  H   VAL A  39      -7.059   9.548  10.012  1.00  0.00           H
ATOM    202  N   VAL A  40     -10.082  12.476   8.665  1.00  0.00           N
ATOM    203  CA  VAL A  40     -10.854  13.009   7.531  1.00  0.00           C
ATOM    204  C   VAL A  40     -10.006  13.964   6.682  1.00  0.00           C
ATOM    205  O   VAL A  40      -9.746  15.082   7.137  1.00  0.00           O
ATOM    206  CB  VAL A  40     -12.155  13.623   8.068  1.00  0.00           C
ATOM    207  CG1 VAL A  40     -12.969  14.276   6.959  1.00  0.00           C
ATOM    208  CG2 VAL A  40     -13.021  12.562   8.743  1.00  0.00           C
ATOM    209  H   VAL A  40     -10.336  12.813   9.564  1.00  0.00           H
ATOM    210  N   ILE A  41      -9.884  13.657   5.395  1.00  0.00           N
ATOM    211  CA  ILE A  41      -9.022  14.422   4.487  1.00  0.00           C
ATOM    212  C   ILE A  41      -9.681  15.751   4.125  1.00  0.00           C
ATOM    213  O   ILE A  41     -10.906  15.850   4.090  1.00  0.00           O
ATOM    214  CB  ILE A  41      -8.505  13.662   3.256  1.00  0.00           C
ATOM    215  CG1 ILE A  41      -9.450  12.732   2.500  1.00  0.00           C
ATOM    216  CG2 ILE A  41      -7.216  12.991   3.730  1.00  0.00           C
ATOM    217  CD  ILE A  41     -10.269  13.605   1.542  1.00  0.00           C
ATOM    218  H   ILE A  41     -10.530  13.032   4.954  1.00  0.00           H
ATOM    219  N   ALA A  42      -8.840  16.705   3.746  1.00  0.00           N
ATOM    220  CA  ALA A  42      -9.276  18.084   3.467  1.00  0.00           C
ATOM    221  C   ALA A  42     -10.180  18.406   2.274  1.00  0.00           C
ATOM    222  CB  ALA A  42      -8.095  19.041   3.543  1.00  0.00           C
ATOM    223  O1  ALA A  42      -9.966  17.964   1.124  1.00  0.00           O
ATOM    224  O2  ALA A  42     -10.953  19.361   2.489  1.00  0.00           O
ATOM    225  H   ALA A  42      -7.877  16.533   3.531  1.00  0.00           H
ATOM    226  N   LEU B  17     -13.983  -8.400   7.963  1.00  0.00           N
ATOM    227  CA  LEU B  17     -13.620  -8.107   6.565  1.00  0.00           C
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ATOM    228  C   LEU B  17     -12.277  -7.388   6.487  1.00  0.00           C
ATOM    229  O   LEU B  17     -12.157  -6.495   7.331  1.00  0.00           O
ATOM    230  CB  LEU B  17     -14.717  -7.295   5.882  1.00  0.00           C
ATOM    231  CG  LEU B  17     -14.784  -7.505   4.369  1.00  0.00           C
ATOM    232  CD1 LEU B  17     -14.985  -8.972   3.965  1.00  0.00           C
ATOM    233  CD2 LEU B  17     -15.939  -6.707   3.765  1.00  0.00           C
ATOM    234  H1  LEU B  17     -13.179  -8.810   8.383  1.00  0.00           H
ATOM    235  H2  LEU B  17     -14.199  -7.581   8.507  1.00  0.00           H
ATOM    236  H3  LEU B  17     -14.740  -9.059   7.991  1.00  0.00           H
ATOM    237  N   VAL B  18     -11.300  -8.158   6.019  1.00  0.00           N
ATOM    238  CA  VAL B  18      -9.900  -7.729   5.909  1.00  0.00           C
ATOM    239  C   VAL B  18      -9.630  -6.682   4.831  1.00  0.00           C
ATOM    240  O   VAL B  18     -10.466  -6.467   3.960  1.00  0.00           O
ATOM    241  CB  VAL B  18      -8.920  -8.906   5.829  1.00  0.00           C
ATOM    242  CG1 VAL B  18      -8.984  -9.727   7.112  1.00  0.00           C
ATOM    243  CG2 VAL B  18      -8.908  -9.686   4.512  1.00  0.00           C
ATOM    244  H   VAL B  18     -11.410  -9.029   5.536  1.00  0.00           H
ATOM    245  N   PHE B  19      -8.458  -6.075   5.007  1.00  0.00           N
ATOM    246  CA  PHE B  19      -7.902  -5.139   4.023  1.00  0.00           C
ATOM    247  C   PHE B  19      -6.404  -5.146   4.314  1.00  0.00           C
ATOM    248  O   PHE B  19      -5.950  -4.483   5.246  1.00  0.00           O
ATOM    249  CB  PHE B  19      -8.465  -3.722   4.176  1.00  0.00           C
ATOM    250  CG  PHE B  19      -8.105  -2.703   3.092  1.00  0.00           C
ATOM    251  CD1 PHE B  19      -6.828  -2.173   3.133  1.00  0.00           C
ATOM    252  CD2 PHE B  19      -9.093  -2.206   2.238  1.00  0.00           C
ATOM    253  CE1 PHE B  19      -6.498  -1.265   2.129  1.00  0.00           C
ATOM    254  CE2 PHE B  19      -8.759  -1.217   1.328  1.00  0.00           C
ATOM    255  CZ  PHE B  19      -7.429  -0.820   1.206  1.00  0.00           C
ATOM    256  H   PHE B  19      -8.181  -5.899   5.960  1.00  0.00           H
ATOM    257  HD1 PHE B  19      -6.030  -2.650   3.709  1.00  0.00           H
ATOM    258  HD2 PHE B  19     -10.091  -2.547   2.516  1.00  0.00           H
ATOM    259  HE1 PHE B  19      -5.468  -1.047   1.840  1.00  0.00           H
ATOM    260  HE2 PHE B  19      -9.525  -0.702   0.743  1.00  0.00           H
ATOM    261  HZ  PHE B  19      -7.126  -0.385   0.254  1.00  0.00           H
ATOM    262  N   PHE B  20      -5.662  -5.830   3.446  1.00  0.00           N
ATOM    263  CA  PHE B  20      -4.312  -6.321   3.803  1.00  0.00           C
ATOM    264  C   PHE B  20      -3.126  -5.673   3.092  1.00  0.00           C
ATOM    265  O   PHE B  20      -3.129  -5.462   1.880  1.00  0.00           O
ATOM    266  CB  PHE B  20      -4.161  -7.808   3.495  1.00  0.00           C
ATOM    267  CG  PHE B  20      -3.336  -8.556   4.548  1.00  0.00           C
ATOM    268  CD1 PHE B  20      -3.989  -9.123   5.639  1.00  0.00           C
ATOM    269  CD2 PHE B  20      -1.956  -8.618   4.383  1.00  0.00           C
ATOM    270  CE1 PHE B  20      -3.163  -9.624   6.643  1.00  0.00           C
ATOM    271  CE2 PHE B  20      -1.147  -9.110   5.392  1.00  0.00           C
ATOM    272  CZ  PHE B  20      -1.774  -9.544   6.551  1.00  0.00           C
ATOM    273  H   PHE B  20      -5.945  -6.046   2.515  1.00  0.00           H
ATOM    274  HD1 PHE B  20      -5.038  -9.388   5.673  1.00  0.00           H
ATOM    275  HD2 PHE B  20      -1.509  -8.568   3.394  1.00  0.00           H
ATOM    276  HE1 PHE B  20      -3.556 -10.085   7.548  1.00  0.00           H
ATOM    277  HE2 PHE B  20      -0.064  -9.056   5.293  1.00  0.00           H
ATOM    278  HZ  PHE B  20      -1.147 -10.002   7.322  1.00  0.00           H
ATOM    279  N   ALA B  21      -1.967  -5.535   3.732  1.00  0.00           N
ATOM    280  CA  ALA B  21      -0.732  -5.168   3.023  1.00  0.00           C
ATOM    281  C   ALA B  21       0.443  -5.945   3.611  1.00  0.00           C
ATOM    282  O   ALA B  21       0.593  -5.892   4.827  1.00  0.00           O
ATOM    283  CB  ALA B  21      -0.429  -3.681   3.242  1.00  0.00           C
ATOM    284  H   ALA B  21      -2.008  -5.363   4.713  1.00  0.00           H
ATOM    285  N   GLU B  22       1.354  -6.410   2.751  1.00  0.00           N
ATOM    286  CA  GLU B  22       2.534  -7.147   3.235  1.00  0.00           C
ATOM    287  C   GLU B  22       3.779  -6.588   2.537  1.00  0.00           C
ATOM    288  O   GLU B  22       3.689  -6.170   1.384  1.00  0.00           O
ATOM    289  CB  GLU B  22       2.409  -8.627   2.871  1.00  0.00           C
ATOM    290  CG  GLU B  22       3.311  -9.459   3.786  1.00  0.00           C
ATOM    291  CD  GLU B  22       3.118 -10.980   3.763  1.00  0.00           C
ATOM    292  OE1 GLU B  22       3.796 -11.705   3.007  1.00  0.00           O
ATOM    293  OE2 GLU B  22       2.122 -11.451   4.350  1.00  0.00           O1-
ATOM    294  H   GLU B  22       1.403  -6.323   1.762  1.00  0.00           H
ATOM    295  N   ASP B  23       4.809  -6.456   3.359  1.00  0.00           N
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ATOM    296  CA  ASP B  23       6.062  -5.942   2.783  1.00  0.00           C
ATOM    297  C   ASP B  23       7.129  -7.030   2.939  1.00  0.00           C
ATOM    298  O   ASP B  23       7.753  -7.170   3.996  1.00  0.00           O
ATOM    299  CB  ASP B  23       6.556  -4.649   3.433  1.00  0.00           C
ATOM    300  CG  ASP B  23       7.788  -3.951   2.856  1.00  0.00           C
ATOM    301  OD1 ASP B  23       8.388  -4.595   1.957  1.00  0.00           O
ATOM    302  OD2 ASP B  23       8.183  -2.850   3.313  1.00  0.00           O1-
ATOM    303  H   ASP B  23       4.812  -6.653   4.342  1.00  0.00           H
ATOM    304  N   VAL B  24       7.349  -7.531   1.724  1.00  0.00           N
ATOM    305  CA  VAL B  24       8.386  -8.519   1.413  1.00  0.00           C
ATOM    306  C   VAL B  24       9.401  -7.955   0.416  1.00  0.00           C
ATOM    307  O   VAL B  24      10.137  -8.697  -0.232  1.00  0.00           O
ATOM    308  CB  VAL B  24       7.704  -9.800   0.919  1.00  0.00           C
ATOM    309  CG1 VAL B  24       6.731 -10.357   1.966  1.00  0.00           C
ATOM    310  CG2 VAL B  24       6.889  -9.573  -0.353  1.00  0.00           C
ATOM    311  H   VAL B  24       6.792  -7.238   0.952  1.00  0.00           H
ATOM    312  N   GLY B  25       9.572  -6.648   0.306  1.00  0.00           N
ATOM    313  CA  GLY B  25      10.587  -5.941  -0.490  1.00  0.00           C
ATOM    314  C   GLY B  25      12.040  -6.093  -0.022  1.00  0.00           C
ATOM    315  O   GLY B  25      12.256  -6.111   1.195  1.00  0.00           O
ATOM    316  H   GLY B  25       9.030  -6.016   0.856  1.00  0.00           H
ATOM    317  N   SER B  26      12.910  -5.593  -0.895  1.00  0.00           N
ATOM    318  CA  SER B  26      14.371  -5.754  -0.867  1.00  0.00           C
ATOM    319  C   SER B  26      15.115  -4.607  -0.175  1.00  0.00           C
ATOM    320  O   SER B  26      14.825  -3.425  -0.374  1.00  0.00           O
ATOM    321  CB  SER B  26      14.902  -5.960  -2.279  1.00  0.00           C
ATOM    322  OG  SER B  26      14.131  -6.895  -3.043  1.00  0.00           O
ATOM    323  H   SER B  26      12.598  -4.889  -1.543  1.00  0.00           H
ATOM    324  HG  SER B  26      14.553  -6.911  -3.943  1.00  0.00           H
ATOM    325  N   ASN B  27      16.224  -4.909   0.492  1.00  0.00           N
ATOM    326  CA  ASN B  27      17.314  -4.041   0.967  1.00  0.00           C
ATOM    327  C   ASN B  27      16.837  -2.880   1.850  1.00  0.00           C
ATOM    328  O   ASN B  27      16.716  -1.731   1.436  1.00  0.00           O
ATOM    329  CB  ASN B  27      18.175  -3.504  -0.174  1.00  0.00           C
ATOM    330  CG  ASN B  27      19.068  -4.497  -0.923  1.00  0.00           C
ATOM    331  ND2 ASN B  27      20.376  -4.367  -0.741  1.00  0.00           N
ATOM    332  OD1 ASN B  27      18.587  -5.477  -1.510  1.00  0.00           O
ATOM    333  H   ASN B  27      16.235  -5.779   0.984  1.00  0.00           H
ATOM    334 1HD2 ASN B  27      20.741  -3.645  -0.147  1.00  0.00           H
ATOM    335 2HD2 ASN B  27      20.910  -5.120  -1.114  1.00  0.00           H
ATOM    336  N   LYS B  28      16.313  -3.231   3.022  1.00  0.00           N
ATOM    337  CA  LYS B  28      15.583  -2.301   3.880  1.00  0.00           C
ATOM    338  C   LYS B  28      16.504  -1.415   4.725  1.00  0.00           C
ATOM    339  O   LYS B  28      17.505  -1.832   5.296  1.00  0.00           O
ATOM    340  CB  LYS B  28      14.713  -3.192   4.768  1.00  0.00           C
ATOM    341  CG  LYS B  28      13.668  -3.950   3.939  1.00  0.00           C
ATOM    342  CD  LYS B  28      12.283  -4.026   4.571  1.00  0.00           C
ATOM    343  CE  LYS B  28      11.408  -5.162   4.021  1.00  0.00           C
ATOM    344  NZ  LYS B  28      10.062  -5.092   4.612  1.00  0.00           N1+
ATOM    345  H   LYS B  28      16.414  -4.093   3.520  1.00  0.00           H
ATOM    346  HZ1 LYS B  28      10.243  -5.032   5.592  1.00  0.00           H
ATOM    347  HZ2 LYS B  28       9.598  -4.268   4.301  1.00  0.00           H
ATOM    348  HZ3 LYS B  28       9.583  -5.942   4.381  1.00  0.00           H
ATOM    349  N   GLY B  29      15.959  -0.200   4.818  1.00  0.00           N
ATOM    350  CA  GLY B  29      16.327   0.938   5.678  1.00  0.00           C
ATOM    351  C   GLY B  29      16.035   1.058   7.178  1.00  0.00           C
ATOM    352  O   GLY B  29      16.010   0.082   7.927  1.00  0.00           O
ATOM    353  H   GLY B  29      15.433   0.108   4.037  1.00  0.00           H
ATOM    354  N   ALA B  30      15.755   2.261   7.663  1.00  0.00           N
ATOM    355  CA  ALA B  30      15.450   2.704   9.036  1.00  0.00           C
ATOM    356  C   ALA B  30      14.107   2.159   9.533  1.00  0.00           C
ATOM    357  O   ALA B  30      14.115   1.070  10.095  1.00  0.00           O
ATOM    358  CB  ALA B  30      15.577   4.228   9.150  1.00  0.00           C
ATOM    359  H   ALA B  30      15.754   3.050   7.042  1.00  0.00           H
ATOM    360  N   ILE B  31      13.007   2.829   9.213  1.00  0.00           N
ATOM    361  CA  ILE B  31      11.787   2.331   9.873  1.00  0.00           C
ATOM    362  C   ILE B  31      10.670   1.747   9.017  1.00  0.00           C
ATOM    363  O   ILE B  31      10.242   2.404   8.068  1.00  0.00           O
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ATOM    364  CB  ILE B  31      11.267   3.458  10.758  1.00  0.00           C
ATOM    365  CG1 ILE B  31      11.046   4.829  10.127  1.00  0.00           C
ATOM    366  CG2 ILE B  31      12.022   3.651  12.075  1.00  0.00           C
ATOM    367  CD  ILE B  31      10.133   5.729  10.953  1.00  0.00           C
ATOM    368  H   ILE B  31      12.940   3.608   8.590  1.00  0.00           H
ATOM    369  N   ILE B  32      10.092   0.598   9.380  1.00  0.00           N
ATOM    370  CA  ILE B  32       8.920   0.057   8.695  1.00  0.00           C
ATOM    371  C   ILE B  32       7.694   0.711   9.326  1.00  0.00           C
ATOM    372  O   ILE B  32       7.475   0.540  10.518  1.00  0.00           O
ATOM    373  CB  ILE B  32       8.915  -1.474   8.764  1.00  0.00           C
ATOM    374  CG1 ILE B  32       7.670  -2.087   8.099  1.00  0.00           C
ATOM    375  CG2 ILE B  32       9.242  -2.162  10.084  1.00  0.00           C
ATOM    376  CD  ILE B  32       7.654  -2.085   6.575  1.00  0.00           C
ATOM    377  H   ILE B  32      10.541   0.146  10.149  1.00  0.00           H
ATOM    378  N   GLY B  33       7.312   1.809   8.662  1.00  0.00           N
ATOM    379  CA  GLY B  33       6.174   2.592   9.166  1.00  0.00           C
ATOM    380  C   GLY B  33       4.823   1.977   8.801  1.00  0.00           C
ATOM    381  O   GLY B  33       4.312   2.415   7.769  1.00  0.00           O
ATOM    382  H   GLY B  33       7.695   2.132   7.800  1.00  0.00           H
ATOM    383  N   LEU B  34       4.188   1.324   9.761  1.00  0.00           N
ATOM    384  CA  LEU B  34       2.830   0.794   9.566  1.00  0.00           C
ATOM    385  C   LEU B  34       1.693   1.788   9.771  1.00  0.00           C
ATOM    386  O   LEU B  34       1.194   1.902  10.903  1.00  0.00           O
ATOM    387  CB  LEU B  34       2.716  -0.458  10.451  1.00  0.00           C
ATOM    388  CG  LEU B  34       3.892  -1.405  10.246  1.00  0.00           C
ATOM    389  CD1 LEU B  34       3.820  -2.400  11.404  1.00  0.00           C
ATOM    390  CD2 LEU B  34       3.732  -2.170   8.927  1.00  0.00           C
ATOM    391  H   LEU B  34       4.506   1.153  10.697  1.00  0.00           H
ATOM    392  N   MET B  35       1.449   2.546   8.710  1.00  0.00           N
ATOM    393  CA  MET B  35       0.525   3.684   8.732  1.00  0.00           C
ATOM    394  C   MET B  35      -0.933   3.254   8.526  1.00  0.00           C
ATOM    395  O   MET B  35      -1.587   3.486   7.510  1.00  0.00           O
ATOM    396  CB  MET B  35       0.936   4.700   7.666  1.00  0.00           C
ATOM    397  CG  MET B  35       2.220   5.453   8.010  1.00  0.00           C
ATOM    398  SD  MET B  35       2.827   6.619   6.734  1.00  0.00           S
ATOM    399  CE  MET B  35       4.574   6.584   7.068  1.00  0.00           C
ATOM    400  H   MET B  35       1.783   2.213   7.829  1.00  0.00           H
ATOM    401  N   VAL B  36      -1.364   2.455   9.498  1.00  0.00           N
ATOM    402  CA  VAL B  36      -2.639   1.719   9.391  1.00  0.00           C
ATOM    403  C   VAL B  36      -3.929   2.538   9.470  1.00  0.00           C
ATOM    404  O   VAL B  36      -4.140   3.222  10.467  1.00  0.00           O
ATOM    405  CB  VAL B  36      -2.626   0.575  10.407  1.00  0.00           C
ATOM    406  CG1 VAL B  36      -1.520  -0.381   9.941  1.00  0.00           C
ATOM    407  CG2 VAL B  36      -2.414   0.997  11.862  1.00  0.00           C
ATOM    408  H   VAL B  36      -1.103   2.502  10.454  1.00  0.00           H
ATOM    409  N   GLY B  37      -4.864   2.131   8.627  1.00  0.00           N
ATOM    410  CA  GLY B  37      -6.170   2.804   8.583  1.00  0.00           C
ATOM    411  C   GLY B  37      -6.257   3.781   7.408  1.00  0.00           C
ATOM    412  O   GLY B  37      -5.384   4.649   7.351  1.00  0.00           O
ATOM    413  H   GLY B  37      -4.692   1.692   7.738  1.00  0.00           H
ATOM    414  N   GLY B  38      -7.268   3.599   6.549  1.00  0.00           N
ATOM    415  CA  GLY B  38      -7.460   4.502   5.413  1.00  0.00           C
ATOM    416  C   GLY B  38      -8.037   5.893   5.652  1.00  0.00           C
ATOM    417  O   GLY B  38      -8.755   6.073   6.640  1.00  0.00           O
ATOM    418  H   GLY B  38      -7.949   2.873   6.480  1.00  0.00           H
ATOM    419  N   VAL B  39      -7.571   6.874   4.881  1.00  0.00           N
ATOM    420  CA  VAL B  39      -8.105   8.227   5.098  1.00  0.00           C
ATOM    421  C   VAL B  39      -9.495   8.528   4.542  1.00  0.00           C
ATOM    422  O   VAL B  39      -9.931   8.079   3.483  1.00  0.00           O
ATOM    423  CB  VAL B  39      -7.097   9.350   4.861  1.00  0.00           C
ATOM    424  CG1 VAL B  39      -5.881   9.243   5.782  1.00  0.00           C
ATOM    425  CG2 VAL B  39      -6.619   9.399   3.406  1.00  0.00           C
ATOM    426  H   VAL B  39      -7.188   6.583   3.998  1.00  0.00           H
ATOM    427  N   VAL B  40     -10.299   9.215   5.354  1.00  0.00           N
ATOM    428  CA  VAL B  40     -11.756   9.340   5.167  1.00  0.00           C
ATOM    429  C   VAL B  40     -12.236  10.587   4.441  1.00  0.00           C
ATOM    430  O   VAL B  40     -11.852  11.694   4.808  1.00  0.00           O
ATOM    431  CB  VAL B  40     -12.499   9.249   6.500  1.00  0.00           C
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ATOM    432  CG1 VAL B  40     -13.997   8.907   6.432  1.00  0.00           C
ATOM    433  CG2 VAL B  40     -11.916   8.153   7.397  1.00  0.00           C
ATOM    434  H   VAL B  40      -9.964   9.831   6.059  1.00  0.00           H
ATOM    435  N   ILE B  41     -13.114  10.294   3.480  1.00  0.00           N
ATOM    436  CA  ILE B  41     -14.028  11.315   2.956  1.00  0.00           C
ATOM    437  C   ILE B  41     -15.281  11.684   3.745  1.00  0.00           C
ATOM    438  O   ILE B  41     -15.860  10.929   4.532  1.00  0.00           O
ATOM    439  CB  ILE B  41     -14.478  11.073   1.510  1.00  0.00           C
ATOM    440  CG1 ILE B  41     -15.095   9.685   1.329  1.00  0.00           C
ATOM    441  CG2 ILE B  41     -13.238  11.216   0.619  1.00  0.00           C
ATOM    442  CD  ILE B  41     -15.972   9.602   0.070  1.00  0.00           C
ATOM    443  H   ILE B  41     -13.175   9.317   3.252  1.00  0.00           H
ATOM    444  N   ALA B  42     -15.599  12.975   3.723  1.00  0.00           N
ATOM    445  CA  ALA B  42     -16.731  13.628   4.388  1.00  0.00           C
ATOM    446  C   ALA B  42     -16.842  15.090   3.946  1.00  0.00           C
ATOM    447  CB  ALA B  42     -16.761  13.754   5.907  1.00  0.00           C
ATOM    448  O1  ALA B  42     -18.013  15.526   3.818  1.00  0.00           O
ATOM    449  O2  ALA B  42     -15.848  15.695   3.486  1.00  0.00           O
ATOM    450  H   ALA B  42     -14.887  13.547   3.311  1.00  0.00           H
ATOM    451  N   LEU C  17     -14.801  -2.132   0.566  1.00  0.00           N
ATOM    452  CA  LEU C  17     -14.129  -2.999  -0.409  1.00  0.00           C
ATOM    453  C   LEU C  17     -12.781  -3.544   0.051  1.00  0.00           C
ATOM    454  O   LEU C  17     -12.204  -2.974   0.978  1.00  0.00           O
ATOM    455  CB  LEU C  17     -14.013  -2.248  -1.739  1.00  0.00           C
ATOM    456  CG  LEU C  17     -15.298  -1.819  -2.448  1.00  0.00           C
ATOM    457  CD1 LEU C  17     -15.317  -0.438  -3.105  1.00  0.00           C
ATOM    458  CD2 LEU C  17     -15.491  -2.788  -3.626  1.00  0.00           C
ATOM    459  H1  LEU C  17     -14.322  -1.255   0.663  1.00  0.00           H
ATOM    460  H2  LEU C  17     -15.721  -1.872   0.261  1.00  0.00           H
ATOM    461  H3  LEU C  17     -14.795  -2.647   1.429  1.00  0.00           H
ATOM    462  N   VAL C  18     -12.442  -4.742  -0.409  1.00  0.00           N
ATOM    463  CA  VAL C  18     -11.237  -5.494  -0.016  1.00  0.00           C
ATOM    464  C   VAL C  18     -10.072  -5.391  -1.000  1.00  0.00           C
ATOM    465  O   VAL C  18     -10.064  -5.835  -2.154  1.00  0.00           O
ATOM    466  CB  VAL C  18     -11.566  -6.957   0.240  1.00  0.00           C
ATOM    467  CG1 VAL C  18     -10.339  -7.764   0.657  1.00  0.00           C
ATOM    468  CG2 VAL C  18     -12.551  -6.914   1.415  1.00  0.00           C
ATOM    469  H   VAL C  18     -13.076  -5.224  -1.016  1.00  0.00           H
ATOM    470  N   PHE C  19      -8.934  -4.916  -0.505  1.00  0.00           N
ATOM    471  CA  PHE C  19      -7.696  -4.862  -1.303  1.00  0.00           C
ATOM    472  C   PHE C  19      -6.642  -5.704  -0.588  1.00  0.00           C
ATOM    473  O   PHE C  19      -6.559  -5.749   0.646  1.00  0.00           O
ATOM    474  CB  PHE C  19      -7.421  -3.360  -1.169  1.00  0.00           C
ATOM    475  CG  PHE C  19      -6.062  -2.960  -1.725  1.00  0.00           C
ATOM    476  CD1 PHE C  19      -4.999  -2.803  -0.839  1.00  0.00           C
ATOM    477  CD2 PHE C  19      -5.911  -2.950  -3.109  1.00  0.00           C
ATOM    478  CE1 PHE C  19      -3.726  -2.555  -1.343  1.00  0.00           C
ATOM    479  CE2 PHE C  19      -4.640  -2.675  -3.591  1.00  0.00           C
ATOM    480  CZ  PHE C  19      -3.578  -2.451  -2.724  1.00  0.00           C
ATOM    481  H   PHE C  19      -8.933  -4.733   0.475  1.00  0.00           H
ATOM    482  HD1 PHE C  19      -5.094  -3.219   0.168  1.00  0.00           H
ATOM    483  HD2 PHE C  19      -6.760  -3.169  -3.755  1.00  0.00           H
ATOM    484  HE1 PHE C  19      -2.982  -2.177  -0.643  1.00  0.00           H
ATOM    485  HE2 PHE C  19      -4.477  -2.581  -4.655  1.00  0.00           H
ATOM    486  HZ  PHE C  19      -2.579  -2.280  -3.141  1.00  0.00           H
ATOM    487  N   PHE C  20      -5.670  -6.168  -1.361  1.00  0.00           N
ATOM    488  CA  PHE C  20      -4.551  -6.941  -0.808  1.00  0.00           C
ATOM    489  C   PHE C  20      -3.261  -6.649  -1.586  1.00  0.00           C
ATOM    490  O   PHE C  20      -3.256  -6.698  -2.815  1.00  0.00           O
ATOM    491  CB  PHE C  20      -4.943  -8.388  -1.085  1.00  0.00           C
ATOM    492  CG  PHE C  20      -4.902  -9.309   0.145  1.00  0.00           C
ATOM    493  CD1 PHE C  20      -6.086  -9.415   0.865  1.00  0.00           C
ATOM    494  CD2 PHE C  20      -3.768  -9.980   0.581  1.00  0.00           C
ATOM    495  CE1 PHE C  20      -6.153 -10.285   1.951  1.00  0.00           C
ATOM    496  CE2 PHE C  20      -3.837 -10.734   1.752  1.00  0.00           C
ATOM    497  CZ  PHE C  20      -5.044 -10.999   2.392  1.00  0.00           C
ATOM    498  H   PHE C  20      -5.675  -5.993  -2.344  1.00  0.00           H
ATOM    499  HD1 PHE C  20      -7.044  -9.067   0.457  1.00  0.00           H
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ATOM    500  HD2 PHE C  20      -2.795  -9.826   0.109  1.00  0.00           H
ATOM    501  HE1 PHE C  20      -7.116 -10.430   2.440  1.00  0.00           H
ATOM    502  HE2 PHE C  20      -2.912 -10.833   2.319  1.00  0.00           H
ATOM    503  HZ  PHE C  20      -5.108 -11.713   3.210  1.00  0.00           H
ATOM    504  N   ALA C  21      -2.253  -6.301  -0.786  1.00  0.00           N
ATOM    505  CA  ALA C  21      -0.959  -5.964  -1.397  1.00  0.00           C
ATOM    506  C   ALA C  21       0.302  -6.759  -1.094  1.00  0.00           C
ATOM    507  O   ALA C  21       0.573  -7.201   0.028  1.00  0.00           O
ATOM    508  CB  ALA C  21      -0.511  -4.503  -1.365  1.00  0.00           C
ATOM    509  H   ALA C  21      -2.450  -5.904   0.109  1.00  0.00           H
ATOM    510  N   GLU C  22       1.031  -6.949  -2.188  1.00  0.00           N
ATOM    511  CA  GLU C  22       2.387  -7.486  -2.042  1.00  0.00           C
ATOM    512  C   GLU C  22       3.447  -6.616  -2.734  1.00  0.00           C
ATOM    513  O   GLU C  22       3.306  -6.383  -3.928  1.00  0.00           O
ATOM    514  CB  GLU C  22       2.365  -8.945  -2.508  1.00  0.00           C
ATOM    515  CG  GLU C  22       3.558  -9.798  -2.071  1.00  0.00           C
ATOM    516  CD  GLU C  22       3.465 -11.285  -2.434  1.00  0.00           C
ATOM    517  OE1 GLU C  22       3.853 -12.078  -1.549  1.00  0.00           O
ATOM    518  OE2 GLU C  22       2.767 -11.633  -3.406  1.00  0.00           O1-
ATOM    519  H   GLU C  22       0.698  -6.921  -3.133  1.00  0.00           H
ATOM    520  N   ASP C  23       4.126  -5.827  -1.905  1.00  0.00           N
ATOM    521  CA  ASP C  23       5.276  -5.016  -2.333  1.00  0.00           C
ATOM    522  C   ASP C  23       6.600  -5.783  -2.400  1.00  0.00           C
ATOM    523  O   ASP C  23       7.033  -6.257  -1.357  1.00  0.00           O
ATOM    524  CB  ASP C  23       5.420  -3.802  -1.407  1.00  0.00           C
ATOM    525  CG  ASP C  23       6.481  -2.797  -1.879  1.00  0.00           C
ATOM    526  OD1 ASP C  23       6.144  -1.599  -1.898  1.00  0.00           O
ATOM    527  OD2 ASP C  23       7.643  -3.134  -2.226  1.00  0.00           O1-
ATOM    528  H   ASP C  23       4.135  -5.993  -0.923  1.00  0.00           H
ATOM    529  N   VAL C  24       7.006  -6.044  -3.633  1.00  0.00           N
ATOM    530  CA  VAL C  24       8.250  -6.784  -3.906  1.00  0.00           C
ATOM    531  C   VAL C  24       9.478  -6.013  -4.398  1.00  0.00           C
ATOM    532  O   VAL C  24      10.426  -6.669  -4.824  1.00  0.00           O
ATOM    533  CB  VAL C  24       7.910  -8.063  -4.673  1.00  0.00           C
ATOM    534  CG1 VAL C  24       6.917  -8.883  -3.853  1.00  0.00           C
ATOM    535  CG2 VAL C  24       7.515  -7.806  -6.126  1.00  0.00           C
ATOM    536  H   VAL C  24       6.393  -5.976  -4.424  1.00  0.00           H
ATOM    537  N   GLY C  25       9.575  -4.738  -4.040  1.00  0.00           N
ATOM    538  CA  GLY C  25      10.478  -3.845  -4.780  1.00  0.00           C
ATOM    539  C   GLY C  25      11.889  -3.673  -4.212  1.00  0.00           C
ATOM    540  O   GLY C  25      12.154  -4.051  -3.077  1.00  0.00           O
ATOM    541  H   GLY C  25       9.274  -4.389  -3.158  1.00  0.00           H
ATOM    542  N   SER C  26      12.810  -3.569  -5.168  1.00  0.00           N
ATOM    543  CA  SER C  26      14.228  -3.307  -4.839  1.00  0.00           C
ATOM    544  C   SER C  26      14.549  -1.992  -4.129  1.00  0.00           C
ATOM    545  O   SER C  26      13.710  -1.100  -4.218  1.00  0.00           O
ATOM    546  CB  SER C  26      15.025  -3.604  -6.100  1.00  0.00           C
ATOM    547  OG  SER C  26      14.957  -2.395  -6.861  1.00  0.00           O
ATOM    548  H   SER C  26      12.574  -3.779  -6.114  1.00  0.00           H
ATOM    549  HG  SER C  26      15.723  -2.404  -7.506  1.00  0.00           H
ATOM    550  N   ASN C  27      15.600  -2.022  -3.315  1.00  0.00           N
ATOM    551  CA  ASN C  27      16.098  -0.914  -2.481  1.00  0.00           C
ATOM    552  C   ASN C  27      15.093  -0.174  -1.601  1.00  0.00           C
ATOM    553  O   ASN C  27      15.009   1.045  -1.702  1.00  0.00           O
ATOM    554  CB  ASN C  27      17.249  -0.134  -3.128  1.00  0.00           C
ATOM    555  CG  ASN C  27      18.475  -1.048  -3.233  1.00  0.00           C
ATOM    556  ND2 ASN C  27      19.616  -0.658  -2.677  1.00  0.00           N
ATOM    557  OD1 ASN C  27      18.424  -2.061  -3.922  1.00  0.00           O
ATOM    558  H   ASN C  27      16.279  -2.720  -3.551  1.00  0.00           H
ATOM    559 1HD2 ASN C  27      19.652   0.191  -2.153  1.00  0.00           H
ATOM    560 2HD2 ASN C  27      20.396  -1.286  -2.670  1.00  0.00           H
ATOM    561  N   LYS C  28      14.595  -0.885  -0.588  1.00  0.00           N
ATOM    562  CA  LYS C  28      13.571  -0.350   0.316  1.00  0.00           C
ATOM    563  C   LYS C  28      14.196   0.661   1.289  1.00  0.00           C
ATOM    564  O   LYS C  28      14.755   0.373   2.342  1.00  0.00           O
ATOM    565  CB  LYS C  28      12.876  -1.497   1.055  1.00  0.00           C
ATOM    566  CG  LYS C  28      11.912  -2.336   0.213  1.00  0.00           C
ATOM    567  CD  LYS C  28      10.592  -1.860  -0.381  1.00  0.00           C
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ATOM    568  CE  LYS C  28       9.527  -1.404   0.627  1.00  0.00           C
ATOM    569  NZ  LYS C  28       8.179  -1.934   0.387  1.00  0.00           N1+
ATOM    570  H   LYS C  28      14.823  -1.834  -0.377  1.00  0.00           H
ATOM    571  HZ1 LYS C  28       8.113  -2.105  -0.595  1.00  0.00           H
ATOM    572  HZ2 LYS C  28       8.168  -2.848   0.812  1.00  0.00           H
ATOM    573  HZ3 LYS C  28       7.418  -1.375   0.707  1.00  0.00           H
ATOM    574  N   GLY C  29      14.024   1.912   0.902  1.00  0.00           N
ATOM    575  CA  GLY C  29      14.662   3.039   1.602  1.00  0.00           C
ATOM    576  C   GLY C  29      14.374   3.316   3.082  1.00  0.00           C
ATOM    577  O   GLY C  29      14.027   2.444   3.873  1.00  0.00           O
ATOM    578  H   GLY C  29      13.835   2.112  -0.060  1.00  0.00           H
ATOM    579  N   ALA C  30      14.726   4.513   3.564  1.00  0.00           N
ATOM    580  CA  ALA C  30      14.789   4.953   4.968  1.00  0.00           C
ATOM    581  C   ALA C  30      13.428   4.965   5.667  1.00  0.00           C
ATOM    582  O   ALA C  30      13.383   4.577   6.827  1.00  0.00           O
ATOM    583  CB  ALA C  30      15.380   6.360   5.021  1.00  0.00           C
ATOM    584  H   ALA C  30      15.342   5.019   2.961  1.00  0.00           H
ATOM    585  N   ILE C  31      12.390   5.420   4.971  1.00  0.00           N
ATOM    586  CA  ILE C  31      11.048   5.395   5.561  1.00  0.00           C
ATOM    587  C   ILE C  31      10.134   4.463   4.755  1.00  0.00           C
ATOM    588  O   ILE C  31       9.496   4.927   3.811  1.00  0.00           O
ATOM    589  CB  ILE C  31      10.423   6.740   5.938  1.00  0.00           C
ATOM    590  CG1 ILE C  31      11.221   7.194   7.154  1.00  0.00           C
ATOM    591  CG2 ILE C  31       8.944   6.606   6.284  1.00  0.00           C
ATOM    592  CD  ILE C  31      12.031   8.392   6.663  1.00  0.00           C
ATOM    593  H   ILE C  31      12.542   5.931   4.126  1.00  0.00           H
ATOM    594  N   ILE C  32      10.066   3.217   5.210  1.00  0.00           N
ATOM    595  CA  ILE C  32       9.121   2.292   4.569  1.00  0.00           C
ATOM    596  C   ILE C  32       7.685   2.478   5.064  1.00  0.00           C
ATOM    597  O   ILE C  32       7.189   1.678   5.857  1.00  0.00           O
ATOM    598  CB  ILE C  32       9.654   0.872   4.768  1.00  0.00           C
ATOM    599  CG1 ILE C  32      11.169   0.855   4.565  1.00  0.00           C
ATOM    600  CG2 ILE C  32       8.904  -0.038   3.780  1.00  0.00           C
ATOM    601  CD  ILE C  32      11.957  -0.271   5.237  1.00  0.00           C
ATOM    602  H   ILE C  32      10.504   2.909   6.058  1.00  0.00           H
ATOM    603  N   GLY C  33       7.111   3.637   4.727  1.00  0.00           N
ATOM    604  CA  GLY C  33       5.785   4.117   5.123  1.00  0.00           C
ATOM    605  C   GLY C  33       4.668   3.408   4.357  1.00  0.00           C
ATOM    606  O   GLY C  33       4.139   3.918   3.362  1.00  0.00           O
ATOM    607  H   GLY C  33       7.571   4.286   4.118  1.00  0.00           H
ATOM    608  N   LEU C  34       4.314   2.187   4.770  1.00  0.00           N
ATOM    609  CA  LEU C  34       3.184   1.331   4.380  1.00  0.00           C
ATOM    610  C   LEU C  34       1.860   1.874   4.901  1.00  0.00           C
ATOM    611  O   LEU C  34       1.492   1.725   6.074  1.00  0.00           O
ATOM    612  CB  LEU C  34       3.390  -0.173   4.577  1.00  0.00           C
ATOM    613  CG  LEU C  34       4.117  -0.950   3.483  1.00  0.00           C
ATOM    614  CD1 LEU C  34       5.630  -0.770   3.524  1.00  0.00           C
ATOM    615  CD2 LEU C  34       3.694  -2.417   3.506  1.00  0.00           C
ATOM    616  H   LEU C  34       4.923   1.784   5.453  1.00  0.00           H
ATOM    617  N   MET C  35       1.160   2.641   4.073  1.00  0.00           N
ATOM    618  CA  MET C  35      -0.126   3.294   4.377  1.00  0.00           C
ATOM    619  C   MET C  35      -1.252   2.406   3.861  1.00  0.00           C
ATOM    620  O   MET C  35      -1.485   2.433   2.649  1.00  0.00           O
ATOM    621  CB  MET C  35      -0.275   4.718   3.841  1.00  0.00           C
ATOM    622  CG  MET C  35       1.035   5.502   3.929  1.00  0.00           C
ATOM    623  SD  MET C  35       0.694   7.215   3.379  1.00  0.00           S
ATOM    624  CE  MET C  35       2.258   7.970   3.779  1.00  0.00           C
ATOM    625  H   MET C  35       1.442   2.777   3.122  1.00  0.00           H
ATOM    626  N   VAL C  36      -1.844   1.562   4.701  1.00  0.00           N
ATOM    627  CA  VAL C  36      -2.843   0.536   4.365  1.00  0.00           C
ATOM    628  C   VAL C  36      -4.237   1.169   4.346  1.00  0.00           C
ATOM    629  O   VAL C  36      -4.893   1.252   5.376  1.00  0.00           O
ATOM    630  CB  VAL C  36      -2.891  -0.568   5.420  1.00  0.00           C
ATOM    631  CG1 VAL C  36      -3.554  -1.873   4.994  1.00  0.00           C
ATOM    632  CG2 VAL C  36      -1.475  -0.955   5.874  1.00  0.00           C
ATOM    633  H   VAL C  36      -1.673   1.605   5.683  1.00  0.00           H
ATOM    634  N   GLY C  37      -4.595   1.674   3.167  1.00  0.00           N
ATOM    635  CA  GLY C  37      -5.916   2.271   2.939  1.00  0.00           C
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ATOM    636  C   GLY C  37      -6.052   3.023   1.608  1.00  0.00           C
ATOM    637  O   GLY C  37      -6.771   2.582   0.713  1.00  0.00           O
ATOM    638  H   GLY C  37      -4.126   1.333   2.352  1.00  0.00           H
ATOM    639  N   GLY C  38      -5.289   4.112   1.544  1.00  0.00           N
ATOM    640  CA  GLY C  38      -5.460   5.256   0.645  1.00  0.00           C
ATOM    641  C   GLY C  38      -6.767   5.946   1.050  1.00  0.00           C
ATOM    642  O   GLY C  38      -7.142   5.869   2.216  1.00  0.00           O
ATOM    643  H   GLY C  38      -4.596   4.264   2.244  1.00  0.00           H
ATOM    644  N   VAL C  39      -7.296   6.640   0.047  1.00  0.00           N
ATOM    645  CA  VAL C  39      -8.612   7.241   0.276  1.00  0.00           C
ATOM    646  C   VAL C  39      -9.729   6.195   0.233  1.00  0.00           C
ATOM    647  O   VAL C  39     -10.207   6.004  -0.882  1.00  0.00           O
ATOM    648  CB  VAL C  39      -8.820   8.463  -0.622  1.00  0.00           C
ATOM    649  CG1 VAL C  39     -10.088   9.285  -0.351  1.00  0.00           C
ATOM    650  CG2 VAL C  39      -7.672   9.476  -0.608  1.00  0.00           C
ATOM    651  H   VAL C  39      -7.215   6.457  -0.935  1.00  0.00           H
ATOM    652  N   VAL C  40     -10.322   5.867   1.373  1.00  0.00           N
ATOM    653  CA  VAL C  40     -11.461   4.948   1.567  1.00  0.00           C
ATOM    654  C   VAL C  40     -12.836   5.615   1.543  1.00  0.00           C
ATOM    655  O   VAL C  40     -12.993   6.731   2.054  1.00  0.00           O
ATOM    656  CB  VAL C  40     -11.513   4.108   2.846  1.00  0.00           C
ATOM    657  CG1 VAL C  40     -10.831   2.756   2.640  1.00  0.00           C
ATOM    658  CG2 VAL C  40     -10.940   4.858   4.048  1.00  0.00           C
ATOM    659  H   VAL C  40     -10.240   6.516   2.130  1.00  0.00           H
ATOM    660  N   ILE C  41     -13.796   4.892   0.972  1.00  0.00           N
ATOM    661  CA  ILE C  41     -15.212   5.275   0.809  1.00  0.00           C
ATOM    662  C   ILE C  41     -16.034   5.506   2.076  1.00  0.00           C
ATOM    663  O   ILE C  41     -16.849   6.427   2.053  1.00  0.00           O
ATOM    664  CB  ILE C  41     -15.890   4.285  -0.138  1.00  0.00           C
ATOM    665  CG1 ILE C  41     -15.218   4.044  -1.487  1.00  0.00           C
ATOM    666  CG2 ILE C  41     -17.403   4.490  -0.307  1.00  0.00           C
ATOM    667  CD  ILE C  41     -14.384   2.759  -1.517  1.00  0.00           C
ATOM    668  H   ILE C  41     -13.753   3.899   1.047  1.00  0.00           H
ATOM    669  N   ALA C  42     -15.615   4.774   3.109  1.00  0.00           N
ATOM    670  CA  ALA C  42     -16.161   4.715   4.470  1.00  0.00           C
ATOM    671  C   ALA C  42     -15.249   3.793   5.276  1.00  0.00           C
ATOM    672  CB  ALA C  42     -17.567   4.103   4.485  1.00  0.00           C
ATOM    673  O1  ALA C  42     -14.946   2.655   4.859  1.00  0.00           O
ATOM    674  O2  ALA C  42     -14.839   4.270   6.353  1.00  0.00           O
ATOM    675  H   ALA C  42     -14.869   4.130   2.949  1.00  0.00           H
ATOM    676  N   LEU D  17     -15.876  -7.084  -6.106  1.00  0.00           N
ATOM    677  CA  LEU D  17     -14.613  -7.556  -6.692  1.00  0.00           C
ATOM    678  C   LEU D  17     -13.396  -7.242  -5.805  1.00  0.00           C
ATOM    679  O   LEU D  17     -13.261  -6.094  -5.387  1.00  0.00           O
ATOM    680  CB  LEU D  17     -14.476  -6.941  -8.082  1.00  0.00           C
ATOM    681  CG  LEU D  17     -13.221  -7.256  -8.892  1.00  0.00           C
ATOM    682  CD1 LEU D  17     -12.898  -8.753  -8.926  1.00  0.00           C
ATOM    683  CD2 LEU D  17     -13.334  -6.787 -10.349  1.00  0.00           C
ATOM    684  H1  LEU D  17     -16.367  -6.602  -6.831  1.00  0.00           H
ATOM    685  H2  LEU D  17     -16.536  -7.784  -5.826  1.00  0.00           H
ATOM    686  H3  LEU D  17     -15.768  -6.521  -5.285  1.00  0.00           H
ATOM    687  N   VAL D  18     -12.608  -8.238  -5.433  1.00  0.00           N
ATOM    688  CA  VAL D  18     -11.374  -8.028  -4.647  1.00  0.00           C
ATOM    689  C   VAL D  18     -10.223  -7.535  -5.527  1.00  0.00           C
ATOM    690  O   VAL D  18      -9.877  -8.312  -6.409  1.00  0.00           O
ATOM    691  CB  VAL D  18     -11.116  -9.334  -3.900  1.00  0.00           C
ATOM    692  CG1 VAL D  18      -9.855  -9.345  -3.022  1.00  0.00           C
ATOM    693  CG2 VAL D  18     -12.281  -9.651  -2.971  1.00  0.00           C
ATOM    694  H   VAL D  18     -12.792  -9.186  -5.688  1.00  0.00           H
ATOM    695  N   PHE D  19      -9.334  -6.786  -4.884  1.00  0.00           N
ATOM    696  CA  PHE D  19      -8.186  -6.221  -5.596  1.00  0.00           C
ATOM    697  C   PHE D  19      -6.818  -6.650  -5.056  1.00  0.00           C
ATOM    698  O   PHE D  19      -6.344  -6.051  -4.089  1.00  0.00           O
ATOM    699  CB  PHE D  19      -8.314  -4.695  -5.575  1.00  0.00           C
ATOM    700  CG  PHE D  19      -7.477  -3.932  -6.600  1.00  0.00           C
ATOM    701  CD1 PHE D  19      -8.045  -3.410  -7.751  1.00  0.00           C
ATOM    702  CD2 PHE D  19      -6.098  -3.758  -6.470  1.00  0.00           C
ATOM    703  CE1 PHE D  19      -7.325  -2.789  -8.766  1.00  0.00           C
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ATOM    704  CE2 PHE D  19      -5.348  -3.138  -7.463  1.00  0.00           C
ATOM    705  CZ  PHE D  19      -5.943  -2.660  -8.617  1.00  0.00           C
ATOM    706  H   PHE D  19      -9.458  -6.425  -3.958  1.00  0.00           H
ATOM    707  HD1 PHE D  19      -9.106  -3.595  -7.920  1.00  0.00           H
ATOM    708  HD2 PHE D  19      -5.584  -4.200  -5.625  1.00  0.00           H
ATOM    709  HE1 PHE D  19      -7.815  -2.523  -9.704  1.00  0.00           H
ATOM    710  HE2 PHE D  19      -4.291  -2.936  -7.261  1.00  0.00           H
ATOM    711  HZ  PHE D  19      -5.412  -2.027  -9.318  1.00  0.00           H
ATOM    712  N   PHE D  20      -6.101  -7.516  -5.763  1.00  0.00           N
ATOM    713  CA  PHE D  20      -4.706  -7.840  -5.427  1.00  0.00           C
ATOM    714  C   PHE D  20      -3.725  -6.921  -6.159  1.00  0.00           C
ATOM    715  O   PHE D  20      -3.946  -6.544  -7.306  1.00  0.00           O
ATOM    716  CB  PHE D  20      -4.408  -9.313  -5.714  1.00  0.00           C
ATOM    717  CG  PHE D  20      -3.160  -9.736  -4.943  1.00  0.00           C
ATOM    718  CD1 PHE D  20      -3.317 -10.166  -3.626  1.00  0.00           C
ATOM    719  CD2 PHE D  20      -1.917  -9.625  -5.554  1.00  0.00           C
ATOM    720  CE1 PHE D  20      -2.154 -10.436  -2.922  1.00  0.00           C
ATOM    721  CE2 PHE D  20      -0.788  -9.937  -4.799  1.00  0.00           C
ATOM    722  CZ  PHE D  20      -0.879 -10.358  -3.481  1.00  0.00           C
ATOM    723  H   PHE D  20      -6.464  -7.741  -6.662  1.00  0.00           H
ATOM    724  HD1 PHE D  20      -4.264 -10.452  -3.165  1.00  0.00           H
ATOM    725  HD2 PHE D  20      -1.863  -9.233  -6.572  1.00  0.00           H
ATOM    726  HE1 PHE D  20      -2.214 -10.679  -1.859  1.00  0.00           H
ATOM    727  HE2 PHE D  20       0.209  -9.848  -5.227  1.00  0.00           H
ATOM    728  HZ  PHE D  20       0.030 -10.362  -2.876  1.00  0.00           H
ATOM    729  N   ALA D  21      -2.731  -6.423  -5.424  1.00  0.00           N
ATOM    730  CA  ALA D  21      -1.623  -5.686  -6.049  1.00  0.00           C
ATOM    731  C   ALA D  21      -0.230  -6.292  -5.842  1.00  0.00           C
ATOM    732  O   ALA D  21       0.219  -6.404  -4.703  1.00  0.00           O
ATOM    733  CB  ALA D  21      -1.572  -4.256  -5.509  1.00  0.00           C
ATOM    734  H   ALA D  21      -2.782  -6.569  -4.445  1.00  0.00           H
ATOM    735  N   GLU D  22       0.588  -6.259  -6.885  1.00  0.00           N
ATOM    736  CA  GLU D  22       1.967  -6.778  -6.860  1.00  0.00           C
ATOM    737  C   GLU D  22       2.888  -5.748  -7.531  1.00  0.00           C
ATOM    738  O   GLU D  22       2.869  -5.491  -8.727  1.00  0.00           O
ATOM    739  CB  GLU D  22       2.043  -8.194  -7.446  1.00  0.00           C
ATOM    740  CG  GLU D  22       3.285  -8.988  -7.044  1.00  0.00           C
ATOM    741  CD  GLU D  22       3.460 -10.319  -7.792  1.00  0.00           C
ATOM    742  OE1 GLU D  22       2.963 -11.392  -7.388  1.00  0.00           O
ATOM    743  OE2 GLU D  22       4.216 -10.291  -8.786  1.00  0.00           O1-
ATOM    744  H   GLU D  22       0.269  -5.980  -7.798  1.00  0.00           H
ATOM    745  N   ASP D  23       3.179  -4.784  -6.661  1.00  0.00           N
ATOM    746  CA  ASP D  23       4.096  -3.713  -7.060  1.00  0.00           C
ATOM    747  C   ASP D  23       5.511  -4.266  -7.212  1.00  0.00           C
ATOM    748  O   ASP D  23       6.380  -4.053  -6.364  1.00  0.00           O
ATOM    749  CB  ASP D  23       3.973  -2.510  -6.121  1.00  0.00           C
ATOM    750  CG  ASP D  23       4.792  -1.321  -6.645  1.00  0.00           C
ATOM    751  OD1 ASP D  23       4.540  -0.227  -6.087  1.00  0.00           O
ATOM    752  OD2 ASP D  23       5.597  -1.507  -7.574  1.00  0.00           O1-
ATOM    753  H   ASP D  23       2.859  -4.739  -5.717  1.00  0.00           H
ATOM    754  N   VAL D  24       5.796  -4.690  -8.444  1.00  0.00           N
ATOM    755  CA  VAL D  24       7.099  -5.147  -8.926  1.00  0.00           C
ATOM    756  C   VAL D  24       8.131  -4.051  -9.191  1.00  0.00           C
ATOM    757  O   VAL D  24       9.174  -4.255  -9.803  1.00  0.00           O
ATOM    758  CB  VAL D  24       6.955  -6.079 -10.138  1.00  0.00           C
ATOM    759  CG1 VAL D  24       6.399  -7.462  -9.796  1.00  0.00           C
ATOM    760  CG2 VAL D  24       6.324  -5.405 -11.362  1.00  0.00           C
ATOM    761  H   VAL D  24       5.066  -4.669  -9.130  1.00  0.00           H
ATOM    762  N   GLY D  25       7.699  -2.839  -8.829  1.00  0.00           N
ATOM    763  CA  GLY D  25       8.396  -1.558  -9.016  1.00  0.00           C
ATOM    764  C   GLY D  25       9.712  -1.510  -8.235  1.00  0.00           C
ATOM    765  O   GLY D  25       9.838  -1.818  -7.059  1.00  0.00           O
ATOM    766  H   GLY D  25       6.968  -2.743  -8.162  1.00  0.00           H
ATOM    767  N   SER D  26      10.748  -1.091  -8.949  1.00  0.00           N
ATOM    768  CA  SER D  26      12.118  -1.104  -8.392  1.00  0.00           C
ATOM    769  C   SER D  26      12.653   0.276  -8.022  1.00  0.00           C
ATOM    770  O   SER D  26      12.171   1.343  -8.397  1.00  0.00           O
ATOM    771  CB  SER D  26      13.025  -1.869  -9.349  1.00  0.00           C
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ATOM    772  OG  SER D  26      13.076  -1.200 -10.611  1.00  0.00           O
ATOM    773  H   SER D  26      10.610  -0.567  -9.784  1.00  0.00           H
ATOM    774  HG  SER D  26      14.001  -0.824 -10.680  1.00  0.00           H
ATOM    775  N   ASN D  27      13.731   0.132  -7.250  1.00  0.00           N
ATOM    776  CA  ASN D  27      14.492   1.189  -6.564  1.00  0.00           C
ATOM    777  C   ASN D  27      13.641   2.157  -5.744  1.00  0.00           C
ATOM    778  O   ASN D  27      13.246   3.237  -6.175  1.00  0.00           O
ATOM    779  CB  ASN D  27      15.487   1.825  -7.533  1.00  0.00           C
ATOM    780  CG  ASN D  27      16.298   2.969  -6.933  1.00  0.00           C
ATOM    781  ND2 ASN D  27      16.651   4.006  -7.671  1.00  0.00           N
ATOM    782  OD1 ASN D  27      16.875   2.895  -5.840  1.00  0.00           O
ATOM    783  H   ASN D  27      14.061  -0.761  -6.974  1.00  0.00           H
ATOM    784 1HD2 ASN D  27      16.413   4.047  -8.642  1.00  0.00           H
ATOM    785 2HD2 ASN D  27      17.128   4.780  -7.253  1.00  0.00           H
ATOM    786  N   LYS D  28      13.098   1.583  -4.674  1.00  0.00           N
ATOM    787  CA  LYS D  28      12.143   2.167  -3.717  1.00  0.00           C
ATOM    788  C   LYS D  28      12.879   2.948  -2.634  1.00  0.00           C
ATOM    789  O   LYS D  28      12.688   2.668  -1.451  1.00  0.00           O
ATOM    790  CB  LYS D  28      11.191   1.049  -3.299  1.00  0.00           C
ATOM    791  CG  LYS D  28       9.950   1.082  -4.193  1.00  0.00           C
ATOM    792  CD  LYS D  28       9.053  -0.111  -3.844  1.00  0.00           C
ATOM    793  CE  LYS D  28       7.995  -0.152  -4.947  1.00  0.00           C
ATOM    794  NZ  LYS D  28       7.237  -1.407  -4.899  1.00  0.00           N1+
ATOM    795  H   LYS D  28      13.313   0.634  -4.429  1.00  0.00           H
ATOM    796  HZ1 LYS D  28       7.595  -2.283  -5.213  1.00  0.00           H
ATOM    797  HZ2 LYS D  28       6.863  -1.520  -3.983  1.00  0.00           H
ATOM    798  HZ3 LYS D  28       6.448  -1.298  -5.515  1.00  0.00           H
ATOM    799  N   GLY D  29      13.634   3.970  -3.039  1.00  0.00           N
ATOM    800  CA  GLY D  29      14.428   4.811  -2.127  1.00  0.00           C
ATOM    801  C   GLY D  29      13.765   5.624  -1.010  1.00  0.00           C
ATOM    802  O   GLY D  29      12.645   6.106  -1.099  1.00  0.00           O
ATOM    803  H   GLY D  29      13.523   4.304  -3.969  1.00  0.00           H
ATOM    804  N   ALA D  30      14.627   6.079  -0.104  1.00  0.00           N
ATOM    805  CA  ALA D  30      14.296   7.147   0.851  1.00  0.00           C
ATOM    806  C   ALA D  30      12.891   7.184   1.469  1.00  0.00           C
ATOM    807  O   ALA D  30      12.450   6.210   2.067  1.00  0.00           O
ATOM    808  CB  ALA D  30      14.748   8.451   0.193  1.00  0.00           C
ATOM    809  H   ALA D  30      15.550   5.725   0.033  1.00  0.00           H
ATOM    810  N   ILE D  31      12.207   8.321   1.371  1.00  0.00           N
ATOM    811  CA  ILE D  31      10.928   8.629   2.031  1.00  0.00           C
ATOM    812  C   ILE D  31       9.707   8.011   1.339  1.00  0.00           C
ATOM    813  O   ILE D  31       8.656   8.632   1.201  1.00  0.00           O
ATOM    814  CB  ILE D  31      10.799  10.101   2.405  1.00  0.00           C
ATOM    815  CG1 ILE D  31      11.012  11.115   1.280  1.00  0.00           C
ATOM    816  CG2 ILE D  31      11.661  10.418   3.631  1.00  0.00           C
ATOM    817  CD  ILE D  31       9.655  11.459   0.664  1.00  0.00           C
ATOM    818  H   ILE D  31      12.340   9.066   0.722  1.00  0.00           H
ATOM    819  N   ILE D  32       9.743   6.732   0.995  1.00  0.00           N
ATOM    820  CA  ILE D  32       8.554   6.170   0.336  1.00  0.00           C
ATOM    821  C   ILE D  32       7.289   5.988   1.181  1.00  0.00           C
ATOM    822  O   ILE D  32       7.064   5.043   1.925  1.00  0.00           O
ATOM    823  CB  ILE D  32       9.055   4.887  -0.338  1.00  0.00           C
ATOM    824  CG1 ILE D  32       9.827   3.905   0.559  1.00  0.00           C
ATOM    825  CG2 ILE D  32       9.707   5.284  -1.661  1.00  0.00           C
ATOM    826  CD  ILE D  32       9.234   2.538   0.215  1.00  0.00           C
ATOM    827  H   ILE D  32      10.301   6.108   1.543  1.00  0.00           H
ATOM    828  N   GLY D  33       6.288   6.782   0.824  1.00  0.00           N
ATOM    829  CA  GLY D  33       4.894   6.805   1.304  1.00  0.00           C
ATOM    830  C   GLY D  33       4.054   5.810   0.507  1.00  0.00           C
ATOM    831  O   GLY D  33       3.408   6.131  -0.500  1.00  0.00           O
ATOM    832  H   GLY D  33       6.372   7.449   0.084  1.00  0.00           H
ATOM    833  N   LEU D  34       4.108   4.526   0.844  1.00  0.00           N
ATOM    834  CA  LEU D  34       3.490   3.416   0.097  1.00  0.00           C
ATOM    835  C   LEU D  34       1.984   3.356   0.368  1.00  0.00           C
ATOM    836  O   LEU D  34       1.533   2.714   1.317  1.00  0.00           O
ATOM    837  CB  LEU D  34       4.121   2.053   0.351  1.00  0.00           C
ATOM    838  CG  LEU D  34       5.155   1.907  -0.777  1.00  0.00           C
ATOM    839  CD1 LEU D  34       6.224   0.940  -0.245  1.00  0.00           C
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ATOM    840  CD2 LEU D  34       4.729   1.664  -2.220  1.00  0.00           C
ATOM    841  H   LEU D  34       4.380   4.263   1.771  1.00  0.00           H
ATOM    842  N   MET D  35       1.219   4.162  -0.358  1.00  0.00           N
ATOM    843  CA  MET D  35      -0.238   4.306  -0.253  1.00  0.00           C
ATOM    844  C   MET D  35      -0.953   3.089  -0.829  1.00  0.00           C
ATOM    845  O   MET D  35      -1.341   3.072  -1.988  1.00  0.00           O
ATOM    846  CB  MET D  35      -0.751   5.577  -0.938  1.00  0.00           C
ATOM    847  CG  MET D  35      -0.444   6.835  -0.120  1.00  0.00           C
ATOM    848  SD  MET D  35      -1.013   8.482  -0.658  1.00  0.00           S
ATOM    849  CE  MET D  35      -2.756   8.364  -0.341  1.00  0.00           C
ATOM    850  H   MET D  35       1.583   4.580  -1.192  1.00  0.00           H
ATOM    851  N   VAL D  36      -0.979   2.002  -0.060  1.00  0.00           N
ATOM    852  CA  VAL D  36      -1.333   0.625  -0.430  1.00  0.00           C
ATOM    853  C   VAL D  36      -2.862   0.642  -0.359  1.00  0.00           C
ATOM    854  O   VAL D  36      -3.410   0.799   0.725  1.00  0.00           O
ATOM    855  CB  VAL D  36      -0.558  -0.518   0.234  1.00  0.00           C
ATOM    856  CG1 VAL D  36       0.768  -0.788  -0.469  1.00  0.00           C
ATOM    857  CG2 VAL D  36      -0.257  -0.281   1.713  1.00  0.00           C
ATOM    858  H   VAL D  36      -0.736   2.050   0.911  1.00  0.00           H
ATOM    859  N   GLY D  37      -3.554   0.786  -1.491  1.00  0.00           N
ATOM    860  CA  GLY D  37      -5.004   0.983  -1.470  1.00  0.00           C
ATOM    861  C   GLY D  37      -5.687   1.767  -2.604  1.00  0.00           C
ATOM    862  O   GLY D  37      -5.125   1.820  -3.699  1.00  0.00           O
ATOM    863  H   GLY D  37      -3.157   0.490  -2.357  1.00  0.00           H
ATOM    864  N   GLY D  38      -6.902   2.205  -2.313  1.00  0.00           N
ATOM    865  CA  GLY D  38      -7.794   2.930  -3.222  1.00  0.00           C
ATOM    866  C   GLY D  38      -7.836   4.451  -3.060  1.00  0.00           C
ATOM    867  O   GLY D  38      -7.248   4.940  -2.096  1.00  0.00           O
ATOM    868  H   GLY D  38      -7.225   2.139  -1.360  1.00  0.00           H
ATOM    869  N   VAL D  39      -8.249   5.116  -4.137  1.00  0.00           N
ATOM    870  CA  VAL D  39      -8.584   6.556  -4.153  1.00  0.00           C
ATOM    871  C   VAL D  39      -9.907   6.943  -4.820  1.00  0.00           C
ATOM    872  O   VAL D  39     -10.248   6.484  -5.906  1.00  0.00           O
ATOM    873  CB  VAL D  39      -7.491   7.504  -4.645  1.00  0.00           C
ATOM    874  CG1 VAL D  39      -6.345   7.679  -3.637  1.00  0.00           C
ATOM    875  CG2 VAL D  39      -6.872   7.267  -6.021  1.00  0.00           C
ATOM    876  H   VAL D  39      -8.127   4.670  -5.022  1.00  0.00           H
ATOM    877  N   VAL D  40     -10.692   7.633  -3.992  1.00  0.00           N
ATOM    878  CA  VAL D  40     -12.066   7.996  -4.375  1.00  0.00           C
ATOM    879  C   VAL D  40     -12.193   9.065  -5.464  1.00  0.00           C
ATOM    880  O   VAL D  40     -11.767  10.196  -5.244  1.00  0.00           O
ATOM    881  CB  VAL D  40     -12.873   8.365  -3.131  1.00  0.00           C
ATOM    882  CG1 VAL D  40     -14.311   8.821  -3.432  1.00  0.00           C
ATOM    883  CG2 VAL D  40     -12.955   7.174  -2.181  1.00  0.00           C
ATOM    884  H   VAL D  40     -10.551   7.638  -2.992  1.00  0.00           H
ATOM    885  N   ILE D  41     -13.001   8.629  -6.427  1.00  0.00           N
ATOM    886  CA  ILE D  41     -13.266   9.487  -7.596  1.00  0.00           C
ATOM    887  C   ILE D  41     -14.748   9.856  -7.625  1.00  0.00           C
ATOM    888  O   ILE D  41     -15.602   9.297  -6.945  1.00  0.00           O
ATOM    889  CB  ILE D  41     -12.976   8.750  -8.907  1.00  0.00           C
ATOM    890  CG1 ILE D  41     -13.766   7.470  -9.162  1.00  0.00           C
ATOM    891  CG2 ILE D  41     -11.486   8.425  -9.025  1.00  0.00           C
ATOM    892  CD  ILE D  41     -14.153   7.431 -10.643  1.00  0.00           C
ATOM    893  H   ILE D  41     -13.403   7.717  -6.474  1.00  0.00           H
ATOM    894  N   ALA D  42     -14.972  10.949  -8.354  1.00  0.00           N
ATOM    895  CA  ALA D  42     -16.312  11.525  -8.566  1.00  0.00           C
ATOM    896  C   ALA D  42     -16.271  12.271  -9.896  1.00  0.00           C
ATOM    897  CB  ALA D  42     -16.743  12.432  -7.420  1.00  0.00           C
ATOM    898  O1  ALA D  42     -15.487  13.238 -10.009  1.00  0.00           O
ATOM    899  O2  ALA D  42     -16.961  11.873 -10.861  1.00  0.00           O
ATOM    900  H   ALA D  42     -14.271  11.406  -8.899  1.00  0.00           H
ATOM    901  N   LEU E  17     -13.196 -14.492  -9.448  1.00  0.00           N
ATOM    902  CA  LEU E  17     -11.750 -14.693  -9.270  1.00  0.00           C
ATOM    903  C   LEU E  17     -11.184 -13.302  -8.940  1.00  0.00           C
ATOM    904  O   LEU E  17     -11.792 -12.316  -9.332  1.00  0.00           O
ATOM    905  CB  LEU E  17     -11.042 -15.334 -10.460  1.00  0.00           C
ATOM    906  CG  LEU E  17     -11.309 -16.837 -10.482  1.00  0.00           C
ATOM    907  CD1 LEU E  17     -10.778 -17.463 -11.777  1.00  0.00           C
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ATOM    908  CD2 LEU E  17     -10.604 -17.676  -9.408  1.00  0.00           C
ATOM    909  H1  LEU E  17     -13.440 -14.741 -10.381  1.00  0.00           H
ATOM    910  H2  LEU E  17     -13.715 -14.968  -8.737  1.00  0.00           H
ATOM    911  H3  LEU E  17     -13.448 -13.532  -9.350  1.00  0.00           H
ATOM    912  N   VAL E  18     -10.052 -13.278  -8.242  1.00  0.00           N
ATOM    913  CA  VAL E  18      -9.368 -12.006  -7.968  1.00  0.00           C
ATOM    914  C   VAL E  18      -8.790 -11.278  -9.191  1.00  0.00           C
ATOM    915  O   VAL E  18      -8.469 -11.919 -10.187  1.00  0.00           O
ATOM    916  CB  VAL E  18      -8.290 -12.392  -6.950  1.00  0.00           C
ATOM    917  CG1 VAL E  18      -7.134 -13.207  -7.532  1.00  0.00           C
ATOM    918  CG2 VAL E  18      -7.880 -11.157  -6.141  1.00  0.00           C
ATOM    919  H   VAL E  18      -9.537 -14.093  -7.986  1.00  0.00           H
ATOM    920  N   PHE E  19      -8.945  -9.965  -9.072  1.00  0.00           N
ATOM    921  CA  PHE E  19      -8.307  -8.994  -9.975  1.00  0.00           C
ATOM    922  C   PHE E  19      -6.930  -8.694  -9.374  1.00  0.00           C
ATOM    923  O   PHE E  19      -6.732  -8.177  -8.278  1.00  0.00           O
ATOM    924  CB  PHE E  19      -9.238  -7.784  -9.960  1.00  0.00           C
ATOM    925  CG  PHE E  19      -8.961  -6.769 -11.072  1.00  0.00           C
ATOM    926  CD1 PHE E  19      -9.797  -6.680 -12.174  1.00  0.00           C
ATOM    927  CD2 PHE E  19      -7.903  -5.881 -10.911  1.00  0.00           C
ATOM    928  CE1 PHE E  19      -9.617  -5.812 -13.240  1.00  0.00           C
ATOM    929  CE2 PHE E  19      -7.671  -5.084 -12.024  1.00  0.00           C
ATOM    930  CZ  PHE E  19      -8.471  -5.019 -13.157  1.00  0.00           C
ATOM    931  H   PHE E  19      -9.526  -9.555  -8.370  1.00  0.00           H
ATOM    932  HD1 PHE E  19     -10.643  -7.369 -12.226  1.00  0.00           H
ATOM    933  HD2 PHE E  19      -7.287  -5.685 -10.032  1.00  0.00           H
ATOM    934  HE1 PHE E  19     -10.135  -5.947 -14.197  1.00  0.00           H
ATOM    935  HE2 PHE E  19      -6.724  -4.566 -12.139  1.00  0.00           H
ATOM    936  HZ  PHE E  19      -8.337  -4.202 -13.868  1.00  0.00           H
ATOM    937  N   PHE E  20      -6.002  -8.582 -10.322  1.00  0.00           N
ATOM    938  CA  PHE E  20      -4.568  -8.361 -10.061  1.00  0.00           C
ATOM    939  C   PHE E  20      -4.068  -7.056 -10.680  1.00  0.00           C
ATOM    940  O   PHE E  20      -4.615  -6.468 -11.606  1.00  0.00           O
ATOM    941  CB  PHE E  20      -3.827  -9.542 -10.698  1.00  0.00           C
ATOM    942  CG  PHE E  20      -2.549  -9.927  -9.944  1.00  0.00           C
ATOM    943  CD1 PHE E  20      -1.350  -9.656 -10.582  1.00  0.00           C
ATOM    944  CD2 PHE E  20      -2.572 -10.772  -8.840  1.00  0.00           C
ATOM    945  CE1 PHE E  20      -0.143 -10.125 -10.060  1.00  0.00           C
ATOM    946  CE2 PHE E  20      -1.363 -11.184  -8.307  1.00  0.00           C
ATOM    947  CZ  PHE E  20      -0.138 -10.861  -8.878  1.00  0.00           C
ATOM    948  H   PHE E  20      -6.257  -8.258 -11.232  1.00  0.00           H
ATOM    949  HD1 PHE E  20      -1.335  -9.119 -11.534  1.00  0.00           H
ATOM    950  HD2 PHE E  20      -3.482 -10.948  -8.272  1.00  0.00           H
ATOM    951  HE1 PHE E  20       0.791  -9.759 -10.486  1.00  0.00           H
ATOM    952  HE2 PHE E  20      -1.363 -12.004  -7.583  1.00  0.00           H
ATOM    953  HZ  PHE E  20       0.821 -11.038  -8.405  1.00  0.00           H
ATOM    954  N   ALA E  21      -2.975  -6.587 -10.079  1.00  0.00           N
ATOM    955  CA  ALA E  21      -2.225  -5.403 -10.500  1.00  0.00           C
ATOM    956  C   ALA E  21      -0.709  -5.518 -10.341  1.00  0.00           C
ATOM    957  O   ALA E  21      -0.081  -5.206  -9.329  1.00  0.00           O
ATOM    958  CB  ALA E  21      -2.943  -4.174  -9.922  1.00  0.00           C
ATOM    959  H   ALA E  21      -2.583  -7.049  -9.283  1.00  0.00           H
ATOM    960  N   GLU E  22      -0.172  -6.230 -11.317  1.00  0.00           N
ATOM    961  CA  GLU E  22       1.271  -6.342 -11.573  1.00  0.00           C
ATOM    962  C   GLU E  22       1.729  -4.993 -12.138  1.00  0.00           C
ATOM    963  O   GLU E  22       2.009  -4.843 -13.327  1.00  0.00           O
ATOM    964  CB  GLU E  22       1.546  -7.535 -12.503  1.00  0.00           C
ATOM    965  CG  GLU E  22       3.017  -7.666 -12.872  1.00  0.00           C
ATOM    966  CD  GLU E  22       3.242  -8.866 -13.798  1.00  0.00           C
ATOM    967  OE1 GLU E  22       2.600  -9.016 -14.856  1.00  0.00           O
ATOM    968  OE2 GLU E  22       4.097  -9.673 -13.379  1.00  0.00           O1-
ATOM    969  H   GLU E  22      -0.823  -6.456 -12.050  1.00  0.00           H
ATOM    970  N   ASP E  23       1.912  -4.054 -11.217  1.00  0.00           N
ATOM    971  CA  ASP E  23       2.320  -2.658 -11.476  1.00  0.00           C
ATOM    972  C   ASP E  23       3.798  -2.466 -11.820  1.00  0.00           C
ATOM    973  O   ASP E  23       4.601  -2.254 -10.911  1.00  0.00           O
ATOM    974  CB  ASP E  23       1.807  -1.723 -10.378  1.00  0.00           C
ATOM    975  CG  ASP E  23       1.315  -0.368 -10.881  1.00  0.00           C
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ATOM    976  OD1 ASP E  23       2.003   0.640 -10.664  1.00  0.00           O
ATOM    977  OD2 ASP E  23       0.341  -0.365 -11.664  1.00  0.00           O1-
ATOM    978  H   ASP E  23       1.841  -4.306 -10.255  1.00  0.00           H
ATOM    979  N   VAL E  24       4.094  -2.246 -13.096  1.00  0.00           N
ATOM    980  CA  VAL E  24       5.414  -2.076 -13.729  1.00  0.00           C
ATOM    981  C   VAL E  24       5.805  -0.598 -13.721  1.00  0.00           C
ATOM    982  O   VAL E  24       4.992   0.282 -14.026  1.00  0.00           O
ATOM    983  CB  VAL E  24       5.323  -2.586 -15.167  1.00  0.00           C
ATOM    984  CG1 VAL E  24       6.612  -2.352 -15.956  1.00  0.00           C
ATOM    985  CG2 VAL E  24       5.037  -4.088 -15.257  1.00  0.00           C
ATOM    986  H   VAL E  24       3.394  -1.837 -13.691  1.00  0.00           H
ATOM    987  N   GLY E  25       7.029  -0.307 -13.295  1.00  0.00           N
ATOM    988  CA  GLY E  25       7.563   1.050 -13.091  1.00  0.00           C
ATOM    989  C   GLY E  25       8.947   1.054 -12.434  1.00  0.00           C
ATOM    990  O   GLY E  25       9.036   0.923 -11.214  1.00  0.00           O
ATOM    991  H   GLY E  25       7.586  -1.066 -12.967  1.00  0.00           H
ATOM    992  N   SER E  26       9.985   1.182 -13.247  1.00  0.00           N
ATOM    993  CA  SER E  26      11.391   1.211 -12.815  1.00  0.00           C
ATOM    994  C   SER E  26      11.658   2.580 -12.192  1.00  0.00           C
ATOM    995  O   SER E  26      10.970   3.552 -12.499  1.00  0.00           O
ATOM    996  CB  SER E  26      12.252   0.996 -14.062  1.00  0.00           C
ATOM    997  OG  SER E  26      13.650   1.026 -13.741  1.00  0.00           O
ATOM    998  H   SER E  26       9.885   1.121 -14.239  1.00  0.00           H
ATOM    999  HG  SER E  26      14.123   1.182 -14.611  1.00  0.00           H
ATOM   1000  N   ASN E  27      12.470   2.532 -11.134  1.00  0.00           N
ATOM   1001  CA  ASN E  27      12.726   3.735 -10.334  1.00  0.00           C
ATOM   1002  C   ASN E  27      11.566   4.412  -9.608  1.00  0.00           C
ATOM   1003  O   ASN E  27      11.246   5.546  -9.934  1.00  0.00           O
ATOM   1004  CB  ASN E  27      13.497   4.770 -11.159  1.00  0.00           C
ATOM   1005  CG  ASN E  27      14.987   4.432 -11.287  1.00  0.00           C
ATOM   1006  ND2 ASN E  27      15.556   4.749 -12.442  1.00  0.00           N
ATOM   1007  OD1 ASN E  27      15.604   4.284 -10.238  1.00  0.00           O
ATOM   1008  H   ASN E  27      12.997   1.721 -10.882  1.00  0.00           H
ATOM   1009 1HD2 ASN E  27      15.015   5.125 -13.207  1.00  0.00           H
ATOM   1010 2HD2 ASN E  27      16.526   4.956 -12.548  1.00  0.00           H
ATOM   1011  N   LYS E  28      10.930   3.723  -8.659  1.00  0.00           N
ATOM   1012  CA  LYS E  28       9.825   4.213  -7.816  1.00  0.00           C
ATOM   1013  C   LYS E  28      10.175   4.734  -6.420  1.00  0.00           C
ATOM   1014  O   LYS E  28       9.339   4.644  -5.529  1.00  0.00           O
ATOM   1015  CB  LYS E  28       8.817   3.071  -7.622  1.00  0.00           C
ATOM   1016  CG  LYS E  28       8.076   2.792  -8.923  1.00  0.00           C
ATOM   1017  CD  LYS E  28       7.005   1.717  -8.668  1.00  0.00           C
ATOM   1018  CE  LYS E  28       6.011   1.543  -9.813  1.00  0.00           C
ATOM   1019  NZ  LYS E  28       4.859   0.660  -9.573  1.00  0.00           N1+
ATOM   1020  H   LYS E  28      11.258   2.817  -8.403  1.00  0.00           H
ATOM   1021  HZ1 LYS E  28       5.336  -0.214  -9.485  1.00  0.00           H
ATOM   1022  HZ2 LYS E  28       4.304   0.961  -8.807  1.00  0.00           H
ATOM   1023  HZ3 LYS E  28       4.329   0.674 -10.421  1.00  0.00           H
ATOM   1024  N   GLY E  29      11.330   5.383  -6.259  1.00  0.00           N
ATOM   1025  CA  GLY E  29      11.707   6.149  -5.064  1.00  0.00           C
ATOM   1026  C   GLY E  29      11.060   7.535  -4.970  1.00  0.00           C
ATOM   1027  O   GLY E  29      11.882   8.450  -4.970  1.00  0.00           O
ATOM   1028  H   GLY E  29      12.109   5.091  -6.818  1.00  0.00           H
ATOM   1029  N   ALA E  30       9.742   7.675  -4.833  1.00  0.00           N
ATOM   1030  CA  ALA E  30       8.952   8.895  -5.013  1.00  0.00           C
ATOM   1031  C   ALA E  30       9.148   9.891  -3.877  1.00  0.00           C
ATOM   1032  O   ALA E  30       9.036   9.494  -2.719  1.00  0.00           O
ATOM   1033  CB  ALA E  30       7.507   8.402  -4.964  1.00  0.00           C
ATOM   1034  H   ALA E  30       9.234   6.965  -4.347  1.00  0.00           H
ATOM   1035  N   ILE E  31       8.778  11.131  -4.219  1.00  0.00           N
ATOM   1036  CA  ILE E  31       8.639  12.241  -3.266  1.00  0.00           C
ATOM   1037  C   ILE E  31       7.253  12.237  -2.623  1.00  0.00           C
ATOM   1038  O   ILE E  31       7.195  11.796  -1.480  1.00  0.00           O
ATOM   1039  CB  ILE E  31       8.961  13.566  -3.959  1.00  0.00           C
ATOM   1040  CG1 ILE E  31      10.121  13.566  -4.955  1.00  0.00           C
ATOM   1041  CG2 ILE E  31       9.095  14.696  -2.938  1.00  0.00           C
ATOM   1042  CD  ILE E  31      11.507  13.158  -4.440  1.00  0.00           C
ATOM   1043  H   ILE E  31       8.699  11.338  -5.191  1.00  0.00           H
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ATOM   1044  N   ILE E  32       6.163  12.404  -3.360  1.00  0.00           N
ATOM   1045  CA  ILE E  32       4.756  12.226  -2.963  1.00  0.00           C
ATOM   1046  C   ILE E  32       4.359  10.775  -2.719  1.00  0.00           C
ATOM   1047  O   ILE E  32       5.098   9.836  -3.038  1.00  0.00           O
ATOM   1048  CB  ILE E  32       3.830  12.935  -3.956  1.00  0.00           C
ATOM   1049  CG1 ILE E  32       4.169  12.566  -5.400  1.00  0.00           C
ATOM   1050  CG2 ILE E  32       3.748  14.422  -3.616  1.00  0.00           C
ATOM   1051  CD  ILE E  32       3.003  12.957  -6.320  1.00  0.00           C
ATOM   1052  H   ILE E  32       6.279  13.025  -4.141  1.00  0.00           H
ATOM   1053  N   GLY E  33       3.172  10.580  -2.156  1.00  0.00           N
ATOM   1054  CA  GLY E  33       2.738   9.208  -1.827  1.00  0.00           C
ATOM   1055  C   GLY E  33       2.526   8.302  -3.040  1.00  0.00           C
ATOM   1056  O   GLY E  33       1.640   8.623  -3.843  1.00  0.00           O
ATOM   1057  H   GLY E  33       2.703  11.284  -1.625  1.00  0.00           H
ATOM   1058  N   LEU E  34       3.172   7.145  -3.067  1.00  0.00           N
ATOM   1059  CA  LEU E  34       3.151   6.223  -4.210  1.00  0.00           C
ATOM   1060  C   LEU E  34       2.009   5.224  -4.027  1.00  0.00           C
ATOM   1061  O   LEU E  34       1.933   4.583  -2.987  1.00  0.00           O
ATOM   1062  CB  LEU E  34       4.505   5.504  -4.150  1.00  0.00           C
ATOM   1063  CG  LEU E  34       4.651   4.689  -5.432  1.00  0.00           C
ATOM   1064  CD1 LEU E  34       4.981   5.441  -6.729  1.00  0.00           C
ATOM   1065  CD2 LEU E  34       5.635   3.543  -5.191  1.00  0.00           C
ATOM   1066  H   LEU E  34       3.522   6.748  -2.216  1.00  0.00           H
ATOM   1067  N   MET E  35       0.929   5.525  -4.754  1.00  0.00           N
ATOM   1068  CA  MET E  35      -0.377   4.862  -4.789  1.00  0.00           C
ATOM   1069  C   MET E  35      -0.249   3.542  -5.555  1.00  0.00           C
ATOM   1070  O   MET E  35       0.437   3.444  -6.573  1.00  0.00           O
ATOM   1071  CB  MET E  35      -1.461   5.607  -5.571  1.00  0.00           C
ATOM   1072  CG  MET E  35      -2.840   5.302  -4.986  1.00  0.00           C
ATOM   1073  SD  MET E  35      -3.094   6.427  -3.563  1.00  0.00           S
ATOM   1074  CE  MET E  35      -4.105   5.241  -2.714  1.00  0.00           C
ATOM   1075  H   MET E  35       0.991   6.386  -5.267  1.00  0.00           H
ATOM   1076  N   VAL E  36      -0.533   2.506  -4.785  1.00  0.00           N
ATOM   1077  CA  VAL E  36      -0.598   1.099  -5.217  1.00  0.00           C
ATOM   1078  C   VAL E  36      -2.024   0.559  -5.174  1.00  0.00           C
ATOM   1079  O   VAL E  36      -2.575   0.143  -4.161  1.00  0.00           O
ATOM   1080  CB  VAL E  36       0.279   0.272  -4.274  1.00  0.00           C
ATOM   1081  CG1 VAL E  36       0.237  -1.240  -4.537  1.00  0.00           C
ATOM   1082  CG2 VAL E  36       1.723   0.761  -4.115  1.00  0.00           C
ATOM   1083  H   VAL E  36      -0.781   2.663  -3.828  1.00  0.00           H
ATOM   1084  N   GLY E  37      -2.656   0.642  -6.344  1.00  0.00           N
ATOM   1085  CA  GLY E  37      -4.065   0.276  -6.553  1.00  0.00           C
ATOM   1086  C   GLY E  37      -4.806   1.104  -7.607  1.00  0.00           C
ATOM   1087  O   GLY E  37      -5.098   0.584  -8.687  1.00  0.00           O
ATOM   1088  H   GLY E  37      -2.191   0.803  -7.212  1.00  0.00           H
ATOM   1089  N   GLY E  38      -5.323   2.272  -7.243  1.00  0.00           N
ATOM   1090  CA  GLY E  38      -5.972   3.166  -8.197  1.00  0.00           C
ATOM   1091  C   GLY E  38      -7.339   3.738  -7.799  1.00  0.00           C
ATOM   1092  O   GLY E  38      -7.727   3.783  -6.637  1.00  0.00           O
ATOM   1093  H   GLY E  38      -5.376   2.552  -6.277  1.00  0.00           H
ATOM   1094  N   VAL E  39      -8.121   4.098  -8.818  1.00  0.00           N
ATOM   1095  CA  VAL E  39      -9.526   4.489  -8.713  1.00  0.00           C
ATOM   1096  C   VAL E  39     -10.541   3.545  -8.045  1.00  0.00           C
ATOM   1097  O   VAL E  39     -10.355   2.333  -8.140  1.00  0.00           O
ATOM   1098  CB  VAL E  39      -9.975   4.874 -10.118  1.00  0.00           C
ATOM   1099  CG1 VAL E  39      -9.114   5.980 -10.739  1.00  0.00           C
ATOM   1100  CG2 VAL E  39     -10.056   3.769 -11.174  1.00  0.00           C
ATOM   1101  H   VAL E  39      -7.629   4.258  -9.673  1.00  0.00           H
ATOM   1102  N   VAL E  40     -11.495   4.169  -7.368  1.00  0.00           N
ATOM   1103  CA  VAL E  40     -12.648   3.462  -6.793  1.00  0.00           C
ATOM   1104  C   VAL E  40     -13.863   4.379  -6.702  1.00  0.00           C
ATOM   1105  O   VAL E  40     -13.717   5.549  -6.328  1.00  0.00           O
ATOM   1106  CB  VAL E  40     -12.258   2.847  -5.448  1.00  0.00           C
ATOM   1107  CG1 VAL E  40     -11.711   3.666  -4.269  1.00  0.00           C
ATOM   1108  CG2 VAL E  40     -13.295   1.895  -4.837  1.00  0.00           C
ATOM   1109  H   VAL E  40     -11.422   5.110  -7.030  1.00  0.00           H
ATOM   1110  N   ILE E  41     -15.025   3.748  -6.840  1.00  0.00           N
ATOM   1111  CA  ILE E  41     -16.277   4.512  -6.928  1.00  0.00           C
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ATOM   1112  C   ILE E  41     -17.171   4.595  -5.685  1.00  0.00           C
ATOM   1113  O   ILE E  41     -17.122   3.655  -4.883  1.00  0.00           O
ATOM   1114  CB  ILE E  41     -17.081   4.071  -8.152  1.00  0.00           C
ATOM   1115  CG1 ILE E  41     -17.245   2.553  -8.204  1.00  0.00           C
ATOM   1116  CG2 ILE E  41     -16.509   4.866  -9.331  1.00  0.00           C
ATOM   1117  CD  ILE E  41     -18.682   2.207  -8.633  1.00  0.00           C
ATOM   1118  H   ILE E  41     -15.127   2.760  -6.734  1.00  0.00           H
ATOM   1119  N   ALA E  42     -17.877   5.689  -5.444  1.00  0.00           N
ATOM   1120  CA  ALA E  42     -18.636   5.894  -4.196  1.00  0.00           C
ATOM   1121  C   ALA E  42     -19.917   6.730  -4.285  1.00  0.00           C
ATOM   1122  CB  ALA E  42     -17.729   6.562  -3.163  1.00  0.00           C
ATOM   1123  O1  ALA E  42     -19.838   7.694  -5.071  1.00  0.00           O
ATOM   1124  O2  ALA E  42     -20.954   6.585  -3.597  1.00  0.00           O
ATOM   1125  H   ALA E  42     -17.765   6.578  -5.887  1.00  0.00           H
ATOM   1126  C1  6n  F  43     -13.676  -1.755  -8.856  1.00  0.00           C
ATOM   1127  N1  6n  F  43     -14.464   1.661 -11.433  1.00  0.00           N
ATOM   1128  O1  6n  F  43     -15.597  -3.134  -9.445  1.00  0.00           O
ATOM   1129  C2  6n  F  43     -14.485  -0.471  -8.490  1.00  0.00           C
ATOM   1130  N2  6n  F  43     -13.598   2.363 -10.648  1.00  0.00           N
ATOM   1131  O2  6n  F  43     -14.296  -2.578 -11.168  1.00  0.00           O
ATOM   1132  C3  6n  F  43     -14.283   0.615  -9.475  1.00  0.00           C
ATOM   1133  N3  6n  F  43     -13.423   1.738  -9.565  1.00  0.00           N
ATOM   1134  O3  6n  F  43     -10.532  -1.548 -10.464  1.00  0.00           O
ATOM   1135  C4  6n  F  43     -14.972   0.571 -10.704  1.00  0.00           C
ATOM   1136  N4  6n  F  43     -11.328  -1.020  -5.185  1.00  0.00           N
ATOM   1137  C5  6n  F  43     -14.541   1.666 -12.846  1.00  0.00           C
ATOM   1138  N5  6n  F  43     -11.703  -2.150  -4.537  1.00  0.00           N
ATOM   1139  C6  6n  F  43     -14.776   0.466 -13.538  1.00  0.00           C
ATOM   1140  N6  6n  F  43     -12.690  -2.687  -5.128  1.00  0.00           N
ATOM   1141  C7  6n  F  43     -14.912   0.439 -14.924  1.00  0.00           C
ATOM   1142  N7  6n  F  43     -12.409  -1.475  -9.482  1.00  0.00           N
ATOM   1143  C8  6n  F  43     -14.818   1.594 -15.680  1.00  0.00           C
ATOM   1144  C9  6n  F  43     -14.704   2.765 -14.933  1.00  0.00           C
ATOM   1145  C10 6n  F  43     -14.611   2.885 -13.554  1.00  0.00           C
ATOM   1146  C11 6n  F  43     -14.523   4.317 -13.014  1.00  0.00           C
ATOM   1147  C12 6n  F  43     -14.563  -2.576  -9.834  1.00  0.00           C
ATOM   1148  C13 6n  F  43     -15.041  -3.421 -12.073  1.00  0.00           C
ATOM   1149  C14 6n  F  43     -14.506  -3.317 -13.481  1.00  0.00           C
ATOM   1150  C15 6n  F  43     -13.643  -2.590  -7.538  1.00  0.00           C
ATOM   1151  C16 6n  F  43     -12.914  -2.060  -6.384  1.00  0.00           C
ATOM   1152  C17 6n  F  43     -12.068  -0.927  -6.377  1.00  0.00           C
ATOM   1153  C18 6n  F  43     -10.011  -0.492  -5.083  1.00  0.00           C
ATOM   1154  C19 6n  F  43      -9.386  -0.758  -3.851  1.00  0.00           C
ATOM   1155  C20 6n  F  43      -7.999  -0.843  -3.904  1.00  0.00           C
ATOM   1156  C21 6n  F  43      -7.284  -0.598  -5.070  1.00  0.00           C
ATOM   1157  C22 6n  F  43      -7.909  -0.234  -6.259  1.00  0.00           C
ATOM   1158  C23 6n  F  43      -9.289  -0.171  -6.260  1.00  0.00           C
ATOM   1159  C24 6n  F  43     -10.036  -0.438  -2.507  1.00  0.00           C
ATOM   1160  C25 6n  F  43     -11.405  -2.295  -9.958  1.00  0.00           C
ATOM   1161  C26 6n  F  43     -11.158  -3.756  -9.710  1.00  0.00           C
ATOM   1162  F1  6n  F  43     -13.547   4.632 -12.090  1.00  0.00           F
ATOM   1163  F2  6n  F  43     -14.362   5.486 -13.736  1.00  0.00           F
ATOM   1164  F3  6n  F  43     -15.703   4.785 -12.462  1.00  0.00           F
ATOM   1165  F4  6n  F  43      -9.198  -0.089  -1.471  1.00  0.00           F
ATOM   1166  F5  6n  F  43     -10.817   0.692  -2.390  1.00  0.00           F
ATOM   1167  F6  6n  F  43     -10.806  -1.410  -1.888  1.00  0.00           F
ATOM   1168  H1  6n  F  43     -12.231  -0.486  -9.453  1.00  0.00           H
ATOM   1169  H03 6n  F  43     -15.600  -0.136 -11.244  1.00  0.00           H
ATOM   1170  H04 6n  F  43     -14.910  -0.489 -12.996  1.00  0.00           H
ATOM   1171  H05 6n  F  43     -15.241  -0.487 -15.429  1.00  0.00           H
ATOM   1172  H06 6n  F  43     -15.129   1.550 -16.726  1.00  0.00           H
ATOM   1173  H07 6n  F  43     -14.247   3.639 -15.433  1.00  0.00           H
ATOM   1174  H11 6n  F  43     -12.095  -0.060  -7.041  1.00  0.00           H
ATOM   1175  H12 6n  F  43      -7.448  -1.064  -2.973  1.00  0.00           H
ATOM   1176  H13 6n  F  43      -6.258  -1.003  -5.130  1.00  0.00           H
ATOM   1177  H14 6n  F  43      -7.327   0.019  -7.158  1.00  0.00           H
ATOM   1178  H15 6n  F  43      -9.795   0.092  -7.204  1.00  0.00           H
END
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## Reference

1. A. Kaur, S. Mann, A. Kaur, N. Priyadarshi, B. Goyal, N. K. Singhal and D. Goyal, *Bioorg. Chem*., 2019, **87**, 572–584.