# Class 11

# Introduction to the RCSB Protein Data Bank (PDB)

## PDB Statistics

Importing CSV

```
pdb_csv <- read.csv("Data Export Summary.csv", row.names = 1)
head(pdb_csv)
```

```
##                           X.ray   NMR   EM Multiple.methods Neutron Other  Total
## Protein (only)          142419 11807 6038              177      70    32 160543
## Protein/Oligosaccharide   8426    31  991                5       0     0   9453
## Protein/NA                7498   274 2000                3       0     0   9775
## Nucleic acid (only)       2368  1378   60                8       2     1   3817
## Other                      149    31    3                0       0     0    183
## Oligosaccharide (only)      11     6    0                1       0     4     22
```

> Q1: What percentage of structures in the PDB are solved by X-Ray and Electron Microscopy.

Percentage using X-ray

```
perc_xray <- (sum(pdb_csv$X.ray)/sum(pdb_csv$Total))*100
perc_xray
```

```
## [1] 87.52836
```

Percentage using EM

```
perc_em <- (sum(pdb_csv$EM)/sum(pdb_csv$Total))*100
perc_em
```

```
## [1] 4.94687
```

> Q2: What proportion of structures in the PDB are protein?

```
perc_protein <- (pdb_csv[1,7]/sum(pdb_csv$Total))*100
perc_protein
```

```
## [1] 87.3499
```

> Q3: Type HIV in the PDB website search box on the home page and determine how many HIV-1 protease structures are in the current PDB?

I found 1205 HIV-1 Proteases in my search

# The PDB Format

Importing specific PDB File for HIV-1 into VMD

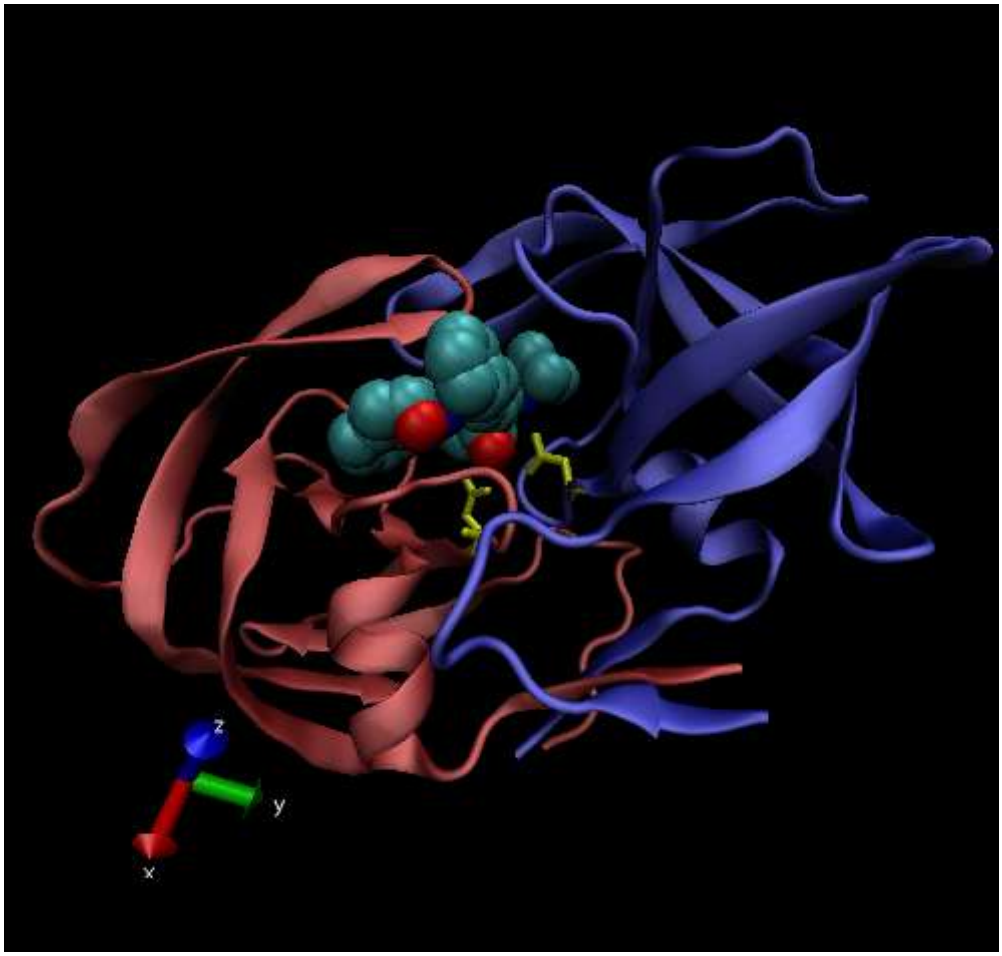
> Q4: Water molecules normally have 3 atoms. Why do we see just one atom per water molecule in this structure?

The EM resolution is 2 angstroms which is not fine enough to see the hydrogen atoms

> Q5: There is a conserved water molecule in the binding site. Can you identify this water molecule? What residue number does this water molecule have (see note below)?

The water molecule with residue number 308 is in the binding site, best seen when the drug is in the binding site.

## Import image into R




# Using Bio3D in R for Structural Bioinformatics

```
library("bio3d")

pdb <- read.pdb("1hel")


##   Note: Accessing on-line PDB file


pdb


##
##  Call:  read.pdb(file = "1hel")
##
##    Total Models#: 1
##      Total Atoms#: 1186,  XYZs#: 3558  Chains#: 1  (values: A)
```

```
##
##      Protein Atoms#: 1001  (residues/Calpha atoms#: 129)
##      Nucleic acid Atoms#: 0  (residues/phosphate atoms#: 0)
##
##      Non-protein/nucleic Atoms#: 185  (residues: 185)
##      Non-protein/nucleic resid values: [ HOH (185) ]
##
##    Protein sequence:
##       KVFGRCELAAAMKRHGLDNYRGYSLGNWVCAAKFESNFNTQATNRNTDGSTDYGILQINS
##       RWWCNDGRTPGSRNLCNIPCSALLSSDITASVNCAKKIVSDGNGMNAWVAWRNRCKGTDV
##       QAWIRGCRL
##
## + attr: atom, xyz, seqres, helix, sheet,
##         calpha, remark, call
```

```
pdb$atom
```

```
##        type eleno elety  alt resid chain resno insert       x      y      z   o
## 1      ATOM     1     N <NA>   LYS     A     1   <NA>   3.294 10.164 10.266 1.0
## 2      ATOM     2    CA <NA>   LYS     A     1   <NA>   2.388 10.533  9.168 1.0
## 3      ATOM     3     C <NA>   LYS     A     1   <NA>   2.438 12.049  8.889 1.0
## 4      ATOM     4     O <NA>   LYS     A     1   <NA>   2.406 12.898  9.815 1.0
## 5      ATOM     5    CB <NA>   LYS     A     1   <NA>   0.949 10.101  9.559 1.0
## 6      ATOM     6    CG <NA>   LYS     A     1   <NA>  -0.050 10.621  8.573 1.0
## 7      ATOM     7    CD <NA>   LYS     A     1   <NA>  -1.425 10.081  8.720 1.0
## 8      ATOM     8    CE <NA>   LYS     A     1   <NA>  -2.370 10.773  7.722 1.0
## 9      ATOM     9    NZ <NA>   LYS     A     1   <NA>  -3.776 10.439  7.933 1.0
## 10     ATOM    10     N <NA>   VAL     A     2   <NA>   2.552 12.428  7.626 1.0
## 11     ATOM    11    CA <NA>   VAL     A     2   <NA>   2.524 13.840  7.282 1.0
## 12     ATOM    12     C <NA>   VAL     A     2   <NA>   1.120 14.180  6.770 1.0
## 13     ATOM    13     O <NA>   VAL     A     2   <NA>   0.737 13.798  5.675 1.0
## 14     ATOM    14    CB <NA>   VAL     A     2   <NA>   3.529 14.264  6.240 1.0
## 15     ATOM    15   CG1 <NA>   VAL     A     2   <NA>   3.313 15.765  5.983 1.0
## 16     ATOM    16   CG2 <NA>   VAL     A     2   <NA>   4.928 14.016  6.810 1.0
## 17     ATOM    17     N <NA>   PHE     A     3   <NA>   0.333 14.851  7.573 1.0
## 18     ATOM    18    CA <NA>   PHE     A     3   <NA>  -1.021 15.173  7.169 1.0
## 19     ATOM    19     C <NA>   PHE     A     3   <NA>  -1.097 16.285  6.126 1.0
## 20     ATOM    20     O <NA>   PHE     A     3   <NA>  -0.261 17.203  6.054 1.0
## 21     ATOM    21    CB <NA>   PHE     A     3   <NA>  -1.867 15.710  8.361 1.0
## 22     ATOM    22    CG <NA>   PHE     A     3   <NA>  -2.412 14.638  9.295 1.0
## 23     ATOM    23   CD1 <NA>   PHE     A     3   <NA>  -1.575 14.049 10.240 1.0
## 24     ATOM    24   CD2 <NA>   PHE     A     3   <NA>  -3.757 14.285  9.274 1.0
## 25     ATOM    25   CE1 <NA>   PHE     A     3   <NA>  -2.065 13.116 11.135 1.0
## 26     ATOM    26   CE2 <NA>   PHE     A     3   <NA>  -4.263 13.332 10.178 1.0
## 27     ATOM    27    CZ <NA>   PHE     A     3   <NA>  -3.413 12.758 11.132 1.0
## 28     ATOM    28     N <NA>   GLY     A     4   <NA>  -2.229 16.228  5.393 1.0
## 29     ATOM    29    CA <NA>   GLY     A     4   <NA>  -2.645 17.273  4.511 1.0
## 30     ATOM    30     C <NA>   GLY     A     4   <NA>  -3.456 18.261  5.350 1.0
```

```
## 31     ATOM     31     O <NA>   GLY     A     4   <NA>  -4.070 17.876  6.282 1.0
## 32     ATOM     32     N <NA>   ARG     A     5   <NA>  -3.414 19.518  5.009 1.0
## 33     ATOM     33    CA <NA>   ARG     A     5   <NA>  -4.106 20.560  5.674 1.0
## 34     ATOM     34     C <NA>   ARG     A     5   <NA>  -5.540 20.226  5.992 1.0
## 35     ATOM     35     O <NA>   ARG     A     5   <NA>  -5.963 20.258  7.138 1.0
## 36     ATOM     36    CB <NA>   ARG     A     5   <NA>  -3.952 21.857  4.900 1.0
## 37     ATOM     37    CG <NA>   ARG     A     5   <NA>  -4.508 23.053  5.610 1.0
## 38     ATOM     38    CD <NA>   ARG     A     5   <NA>  -4.414 24.335  4.775 1.0
## 39     ATOM     39    NE <NA>   ARG     A     5   <NA>  -5.013 24.223  3.447 1.0
## 40     ATOM     40    CZ <NA>   ARG     A     5   <NA>  -6.287 24.522  3.048 1.0
## 41     ATOM     41   NH1 <NA>   ARG     A     5   <NA>  -7.248 25.009  3.841 1.0
## 42     ATOM     42   NH2 <NA>   ARG     A     5   <NA>  -6.619 24.303  1.767 1.0
## 43     ATOM     43     N <NA>   CYS     A     6   <NA>  -6.327 19.866  4.967 1.0
## 44     ATOM     44    CA <NA>   CYS     A     6   <NA>  -7.767 19.572  5.189 1.0
## 45     ATOM     45     C <NA>   CYS     A     6   <NA>  -7.997 18.269  5.916 1.0
## 46     ATOM     46     O <NA>   CYS     A     6   <NA>  -8.992 18.125  6.630 1.0
## 47     ATOM     47    CB <NA>   CYS     A     6   <NA>  -8.607 19.637  3.859 1.0
## 48     ATOM     48    SG <NA>   CYS     A     6   <NA>  -8.669 21.273  3.104 1.0
## 49     ATOM     49     N <NA>   GLU     A     7   <NA>  -7.142 17.274  5.653 1.0
## 50     ATOM     50    CA <NA>   GLU     A     7   <NA>  -7.309 15.981  6.323 1.0
## 51     ATOM     51     C <NA>   GLU     A     7   <NA>  -7.129 16.181  7.848 1.0
## 52     ATOM     52     O <NA>   GLU     A     7   <NA>  -7.835 15.638  8.657 1.0
## 53     ATOM     53    CB <NA>   GLU     A     7   <NA>  -6.187 15.048  5.880 1.0
## 54     ATOM     54    CG <NA>   GLU     A     7   <NA>  -6.206 13.614  6.496 1.0
## 55     ATOM     55    CD <NA>   GLU     A     7   <NA>  -4.952 12.864  6.030 1.0
## 56     ATOM     56   OE1 <NA>   GLU     A     7   <NA>  -4.003 13.411  5.480 1.0
## 57     ATOM     57   OE2 <NA>   GLU     A     7   <NA>  -4.992 11.578  6.219 1.0
## 58     ATOM     58     N <NA>   LEU     A     8   <NA>  -6.148 16.987  8.221 1.0
## 59     ATOM     59    CA <NA>   LEU     A     8   <NA>  -5.919 17.285  9.637 1.0
## 60     ATOM     60     C <NA>   LEU     A     8   <NA>  -7.068 18.103 10.254 1.0
## 61     ATOM     61     O <NA>   LEU     A     8   <NA>  -7.500 17.827 11.353 1.0
## 62     ATOM     62    CB <NA>   LEU     A     8   <NA>  -4.607 18.084  9.809 1.0
## 63     ATOM     63    CG <NA>   LEU     A     8   <NA>  -4.384 18.432 11.299 1.0
## 64     ATOM     64   CD1 <NA>   LEU     A     8   <NA>  -4.110 17.104 12.053 1.0
## 65     ATOM     65   CD2 <NA>   LEU     A     8   <NA>  -3.147 19.299 11.372 1.0
## 66     ATOM     66     N <NA>   ALA     A     9   <NA>  -7.524 19.122  9.561 1.0
## 67     ATOM     67    CA <NA>   ALA     A     9   <NA>  -8.664 19.896  9.982 1.0
## 68     ATOM     68     C <NA>   ALA     A     9   <NA>  -9.841 18.971 10.304 1.0
## 69     ATOM     69     O <NA>   ALA     A     9   <NA> -10.469 19.046 11.359 1.0
## 70     ATOM     70    CB <NA>   ALA     A     9   <NA>  -9.039 21.012  8.954 1.0
## 71     ATOM     71     N <NA>   ALA     A    10   <NA> -10.124 18.049  9.425 1.0
## 72     ATOM     72    CA <NA>   ALA     A    10   <NA> -11.262 17.129  9.595 1.0
## 73     ATOM     73     C <NA>   ALA     A    10   <NA> -11.034 16.206 10.780 1.0
## 74     ATOM     74     O <NA>   ALA     A    10   <NA> -11.932 15.902 11.522 1.0
## 75     ATOM     75    CB <NA>   ALA     A    10   <NA> -11.457 16.297  8.313 1.0
## 76     ATOM     76     N <NA>   ALA     A    11   <NA>  -9.815 15.771 10.988 1.0
## 77     ATOM     77    CA <NA>   ALA     A    11   <NA>  -9.544 14.908 12.136 1.0
## 78     ATOM     78     C <NA>   ALA     A    11   <NA>  -9.651 15.641 13.494 1.0
## 79     ATOM     79     O <NA>   ALA     A    11   <NA> -10.088 15.066 14.457 1.0
## 80     ATOM     80    CB <NA>   ALA     A    11   <NA>  -8.153 14.250 12.041 1.0
## 81     ATOM     81     N <NA>   MET     A    12   <NA>  -9.107 16.884 13.529 1.0
```

```
## 82     ATOM    82    CA <NA>   MET     A    12   <NA>  -9.160 17.683 14.710 1.0
## 83     ATOM    83     C <NA>   MET     A    12   <NA> -10.599 17.988 15.028 1.0
## 84     ATOM    84     O <NA>   MET     A    12   <NA> -10.964 17.966 16.195 1.0
## 85     ATOM    85    CB <NA>   MET     A    12   <NA>  -8.385 18.996 14.563 1.0
## 86     ATOM    86    CG <NA>   MET     A    12   <NA>  -6.872 18.717 14.593 1.0
## 87     ATOM    87    SD <NA>   MET     A    12   <NA>  -5.971 20.286 14.351 1.0
## 88     ATOM    88    CE <NA>   MET     A    12   <NA>  -4.392 19.972 15.137 1.0
## 89     ATOM    89     N <NA>   LYS     A    13   <NA> -11.421 18.239 13.985 1.0
## 90     ATOM    90    CA <NA>   LYS     A    13   <NA> -12.844 18.554 14.146 1.0
## 91     ATOM    91     C <NA>   LYS     A    13   <NA> -13.552 17.402 14.762 1.0
## 92     ATOM    92     O <NA>   LYS     A    13   <NA> -14.278 17.533 15.704 1.0
## 93     ATOM    93    CB <NA>   LYS     A    13   <NA> -13.505 18.908 12.852 1.0
## 94     ATOM    94    CG <NA>   LYS     A    13   <NA> -14.874 19.457 13.096 1.0
## 95     ATOM    95    CD <NA>   LYS     A    13   <NA> -15.519 20.062 11.867 1.0
## 96     ATOM    96    CE <NA>   LYS     A    13   <NA> -17.062 20.060 11.971 1.0
## 97     ATOM    97    NZ <NA>   LYS     A    13   <NA> -17.725 20.836 10.899 1.0
## 98     ATOM    98     N <NA>   ARG     A    14   <NA> -13.273 16.240 14.220 1.0
## 99     ATOM    99    CA <NA>   ARG     A    14   <NA> -13.878 15.021 14.667 1.0
## 100    ATOM   100     C <NA>   ARG     A    14   <NA> -13.480 14.746 16.099 1.0
## 101    ATOM   101     O <NA>   ARG     A    14   <NA> -14.217 14.129 16.823 1.0
## 102    ATOM   102    CB <NA>   ARG     A    14   <NA> -13.448 13.876 13.756 1.0
## 103    ATOM   103    CG <NA>   ARG     A    14   <NA> -14.102 12.553 14.162 1.0
## 104    ATOM   104    CD <NA>   ARG     A    14   <NA> -13.875 11.424 13.160 1.0
## 105    ATOM   105    NE <NA>   ARG     A    14   <NA> -12.616 10.730 13.354 1.0
## 106    ATOM   106    CZ <NA>   ARG     A    14   <NA> -12.406  9.681 14.156 1.0
## 107    ATOM   107   NH1 <NA>   ARG     A    14   <NA> -13.357  9.121 14.898 1.0
## 108    ATOM   108   NH2 <NA>   ARG     A    14   <NA> -11.177  9.169 14.196 1.0
## 109    ATOM   109     N <NA>   HIS     A    15   <NA> -12.300 15.219 16.498 1.0
## 110    ATOM   110    CA <NA>   HIS     A    15   <NA> -11.791 15.016 17.846 1.0
## 111    ATOM   111     C <NA>   HIS     A    15   <NA> -12.221 16.074 18.888 1.0
## 112    ATOM   112     O <NA>   HIS     A    15   <NA> -11.689 16.060 19.970 1.0
## 113    ATOM   113    CB <NA>   HIS     A    15   <NA> -10.268 14.799 17.851 1.0
## 114    ATOM   114    CG <NA>   HIS     A    15   <NA>  -9.906 13.364 17.563 1.0
## 115    ATOM   115   ND1 <NA>   HIS     A    15   <NA>  -9.721 12.896 16.256 1.0
## 116    ATOM   116   CD2 <NA>   HIS     A    15   <NA>  -9.723 12.308 18.413 1.0
## 117    ATOM   117   CE1 <NA>   HIS     A    15   <NA>  -9.422 11.580 16.350 1.0
## 118    ATOM   118   NE2 <NA>   HIS     A    15   <NA>  -9.412 11.213 17.627 1.0
## 119    ATOM   119     N <NA>   GLY     A    16   <NA> -13.146 16.952 18.551 1.0
## 120    ATOM   120    CA <NA>   GLY     A    16   <NA> -13.687 17.956 19.401 1.0
## 121    ATOM   121     C <NA>   GLY     A    16   <NA> -12.871 19.227 19.554 1.0
## 122    ATOM   122     O <NA>   GLY     A    16   <NA> -13.121 20.016 20.460 1.0
## 123    ATOM   123     N <NA>   LEU     A    17   <NA> -11.922 19.491 18.685 1.0
## 124    ATOM   124    CA <NA>   LEU     A    17   <NA> -11.134 20.695 18.826 1.0
## 125    ATOM   125     C <NA>   LEU     A    17   <NA> -11.728 21.961 18.295 1.0
## 126    ATOM   126     O <NA>   LEU     A    17   <NA> -11.276 23.016 18.657 1.0
## 127    ATOM   127    CB <NA>   LEU     A    17   <NA>  -9.749 20.538 18.218 1.0
## 128    ATOM   128    CG <NA>   LEU     A    17   <NA>  -8.792 19.745 19.031 1.0
## 129    ATOM   129   CD1 <NA>   LEU     A    17   <NA>  -7.483 19.876 18.293 1.0
## 130    ATOM   130   CD2 <NA>   LEU     A    17   <NA>  -8.675 20.282 20.474 1.0
## 131    ATOM   131     N <NA>   ASP     A    18   <NA> -12.704 21.930 17.405 1.0
## 132    ATOM   132    CA <NA>   ASP     A    18   <NA> -13.261 23.178 16.884 1.0
```

```
## 133   ATOM   133     C <NA>   ASP     A    18   <NA> -13.986 23.912 17.979 1.0
## 134   ATOM   134     O <NA>   ASP     A    18   <NA> -14.952 23.375 18.512 1.0
## 135   ATOM   135    CB <NA>   ASP     A    18   <NA> -14.275 23.002 15.717 1.0
## 136   ATOM   136    CG <NA>   ASP     A    18   <NA> -14.712 24.288 15.010 1.0
## 137   ATOM   137   OD1 <NA>   ASP     A    18   <NA> -14.134 25.393 15.038 1.0
## 138   ATOM   138   OD2 <NA>   ASP     A    18   <NA> -15.751 24.055 14.248 1.0
## 139   ATOM   139     N <NA>   ASN     A    19   <NA> -13.542 25.130 18.229 1.0
## 140   ATOM   140    CA <NA>   ASN     A    19   <NA> -14.046 26.010 19.253 1.0
## 141   ATOM   141     C <NA>   ASN     A    19   <NA> -13.851 25.507 20.671 1.0
## 142   ATOM   142     O <NA>   ASN     A    19   <NA> -14.534 25.975 21.595 1.0
## 143   ATOM   143    CB <NA>   ASN     A    19   <NA> -15.518 26.259 19.032 1.0
## 144   ATOM   144    CG <NA>   ASN     A    19   <NA> -15.706 27.052 17.774 1.0
## 145   ATOM   145   OD1 <NA>   ASN     A    19   <NA> -15.227 28.183 17.693 1.0
## 146   ATOM   146   ND2 <NA>   ASN     A    19   <NA> -16.402 26.456 16.811 1.0
## 147   ATOM   147     N <NA>   TYR     A    20   <NA> -12.956 24.552 20.827 1.0
## 148   ATOM   148    CA <NA>   TYR     A    20   <NA> -12.652 24.027 22.106 1.0
## 149   ATOM   149     C <NA>   TYR     A    20   <NA> -12.037 25.159 22.929 1.0
## 150   ATOM   150     O <NA>   TYR     A    20   <NA> -10.978 25.687 22.602 1.0
## 151   ATOM   151    CB <NA>   TYR     A    20   <NA> -11.717 22.810 22.005 1.0
## 152   ATOM   152    CG <NA>   TYR     A    20   <NA> -11.532 22.151 23.355 1.0
## 153   ATOM   153   CD1 <NA>   TYR     A    20   <NA> -12.444 21.206 23.832 1.0
## 154   ATOM   154   CD2 <NA>   TYR     A    20   <NA> -10.475 22.556 24.184 1.0
## 155   ATOM   155   CE1 <NA>   TYR     A    20   <NA> -12.311 20.657 25.111 1.0
## 156   ATOM   156   CE2 <NA>   TYR     A    20   <NA> -10.331 22.023 25.461 1.0
## 157   ATOM   157    CZ <NA>   TYR     A    20   <NA> -11.259 21.078 25.922 1.0
## 158   ATOM   158    OH <NA>   TYR     A    20   <NA> -11.104 20.560 27.183 1.0
## 159   ATOM   159     N <NA>   ARG     A    21   <NA> -12.721 25.593 23.977 1.0
## 160   ATOM   160    CA <NA>   ARG     A    21   <NA> -12.250 26.715 24.791 1.0
## 161   ATOM   161     C <NA>   ARG     A    21   <NA> -12.264 27.987 24.017 1.0
## 162   ATOM   162     O <NA>   ARG     A    21   <NA> -11.450 28.877 24.295 1.0
## 163   ATOM   163    CB <NA>   ARG     A    21   <NA> -10.847 26.601 25.387 1.0
## 164   ATOM   164    CG <NA>   ARG     A    21   <NA> -10.694 25.514 26.442 1.0
## 165   ATOM   165    CD <NA>   ARG     A    21   <NA> -11.577 25.864 27.598 1.0
## 166   ATOM   166    NE <NA>   ARG     A    21   <NA> -11.597 24.902 28.676 1.0
## 167   ATOM   167    CZ <NA>   ARG     A    21   <NA> -11.253 25.330 29.884 1.0
## 168   ATOM   168   NH1 <NA>   ARG     A    21   <NA> -10.859 26.593 30.049 1.0
## 169   ATOM   169   NH2 <NA>   ARG     A    21   <NA> -11.283 24.508 30.937 1.0
## 170   ATOM   170     N <NA>   GLY     A    22   <NA> -13.173 28.076 23.045 1.0
## 171   ATOM   171    CA <NA>   GLY     A    22   <NA> -13.290 29.312 22.253 1.0
## 172   ATOM   172     C <NA>   GLY     A    22   <NA> -12.276 29.499 21.125 1.0
## 173   ATOM   173     O <NA>   GLY     A    22   <NA> -12.274 30.537 20.508 1.0
## 174   ATOM   174     N <NA>   TYR     A    23   <NA> -11.414 28.511 20.863 1.0
## 175   ATOM   175    CA <NA>   TYR     A    23   <NA> -10.419 28.584 19.787 1.0
## 176   ATOM   176     C <NA>   TYR     A    23   <NA> -10.964 27.832 18.564 1.0
## 177   ATOM   177     O <NA>   TYR     A    23   <NA> -11.097 26.573 18.581 1.0
## 178   ATOM   178    CB <NA>   TYR     A    23   <NA>  -9.059 27.910 20.217 1.0
## 179   ATOM   179    CG <NA>   TYR     A    23   <NA>  -8.358 28.702 21.299 1.0
## 180   ATOM   180   CD1 <NA>   TYR     A    23   <NA>  -7.560 29.766 20.910 1.0
## 181   ATOM   181   CD2 <NA>   TYR     A    23   <NA>  -8.534 28.427 22.652 1.0
## 182   ATOM   182   CE1 <NA>   TYR     A    23   <NA>  -6.879 30.557 21.846 1.0
## 183   ATOM   183   CE2 <NA>   TYR     A    23   <NA>  -7.907 29.219 23.612 1.0
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## 185    ATOM   185    OH <NA>   TYR     A     23   <NA>  -6.411 31.069 24.111 1.0
## 186    ATOM   186     N <NA>   SER     A     24   <NA> -11.219 28.590 17.517 1.0
## 187    ATOM   187    CA <NA>   SER     A     24   <NA> -11.730 28.032 16.253 1.0
## 188    ATOM   188     C <NA>   SER     A     24   <NA> -10.726 27.075 15.616 1.0
## 189    ATOM   189     O <NA>   SER     A     24   <NA>  -9.487 27.191 15.841 1.0
## 190    ATOM   190    CB <NA>   SER     A     24   <NA> -12.060 29.179 15.305 1.0
## 191    ATOM   191    OG <NA>   SER     A     24   <NA> -10.830 29.750 14.853 1.0
## 192    ATOM   192     N <NA>   LEU     A     25   <NA> -11.267 26.110 14.822 1.0
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## 196    ATOM   196    CB <NA>   LEU     A     25   <NA> -11.293 24.412 12.993 1.0
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## 199    ATOM   199   CD2 <NA>   LEU     A     25   <NA> -12.018 22.437 11.805 1.0
## 200    ATOM   200     N <NA>   GLY     A     26   <NA>  -9.311 26.836 12.758 1.0
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## 210    ATOM   210   OD1 <NA>   ASN     A     27   <NA>  -6.292 30.979 16.582 1.0
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## 222    ATOM   222   CE3 <NA>   TRP     A     28   <NA>  -5.321 23.121 19.249 1.0
## 223    ATOM   223   CZ2 <NA>   TRP     A     28   <NA>  -7.187 24.066 21.210 1.0
## 224    ATOM   224   CZ3 <NA>   TRP     A     28   <NA>  -5.059 23.060 20.609 1.0
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## 231    ATOM   231   CG1 <NA>   VAL     A     29   <NA>  -4.630 23.646  9.743 1.0
## 232    ATOM   232   CG2 <NA>   VAL     A     29   <NA>  -6.516 22.751 11.149 1.0
## 233    ATOM   233     N <NA>   CYS     A     30   <NA>  -3.372 26.060 12.262 1.0
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## 388    ATOM   388     O <NA>   SER     A     50   <NA>  14.085 19.016 25.374 1.0
## 389    ATOM   389    CB <NA>   SER     A     50   <NA>  12.113 19.490 28.182 1.0
## 390    ATOM   390    OG <NA>   SER     A     50   <NA>  12.074 20.716 27.461 1.0
## 391    ATOM   391     N <NA>   THR     A     51   <NA>  12.150 17.857 25.646 1.0
## 392    ATOM   392    CA <NA>   THR     A     51   <NA>  11.958 17.610 24.179 1.0
## 393    ATOM   393     C <NA>   THR     A     51   <NA>  10.485 17.806 23.917 1.0
## 394    ATOM   394     O <NA>   THR     A     51   <NA>   9.677 17.499 24.825 1.0
## 395    ATOM   395    CB <NA>   THR     A     51   <NA>  12.363 16.177 23.757 1.0
## 396    ATOM   396   OG1 <NA>   THR     A     51   <NA>  13.711 15.986 24.120 1.0
## 397    ATOM   397   CG2 <NA>   THR     A     51   <NA>  12.234 15.930 22.227 1.0
## 398    ATOM   398     N <NA>   ASP     A     52   <NA>  10.158 18.354 22.701 1.0
## 399    ATOM   399    CA <NA>   ASP     A     52   <NA>   8.767 18.608 22.181 1.0
## 400    ATOM   400     C <NA>   ASP     A     52   <NA>   8.451 17.463 21.198 1.0
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## 403    ATOM   403    CG <NA>   ASP     A     52   <NA>   9.014 21.046 22.449 1.0
## 404    ATOM   404   OD1 <NA>   ASP     A     52   <NA>   8.778 20.978 23.593 1.0
## 405    ATOM   405   OD2 <NA>   ASP     A     52   <NA>   9.531 22.065 21.923 1.0
## 406    ATOM   406     N <NA>   TYR     A     53   <NA>   7.279 16.908 21.280 1.0
## 407    ATOM   407    CA <NA>   TYR     A     53   <NA>   6.899 15.745 20.548 1.0
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## 409    ATOM   409     O <NA>   TYR     A     53   <NA>   4.554 16.399 20.326 1.0
## 410    ATOM   410    CB <NA>   TYR     A     53   <NA>   6.630 14.562 21.517 1.0
## 411    ATOM   411    CG <NA>   TYR     A     53   <NA>   7.865 14.099 22.242 1.0
## 412    ATOM   412   CD1 <NA>   TYR     A     53   <NA>   8.335 14.742 23.399 1.0
## 413    ATOM   413   CD2 <NA>   TYR     A     53   <NA>   8.618 13.027 21.749 1.0
## 414    ATOM   414   CE1 <NA>   TYR     A     53   <NA>   9.548 14.382 24.006 1.0
## 415    ATOM   415   CE2 <NA>   TYR     A     53   <NA>   9.846 12.646 22.351 1.0
## 416    ATOM   416    CZ <NA>   TYR     A     53   <NA>  10.229 13.264 23.534 1.0
## 417    ATOM   417    OH <NA>   TYR     A     53   <NA>  11.374 12.889 24.151 1.0
## 418    ATOM   418     N <NA>   GLY     A     54   <NA>   5.598 15.446 18.516 1.0
## 419    ATOM   419    CA <NA>   GLY     A     54   <NA>   4.390 15.347 17.710 1.0
## 420    ATOM   420     C <NA>   GLY     A     54   <NA>   3.939 16.599 17.020 1.0
## 421    ATOM   421     O <NA>   GLY     A     54   <NA>   4.535 17.621 17.017 1.0
## 422    ATOM   422     N <NA>   ILE     A     55   <NA>   2.748 16.458 16.496 1.0
## 423    ATOM   423    CA <NA>   ILE     A     55   <NA>   2.096 17.435 15.686 1.0
## 424    ATOM   424     C <NA>   ILE     A     55   <NA>   1.893 18.749 16.386 1.0
## 425    ATOM   425     O <NA>   ILE     A     55   <NA>   1.904 19.805 15.761 1.0
## 426    ATOM   426    CB <NA>   ILE     A     55   <NA>   0.838 16.805 15.068 1.0
## 427    ATOM   427   CG1 <NA>   ILE     A     55   <NA>   0.390 17.438 13.734 1.0
## 428    ATOM   428   CG2 <NA>   ILE     A     55   <NA>  -0.262 16.528 16.106 1.0
## 429    ATOM   429   CD1 <NA>   ILE     A     55   <NA>  -0.353 16.483 12.846 1.0
## 430    ATOM   430     N <NA>   LEU     A     56   <NA>   1.765 18.677 17.706 1.0
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## 432    ATOM   432     C <NA>   LEU     A     56   <NA>   2.735 20.173 19.390 1.0
## 433    ATOM   433     O <NA>   LEU     A     56   <NA>   2.660 21.074 20.200 1.0
## 434    ATOM   434    CB <NA>   LEU     A     56   <NA>   0.216 19.957 19.205 1.0
## 435    ATOM   435    CG <NA>   LEU     A     56   <NA>  -0.990 20.157 18.283 1.0
## 436    ATOM   436   CD1 <NA>   LEU     A     56   <NA>  -2.255 19.795 19.036 1.0
## 437    ATOM   437   CD2 <NA>   LEU     A     56   <NA>  -1.074 21.607 17.850 1.0
## 438    ATOM   438     N <NA>   GLN     A     57   <NA>   3.804 19.441 19.202 1.0
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## 439    ATOM   439    CA <NA>   GLN     A     57   <NA>   5.029 19.733 19.898 1.0
## 440    ATOM   440     C <NA>   GLN     A     57   <NA>   4.883 19.918 21.451 1.0
## 441    ATOM   441     O <NA>   GLN     A     57   <NA>   5.272 20.968 22.020 1.0
## 442    ATOM   442    CB <NA>   GLN     A     57   <NA>   5.767 20.937 19.263 1.0
## 443    ATOM   443    CG <NA>   GLN     A     57   <NA>   6.362 20.658 17.863 1.0
## 444    ATOM   444    CD <NA>   GLN     A     57   <NA>   7.544 19.747 17.936 1.0
## 445    ATOM   445   OE1 <NA>   GLN     A     57   <NA>   8.676 20.257 18.147 1.0
## 446    ATOM   446   NE2 <NA>   GLN     A     57   <NA>   7.279 18.413 17.746 1.0
## 447    ATOM   447     N <NA>   ILE     A     58   <NA>   4.303 18.898 22.061 1.0
## 448    ATOM   448    CA <NA>   ILE     A     58   <NA>   4.031 18.814 23.487 1.0
## 449    ATOM   449     C <NA>   ILE     A     58   <NA>   5.301 18.482 24.282 1.0
## 450    ATOM   450     O <NA>   ILE     A     58   <NA>   6.055 17.583 23.982 1.0
## 451    ATOM   451    CB <NA>   ILE     A     58   <NA>   2.839 17.923 23.711 1.0
## 452    ATOM   452   CG1 <NA>   ILE     A     58   <NA>   1.599 18.614 23.110 1.0
## 453    ATOM   453   CG2 <NA>   ILE     A     58   <NA>   2.704 17.544 25.215 1.0
## 454    ATOM   454   CD1 <NA>   ILE     A     58   <NA>   0.329 17.770 23.138 1.0
## 455    ATOM   455     N <NA>   ASN     A     59   <NA>   5.556 19.297 25.282 1.0
## 456    ATOM   456    CA <NA>   ASN     A     59   <NA>   6.797 19.305 26.034 1.0
## 457    ATOM   457     C <NA>   ASN     A     59   <NA>   6.893 18.239 27.099 1.0
## 458    ATOM   458     O <NA>   ASN     A     59   <NA>   5.904 18.002 27.761 1.0
## 459    ATOM   459    CB <NA>   ASN     A     59   <NA>   7.045 20.721 26.565 1.0
## 460    ATOM   460    CG <NA>   ASN     A     59   <NA>   8.434 20.839 27.178 1.0
## 461    ATOM   461   OD1 <NA>   ASN     A     59   <NA>   8.578 20.809 28.411 1.0
## 462    ATOM   462   ND2 <NA>   ASN     A     59   <NA>   9.469 20.939 26.342 1.0
## 463    ATOM   463     N <NA>   SER     A     60   <NA>   8.096 17.590 27.218 1.0
## 464    ATOM   464    CA <NA>   SER     A     60   <NA>   8.333 16.496 28.162 1.0
## 465    ATOM   465     C <NA>   SER     A     60   <NA>   8.586 17.015 29.647 1.0
## 466    ATOM   466     O <NA>   SER     A     60   <NA>   8.559 16.218 30.620 1.0
## 467    ATOM   467    CB <NA>   SER     A     60   <NA>   9.448 15.619 27.698 1.0
## 468    ATOM   468    OG <NA>   SER     A     60   <NA>  10.642 16.390 27.790 1.0
## 469    ATOM   469     N <NA>   ARG     A     61   <NA>   8.806 18.347 29.787 1.0
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## 471    ATOM   471     C <NA>   ARG     A     61   <NA>   7.701 18.806 31.935 1.0
## 472    ATOM   472     O <NA>   ARG     A     61   <NA>   7.730 18.363 33.063 1.0
## 473    ATOM   473    CB <NA>   ARG     A     61   <NA>   9.507 20.347 31.068 1.0
## 474    ATOM   474    CG <NA>   ARG     A     61   <NA>   9.259 21.125 32.338 1.0
## 475    ATOM   475    CD <NA>   ARG     A     61   <NA>  10.511 21.648 33.063 1.0
## 476    ATOM   476    NE <NA>   ARG     A     61   <NA>  11.777 21.523 32.353 1.0
## 477    ATOM   477    CZ <NA>   ARG     A     61   <NA>  12.722 20.587 32.539 1.0
## 478    ATOM   478   NH1 <NA>   ARG     A     61   <NA>  12.610 19.570 33.413 1.0
## 479    ATOM   479   NH2 <NA>   ARG     A     61   <NA>  13.829 20.673 31.795 1.0
## 480    ATOM   480     N <NA>   TRP     A     62   <NA>   6.542 19.071 31.329 1.0
## 481    ATOM   481    CA <NA>   TRP     A     62   <NA>   5.279 18.955 32.026 1.0
## 482    ATOM   482     C <NA>   TRP     A     62   <NA>   4.281 17.916 31.682 1.0
## 483    ATOM   483     O <NA>   TRP     A     62   <NA>   3.526 17.478 32.563 1.0
## 484    ATOM   484    CB <NA>   TRP     A     62   <NA>   4.455 20.234 31.875 1.0
## 485    ATOM   485    CG <NA>   TRP     A     62   <NA>   5.346 21.376 31.920 1.0
## 486    ATOM   486   CD1 <NA>   TRP     A     62   <NA>   5.937 21.965 30.857 1.0
## 487    ATOM   487   CD2 <NA>   TRP     A     62   <NA>   5.859 21.980 33.091 1.0
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## 493    ATOM   493   CH2 <NA>   TRP     A     62   <NA>   7.122 23.609 34.923 1.0
## 494    ATOM   494     N <NA>   TRP     A     63   <NA>   4.152 17.600 30.385 1.0
## 495    ATOM   495    CA <NA>   TRP     A     63   <NA>   3.036 16.858 29.848 1.0
## 496    ATOM   496     C <NA>   TRP     A     63   <NA>   3.155 15.396 29.592 1.0
## 497    ATOM   497     O <NA>   TRP     A     63   <NA>   2.183 14.725 29.581 1.0
## 498    ATOM   498    CB <NA>   TRP     A     63   <NA>   2.652 17.635 28.566 1.0
## 499    ATOM   499    CG <NA>   TRP     A     63   <NA>   2.429 19.101 28.874 1.0
## 500    ATOM   500   CD1 <NA>   TRP     A     63   <NA>   3.223 20.140 28.615 1.0
## 501    ATOM   501   CD2 <NA>   TRP     A     63   <NA>   1.364 19.632 29.695 1.0
## 502    ATOM   502   NE1 <NA>   TRP     A     63   <NA>   2.675 21.309 29.075 1.0
## 503    ATOM   503   CE2 <NA>   TRP     A     63   <NA>   1.567 21.028 29.780 1.0
## 504    ATOM   504   CE3 <NA>   TRP     A     63   <NA>   0.230 19.055 30.324 1.0
## 505    ATOM   505   CZ2 <NA>   TRP     A     63   <NA>   0.682 21.862 30.488 1.0
## 506    ATOM   506   CZ3 <NA>   TRP     A     63   <NA>  -0.678 19.891 30.985 1.0
## 507    ATOM   507   CH2 <NA>   TRP     A     63   <NA>  -0.421 21.271 31.057 1.0
## 508    ATOM   508     N <NA>   CYS     A     64   <NA>   4.324 14.905 29.353 1.0
## 509    ATOM   509    CA <NA>   CYS     A     64   <NA>   4.448 13.469 29.032 1.0
## 510    ATOM   510     C <NA>   CYS     A     64   <NA>   5.785 12.968 29.569 1.0
## 511    ATOM   511     O <NA>   CYS     A     64   <NA>   6.694 13.742 29.793 1.0
## 512    ATOM   512    CB <NA>   CYS     A     64   <NA>   4.366 13.241 27.432 1.0
## 513    ATOM   513    SG <NA>   CYS     A     64   <NA>   5.695 14.086 26.427 1.0
## 514    ATOM   514     N <NA>   ASN     A     65   <NA>   5.913 11.651 29.720 1.0
## 515    ATOM   515    CA <NA>   ASN     A     65   <NA>   7.127 11.114 30.200 1.0
## 516    ATOM   516     C <NA>   ASN     A     65   <NA>   7.999 10.547 29.073 1.0
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## 519    ATOM   519    CG <NA>   ASN     A     65   <NA>   8.120  9.322 31.715 1.0
## 520    ATOM   520   OD1 <NA>   ASN     A     65   <NA>   9.033 10.017 32.182 1.0
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## 527    ATOM   527    CG <NA>   ASP     A     66   <NA>  11.480 12.554 27.535 1.0
## 528    ATOM   528   OD1 <NA>   ASP     A     66   <NA>  11.787 12.613 28.717 1.0
## 529    ATOM   529   OD2 <NA>   ASP     A     66   <NA>  11.850 13.432 26.659 1.0
## 530    ATOM   530     N <NA>   GLY     A     67   <NA>  11.395  9.644 29.920 1.0
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## 537    ATOM   537     O <NA>   ARG     A     68   <NA>  15.995 13.645 30.281 1.0
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## 547    ATOM   547     C <NA>   THR     A     69   <NA>  13.372 14.770 33.144 1.0
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## 550    ATOM   550   OG1 <NA>   THR     A     69   <NA>  12.589 15.107 29.412 1.0
## 551    ATOM   551   CG2 <NA>   THR     A     69   <NA>  12.392 16.932 30.990 1.0
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## 553    ATOM   553    CA <NA>   PRO     A     70   <NA>  14.563 14.964 35.315 1.0
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## 555    ATOM   555     O <NA>   PRO     A     70   <NA>  13.699 17.188 35.594 1.0
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## 578    ATOM   578   NH1 <NA>   ARG     A     73   <NA>   3.742 21.891 38.705 1.0
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## 594    ATOM   594   CD1 <NA>   LEU     A     75   <NA>   0.889 19.358 34.725 1.0
## 595    ATOM   595   CD2 <NA>   LEU     A     75   <NA>   0.238 17.306 35.969 1.0
## 596    ATOM   596     N <NA>   CYS     A     76   <NA>  -0.146 14.663 31.359 1.0
## 597    ATOM   597    CA <NA>   CYS     A     76   <NA>  -1.153 13.970 30.513 1.0
## 598    ATOM   598     C <NA>   CYS     A     76   <NA>  -1.137 12.463 30.738 1.0
## 599    ATOM   599     O <NA>   CYS     A     76   <NA>  -1.935 11.725 30.131 1.0
## 600    ATOM   600    CB <NA>   CYS     A     76   <NA>  -1.094 14.295 28.984 1.0
## 601    ATOM   601    SG <NA>   CYS     A     76   <NA>  -1.329 16.050 28.713 1.0
## 602    ATOM   602     N <NA>   ASN     A     77   <NA>  -0.194 12.038 31.586 1.0
## 603    ATOM   603    CA <NA>   ASN     A     77   <NA>  -0.117 10.607 31.926 1.0
## 604    ATOM   604     C <NA>   ASN     A     77   <NA>   0.099  9.697 30.747 1.0
## 605    ATOM   605     O <NA>   ASN     A     77   <NA>  -0.626  8.715 30.538 1.0
## 606    ATOM   606    CB <NA>   ASN     A     77   <NA>  -1.421 10.174 32.620 1.0
## 607    ATOM   607    CG <NA>   ASN     A     77   <NA>  -1.361  8.783 33.215 1.0
## 608    ATOM   608   OD1 <NA>   ASN     A     77   <NA>  -2.358  8.042 33.188 1.0
## 609    ATOM   609   ND2 <NA>   ASN     A     77   <NA>  -0.186  8.412 33.715 1.0
## 610    ATOM   610     N <NA>   ILE     A     78   <NA>   1.114 10.006 29.979 1.0
## 611    ATOM   611    CA <NA>   ILE     A     78   <NA>   1.373  9.191 28.838 1.0
## 612    ATOM   612     C <NA>   ILE     A     78   <NA>   2.873  9.258 28.499 1.0
## 613    ATOM   613     O <NA>   ILE     A     78   <NA>   3.568 10.265 28.718 1.0
## 614    ATOM   614    CB <NA>   ILE     A     78   <NA>   0.764  9.855 27.598 1.0
## 615    ATOM   615   CG1 <NA>   ILE     A     78   <NA>   0.764 11.376 27.743 1.0
## 616    ATOM   616   CG2 <NA>   ILE     A     78   <NA>  -0.461  9.195 26.985 1.0
## 617    ATOM   617   CD1 <NA>   ILE     A     78   <NA>   0.735 12.094 26.406 1.0
## 618    ATOM   618     N <NA>   PRO     A     79   <NA>   3.343  8.210 27.843 1.0
## 619    ATOM   619    CA <NA>   PRO     A     79   <NA>   4.715  8.229 27.362 1.0
## 620    ATOM   620     C <NA>   PRO     A     79   <NA>   4.738  9.234 26.187 1.0
## 621    ATOM   621     O <NA>   PRO     A     79   <NA>   3.762  9.304 25.359 1.0
## 622    ATOM   622    CB <NA>   PRO     A     79   <NA>   4.962  6.830 26.843 1.0
## 623    ATOM   623    CG <NA>   PRO     A     79   <NA>   3.631  6.096 26.844 1.0
## 624    ATOM   624    CD <NA>   PRO     A     79   <NA>   2.621  6.951 27.581 1.0
## 625    ATOM   625     N <NA>   CYS     A     80   <NA>   5.798 10.020 26.078 1.0
## 626    ATOM   626    CA <NA>   CYS     A     80   <NA>   5.870 11.003 24.969 1.0
## 627    ATOM   627     C <NA>   CYS     A     80   <NA>   5.782 10.359 23.546 1.0
## 628    ATOM   628     O <NA>   CYS     A     80   <NA>   5.284 10.950 22.568 1.0
## 629    ATOM   629    CB <NA>   CYS     A     80   <NA>   7.126 11.894 25.061 1.0
## 630    ATOM   630    SG <NA>   CYS     A     80   <NA>   7.251 12.847 26.592 1.0
## 631    ATOM   631     N <NA>   SER     A     81   <NA>   6.259  9.115 23.442 1.0
## 632    ATOM   632    CA <NA>   SER     A     81   <NA>   6.242  8.432 22.154 1.0
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## 634    ATOM   634     O <NA>   SER     A     81   <NA>   4.554  8.156 20.510 1.0
## 635    ATOM   635    CB <NA>   SER     A     81   <NA>   6.995  7.111 22.234 1.0
## 636    ATOM   636    OG <NA>   SER     A     81   <NA>   6.295  6.245 23.119 1.0
## 637    ATOM   637     N <NA>   ALA     A     82   <NA>   3.857  8.169 22.598 1.0
## 638    ATOM   638    CA <NA>   ALA     A     82   <NA>   2.452  8.033 22.185 1.0
## 639    ATOM   639     C <NA>   ALA     A     82   <NA>   2.000  9.216 21.325 1.0
## 640    ATOM   640     O <NA>   ALA     A     82   <NA>   1.033  9.113 20.571 1.0
## 641    ATOM   641    CB <NA>   ALA     A     82   <NA>   1.481  8.009 23.384 1.0
## 642    ATOM   642     N <NA>   LEU     A     83   <NA>   2.659 10.349 21.528 1.0
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## 643    ATOM   643    CA <NA>   LEU     A     83   <NA>   2.329 11.589 20.867 1.0
## 644    ATOM   644     C <NA>   LEU     A     83   <NA>   2.834 11.627 19.385 1.0
## 645    ATOM   645     O <NA>   LEU     A     83   <NA>   2.626 12.620 18.685 1.0
## 646    ATOM   646    CB <NA>   LEU     A     83   <NA>   2.986 12.761 21.651 1.0
## 647    ATOM   647    CG <NA>   LEU     A     83   <NA>   2.370 12.966 23.055 1.0
## 648    ATOM   648   CD1 <NA>   LEU     A     83   <NA>   3.076 14.069 23.849 1.0
## 649    ATOM   649   CD2 <NA>   LEU     A     83   <NA>   0.843 13.174 22.965 1.0
## 650    ATOM   650     N <NA>   LEU     A     84   <NA>   3.542 10.556 18.940 1.0
## 651    ATOM   651    CA <NA>   LEU     A     84   <NA>   4.131 10.512 17.618 1.0
## 652    ATOM   652     C <NA>   LEU     A     84   <NA>   3.361  9.657 16.630 1.0
## 653    ATOM   653     O <NA>   LEU     A     84   <NA>   3.704  9.570 15.475 1.0
## 654    ATOM   654    CB <NA>   LEU     A     84   <NA>   5.630 10.044 17.645 1.0
## 655    ATOM   655    CG <NA>   LEU     A     84   <NA>   6.546 10.859 18.552 1.0
## 656    ATOM   656   CD1 <NA>   LEU     A     84   <NA>   7.978 10.414 18.359 1.0
## 657    ATOM   657   CD2 <NA>   LEU     A     84   <NA>   6.513 12.306 18.116 1.0
## 658    ATOM   658     N <NA>   SER     A     85   <NA>   2.332  9.023 17.096 1.0
## 659    ATOM   659    CA <NA>   SER     A     85   <NA>   1.485  8.148 16.333 1.0
## 660    ATOM   660     C <NA>   SER     A     85   <NA>   0.792  8.827 15.194 1.0
## 661    ATOM   661     O <NA>   SER     A     85   <NA>   0.519 10.007 15.280 1.0
## 662    ATOM   662    CB <NA>   SER     A     85   <NA>   0.376  7.776 17.295 1.0
## 663    ATOM   663    OG <NA>   SER     A     85   <NA>  -0.373  6.761 16.741 1.0
## 664    ATOM   664     N <NA>   SER     A     86   <NA>   0.371  8.039 14.186 1.0
## 665    ATOM   665    CA <NA>   SER     A     86   <NA>  -0.430  8.505 13.025 1.0
## 666    ATOM   666     C <NA>   SER     A     86   <NA>  -1.827  8.884 13.487 1.0
## 667    ATOM   667     O <NA>   SER     A     86   <NA>  -2.481  9.696 12.857 1.0
## 668    ATOM   668    CB <NA>   SER     A     86   <NA>  -0.584  7.358 12.026 1.0
## 669    ATOM   669    OG <NA>   SER     A     86   <NA>   0.687  7.146 11.467 1.0
## 670    ATOM   670     N <NA>   ASP     A     87   <NA>  -2.288  8.227 14.575 1.0
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## 676    ATOM   676   OD1 <NA>   ASP     A     87   <NA>  -5.875  8.512 16.868 1.0
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## 678    ATOM   678     N <NA>   ILE     A     88   <NA>  -4.037 10.803 15.879 1.0
## 679    ATOM   679    CA <NA>   ILE     A     88   <NA>  -3.749 11.974 16.722 1.0
## 680    ATOM   680     C <NA>   ILE     A     88   <NA>  -4.490 12.067 18.055 1.0
## 681    ATOM   681     O <NA>   ILE     A     88   <NA>  -4.393 13.081 18.780 1.0
## 682    ATOM   682    CB <NA>   ILE     A     88   <NA>  -4.014 13.293 15.954 1.0
## 683    ATOM   683   CG1 <NA>   ILE     A     88   <NA>  -5.565 13.392 15.634 1.0
## 684    ATOM   684   CG2 <NA>   ILE     A     88   <NA>  -3.104 13.384 14.694 1.0
## 685    ATOM   685   CD1 <NA>   ILE     A     88   <NA>  -6.065 14.738 15.196 1.0
## 686    ATOM   686     N <NA>   THR     A     89   <NA>  -5.257 11.069 18.381 1.0
## 687    ATOM   687    CA <NA>   THR     A     89   <NA>  -6.058 11.103 19.584 1.0
## 688    ATOM   688     C <NA>   THR     A     89   <NA>  -5.326 11.520 20.907 1.0
## 689    ATOM   689     O <NA>   THR     A     89   <NA>  -5.777 12.403 21.614 1.0
## 690    ATOM   690    CB <NA>   THR     A     89   <NA>  -6.717  9.735 19.716 1.0
## 691    ATOM   691   OG1 <NA>   THR     A     89   <NA>  -7.492  9.539 18.564 1.0
## 692    ATOM   692   CG2 <NA>   THR     A     89   <NA>  -7.642  9.724 20.953 1.0
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## 694    ATOM   694    CA <NA>   ALA     A    90   <NA>  -3.483 11.250 22.444 1.0
## 695    ATOM   695     C <NA>   ALA     A    90   <NA>  -2.971 12.685 22.412 1.0
## 696    ATOM   696     O <NA>   ALA     A    90   <NA>  -2.981 13.344 23.413 1.0
## 697    ATOM   697    CB <NA>   ALA     A    90   <NA>  -2.331 10.290 22.751 1.0
## 698    ATOM   698     N <NA>   SER     A    91   <NA>  -2.504 13.185 21.257 1.0
## 699    ATOM   699    CA <NA>   SER     A    91   <NA>  -2.032 14.567 21.163 1.0
## 700    ATOM   700     C <NA>   SER     A    91   <NA>  -3.155 15.522 21.418 1.0
## 701    ATOM   701     O <NA>   SER     A    91   <NA>  -3.033 16.547 22.059 1.0
## 702    ATOM   702    CB <NA>   SER     A    91   <NA>  -1.445 14.870 19.783 1.0
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## 704    ATOM   704     N <NA>   VAL     A    92   <NA>  -4.289 15.234 20.839 1.0
## 705    ATOM   705    CA <NA>   VAL     A    92   <NA>  -5.449 16.101 21.004 1.0
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## 707    ATOM   707     O <NA>   VAL     A    92   <NA>  -6.254 17.195 23.018 1.0
## 708    ATOM   708    CB <NA>   VAL     A    92   <NA>  -6.523 15.597 19.994 1.0
## 709    ATOM   709   CG1 <NA>   VAL     A    92   <NA>  -7.936 16.117 20.303 1.0
## 710    ATOM   710   CG2 <NA>   VAL     A    92   <NA>  -6.110 15.987 18.555 1.0
## 711    ATOM   711     N <NA>   ASN     A    93   <NA>  -6.047 14.973 23.140 1.0
## 712    ATOM   712    CA <NA>   ASN     A    93   <NA>  -6.511 14.862 24.536 1.0
## 713    ATOM   713     C <NA>   ASN     A    93   <NA>  -5.602 15.647 25.472 1.0
## 714    ATOM   714     O <NA>   ASN     A    93   <NA>  -6.049 16.390 26.310 1.0
## 715    ATOM   715    CB <NA>   ASN     A    93   <NA>  -6.580 13.395 24.989 1.0
## 716    ATOM   716    CG <NA>   ASN     A    93   <NA>  -7.781 12.668 24.406 1.0
## 717    ATOM   717   OD1 <NA>   ASN     A    93   <NA>  -7.842 11.422 24.426 1.0
## 718    ATOM   718   ND2 <NA>   ASN     A    93   <NA>  -8.682 13.436 23.835 1.0
## 719    ATOM   719     N <NA>   CYS     A    94   <NA>  -4.284 15.477 25.249 1.0
## 720    ATOM   720    CA <NA>   CYS     A    94   <NA>  -3.267 16.178 25.984 1.0
## 721    ATOM   721     C <NA>   CYS     A    94   <NA>  -3.353 17.649 25.690 1.0
## 722    ATOM   722     O <NA>   CYS     A    94   <NA>  -3.298 18.462 26.598 1.0
## 723    ATOM   723    CB <NA>   CYS     A    94   <NA>  -1.875 15.620 25.709 1.0
## 724    ATOM   724    SG <NA>   CYS     A    94   <NA>  -0.613 16.312 26.762 1.0
## 725    ATOM   725     N <NA>   ALA     A    95   <NA>  -3.546 18.041 24.407 1.0
## 726    ATOM   726    CA <NA>   ALA     A    95   <NA>  -3.656 19.481 24.142 1.0
## 727    ATOM   727     C <NA>   ALA     A    95   <NA>  -4.864 20.156 24.849 1.0
## 728    ATOM   728     O <NA>   ALA     A    95   <NA>  -4.867 21.353 25.215 1.0
## 729    ATOM   729    CB <NA>   ALA     A    95   <NA>  -3.774 19.698 22.627 1.0
## 730    ATOM   730     N <NA>   LYS     A    96   <NA>  -5.932 19.405 24.966 1.0
## 731    ATOM   731    CA <NA>   LYS     A    96   <NA>  -7.108 19.927 25.596 1.0
## 732    ATOM   732     C <NA>   LYS     A    96   <NA>  -6.804 20.229 27.091 1.0
## 733    ATOM   733     O <NA>   LYS     A    96   <NA>  -7.271 21.199 27.627 1.0
## 734    ATOM   734    CB <NA>   LYS     A    96   <NA>  -8.195 18.868 25.472 1.0
## 735    ATOM   735    CG <NA>   LYS     A    96   <NA>  -8.927 18.820 24.137 1.0
## 736    ATOM   736    CD <NA>   LYS     A    96   <NA>  -9.976 17.699 24.147 1.0
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## 739    ATOM   739     N <NA>   LYS     A    97   <NA>  -5.944 19.447 27.750 1.0
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## 746   ATOM   746    CE <NA>   LYS     A    97   <NA>  -7.073 16.369 31.886 1.0
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## 748   ATOM   748     N <NA>   ILE     A    98   <NA>  -3.760 21.072 28.264 1.0
## 749   ATOM   749    CA <NA>   ILE     A    98   <NA>  -2.856 22.204 28.161 1.0
## 750   ATOM   750     C <NA>   ILE     A    98   <NA>  -3.607 23.536 27.991 1.0
## 751   ATOM   751     O <NA>   ILE     A    98   <NA>  -3.322 24.532 28.701 1.0
## 752   ATOM   752    CB <NA>   ILE     A    98   <NA>  -1.778 22.026 27.022 1.0
## 753   ATOM   753   CG1 <NA>   ILE     A    98   <NA>  -0.899 20.798 27.234 1.0
## 754   ATOM   754   CG2 <NA>   ILE     A    98   <NA>  -0.932 23.292 26.811 1.0
## 755   ATOM   755   CD1 <NA>   ILE     A    98   <NA>  -0.035 20.440 26.059 1.0
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## 762   ATOM   762   CG2 <NA>   VAL     A    99   <NA>  -6.203 26.159 24.648 1.0
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## 764   ATOM   764    CA <NA>   SER     A   100   <NA>  -7.469 24.559 29.728 1.0
## 765   ATOM   765     C <NA>   SER     A   100   <NA>  -6.810 25.233 30.952 1.0
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## 770   ATOM   770    CA <NA>   ASP     A   101   <NA>  -4.485 25.414 31.955 1.0
## 771   ATOM   771     C <NA>   ASP     A   101   <NA>  -4.239 26.879 32.265 1.0
## 772   ATOM   772     O <NA>   ASP     A   101   <NA>  -3.422 27.194 33.137 1.0
## 773   ATOM   773    CB <NA>   ASP     A   101   <NA>  -3.173 24.648 31.624 1.0
## 774   ATOM   774    CG <NA>   ASP     A   101   <NA>  -2.133 24.566 32.715 1.0
## 775   ATOM   775   OD1 <NA>   ASP     A   101   <NA>  -2.482 23.821 33.747 1.0
## 776   ATOM   776   OD2 <NA>   ASP     A   101   <NA>  -1.045 25.095 32.609 1.0
## 777   ATOM   777     N <NA>   GLY     A   102   <NA>  -4.876 27.820 31.617 1.0
## 778   ATOM   778    CA <NA>   GLY     A   102   <NA>  -4.525 29.170 32.093 1.0
## 779   ATOM   779     C <NA>   GLY     A   102   <NA>  -4.082 30.192 31.049 1.0
## 780   ATOM   780     O <NA>   GLY     A   102   <NA>  -4.713 31.264 30.990 1.0
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## 783   ATOM   783     C <NA>   ASN     A   103   <NA>  -3.176 30.497 27.876 1.0
## 784   ATOM   784     O <NA>   ASN     A   103   <NA>  -2.905 31.106 26.860 1.0
## 785   ATOM   785    CB <NA>   ASN     A   103   <NA>  -1.070 31.114 29.177 1.0
## 786   ATOM   786    CG <NA>   ASN     A   103   <NA>  -0.638 31.476 30.587 1.0
## 787   ATOM   787   OD1 <NA>   ASN     A   103   <NA>   0.384 30.993 31.105 1.0
## 788   ATOM   788   ND2 <NA>   ASN     A   103   <NA>  -1.509 32.224 31.271 1.0
## 789   ATOM   789     N <NA>   GLY     A   104   <NA>  -4.070 29.522 27.865 1.0
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## 792   ATOM   792     O <NA>   GLY     A   104   <NA>  -2.766 27.947 25.892 1.0
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## 795   ATOM   795     C <NA>   MET     A   105   <NA>  -1.637 29.372 23.232 1.0
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## 796    ATOM   796     O <NA>   MET     A   105   <NA>  -0.727 29.013 22.506 1.0
## 797    ATOM   797    CB <NA>   MET     A   105   <NA>  -3.739 28.882 21.838 1.0
## 798    ATOM   798    CG <NA>   MET     A   105   <NA>  -4.790 27.788 21.646 1.0
## 799    ATOM   799    SD <NA>   MET     A   105   <NA>  -5.184 27.455 19.852 1.0
## 800    ATOM   800    CE <NA>   MET     A   105   <NA>  -3.617 26.757 19.326 1.0
## 801    ATOM   801     N <NA>   ASN     A   106   <NA>  -1.509 30.373 24.105 1.0
## 802    ATOM   802    CA <NA>   ASN     A   106   <NA>  -0.270 31.037 24.269 1.0
## 803    ATOM   803     C <NA>   ASN     A   106   <NA>   0.809 30.046 24.765 1.0
## 804    ATOM   804     O <NA>   ASN     A   106   <NA>   2.030 30.336 24.608 1.0
## 805    ATOM   805    CB <NA>   ASN     A   106   <NA>  -0.396 32.190 25.241 1.0
## 806    ATOM   806    CG <NA>   ASN     A   106   <NA>  -1.239 33.309 24.682 1.0
## 807    ATOM   807   OD1 <NA>   ASN     A   106   <NA>  -0.864 33.972 23.658 1.0
## 808    ATOM   808   ND2 <NA>   ASN     A   106   <NA>  -2.372 33.492 25.355 1.0
## 809    ATOM   809     N <NA>   ALA     A   107   <NA>   0.360 28.870 25.250 1.0
## 810    ATOM   810    CA <NA>   ALA     A   107   <NA>   1.308 27.840 25.625 1.0
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## 813    ATOM   813    CB <NA>   ALA     A   107   <NA>   0.585 26.599 26.143 1.0
## 814    ATOM   814     N <NA>   TRP     A   108   <NA>   1.577 27.639 23.205 1.0
## 815    ATOM   815    CA <NA>   TRP     A   108   <NA>   2.303 27.285 21.966 1.0
## 816    ATOM   816     C <NA>   TRP     A   108   <NA>   2.970 28.504 21.404 1.0
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## 818    ATOM   818    CB <NA>   TRP     A   108   <NA>   1.398 26.569 20.912 1.0
## 819    ATOM   819    CG <NA>   TRP     A   108   <NA>   1.005 25.176 21.256 1.0
## 820    ATOM   820   CD1 <NA>   TRP     A   108   <NA>   1.760 24.069 21.021 1.0
## 821    ATOM   821   CD2 <NA>   TRP     A   108   <NA>  -0.146 24.722 21.926 1.0
## 822    ATOM   822   NE1 <NA>   TRP     A   108   <NA>   1.131 22.972 21.471 1.0
## 823    ATOM   823   CE2 <NA>   TRP     A   108   <NA>  -0.048 23.321 22.045 1.0
## 824    ATOM   824   CE3 <NA>   TRP     A   108   <NA>  -1.256 25.348 22.436 1.0
## 825    ATOM   825   CZ2 <NA>   TRP     A   108   <NA>  -1.038 22.520 22.626 1.0
## 826    ATOM   826   CZ3 <NA>   TRP     A   108   <NA>  -2.220 24.549 23.074 1.0
## 827    ATOM   827   CH2 <NA>   TRP     A   108   <NA>  -2.156 23.123 23.101 1.0
## 828    ATOM   828     N <NA>   VAL     A   109   <NA>   4.320 28.523 21.508 1.0
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## 830    ATOM   830     C <NA>   VAL     A   109   <NA>   4.800 30.025 19.545 1.0
## 831    ATOM   831     O <NA>   VAL     A   109   <NA>   4.617 31.199 19.228 1.0
## 832    ATOM   832    CB <NA>   VAL     A   109   <NA>   6.549 29.491 21.342 1.0
## 833    ATOM   833   CG1 <NA>   VAL     A   109   <NA>   7.068 28.242 20.605 1.0
## 834    ATOM   834   CG2 <NA>   VAL     A   109   <NA>   7.327 30.751 20.898 1.0
## 835    ATOM   835     N <NA>   ALA     A   110   <NA>   4.761 28.998 18.662 1.0
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## 838    ATOM   838     O <NA>   ALA     A   110   <NA>   2.902 30.659 16.125 1.0
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## 840    ATOM   840     N <NA>   TRP     A   111   <NA>   2.190 29.398 17.892 1.0
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## 844    ATOM   844    CB <NA>   TRP     A   111   <NA>  -0.240 29.136 18.618 1.0
## 845    ATOM   845    CG <NA>   TRP     A   111   <NA>  -1.589 29.763 18.461 1.0
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## 847    ATOM   847   CD2 <NA>   TRP     A   111   <NA>  -2.190 30.781 19.295 1.0
## 848    ATOM   848   NE1 <NA>   TRP     A   111   <NA>  -3.642 30.322 17.597 1.0
## 849    ATOM   849   CE2 <NA>   TRP     A   111   <NA>  -3.471 31.090 18.728 1.0
## 850    ATOM   850   CE3 <NA>   TRP     A   111   <NA>  -1.805 31.432 20.511 1.0
## 851    ATOM   851   CZ2 <NA>   TRP     A   111   <NA>  -4.306 32.057 19.314 1.0
## 852    ATOM   852   CZ3 <NA>   TRP     A   111   <NA>  -2.658 32.382 21.061 1.0
## 853    ATOM   853   CH2 <NA>   TRP     A   111   <NA>  -3.906 32.666 20.489 1.0
## 854    ATOM   854     N <NA>   ARG     A   112   <NA>   1.497 31.701 19.218 1.0
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## 863    ATOM   863   NH1 <NA>   ARG     A   112   <NA>   5.612 34.286 23.535 1.0
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## 872    ATOM   872   ND2 <NA>   ASN     A   113   <NA>   7.179 33.595 19.091 1.0
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## 890    ATOM   890     N <NA>   LYS     A   116   <NA>  -1.630 33.796 16.196 1.0
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## 909    ATOM   909   CG2 <NA>   THR     A   118   <NA>  -1.455 36.072 12.193 1.0
## 910    ATOM   910     N <NA>   ASP     A   119   <NA>  -5.573 35.973 10.102 1.0
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## 915    ATOM   915    CG <NA>   ASP     A   119   <NA>  -8.359 35.154  7.625 1.0
## 916    ATOM   916   OD1 <NA>   ASP     A   119   <NA>  -9.168 34.529  8.288 1.0
## 917    ATOM   917   OD2 <NA>   ASP     A   119   <NA>  -8.349 35.190  6.315 1.0
## 918    ATOM   918     N <NA>   VAL     A   120   <NA>  -6.836 33.291 10.750 1.0
## 919    ATOM   919    CA <NA>   VAL     A   120   <NA>  -6.637 31.835 10.895 1.0
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## 923    ATOM   923   CG1 <NA>   VAL     A   120   <NA>  -5.271 32.055 13.060 1.0
## 924    ATOM   924   CG2 <NA>   VAL     A   120   <NA>  -7.761 31.691 13.097 1.0
## 925    ATOM   925     N <NA>   GLN     A   121   <NA>  -8.761 31.679  9.776 1.0
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## 927    ATOM   927     C <NA>   GLN     A   121   <NA>  -9.285 30.499  7.694 1.0
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## 930    ATOM   930    CG <NA>   GLN     A   121   <NA> -12.076 31.743  9.628 1.0
## 931    ATOM   931    CD <NA>   GLN     A   121   <NA> -13.286 31.887  8.785 1.0
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## 933    ATOM   933   NE2 <NA>   GLN     A   121   <NA> -13.757 33.131  8.683 1.0
## 934    ATOM   934     N <NA>   ALA     A   122   <NA>  -8.222 31.161  7.229 1.0
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## 945    ATOM   945   CD1 <NA>   TRP     A   123   <NA>  -4.115 29.310  9.238 1.0
## 946    ATOM   946   CD2 <NA>   TRP     A   123   <NA>  -3.066 27.733  8.045 1.0
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## 966    ATOM   966    CG <NA>   ARG     A   125   <NA> -10.586 29.089  1.669 1.0
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## 974    ATOM   974     C <NA>   GLY     A   126   <NA> -11.903 23.570  1.356 1.0
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## 995    ATOM   995     C <NA>   LEU     A   129   <NA> -17.449 19.906  7.141 1.0
## 996    ATOM   996     O <NA>   LEU     A   129   <NA> -18.191 20.465  6.277 1.0
## 997    ATOM   997    CB <NA>   LEU     A   129   <NA> -15.235 20.742  7.845 1.0
## 998    ATOM   998    CG <NA>   LEU     A   129   <NA> -13.711 20.917  7.641 1.0
## 999    ATOM   999   CD1 <NA>   LEU     A   129   <NA> -13.308 22.315  8.150 1.0
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## 1000   ATOM  1000   CD2 <NA>   LEU     A   129   <NA> -12.970 19.868  8.434 1.0
## 1001   ATOM  1001   OXT <NA>   LEU     A   129   <NA> -17.769 19.416  8.251 1.0
## 1002 HETATM  1003     O <NA>   HOH     A   131   <NA>  10.467 23.310 29.307 1.0
## 1003 HETATM  1004     O <NA>   HOH     A   132   <NA>  -1.176 15.339  1.263 1.0
## 1004 HETATM  1005     O <NA>   HOH     A   133   <NA>  -2.951 23.272  0.888 1.0
## 1005 HETATM  1006     O <NA>   HOH     A   134   <NA>   1.217 11.752 36.245 1.0
## 1006 HETATM  1007     O <NA>   HOH     A   135   <NA>  -5.565 19.565  2.145 1.0
## 1007 HETATM  1008     O <NA>   HOH     A   136   <NA>  -8.561 15.857  2.186 1.0
## 1008 HETATM  1009     O <NA>   HOH     A   137   <NA> -11.371 18.534  1.797 1.0
## 1009 HETATM  1010     O <NA>   HOH     A   138   <NA>  -5.769 17.371  2.752 1.0
## 1010 HETATM  1011     O <NA>   HOH     A   139   <NA>  -1.154 20.600  3.261 1.0
## 1011 HETATM  1012     O <NA>   HOH     A   140   <NA> -14.391 27.317  2.971 1.0
## 1012 HETATM  1013     O <NA>   HOH     A   141   <NA>   9.925 21.314  4.349 1.0
## 1013 HETATM  1014     O <NA>   HOH     A   142   <NA>  -3.255 29.381  4.245 1.0
## 1014 HETATM  1015     O <NA>   HOH     A   143   <NA>  -1.469 12.396  4.494 1.0
## 1015 HETATM  1016     O <NA>   HOH     A   144   <NA>   1.369 18.410  4.770 1.0
## 1016 HETATM  1017     O <NA>   HOH     A   145   <NA> -13.995 24.766  5.080 1.0
## 1017 HETATM  1018     O <NA>   HOH     A   146   <NA> -11.877 17.908  5.201 1.0
## 1018 HETATM  1019     O <NA>   HOH     A   147   <NA>   3.579 19.755  5.269 1.0
## 1019 HETATM  1020     O <NA>   HOH     A   148   <NA>  -0.938 23.757  3.720 1.0
## 1020 HETATM  1021     O <NA>   HOH     A   149   <NA>   2.851 10.418  5.675 1.0
## 1021 HETATM  1022     O <NA>   HOH     A   150   <NA>   6.153 10.387  6.792 1.0
## 1022 HETATM  1023     O <NA>   HOH     A   151   <NA>  -4.154 33.433  7.551 1.0
## 1023 HETATM  1024     O <NA>   HOH     A   152   <NA>  -2.892 31.523  5.422 1.0
## 1024 HETATM  1025     O <NA>   HOH     A   153   <NA>   8.184 17.799  8.234 1.0
## 1025 HETATM  1026     O <NA>   HOH     A   154   <NA>   7.851 28.286  8.261 1.0
## 1026 HETATM  1027     O <NA>   HOH     A   155   <NA>  -0.327 32.726  8.576 1.0
## 1027 HETATM  1028     O <NA>   HOH     A   156   <NA>  -7.096 11.131  8.405 1.0
## 1028 HETATM  1029     O <NA>   HOH     A   157   <NA>  -3.462 37.549  8.393 1.0
## 1029 HETATM  1030     O <NA>   HOH     A   158   <NA>  -8.809 13.307  8.142 1.0
## 1030 HETATM  1031     O <NA>   HOH     A   159   <NA>  -0.082 35.568  8.883 1.0
## 1031 HETATM  1032     O <NA>   HOH     A   160   <NA>   5.759 11.110  9.448 1.0
## 1032 HETATM  1033     O <NA>   HOH     A   161   <NA>   1.655 33.826  9.694 1.0
## 1033 HETATM  1034     O <NA>   HOH     A   162   <NA>  -2.547 32.477  9.746 1.0
## 1034 HETATM  1035     O <NA>   HOH     A   163   <NA>   4.474 33.152  9.881 1.0
## 1035 HETATM  1036     O <NA>   HOH     A   164   <NA>   3.338  7.494 10.654 1.0
## 1036 HETATM  1037     O <NA>   HOH     A   165   <NA>   8.193 18.034 10.710 1.0
## 1037 HETATM  1038     O <NA>   HOH     A   166   <NA>   7.329 25.034 11.046 1.0
## 1038 HETATM  1039     O <NA>   HOH     A   167   <NA> -14.609 15.459 10.822 1.0
## 1039 HETATM  1040     O <NA>   HOH     A   168   <NA> -10.475 34.131 10.612 1.0
## 1040 HETATM  1041     O <NA>   HOH     A   169   <NA>   2.254  4.105 11.205 1.0
## 1041 HETATM  1042     O <NA>   HOH     A   170   <NA>   8.719 22.583 10.964 1.0
## 1042 HETATM  1043     O <NA>   HOH     A   171   <NA> -11.115 29.055 11.946 1.0
## 1043 HETATM  1044     O <NA>   HOH     A   172   <NA> -13.874 27.050 11.990 1.0
## 1044 HETATM  1045     O <NA>   HOH     A   173   <NA>  -5.674 10.727 13.313 1.0
## 1045 HETATM  1046     O <NA>   HOH     A   174   <NA> -11.999 31.072 12.630 1.0
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## 1047 HETATM  1048     O <NA>   HOH     A   176   <NA>  10.318 19.087 12.648 1.0
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## 1057 HETATM  1058     O <NA>   HOH     A   186   <NA>  11.590 13.479 14.940 1.0
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## 1059 HETATM  1060     O <NA>   HOH     A   188   <NA>  -4.892 -0.201 15.033 1.0
## 1060 HETATM  1061     O <NA>   HOH     A   189   <NA>   1.858 30.674  4.862 1.0
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## 1062 HETATM  1063     O <NA>   HOH     A   191   <NA>   0.992 36.275 15.433 1.0
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## 1077 HETATM  1078     O <NA>   HOH     A   206   <NA>   3.768  6.469 18.636 1.0
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## 1084 HETATM  1085     O <NA>   HOH     A   213   <NA>  -3.235  8.498 19.677 1.0
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## 1089 HETATM  1090     O <NA>   HOH     A   219   <NA> -11.306 12.254 20.909 1.0
## 1090 HETATM  1091     O <NA>   HOH     A   220   <NA> -15.497 22.071 20.968 1.0
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## 1092 HETATM  1093     O <NA>   HOH     A   222   <NA>   5.919 23.529 21.973 1.0
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## 1094 HETATM  1095     O <NA>   HOH     A   224   <NA>   8.793 23.775 23.737 1.0
## 1095 HETATM  1096     O <NA>   HOH     A   225   <NA> -14.958 24.195 25.086 1.0
## 1096 HETATM  1097     O <NA>   HOH     A   226   <NA> -14.258 17.077 24.576 1.0
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## 1098 HETATM  1099     O <NA>   HOH     A   228   <NA> -17.138 15.370 26.017 1.0
## 1099 HETATM  1100     O <NA>   HOH     A   229   <NA>   1.041 39.543 25.118 1.0
## 1100 HETATM  1101     O <NA>   HOH     A   230   <NA> -18.171 19.097 19.147 1.0
## 1101 HETATM  1102     O <NA>   HOH     A   231   <NA>  19.800 18.720 25.766 1.0
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## 1102 HETATM  1103     O <NA>   HOH     A   232   <NA>  13.910 14.986 26.681 1.0
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## 1106 HETATM  1107     O <NA>   HOH     A   236   <NA>  -8.227 15.787 27.736 1.0
## 1107 HETATM  1108     O <NA>   HOH     A   237   <NA>  11.129 29.398 26.784 1.0
## 1108 HETATM  1109     O <NA>   HOH     A   238   <NA>  -2.152 26.984 28.613 1.0
## 1109 HETATM  1110     O <NA>   HOH     A   239   <NA> -12.126 14.584 29.332 1.0
## 1110 HETATM  1111     O <NA>   HOH     A   240   <NA>  -6.410 28.639 29.739 1.0
## 1111 HETATM  1112     O <NA>   HOH     A   241   <NA>  -9.363 18.929 29.236 1.0
## 1112 HETATM  1113     O <NA>   HOH     A   242   <NA>   7.290  6.035 29.744 1.0
## 1113 HETATM  1114     O <NA>   HOH     A   243   <NA>   0.532  4.323 25.856 1.0
## 1114 HETATM  1115     O <NA>   HOH     A   244   <NA>  -5.527 11.769 31.278 1.0
## 1115 HETATM  1116     O <NA>   HOH     A   245   <NA>   9.709 13.211 30.865 1.0
## 1116 HETATM  1117     O <NA>   HOH     A   246   <NA>  -5.539 14.098 29.938 1.0
## 1117 HETATM  1118     O <NA>   HOH     A   247   <NA>   2.285  7.164 31.744 1.0
## 1118 HETATM  1119     O <NA>   HOH     A   249   <NA>   2.557 37.778 32.502 1.0
## 1119 HETATM  1120     O <NA>   HOH     A   250   <NA>  11.653 11.933 32.683 1.0
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## 1121 HETATM  1122     O <NA>   HOH     A   252   <NA>   7.578 12.160 33.759 1.0
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## 1124 HETATM  1125     O <NA>   HOH     A   255   <NA>  13.552 10.709 34.982 1.0
## 1125 HETATM  1126     O <NA>   HOH     A   256   <NA>  -0.456 24.995 36.970 1.0
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## 1127 HETATM  1128     O <NA>   HOH     A   258   <NA>  -7.483 20.739 37.397 1.0
## 1128 HETATM  1129     O <NA>   HOH     A   259   <NA>  16.885 30.334 28.147 1.0
## 1129 HETATM  1130     O <NA>   HOH     A   260   <NA>  -2.189 19.144  1.123 1.0
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## 1131 HETATM  1132     O <NA>   HOH     A   264   <NA>   0.167 38.321 22.074 1.0
## 1132 HETATM  1133     O <NA>   HOH     A   265   <NA>   2.643 23.311 24.222 1.0
## 1133 HETATM  1134     O <NA>   HOH     A   266   <NA>  -3.261 12.368 26.079 1.0
## 1134 HETATM  1135     O <NA>   HOH     A   267   <NA>  -8.163 28.523 28.227 1.0
## 1135 HETATM  1136     O <NA>   HOH     A   268   <NA>  11.314 34.308 29.649 1.0
## 1136 HETATM  1137     O <NA>   HOH     A   269   <NA>  -8.925 18.710 -0.425 1.0
## 1137 HETATM  1138     O <NA>   HOH     A   270   <NA>   1.106  7.975  2.503 1.0
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## 1139 HETATM  1140     O <NA>   HOH     A   272   <NA>   5.462 18.910  4.058 1.0
## 1140 HETATM  1141     O <NA>   HOH     A   273   <NA> -12.194 34.778  7.299 1.0
## 1141 HETATM  1142     O <NA>   HOH     A   274   <NA>  -1.696  6.065  8.495 1.0
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## 1145 HETATM  1146     O <NA>   HOH     A   278   <NA> -18.106  6.723 19.155 1.0
## 1146 HETATM  1147     O <NA>   HOH     A   279   <NA> -10.523  7.855 18.757 1.0
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## 1148 HETATM  1149     O <NA>   HOH     A   281   <NA>   4.973 30.366 26.631 1.0
## 1149 HETATM  1150     O <NA>   HOH     A   282   <NA> -14.163 23.294 27.041 1.0
## 1150 HETATM  1151     O <NA>   HOH     A   283   <NA>   4.190 23.920 28.202 1.0
## 1151 HETATM  1152     O <NA>   HOH     A   284   <NA>   1.927 24.235 28.261 1.0
## 1152 HETATM  1153     O <NA>   HOH     A   285   <NA>   8.469 24.914 28.323 1.0
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## 1153 HETATM  1154     O <NA>   HOH     A   286   <NA>   0.504 26.234 30.223 1.0
## 1154 HETATM  1155     O <NA>   HOH     A   287   <NA>   4.961  6.376 30.326 1.0
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## 1159 HETATM  1160     O <NA>   HOH     A   292   <NA>  11.050  6.576 33.893 1.0
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## 1168 HETATM  1169     O <NA>   HOH     A   301   <NA>   3.836 11.760  3.259 1.0
## 1169 HETATM  1170     O <NA>   HOH     A   302   <NA>  -9.211  4.115 14.687 1.0
## 1170 HETATM  1171     O <NA>   HOH     A   303   <NA>  16.205 21.210 16.009 1.0
## 1171 HETATM  1172     O <NA>   HOH     A   304   <NA> -14.845  6.428 21.717 1.0
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## 1175 HETATM  1176     O <NA>   HOH     A   308   <NA> -32.793  6.518 16.878 1.0
## 1176 HETATM  1177     O <NA>   HOH     A   309   <NA> -10.109 33.422  4.951 1.0
## 1177 HETATM  1178     O <NA>   HOH     A   310   <NA>  -6.930 35.720  3.927 1.0
## 1178 HETATM  1179     O <NA>   HOH     A   311   <NA>  -1.458 29.021 31.741 1.0
## 1179 HETATM  1180     O <NA>   HOH     A   312   <NA>  -7.776 27.408 33.976 1.0
## 1180 HETATM  1181     O <NA>   HOH     A   313   <NA>   2.002 13.196  3.708 1.0
## 1181 HETATM  1182     O <NA>   HOH     A   314   <NA>   7.005 28.792 27.719 1.0
## 1182 HETATM  1183     O <NA>   HOH     A   315   <NA> -14.736 20.042 16.788 1.0
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## 1185 HETATM  1186     O <NA>   HOH     A   318   <NA>  12.884 12.733 37.805 0.5
## 1186 HETATM  1187     O <NA>   HOH     A   319   <NA>   7.795 26.278 15.645 1.0
##          b segid elesy charge
## 1    11.18  <NA>     N   <NA>
## 2     9.68  <NA>     C   <NA>
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## 457   8.46  <NA>     C   <NA>
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## 890  10.46  <NA>     N   <NA>
## 891   9.75  <NA>     C   <NA>
## 892   9.63  <NA>     C   <NA>
## 893  13.85  <NA>     O   <NA>
## 894  12.72  <NA>     C   <NA>
## 895   7.87  <NA>     C   <NA>
## 896  15.62  <NA>     C   <NA>
## 897  17.04  <NA>     C   <NA>
## 898  11.32  <NA>     N   <NA>
## 899   9.19  <NA>     N   <NA>
## 900  22.87  <NA>     C   <NA>
## 901  33.97  <NA>     C   <NA>
## 902  28.79  <NA>     O   <NA>
## 903  15.57  <NA>     N   <NA>
## 904  20.24  <NA>     C   <NA>
## 905  18.25  <NA>     C   <NA>
## 906  18.09  <NA>     O   <NA>
## 907  13.62  <NA>     C   <NA>
## 908  12.88  <NA>     O   <NA>
## 909  12.89  <NA>     C   <NA>
## 910  20.97  <NA>     N   <NA>
## 911  17.43  <NA>     C   <NA>
## 912  19.50  <NA>     C   <NA>
## 913  24.87  <NA>     O   <NA>
## 914  27.62  <NA>     C   <NA>
## 915  57.62  <NA>     C   <NA>
## 916  36.72  <NA>     O   <NA>
## 917  41.26  <NA>     O   <NA>
## 918  20.10  <NA>     N   <NA>
## 919  24.77  <NA>     C   <NA>
## 920  16.15  <NA>     C   <NA>
## 921  13.85  <NA>     O   <NA>
## 922  15.61  <NA>     C   <NA>
## 923  17.17  <NA>     C   <NA>
## 924  18.96  <NA>     C   <NA>
## 925  18.05  <NA>     N   <NA>
## 926  20.34  <NA>     C   <NA>
## 927  14.19  <NA>     C   <NA>
## 928  15.61  <NA>     O   <NA>
## 929  39.58  <NA>     C   <NA>
## 930  39.30  <NA>     C   <NA>
## 931  58.93  <NA>     C   <NA>
## 932  64.91  <NA>     O   <NA>
## 933  55.29  <NA>     N   <NA>
## 934  14.53  <NA>     N   <NA>
```

```
## 935  13.31  <NA>     C   <NA>
## 936  18.32  <NA>     C   <NA>
## 937  14.96  <NA>     O   <NA>
## 938  18.92  <NA>     C   <NA>
## 939  14.16  <NA>     N   <NA>
## 940  21.27  <NA>     C   <NA>
## 941  12.05  <NA>     C   <NA>
## 942  15.94  <NA>     O   <NA>
## 943  14.43  <NA>     C   <NA>
## 944  16.32  <NA>     C   <NA>
## 945  16.23  <NA>     C   <NA>
## 946   6.26  <NA>     C   <NA>
## 947  13.70  <NA>     N   <NA>
## 948  10.20  <NA>     C   <NA>
## 949  14.76  <NA>     C   <NA>
## 950  21.80  <NA>     C   <NA>
## 951  21.47  <NA>     C   <NA>
## 952  22.40  <NA>     C   <NA>
## 953  10.36  <NA>     N   <NA>
## 954  14.89  <NA>     C   <NA>
## 955  16.52  <NA>     C   <NA>
## 956  16.40  <NA>     O   <NA>
## 957  15.33  <NA>     C   <NA>
## 958  15.55  <NA>     C   <NA>
## 959  15.50  <NA>     C   <NA>
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## 964  24.03  <NA>     O   <NA>
## 965  29.23  <NA>     C   <NA>
## 966  46.98  <NA>     C   <NA>
## 967  51.79  <NA>     C   <NA>
## 968  80.40  <NA>     N   <NA>
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## 970  50.97  <NA>     N   <NA>
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## 974  22.07  <NA>     C   <NA>
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## 978  13.96  <NA>     C   <NA>
## 979  19.22  <NA>     O   <NA>
## 980  16.08  <NA>     C   <NA>
## 981  17.92  <NA>     S   <NA>
## 982  19.23  <NA>     N   <NA>
## 983  29.52  <NA>     C   <NA>
## 984  19.23  <NA>     C   <NA>
## 985  29.24  <NA>     O   <NA>
```

```
## 986  35.15  <NA>     C   <NA>
## 987  32.92  <NA>     C   <NA>
## 988  38.70  <NA>     C   <NA>
## 989  50.55  <NA>     N   <NA>
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## 991  46.94  <NA>     N   <NA>
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## 994  33.38  <NA>     C   <NA>
## 995  72.70  <NA>     C   <NA>
## 996  49.87  <NA>     O   <NA>
## 997  23.67  <NA>     C   <NA>
## 998  28.34  <NA>     C   <NA>
## 999  36.38  <NA>     C   <NA>
## 1000 43.93  <NA>     C   <NA>
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## 1002 39.80  <NA>     O   <NA>
## 1003 49.26  <NA>     O   <NA>
## 1004 44.65  <NA>     O   <NA>
## 1005 47.43  <NA>     O   <NA>
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## 1008 29.55  <NA>     O   <NA>
## 1009 20.51  <NA>     O   <NA>
## 1010 38.26  <NA>     O   <NA>
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## 1018 28.71  <NA>     O   <NA>
## 1019 71.21  <NA>     O   <NA>
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## 1021 23.16  <NA>     O   <NA>
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## 1023 70.64  <NA>     O   <NA>
## 1024 52.27  <NA>     O   <NA>
## 1025 20.33  <NA>     O   <NA>
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## 1033 26.29  <NA>     O   <NA>
## 1034 17.58  <NA>     O   <NA>
## 1035 33.32  <NA>     O   <NA>
## 1036 21.87  <NA>     O   <NA>
```

```
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## 1038 40.68  <NA>     O   <NA>
## 1039 52.70  <NA>     O   <NA>
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## 1085 35.14  <NA>     O   <NA>
## 1086  9.12  <NA>     O   <NA>
## 1087 44.08  <NA>     O   <NA>
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## 1089 58.87  <NA>     O   <NA>
## 1090 42.59  <NA>     O   <NA>
## 1091 59.61  <NA>     O   <NA>
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## 1137 57.87  <NA>     O   <NA>
## 1138 58.10  <NA>     O   <NA>
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## 1140 56.09  <NA>     0   <NA>
## 1141 68.76  <NA>     0   <NA>
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## 1148 56.27  <NA>     0   <NA>
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## 1161 55.95  <NA>     0   <NA>
## 1162 70.62  <NA>     0   <NA>
## 1163 49.79  <NA>     0   <NA>
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## 1166 52.55  <NA>     0   <NA>
## 1167 74.82  <NA>     0   <NA>
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## 1170 69.59  <NA>     0   <NA>
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## 1182 37.49  <NA>     0   <NA>
## 1183 36.58  <NA>     0   <NA>
## 1184 42.27  <NA>     0   <NA>
## 1185 65.31  <NA>     0   <NA>
## 1186 44.16  <NA>     0   <NA>
```
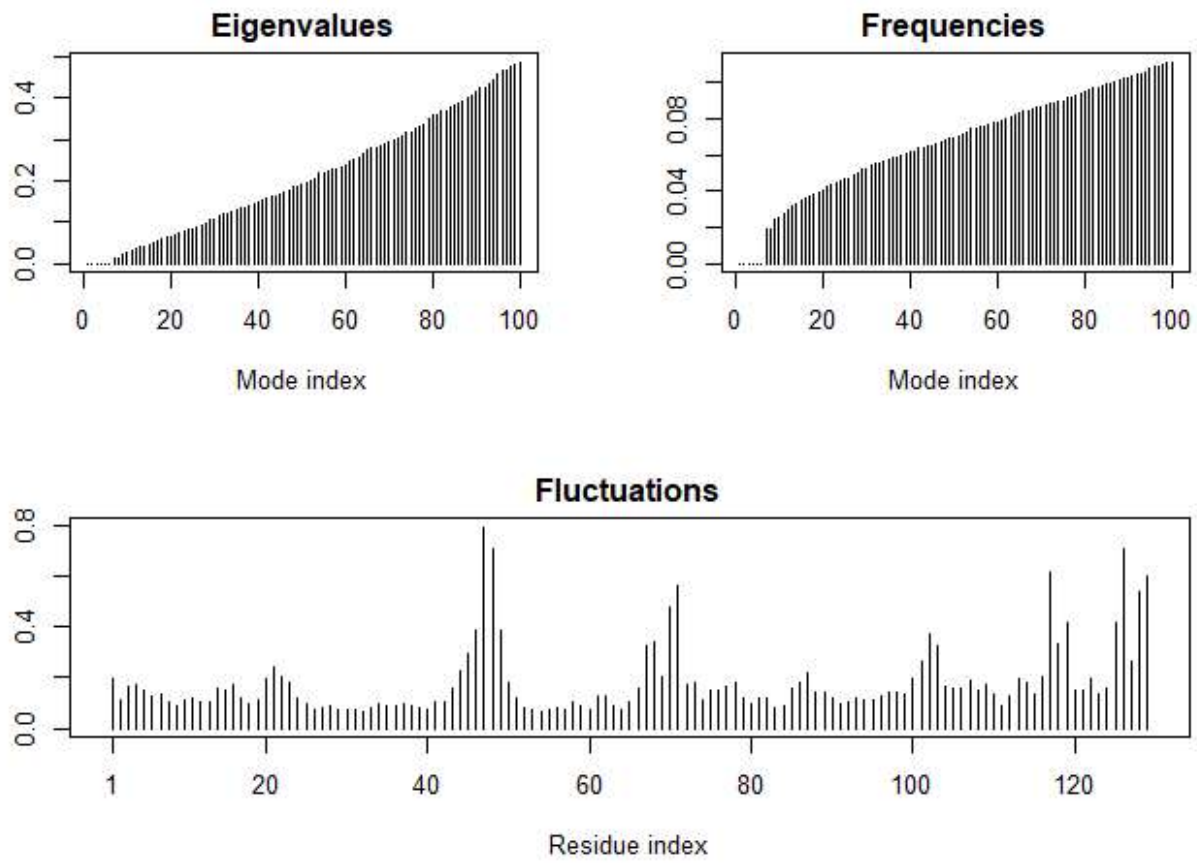

Normal Mode Analysis (nma) is a prediction of the conformational variability and intrinsic dynamics of this protein

```
m <- nma(pdb)
```

```
##  Building Hessian...     Done in 0.03 seconds.
##  Diagonalizing Hessian...    Done in 0.16 seconds.
```

```
plot(m)
```




Saving the file to make a movie

```
mktrj(m, file = "nma.pdb")
```

Can open in VMD. There will be 34 frames, can press play to watch