Load the BINANA module

This notebook was tested in Jupyter Notebook 5.7.8. It did not work when tested in Jupyter Lab. We have confirmed that similar usage works in HTML/JavaScript web pages.

In [31]:
```
%%html
<script type="module">
    window.binana = undefined
    import * as bnana from './binana.js';
    window.binana = bnana;
</script>
```

Define a JavaScript function to output formatted results

In [32]:
```
%%javascript

window.output = function(element, txt) {
    element.html("<pre style='font-size:80%;'>" + txt + "</pre>");
};
```

Define ligand PDBQT text

In [33]:

```
%%javascript

window.ligPDBTxt = `REMARK  8 active torsions:
REMARK  status: ('A' for Active; 'I' for Inactive)
REMARK    1  A    between atoms: C4_1  and  C5_2
REMARK    2  A    between atoms: C4_1  and  N1_7
REMARK    3  A    between atoms: C4_1  and  O6_5
REMARK    4  A    between atoms: C5_2  and  N1_6
REMARK    5  A    between atoms: C7_4  and  N1_6
REMARK    6  A    between atoms: C7_4  and  C1_8
REMARK    7  A    between atoms: N1_6  and  C6_14
REMARK    8  A    between atoms: N1_7  and  C2_9
ROOT
HETATM    1  C5  CHT A   1      16.376   2.063   7.151  1.00  6.35      0.30
ENDROOT
BRANCH   1   2
HETATM    2  N1  CHT A   1      15.723   3.326   7.619  1.00  6.17     -0.00
HETATM    3  C6  CHT A   1      15.386   3.121   9.043  1.00  5.88      0.28
BRANCH   2   4
HETATM    4  C6  CHT A   1      14.451   3.555   6.881  1.00  0.00      0.24
HETATM    5  C7  CHT A   1      14.179   3.052   5.671  1.00  0.00      0.06
HETATM    6  C8  CHT A   1      12.835   3.506   5.294  1.00  0.00      0.02
HETATM    7  C9  CHT A   1      12.365   4.258   6.295  1.00  0.00      0.14
HETATM    8  O2  CHT A   1      13.332   4.389   7.437  1.00  0.00     -0.30
ENDBRANCH   2   4
BRANCH   2   9
HETATM    9  C7  CHT A   1      16.663   4.518   7.461  1.00  4.71      0.35
BRANCH   9  10
HETATM   10  C1  CHT A   1      17.243   5.230   8.677  1.00  0.00      0.20
HETATM   11  O4  CHT A   1      16.818   5.027   9.728  1.00  0.00     -0.64
HETATM   12  O3  CHT A   1      18.046   6.106   8.908  1.00  0.00     -0.64
ENDBRANCH   9  10
ENDBRANCH   2   9
ENDBRANCH   1   2
BRANCH   1  13
HETATM   13  C4  CHT A   1      17.023   2.039   5.749  1.00  7.51      0.35
BRANCH  13  14
HETATM   14  N1  CHT A   1      17.117   0.715   5.182  1.00  0.00      0.00
HETATM   15  H2  CHT A   1      16.240   0.227   5.182  1.00  0.00      0.28
HETATM   16  H1  CHT A   1      17.432   0.801   4.195  1.00  0.00      0.28
BRANCH  14  17
HETATM   17  C2  CHT A   1      18.204  -0.049   5.920  1.00  0.00      0.24
HETATM   18  O1  CHT A   1      19.656   0.045   5.545  1.00  0.00     -0.30
HETATM   19  C5  CHT A   1      20.217  -0.885   6.582  1.00  0.00      0.14
HETATM   20  C4  CHT A   1      19.280  -1.403   7.384  1.00  0.00      0.02
HETATM   21  C3  CHT A   1      17.983  -0.864   6.957  1.00  0.00      0.06
ENDBRANCH  14  17
ENDBRANCH  13  14
BRANCH  13  22
HETATM   22  O6  CHT A   1      18.398   2.270   5.897  1.00  8.52     -0.36
HETATM   23  HO6 CHT A   1      18.813   2.276   5.007  1.00  0.00      0.21
ENDBRANCH  13  22
ENDBRANCH   1  13
TORSDOF 8`;
```

Define protein PDBQT text

In [34]:

```
%%javascript

window.recepPDBTxt = `ATOM      1  N   ASP A  40      23.366  -3.399  14.66
ATOM      2  CA  ASP A  40      22.530  -2.226  14.843  1.00 15.81      0.20
ATOM      3  C   ASP A  40      23.197  -1.095  14.078  1.00 15.68      0.24
ATOM      4  O   ASP A  40      24.256  -0.613  14.476  1.00 15.64     -0.27
ATOM      5  CB  ASP A  40      22.432  -1.893  16.332  1.00 15.92      0.14
ATOM      6  CG  ASP A  40      21.603  -0.652  16.619  1.00 16.79      0.17
ATOM      7  OD1 ASP A  40      21.101   0.007  15.681  1.00 17.82     -0.64
ATOM      8  OD2 ASP A  40      21.413  -0.255  17.786  1.00 19.39     -0.64
ATOM      9  H   ASP A  40      24.353  -3.311  14.877  1.00  0.00      0.18
ATOM     10  N   VAL A  41      22.581  -0.683  12.973  1.00 15.78     -0.34
ATOM     11  CA  VAL A  41      23.169   0.349  12.110  1.00 15.92      0.18
ATOM     12  C   VAL A  41      23.137   1.720  12.785  1.00 16.19      0.24
ATOM     13  O   VAL A  41      23.963   2.596  12.486  1.00 16.57     -0.27
ATOM     14  CB  VAL A  41      22.514   0.374  10.712  1.00 15.84      0.00
ATOM     15  CG1 VAL A  41      23.234   1.342   9.761  1.00 15.67      0.01
ATOM     16  CG2 VAL A  41      22.531  -1.022  10.096  1.00 16.11      0.01
ATOM     17  H   VAL A  41      21.709  -1.109  12.695  1.00  0.00      0.16
ATOM     18  N   GLY A  42      22.202   1.885  13.713  1.00 15.88     -0.35
ATOM     19  CA  GLY A  42      22.136   3.082  14.535  1.00 15.70      0.22
ATOM     20  C   GLY A  42      20.886   3.924  14.379  1.00 15.32      0.23
ATOM     21  O   GLY A  42      20.671   4.848  15.172  1.00 15.23     -0.27
ATOM     22  H   GLY A  42      21.603   1.109  13.966  1.00  0.00      0.16
ATOM     23  N   TRP A  43      20.067   3.630  13.366  1.00 14.72     -0.34
ATOM     24  CA  TRP A  43      18.778   4.311  13.226  1.00 14.44      0.18
ATOM     25  C   TRP A  43      17.932   3.984  14.459  1.00 14.06      0.24
ATOM     26  O   TRP A  43      18.069   2.906  15.035  1.00 14.14     -0.27
ATOM     27  CB  TRP A  43      18.028   3.887  11.955  1.00 14.50      0.07
ATOM     28  CG  TRP A  43      18.852   3.543  10.764  1.00 14.78     -0.02
ATOM     29  CD1 TRP A  43      19.772   4.326  10.159  1.00 14.91      0.09
ATOM     30  CD2 TRP A  43      18.860   2.280  10.050  1.00 14.20     -0.00
ATOM     31  NE1 TRP A  43      20.356   3.632   9.123  1.00 14.90     -0.36
ATOM     32  CE2 TRP A  43      19.833   2.360   9.011  1.00 14.43      0.04
ATOM     33  CE3 TRP A  43      18.124   1.077  10.178  1.00 14.13      0.01
ATOM     34  CZ2 TRP A  43      20.063   1.286   8.142  1.00 14.63      0.03
ATOM     35  CZ3 TRP A  43      18.350  -0.008   9.313  1.00 14.56      0.00
ATOM     36  CH2 TRP A  43      19.316   0.106   8.298  1.00 14.58      0.00
ATOM     37  H   TRP A  43      20.294   2.873  12.738  1.00  0.00      0.16
ATOM     38  HE1 TRP A  43      21.179   4.024   8.621  1.00  0.00      0.16
ATOM     39  N   THR A  44      17.062   4.907  14.857  1.00 13.58     -0.34
ATOM     40  CA  THR A  44      16.229   4.697  16.050  1.00 13.07      0.20
ATOM     41  C   THR A  44      15.366   3.431  15.946  1.00 12.89      0.24
ATOM     42  O   THR A  44      15.203   2.719  16.929  1.00 12.25     -0.27
ATOM     43  CB  THR A  44      15.358   5.934  16.326  1.00 13.11      0.14
ATOM     44  OG1 THR A  44      16.191   7.100  16.371  1.00 12.54     -0.39
ATOM     45  CG2 THR A  44      14.740   5.865  17.735  1.00 13.56      0.04
ATOM     46  H   THR A  44      16.968   5.767  14.327  1.00  0.00      0.16
ATOM     47  HG1 THR A  44      16.365   7.406  15.487  1.00  0.00      0.21
ATOM     48  N   ASP A  45      14.834   3.144  14.756  1.00 12.67     -0.34
ATOM     49  CA  ASP A  45      13.958   1.979  14.592  1.00 12.87      0.18
ATOM     50  C   ASP A  45      14.693   0.650  14.775  1.00 13.06      0.24
ATOM     51  O   ASP A  45      14.203  -0.233  15.477  1.00 13.06     -0.27
ATOM     52  CB  ASP A  45      13.196   2.016  13.235  1.00 13.01      0.14
ATOM     53  CG  ASP A  45      14.042   1.759  11.988  1.00 13.25      0.17
ATOM     54  OD1 ASP A  45      15.013   2.526  11.815  1.00 14.05     -0.64
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ATOM     55  OD2 ASP A  45      13.740   0.837  11.196  1.00 13.00    -0.64
ATOM     56  H   ASP A  45      15.036   3.719  13.950  1.00  0.00     0.16
ATOM     57  N   ILE A  46      15.868   0.512  14.158  1.00 13.12    -0.34
ATOM     58  CA  ILE A  46      16.648  -0.722  14.301  1.00 13.55     0.18
ATOM     59  C   ILE A  46      17.199  -0.860  15.723  1.00 13.70     0.24
ATOM     60  O   ILE A  46      17.346  -1.969  16.223  1.00 13.30    -0.27
ATOM     61  CB  ILE A  46      17.763  -0.847  13.206  1.00 13.63     0.01
ATOM     62  CG1 ILE A  46      18.452  -2.215  13.258  1.00 13.94     0.00
ATOM     63  CG2 ILE A  46      18.797   0.261  13.335  1.00 14.03     0.01
ATOM     64  CD1 ILE A  46      17.523  -3.407  13.070  1.00 13.44     0.00
ATOM     65  H   ILE A  46      16.218   1.256  13.569  1.00  0.00     0.16
ATOM     66  N   THR A  47      17.474   0.267  16.384  1.00 14.15    -0.34
ATOM     67  CA  THR A  47      17.887   0.227  17.788  1.00 14.72     0.20
ATOM     68  C   THR A  47      16.727  -0.263  18.660  1.00 14.48     0.24
ATOM     69  O   THR A  47      16.931  -1.016  19.615  1.00 14.70    -0.27
ATOM     70  CB  THR A  47      18.408   1.604  18.247  1.00 14.88     0.14
ATOM     71  OG1 THR A  47      19.530   1.978  17.436  1.00 15.66    -0.39
ATOM     72  CG2 THR A  47      19.022   1.523  19.646  1.00 16.13     0.04
ATOM     73  H   THR A  47      17.394   1.166  15.925  1.00  0.00     0.16
ATOM     74  HG1 THR A  47      20.171   1.276  17.456  1.00  0.00     0.21
ATOM     75  N   ALA A  48      15.515   0.167  18.315  1.00 14.28    -0.34
ATOM     76  CA  ALA A  48      14.303  -0.202  19.046  1.00 14.12     0.17
ATOM     77  C   ALA A  48      13.950  -1.678  18.886  1.00 13.83     0.24
ATOM     78  O   ALA A  48      13.683  -2.357  19.877  1.00 13.54    -0.27
ATOM     79  CB  ALA A  48      13.129   0.678  18.618  1.00 14.05     0.04
ATOM     80  H   ALA A  48      15.423   0.801  17.531  1.00  0.00     0.16
ATOM     81  N   THR A  49      13.951  -2.172  17.648  1.00 13.66    -0.34
ATOM     82  CA  THR A  49      13.629  -3.581  17.402  1.00 13.40     0.19
ATOM     83  C   THR A  49      14.694  -4.504  17.988  1.00 13.28     0.22
ATOM     84  O   THR A  49      14.371  -5.555  18.535  1.00 13.49    -0.28
ATOM     85  CB  THR A  49      13.441  -3.883  15.900  1.00 13.46     0.14
ATOM     86  OG1 THR A  49      14.556  -3.379  15.153  1.00 13.38    -0.39
ATOM     87  CG2 THR A  49      12.238  -3.145  15.346  1.00 13.62     0.04
ATOM     88  H   THR A  49      14.157  -1.564  16.866  1.00  0.00     0.16
ATOM     89  HG1 THR A  49      14.546  -2.434  15.199  1.00  0.00     0.21
ATOM     90  N   GLY A  88      17.040  -5.422  10.405  1.00 12.46    -0.33
ATOM     91  CA  GLY A  88      16.804  -4.172   9.687  1.00 12.42     0.22
ATOM     92  C   GLY A  88      16.909  -4.259   8.184  1.00 12.27     0.21
ATOM     93  O   GLY A  88      17.363  -3.303   7.556  1.00 12.16    -0.28
ATOM     94  H   GLY A  88      17.987  -5.765  10.479  1.00  0.00     0.18
ATOM     95  N   TRP A  90      15.564  -3.624   5.029  1.00 12.20    -0.32
ATOM     96  CA  TRP A  90      14.502  -2.864   4.372  1.00 12.40     0.19
ATOM     97  C   TRP A  90      14.476  -3.199   2.875  1.00 12.75     0.24
ATOM     98  O   TRP A  90      15.493  -3.151   2.174  1.00 13.02    -0.27
ATOM     99  CB  TRP A  90      14.718  -1.367   4.573  1.00 12.16     0.07
ATOM    100  CG  TRP A  90      14.277  -0.849   5.935  1.00 11.70    -0.02
ATOM    101  CD1 TRP A  90      15.070  -0.651   7.015  1.00 11.86     0.09
ATOM    102  CD2 TRP A  90      12.935  -0.486   6.377  1.00 12.11    -0.00
ATOM    103  NE1 TRP A  90      14.322  -0.196   8.083  1.00 11.22    -0.36
ATOM    104  CE2 TRP A  90      12.995  -0.100   7.753  1.00 11.58     0.04
ATOM    105  CE3 TRP A  90      11.664  -0.452   5.762  1.00 12.22     0.01
ATOM    106  CZ2 TRP A  90      11.867   0.303   8.478  1.00 11.72     0.03
ATOM    107  CZ3 TRP A  90      10.522  -0.035   6.478  1.00 11.86     0.00
ATOM    108  CH2 TRP A  90      10.627   0.353   7.827  1.00 11.69     0.00
ATOM    109  H   TRP A  90      16.500  -3.228   5.095  1.00  0.00     0.18
ATOM    110  HE1 TRP A  90      14.655  -0.008   9.037  1.00  0.00     0.16
ATOM    111  N   MET A  91      13.288  -3.554   2.389  1.00 13.09    -0.34
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ATOM    112  CA  MET A  91      13.056  -3.901   0.997  1.00 13.24      0.17
ATOM    113  C   MET A  91      11.899  -3.053   0.465  1.00 13.24      0.24
ATOM    114  O   MET A  91      10.902  -2.887   1.164  1.00 13.54     -0.27
ATOM    115  CB  MET A  91      12.752  -5.398   0.858  1.00 13.31      0.04
ATOM    116  CG  MET A  91      13.889  -6.315   1.325  1.00 14.49      0.07
ATOM    117  SD  MET A  91      15.369  -6.218   0.294  1.00 15.59     -0.17
ATOM    118  CE  MET A  91      14.916  -7.321  -1.041  1.00 16.54      0.08
ATOM    119  H   MET A  91      12.484  -3.598   3.016  1.00  0.00      0.16
ATOM    120  N   PRO A  92      11.985  -2.553  -0.771  1.00 13.31     -0.33
ATOM    121  CA  PRO A  92      12.964  -2.988  -1.772  1.00 13.27      0.17
ATOM    122  C   PRO A  92      14.346  -2.294  -1.822  1.00 13.10      0.24
ATOM    123  O   PRO A  92      15.187  -2.715  -2.602  1.00 12.78     -0.27
ATOM    124  CB  PRO A  92      12.229  -2.707  -3.080  1.00 13.32      0.03
ATOM    125  CG  PRO A  92      11.445  -1.452  -2.784  1.00 13.37      0.02
ATOM    126  CD  PRO A  92      11.080  -1.519  -1.310  1.00 13.30      0.12
ATOM    127  N   THR A  93      14.665  -1.240  -1.077  1.00 13.14     -0.34
ATOM    128  CA  THR A  93      15.904  -0.503  -1.373  1.00 13.15      0.20
ATOM    129  C   THR A  93      17.214  -1.240  -1.093  1.00 13.41      0.24
ATOM    130  O   THR A  93      18.231  -0.857  -1.689  1.00 13.68     -0.27
ATOM    131  CB  THR A  93      15.853   0.835  -0.661  1.00 12.81      0.14
ATOM    132  OG1 THR A  93      15.589   0.602   0.721  1.00 12.43     -0.39
ATOM    133  CG2 THR A  93      14.783   1.692  -1.378  1.00 12.91      0.04
ATOM    134  H   THR A  93      14.063  -0.836  -0.375  1.00  0.00      0.16
ATOM    135  HG1 THR A  93      16.413   0.539   1.229  1.00  0.00      0.21
ATOM    136  N   LYS A  94      17.186  -2.333  -0.311  1.00 13.91     -0.34
ATOM    137  CA  LYS A  94      18.430  -3.076  -0.092  1.00 14.19      0.16
ATOM    138  C   LYS A  94      18.718  -4.139  -1.030  1.00 14.32      0.21
ATOM    139  O   LYS A  94      19.695  -4.858  -0.825  1.00 14.35     -0.28
ATOM    140  CB  LYS A  94      18.294  -3.889   1.138  1.00  0.00      0.03
ATOM    141  CG  LYS A  94      18.731  -2.873   2.065  1.00  0.00      0.00
ATOM    142  CD  LYS A  94      18.597  -3.520   3.332  1.00  0.00      0.02
ATOM    143  CE  LYS A  94      18.768  -2.336   4.134  1.00  0.00      0.22
ATOM    144  NZ  LYS A  94      18.930  -2.951   5.358  1.00  0.00     -0.07
ATOM    145  H   LYS A  94      16.341  -2.663   0.188  1.00  0.00      0.16
ATOM    146  HZ1 LYS A  94      18.102  -3.274   5.843  1.00  0.00      0.27
ATOM    147  HZ2 LYS A  94      19.613  -3.692   5.269  1.00  0.00      0.27
ATOM    148  HZ3 LYS A  94      19.331  -2.252   5.977  1.00  0.00      0.27
ATOM    149  N   LEU A 114       8.111  -6.486   9.691  1.00 12.35     -0.32
ATOM    150  CA  LEU A 114       7.316  -5.252   9.629  1.00 11.61      0.17
ATOM    151  C   LEU A 114       6.731  -5.002   8.242  1.00 11.30      0.22
ATOM    152  O   LEU A 114       7.458  -4.994   7.244  1.00 10.95     -0.28
ATOM    153  CB  LEU A 114       8.136  -4.028  10.079  1.00 11.79      0.03
ATOM    154  CG  LEU A 114       7.343  -2.710  10.162  1.00 11.19     -0.02
ATOM    155  CD1 LEU A 114       6.399  -2.729  11.361  1.00 11.81      0.00
ATOM    156  CD2 LEU A 114       8.291  -1.514  10.220  1.00 11.64      0.00
ATOM    157  H   LEU A 114       8.559  -6.809   8.844  1.00  0.00      0.18
ATOM    158  N   GLY A 116       3.931  -2.315   5.960  1.00  9.85     -0.33
ATOM    159  CA  GLY A 116       3.287  -0.999   5.932  1.00  9.60      0.24
ATOM    160  C   GLY A 116       4.183   0.158   6.288  1.00  9.85      0.23
ATOM    161  O   GLY A 116       3.757   1.287   6.463  1.00  9.67     -0.27
ATOM    162  H   GLY A 116       4.157  -2.755   5.076  1.00  0.00      0.18
ATOM    163  N   ALA A 117       5.465  -0.095   6.369  1.00  9.43     -0.34
ATOM    164  CA  ALA A 117       6.400   0.972   6.488  1.00  9.61      0.17
ATOM    165  C   ALA A 117       6.764   1.450   5.080  1.00  9.59      0.24
ATOM    166  O   ALA A 117       6.680   0.701   4.106  1.00  9.45     -0.27
ATOM    167  CB  ALA A 117       7.545   0.353   7.198  1.00  9.53      0.04
ATOM    168  H   ALA A 117       5.800  -1.018   6.144  1.00  0.00      0.16
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ATOM    169  N   LYS A 118       7.055   2.741   4.970  1.00  9.92    -0.34
ATOM    170  CA  LYS A 118       7.014   3.486   3.722  1.00  9.68     0.17
ATOM    171  C   LYS A 118       7.838   4.751   3.874  1.00  9.08     0.24
ATOM    172  O   LYS A 118       7.817   5.367   4.944  1.00  8.87    -0.27
ATOM    173  CB  LYS A 118       5.544   3.795   3.317  1.00 10.07     0.03
ATOM    174  CG  LYS A 118       4.652   4.446   4.405  1.00 11.88     0.00
ATOM    175  CD  LYS A 118       4.097   5.851   4.088  1.00 15.78     0.02
ATOM    176  CE  LYS A 118       5.113   7.010   4.110  1.00 17.52     0.22
ATOM    177  NZ  LYS A 118       5.813   7.122   5.402  1.00 19.32    -0.07
ATOM    178  H   LYS A 118       7.240   3.259   5.820  1.00  0.00     0.16
ATOM    179  HZ1 LYS A 118       6.491   6.364   5.479  1.00  0.00     0.27
ATOM    180  HZ2 LYS A 118       6.350   7.980   5.469  1.00  0.00     0.27
ATOM    181  HZ3 LYS A 118       5.185   7.084   6.193  1.00  0.00     0.27
ATOM    182  N   GLY A 119       8.457   5.215   2.797  1.00  8.22    -0.35
ATOM    183  CA  GLY A 119       9.061   6.528   2.736  1.00  7.98     0.22
ATOM    184  C   GLY A 119       9.867   6.728   1.468  1.00  8.26     0.23
ATOM    185  O   GLY A 119       9.973   5.818   0.662  1.00  8.10    -0.27
ATOM    186  H   GLY A 119       8.483   4.677   1.931  1.00  0.00     0.16
ATOM    187  N   THR A 120      10.466   7.880   1.245  1.00  8.66    -0.34
ATOM    188  CA  THR A 120      11.225   8.115   0.031  1.00  9.18     0.20
ATOM    189  C   THR A 120      12.042   9.380   0.302  1.00  9.49     0.24
ATOM    190  O   THR A 120      12.297   9.711   1.470  1.00  9.35    -0.27
ATOM    191  CB  THR A 120      10.256   8.056  -1.205  1.00  9.02     0.14
ATOM    192  OG1 THR A 120      10.933   8.229  -2.416  1.00  9.63    -0.39
ATOM    193  CG2 THR A 120       9.048   9.002  -1.172  1.00  8.63     0.04
ATOM    194  H   THR A 120      10.595   8.555   1.989  1.00  0.00     0.16
ATOM    195  HG1 THR A 120      10.295   8.230  -3.115  1.00  0.00     0.21
ATOM    196  N   LEU A 121      12.404  10.131  -0.741  1.00 10.01    -0.34
ATOM    197  CA  LEU A 121      12.752  11.533  -0.558  1.00 10.62     0.17
ATOM    198  C   LEU A 121      11.499  12.279  -0.068  1.00 10.95     0.24
ATOM    199  O   LEU A 121      10.398  12.075  -0.578  1.00 11.41    -0.27
ATOM    200  CB  LEU A 121      13.317  12.169  -1.842  1.00 10.89     0.03
ATOM    201  CG  LEU A 121      14.734  11.686  -2.226  1.00 10.87    -0.02
ATOM    202  CD1 LEU A 121      15.183  12.340  -3.537  1.00 11.50     0.00
ATOM    203  CD2 LEU A 121      15.780  11.983  -1.137  1.00 11.42     0.00
ATOM    204  H   LEU A 121      12.110   9.811  -1.656  1.00  0.00     0.16
ATOM    205  N   ALA A 122      11.665  13.085   0.971  1.00 11.13    -0.34
ATOM    206  CA  ALA A 122      10.648  13.926   1.569  1.00 11.41     0.17
ATOM    207  C   ALA A 122      11.131  15.364   1.571  1.00 11.61     0.24
ATOM    208  O   ALA A 122      12.323  15.632   1.403  1.00 11.78    -0.27
ATOM    209  CB  ALA A 122      10.348  13.478   2.998  1.00 10.72     0.04
ATOM    210  H   ALA A 122      12.621  13.193   1.315  1.00  0.00     0.16
ATOM    211  N   THR A 123      10.196  16.283   1.776  1.00 11.79    -0.34
ATOM    212  CA  THR A 123      10.534  17.686   1.953  1.00 11.84     0.19
ATOM    213  C   THR A 123       9.774  18.241   3.152  1.00 12.05     0.22
ATOM    214  O   THR A 123       8.868  17.586   3.671  1.00 12.08    -0.28
ATOM    215  CB  THR A 123      10.273  18.491   0.649  1.00 12.02     0.14
ATOM    216  OG1 THR A 123      10.808  19.813   0.790  1.00 11.74    -0.39
ATOM    217  CG2 THR A 123       8.779  18.723   0.409  1.00 11.30     0.04
ATOM    218  H   THR A 123       9.229  16.002   1.885  1.00  0.00     0.16
ATOM    219  HG1 THR A 123      11.739  19.741   0.956  1.00  0.00     0.21
ATOM    220  N   ILE A 149      21.031  17.360  -1.244  1.00 11.50    -0.32
ATOM    221  CA  ILE A 149      20.030  16.443  -0.695  1.00 11.16     0.19
ATOM    222  C   ILE A 149      20.669  15.806   0.527  1.00 11.40     0.24
ATOM    223  O   ILE A 149      21.818  15.372   0.464  1.00 11.23    -0.27
ATOM    224  CB  ILE A 149      19.635  15.356  -1.721  1.00 11.30     0.01
ATOM    225  CG1 ILE A 149      18.877  15.979  -2.895  1.00 10.65     0.00
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ATOM    226  CG2 ILE A 149      18.794  14.248  -1.046  1.00 11.03      0.01
ATOM    227  CD1 ILE A 149      18.826  15.097  -4.137  1.00 12.78      0.00
ATOM    228  H   ILE A 149      21.989  17.032  -1.278  1.00  0.00      0.18
ATOM    229  N   TYR A 150      19.930  15.761   1.631  1.00 11.16     -0.34
ATOM    230  CA  TYR A 150      20.458  15.239   2.889  1.00 11.90      0.18
ATOM    231  C   TYR A 150      20.104  13.785   3.133  1.00 11.90      0.24
ATOM    232  O   TYR A 150      18.926  13.422   3.221  1.00 12.35     -0.27
ATOM    233  CB  TYR A 150      20.001  16.110   4.058  1.00 11.76      0.07
ATOM    234  CG  TYR A 150      20.682  17.447   4.050  1.00 12.50     -0.05
ATOM    235  CD1 TYR A 150      20.163  18.512   3.312  1.00 12.40      0.01
ATOM    236  CD2 TYR A 150      21.872  17.642   4.751  1.00 13.12      0.01
ATOM    237  CE1 TYR A 150      20.801  19.742   3.289  1.00 13.12      0.03
ATOM    238  CE2 TYR A 150      22.521  18.865   4.731  1.00 13.87      0.03
ATOM    239  CZ  TYR A 150      21.980  19.910   4.001  1.00 13.21      0.06
ATOM    240  OH  TYR A 150      22.616  21.125   3.984  1.00 13.02     -0.36
ATOM    241  H   TYR A 150      18.982  16.116   1.615  1.00  0.00      0.16
ATOM    242  HH  TYR A 150      23.394  21.145   4.520  1.00  0.00      0.21
ATOM    243  N   GLY A 151      21.131  12.941   3.228  1.00 11.78     -0.35
ATOM    244  CA  GLY A 151      20.991  11.520   3.503  1.00 11.88      0.22
ATOM    245  C   GLY A 151      21.339  11.195   4.955  1.00 11.73      0.23
ATOM    246  O   GLY A 151      21.381  12.069   5.820  1.00 11.48     -0.27
ATOM    247  H   GLY A 151      22.083  13.319   3.195  1.00  0.00      0.16
ATOM    248  N   ILE A 152      21.627   9.925   5.232  1.00 11.73     -0.34
ATOM    249  CA  ILE A 152      21.999   9.437   6.555  1.00 11.80      0.18
ATOM    250  C   ILE A 152      23.412   8.862   6.484  1.00 11.89      0.24
ATOM    251  O   ILE A 152      24.271   9.503   5.869  1.00 11.83     -0.27
ATOM    252  CB  ILE A 152      20.904   8.523   7.143  1.00 11.64      0.01
ATOM    253  CG1 ILE A 152      20.536   7.372   6.203  1.00 11.72      0.00
ATOM    254  CG2 ILE A 152      19.656   9.335   7.510  1.00 13.03      0.01
ATOM    255  CD1 ILE A 152      19.482   6.459   6.807  1.00 11.33      0.00
ATOM    256  H   ILE A 152      21.670   9.250   4.470  1.00  0.00      0.16
ATOM    257  N   GLU A 153      23.706   7.755   7.177  1.00 12.00     -0.34
ATOM    258  CA  GLU A 153      25.072   7.301   7.365  1.00 12.14      0.16
ATOM    259  C   GLU A 153      25.688   6.748   6.073  1.00 12.25      0.21
ATOM    260  O   GLU A 153      24.985   6.183   5.227  1.00 12.49     -0.28
ATOM    261  CB  GLU A 153      25.167   6.305   8.535  1.00 12.26      0.04
ATOM    262  CG  GLU A 153      24.804   4.831   8.230  1.00 12.09      0.11
ATOM    263  CD  GLU A 153      23.324   4.579   7.940  1.00 11.17      0.17
ATOM    264  OE1 GLU A 153      22.996   3.503   7.395  1.00 11.67     -0.64
ATOM    265  OE2 GLU A 153      22.476   5.444   8.253  1.00 12.22     -0.64
ATOM    266  H   GLU A 153      22.981   7.133   7.544  1.00  0.00      0.16
ATOM    267  N   ASN A 156      24.620   3.641   3.511  1.00 11.56     -0.32
ATOM    268  CA  ASN A 156      23.174   3.426   3.553  1.00 11.42      0.19
ATOM    269  C   ASN A 156      22.553   3.137   2.159  1.00 11.44      0.24
ATOM    270  O   ASN A 156      22.966   3.688   1.134  1.00 11.29     -0.27
ATOM    271  CB  ASN A 156      22.493   4.626   4.218  1.00 11.60      0.13
ATOM    272  CG  ASN A 156      21.085   4.270   4.620  1.00 11.51      0.21
ATOM    273  OD1 ASN A 156      20.164   4.472   3.840  1.00 10.74     -0.27
ATOM    274  ND2 ASN A 156      20.916   3.707   5.804  1.00 11.00     -0.37
ATOM    275  H   ASN A 156      25.016   4.493   3.924  1.00  0.00      0.18
ATOM    276 2HD2 ASN A 156      19.999   3.479   6.150  1.00  0.00      0.15
ATOM    277 1HD2 ASN A 156      21.740   3.622   6.443  1.00  0.00      0.15
ATOM    278  N   ASP A 157      21.519   2.288   2.150  1.00 11.51     -0.34
ATOM    279  CA  ASP A 157      20.731   1.845   0.999  1.00 11.62      0.18
ATOM    280  C   ASP A 157      19.943   3.001   0.369  1.00 12.02      0.24
ATOM    281  O   ASP A 157      19.759   3.023  -0.847  1.00 11.71     -0.27
ATOM    282  CB  ASP A 157      19.723   0.735   1.415  1.00 11.55      0.14
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ATOM    283  CG  ASP A 157      18.765   1.054   2.564  1.00 11.89      0.17
ATOM    284  OD1 ASP A 157      19.182   1.675   3.557  1.00 10.60     -0.64
ATOM    285  OD2 ASP A 157      17.582   0.644   2.574  1.00 12.39     -0.64
ATOM    286  H   ASP A 157      21.161   1.985   3.048  1.00  0.00      0.16
ATOM    287  N   GLY A 158      19.492   3.973   1.169  1.00 11.98     -0.35
ATOM    288  CA  GLY A 158      18.846   5.178   0.677  1.00 12.21      0.22
ATOM    289  C   GLY A 158      19.858   6.139   0.087  1.00 12.14      0.23
ATOM    290  O   GLY A 158      19.643   6.612  -1.023  1.00 12.46     -0.27
ATOM    291  H   GLY A 158      19.709   3.906   2.166  1.00  0.00      0.16
ATOM    292  N   ASN A 159      20.985   6.349   0.784  1.00 11.91     -0.34
ATOM    293  CA  ASN A 159      22.128   7.158   0.336  1.00 11.69      0.17
ATOM    294  C   ASN A 159      22.619   6.733  -1.034  1.00 11.98      0.22
ATOM    295  O   ASN A 159      22.738   7.558  -1.935  1.00 11.83     -0.28
ATOM    296  CB  ASN A 159      23.309   7.088   1.319  1.00 11.90      0.13
ATOM    297  CG  ASN A 159      23.088   7.968   2.533  1.00 11.42      0.21
ATOM    298  OD1 ASN A 159      21.971   8.144   3.023  1.00 14.57     -0.27
ATOM    299  ND2 ASN A 159      24.150   8.541   3.040  1.00  8.90     -0.37
ATOM    300  H   ASN A 159      21.061   5.916   1.694  1.00  0.00      0.16
ATOM    301 2HD2 ASN A 159      24.040   9.116   3.865  1.00  0.00      0.15
ATOM    302 1HD2 ASN A 159      25.077   8.400   2.642  1.00  0.00      0.15
ATOM    303  N   ILE A 162      20.190   7.710  -3.901  1.00 12.21     -0.32
ATOM    304  CA  ILE A 162      20.287   9.128  -4.228  1.00 12.29      0.18
ATOM    305  C   ILE A 162      21.598   9.426  -4.950  1.00 12.35      0.22
ATOM    306  O   ILE A 162      21.601  10.142  -5.954  1.00 12.59     -0.28
ATOM    307  CB  ILE A 162      20.179  10.043  -2.985  1.00 12.46      0.01
ATOM    308  CG1 ILE A 162      18.987   9.672  -2.097  1.00 12.46      0.00
ATOM    309  CG2 ILE A 162      20.090  11.519  -3.416  1.00 12.03      0.01
ATOM    310  CD1 ILE A 162      19.075  10.291  -0.707  1.00 12.48      0.00
ATOM    311  H   ILE A 162      20.304   7.420  -2.936  1.00  0.00      0.18
ATOM    312  N   VAL A 179      24.564  14.939   1.077  1.00 12.38     -0.32
ATOM    313  CA  VAL A 179      25.237  15.236   2.332  1.00 12.08      0.19
ATOM    314  C   VAL A 179      24.992  14.066   3.276  1.00 11.87      0.24
ATOM    315  O   VAL A 179      23.853  13.796   3.663  1.00 11.45     -0.27
ATOM    316  CB  VAL A 179      24.745  16.552   2.969  1.00 12.10      0.01
ATOM    317  CG1 VAL A 179      25.613  16.914   4.169  1.00 12.06      0.01
ATOM    318  CG2 VAL A 179      24.731  17.691   1.945  1.00 11.62      0.01
ATOM    319  H   VAL A 179      23.624  15.286   0.930  1.00  0.00      0.18
ATOM    320  N   GLU A 180      26.065  13.362   3.618  1.00 11.81     -0.34
ATOM    321  CA  GLU A 180      25.960  12.170   4.465  1.00 12.14      0.17
ATOM    322  C   GLU A 180      26.339  12.483   5.900  1.00 12.10      0.24
ATOM    323  O   GLU A 180      27.287  13.227   6.153  1.00 11.96     -0.27
ATOM    324  CB  GLU A 180      26.857  11.051   3.937  1.00 12.46      0.04
ATOM    325  CG  GLU A 180      26.711  10.790   2.450  1.00 12.39      0.11
ATOM    326  CD  GLU A 180      27.369   9.494   2.039  1.00 13.53      0.17
ATOM    327  OE1 GLU A 180      28.620   9.469   1.955  1.00 13.91     -0.64
ATOM    328  OE2 GLU A 180      26.635   8.505   1.809  1.00 12.09     -0.64
ATOM    329  H   GLU A 180      26.974  13.621   3.263  1.00  0.00      0.16
ATOM    330  N   SER A 181      25.594  11.907   6.839  1.00 12.07     -0.34
ATOM    331  CA  SER A 181      25.902  12.055   8.257  1.00 11.98      0.20
ATOM    332  C   SER A 181      25.385  10.843   9.014  1.00 11.98      0.24
ATOM    333  O   SER A 181      26.126   9.883   9.248  1.00 11.67     -0.27
ATOM    334  CB  SER A 181      25.316  13.358   8.823  1.00 12.16      0.19
ATOM    335  OG  SER A 181      23.935  13.488   8.521  1.00 12.06     -0.39
ATOM    336  H   SER A 181      24.851  11.275   6.570  1.00  0.00      0.16
ATOM    337  HG  SER A 181      23.837  13.530   7.581  1.00  0.00      0.20
ATOM    338  N   SER A 182      24.101  10.901   9.361  1.00 11.98     -0.34
ATOM    339  CA  SER A 182      23.399   9.874  10.128  1.00 11.77      0.20
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ATOM    340  C   SER A 182      21.911  10.313  10.165  1.00 11.89     0.24
ATOM    341  O   SER A 182      21.610  11.434   9.858  1.00 11.39    -0.27
ATOM    342  CB  SER A 182      23.983   9.754  11.538  1.00 12.24     0.19
ATOM    343  OG  SER A 182      23.845  10.974  12.255  1.00 11.50    -0.39
ATOM    344  H   SER A 182      23.581  11.740   9.131  1.00  0.00     0.16
ATOM    345  HG  SER A 182      24.214  10.852  13.117  1.00  0.00     0.20
ATOM    346  N   LYS A 183      20.859   9.606  10.560  1.00 11.60    -0.34
ATOM    347  CA  LYS A 183      19.583  10.376  10.752  1.00 11.68     0.17
ATOM    348  C   LYS A 183      19.576  11.281  11.939  1.00 11.59     0.24
ATOM    349  O   LYS A 183      18.733  12.171  11.953  1.00 11.49    -0.27
ATOM    350  CB  LYS A 183      18.309   9.610  10.723  1.00  0.00     0.03
ATOM    351  CG  LYS A 183      17.455   9.308  11.973  1.00  0.00     0.00
ATOM    352  CD  LYS A 183      18.177   8.493  13.020  1.00  0.00     0.02
ATOM    353  CE  LYS A 183      19.161   7.537  12.364  1.00  0.00     0.22
ATOM    354  NZ  LYS A 183      18.466   6.708  11.341  1.00  0.00    -0.07
ATOM    355  H   LYS A 183      20.943   8.613  10.692  1.00  0.00     0.16
ATOM    356  HZ1 LYS A 183      18.878   5.799  11.152  1.00  0.00     0.27
ATOM    357  HZ2 LYS A 183      17.490   6.496  11.464  1.00  0.00     0.27
ATOM    358  HZ3 LYS A 183      18.465   7.012  10.355  1.00  0.00     0.27
ATOM    359  N   GLN A 184      20.465  11.086  12.922  0.70 11.69    -0.34
ATOM    360  CA  GLN A 184      20.556  12.140  13.886  0.70 11.77     0.17
ATOM    361  C   GLN A 184      21.042  13.457  13.247  0.70 11.78     0.24
ATOM    362  O   GLN A 184      20.450  14.518  13.468  0.70 11.77    -0.27
ATOM    363  CB  GLN A 184      21.433  11.685  15.064  0.70 11.86     0.04
ATOM    364  CG  GLN A 184      20.881  10.449  15.859  0.70 12.45     0.08
ATOM    365  CD  GLN A 184      21.005   9.079  15.141  0.70 12.58     0.14
ATOM    366  OE1 GLN A 184      21.931   8.974  14.196  0.70 13.41    -0.17
ATOM    367  NE2 GLN A 184      20.269   8.128  15.467  0.70  8.45    -0.38
ATOM    368  H   GLN A 184      21.090  10.271  13.055  0.70  0.00     0.16
ATOM    369 2HE2 GLN A 184      20.381   7.228  15.019  0.70  0.00     0.15
ATOM    370 1HE2 GLN A 184      19.570   8.248  16.186  0.70  0.00     0.15
ATOM    371  N   GLY A 185      22.087  13.371  12.424  1.00 11.76    -0.35
ATOM    372  CA  GLY A 185      22.617  14.520  11.671  1.00 11.69     0.22
ATOM    373  C   GLY A 185      21.616  15.109  10.689  1.00 12.00     0.23
ATOM    374  O   GLY A 185      21.431  16.328  10.635  1.00 11.70    -0.27
ATOM    375  H   GLY A 185      22.521  12.468  12.274  1.00  0.00     0.16
ATOM    376  N   MET A 186      20.961  14.236   9.921  1.00 12.04    -0.34
ATOM    377  CA  MET A 186      19.958  14.648   8.934  1.00 12.23     0.17
ATOM    378  C   MET A 186      18.794  15.386   9.603  1.00 12.44     0.24
ATOM    379  O   MET A 186      18.417  16.470   9.174  1.00 11.89    -0.27
ATOM    380  CB  MET A 186      19.446  13.428   8.149  1.00 12.10     0.04
ATOM    381  CG  MET A 186      18.412  13.746   7.082  1.00 11.58     0.07
ATOM    382  SD  MET A 186      17.457  12.312   6.525  1.00 12.65    -0.17
ATOM    383  CE  MET A 186      16.449  12.014   7.980  1.00 12.54     0.08
ATOM    384  H   MET A 186      21.167  13.248  10.008  1.00  0.00     0.16
ATOM    385  N   LEU A 187      18.255  14.803  10.673  1.00 12.67    -0.34
ATOM    386  CA  LEU A 187      17.145  15.418  11.407  1.00 13.26     0.17
ATOM    387  C   LEU A 187      17.502  16.724  12.101  1.00 13.07     0.24
ATOM    388  O   LEU A 187      16.641  17.590  12.264  1.00 12.98    -0.27
ATOM    389  CB  LEU A 187      16.536  14.433  12.407  1.00 13.37     0.03
ATOM    390  CG  LEU A 187      15.819  13.247  11.752  1.00 14.61    -0.02
ATOM    391  CD1 LEU A 187      15.477  12.202  12.791  1.00 14.72     0.00
ATOM    392  CD2 LEU A 187      14.568  13.676  10.985  1.00 16.49     0.00
ATOM    393  H   LEU A 187      18.608  13.909  10.990  1.00  0.00     0.16
ATOM    394  N   ALA A 188      18.762  16.859  12.512  1.00 13.21    -0.34
ATOM    395  CA  ALA A 188      19.264  18.111  13.072  1.00 13.31     0.17
ATOM    396  C   ALA A 188      19.209  19.213  12.011  1.00 13.46     0.24
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ATOM    397  O   ALA A 188      18.840  20.350  12.299  1.00 13.24    -0.27
ATOM    398  CB  ALA A 188      20.685  17.930  13.583  1.00 13.23     0.04
ATOM    399  H   ALA A 188      19.411  16.093  12.388  1.00  0.00     0.16
ATOM    400  N   GLN A 189      19.569  18.851  10.782  1.00 13.81    -0.34
ATOM    401  CA  GLN A 189      19.539  19.765   9.646  1.00 13.98     0.17
ATOM    402  C   GLN A 189      18.104  20.136   9.254  1.00 13.85     0.24
ATOM    403  O   GLN A 189      17.820  21.294   8.937  1.00 13.52    -0.27
ATOM    404  CB  GLN A 189      20.294  19.145   8.459  1.00 14.41     0.04
ATOM    405  CG  GLN A 189      20.443  20.049   7.239  1.00 15.38     0.08
ATOM    406  CD  GLN A 189      21.258  21.307   7.500  1.00 17.22     0.14
ATOM    407  OE1 GLN A 189      22.257  21.210   8.371  1.00 19.78    -0.17
ATOM    408  NE2 GLN A 189      20.984  22.354   6.912  1.00 17.35    -0.38
ATOM    409  H   GLN A 189      19.860  17.896  10.617  1.00  0.00     0.16
ATOM    410 2HE2 GLN A 189      21.534  23.184   7.080  1.00  0.00     0.15
ATOM    411 1HE2 GLN A 189      20.219  22.378   6.252  1.00  0.00     0.15
ATOM    412  N   VAL A 190      17.202  19.156   9.284  1.00 13.86    -0.34
ATOM    413  CA  VAL A 190      15.775  19.417   9.064  1.00 14.02     0.16
ATOM    414  C   VAL A 190      15.253  20.421  10.102  1.00 14.30     0.21
ATOM    415  O   VAL A 190      14.514  21.350   9.762  1.00 14.13    -0.28
ATOM    416  CB  VAL A 190      14.948  18.102   9.099  1.00 14.45     0.00
ATOM    417  CG1 VAL A 190      13.451  18.376   9.064  1.00 14.20     0.01
ATOM    418  CG2 VAL A 190      15.347  17.192   7.939  1.00 13.67     0.01
ATOM    419  H   VAL A 190      17.494  18.215   9.512  1.00  0.00     0.16
ATOM    420  N   ILE A 200      14.126  22.005   2.370  1.00 11.66    -0.32
ATOM    421  CA  ILE A 200      15.143  20.956   2.466  1.00 11.74     0.19
ATOM    422  C   ILE A 200      14.565  19.673   1.876  1.00 11.78     0.24
ATOM    423  O   ILE A 200      13.363  19.429   1.988  1.00 11.82    -0.27
ATOM    424  CB  ILE A 200      15.617  20.759   3.947  1.00 11.89     0.01
ATOM    425  CG1 ILE A 200      16.806  19.783   4.021  1.00 12.45     0.00
ATOM    426  CG2 ILE A 200      14.454  20.323   4.850  1.00 11.59     0.01
ATOM    427  CD1 ILE A 200      17.373  19.578   5.447  1.00 11.83     0.00
ATOM    428  H   ILE A 200      13.155  21.726   2.409  1.00  0.00     0.18
ATOM    429  N   VAL A 201      15.414  18.885   1.216  1.00 11.57    -0.34
ATOM    430  CA  VAL A 201      15.025  17.581   0.684  1.00 11.51     0.18
ATOM    431  C   VAL A 201      15.910  16.521   1.329  1.00 11.35     0.24
ATOM    432  O   VAL A 201      17.133  16.668   1.379  1.00 11.16    -0.27
ATOM    433  CB  VAL A 201      15.104  17.529  -0.869  1.00 11.76     0.00
ATOM    434  CG1 VAL A 201      14.802  16.125  -1.396  1.00 11.62     0.01
ATOM    435  CG2 VAL A 201      14.138  18.538  -1.481  1.00 11.93     0.01
ATOM    436  H   VAL A 201      16.386  19.150   1.143  1.00  0.00     0.16
ATOM    437  N   PHE A 202      15.276  15.463   1.834  1.00 11.11    -0.34
ATOM    438  CA  PHE A 202      15.958  14.470   2.661  1.00 11.22     0.18
ATOM    439  C   PHE A 202      15.260  13.108   2.608  1.00 11.29     0.24
ATOM    440  O   PHE A 202      14.198  12.967   2.006  1.00 11.42    -0.27
ATOM    441  CB  PHE A 202      16.048  14.978   4.104  1.00 10.67     0.07
ATOM    442  CG  PHE A 202      14.707  15.211   4.742  1.00 11.26    -0.05
ATOM    443  CD1 PHE A 202      14.137  14.244   5.570  1.00 10.85     0.00
ATOM    444  CD2 PHE A 202      14.007  16.397   4.515  1.00 10.34     0.00
ATOM    445  CE1 PHE A 202      12.885  14.447   6.150  1.00 11.52     0.00
ATOM    446  CE2 PHE A 202      12.762  16.608   5.087  1.00 11.79     0.00
ATOM    447  CZ  PHE A 202      12.200  15.634   5.915  1.00 10.91     0.00
ATOM    448  H   PHE A 202      14.270  15.390   1.740  1.00  0.00     0.16
ATOM    449  N   LEU A 203      15.807  12.099   3.287  1.00 11.71    -0.34
ATOM    450  CA  LEU A 203      15.183  10.789   3.407  1.00 11.70     0.17
ATOM    451  C   LEU A 203      14.185  10.764   4.578  1.00 12.11     0.24
ATOM    452  O   LEU A 203      14.587  10.842   5.733  1.00 11.90    -0.27
ATOM    453  CB  LEU A 203      16.291   9.766   3.700  1.00 11.94     0.03
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ATOM    454  CG  LEU A 203      17.258   9.512   2.526  1.00 11.83    -0.02
ATOM    455  CD1 LEU A 203      18.461   8.692   3.005  1.00 11.18     0.00
ATOM    456  CD2 LEU A 203      16.553   8.802   1.372  1.00 12.06     0.00
ATOM    457  H   LEU A 203      16.661  12.260   3.809  1.00  0.00     0.16
ATOM    458  N   GLY A 204      12.888  10.612   4.300  1.00 11.84    -0.35
ATOM    459  CA  GLY A 204      11.849  10.477   5.320  1.00 12.11     0.22
ATOM    460  C   GLY A 204      11.388   9.026   5.381  1.00 11.88     0.23
ATOM    461  O   GLY A 204      11.330   8.386   4.331  1.00 12.39    -0.27
ATOM    462  H   GLY A 204      12.610  10.410   3.346  1.00  0.00     0.16
ATOM    463  N   TRP A 205      11.021   8.500   6.557  1.00 11.68    -0.34
ATOM    464  CA  TRP A 205      10.469   7.153   6.724  1.00 11.68     0.18
ATOM    465  C   TRP A 205       9.365   7.085   7.764  1.00 11.46     0.24
ATOM    466  O   TRP A 205       9.364   7.863   8.715  1.00 11.65    -0.27
ATOM    467  CB  TRP A 205      11.527   6.078   7.034  1.00 11.18     0.07
ATOM    468  CG  TRP A 205      12.368   6.231   8.252  1.00 11.52    -0.02
ATOM    469  CD1 TRP A 205      12.279   5.486   9.374  1.00 11.31     0.09
ATOM    470  CD2 TRP A 205      13.567   7.039   8.396  1.00 11.04    -0.00
ATOM    471  NE1 TRP A 205      13.351   5.771  10.193  1.00 11.88    -0.36
ATOM    472  CE2 TRP A 205      14.223   6.652   9.595  1.00 12.12     0.04
ATOM    473  CE3 TRP A 205      14.210   8.013   7.600  1.00 12.40     0.01
ATOM    474  CZ2 TRP A 205      15.502   7.114   9.918  1.00 11.27     0.03
ATOM    475  CZ3 TRP A 205      15.512   8.457   7.895  1.00 11.78     0.00
ATOM    476  CH2 TRP A 205      16.163   8.000   9.051  1.00 11.54     0.00
ATOM    477  H   TRP A 205      10.990   9.082   7.386  1.00  0.00     0.16
ATOM    478  HE1 TRP A 205      13.509   5.279  11.068  1.00  0.00     0.16
ATOM    479  N   GLU A 206       8.490   6.088   7.602  1.00 11.69    -0.34
ATOM    480  CA  GLU A 206       7.671   5.520   8.669  1.00 12.08     0.17
ATOM    481  C   GLU A 206       8.153   4.070   8.875  1.00 12.10     0.24
ATOM    482  O   GLU A 206       8.390   3.397   7.862  1.00 11.88    -0.27
ATOM    483  CB  GLU A 206       6.196   5.468   8.240  1.00 12.38     0.04
ATOM    484  CG  GLU A 206       5.479   6.814   8.423  1.00 13.95     0.11
ATOM    485  CD  GLU A 206       4.975   7.074   9.850  1.00 16.11     0.17
ATOM    486  OE1 GLU A 206       5.484   6.468  10.816  1.00 16.70    -0.64
ATOM    487  OE2 GLU A 206       4.058   7.900   9.967  1.00 16.69    -0.64
ATOM    488  H   GLU A 206       8.642   5.490   6.801  1.00  0.00     0.16
ATOM    489  N   PRO A 207       8.249   3.566  10.124  1.00 11.89    -0.33
ATOM    490  CA  PRO A 207       7.910   4.294  11.345  1.00 11.84     0.17
ATOM    491  C   PRO A 207       9.056   5.215  11.760  1.00 11.79     0.24
ATOM    492  O   PRO A 207      10.214   4.800  11.728  1.00 11.40    -0.27
ATOM    493  CB  PRO A 207       7.688   3.228  12.408  1.00 11.84     0.03
ATOM    494  CG  PRO A 207       8.590   2.088  11.972  1.00 11.93     0.02
ATOM    495  CD  PRO A 207       8.654   2.197  10.443  1.00 12.02     0.12
ATOM    496  N   HIS A 208       8.726   6.447  12.151  1.00 12.04    -0.34
ATOM    497  CA  HIS A 208       9.643   7.356  12.820  1.00 11.94     0.18
ATOM    498  C   HIS A 208       8.886   8.540  13.444  1.00 12.48     0.24
ATOM    499  O   HIS A 208       7.987   9.094  12.797  1.00 12.92    -0.27
ATOM    500  CB  HIS A 208      10.759   7.825  11.868  1.00 11.83     0.09
ATOM    501  CG  HIS A 208      11.908   8.495  12.555  1.00 10.74     0.05
ATOM    502  ND1 HIS A 208      11.850   9.779  13.050  1.00  9.65    -0.24
ATOM    503  CD2 HIS A 208      13.142   8.027  12.872  1.00 10.15     0.11
ATOM    504  CE1 HIS A 208      13.005  10.088  13.611  1.00 10.80     0.20
ATOM    505  NE2 HIS A 208      13.804   9.039  13.526  1.00 10.24    -0.35
ATOM    506  H   HIS A 208       7.737   6.684  12.198  1.00  0.00     0.16
ATOM    507  HE2 HIS A 208      14.757   8.986  13.877  1.00  0.00     0.16
ATOM    508  N   PRO A 209       9.273   9.014  14.650  1.00 12.66    -0.33
ATOM    509  CA  PRO A 209       8.702  10.234  15.252  1.00 12.90     0.17
ATOM    510  C   PRO A 209       8.732  11.505  14.381  1.00 12.86     0.24
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ATOM    511  O   PRO A 209       7.979  12.443  14.655  1.00 12.39    -0.27
ATOM    512  CB  PRO A 209       9.555  10.433  16.514  1.00 12.90     0.03
ATOM    513  CG  PRO A 209       9.994   9.054  16.884  1.00 12.51     0.02
ATOM    514  CD  PRO A 209      10.225   8.356  15.564  1.00 12.51     0.12
ATOM    515  N   MET A 210       9.577  11.536  13.351  1.00 13.34    -0.34
ATOM    516  CA  MET A 210       9.678  12.706  12.465  1.00 13.73     0.17
ATOM    517  C   MET A 210       8.332  13.063  11.830  1.00 14.03     0.24
ATOM    518  O   MET A 210       8.060  14.232  11.540  1.00 13.99    -0.27
ATOM    519  CB  MET A 210      10.755  12.508  11.383  1.00 13.78     0.04
ATOM    520  CG  MET A 210      10.444  11.440  10.331  1.00 13.35     0.07
ATOM    521  SD  MET A 210      11.648  11.392   8.987  1.00 13.72    -0.17
ATOM    522  CE  MET A 210      12.812  10.171   9.605  1.00 10.69     0.08
ATOM    523  H   MET A 210      10.203  10.757  13.190  1.00  0.00     0.16
ATOM    524  N   ASN A 211       7.501  12.044  11.628  1.00 14.68    -0.34
ATOM    525  CA  ASN A 211       6.192  12.192  11.003  1.00 15.25     0.18
ATOM    526  C   ASN A 211       5.215  12.979  11.868  1.00 15.79     0.24
ATOM    527  O   ASN A 211       4.373  13.721  11.351  1.00 16.01    -0.27
ATOM    528  CB  ASN A 211       5.634  10.808  10.646  1.00 15.10     0.13
ATOM    529  CG  ASN A 211       6.515  10.136   9.590  1.00 15.00     0.21
ATOM    530  OD1 ASN A 211       6.447  10.437   8.397  1.00 14.34    -0.27
ATOM    531  ND2 ASN A 211       7.416   9.268  10.031  1.00 14.70    -0.37
ATOM    532  H   ASN A 211       7.791  11.117  11.908  1.00  0.00     0.16
ATOM    533 2HD2 ASN A 211       8.056   8.781   9.405  1.00  0.00     0.15
ATOM    534 1HD2 ASN A 211       7.396   8.986  11.009  1.00  0.00     0.15
ATOM    535  N   ALA A 212       5.351  12.819  13.183  1.00 16.30    -0.34
ATOM    536  CA  ALA A 212       4.566  13.559  14.160  1.00 17.03     0.17
ATOM    537  C   ALA A 212       5.251  14.856  14.600  1.00 17.66     0.24
ATOM    538  O   ALA A 212       4.579  15.846  14.906  1.00 17.51    -0.27
ATOM    539  CB  ALA A 212       4.280  12.682  15.367  1.00 16.99     0.04
ATOM    540  H   ALA A 212       6.074  12.202  13.526  1.00  0.00     0.16
ATOM    541  N   ASN A 213       6.583  14.838  14.643  1.00 18.15    -0.34
ATOM    542  CA  ASN A 213       7.367  15.976  15.132  1.00 18.84     0.18
ATOM    543  C   ASN A 213       7.540  17.082  14.089  1.00 19.09     0.24
ATOM    544  O   ASN A 213       7.701  18.250  14.440  1.00 19.34    -0.27
ATOM    545  CB  ASN A 213       8.735  15.512  15.658  1.00 18.73     0.12
ATOM    546  CG  ASN A 213       8.626  14.642  16.904  1.00 19.14     0.15
ATOM    547  OD1 ASN A 213       9.693  13.908  17.211  1.00 19.76    -0.17
ATOM    548  ND2 ASN A 213       7.602  14.634  17.585  1.00 19.07    -0.38
ATOM    549  H   ASN A 213       7.075  13.984  14.409  1.00  0.00     0.16
ATOM    550 2HD2 ASN A 213       7.557  14.053  18.409  1.00  0.00     0.15
ATOM    551 1HD2 ASN A 213       6.808  15.197  17.317  1.00  0.00     0.15
ATOM    552  N   PHE A 214       7.515  16.707  12.814  1.00 19.61    -0.34
ATOM    553  CA  PHE A 214       7.601  17.666  11.715  1.00 20.09     0.16
ATOM    554  C   PHE A 214       6.430  17.453  10.761  1.00 20.31     0.21
ATOM    555  O   PHE A 214       5.840  16.373  10.722  1.00 20.32    -0.28
ATOM    556  CB  PHE A 214       8.921  17.504  10.943  1.00 20.30     0.07
ATOM    557  CG  PHE A 214      10.155  17.721  11.777  1.00 21.29    -0.05
ATOM    558  CD1 PHE A 214      10.861  16.640  12.294  1.00 21.40     0.00
ATOM    559  CD2 PHE A 214      10.622  19.012  12.032  1.00 21.88     0.00
ATOM    560  CE1 PHE A 214      12.010  16.838  13.068  1.00 22.57     0.00
ATOM    561  CE2 PHE A 214      11.766  19.222  12.799  1.00 22.36     0.00
ATOM    562  CZ  PHE A 214      12.462  18.130  13.321  1.00 21.63     0.00
ATOM    563  H   PHE A 214       7.399  15.730  12.576  1.00  0.00     0.16
ATOM    564  N   LEU A 216       6.041  16.869   7.274  1.00 19.67    -0.32
ATOM    565  CA  LEU A 216       6.729  16.537   6.027  1.00 19.02     0.19
ATOM    566  C   LEU A 216       5.797  16.085   4.919  1.00 18.22     0.24
ATOM    567  O   LEU A 216       4.675  15.632   5.162  1.00 17.79    -0.27
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ATOM    568  CB  LEU A 216       7.871  15.519   6.222  1.00 19.59      0.04
ATOM    569  CG  LEU A 216       7.897  14.407   7.273  1.00 20.61     -0.02
ATOM    570  CD1 LEU A 216       8.706  13.221   6.785  1.00 21.08      0.00
ATOM    571  CD2 LEU A 216       8.500  14.944   8.534  1.00 21.36      0.00
ATOM    572  H   LEU A 216       5.723  16.117   7.868  1.00  0.00      0.18
ATOM    573  N   THR A 217       6.292  16.218   3.695  1.00 17.08     -0.34
ATOM    574  CA  THR A 217       5.601  15.759   2.509  1.00 16.40      0.20
ATOM    575  C   THR A 217       6.513  14.767   1.824  1.00 15.65      0.24
ATOM    576  O   THR A 217       7.617  15.126   1.414  1.00 15.57     -0.27
ATOM    577  CB  THR A 217       5.316  16.946   1.571  1.00 16.32      0.14
ATOM    578  OG1 THR A 217       4.391  17.841   2.196  1.00 16.48     -0.39
ATOM    579  CG2 THR A 217       4.583  16.486   0.307  1.00 16.97      0.04
ATOM    580  H   THR A 217       7.218  16.611   3.580  1.00  0.00      0.16
ATOM    581  HG1 THR A 217       4.783  18.165   2.993  1.00  0.00      0.21
ATOM    582  N   TYR A 218       6.064  13.517   1.725  1.00 14.71     -0.34
ATOM    583  CA  TYR A 218       6.770  12.515   0.931  1.00 14.01      0.18
ATOM    584  C   TYR A 218       6.542  12.836  -0.540  1.00 13.78      0.24
ATOM    585  O   TYR A 218       5.423  13.176  -0.938  1.00 13.09     -0.27
ATOM    586  CB  TYR A 218       6.261  11.105   1.257  1.00 14.04      0.07
ATOM    587  CG  TYR A 218       6.642  10.605   2.630  1.00 13.76     -0.05
ATOM    588  CD1 TYR A 218       5.848  10.920   3.752  1.00 14.23      0.01
ATOM    589  CD2 TYR A 218       7.812   9.841   2.793  1.00 13.15      0.01
ATOM    590  CE1 TYR A 218       6.228  10.480   5.031  1.00 13.99      0.03
ATOM    591  CE2 TYR A 218       8.146   9.344   4.061  1.00 13.75      0.03
ATOM    592  CZ  TYR A 218       7.370   9.681   5.180  1.00 14.52      0.06
ATOM    593  OH  TYR A 218       7.739   9.248   6.408  1.00 14.08     -0.36
ATOM    594  H   TYR A 218       5.156  13.281   2.098  1.00  0.00      0.16
ATOM    595  HH  TYR A 218       7.261   9.670   7.135  1.00  0.00      0.21
ATOM    596  N   LEU A 219       7.606  12.747  -1.333  1.00 13.49     -0.34
ATOM    597  CA  LEU A 219       7.539  13.103  -2.750  1.00 13.58      0.16
ATOM    598  C   LEU A 219       7.068  11.931  -3.600  1.00 13.70      0.21
ATOM    599  O   LEU A 219       7.506  10.795  -3.399  1.00 14.22     -0.28
ATOM    600  CB  LEU A 219       8.900  13.591  -3.263  1.00 13.42      0.03
ATOM    601  CG  LEU A 219       9.700  14.634  -2.477  1.00 13.48     -0.02
ATOM    602  CD1 LEU A 219      10.969  14.992  -3.250  1.00 12.46      0.00
ATOM    603  CD2 LEU A 219       8.871  15.885  -2.180  1.00 12.90      0.00
ATOM    604  H   LEU A 219       8.499  12.455  -0.955  1.00  0.00      0.16
ATOM    605  N   PHE A 226      12.861   4.334  -5.313  1.00 14.13     -0.32
ATOM    606  CA  PHE A 226      12.601   3.909  -3.940  1.00 14.03      0.18
ATOM    607  C   PHE A 226      11.393   2.978  -3.869  1.00 14.36      0.22
ATOM    608  O   PHE A 226      11.123   2.414  -2.810  1.00 14.92     -0.28
ATOM    609  CB  PHE A 226      12.357   5.152  -3.075  1.00 13.66      0.07
ATOM    610  CG  PHE A 226      13.663   5.772  -2.622  1.00 13.26     -0.05
ATOM    611  CD1 PHE A 226      14.335   6.684  -3.442  1.00 14.02      0.00
ATOM    612  CD2 PHE A 226      14.256   5.398  -1.408  1.00 13.56      0.00
ATOM    613  CE1 PHE A 226      15.548   7.255  -3.039  1.00 13.78      0.00
ATOM    614  CE2 PHE A 226      15.494   5.966  -1.037  1.00 13.49      0.00
ATOM    615  CZ  PHE A 226      16.124   6.922  -1.819  1.00 13.23      0.00
ATOM    616  H   PHE A 226      12.280   5.058  -5.717  1.00  0.00      0.18
ATOM    617  N   ASN A 229       4.060   3.896  -4.348  1.00 15.61     -0.32
ATOM    618  CA  ASN A 229       3.325   4.282  -3.132  0.50 15.59      0.19
ATOM    619  C   ASN A 229       4.217   4.992  -2.096  1.00 15.45      0.24
ATOM    620  O   ASN A 229       4.172   4.715  -0.899  1.00 15.17     -0.27
ATOM    621  CB  ASN A 229       2.574   3.070  -2.527  0.50 15.73      0.13
ATOM    622  CG  ASN A 229       1.576   3.420  -1.429  0.50 16.09      0.21
ATOM    623  OD1 ASN A 229       1.441   2.713  -0.440  0.50 16.12     -0.27
ATOM    624  ND2 ASN A 229       0.872   4.529  -1.588  0.50 16.05     -0.37
```

```
ATOM    625  H   ASN A 229       3.729   4.255  -5.233  1.00  0.00      0.18
ATOM    626 2HD2 ASN A 229       0.237   4.765  -0.855  0.50  0.00      0.15
ATOM    627 1HD2 ASN A 229       0.988   5.101  -2.401  0.50  0.00      0.15
ATOM    628  N   TYR A 230       5.040   5.932  -2.567  1.00 15.19     -0.34
ATOM    629  CA  TYR A 230       5.957   6.704  -1.727  1.00 15.12      0.18
ATOM    630  C   TYR A 230       7.011   5.819  -1.054  1.00 14.50      0.24
ATOM    631  O   TYR A 230       7.331   6.021   0.119  1.00 14.95     -0.27
ATOM    632  CB  TYR A 230       5.191   7.609  -0.741  1.00 15.62      0.07
ATOM    633  CG  TYR A 230       4.178   8.485  -1.451  1.00 15.84     -0.05
ATOM    634  CD1 TYR A 230       2.846   8.081  -1.591  1.00 16.47      0.01
ATOM    635  CD2 TYR A 230       4.556   9.704  -2.011  1.00 15.72      0.01
ATOM    636  CE1 TYR A 230       1.918   8.877  -2.265  1.00 16.79      0.03
ATOM    637  CE2 TYR A 230       3.637  10.506  -2.680  1.00 16.29      0.03
ATOM    638  CZ  TYR A 230       2.324  10.088  -2.808  1.00 16.84      0.06
ATOM    639  OH  TYR A 230       1.414  10.887  -3.477  1.00 17.19     -0.36
ATOM    640  H   TYR A 230       4.930   6.214  -3.530  1.00  0.00      0.16
ATOM    641  HH  TYR A 230       1.789  11.695  -3.794  1.00  0.00      0.21
ATOM    642  N   GLY A 231       7.522   4.842  -1.810  1.00 13.90     -0.35
ATOM    643  CA  GLY A 231       8.501   3.873  -1.359  1.00 13.24      0.22
ATOM    644  C   GLY A 231       7.925   2.911  -0.334  1.00 12.81      0.23
ATOM    645  O   GLY A 231       8.544   2.719   0.704  1.00 13.23     -0.27
ATOM    646  H   GLY A 231       7.184   4.704  -2.752  1.00  0.00      0.16
ATOM    647  N   GLY A 232       6.726   2.358  -0.568  1.00 12.46     -0.35
ATOM    648  CA  GLY A 232       6.094   1.385   0.326  1.00 11.86      0.20
ATOM    649  C   GLY A 232       7.021   0.184   0.542  1.00 11.80      0.21
ATOM    650  O   GLY A 232       7.466  -0.424  -0.430  1.00 11.70     -0.28
ATOM    651  H   GLY A 232       6.295   2.507  -1.473  1.00  0.00      0.16
ATOM    652  N   PHE A 233       8.707   0.229   2.260  1.00 11.20     -0.33
ATOM    653  CA  PHE A 233       9.921  -0.550   2.441  1.00 11.33      0.17
ATOM    654  C   PHE A 233       9.604  -1.911   3.048  1.00 11.26      0.37
ATOM    655  O   PHE A 233       8.608  -2.080   3.758  1.00 11.40     -0.14
ATOM    656  CB  PHE A 233      10.913   0.218   3.309  1.00  0.00      0.07
ATOM    657  CG  PHE A 233      11.526   1.445   2.670  1.00  0.00     -0.05
ATOM    658  CD1 PHE A 233      10.898   2.695   2.811  1.00  0.00      0.00
ATOM    659  CD2 PHE A 233      12.719   1.337   1.936  1.00  0.00      0.00
ATOM    660  CE1 PHE A 233      11.467   3.838   2.224  1.00  0.00      0.00
ATOM    661  CE2 PHE A 233      13.288   2.481   1.347  1.00  0.00      0.00
ATOM    662  CZ  PHE A 233      12.662   3.731   1.492  1.00  0.00      0.00
ATOM    663  H   PHE A 233       8.130   0.337   3.095  1.00  0.00      0.18
ATOM    664  N   THR A 234       8.824  -3.031   3.305  1.00 11.58      0.10
ATOM    665  CA  THR A 234       8.732  -4.052   4.330  1.00 11.51      0.34
ATOM    666  C   THR A 234      10.106  -4.205   4.975  1.00 11.65      0.25
ATOM    667  O   THR A 234      11.134  -3.940   4.335  1.00 11.46     -0.27
ATOM    668  CB  THR A 234       8.189  -5.364   3.720  1.00 11.81      0.15
ATOM    669  OG1 THR A 234       9.060  -5.796   2.686  1.00 11.15     -0.39
ATOM    670  CG2 THR A 234       6.802  -5.192   3.085  1.00 10.62      0.04
ATOM    671  H   THR A 234       9.550  -3.189   2.611  1.00  0.00      0.32
ATOM    672  HG1 THR A 234       9.798  -6.260   3.060  1.00  0.00      0.21
ATOM    673  N   VAL A 235      10.108  -4.660   6.230  1.00 11.95     -0.34
ATOM    674  CA  VAL A 235      11.367  -4.886   6.948  1.00 11.76      0.16
ATOM    675  C   VAL A 235      11.463  -6.360   7.311  1.00 11.88      0.21
ATOM    676  O   VAL A 235      10.480  -6.965   7.733  1.00 11.90     -0.28
ATOM    677  CB  VAL A 235      11.531  -3.986   8.187  1.00 12.06      0.00
ATOM    678  CG1 VAL A 235      12.976  -4.039   8.712  1.00 11.43      0.01
ATOM    679  CG2 VAL A 235      11.131  -2.537   7.884  1.00 11.50      0.01
ATOM    680  H   VAL A 235       9.235  -4.847   6.709  1.00  0.00      0.16
ATOM    681  N   LEU A 261       3.944  -0.771  12.958  1.00 15.84     -0.32
```

```
ATOM    682  CA  LEU A 261       4.265   0.662  12.953  1.00 16.28      0.17
ATOM    683  C   LEU A 261       3.910   1.328  14.281  1.00 16.27      0.22
ATOM    684  O   LEU A 261       4.682   2.141  14.791  1.00 16.48     -0.28
ATOM    685  CB  LEU A 261       3.538   1.374  11.790  1.00 16.36      0.03
ATOM    686  CG  LEU A 261       4.396   1.901  10.631  1.00 16.91     -0.02
ATOM    687  CD1 LEU A 261       5.111   0.771   9.892  1.00 17.91      0.00
ATOM    688  CD2 LEU A 261       3.543   2.737   9.671  1.00 16.66      0.00
ATOM    689  H   LEU A 261       3.306  -1.122  12.259  1.00  0.00      0.18
ATOM    690  N   GLU A 264       6.456   0.248  17.052  1.00 15.33     -0.32
ATOM    691  CA  GLU A 264       7.770   0.832  16.793  1.00 14.94      0.19
ATOM    692  C   GLU A 264       7.792   2.338  17.071  1.00 15.03      0.24
ATOM    693  O   GLU A 264       8.703   2.829  17.735  1.00 14.99     -0.27
ATOM    694  CB  GLU A 264       8.261   0.501  15.383  1.00 14.44      0.04
ATOM    695  CG  GLU A 264       8.629  -0.971  15.218  1.00 13.96      0.11
ATOM    696  CD  GLU A 264       9.489  -1.245  14.004  1.00 13.50      0.13
ATOM    697  OE1 GLU A 264       9.419  -2.371  13.465  1.00 12.57     -0.65
ATOM    698  OE2 GLU A 264      10.247  -0.346  13.605  1.00 13.37     -0.77
ATOM    699  H   GLU A 264       5.857   0.013  16.271  1.00  0.00      0.18
ATOM    700  HE2 GLU A 264      10.753  -0.613  12.853  1.00  0.00      0.16
ATOM    701  N   ASN A 265       6.773   3.048  16.590  1.00 15.07     -0.34
ATOM    702  CA  ASN A 265       6.625   4.478  16.858  1.00 15.63      0.17
ATOM    703  C   ASN A 265       6.558   4.785  18.360  1.00 15.73      0.22
ATOM    704  O   ASN A 265       7.099   5.797  18.811  1.00 15.76     -0.28
ATOM    705  CB  ASN A 265       5.410   5.062  16.111  1.00 15.30      0.13
ATOM    706  CG  ASN A 265       5.764   5.584  14.718  1.00 16.37      0.21
ATOM    707  OD1 ASN A 265       6.804   6.214  14.522  1.00 16.85     -0.27
ATOM    708  ND2 ASN A 265       4.883   5.339  13.747  1.00 17.05     -0.37
ATOM    709  H   ASN A 265       6.053   2.587  16.047  1.00  0.00      0.16
ATOM    710 2HD2 ASN A 265       5.059   5.688  12.811  1.00  0.00      0.15
ATOM    711 1HD2 ASN A 265       4.043   4.816  13.944  1.00  0.00      0.15
ATOM    712  N   MET A 268      10.217   4.159  19.769  1.00 14.93     -0.32
ATOM    713  CA  MET A 268      11.076   5.197  19.191  1.00 15.12      0.19
ATOM    714  C   MET A 268      10.774   6.571  19.788  1.00 14.84      0.24
ATOM    715  O   MET A 268      11.677   7.386  19.971  1.00 14.58     -0.27
ATOM    716  CB  MET A 268      10.928   5.241  17.673  1.00 15.11      0.04
ATOM    717  CG  MET A 268      11.388   3.992  16.945  1.00 15.05      0.07
ATOM    718  SD  MET A 268      10.868   4.027  15.206  1.00 16.23     -0.17
ATOM    719  CE  MET A 268      12.024   5.261  14.568  1.00 15.55      0.08
ATOM    720  H   MET A 268       9.566   3.678  19.160  1.00  0.00      0.18
ATOM    721  N   GLY A 269       9.501   6.817  20.096  1.00 14.94     -0.35
ATOM    722  CA  GLY A 269       9.095   8.028  20.807  1.00 14.74      0.20
ATOM    723  C   GLY A 269       9.757   8.159  22.175  1.00 15.10      0.21
ATOM    724  O   GLY A 269      10.238   9.235  22.534  1.00 14.86     -0.28
ATOM    725  H   GLY A 269       8.792   6.126  19.888  1.00  0.00      0.16
ATOM    726  N   ILE A 271      12.583   6.748  23.091  1.00 15.79     -0.32
ATOM    727  CA  ILE A 271      14.009   6.921  22.831  1.00 16.20      0.19
ATOM    728  C   ILE A 271      14.317   8.346  22.372  1.00 16.57      0.24
ATOM    729  O   ILE A 271      15.183   9.015  22.942  1.00 16.13     -0.27
ATOM    730  CB  ILE A 271      14.500   5.884  21.777  1.00 16.36      0.01
ATOM    731  CG1 ILE A 271      14.422   4.465  22.350  1.00 16.05      0.00
ATOM    732  CG2 ILE A 271      15.922   6.229  21.286  1.00 16.38      0.01
ATOM    733  CD1 ILE A 271      14.458   3.361  21.301  1.00 16.35      0.00
ATOM    734  H   ILE A 271      12.062   6.121  22.492  1.00  0.00      0.18
ATOM    735  N   LEU A 272      13.599   8.807  21.350  1.00 16.95     -0.34
ATOM    736  CA  LEU A 272      13.916  10.080  20.710  1.00 17.45      0.16
ATOM    737  C   LEU A 272      13.363  11.310  21.411  1.00 17.47      0.21
ATOM    738  O   LEU A 272      14.100  12.274  21.650  1.00 17.52     -0.28
```

```
ATOM    739  CB  LEU A 272      13.486  10.073  19.242  1.00 17.86      0.03
ATOM    740  CG  LEU A 272      14.551   9.701  18.218  1.00 18.82     -0.02
ATOM    741  CD1 LEU A 272      13.991   9.912  16.822  1.00 19.34      0.00
ATOM    742  CD2 LEU A 272      15.808  10.535  18.401  1.00 19.73      0.00
ATOM    743  H   LEU A 272      12.883   8.223  20.933  1.00  0.00      0.16
TER     744      LEU A 272 `;
```

Load the PDB texts into models

In [35]:
```
%%javascript

let models = binana.load_ligand_receptor.from_texts(
    ligPDBTxt, recepPDBTxt
);
window.ligand = models[0];
window.receptor = models[1];
```

Get information about the hydrogen bonds (example)

In [36]:
```
%%javascript

window.hbondInf = binana.interactions.get_hydrogen_bonds(
    ligand, receptor
);
```

In [37]:
```
%%javascript

// Counting/characterizing the acceptors and donors (counts)
output(
    element,
    JSON.stringify(
        hbondInf["counts"],
        null, 2
    )
);
```

```
{
  "HDONOR_LIGAND_SIDECHAIN_OTHER": 2,
  "HDONOR_RECEPTOR_SIDECHAIN_OTHER": 1
}
```

In [38]:
```
%%javascript

// List the atoms involved in each hydrogen bond, and the
// angles/distances
let toShow = "";
for(let hbondLabel of hbondInf["labels"]) {
    toShow += JSON.stringify(
        hbondLabel, null, 2
    ) + "\n";
}
output(element, toShow);
```


```
[
  "A:CHT(1):N1(14)",
  "A:CHT(1):H1(16)",
  "A:ASP(157):OD2(285)",
  "LIGAND",
  {
    "distance": 2.6500811308335455,
    "angle": 16.087842801376098
  }
]
[
  "A:CHT(1):O6(22)",
  "A:ASN(156):2HD2(276)",
  "A:ASN(156):ND2(274)",
  "RECEPTOR",
  {
    "distance": 2.9006795755477723,
    "angle": 35.51562311681741
  }
]
[
  "A:CHT(1):O6(22)",
  "A:CHT(1):HO6(23)",
  "A:ASP(157):OD1(284)",
  "LIGAND",
  {
    "distance": 2.538558843123397,
    "angle": 24.57128175960105
  }
]
```


Get information about the cation-pi interactions (example)

In [39]:
```
%%javascript

window.cationPiInf = binana.interactions.get_cation_pi(
    ligand,
    receptor
);
```

In [40]:
```
%%javascript

// Counting/characterizing the acceptors and donors (counts)
output(
    element,
    JSON.stringify(
        cationPiInf["counts"],
        null, 2
    )
);
```


```
{
  "PI-CATION_LIGAND-CHARGED_OTHER": 2,
  "PI-CATION_LIGAND-CHARGED_BETA": 2,
  "PI-CATION_RECEPTOR-CHARGED_OTHER": 5
}
```

In [41]:

```
%%javascript

// List the atoms involved in each cation-pi interaction
let toShow = "";
for(let cationPiLabel of cationPiInf["labels"]) {
    toShow += JSON.stringify(
        cationPiLabel, null, 2
    ) + "\n";
}
output(element, toShow);
```


```
[
  "[A:CHT(1):N1(2) / A:CHT(1):C5(1) / A:CHT(1):C6(3) / A:CHT(1):C6(4) / A:CHT(1):C7(9)]",
  "[A:TRP(43):CG(28) / A:TRP(43):CD1(29) / A:TRP(43):NE1(31) / A:TRP(43):CE2(32) / A:TRP(43):CD2(30)]",
  {
    "distance": 4.403228947034208
  }
]
[
  "[A:CHT(1):N1(2) / A:CHT(1):C5(1) / A:CHT(1):C6(3) / A:CHT(1):C6(4) / A:CHT(1):C7(9)]",
  "[A:TRP(43):CE2(32) / A:TRP(43):CD2(30) / A:TRP(43):CE3(33) / A:TRP(43):CZ3(35) / A:TRP(43):CH2(36) / A:TRP(43):CZ2(34)]",
  {
    "distance": 4.280756595250165
  }
]
[
  "[A:CHT(1):N1(2) / A:CHT(1):C5(1) / A:CHT(1):C6(3) / A:CHT(1):C6(4) / A:CHT(1):C7(9)]",
  "[A:TRP(205):CG(468) / A:TRP(205):CD1(469) / A:TRP(205):NE1(471) / A:TRP(205):CE2(472) / A:TRP(205):CD2(470)]",
  {
    "distance": 4.1748128341280175
  }
]
[
  "[A:CHT(1):N1(2) / A:CHT(1):C5(1) / A:CHT(1):C6(3) / A:CHT(1):C6(4) / A:CHT(1):C7(9)]",
  "[A:TRP(205):CE2(472) / A:TRP(205):CD2(470) / A:TRP(205):CE3(473) / A:TRP(205):CZ3(475) / A:TRP(205):CH2(476) / A:TRP(205):CZ2(474)]",
  {
    "distance": 4.45074514048553
  }
]
[
  "[A:CHT(1):C2(17) / A:CHT(1):O1(18) / A:CHT(1):C5(19) / A:CHT(1):C4(20) / A:CHT(1):C3(21)]",
  "[A:LYS(94):NZ(144) / A:LYS(94):HZ1(146) / A:LYS(94):HZ2(147) / A:LYS(94):HZ3(148)]",
  {
    "distance": 2.57953875721998
  }
```

```
]
[
  "[A:CHT(1):O1(18) / A:CHT(1):C2(17) / A:CHT(1):C3(21) / A:CHT(1):C4(20) / A:CHT(1):C5(1
9)]",
  "[A:LYS(94):NZ(144) / A:LYS(94):HZ1(146) / A:LYS(94):HZ2(147) / A:LYS(94):HZ3(148)]",
  {
    "distance": 2.57953875721998
  }
]
[
  "[A:CHT(1):C5(19) / A:CHT(1):O1(18) / A:CHT(1):C2(17) / A:CHT(1):C3(21) / A:CHT(1):C4(2
0)]",
  "[A:LYS(94):NZ(144) / A:LYS(94):HZ1(146) / A:LYS(94):HZ2(147) / A:LYS(94):HZ3(148)]",
  {
    "distance": 2.57953875721998
  }
]
[
  "[A:CHT(1):C4(20) / A:CHT(1):C5(19) / A:CHT(1):O1(18) / A:CHT(1):C2(17) / A:CHT(1):C3(2
1)]",
  "[A:LYS(94):NZ(144) / A:LYS(94):HZ1(146) / A:LYS(94):HZ2(147) / A:LYS(94):HZ3(148)]",
  {
    "distance": 2.5795387572199804
  }
]
[
  "[A:CHT(1):C3(21) / A:CHT(1):C2(17) / A:CHT(1):O1(18) / A:CHT(1):C5(19) / A:CHT(1):C4(2
0)]",
  "[A:LYS(94):NZ(144) / A:LYS(94):HZ1(146) / A:LYS(94):HZ2(147) / A:LYS(94):HZ3(148)]",
  {
    "distance": 2.57953875721998
  }
]
```


Other interactions are also available

In [42]:
```
%%javascript

let toShow = "";
toShow += "Available functions for detecting interactions:\n";
let funcNames = Object.keys(binana.interactions).filter(
    n => n.startsWith("get_")
);
toShow += funcNames.join("\n");
output(element, toShow);
```

```
Available functions for detecting interactions:
get_active_site_flexibility
get_all_interactions
get_cation_pi
get_close
get_closest
get_electrostatic_energies
get_halogen_bonds
get_hydrogen_bonds
get_hydrophobics
get_ligand_atom_types
get_metal_coordinations
get_pi_pi
get_salt_bridges
```

Get PDB-formatted text

In [43]:

```
%%javascript

window.pdbTxt = binana.output.pdb_file.write(
    ligand,
    receptor,
    null,          // closest
    null,          // close
    null,          // hydrophobics
    hbondInf,      // hydrogen bonds
    null,          // halogen bonds
    null,          // salt_bridges
    null,          // metal_coordinations
    null,          // pi_pi
    cationPiInf,   // cat_pi
    null,          // active_site_flexibility
    null,          // log_output
    true,          // as_str
)

let pdbRemarkLines = pdbTxt.split("\n")
    .filter(l => l.startsWith("REMARK") && l !== 'REMARK');
let pdbRemarkTxt = pdbRemarkLines.join(",")
    .replace(/REMARK {0,1}/g, "")
    .replace(".,", ".");
output(element, pdbRemarkTxt);
```

```
The residue named "CCN" contains the closest contacts between the protein and receptor. "CO
N" indicates close contacts. "ALP", "BET", and "OTH" indicate receptor contacts whose respe
ctive protein residues have the alpha-helix, beta-sheet, or "other" secondary structure. "B
AC" and "SID" indicate receptor contacts that are part of the protein backbone and sidechai
n, respectively. "HYD" indicates hydrophobic contacts between the protein and ligand. "HBN"
indicates hydrogen bonds. "HAL" indicates halogen bonds. "SAL" indicates salt bridges. "PI
S" indicates pi-pi stacking interactions, "PIT" indicates T-stacking interactions, and "PI
C" indicates cation-pi interactions. "MTL" indicates metal-coordination interactions. Prote
in residue names are unchanged, but the ligand residue is now named "LIG".
```

In [44]:
```
%%javascript

output(element, pdbTxt);
```

```
REMARK
REMARK The residue named "CCN" contains the closest contacts between the protein and recept
or. "CON" indicates close contacts. "ALP", "BET", and "OTH" indicate receptor contacts whos
e respective protein residues have the alpha-helix, beta-sheet, or "other" secondary struct
ure. "BAC" and "SID" indicate receptor contacts that are part of the protein backbone and s
idechain, respectively. "HYD" indicates hydrophobic contacts between the protein and ligan
d. "HBN" indicates hydrogen bonds. "HAL" indicates halogen bonds. "SAL" indicates salt brid
ges. "PIS" indicates pi-pi stacking interactions, "PIT" indicates T-stacking interactions,
and "PIC" indicates cation-pi interactions. "MTL" indicates metal-coordination interaction
s. Protein residue names are unchanged, but the ligand residue is now named "LIG".
REMARK
ATOM      1  N   ASP A  40      23.366  -3.399  14.662                       N
ATOM      2  CA  ASP A  40      22.530  -2.226  14.843                       C
ATOM      3  C   ASP A  40      23.197  -1.095  14.078                       C
ATOM      4  O   ASP A  40      24.256  -0.613  14.476                       O
ATOM      5  CB  ASP A  40      22.432  -1.893  16.332                       C
ATOM      6  CG  ASP A  40      21.603  -0.652  16.619                       C
```

Get the interactions as a dictionary for easier big-data analysis

In [45]:

```
%%javascript

window.data = binana.output.dictionary.collect(
    null,          // closest
    null,          // close
    null,          // hydrophobics
    hbondInf,      // hydrogen_bonds
    null,          // halogen_bonds
    null,          // salt_bridges
    null,          // metal_coordinations
    null,          // pi_pi
    cationPiInf,   // cat_pi
    null,          // electrostatic_energies
    null,          // active_site_flexibility
    null,          // ligand_atom_types
    null,          // ligand_rotatable_bonds
)

let toShow = "KEYS: ";
toShow += Object.keys(window.data).join(", ") + ". ";
toShow += "\n\nHYDROGEN-BOND DATA (EXAMPLE):\n\n";
toShow += JSON.stringify(window.data["hydrogenBonds"], null, 2);

output(element, toShow);
```

```
KEYS: hydrogenBonds, cationPiInteractions.


HYDROGEN-BOND DATA (EXAMPLE):


[
  {
    "ligandAtoms": [
      {
        "chain": "A",
        "resID": 1,
        "resName": "CHT",
        "atomName": "N1",
        "atomIndex": 14
      },
      {
        "chain": "A",
        "resID": 1,
```

Some prefer CSV-formatted data

In [46]:
```
%%javascript

let csv = binana.output.csv.collect(window.data).slice(0, 500) + "\n\n..."

output(element, csv);
```

```
cationPiInteractions
,cationPiInteractions.1
,,ligandAtoms
,,,ligandAtoms.1
,,,,atomIndex,2
,,,,atomName,N1
,,,,chain,A
,,,,resID,1
,,,,resName,CHT
,,,ligandAtoms.2
,,,,atomIndex,1
,,,,atomName,C5
,,,,chain,A
,,,,resID,1
,,,,resName,CHT
,,,ligandAtoms.3
,,,,atomIndex,3
,,,,atomName,C6
,,,,chain,A
,,,,resID,1
,,,,resName,CHT
,,,ligandAtoms.4
,,,,atomIndex,4
,,,,atomName,C6
,,,,chain,A
,,,,resID,1
,,,,resName,CHT
,,,ligandAtoms.5
,,,,atomIndex,9
,,,,atomName,C7
,,,,chain,A
,,,,resID,1
,,,,resName,

...
```

Get all the interactions at once

In [47]:
```
%%javascript

window.allInf = binana.interactions.get_all_interactions(
    ligand, receptor
);
```

In [48]:
```
%%javascript

output(
    element,
    JSON.stringify(
        Object.keys(allInf), null, 2
    )
);
```


```
[
  "closest",
  "close",
  "electrostatic_energies",
  "active_site_flexibility",
  "hydrophobics",
  "hydrogen_bonds",
  "halogen_bonds",
  "ligand_atom_types",
  "pi_pi",
  "cat_pi",
  "salt_bridges",
  "metal_coordinations",
  "ligand_rotatable_bonds"
]
```


Get and display PDB-formatted text containing all interactions

In [49]:
```
%%javascript

window.pdbTxt = binana.output.pdb_file.write_all(
    ligand, receptor,
    allInf,
    null,  // log_output
    true   // as_str
);

output(
    element,
    pdbTxt
);
```

```
REMARK
REMARK The residue named "CCN" contains the closest contacts between the protein and recept
or. "CON" indicates close contacts. "ALP", "BET", and "OTH" indicate receptor contacts whos
e respective protein residues have the alpha-helix, beta-sheet, or "other" secondary struct
ure. "BAC" and "SID" indicate receptor contacts that are part of the protein backbone and s
idechain, respectively. "HYD" indicates hydrophobic contacts between the protein and ligan
d. "HBN" indicates hydrogen bonds. "HAL" indicates halogen bonds. "SAL" indicates salt brid
ges. "PIS" indicates pi-pi stacking interactions, "PIT" indicates T-stacking interactions,
and "PIC" indicates cation-pi interactions. "MTL" indicates metal-coordination interaction
s. Protein residue names are unchanged, but the ligand residue is now named "LIG".
REMARK
ATOM      1  N   ASP A  40      23.366  -3.399  14.662                       N
ATOM      2  CA  ASP A  40      22.530  -2.226  14.843                       C
ATOM      3  C   ASP A  40      23.197  -1.095  14.078                       C
ATOM      4  O   ASP A  40      24.256  -0.613  14.476                       O
ATOM      5  CB  ASP A  40      22.432  -1.893  16.332                       C
ATOM      6  CG  ASP A  40      21.603  -0.652  16.619                       C
```

Get all interactions as a single dictionary

In [51]:

```
%%javascript

let allData = binana.output.dictionary.collect_all(allInf)

let out = JSON.stringify(Object.keys(allData))
out += "\n\nHydrogen bonds (example):\n\n";
out += JSON.stringify(allData["hydrogenBonds"], null, 4)

output(
    element,
    out
);
```


```
["closestContacts","closeContacts","hydrophobicContacts","hydrogenBonds","halogenBonds","piPiStackingInteractions","tStackingInteractions","cationPiInteractions","saltBridges","metalCoordinations","activeSiteFlexibility","electrostaticEnergies","ligandAtomTypes","ligandRotatableBonds"]

Hydrogen bonds (example):

[
    {
        "ligandAtoms": [
            {
                "chain": "A",
                "resID": 1,
                "resName": "LIG",
                "atomName": "N1",
                "atomIndex": 14
            `
```