Untitled

1. Intro to the PDB database

```
pdb.stats <- read.csv("Data_Export_Summary.csv", row.names = 1)
View(pdb.stats)
```

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

Microscopy.

```
# for x-ray:
sum(pdb.stats$X.ray) / sum(pdb.stats$Total) * 100
```

```
## [1] 87.19655
```

```
# for EM:
sum(pdb.stats$EM) / sum(pdb.stats$Total) * 100
```

```
## [1] 5.354296
```

```
# alternatively, use colSums()
tot.method <- colSums(pdb.stats)
signif(tot.method / tot.method["Total"] * 100, 3)
```

```
##            X.ray              NMR               EM Multiple.methods
##          87.2000           7.2800           5.3500           0.1060
##          Neutron            Other            Total
##           0.0385           0.0198         100.0000
```

87.2% are solved by X-ray, 5.35% are solved by EM.

Q2. What proportion of structures in the PDB are protein?

```
signif(pdb.stats$Total[1] / sum(pdb.stats$Total), 3) * 100
```

```
## [1] 87.3
```

87.3% of structures are proteins.

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?

There are 836 protease structures.

2. Visualizing the HIV-1 protease structure

Bio3D package for bioinformatics

```
# install.packages("bio3d")
library(bio3d)
pdb <- read.pdb("1hsg")
```

```
##   Note: Accessing on-line PDB file
```

```
pdb
```

```
##
##  Call:  read.pdb(file = "1hsg")
##
##    Total Models#: 1
##      Total Atoms#: 1686,  XYZs#: 5058  Chains#: 2  (values: A B)
##
##      Protein Atoms#: 1514  (residues/Calpha atoms#: 198)
##      Nucleic acid Atoms#: 0  (residues/phosphate atoms#: 0)
```

```
##      Nucleic acid Atoms#: 0  (residues/phosphate atoms#: 0)
##
##      Non-protein/nucleic Atoms#: 172  (residues: 128)
##      Non-protein/nucleic resid values: [ HOH (127), MK1 (1) ]
##
##    Protein sequence:
##       PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGIGGFIKVRQYD
##       QILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFPQITLWQRPLVTIKIGGQLKE
##       ALLDTGADDTVLEEMSLPGRWKPKMIGGIGGFIKVRQYDQILIEICGHKAIGTVLVGPTP
##       VNIIGRNLLTQIGCTLNF

##
## + 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>   PRO     A     1   <NA> 29.361  39.686   5.862 1
## 2      ATOM     2    CA <NA>   PRO     A     1   <NA> 30.307  38.663   5.319 1
## 3      ATOM     3     C <NA>   PRO     A     1   <NA> 29.760  38.071   4.022 1
## 4      ATOM     4     O <NA>   PRO     A     1   <NA> 28.600  38.302   3.676 1
## 5      ATOM     5    CB <NA>   PRO     A     1   <NA> 30.508  37.541   6.342 1
## 6      ATOM     6    CG <NA>   PRO     A     1   <NA> 29.296  37.591   7.162 1
## 7      ATOM     7    CD <NA>   PRO     A     1   <NA> 28.778  39.015   7.019 1
## 8      ATOM     8     N <NA>   GLN     A     2   <NA> 30.607  37.334   3.305 1
## 9      ATOM     9    CA <NA>   GLN     A     2   <NA> 30.158  36.492   2.199 1
## 10     ATOM    10     C <NA>   GLN     A     2   <NA> 30.298  35.041   2.643 1
## 11     ATOM    11     O <NA>   GLN     A     2   <NA> 31.401  34.494   2.763 1
## 12     ATOM    12    CB <NA>   GLN     A     2   <NA> 30.970  36.738   0.926 1
## 13     ATOM    13    CG <NA>   GLN     A     2   <NA> 30.625  35.783  -0.201 1
## 14     ATOM    14    CD <NA>   GLN     A     2   <NA> 31.184  36.217  -1.549 1
## 15     ATOM    15   OE1 <NA>   GLN     A     2   <NA> 32.006  35.518  -2.156 1
## 16     ATOM    16   NE2 <NA>   GLN     A     2   <NA> 30.684  37.339  -2.061 1
## 17     ATOM    17     N <NA>   ILE     A     3   <NA> 29.160  34.436   2.919 1
## 18     ATOM    18    CA <NA>   ILE     A     3   <NA> 29.123  33.098   3.397 1
## 19     ATOM    19     C <NA>   ILE     A     3   <NA> 28.968  32.155   2.198 1
## 20     ATOM    20     O <NA>   ILE     A     3   <NA> 28.088  32.330   1.368 1
## 21     ATOM    21    CB <NA>   ILE     A     3   <NA> 27.977  32.995   4.409 1
## 22     ATOM    22   CG1 <NA>   ILE     A     3   <NA> 28.341  33.820   5.652 1
## 23     ATOM    23   CG2 <NA>   ILE     A     3   <NA> 27.692  31.548   4.745 1
## 24     ATOM    24   CD1 <NA>   ILE     A     3   <NA> 27.264  33.884   6.696 1
## 25     ATOM    25     N <NA>   THR     A     4   <NA> 29.891  31.210   2.066 1
## 26     ATOM    26    CA <NA>   THR     A     4   <NA> 29.774  30.143   1.062 1
## 27     ATOM    27     C <NA>   THR     A     4   <NA> 28.986  28.975   1.658 1
## 28     ATOM    28     O <NA>   THR     A     4   <NA> 28.690  28.948   2.875 1
## 29     ATOM    29    CB <NA>   THR     A     4   <NA> 31.165  29.618   0.634 1
```

```
## 30     ATOM    30   OG1 <NA>   THR     A     4   <NA> 31.866  29.209   1.815 1
## 31     ATOM    31   CG2 <NA>   THR     A     4   <NA> 31.980  30.688  -0.085 1
## 32     ATOM    32     N <NA>   LEU     A     5   <NA> 28.641  28.019   0.803 1
## 33     ATOM    33    CA <NA>   LEU     A     5   <NA> 27.644  27.003   1.144 1
## 34     ATOM    34     C <NA>   LEU     A     5   <NA> 28.204  25.559   1.071 1
## 35     ATOM    35     O <NA>   LEU     A     5   <NA> 27.446  24.583   0.969 1
## 36     ATOM    36    CB <NA>   LEU     A     5   <NA> 26.411  27.139   0.226 1
## 37     ATOM    37    CG <NA>   LEU     A     5   <NA> 25.676  28.479   0.352 1
## 38     ATOM    38   CD1 <NA>   LEU     A     5   <NA> 24.624  28.624  -0.753 1
## 39     ATOM    39   CD2 <NA>   LEU     A     5   <NA> 25.088  28.590   1.745 1
## 40     ATOM    40     N <NA>   TRP     A     6   <NA> 29.528  25.436   1.146 1
## 41     ATOM    41    CA <NA>   TRP     A     6   <NA> 30.177  24.150   1.279 1
## 42     ATOM    42     C <NA>   TRP     A     6   <NA> 29.837  23.488   2.611 1
## 43     ATOM    43     O <NA>   TRP     A     6   <NA> 29.706  22.271   2.673 1
## 44     ATOM    44    CB <NA>   TRP     A     6   <NA> 31.685  24.301   1.109 1
## 45     ATOM    45    CG <NA>   TRP     A     6   <NA> 32.152  24.955  -0.189 1
## 46     ATOM    46   CD1 <NA>   TRP     A     6   <NA> 32.681  26.216  -0.345 1
## 47     ATOM    47   CD2 <NA>   TRP     A     6   <NA> 32.274  24.314  -1.478 1
## 48     ATOM    48   NE1 <NA>   TRP     A     6   <NA> 33.102  26.385  -1.655 1
## 49     ATOM    49   CE2 <NA>   TRP     A     6   <NA> 32.864  25.258  -2.369 1
## 50     ATOM    50   CE3 <NA>   TRP     A     6   <NA> 31.949  23.035  -1.986 1
## 51     ATOM    51   CZ2 <NA>   TRP     A     6   <NA> 33.093  24.968  -3.717 1
## 52     ATOM    52   CZ3 <NA>   TRP     A     6   <NA> 32.195  22.755  -3.294 1
## 53     ATOM    53   CH2 <NA>   TRP     A     6   <NA> 32.754  23.722  -4.169 1
## 54     ATOM    54     N <NA>   GLN     A     7   <NA> 29.667  24.280   3.667 1
## 55     ATOM    55    CA <NA>   GLN     A     7   <NA> 29.141  23.799   4.960 1
## 56     ATOM    56     C <NA>   GLN     A     7   <NA> 27.747  24.395   5.208 1
## 57     ATOM    57     O <NA>   GLN     A     7   <NA> 27.349  25.330   4.547 1
## 58     ATOM    58    CB <NA>   GLN     A     7   <NA> 30.072  24.227   6.100 1
## 59     ATOM    59    CG <NA>   GLN     A     7   <NA> 31.512  23.694   5.995 1
## 60     ATOM    60    CD <NA>   GLN     A     7   <NA> 32.521  24.750   5.469 1
## 61     ATOM    61   OE1 <NA>   GLN     A     7   <NA> 32.666  25.860   6.038 1
## 62     ATOM    62   NE2 <NA>   GLN     A     7   <NA> 33.268  24.374   4.419 1

## 63     ATOM    63     N <NA>   ARG     A     8   <NA> 26.992  23.877   6.169 1
## 64     ATOM    64    CA <NA>   ARG     A     8   <NA> 25.757  24.566   6.593 1
## 65     ATOM    65     C <NA>   ARG     A     8   <NA> 26.029  26.025   6.996 1
## 66     ATOM    66     O <NA>   ARG     A     8   <NA> 26.947  26.291   7.775 1
## 67     ATOM    67    CB <NA>   ARG     A     8   <NA> 25.087  23.849   7.776 1
## 68     ATOM    68    CG <NA>   ARG     A     8   <NA> 24.646  22.409   7.505 1
## 69     ATOM    69    CD <NA>   ARG     A     8   <NA> 23.728  21.896   8.637 1
## 70     ATOM    70    NE <NA>   ARG     A     8   <NA> 22.952  20.730   8.230 1
## 71     ATOM    71    CZ <NA>   ARG     A     8   <NA> 22.367  19.871   9.064 1
## 72     ATOM    72   NH1 <NA>   ARG     A     8   <NA> 22.376  20.074  10.370 1
## 73     ATOM    73   NH2 <NA>   ARG     A     8   <NA> 21.776  18.789   8.589 1
## 74     ATOM    74     N <NA>   PRO     A     9   <NA> 25.123  26.955   6.645 1
## 75     ATOM    75    CA <NA>   PRO     A     9   <NA> 25.491  28.352   6.938 1
## 76     ATOM    76     C <NA>   PRO     A     9   <NA> 25.127  28.763   8.364 1
## 77     ATOM    77     O <NA>   PRO     A     9   <NA> 24.136  29.472   8.578 1
## 78     ATOM    78    CB <NA>   PRO     A     9   <NA> 24.719  29.176   5.916 1
```

```
## 79     ATOM    79    CG <NA>   PRO     A     9   <NA> 23.625  28.254   5.407 1
## 80     ATOM    80    CD <NA>   PRO     A     9   <NA> 24.096  26.855   5.591 1
## 81     ATOM    81     N <NA>   LEU     A    10   <NA> 25.905  28.285   9.330 1
## 82     ATOM    82    CA <NA>   LEU     A    10   <NA> 25.653  28.510  10.750 1
## 83     ATOM    83     C <NA>   LEU     A    10   <NA> 26.383  29.770  11.208 1
## 84     ATOM    84     O <NA>   LEU     A    10   <NA> 27.567  29.927  10.938 1
## 85     ATOM    85    CB <NA>   LEU     A    10   <NA> 26.120  27.284  11.573 1
## 86     ATOM    86    CG <NA>   LEU     A    10   <NA> 25.161  26.082  11.544 1
## 87     ATOM    87   CD1 <NA>   LEU     A    10   <NA> 25.895  24.743  11.662 1
## 88     ATOM    88   CD2 <NA>   LEU     A    10   <NA> 24.206  26.196  12.696 1
## 89     ATOM    89     N <NA>   VAL     A    11   <NA> 25.667  30.672  11.872 1
## 90     ATOM    90    CA <NA>   VAL     A    11   <NA> 26.267  31.854  12.497 1
## 91     ATOM    91     C <NA>   VAL     A    11   <NA> 25.818  31.957  13.955 1
## 92     ATOM    92     O <NA>   VAL     A    11   <NA> 24.929  31.184  14.402 1
## 93     ATOM    93    CB <NA>   VAL     A    11   <NA> 25.824  33.131  11.791 1
## 94     ATOM    94   CG1 <NA>   VAL     A    11   <NA> 26.270  33.089  10.323 1
## 95     ATOM    95   CG2 <NA>   VAL     A    11   <NA> 24.333  33.275  11.879 1
## 96     ATOM    96     N <NA>   THR     A    12   <NA> 26.397  32.913  14.700 1
## 97     ATOM    97    CA <NA>   THR     A    12   <NA> 26.001  33.143  16.102 1
## 98     ATOM    98     C <NA>   THR     A    12   <NA> 24.915  34.200  16.204 1
## 99     ATOM    99     O <NA>   THR     A    12   <NA> 25.010  35.279  15.610 1
## 100    ATOM   100    CB <NA>   THR     A    12   <NA> 27.201  33.565  16.998 1
## 101    ATOM   101   OG1 <NA>   THR     A    12   <NA> 28.330  32.709  16.751 1
## 102    ATOM   102   CG2 <NA>   THR     A    12   <NA> 26.827  33.430  18.450 1
## 103    ATOM   103     N <NA>   ILE     A    13   <NA> 23.848  33.868  16.909 1
## 104    ATOM   104    CA <NA>   ILE     A    13   <NA> 22.842  34.875  17.206 1
## 105    ATOM   105     C <NA>   ILE     A    13   <NA> 22.770  35.114  18.707 1
## 106    ATOM   106     O <NA>   ILE     A    13   <NA> 23.328  34.363  19.500 1
## 107    ATOM   107    CB <NA>   ILE     A    13   <NA> 21.413  34.460  16.661 1
## 108    ATOM   108   CG1 <NA>   ILE     A    13   <NA> 20.878  33.229  17.431 1
## 109    ATOM   109   CG2 <NA>   ILE     A    13   <NA> 21.510  34.194  15.162 1
## 110    ATOM   110   CD1 <NA>   ILE     A    13   <NA> 19.353  33.201  17.603 1
## 111    ATOM   111     N <NA>   LYS     A    14   <NA> 22.106  36.199  19.087 1

## 112    ATOM   112    CA <NA>   LYS     A    14   <NA> 21.894  36.545  20.492 1
## 113    ATOM   113     C <NA>   LYS     A    14   <NA> 20.442  36.943  20.615 1
## 114    ATOM   114     O <NA>   LYS     A    14   <NA> 19.960  37.808  19.873 1
## 115    ATOM   115    CB <NA>   LYS     A    14   <NA> 22.777  37.724  20.896 1
## 116    ATOM   116    CG <NA>   LYS     A    14   <NA> 22.727  38.056  22.383 1
## 117    ATOM   117    CD <NA>   LYS     A    14   <NA> 23.270  39.450  22.678 1
## 118    ATOM   118    CE <NA>   LYS     A    14   <NA> 24.814  39.490  22.755 1
## 119    ATOM   119    NZ <NA>   LYS     A    14   <NA> 25.394  40.891  22.572 1
## 120    ATOM   120     N <NA>   ILE     A    15   <NA> 19.739  36.267  21.512 1
## 121    ATOM   121    CA <NA>   ILE     A    15   <NA> 18.345  36.563  21.813 1
## 122    ATOM   122     C <NA>   ILE     A    15   <NA> 18.224  36.327  23.316 1
## 123    ATOM   123     O <NA>   ILE     A    15   <NA> 18.886  35.449  23.864 1
## 124    ATOM   124    CB <NA>   ILE     A    15   <NA> 17.380  35.592  21.022 1
## 125    ATOM   125   CG1 <NA>   ILE     A    15   <NA> 15.935  35.812  21.435 1
## 126    ATOM   126   CG2 <NA>   ILE     A    15   <NA> 17.745  34.137  21.266 1
## 127    ATOM   127   CD1 <NA>   ILE     A    15   <NA> 14.929  35.116  20.526 1
```

```
## 128    ATOM   128     N <NA>   GLY     A    16   <NA> 17.446  37.139  24.012 1
## 129    ATOM   129    CA <NA>   GLY     A    16   <NA> 17.356  36.968  25.459 1
## 130    ATOM   130     C <NA>   GLY     A    16   <NA> 18.711  36.871  26.160 1
## 131    ATOM   131     O <NA>   GLY     A    16   <NA> 18.866  36.162  27.153 1
## 132    ATOM   132     N <NA>   GLY     A    17   <NA> 19.671  37.659  25.697 1
## 133    ATOM   133    CA <NA>   GLY     A    17   <NA> 20.970  37.660  26.340 1
## 134    ATOM   134     C <NA>   GLY     A    17   <NA> 21.680  36.316  26.278 1
## 135    ATOM   135     O <NA>   GLY     A    17   <NA> 22.785  36.163  26.794 1
## 136    ATOM   136     N <NA>   GLN     A    18   <NA> 21.093  35.361  25.572 1
## 137    ATOM   137    CA <NA>   GLN     A    18   <NA> 21.780  34.106  25.263 1
## 138    ATOM   138     C <NA>   GLN     A    18   <NA> 22.500  34.159  23.907 1
## 139    ATOM   139     O <NA>   GLN     A    18   <NA> 21.937  34.624  22.915 1
## 140    ATOM   140    CB <NA>   GLN     A    18   <NA> 20.776  32.957  25.228 1
## 141    ATOM   141    CG <NA>   GLN     A    18   <NA> 19.599  33.116  26.176 1
## 142    ATOM   142    CD <NA>   GLN     A    18   <NA> 19.556  31.997  27.179 1
## 143    ATOM   143   OE1 <NA>   GLN     A    18   <NA> 20.393  31.944  28.082 1
## 144    ATOM   144   NE2 <NA>   GLN     A    18   <NA> 18.647  31.035  26.975 1
## 145    ATOM   145     N <NA>   LEU     A    19   <NA> 23.733  33.672  23.848 1
## 146    ATOM   146    CA <NA>   LEU     A    19   <NA> 24.334  33.365  22.552 1
## 147    ATOM   147     C <NA>   LEU     A    19   <NA> 23.896  31.963  22.106 1
## 148    ATOM   148     O <NA>   LEU     A    19   <NA> 23.975  31.020  22.863 1
## 149    ATOM   149    CB <NA>   LEU     A    19   <NA> 25.869  33.432  22.625 1
## 150    ATOM   150    CG <NA>   LEU     A    19   <NA> 26.561  34.761  22.968 1
## 151    ATOM   151   CD1 <NA>   LEU     A    19   <NA> 28.007  34.629  22.620 1
## 152    ATOM   152   CD2 <NA>   LEU     A    19   <NA> 25.983  35.913  22.194 1
## 153    ATOM   153     N <NA>   LYS     A    20   <NA> 23.416  31.855  20.876 1
## 154    ATOM   154    CA <NA>   LYS     A    20   <NA> 23.006  30.584  20.266 1
## 155    ATOM   155     C <NA>   LYS     A    20   <NA> 23.626  30.463  18.874 1
## 156    ATOM   156     O <NA>   LYS     A    20   <NA> 24.024  31.460  18.283 1
## 157    ATOM   157    CB <NA>   LYS     A    20   <NA> 21.494  30.523  20.107 1
## 158    ATOM   158    CG <NA>   LYS     A    20   <NA> 20.778  29.875  21.264 1
## 159    ATOM   159    CD <NA>   LYS     A    20   <NA> 19.868  30.857  21.939 1
## 160    ATOM   160    CE <NA>   LYS     A    20   <NA> 19.112  30.168  23.043 1

## 161    ATOM   161    NZ <NA>   LYS     A    20   <NA> 18.467  28.892  22.571 1
## 162    ATOM   162     N <NA>   GLU     A    21   <NA> 23.725  29.250  18.342 1
## 163    ATOM   163    CA <NA>   GLU     A    21   <NA> 24.053  29.117  16.931 1
## 164    ATOM   164     C <NA>   GLU     A    21   <NA> 22.822  28.761  16.150 1
## 165    ATOM   165     O <NA>   GLU     A    21   <NA> 21.879  28.136  16.672 1
## 166    ATOM   166    CB <NA>   GLU     A    21   <NA> 25.197  28.130  16.679 1
## 167    ATOM   167    CG <NA>   GLU     A    21   <NA> 25.035  26.716  17.168 1
## 168    ATOM   168    CD <NA>   GLU     A    21   <NA> 25.878  25.743  16.334 1
## 169    ATOM   169   OE1 <NA>   GLU     A    21   <NA> 27.022  26.130  15.972 1
## 170    ATOM   170   OE2 <NA>   GLU     A    21   <NA> 25.379  24.639  15.983 1
## 171    ATOM   171     N <NA>   ALA     A    22   <NA> 22.778  29.268  14.927 1
## 172    ATOM   172    CA <NA>   ALA     A    22   <NA> 21.553  29.189  14.165 1
## 173    ATOM   173     C <NA>   ALA     A    22   <NA> 21.870  29.183  12.682 1
## 174    ATOM   174     O <NA>   ALA     A    22   <NA> 22.975  29.578  12.252 1
## 175    ATOM   175    CB <NA>   ALA     A    22   <NA> 20.625  30.359  14.524 1
## 176    ATOM   176     N <NA>   LEU     A    23   <NA> 20.893  28.726  11.903 1
```

```
## 177    ATOM   177    CA <NA>   LEU     A    23   <NA> 21.047  28.473  10.476 1
## 178    ATOM   178     C <NA>   LEU     A    23   <NA> 20.381  29.596   9.664 1
## 179    ATOM   179     O <NA>   LEU     A    23   <NA> 19.231  29.943   9.912 1
## 180    ATOM   180    CB <NA>   LEU     A    23   <NA> 20.382  27.135  10.174 1
## 181    ATOM   181    CG <NA>   LEU     A    23   <NA> 20.532  26.573   8.786 1
## 182    ATOM   182   CD1 <NA>   LEU     A    23   <NA> 21.939  26.039   8.621 1
## 183    ATOM   183   CD2 <NA>   LEU     A    23   <NA> 19.490  25.490   8.627 1
## 184    ATOM   184     N <NA>   LEU     A    24   <NA> 21.122  30.163   8.715 1
## 185    ATOM   185    CA <NA>   LEU     A    24   <NA> 20.617  31.144   7.775 1
## 186    ATOM   186     C <NA>   LEU     A    24   <NA> 19.940  30.412   6.617 1
## 187    ATOM   187     O <NA>   LEU     A    24   <NA> 20.567  29.833   5.740 1
## 188    ATOM   188    CB <NA>   LEU     A    24   <NA> 21.767  32.023   7.262 1
## 189    ATOM   189    CG <NA>   LEU     A    24   <NA> 22.647  32.673   8.359 1
## 190    ATOM   190   CD1 <NA>   LEU     A    24   <NA> 23.698  33.581   7.738 1
## 191    ATOM   191   CD2 <NA>   LEU     A    24   <NA> 21.797  33.496   9.368 1
## 192    ATOM   192     N <NA>   ASP     A    25   <NA> 18.626  30.444   6.627 1
## 193    ATOM   193    CA <NA>   ASP     A    25   <NA> 17.853  29.516   5.837 1
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## 195    ATOM   195     O <NA>   ASP     A    25   <NA> 15.843  30.678   5.237 1
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## 198    ATOM   198   OD1 <NA>   ASP     A    25   <NA> 16.236  27.458   4.905 1
## 199    ATOM   199   OD2 <NA>   ASP     A    25   <NA> 15.762  26.696   6.882 1
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## 203    ATOM   203     O <NA>   THR     A    26   <NA> 14.412  30.939   1.615 1
## 204    ATOM   204    CB <NA>   THR     A    26   <NA> 17.328  31.419   1.447 1
## 205    ATOM   205   OG1 <NA>   THR     A    26   <NA> 17.693  30.177   0.863 1
## 206    ATOM   206   CG2 <NA>   THR     A    26   <NA> 18.601  32.197   1.773 1
## 207    ATOM   207     N <NA>   GLY     A    27   <NA> 15.213  29.111   2.702 1
## 208    ATOM   208    CA <NA>   GLY     A    27   <NA> 14.043  28.331   2.349 1
## 209    ATOM   209     C <NA>   GLY     A    27   <NA> 12.958  28.456   3.394 1

## 210    ATOM   210     O <NA>   GLY     A    27   <NA> 11.832  28.015   3.171 1
## 211    ATOM   211     N <NA>   ALA     A    28   <NA> 13.301  28.967   4.569 1
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## 216    ATOM   216     N <NA>   ASP     A    29   <NA> 10.296  30.560   5.587 1
## 217    ATOM   217    CA <NA>   ASP     A    29   <NA>  9.512  31.798   5.651 1
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## 237    ATOM   237   OG1 <NA>   THR     A    31   <NA> 13.451  34.082  11.707 1
## 238    ATOM   238   CG2 <NA>   THR     A    31   <NA> 14.027  32.992  13.816 1
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## 253    ATOM   253   CD2 <NA>   LEU     A    33   <NA> 16.139  30.718  16.927 1
## 254    ATOM   254     N <NA>   GLU     A    34   <NA> 14.568  26.722  18.889 1
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## 259    ATOM   259    CG <NA>   GLU     A    34   <NA> 16.297  24.250  18.988 1
## 260    ATOM   260    CD <NA>   GLU     A    34   <NA> 17.726  23.801  19.191 1
## 261    ATOM   261   OE1 <NA>   GLU     A    34   <NA> 18.134  23.657  20.375 1
## 262    ATOM   262   OE2 <NA>   GLU     A    34   <NA> 18.443  23.614  18.182 1
## 263    ATOM   263     N <NA>   GLU     A    35   <NA> 12.865  25.288  21.703 1
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## 270    ATOM   270   OE1 <NA>   GLU     A    35   <NA>  9.134  23.066  23.120 1
## 271    ATOM   271   OE2 <NA>   GLU     A    35   <NA>  8.758  25.047  24.035 1
## 272    ATOM   272     N <NA>   MET     A    36   <NA> 12.495  27.556  24.269 1
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## 300    ATOM   300    CD <NA>   PRO     A    39   <NA> 11.291  37.226  26.725 1
## 301    ATOM   301     N <NA>   GLY     A    40   <NA>  6.601  37.811  27.029 1
## 302    ATOM   302    CA <NA>   GLY     A    40   <NA>  5.419  38.218  26.302 1
## 303    ATOM   303     C <NA>   GLY     A    40   <NA>  4.430  37.094  26.331 1
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## 305    ATOM   305     N <NA>   ARG     A    41   <NA>  3.289  37.341  25.729 1
## 306    ATOM   306    CA <NA>   ARG     A    41   <NA>  2.382  36.252  25.509 1
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## 308    ATOM   308     O <NA>   ARG     A    41   <NA>  3.225  36.383  23.273 1
## 309    ATOM   309    CB <NA>   ARG     A    41   <NA>  0.956  36.719  25.748 1
## 310    ATOM   310    CG <NA>   ARG     A    41   <NA>  0.288  36.021  26.959 1
## 311    ATOM   311    CD <NA>   ARG     A    41   <NA>  0.118  36.953  28.169 1
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## 314    ATOM   314   NH1 <NA>   ARG     A    41   <NA>  1.161  39.450  29.040 1
## 315    ATOM   315   NH2 <NA>   ARG     A    41   <NA>  2.973  38.402  29.994 1
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## 323    ATOM   323   CD2 <NA>   TRP     A    42   <NA>  1.989  30.710  23.857 1
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## 329    ATOM   329   CH2 <NA>   TRP     A    42   <NA>  0.305  28.651  24.686 1
## 330    ATOM   330     N <NA>   LYS     A    43   <NA>  0.781  33.465  20.639 1
## 331    ATOM   331    CA <NA>   LYS     A    43   <NA> -0.305  32.776  19.928 1
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## 338    ATOM   338    NZ <NA>   LYS     A    43   <NA> -0.979  38.292  19.067 1
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## 340    ATOM   340    CA <NA>   PRO     A    44   <NA> -0.088  29.114  18.966 1
## 341    ATOM   341     C <NA>   PRO     A    44   <NA> -0.275  29.085  17.454 1
## 342    ATOM   342     O <NA>   PRO     A    44   <NA> -1.185  29.721  16.929 1
## 343    ATOM   343    CB <NA>   PRO     A    44   <NA> -0.893  28.021  19.667 1
## 344    ATOM   344    CG <NA>   PRO     A    44   <NA> -2.170  28.683  20.012 1
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## 346    ATOM   346     N <NA>   LYS     A    45   <NA>  0.586  28.336  16.762 1
## 347    ATOM   347    CA <NA>   LYS     A    45   <NA>  0.634  28.302  15.290 1
## 348    ATOM   348     C <NA>   LYS     A    45   <NA>  1.025  26.869  14.873 1
## 349    ATOM   349     O <NA>   LYS     A    45   <NA>  1.711  26.163  15.608 1
## 350    ATOM   350    CB <NA>   LYS     A    45   <NA>  1.693  29.299  14.799 1
## 351    ATOM   351    CG <NA>   LYS     A    45   <NA>  1.495  29.822  13.396 1
## 352    ATOM   352    CD <NA>   LYS     A    45   <NA>  2.628  30.791  12.986 1
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## 355    ATOM   355     N <NA>   MET     A    46   <NA>  0.570  26.438  13.707 1
## 356    ATOM   356    CA <NA>   MET     A    46   <NA>  1.091  25.232  13.081 1

## 357    ATOM   357     C <NA>   MET     A    46   <NA>  1.899  25.638  11.874 1
## 358    ATOM   358     O <NA>   MET     A    46   <NA>  1.385  26.292  10.965 1
## 359    ATOM   359    CB <NA>   MET     A    46   <NA> -0.047  24.319  12.624 1
## 360    ATOM   360    CG <NA>   MET     A    46   <NA> -0.970  23.867  13.745 1
## 361    ATOM   361    SD <NA>   MET     A    46   <NA> -0.348  22.459  14.681 1
## 362    ATOM   362    CE <NA>   MET     A    46   <NA> -0.585  21.081  13.426 1
## 363    ATOM   363     N <NA>   ILE     A    47   <NA>  3.167  25.258  11.849 1
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## 366    ATOM   366     O <NA>   ILE     A    47   <NA>  4.667  23.248  10.887 1
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## 368    ATOM   368   CG1 <NA>   ILE     A    47   <NA>  5.959  25.628  12.127 1
## 369    ATOM   369   CG2 <NA>   ILE     A    47   <NA>  4.898  27.703  11.148 1
## 370    ATOM   370   CD1 <NA>   ILE     A    47   <NA>  7.369  26.170  12.291 1
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## 384    ATOM   384   CG1 <NA>   ILE     A    50   <NA> 11.553  18.874   3.682 1
## 385    ATOM   385   CG2 <NA>   ILE     A    50   <NA> 11.521  16.945   5.317 1
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## 391    ATOM   391     N <NA>   GLY     A    52   <NA>  6.141  17.132   7.563 1
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## 402    ATOM   402   CD2 <NA>   PHE     A    53   <NA>  1.556  22.518   9.607 1
## 403    ATOM   403   CE1 <NA>   PHE     A    53   <NA>  1.500  21.332   7.075 1
## 404    ATOM   404   CE2 <NA>   PHE     A    53   <NA>  1.327  23.302   8.496 1
## 405    ATOM   405    CZ <NA>   PHE     A    53   <NA>  1.290  22.718   7.212 1

## 406    ATOM   406     N <NA>   ILE     A    54   <NA>  4.483  20.969  12.792 1
## 407    ATOM   407    CA <NA>   ILE     A    54   <NA>  4.689  21.005  14.248 1
## 408    ATOM   408     C <NA>   ILE     A    54   <NA>  3.921  22.179  14.858 1
## 409    ATOM   409     O <NA>   ILE     A    54   <NA>  3.575  23.139  14.182 1
## 410    ATOM   410    CB <NA>   ILE     A    54   <NA>  6.199  21.155  14.625 1
## 411    ATOM   411   CG1 <NA>   ILE     A    54   <NA>  6.796  22.408  13.939 1
## 412    ATOM   412   CG2 <NA>   ILE     A    54   <NA>  6.967  19.888  14.203 1
## 413    ATOM   413   CD1 <NA>   ILE     A    54   <NA>  8.110  22.821  14.465 1
## 414    ATOM   414     N <NA>   LYS     A    55   <NA>  3.632  22.095  16.145 1
## 415    ATOM   415    CA <NA>   LYS     A    55   <NA>  2.968  23.196  16.823 1
## 416    ATOM   416     C <NA>   LYS     A    55   <NA>  4.038  24.093  17.449 1
## 417    ATOM   417     O <NA>   LYS     A    55   <NA>  4.949  23.610  18.157 1
## 418    ATOM   418    CB <NA>   LYS     A    55   <NA>  2.021  22.661  17.895 1
## 419    ATOM   419    CG <NA>   LYS     A    55   <NA>  0.974  23.665  18.300 1
## 420    ATOM   420    CD <NA>   LYS     A    55   <NA>  0.006  23.101  19.304 1
## 421    ATOM   421    CE <NA>   LYS     A    55   <NA> -0.580  24.217  20.149 1
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## 422    ATOM   422    NZ <NA>   LYS     A    55   <NA>  0.439  24.751  21.104 1
## 423    ATOM   423     N <NA>   VAL     A    56   <NA>  3.953  25.391  17.185 1
## 424    ATOM   424    CA <NA>   VAL     A    56   <NA>  4.927  26.319  17.754 1
## 425    ATOM   425     C <NA>   VAL     A    56   <NA>  4.225  27.378  18.556 1
## 426    ATOM   426     O <NA>   VAL     A    56   <NA>  3.023  27.557  18.455 1
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## 428    ATOM   428   CG1 <NA>   VAL     A    56   <NA>  6.791  26.027  16.120 1
## 429    ATOM   429   CG2 <NA>   VAL     A    56   <NA>  4.881  27.551  15.567 1
## 430    ATOM   430     N <NA>   ARG     A    57   <NA>  4.978  28.079  19.377 1
## 431    ATOM   431    CA <NA>   ARG     A    57   <NA>  4.459  29.271  20.026 1
## 432    ATOM   432     C <NA>   ARG     A    57   <NA>  5.038  30.502  19.335 1
## 433    ATOM   433     O <NA>   ARG     A    57   <NA>  6.242  30.596  19.138 1
## 434    ATOM   434    CB <NA>   ARG     A    57   <NA>  4.824  29.245  21.505 1
## 435    ATOM   435    CG <NA>   ARG     A    57   <NA>  4.168  28.102  22.260 1
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## 439    ATOM   439   NH1 <NA>   ARG     A    57   <NA>  6.825  29.532  24.678 1
## 440    ATOM   440   NH2 <NA>   ARG     A    57   <NA>  8.223  27.723  24.467 1
## 441    ATOM   441     N <NA>   GLN     A    58   <NA>  4.171  31.431  18.958 1
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## 446    ATOM   446    CG <NA>   GLN     A    58   <NA>  3.736  34.104  16.321 1
## 447    ATOM   447    CD <NA>   GLN     A    58   <NA>  2.500  34.473  15.541 1
## 448    ATOM   448   OE1 <NA>   GLN     A    58   <NA>  1.530  33.703  15.489 1
## 449    ATOM   449   NE2 <NA>   GLN     A    58   <NA>  2.508  35.651  14.940 1
## 450    ATOM   450     N <NA>   TYR     A    59   <NA>  5.883  34.378  19.196 1
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## 454    ATOM   454    CB <NA>   TYR     A    59   <NA>  7.354  35.588  20.765 1

## 455    ATOM   455    CG <NA>   TYR     A    59   <NA>  7.213  34.624  21.955 1
## 456    ATOM   456   CD1 <NA>   TYR     A    59   <NA>  7.479  33.237  21.805 1
## 457    ATOM   457   CD2 <NA>   TYR     A    59   <NA>  6.795  35.087  23.223 1
## 458    ATOM   458   CE1 <NA>   TYR     A    59   <NA>  7.345  32.365  22.871 1
## 459    ATOM   459   CE2 <NA>   TYR     A    59   <NA>  6.638  34.224  24.268 1
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## 461    ATOM   461    OH <NA>   TYR     A    59   <NA>  6.967  32.076  25.200 1
## 462    ATOM   462     N <NA>   ASP     A    60   <NA>  5.767  37.940  19.049 1
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## 465    ATOM   465     O <NA>   ASP     A    60   <NA>  7.340  39.951  19.900 1
## 466    ATOM   466    CB <NA>   ASP     A    60   <NA>  4.719  39.777  17.832 1
## 467    ATOM   467    CG <NA>   ASP     A    60   <NA>  3.699  38.899  17.148 1
## 468    ATOM   468   OD1 <NA>   ASP     A    60   <NA>  3.989  38.368  16.050 1
## 469    ATOM   469   OD2 <NA>   ASP     A    60   <NA>  2.570  38.799  17.672 1
## 470    ATOM   470     N <NA>   GLN     A    61   <NA>  7.529  40.913  17.896 1
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## 471    ATOM   471    CA <NA>   GLN     A    61   <NA>  8.337  42.060  18.331 1
## 472    ATOM   472     C <NA>   GLN     A    61   <NA>  9.535  41.630  19.179 1
## 473    ATOM   473     O <NA>   GLN     A    61   <NA>  9.777  42.191  20.264 1
## 474    ATOM   474    CB <NA>   GLN     A    61   <NA>  7.471  43.051  19.131 1
## 475    ATOM   475    CG <NA>   GLN     A    61   <NA>  7.718  44.555  18.814 1
## 476    ATOM   476    CD <NA>   GLN     A    61   <NA>  7.182  45.552  19.907 1
## 477    ATOM   477   OE1 <NA>   GLN     A    61   <NA>  7.936  46.461  20.398 1
## 478    ATOM   478   NE2 <NA>   GLN     A    61   <NA>  5.892  45.377  20.306 1
## 479    ATOM   479     N <NA>   ILE     A    62   <NA> 10.283  40.645  18.676 1
## 480    ATOM   480    CA <NA>   ILE     A    62   <NA> 11.484  40.115  19.328 1
## 481    ATOM   481     C <NA>   ILE     A    62   <NA> 12.745  40.584  18.614 1
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## 484    ATOM   484   CG1 <NA>   ILE     A    62   <NA> 10.152  38.035  19.930 1
## 485    ATOM   485   CG2 <NA>   ILE     A    62   <NA> 12.688  37.973  20.027 1
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## 488    ATOM   488    CA <NA>   LEU     A    63   <NA> 15.038  41.476  18.822 1
## 489    ATOM   489     C <NA>   LEU     A    63   <NA> 16.033  40.304  18.862 1
## 490    ATOM   490     O <NA>   LEU     A    63   <NA> 16.195  39.661  19.897 1
## 491    ATOM   491    CB <NA>   LEU     A    63   <NA> 15.631  42.666  19.619 1
## 492    ATOM   492    CG <NA>   LEU     A    63   <NA> 16.776  43.426  18.914 1
## 493    ATOM   493   CD1 <NA>   LEU     A    63   <NA> 16.560  44.922  18.993 1
## 494    ATOM   494   CD2 <NA>   LEU     A    63   <NA> 18.103  43.062  19.558 1
## 495    ATOM   495     N <NA>   ILE     A    64   <NA> 16.686  40.036  17.738 1
## 496    ATOM   496    CA <NA>   ILE     A    64   <NA> 17.760  39.039  17.653 1
## 497    ATOM   497     C <NA>   ILE     A    64   <NA> 18.991  39.753  17.116 1
## 498    ATOM   498     O <NA>   ILE     A    64   <NA> 18.862  40.632  16.288 1
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## 500    ATOM   500   CG1 <NA>   ILE     A    64   <NA> 16.127  37.137  17.110 1
## 501    ATOM   501   CG2 <NA>   ILE     A    64   <NA> 18.551  36.857  16.518 1
## 502    ATOM   502   CD1 <NA>   ILE     A    64   <NA> 16.194  35.643  16.885 1
## 503    ATOM   503     N <NA>   GLU     A    65   <NA> 20.181  39.387  17.573 1

## 504    ATOM   504    CA <NA>   GLU     A    65   <NA> 21.406  39.983  17.036 1
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## 509    ATOM   509    CD <NA>   GLU     A    65   <NA> 23.228  42.558  19.187 1
## 510    ATOM   510   OE1 <NA>   GLU     A    65   <NA> 24.094  42.925  18.348 1
## 511    ATOM   511   OE2 <NA>   GLU     A    65   <NA> 23.348  42.730  20.429 1
## 512    ATOM   512     N <NA>   ILE     A    66   <NA> 22.148  39.215  14.823 1
## 513    ATOM   513    CA <NA>   ILE     A    66   <NA> 22.818  38.327  13.863 1
## 514    ATOM   514     C <NA>   ILE     A    66   <NA> 24.123  38.945  13.303 1
## 515    ATOM   515     O <NA>   ILE     A    66   <NA> 24.114  39.903  12.521 1
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## 517    ATOM   517   CG1 <NA>   ILE     A    66   <NA> 20.481  37.516  13.278 1
## 518    ATOM   518   CG2 <NA>   ILE     A    66   <NA> 22.444  36.880  11.799 1
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## 524    ATOM   524    CB <NA>   CYS     A    67   <NA> 26.907  38.497  11.905 1
## 525    ATOM   525    SG <NA>   CYS     A    67   <NA> 27.274  36.734  11.705 1
## 526    ATOM   526     N <NA>   GLY     A    68   <NA> 26.239  40.887  14.650 1
## 527    ATOM   527    CA <NA>   GLY     A    68   <NA> 26.319  42.307  14.938 1
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## 535    ATOM   535    CG <NA>   HIS     A    69   <NA> 24.157  43.172  10.639 1
## 536    ATOM   536   ND1 <NA>   HIS     A    69   <NA> 25.294  42.398  10.762 1
## 537    ATOM   537   CD2 <NA>   HIS     A    69   <NA> 24.283  43.886   9.518 1
## 538    ATOM   538   CE1 <NA>   HIS     A    69   <NA> 26.075  42.630   9.723 1
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## 544    ATOM   544    CB <NA>   LYS     A    70   <NA> 19.667  45.075  15.840 1
## 545    ATOM   545    CG <NA>   LYS     A    70   <NA> 20.422  45.141  17.154 1
## 546    ATOM   546    CD <NA>   LYS     A    70   <NA> 19.885  46.281  18.036 1
## 547    ATOM   547    CE <NA>   LYS     A    70   <NA> 20.905  46.699  19.095 1
## 548    ATOM   548    NZ <NA>   LYS     A    70   <NA> 20.376  47.817  19.946 1
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## 553    ATOM   553    CB <NA>   ALA     A    71   <NA> 16.937  41.464  12.683 1
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## 555    ATOM   555    CA <NA>   ILE     A    72   <NA> 13.233  42.663  15.111 1
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## 557    ATOM   557     O <NA>   ILE     A    72   <NA> 12.083  42.266  13.025 1
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## 559    ATOM   559   CG1 <NA>   ILE     A    72   <NA> 13.664  44.777  16.446 1
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## 610    ATOM   610    CB <NA>   THR     A    80   <NA> 13.031  23.467  15.319 1
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## 614    ATOM   614    CA <NA>   PRO     A    81   <NA> 16.233  20.170  15.766 1
## 615    ATOM   615     C <NA>   PRO     A    81   <NA> 17.352  21.205  15.795 1
## 616    ATOM   616     O <NA>   PRO     A    81   <NA> 18.306  21.085  16.567 1
## 617    ATOM   617    CB <NA>   PRO     A    81   <NA> 16.467  19.139  14.669 1
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## 619    ATOM   619    CD <NA>   PRO     A    81   <NA> 14.331  20.114  14.238 1
## 620    ATOM   620     N <NA>   VAL     A    82   <NA> 17.220  22.219  14.948 1
## 621    ATOM   621    CA <NA>   VAL     A    82   <NA> 18.236  23.243  14.762 1
## 622    ATOM   622     C <NA>   VAL     A    82   <NA> 17.549  24.626  14.801 1
## 623    ATOM   623     O <NA>   VAL     A    82   <NA> 16.328  24.735  14.569 1
## 624    ATOM   624    CB <NA>   VAL     A    82   <NA> 18.969  23.017  13.388 1
## 625    ATOM   625   CG1 <NA>   VAL     A    82   <NA> 18.009  22.769  12.263 1
## 626    ATOM   626   CG2 <NA>   VAL     A    82   <NA> 19.843  24.144  13.080 1
## 627    ATOM   627     N <NA>   ASN     A    83   <NA> 18.292  25.671  15.167 1
## 628    ATOM   628    CA <NA>   ASN     A    83   <NA> 17.731  27.051  15.193 1
## 629    ATOM   629     C <NA>   ASN     A    83   <NA> 17.799  27.628  13.799 1
## 630    ATOM   630     O <NA>   ASN     A    83   <NA> 18.794  27.456  13.113 1
## 631    ATOM   631    CB <NA>   ASN     A    83   <NA> 18.508  27.950  16.161 1
## 632    ATOM   632    CG <NA>   ASN     A    83   <NA> 18.236  27.600  17.636 1
## 633    ATOM   633   OD1 <NA>   ASN     A    83   <NA> 17.102  27.381  18.051 1
## 634    ATOM   634   ND2 <NA>   ASN     A    83   <NA> 19.287  27.475  18.398 1
## 635    ATOM   635     N <NA>   ILE     A    84   <NA> 16.729  28.283  13.370 1
## 636    ATOM   636    CA <NA>   ILE     A    84   <NA> 16.588  28.651  11.955 1
## 637    ATOM   637     C <NA>   ILE     A    84   <NA> 16.190  30.132  11.811 1
## 638    ATOM   638     O <NA>   ILE     A    84   <NA> 15.178  30.600  12.384 1
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## 640    ATOM   640   CG1 <NA>   ILE     A    84   <NA> 16.049  26.365  11.040 1
## 641    ATOM   641   CG2 <NA>   ILE     A    84   <NA> 15.081  28.324   9.932 1
## 642    ATOM   642   CD1 <NA>   ILE     A    84   <NA> 14.957  25.345  11.321 1
## 643    ATOM   643     N <NA>   ILE     A    85   <NA> 16.991  30.863  11.053 1
## 644    ATOM   644    CA <NA>   ILE     A    85   <NA> 16.710  32.257  10.821 1
## 645    ATOM   645     C <NA>   ILE     A    85   <NA> 16.155  32.252   9.420 1
## 646    ATOM   646     O <NA>   ILE     A    85   <NA> 16.857  31.950   8.464 1
## 647    ATOM   647    CB <NA>   ILE     A    85   <NA> 17.999  33.119  10.844 1
## 648    ATOM   648   CG1 <NA>   ILE     A    85   <NA> 18.724  32.983  12.207 1
## 649    ATOM   649   CG2 <NA>   ILE     A    85   <NA> 17.653  34.600  10.517 1
## 650    ATOM   650   CD1 <NA>   ILE     A    85   <NA> 17.830  33.204  13.418 1

## 651    ATOM   651     N <NA>   GLY     A    86   <NA> 14.888  32.608   9.302 1
## 652    ATOM   652    CA <NA>   GLY     A    86   <NA> 14.238  32.655   8.011 1
## 653    ATOM   653     C <NA>   GLY     A    86   <NA> 14.181  34.034   7.393 1
## 654    ATOM   654     O <NA>   GLY     A    86   <NA> 14.714  34.991   7.894 1
## 655    ATOM   655     N <NA>   ARG     A    87   <NA> 13.398  34.131   6.334 1
## 656    ATOM   656    CA <NA>   ARG     A    87   <NA> 13.370  35.302   5.456 1
## 657    ATOM   657     C <NA>   ARG     A    87   <NA> 12.931  36.548   6.216 1
## 658    ATOM   658     O <NA>   ARG     A    87   <NA> 13.429  37.633   5.958 1
## 659    ATOM   659    CB <NA>   ARG     A    87   <NA> 12.459  35.018   4.263 1
## 660    ATOM   660    CG <NA>   ARG     A    87   <NA> 13.030  34.044   3.318 1
## 661    ATOM   661    CD <NA>   ARG     A    87   <NA> 12.310  34.101   1.966 1
## 662    ATOM   662    NE <NA>   ARG     A    87   <NA> 10.903  33.713   2.088 1
## 663    ATOM   663    CZ <NA>   ARG     A    87   <NA>  9.899  34.575   2.137 1
## 664    ATOM   664   NH1 <NA>   ARG     A    87   <NA> 10.126  35.860   1.922 1
## 665    ATOM   665   NH2 <NA>   ARG     A    87   <NA>  8.657  34.143   2.300 1
## 666    ATOM   666     N <NA>   ASN     A    88   <NA> 12.063  36.352   7.198 1
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## 667    ATOM   667    CA <NA>   ASN     A    88   <NA> 11.458  37.455   7.919 1
## 668    ATOM   668     C <NA>   ASN     A    88   <NA> 12.511  38.266   8.653 1
## 669    ATOM   669     O <NA>   ASN     A    88   <NA> 12.419  39.481   8.723 1
## 670    ATOM   670    CB <NA>   ASN     A    88   <NA> 10.359  36.959   8.863 1
## 671    ATOM   671    CG <NA>   ASN     A    88   <NA> 10.892  36.309  10.125 1
## 672    ATOM   672   OD1 <NA>   ASN     A    88   <NA> 11.577  35.273  10.065 1
## 673    ATOM   673   ND2 <NA>   ASN     A    88   <NA> 10.446  36.809  11.283 1
## 674    ATOM   674     N <NA>   LEU     A    89   <NA> 13.551  37.601   9.136 1
## 675    ATOM   675    CA <NA>   LEU     A    89   <NA> 14.633  38.337   9.729 1
## 676    ATOM   676     C <NA>   LEU     A    89   <NA> 15.802  38.487   8.783 1
## 677    ATOM   677     O <NA>   LEU     A    89   <NA> 16.580  39.394   8.941 1
## 678    ATOM   678    CB <NA>   LEU     A    89   <NA> 15.096  37.687  11.029 1
## 679    ATOM   679    CG <NA>   LEU     A    89   <NA> 14.146  37.555  12.221 1
## 680    ATOM   680   CD1 <NA>   LEU     A    89   <NA> 14.939  37.022  13.434 1
## 681    ATOM   681   CD2 <NA>   LEU     A    89   <NA> 13.508  38.913  12.527 1
## 682    ATOM   682     N <NA>   LEU     A    90   <NA> 15.910  37.651   7.761 1
## 683    ATOM   683    CA <NA>   LEU     A    90   <NA> 17.078  37.773   6.865 1
## 684    ATOM   684     C <NA>   LEU     A    90   <NA> 17.048  39.068   6.049 1
## 685    ATOM   685     O <NA>   LEU     A    90   <NA> 18.098  39.613   5.652 1
## 686    ATOM   686    CB <NA>   LEU     A    90   <NA> 17.200  36.561   5.913 1
## 687    ATOM   687    CG <NA>   LEU     A    90   <NA> 17.754  35.226   6.440 1
## 688    ATOM   688   CD1 <NA>   LEU     A    90   <NA> 17.798  34.207   5.340 1
## 689    ATOM   689   CD2 <NA>   LEU     A    90   <NA> 19.138  35.441   7.022 1
## 690    ATOM   690     N <NA>   THR     A    91   <NA> 15.835  39.547   5.808 1
## 691    ATOM   691    CA <NA>   THR     A    91   <NA> 15.653  40.738   4.985 1
## 692    ATOM   692     C <NA>   THR     A    91   <NA> 16.137  41.999   5.772 1
## 693    ATOM   693     O <NA>   THR     A    91   <NA> 16.848  42.870   5.252 1
## 694    ATOM   694    CB <NA>   THR     A    91   <NA> 14.157  40.860   4.594 1
## 695    ATOM   695   OG1 <NA>   THR     A    91   <NA> 13.342  40.810   5.786 1
## 696    ATOM   696   CG2 <NA>   THR     A    91   <NA> 13.740  39.709   3.681 1
## 697    ATOM   697     N <NA>   GLN     A    92   <NA> 15.842  42.001   7.064 1
## 698    ATOM   698    CA <NA>   GLN     A    92   <NA> 16.170  43.099   7.967 1
## 699    ATOM   699     C <NA>   GLN     A    92   <NA> 17.650  43.315   8.126 1

## 700    ATOM   700     O <NA>   GLN     A    92   <NA> 18.071  44.440   8.459 1
## 701    ATOM   701    CB <NA>   GLN     A    92   <NA> 15.580  42.837   9.347 1
## 702    ATOM   702    CG <NA>   GLN     A    92   <NA> 14.081  42.603   9.325 1
## 703    ATOM   703    CD <NA>   GLN     A    92   <NA> 13.318  43.811   8.800 1
## 704    ATOM   704   OE1 <NA>   GLN     A    92   <NA> 12.836  43.807   7.683 1
## 705    ATOM   705   NE2 <NA>   GLN     A    92   <NA> 13.349  44.892   9.543 1
## 706    ATOM   706     N <NA>   ILE     A    93   <NA> 18.444  42.266   7.913 1
## 707    ATOM   707    CA <NA>   ILE     A    93   <NA> 19.887  42.417   8.035 1
## 708    ATOM   708     C <NA>   ILE     A    93   <NA> 20.530  42.555   6.677 1
## 709    ATOM   709     O <NA>   ILE     A    93   <NA> 21.744  42.639   6.577 1
## 710    ATOM   710    CB <NA>   ILE     A    93   <NA> 20.557  41.231   8.872 1
## 711    ATOM   711   CG1 <NA>   ILE     A    93   <NA> 20.472  39.878   8.113 1
## 712    ATOM   712   CG2 <NA>   ILE     A    93   <NA> 19.926  41.182  10.272 1
## 713    ATOM   713   CD1 <NA>   ILE     A    93   <NA> 21.520  38.796   8.533 1
## 714    ATOM   714     N <NA>   GLY     A    94   <NA> 19.713  42.563   5.636 1
## 715    ATOM   715    CA <NA>   GLY     A    94   <NA> 20.226  42.870   4.327 1
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## 716    ATOM   716     C <NA>   GLY     A    94   <NA> 20.843  41.689   3.611 1
## 717    ATOM   717     O <NA>   GLY     A    94   <NA> 21.680  41.866   2.723 1
## 718    ATOM   718     N <NA>   CYS     A    95   <NA> 20.294  40.507   3.844 1
## 719    ATOM   719    CA <NA>   CYS     A    95   <NA> 20.890  39.296   3.297 1
## 720    ATOM   720     C <NA>   CYS     A    95   <NA> 20.407  39.005   1.897 1
## 721    ATOM   721     O <NA>   CYS     A    95   <NA> 19.217  39.101   1.606 1
## 722    ATOM   722    CB <NA>   CYS     A    95   <NA> 20.585  38.134   4.215 1
## 723    ATOM   723    SG <NA>   CYS     A    95   <NA> 21.505  36.663   3.848 1
## 724    ATOM   724     N <NA>   THR     A    96   <NA> 21.339  38.698   1.005 1
## 725    ATOM   725    CA <NA>   THR     A    96   <NA> 20.969  38.276  -0.346 1
## 726    ATOM   726     C <NA>   THR     A    96   <NA> 21.721  37.024  -0.758 1
## 727    ATOM   727     O <NA>   THR     A    96   <NA> 22.753  36.645  -0.178 1
## 728    ATOM   728    CB <NA>   THR     A    96   <NA> 21.298  39.331  -1.459 1
## 729    ATOM   729   OG1 <NA>   THR     A    96   <NA> 22.688  39.698  -1.364 1
## 730    ATOM   730   CG2 <NA>   THR     A    96   <NA> 20.405  40.560  -1.303 1
## 731    ATOM   731     N <NA>   LEU     A    97   <NA> 21.183  36.413  -1.805 1
## 732    ATOM   732    CA <NA>   LEU     A    97   <NA> 21.718  35.228  -2.473 1
## 733    ATOM   733     C <NA>   LEU     A    97   <NA> 22.314  35.753  -3.779 1
## 734    ATOM   734     O <NA>   LEU     A    97   <NA> 21.616  36.396  -4.577 1
## 735    ATOM   735    CB <NA>   LEU     A    97   <NA> 20.518  34.349  -2.810 1
## 736    ATOM   736    CG <NA>   LEU     A    97   <NA> 20.318  32.897  -2.464 1
## 737    ATOM   737   CD1 <NA>   LEU     A    97   <NA> 21.285  32.388  -1.422 1
## 738    ATOM   738   CD2 <NA>   LEU     A    97   <NA> 18.896  32.782  -2.010 1
## 739    ATOM   739     N <NA>   ASN     A    98   <NA> 23.577  35.469  -4.026 1
## 740    ATOM   740    CA <NA>   ASN     A    98   <NA> 24.207  35.904  -5.257 1
## 741    ATOM   741     C <NA>   ASN     A    98   <NA> 24.863  34.748  -5.999 1
## 742    ATOM   742     O <NA>   ASN     A    98   <NA> 25.635  33.982  -5.396 1
## 743    ATOM   743    CB <NA>   ASN     A    98   <NA> 25.229  36.991  -4.938 1
## 744    ATOM   744    CG <NA>   ASN     A    98   <NA> 24.609  38.190  -4.212 1
## 745    ATOM   745   OD1 <NA>   ASN     A    98   <NA> 24.263  38.112  -3.019 1
## 746    ATOM   746   ND2 <NA>   ASN     A    98   <NA> 24.354  39.252  -4.955 1
## 747    ATOM   747     N <NA>   PHE     A    99   <NA> 24.539  34.602  -7.287 1
## 748    ATOM   748    CA <NA>   PHE     A    99   <NA> 25.376  33.754  -8.172 1

## 749    ATOM   749     C <NA>   PHE     A    99   <NA> 25.726  34.383  -9.544 1
## 750    ATOM   750     O <NA>   PHE     A    99   <NA> 24.797  34.890 -10.226 1
## 751    ATOM   751    CB <NA>   PHE     A    99   <NA> 24.743  32.354  -8.375 1
## 752    ATOM   752    CG <NA>   PHE     A    99   <NA> 23.328  32.389  -8.856 1
## 753    ATOM   753   CD1 <NA>   PHE     A    99   <NA> 22.303  32.588  -7.961 1
## 754    ATOM   754   CD2 <NA>   PHE     A    99   <NA> 23.029  32.118 -10.181 1
## 755    ATOM   755   CE1 <NA>   PHE     A    99   <NA> 21.000  32.515  -8.357 1
## 756    ATOM   756   CE2 <NA>   PHE     A    99   <NA> 21.730  32.028 -10.613 1
## 757    ATOM   757    CZ <NA>   PHE     A    99   <NA> 20.700  32.221  -9.700 1
## 758    ATOM   759     N <NA>   PRO     B     1   <NA> 22.659  36.727 -10.823 1
## 759    ATOM   760    CA <NA>   PRO     B     1   <NA> 21.708  37.741 -10.269 1
## 760    ATOM   761     C <NA>   PRO     B     1   <NA> 21.931  37.939  -8.779 1
## 761    ATOM   762     O <NA>   PRO     B     1   <NA> 22.755  37.283  -8.190 1
## 762    ATOM   763    CB <NA>   PRO     B     1   <NA> 20.263  37.289 -10.512 1
## 763    ATOM   764    CG <NA>   PRO     B     1   <NA> 20.385  35.811 -10.891 1
## 764    ATOM   765    CD <NA>   PRO     B     1   <NA> 21.753  35.755 -11.555 1
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## 765    ATOM   766     N <NA>   GLN     B     2   <NA> 21.203  38.873  -8.191 1
## 766    ATOM   767    CA <NA>   GLN     B     2   <NA> 21.156  39.043  -6.744 1
## 767    ATOM   768     C <NA>   GLN     B     2   <NA> 19.698  38.882  -6.389 1
## 768    ATOM   769     O <NA>   GLN     B     2   <NA> 18.850  39.538  -6.975 1
## 769    ATOM   770    CB <NA>   GLN     B     2   <NA> 21.625  40.447  -6.329 1
## 770    ATOM   771    CG <NA>   GLN     B     2   <NA> 21.353  40.777  -4.865 1
## 771    ATOM   772    CD <NA>   GLN     B     2   <NA> 22.139  41.975  -4.358 1
## 772    ATOM   773   OE1 <NA>   GLN     B     2   <NA> 21.577  42.881  -3.752 1
## 773    ATOM   774   NE2 <NA>   GLN     B     2   <NA> 23.450  41.976  -4.586 1
## 774    ATOM   775     N <NA>   ILE     B     3   <NA> 19.405  38.008  -5.448 1
## 775    ATOM   776    CA <NA>   ILE     B     3   <NA> 18.037  37.742  -5.100 1
## 776    ATOM   777     C <NA>   ILE     B     3   <NA> 17.832  38.164  -3.660 1
## 777    ATOM   778     O <NA>   ILE     B     3   <NA> 18.457  37.631  -2.746 1
## 778    ATOM   779    CB <NA>   ILE     B     3   <NA> 17.694  36.224  -5.238 1
## 779    ATOM   780   CG1 <NA>   ILE     B     3   <NA> 17.788  35.772  -6.692 1
## 780    ATOM   781   CG2 <NA>   ILE     B     3   <NA> 16.284  35.967  -4.750 1
## 781    ATOM   782   CD1 <NA>   ILE     B     3   <NA> 18.183  34.327  -6.802 1
## 782    ATOM   783     N <NA>   THR     B     4   <NA> 16.960  39.132  -3.461 1
## 783    ATOM   784    CA <NA>   THR     B     4   <NA> 16.635  39.571  -2.117 1
## 784    ATOM   785     C <NA>   THR     B     4   <NA> 15.555  38.634  -1.627 1
## 785    ATOM   786     O <NA>   THR     B     4   <NA> 15.066  37.784  -2.372 1
## 786    ATOM   787    CB <NA>   THR     B     4   <NA> 16.147  41.074  -2.110 1
## 787    ATOM   788   OG1 <NA>   THR     B     4   <NA> 15.093  41.256  -3.079 1
## 788    ATOM   789   CG2 <NA>   THR     B     4   <NA> 17.283  42.019  -2.472 1
## 789    ATOM   790     N <NA>   LEU     B     5   <NA> 15.157  38.761  -0.379 1
## 790    ATOM   791    CA <NA>   LEU     B     5   <NA> 14.466  37.636   0.259 1
## 791    ATOM   792     C <NA>   LEU     B     5   <NA> 13.125  38.065   0.821 1
## 792    ATOM   793     O <NA>   LEU     B     5   <NA> 12.585  37.446   1.733 1
## 793    ATOM   794    CB <NA>   LEU     B     5   <NA> 15.340  37.047   1.374 1
## 794    ATOM   795    CG <NA>   LEU     B     5   <NA> 16.622  36.365   0.892 1
## 795    ATOM   796   CD1 <NA>   LEU     B     5   <NA> 17.455  35.953   2.080 1
## 796    ATOM   797   CD2 <NA>   LEU     B     5   <NA> 16.248  35.136  -0.006 1
## 797    ATOM   798     N <NA>   TRP     B     6   <NA> 12.567  39.127   0.262 1

## 798    ATOM   799    CA <NA>   TRP     B     6   <NA> 11.260  39.582   0.682 1
## 799    ATOM   800     C <NA>   TRP     B     6   <NA> 10.196  38.601   0.218 1
## 800    ATOM   801     O <NA>   TRP     B     6   <NA>  9.192  38.404   0.903 1
## 801    ATOM   802    CB <NA>   TRP     B     6   <NA> 11.004  40.992   0.135 1
## 802    ATOM   803    CG <NA>   TRP     B     6   <NA> 12.065  42.014   0.478 1
## 803    ATOM   804   CD1 <NA>   TRP     B     6   <NA> 13.157  42.366  -0.279 1
## 804    ATOM   805   CD2 <NA>   TRP     B     6   <NA> 12.209  42.716   1.739 1
## 805    ATOM   806   NE1 <NA>   TRP     B     6   <NA> 13.979  43.196   0.470 1
## 806    ATOM   807   CE2 <NA>   TRP     B     6   <NA> 13.433  43.441   1.686 1
## 807    ATOM   808   CE3 <NA>   TRP     B     6   <NA> 11.443  42.805   2.913 1
## 808    ATOM   809   CZ2 <NA>   TRP     B     6   <NA> 13.914  44.211   2.785 1
## 809    ATOM   810   CZ3 <NA>   TRP     B     6   <NA> 11.903  43.585   3.953 1
## 810    ATOM   811   CH2 <NA>   TRP     B     6   <NA> 13.148  44.273   3.896 1
## 811    ATOM   812     N <NA>   GLN     B     7   <NA> 10.396  38.008  -0.958 1
## 812    ATOM   813    CA <NA>   GLN     B     7   <NA>  9.518  36.960  -1.516 1
## 813    ATOM   814     C <NA>   GLN     B     7   <NA> 10.321  35.670  -1.433 1
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## 814    ATOM   815     O <NA>   GLN     B     7   <NA> 11.546  35.694  -1.298 1
## 815    ATOM   816    CB <NA>   GLN     B     7   <NA>  9.215  37.238  -3.000 1
## 816    ATOM   817    CG <NA>   GLN     B     7   <NA>  8.278  38.433  -3.326 1
## 817    ATOM   818    CD <NA>   GLN     B     7   <NA>  7.629  38.332  -4.744 1
## 818    ATOM   819   OE1 <NA>   GLN     B     7   <NA>  8.319  38.100  -5.754 1
## 819    ATOM   820   NE2 <NA>   GLN     B     7   <NA>  6.307  38.532  -4.814 1
## 820    ATOM   821     N <NA>   ARG     B     8   <NA>  9.661  34.528  -1.525 1
## 821    ATOM   822    CA <NA>   ARG     B     8   <NA> 10.385  33.251  -1.642 1
## 822    ATOM   823     C <NA>   ARG     B     8   <NA> 11.348  33.305  -2.780 1
## 823    ATOM   824     O <NA>   ARG     B     8   <NA> 10.964  33.682  -3.906 1
## 824    ATOM   825    CB <NA>   ARG     B     8   <NA>  9.435  32.061  -1.862 1
## 825    ATOM   826    CG <NA>   ARG     B     8   <NA>  8.623  31.716  -0.644 1
## 826    ATOM   827    CD <NA>   ARG     B     8   <NA>  7.828  30.471  -0.844 1
## 827    ATOM   828    NE <NA>   ARG     B     8   <NA>  7.143  30.102   0.378 1
## 828    ATOM   829    CZ <NA>   ARG     B     8   <NA>  6.523  28.938   0.561 1
## 829    ATOM   830   NH1 <NA>   ARG     B     8   <NA>  6.476  28.028  -0.411 1
## 830    ATOM   831   NH2 <NA>   ARG     B     8   <NA>  5.925  28.688   1.719 1
## 831    ATOM   832     N <NA>   PRO     B     9   <NA> 12.533  32.711  -2.598 1
## 832    ATOM   833    CA <NA>   PRO     B     9   <NA> 13.443  32.743  -3.746 1
## 833    ATOM   834     C <NA>   PRO     B     9   <NA> 13.174  31.592  -4.703 1
## 834    ATOM   835     O <NA>   PRO     B     9   <NA> 13.897  30.587  -4.698 1
## 835    ATOM   836    CB <NA>   PRO     B     9   <NA> 14.813  32.658  -3.125 1
## 836    ATOM   837    CG <NA>   PRO     B     9   <NA> 14.564  31.823  -1.917 1
## 837    ATOM   838    CD <NA>   PRO     B     9   <NA> 13.238  32.289  -1.373 1
## 838    ATOM   839     N <NA>   LEU     B    10   <NA> 12.134  31.727  -5.504 1
## 839    ATOM   840    CA <NA>   LEU     B    10   <NA> 11.816  30.740  -6.534 1
## 840    ATOM   841     C <NA>   LEU     B    10   <NA> 12.459  31.075  -7.877 1
## 841    ATOM   842     O <NA>   LEU     B    10   <NA> 12.274  32.150  -8.406 1
## 842    ATOM   843    CB <NA>   LEU     B    10   <NA> 10.303  30.637  -6.738 1
## 843    ATOM   844    CG <NA>   LEU     B    10   <NA>  9.483  30.307  -5.497 1
## 844    ATOM   845   CD1 <NA>   LEU     B    10   <NA>  8.028  30.334  -5.876 1
## 845    ATOM   846   CD2 <NA>   LEU     B    10   <NA>  9.845  28.975  -4.951 1
## 846    ATOM   847     N <NA>   VAL     B    11   <NA> 13.225  30.141  -8.420 1

## 847    ATOM   848    CA <NA>   VAL     B    11   <NA> 13.759  30.227  -9.768 1
## 848    ATOM   849     C <NA>   VAL     B    11   <NA> 13.103  29.153 -10.641 1
## 849    ATOM   850     O <NA>   VAL     B    11   <NA> 12.381  28.285 -10.135 1
## 850    ATOM   851    CB <NA>   VAL     B    11   <NA> 15.253  29.988  -9.735 1
## 851    ATOM   852   CG1 <NA>   VAL     B    11   <NA> 15.898  31.108  -8.939 1
## 852    ATOM   853   CG2 <NA>   VAL     B    11   <NA> 15.573  28.635  -9.104 1
## 853    ATOM   854     N <NA>   THR     B    12   <NA> 13.346  29.214 -11.949 1
## 854    ATOM   855    CA <NA>   THR     B    12   <NA> 12.809  28.220 -12.873 1
## 855    ATOM   856     C <NA>   THR     B    12   <NA> 13.951  27.253 -13.210 1
## 856    ATOM   857     O <NA>   THR     B    12   <NA> 15.089  27.656 -13.442 1
## 857    ATOM   858    CB <NA>   THR     B    12   <NA> 12.259  28.907 -14.158 1
## 858    ATOM   859   OG1 <NA>   THR     B    12   <NA> 11.693  27.933 -15.028 1
## 859    ATOM   860   CG2 <NA>   THR     B    12   <NA> 13.341  29.639 -14.925 1
## 860    ATOM   861     N <NA>   ILE     B    13   <NA> 13.684  25.961 -13.124 1
## 861    ATOM   862    CA <NA>   ILE     B    13   <NA> 14.708  24.966 -13.446 1
## 862    ATOM   863     C <NA>   ILE     B    13   <NA> 14.230  24.165 -14.639 1
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## 863    ATOM   864     O <NA>   ILE     B    13   <NA> 13.014  24.057 -14.918 1
## 864    ATOM   865    CB <NA>   ILE     B    13   <NA> 14.993  23.953 -12.269 1
## 865    ATOM   866   CG1 <NA>   ILE     B    13   <NA> 13.699  23.190 -11.870 1
## 866    ATOM   867   CG2 <NA>   ILE     B    13   <NA> 15.564  24.705 -11.094 1
## 867    ATOM   868   CD1 <NA>   ILE     B    13   <NA> 13.900  22.077 -10.834 1
## 868    ATOM   869     N <NA>   LYS     B    14   <NA> 15.186  23.630 -15.378 1
## 869    ATOM   870    CA <NA>   LYS     B    14   <NA> 14.828  22.733 -16.464 1
## 870    ATOM   871     C <NA>   LYS     B    14   <NA> 15.482  21.387 -16.141 1
## 871    ATOM   872     O <NA>   LYS     B    14   <NA> 16.690  21.305 -15.886 1
## 872    ATOM   873    CB <NA>   LYS     B    14   <NA> 15.340  23.256 -17.814 1
## 873    ATOM   874    CG <NA>   LYS     B    14   <NA> 14.868  22.447 -18.992 1
## 874    ATOM   875    CD <NA>   LYS     B    14   <NA> 14.687  23.295 -20.194 1
## 875    ATOM   876    CE <NA>   LYS     B    14   <NA> 15.979  23.453 -20.922 1
## 876    ATOM   877    NZ <NA>   LYS     B    14   <NA> 15.739  23.451 -22.389 1
## 877    ATOM   878     N <NA>   ILE     B    15   <NA> 14.660  20.354 -16.136 1
## 878    ATOM   879    CA <NA>   ILE     B    15   <NA> 15.108  18.999 -15.906 1
## 879    ATOM   880     C <NA>   ILE     B    15   <NA> 14.188  18.067 -16.702 1
## 880    ATOM   881     O <NA>   ILE     B    15   <NA> 12.968  18.199 -16.719 1
## 881    ATOM   882    CB <NA>   ILE     B    15   <NA> 15.090  18.663 -14.360 1
## 882    ATOM   883   CG1 <NA>   ILE     B    15   <NA> 15.694  17.283 -14.101 1
## 883    ATOM   884   CG2 <NA>   ILE     B    15   <NA> 13.682  18.760 -13.780 1
## 884    ATOM   885   CD1 <NA>   ILE     B    15   <NA> 16.011  17.036 -12.625 1
## 885    ATOM   886     N <NA>   GLY     B    16   <NA> 14.799  17.159 -17.438 1
## 886    ATOM   887    CA <NA>   GLY     B    16   <NA> 14.024  16.279 -18.286 1
## 887    ATOM   888     C <NA>   GLY     B    16   <NA> 13.311  17.029 -19.391 1
## 888    ATOM   889     O <NA>   GLY     B    16   <NA> 12.318  16.549 -19.924 1
## 889    ATOM   890     N <NA>   GLY     B    17   <NA> 13.887  18.145 -19.823 1
## 890    ATOM   891    CA <NA>   GLY     B    17   <NA> 13.243  18.938 -20.850 1
## 891    ATOM   892     C <NA>   GLY     B    17   <NA> 12.009  19.638 -20.345 1
## 892    ATOM   893     O <NA>   GLY     B    17   <NA> 11.392  20.369 -21.084 1
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## 894    ATOM   895    CA <NA>   GLN     B    18   <NA> 10.572  20.249 -18.515 1
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## 896    ATOM   897     O <NA>   GLN     B    18   <NA> 12.196  21.494 -17.175 1
## 897    ATOM   898    CB <NA>   GLN     B    18   <NA>  9.708  19.388 -17.619 1
## 898    ATOM   899    CG <NA>   GLN     B    18   <NA>  8.936  18.297 -18.309 1
## 899    ATOM   900    CD <NA>   GLN     B    18   <NA>  9.088  16.973 -17.566 1
## 900    ATOM   901   OE1 <NA>   GLN     B    18   <NA>  9.813  16.078 -18.014 1
## 901    ATOM   902   NE2 <NA>   GLN     B    18   <NA>  8.488  16.884 -16.371 1
## 902    ATOM   903     N <NA>   LEU     B    19   <NA> 10.186  22.475 -17.590 1
## 903    ATOM   904    CA <NA>   LEU     B    19   <NA> 10.450  23.647 -16.749 1
## 904    ATOM   905     C <NA>   LEU     B    19   <NA>  9.631  23.511 -15.483 1
## 905    ATOM   906     O <NA>   LEU     B    19   <NA>  8.432  23.277 -15.551 1
## 906    ATOM   907    CB <NA>   LEU     B    19   <NA> 10.010  24.932 -17.474 1
## 907    ATOM   908    CG <NA>   LEU     B    19   <NA> 10.775  25.419 -18.723 1
## 908    ATOM   909   CD1 <NA>   LEU     B    19   <NA> 10.226  26.727 -19.190 1
## 909    ATOM   910   CD2 <NA>   LEU     B    19   <NA> 12.241  25.543 -18.395 1
## 910    ATOM   911     N <NA>   LYS     B    20   <NA> 10.273  23.619 -14.329 1
## 911    ATOM   912    CA <NA>   LYS     B    20   <NA>  9.576  23.583 -13.044 1
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## 912    ATOM   913     C <NA>   LYS     B    20   <NA> 10.018  24.784 -12.260 1
## 913    ATOM   914     O <NA>   LYS     B    20   <NA> 10.998  25.429 -12.605 1
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## 916    ATOM   917    CD <NA>   LYS     B    20   <NA>  9.037  20.289 -13.305 1
## 917    ATOM   918    CE <NA>   LYS     B    20   <NA>  9.400  18.836 -13.595 1
## 918    ATOM   919    NZ <NA>   LYS     B    20   <NA>  9.672  18.102 -12.328 1
## 919    ATOM   920     N <NA>   GLU     B    21   <NA>  9.324  25.048 -11.162 1
## 920    ATOM   921    CA <NA>   GLU     B    21   <NA>  9.705  26.075 -10.199 1
## 921    ATOM   922     C <NA>   GLU     B    21   <NA> 10.311  25.408  -8.990 1
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## 925    ATOM   926    CD <NA>   GLU     B    21   <NA>  7.419  29.111 -10.041 1
## 926    ATOM   927   OE1 <NA>   GLU     B    21   <NA>  6.374  28.877  -9.383 1
## 927    ATOM   928   OE2 <NA>   GLU     B    21   <NA>  7.461  29.911 -11.004 1
## 928    ATOM   929     N <NA>   ALA     B    22   <NA> 11.348  26.008  -8.443 1
## 929    ATOM   930    CA <NA>   ALA     B    22   <NA> 12.025  25.431  -7.271 1
## 930    ATOM   931     C <NA>   ALA     B    22   <NA> 12.472  26.569  -6.331 1
## 931    ATOM   932     O <NA>   ALA     B    22   <NA> 12.709  27.701  -6.765 1
## 932    ATOM   933    CB <NA>   ALA     B    22   <NA> 13.248  24.643  -7.708 1
## 933    ATOM   934     N <NA>   LEU     B    23   <NA> 12.560  26.257  -5.054 1
## 934    ATOM   935    CA <NA>   LEU     B    23   <NA> 13.017  27.151  -4.001 1
## 935    ATOM   936     C <NA>   LEU     B    23   <NA> 14.518  27.005  -3.822 1
## 936    ATOM   937     O <NA>   LEU     B    23   <NA> 15.008  25.915  -3.588 1
## 937    ATOM   938    CB <NA>   LEU     B    23   <NA> 12.330  26.721  -2.741 1
## 938    ATOM   939    CG <NA>   LEU     B    23   <NA> 12.592  27.472  -1.469 1
## 939    ATOM   940   CD1 <NA>   LEU     B    23   <NA> 12.006  28.877  -1.562 1
## 940    ATOM   941   CD2 <NA>   LEU     B    23   <NA> 11.917  26.658  -0.379 1
## 941    ATOM   942     N <NA>   LEU     B    24   <NA> 15.266  28.090  -3.963 1
## 942    ATOM   943    CA <NA>   LEU     B    24   <NA> 16.672  28.114  -3.511 1
## 943    ATOM   944     C <NA>   LEU     B    24   <NA> 16.809  28.098  -1.992 1
## 944    ATOM   945     O <NA>   LEU     B    24   <NA> 16.417  29.019  -1.338 1

## 945    ATOM   946    CB <NA>   LEU     B    24   <NA> 17.416  29.342  -4.065 1
## 946    ATOM   947    CG <NA>   LEU     B    24   <NA> 17.444  29.528  -5.585 1
## 947    ATOM   948   CD1 <NA>   LEU     B    24   <NA> 18.151  30.843  -5.884 1
## 948    ATOM   949   CD2 <NA>   LEU     B    24   <NA> 18.170  28.385  -6.270 1
## 949    ATOM   950     N <NA>   ASP     B    25   <NA> 17.407  27.054  -1.437 1
## 950    ATOM   951    CA <NA>   ASP     B    25   <NA> 17.227  26.751  -0.026 1
## 951    ATOM   952     C <NA>   ASP     B    25   <NA> 18.555  26.446   0.653 1
## 952    ATOM   953     O <NA>   ASP     B    25   <NA> 19.003  25.309   0.692 1
## 953    ATOM   954    CB <NA>   ASP     B    25   <NA> 16.258  25.572   0.084 1
## 954    ATOM   955    CG <NA>   ASP     B    25   <NA> 15.759  25.336   1.493 1
## 955    ATOM   956   OD1 <NA>   ASP     B    25   <NA> 16.399  25.780   2.453 1
## 956    ATOM   957   OD2 <NA>   ASP     B    25   <NA> 14.731  24.675   1.645 1
## 957    ATOM   958     N <NA>   THR     B    26   <NA> 19.163  27.455   1.257 1
## 958    ATOM   959    CA <NA>   THR     B    26   <NA> 20.441  27.290   1.920 1
## 959    ATOM   960     C <NA>   THR     B    26   <NA> 20.319  26.393   3.168 1
## 960    ATOM   961     O <NA>   THR     B    26   <NA> 21.316  25.867   3.637 1
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## 961    ATOM   962    CB <NA>   THR     B    26   <NA> 21.063  28.678   2.282 1
## 962    ATOM   963   OG1 <NA>   THR     B    26   <NA> 20.188  29.407   3.146 1
## 963    ATOM   964   CG2 <NA>   THR     B    26   <NA> 21.279  29.499   1.024 1
## 964    ATOM   965     N <NA>   GLY     B    27   <NA> 19.106  26.199   3.688 1
## 965    ATOM   966    CA <NA>   GLY     B    27   <NA> 18.957  25.372   4.876 1
## 966    ATOM   967     C <NA>   GLY     B    27   <NA> 18.845  23.903   4.520 1
## 967    ATOM   968     O <NA>   GLY     B    27   <NA> 18.660  23.054   5.417 1
## 968    ATOM   969     N <NA>   ALA     B    28   <NA> 18.819  23.600   3.217 1
## 969    ATOM   970    CA <NA>   ALA     B    28   <NA> 18.721  22.211   2.738 1
## 970    ATOM   971     C <NA>   ALA     B    28   <NA> 20.089  21.661   2.292 1
## 971    ATOM   972     O <NA>   ALA     B    28   <NA> 20.749  22.243   1.403 1
## 972    ATOM   973    CB <NA>   ALA     B    28   <NA> 17.682  22.117   1.578 1
## 973    ATOM   974     N <NA>   ASP     B    29   <NA> 20.536  20.559   2.918 1
## 974    ATOM   975    CA <NA>   ASP     B    29   <NA> 21.779  19.912   2.496 1
## 975    ATOM   976     C <NA>   ASP     B    29   <NA> 21.693  19.374   1.107 1
## 976    ATOM   977     O <NA>   ASP     B    29   <NA> 22.642  19.502   0.361 1
## 977    ATOM   978    CB <NA>   ASP     B    29   <NA> 22.169  18.827   3.447 1
## 978    ATOM   979    CG <NA>   ASP     B    29   <NA> 22.272  19.337   4.844 1
## 979    ATOM   980   OD1 <NA>   ASP     B    29   <NA> 22.714  20.482   5.029 1
## 980    ATOM   981   OD2 <NA>   ASP     B    29   <NA> 21.836  18.647   5.778 1
## 981    ATOM   982     N <NA>   ASP     B    30   <NA> 20.524  18.868   0.719 1
## 982    ATOM   983    CA <NA>   ASP     B    30   <NA> 20.355  18.227  -0.584 1
## 983    ATOM   984     C <NA>   ASP     B    30   <NA> 19.212  18.807  -1.371 1
## 984    ATOM   985     O <NA>   ASP     B    30   <NA> 18.383  19.523  -0.846 1
## 985    ATOM   986    CB <NA>   ASP     B    30   <NA> 20.084  16.745  -0.413 1
## 986    ATOM   987    CG <NA>   ASP     B    30   <NA> 21.023  16.088   0.586 1
## 987    ATOM   988   OD1 <NA>   ASP     B    30   <NA> 22.233  15.970   0.265 1
## 988    ATOM   989   OD2 <NA>   ASP     B    30   <NA> 20.531  15.682   1.672 1
## 989    ATOM   990     N <NA>   THR     B    31   <NA> 19.152  18.428  -2.643 1
## 990    ATOM   991    CA <NA>   THR     B    31   <NA> 18.113  18.843  -3.603 1
## 991    ATOM   992     C <NA>   THR     B    31   <NA> 17.019  17.743  -3.682 1
## 992    ATOM   993     O <NA>   THR     B    31   <NA> 17.342  16.586  -3.904 1
## 993    ATOM   994    CB <NA>   THR     B    31   <NA> 18.810  19.051  -4.967 1

## 994    ATOM   995   OG1 <NA>   THR     B    31   <NA> 19.740  20.123  -4.831 1
## 995    ATOM   996   CG2 <NA>   THR     B    31   <NA> 17.844  19.330  -6.078 1
## 996    ATOM   997     N <NA>   VAL     B    32   <NA> 15.750  18.102  -3.440 1
## 997    ATOM   998    CA <NA>   VAL     B    32   <NA> 14.628  17.162  -3.514 1
## 998    ATOM   999     C <NA>   VAL     B    32   <NA> 13.618  17.726  -4.436 1
## 999    ATOM  1000     O <NA>   VAL     B    32   <NA> 13.169  18.861  -4.263 1
## 1000   ATOM  1001    CB <NA>   VAL     B    32   <NA> 13.781  17.005  -2.245 1
## 1001   ATOM  1002   CG1 <NA>   VAL     B    32   <NA> 13.297  15.592  -2.184 1
## 1002   ATOM  1003   CG2 <NA>   VAL     B    32   <NA> 14.518  17.455  -1.007 1
## 1003   ATOM  1004     N <NA>   LEU     B    33   <NA> 13.199  16.926  -5.401 1
## 1004   ATOM  1005    CA <NA>   LEU     B    33   <NA> 12.141  17.335  -6.327 1
## 1005   ATOM  1006     C <NA>   LEU     B    33   <NA> 10.876  16.500  -6.065 1
## 1006   ATOM  1007     O <NA>   LEU     B    33   <NA> 10.948  15.389  -5.534 1
## 1007   ATOM  1008    CB <NA>   LEU     B    33   <NA> 12.618  17.139  -7.766 1
## 1008   ATOM  1009    CG <NA>   LEU     B    33   <NA> 13.889  17.846  -8.247 1
## 1009   ATOM  1010   CD1 <NA>   LEU     B    33   <NA> 13.942  17.794  -9.731 1
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## 1010   ATOM  1011   CD2 <NA>   LEU     B    33   <NA> 13.897  19.266  -7.782 1
## 1011   ATOM  1012     N <NA>   GLU     B    34   <NA>  9.719  17.083  -6.361 1
## 1012   ATOM  1013    CA <NA>   GLU     B    34   <NA>  8.442  16.392  -6.346 1
## 1013   ATOM  1014     C <NA>   GLU     B    34   <NA>  8.514  15.172  -7.224 1
## 1014   ATOM  1015     O <NA>   GLU     B    34   <NA>  9.413  15.013  -8.040 1
## 1015   ATOM  1016    CB <NA>   GLU     B    34   <NA>  7.316  17.305  -6.819 1
## 1016   ATOM  1017    CG <NA>   GLU     B    34   <NA>  6.914  18.362  -5.808 1
## 1017   ATOM  1018    CD <NA>   GLU     B    34   <NA>  6.205  19.552  -6.439 1
## 1018   ATOM  1019   OE1 <NA>   GLU     B    34   <NA>  6.323  19.742  -7.666 1
## 1019   ATOM  1020   OE2 <NA>   GLU     B    34   <NA>  5.613  20.369  -5.715 1
## 1020   ATOM  1021     N <NA>   GLU     B    35   <NA>  7.526  14.309  -7.044 1
## 1021   ATOM  1022    CA <NA>   GLU     B    35   <NA>  7.425  13.006  -7.682 1
## 1022   ATOM  1023     C <NA>   GLU     B    35   <NA>  7.528  13.141  -9.172 1
## 1023   ATOM  1024     O <NA>   GLU     B    35   <NA>  6.660  13.711  -9.819 1
## 1024   ATOM  1025    CB <NA>   GLU     B    35   <NA>  6.100  12.361  -7.297 1
## 1025   ATOM  1026    CG <NA>   GLU     B    35   <NA>  5.907  10.953  -7.838 1
## 1026   ATOM  1027    CD <NA>   GLU     B    35   <NA>  7.182  10.093  -7.854 1
## 1027   ATOM  1028   OE1 <NA>   GLU     B    35   <NA>  7.743   9.853  -6.766 1
## 1028   ATOM  1029   OE2 <NA>   GLU     B    35   <NA>  7.521   9.561  -8.946 1
## 1029   ATOM  1030     N <NA>   MET     B    36   <NA>  8.627  12.651  -9.705 1
## 1030   ATOM  1031    CA <NA>   MET     B    36   <NA>  8.791  12.578 -11.145 1
## 1031   ATOM  1032     C <NA>   MET     B    36   <NA>  9.583  11.322 -11.483 1
## 1032   ATOM  1033     O <NA>   MET     B    36   <NA> 10.100  10.637 -10.616 1
## 1033   ATOM  1034    CB <NA>   MET     B    36   <NA>  9.546  13.808 -11.654 1
## 1034   ATOM  1035    CG <NA>   MET     B    36   <NA> 10.867  14.095 -11.014 1
## 1035   ATOM  1036    SD <NA>   MET     B    36   <NA> 11.575  15.547 -11.778 1
## 1036   ATOM  1037    CE <NA>   MET     B    36   <NA> 11.710  15.108 -13.551 1
## 1037   ATOM  1038     N <NA>   SER     B    37   <NA>  9.657  11.016 -12.763 1
## 1038   ATOM  1039    CA <NA>   SER     B    37   <NA> 10.411   9.858 -13.218 1
## 1039   ATOM  1040     C <NA>   SER     B    37   <NA> 11.673  10.374 -13.825 1
## 1040   ATOM  1041     O <NA>   SER     B    37   <NA> 11.636  11.272 -14.685 1
## 1041   ATOM  1042    CB <NA>   SER     B    37   <NA>  9.573   9.049 -14.221 1
## 1042   ATOM  1043    OG <NA>   SER     B    37   <NA>  8.330   8.594 -13.579 1

## 1043   ATOM  1044     N <NA>   LEU     B    38   <NA> 12.793   9.884 -13.330 1
## 1044   ATOM  1045    CA <NA>   LEU     B    38   <NA> 14.091  10.261 -13.857 1
## 1045   ATOM  1046     C <NA>   LEU     B    38   <NA> 14.818   9.018 -14.330 1
## 1046   ATOM  1047     O <NA>   LEU     B    38   <NA> 14.416   7.898 -13.995 1
## 1047   ATOM  1048    CB <NA>   LEU     B    38   <NA> 14.866  10.942 -12.759 1
## 1048   ATOM  1049    CG <NA>   LEU     B    38   <NA> 14.480  12.376 -12.556 1
## 1049   ATOM  1050   CD1 <NA>   LEU     B    38   <NA> 15.159  12.900 -11.300 1
## 1050   ATOM  1051   CD2 <NA>   LEU     B    38   <NA> 14.955  13.131 -13.766 1
## 1051   ATOM  1052     N <NA>   PRO     B    39   <NA> 15.767   9.161 -15.261 1
## 1052   ATOM  1053    CA <NA>   PRO     B    39   <NA> 16.525   8.031 -15.798 1
## 1053   ATOM  1054     C <NA>   PRO     B    39   <NA> 17.366   7.241 -14.777 1
## 1054   ATOM  1055     O <NA>   PRO     B    39   <NA> 17.943   7.817 -13.847 1
## 1055   ATOM  1056    CB <NA>   PRO     B    39   <NA> 17.407   8.673 -16.857 1
## 1056   ATOM  1057    CG <NA>   PRO     B    39   <NA> 17.532  10.100 -16.423 1
## 1057   ATOM  1058    CD <NA>   PRO     B    39   <NA> 16.150  10.405 -15.968 1
## 1058   ATOM  1059     N <NA>   GLY     B    40   <NA> 17.477   5.932 -14.999 1
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## 1059   ATOM  1060    CA <NA>   GLY     B    40   <NA> 18.494   5.171 -14.302 1
## 1060   ATOM  1061     C <NA>   GLY     B    40   <NA> 18.048   4.556 -12.995 1
## 1061   ATOM  1062     O <NA>   GLY     B    40   <NA> 16.865   4.438 -12.729 1
## 1062   ATOM  1063     N <NA>   ARG     B    41   <NA> 19.000   3.939 -12.313 1
## 1063   ATOM  1064    CA <NA>   ARG     B    41   <NA> 18.722   3.282 -11.042 1
## 1064   ATOM  1065     C <NA>   ARG     B    41   <NA> 18.615   4.306  -9.916 1
## 1065   ATOM  1066     O <NA>   ARG     B    41   <NA> 19.168   5.390 -10.018 1
## 1066   ATOM  1067    CB <NA>   ARG     B    41   <NA> 19.852   2.333 -10.662 1
## 1067   ATOM  1068    CG <NA>   ARG     B    41   <NA> 20.359   1.417 -11.726 1
## 1068   ATOM  1069    CD <NA>   ARG     B    41   <NA> 20.905   0.188 -11.023 1
## 1069   ATOM  1070    NE <NA>   ARG     B    41   <NA> 19.927  -0.864 -11.169 1
## 1070   ATOM  1071    CZ <NA>   ARG     B    41   <NA> 19.354  -1.538 -10.177 1
## 1071   ATOM  1072   NH1 <NA>   ARG     B    41   <NA> 19.839  -1.513  -8.939 1
## 1072   ATOM  1073   NH2 <NA>   ARG     B    41   <NA> 18.333  -2.314 -10.472 1
## 1073   ATOM  1074     N <NA>   TRP     B    42   <NA> 17.989   3.918  -8.810 1
## 1074   ATOM  1075    CA <NA>   TRP     B    42   <NA> 17.920   4.766  -7.634 1
## 1075   ATOM  1076     C <NA>   TRP     B    42   <NA> 18.295   3.969  -6.380 1
## 1076   ATOM  1077     O <NA>   TRP     B    42   <NA> 18.163   2.742  -6.361 1
## 1077   ATOM  1078    CB <NA>   TRP     B    42   <NA> 16.525   5.338  -7.459 1
## 1078   ATOM  1079    CG <NA>   TRP     B    42   <NA> 15.444   4.372  -7.312 1
## 1079   ATOM  1080   CD1 <NA>   TRP     B    42   <NA> 14.681   3.834  -8.299 1
## 1080   ATOM  1081   CD2 <NA>   TRP     B    42   <NA> 14.840   3.957  -6.079 1
## 1081   ATOM  1082   NE1 <NA>   TRP     B    42   <NA> 13.640   3.121  -7.756 1
## 1082   ATOM  1083   CE2 <NA>   TRP     B    42   <NA> 13.719   3.166  -6.402 1
## 1083   ATOM  1084   CE3 <NA>   TRP     B    42   <NA> 15.154   4.180  -4.715 1
## 1084   ATOM  1085   CZ2 <NA>   TRP     B    42   <NA> 12.881   2.589  -5.411 1
## 1085   ATOM  1086   CZ3 <NA>   TRP     B    42   <NA> 14.300   3.625  -3.745 1
## 1086   ATOM  1087   CH2 <NA>   TRP     B    42   <NA> 13.168   2.842  -4.106 1
## 1087   ATOM  1088     N <NA>   LYS     B    43   <NA> 18.801   4.689  -5.365 1
## 1088   ATOM  1089    CA <NA>   LYS     B    43   <NA> 19.180   4.182  -4.032 1
## 1089   ATOM  1090     C <NA>   LYS     B    43   <NA> 18.127   4.736  -3.089 1
## 1090   ATOM  1091     O <NA>   LYS     B    43   <NA> 17.442   5.729  -3.400 1
## 1091   ATOM  1092    CB <NA>   LYS     B    43   <NA> 20.561   4.731  -3.581 1

## 1092   ATOM  1093    CG <NA>   LYS     B    43   <NA> 21.777   4.400  -4.445 1
## 1093   ATOM  1094    CD <NA>   LYS     B    43   <NA> 22.996   5.295  -4.048 1
## 1094   ATOM  1095    CE <NA>   LYS     B    43   <NA> 24.193   5.280  -5.063 1
## 1095   ATOM  1096    NZ <NA>   LYS     B    43   <NA> 25.251   6.324  -4.725 1
## 1096   ATOM  1097     N <NA>   PRO     B    44   <NA> 18.053   4.208  -1.878 1
## 1097   ATOM  1098    CA <NA>   PRO     B    44   <NA> 17.102   4.804  -0.946 1
## 1098   ATOM  1099     C <NA>   PRO     B    44   <NA> 17.754   5.853  -0.023 1
## 1099   ATOM  1100     O <NA>   PRO     B    44   <NA> 18.929   5.769   0.330 1
## 1100   ATOM  1101    CB <NA>   PRO     B    44   <NA> 16.596   3.610  -0.171 1
## 1101   ATOM  1102    CG <NA>   PRO     B    44   <NA> 17.803   2.676  -0.117 1
## 1102   ATOM  1103    CD <NA>   PRO     B    44   <NA> 18.649   2.962  -1.335 1
## 1103   ATOM  1104     N <NA>   LYS     B    45   <NA> 16.974   6.847   0.381 1
## 1104   ATOM  1105    CA <NA>   LYS     B    45   <NA> 17.443   7.812   1.371 1
## 1105   ATOM  1106     C <NA>   LYS     B    45   <NA> 16.334   8.328   2.257 1
## 1106   ATOM  1107     O <NA>   LYS     B    45   <NA> 15.192   8.470   1.828 1
## 1107   ATOM  1108    CB <NA>   LYS     B    45   <NA> 18.177   8.988   0.701 1
```

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## 1108   ATOM  1109    CG <NA>   LYS     B    45   <NA> 19.183   9.659   1.670 1
## 1109   ATOM  1110    CD <NA>   LYS     B    45   <NA> 20.095  10.640   1.011 1
## 1110   ATOM  1111    CE <NA>   LYS     B    45   <NA> 20.751  11.491   2.069 1
## 1111   ATOM  1112    NZ <NA>   LYS     B    45   <NA> 21.413  12.705   1.509 1
## 1112   ATOM  1113     N <NA>   MET     B    46   <NA> 16.672   8.585   3.514 1
## 1113   ATOM  1114    CA <NA>   MET     B    46   <NA> 15.755   9.281   4.404 1
## 1114   ATOM  1115     C <NA>   MET     B    46   <NA> 16.373  10.584   4.732 1
## 1115   ATOM  1116     O <NA>   MET     B    46   <NA> 17.542  10.636   5.104 1
## 1116   ATOM  1117    CB <NA>   MET     B    46   <NA> 15.562   8.530   5.708 1
## 1117   ATOM  1118    CG <NA>   MET     B    46   <NA> 14.763   7.266   5.540 1
## 1118   ATOM  1119    SD <NA>   MET     B    46   <NA> 13.357   7.367   6.566 1
## 1119   ATOM  1120    CE <NA>   MET     B    46   <NA> 14.146   6.922   8.167 1
## 1120   ATOM  1121     N <NA>   ILE     B    47   <NA> 15.582  11.636   4.604 1
## 1121   ATOM  1122    CA <NA>   ILE     B    47   <NA> 16.003  12.986   4.955 1
## 1122   ATOM  1123     C <NA>   ILE     B    47   <NA> 15.018  13.507   5.961 1
## 1123   ATOM  1124     O <NA>   ILE     B    47   <NA> 13.822  13.222   5.884 1
## 1124   ATOM  1125    CB <NA>   ILE     B    47   <NA> 16.040  13.915   3.699 1
## 1125   ATOM  1126   CG1 <NA>   ILE     B    47   <NA> 14.745  13.761   2.918 1
## 1126   ATOM  1127   CG2 <NA>   ILE     B    47   <NA> 17.229  13.534   2.782 1
## 1127   ATOM  1128   CD1 <NA>   ILE     B    47   <NA> 14.742  14.561   1.698 1
## 1128   ATOM  1129     N <NA>   GLY     B    48   <NA> 15.542  14.239   6.941 1
## 1129   ATOM  1130    CA <NA>   GLY     B    48   <NA> 14.714  14.799   8.014 1
## 1130   ATOM  1131     C <NA>   GLY     B    48   <NA> 14.762  16.314   8.114 1
## 1131   ATOM  1132     O <NA>   GLY     B    48   <NA> 15.803  16.952   7.888 1
## 1132   ATOM  1133     N <NA>   GLY     B    49   <NA> 13.583  16.896   8.239 1
## 1133   ATOM  1134    CA <NA>   GLY     B    49   <NA> 13.484  18.319   8.459 1
## 1134   ATOM  1135     C <NA>   GLY     B    49   <NA> 12.647  18.565   9.672 1
## 1135   ATOM  1136     O <NA>   GLY     B    49   <NA> 12.880  17.976  10.721 1
## 1136   ATOM  1137     N <NA>   ILE     B    50   <NA> 11.850  19.611   9.584 1
## 1137   ATOM  1138    CA <NA>   ILE     B    50   <NA> 10.858  19.974  10.594 1
## 1138   ATOM  1139     C <NA>   ILE     B    50   <NA>  9.707  18.988  10.393 1
## 1139   ATOM  1140     O <NA>   ILE     B    50   <NA>  9.341  18.670   9.251 1
## 1140   ATOM  1141    CB <NA>   ILE     B    50   <NA> 10.365  21.453  10.316 1

## 1141   ATOM  1142   CG1 <NA>   ILE     B    50   <NA> 11.556  22.421  10.394 1
## 1142   ATOM  1143   CG2 <NA>   ILE     B    50   <NA>  9.299  21.862  11.270 1
## 1143   ATOM  1144   CD1 <NA>   ILE     B    50   <NA> 11.936  22.850  11.773 1
## 1144   ATOM  1145     N <NA>   GLY     B    51   <NA>  9.164  18.455  11.474 1
## 1145   ATOM  1146    CA <NA>   GLY     B    51   <NA>  8.011  17.583  11.313 1
## 1146   ATOM  1147     C <NA>   GLY     B    51   <NA>  8.360  16.130  11.054 1
## 1147   ATOM  1148     O <NA>   GLY     B    51   <NA>  7.494  15.283  11.167 1
## 1148   ATOM  1149     N <NA>   GLY     B    52   <NA>  9.638  15.842  10.818 1
## 1149   ATOM  1150    CA <NA>   GLY     B    52   <NA> 10.123  14.474  10.792 1
## 1150   ATOM  1151     C <NA>   GLY     B    52   <NA> 10.860  14.080   9.524 1
## 1151   ATOM  1152     O <NA>   GLY     B    52   <NA> 11.419  14.930   8.826 1
## 1152   ATOM  1153     N <NA>   PHE     B    53   <NA> 10.878  12.788   9.221 1
## 1153   ATOM  1154    CA <NA>   PHE     B    53   <NA> 11.638  12.302   8.079 1
## 1154   ATOM  1155     C <NA>   PHE     B    53   <NA> 10.739  11.914   6.924 1
## 1155   ATOM  1156     O <NA>   PHE     B    53   <NA>  9.601  11.543   7.137 1
## 1156   ATOM  1157    CB <NA>   PHE     B    53   <NA> 12.458  11.126   8.531 1
```

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## 1157   ATOM  1158    CG <NA>   PHE     B    53   <NA> 13.464  11.471   9.564 1
## 1158   ATOM  1159   CD1 <NA>   PHE     B    53   <NA> 13.092  11.697  10.886 1
## 1159   ATOM  1160   CD2 <NA>   PHE     B    53   <NA> 14.789  11.625   9.189 1
## 1160   ATOM  1161   CE1 <NA>   PHE     B    53   <NA> 14.036  12.076  11.825 1
## 1161   ATOM  1162   CE2 <NA>   PHE     B    53   <NA> 15.753  12.001  10.078 1
## 1162   ATOM  1163    CZ <NA>   PHE     B    53   <NA> 15.392  12.225  11.421 1
## 1163   ATOM  1164     N <NA>   ILE     B    54   <NA> 11.204  12.078   5.695 1
## 1164   ATOM  1165    CA <NA>   ILE     B    54   <NA> 10.538  11.431   4.563 1
## 1165   ATOM  1166     C <NA>   ILE     B    54   <NA> 11.513  10.453   3.866 1
## 1166   ATOM  1167     O <NA>   ILE     B    54   <NA> 12.727  10.529   4.052 1
## 1167   ATOM  1168    CB <NA>   ILE     B    54   <NA>  9.923  12.446   3.500 1
## 1168   ATOM  1169   CG1 <NA>   ILE     B    54   <NA> 10.968  13.414   2.964 1
## 1169   ATOM  1170   CG2 <NA>   ILE     B    54   <NA>  8.754  13.195   4.090 1
## 1170   ATOM  1171   CD1 <NA>   ILE     B    54   <NA> 10.571  14.020   1.616 1
## 1171   ATOM  1172     N <NA>   LYS     B    55   <NA> 10.983   9.503   3.111 1
## 1172   ATOM  1173    CA <NA>   LYS     B    55   <NA> 11.816   8.478   2.482 1
## 1173   ATOM  1174     C <NA>   LYS     B    55   <NA> 11.862   8.988   1.074 1
## 1174   ATOM  1175     O <NA>   LYS     B    55   <NA> 10.827   9.256   0.525 1
## 1175   ATOM  1176    CB <NA>   LYS     B    55   <NA> 11.062   7.136   2.489 1
## 1176   ATOM  1177    CG <NA>   LYS     B    55   <NA> 11.699   5.963   3.273 1
## 1177   ATOM  1178    CD <NA>   LYS     B    55   <NA> 13.070   5.502   2.689 1
## 1178   ATOM  1179    CE <NA>   LYS     B    55   <NA> 12.949   4.923   1.253 1
## 1179   ATOM  1180    NZ <NA>   LYS     B    55   <NA> 13.964   5.445   0.291 1
## 1180   ATOM  1181     N <NA>   VAL     B    56   <NA> 13.024   9.137   0.474 1
## 1181   ATOM  1182    CA <NA>   VAL     B    56   <NA> 13.072   9.652  -0.897 1
## 1182   ATOM  1183     C <NA>   VAL     B    56   <NA> 13.885   8.719  -1.786 1
## 1183   ATOM  1184     O <NA>   VAL     B    56   <NA> 14.547   7.817  -1.279 1
## 1184   ATOM  1185    CB <NA>   VAL     B    56   <NA> 13.757  11.033  -0.959 1
## 1185   ATOM  1186   CG1 <NA>   VAL     B    56   <NA> 12.766  12.134  -0.523 1
## 1186   ATOM  1187   CG2 <NA>   VAL     B    56   <NA> 15.032  11.016  -0.119 1
## 1187   ATOM  1188     N <NA>   ARG     B    57   <NA> 13.889   8.977  -3.102 1
## 1188   ATOM  1189    CA <NA>   ARG     B    57   <NA> 14.697   8.220  -4.083 1
## 1189   ATOM  1190     C <NA>   ARG     B    57   <NA> 15.894   9.023  -4.591 1

## 1190   ATOM  1191     O <NA>   ARG     B    57   <NA> 15.735  10.066  -5.210 1
## 1191   ATOM  1192    CB <NA>   ARG     B    57   <NA> 13.862   7.854  -5.298 1
## 1192   ATOM  1193    CG <NA>   ARG     B    57   <NA> 12.767   6.845  -5.041 1
## 1193   ATOM  1194    CD <NA>   ARG     B    57   <NA> 12.224   6.316  -6.354 1
## 1194   ATOM  1195    NE <NA>   ARG     B    57   <NA> 10.944   6.937  -6.617 1
## 1195   ATOM  1196    CZ <NA>   ARG     B    57   <NA> 10.717   7.776  -7.614 1
## 1196   ATOM  1197   NH1 <NA>   ARG     B    57   <NA> 11.534   7.792  -8.658 1
## 1197   ATOM  1198   NH2 <NA>   ARG     B    57   <NA>  9.555   8.403  -7.678 1
## 1198   ATOM  1199     N <NA>   GLN     B    58   <NA> 17.095   8.516  -4.388 1
## 1199   ATOM  1200    CA <NA>   GLN     B    58   <NA> 18.306   9.218  -4.819 1
## 1200   ATOM  1201     C <NA>   GLN     B    58   <NA> 18.742   8.833  -6.226 1
## 1201   ATOM  1202     O <NA>   GLN     B    58   <NA> 19.157   7.694  -6.438 1
## 1202   ATOM  1203    CB <NA>   GLN     B    58   <NA> 19.465   8.920  -3.861 1
## 1203   ATOM  1204    CG <NA>   GLN     B    58   <NA> 20.738   9.622  -4.271 1
## 1204   ATOM  1205    CD <NA>   GLN     B    58   <NA> 21.825   9.463  -3.248 1
## 1205   ATOM  1206   OE1 <NA>   GLN     B    58   <NA> 21.554   9.424  -2.048 1
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## 1206   ATOM  1207   NE2 <NA>   GLN     B    58   <NA> 23.045   9.365  -3.692 1
## 1207   ATOM  1208     N <NA>   TYR     B    59   <NA> 18.705   9.773  -7.167 1
## 1208   ATOM  1209    CA <NA>   TYR     B    59   <NA> 19.361   9.587  -8.464 1
## 1209   ATOM  1210     C <NA>   TYR     B    59   <NA> 20.689  10.330  -8.544 1
## 1210   ATOM  1211     O <NA>   TYR     B    59   <NA> 20.860  11.368  -7.943 1
## 1211   ATOM  1212    CB <NA>   TYR     B    59   <NA> 18.472  10.082  -9.563 1
## 1212   ATOM  1213    CG <NA>   TYR     B    59   <NA> 17.116   9.383  -9.609 1
## 1213   ATOM  1214   CD1 <NA>   TYR     B    59   <NA> 16.157   9.612  -8.615 1
## 1214   ATOM  1215   CD2 <NA>   TYR     B    59   <NA> 16.814   8.484 -10.637 1
## 1215   ATOM  1216   CE1 <NA>   TYR     B    59   <NA> 14.959   8.977  -8.640 1
## 1216   ATOM  1217   CE2 <NA>   TYR     B    59   <NA> 15.647   7.851 -10.673 1
## 1217   ATOM  1218    CZ <NA>   TYR     B    59   <NA> 14.704   8.066  -9.679 1
## 1218   ATOM  1219    OH <NA>   TYR     B    59   <NA> 13.561   7.307  -9.711 1
## 1219   ATOM  1220     N <NA>   ASP     B    60   <NA> 21.665   9.797  -9.258 1
## 1220   ATOM  1221    CA <NA>   ASP     B    60   <NA> 22.959  10.470  -9.336 1
## 1221   ATOM  1222     C <NA>   ASP     B    60   <NA> 23.303  10.921 -10.737 1
## 1222   ATOM  1223     O <NA>   ASP     B    60   <NA> 22.793  10.396 -11.707 1
## 1223   ATOM  1224    CB <NA>   ASP     B    60   <NA> 24.042   9.554  -8.834 1
## 1224   ATOM  1225    CG <NA>   ASP     B    60   <NA> 23.843   9.184  -7.407 1
## 1225   ATOM  1226   OD1 <NA>   ASP     B    60   <NA> 23.463  10.074  -6.620 1
## 1226   ATOM  1227   OD2 <NA>   ASP     B    60   <NA> 24.107   8.012  -7.044 1
## 1227   ATOM  1228     N <NA>   GLN     B    61   <NA> 24.189  11.897 -10.837 1
## 1228   ATOM  1229    CA <NA>   GLN     B    61   <NA> 24.622  12.478 -12.111 1
## 1229   ATOM  1230     C <NA>   GLN     B    61   <NA> 23.474  12.903 -13.022 1
## 1230   ATOM  1231     O <NA>   GLN     B    61   <NA> 23.492  12.665 -14.229 1
## 1231   ATOM  1232    CB <NA>   GLN     B    61   <NA> 25.596  11.549 -12.869 1
## 1232   ATOM  1233    CG <NA>   GLN     B    61   <NA> 26.892  12.283 -13.369 1
## 1233   ATOM  1234    CD <NA>   GLN     B    61   <NA> 28.007  11.392 -13.985 1
## 1234   ATOM  1235   OE1 <NA>   GLN     B    61   <NA> 28.747  11.845 -14.875 1
## 1235   ATOM  1236   NE2 <NA>   GLN     B    61   <NA> 28.197  10.173 -13.442 1
## 1236   ATOM  1237     N <NA>   ILE     B    62   <NA> 22.493  13.589 -12.452 1
## 1237   ATOM  1238    CA <NA>   ILE     B    62   <NA> 21.380  14.141 -13.224 1
## 1238   ATOM  1239     C <NA>   ILE     B    62   <NA> 21.710  15.575 -13.686 1

## 1239   ATOM  1240     O <NA>   ILE     B    62   <NA> 22.247  16.373 -12.924 1
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## 1241   ATOM  1242   CG1 <NA>   ILE     B    62   <NA> 19.709  12.702 -11.952 1
## 1242   ATOM  1243   CG2 <NA>   ILE     B    62   <NA> 18.950  14.826 -13.045 1
## 1243   ATOM  1244   CD1 <NA>   ILE     B    62   <NA> 19.068  11.933 -13.057 1
## 1244   ATOM  1245     N <NA>   LEU     B    63   <NA> 21.400  15.900 -14.931 1
## 1245   ATOM  1246    CA <NA>   LEU     B    63   <NA> 21.600  17.263 -15.431 1
## 1246   ATOM  1247     C <NA>   LEU     B    63   <NA> 20.386  18.085 -15.052 1
## 1247   ATOM  1248     O <NA>   LEU     B    63   <NA> 19.260  17.703 -15.355 1
## 1248   ATOM  1249    CB <NA>   LEU     B    63   <NA> 21.769  17.265 -16.962 1
## 1249   ATOM  1250    CG <NA>   LEU     B    63   <NA> 21.792  18.587 -17.759 1
## 1250   ATOM  1251   CD1 <NA>   LEU     B    63   <NA> 22.903  19.529 -17.300 1
## 1251   ATOM  1252   CD2 <NA>   LEU     B    63   <NA> 21.997  18.246 -19.205 1
## 1252   ATOM  1253     N <NA>   ILE     B    64   <NA> 20.626  19.203 -14.381 1
## 1253   ATOM  1254    CA <NA>   ILE     B    64   <NA> 19.548  20.111 -14.029 1
## 1254   ATOM  1255     C <NA>   ILE     B    64   <NA> 20.089  21.523 -14.223 1
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## 1255   ATOM  1256     O <NA>   ILE     B    64   <NA> 21.175  21.858 -13.763 1
## 1256   ATOM  1257    CB <NA>   ILE     B    64   <NA> 19.107  19.880 -12.540 1
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## 1259   ATOM  1260   CD1 <NA>   ILE     B    64   <NA> 17.324  20.544 -10.930 1
## 1260   ATOM  1261     N <NA>   GLU     B    65   <NA> 19.327  22.330 -14.953 1
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## 1267   ATOM  1268   OE1 <NA>   GLU     B    65   <NA> 19.601  24.094 -19.445 1
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## 1269   ATOM  1270     N <NA>   ILE     B    66   <NA> 19.709  25.427 -13.547 1
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## 1274   ATOM  1275   CG1 <NA>   ILE     B    66   <NA> 19.566  24.717 -10.848 1
## 1275   ATOM  1276   CG2 <NA>   ILE     B    66   <NA> 18.824  27.018 -10.232 1
## 1276   ATOM  1277   CD1 <NA>   ILE     B    66   <NA> 20.510  24.280  -9.745 1
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## 1280   ATOM  1281     O <NA>   CYS     B    67   <NA> 20.565  30.852 -15.294 1
## 1281   ATOM  1282    CB <NA>   CYS     B    67   <NA> 19.124  30.970 -13.037 1
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## 1287   ATOM  1288     N <NA>   HIS     B    69   <NA> 22.059  28.002 -15.633 1

## 1288   ATOM  1289    CA <NA>   HIS     B    69   <NA> 23.354  27.479 -15.197 1
## 1289   ATOM  1290     C <NA>   HIS     B    69   <NA> 23.178  25.984 -15.087 1
## 1290   ATOM  1291     O <NA>   HIS     B    69   <NA> 22.307  25.523 -14.354 1
## 1291   ATOM  1292    CB <NA>   HIS     B    69   <NA> 23.711  27.993 -13.810 1
## 1292   ATOM  1293    CG <NA>   HIS     B    69   <NA> 23.976  29.473 -13.740 1
## 1293   ATOM  1294   ND1 <NA>   HIS     B    69   <NA> 25.177  29.994 -13.361 1
## 1294   ATOM  1295   CD2 <NA>   HIS     B    69   <NA> 23.114  30.512 -13.920 1
## 1295   ATOM  1296   CE1 <NA>   HIS     B    69   <NA> 25.058  31.325 -13.286 1
## 1296   ATOM  1297   NE2 <NA>   HIS     B    69   <NA> 23.849  31.652 -13.613 1
## 1297   ATOM  1298     N <NA>   LYS     B    70   <NA> 23.995  25.240 -15.820 1
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## 1299   ATOM  1300     C <NA>   LYS     B    70   <NA> 24.749  23.243 -14.652 1
## 1300   ATOM  1301     O <NA>   LYS     B    70   <NA> 25.875  23.676 -14.403 1
## 1301   ATOM  1302    CB <NA>   LYS     B    70   <NA> 24.423  23.212 -17.115 1
## 1302   ATOM  1303    CG <NA>   LYS     B    70   <NA> 23.463  23.445 -18.279 1
## 1303   ATOM  1304    CD <NA>   LYS     B    70   <NA> 24.261  23.524 -19.576 1
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## 1304   ATOM  1305    CE <NA>   LYS     B    70   <NA> 23.377  23.737 -20.816 1
## 1305   ATOM  1306    NZ <NA>   LYS     B    70   <NA> 22.863  22.443 -21.404 1
## 1306   ATOM  1307     N <NA>   ALA     B    71   <NA> 24.104  22.353 -13.909 1
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## 1309   ATOM  1310     O <NA>   ALA     B    71   <NA> 23.339  19.865 -13.735 1
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## 1311   ATOM  1312     N <NA>   ILE     B    72   <NA> 25.330  19.253 -12.902 1
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## 1313   ATOM  1314     C <NA>   ILE     B    72   <NA> 25.312  17.246 -11.637 1
## 1314   ATOM  1315     O <NA>   ILE     B    72   <NA> 26.442  17.315 -11.167 1
## 1315   ATOM  1316    CB <NA>   ILE     B    72   <NA> 26.029  17.094 -13.983 1
## 1316   ATOM  1317   CG1 <NA>   ILE     B    72   <NA> 26.092  17.805 -15.333 1
## 1317   ATOM  1318   CG2 <NA>   ILE     B    72   <NA> 25.615  15.649 -14.171 1
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## 1319   ATOM  1320     N <NA>   GLY     B    73   <NA> 24.303  16.690 -10.975 1
## 1320   ATOM  1321    CA <NA>   GLY     B    73   <NA> 24.545  16.248  -9.616 1
## 1321   ATOM  1322     C <NA>   GLY     B    73   <NA> 23.470  15.337  -9.095 1
## 1322   ATOM  1323     O <NA>   GLY     B    73   <NA> 22.674  14.852  -9.881 1
## 1323   ATOM  1324     N <NA>   THR     B    74   <NA> 23.517  15.041  -7.794 1
## 1324   ATOM  1325    CA <NA>   THR     B    74   <NA> 22.568  14.162  -7.116 1
## 1325   ATOM  1326     C <NA>   THR     B    74   <NA> 21.280  14.889  -6.829 1
## 1326   ATOM  1327     O <NA>   THR     B    74   <NA> 21.299  16.005  -6.275 1
## 1327   ATOM  1328    CB <NA>   THR     B    74   <NA> 23.128  13.638  -5.748 1
## 1328   ATOM  1329   OG1 <NA>   THR     B    74   <NA> 24.323  12.880  -5.961 1
## 1329   ATOM  1330   CG2 <NA>   THR     B    74   <NA> 22.071  12.763  -5.030 1
## 1330   ATOM  1331     N <NA>   VAL     B    75   <NA> 20.177  14.227  -7.192 1
## 1331   ATOM  1332    CA <NA>   VAL     B    75   <NA> 18.832  14.773  -7.068 1
## 1332   ATOM  1333     C <NA>   VAL     B    75   <NA> 17.989  13.688  -6.360 1
## 1333   ATOM  1334     O <NA>   VAL     B    75   <NA> 17.993  12.504  -6.743 1
## 1334   ATOM  1335    CB <NA>   VAL     B    75   <NA> 18.229  15.113  -8.501 1
## 1335   ATOM  1336   CG1 <NA>   VAL     B    75   <NA> 16.760  15.421  -8.434 1
## 1336   ATOM  1337   CG2 <NA>   VAL     B    75   <NA> 18.967  16.317  -9.099 1

## 1337   ATOM  1338     N <NA>   LEU     B    76   <NA> 17.295  14.086  -5.303 1
## 1338   ATOM  1339    CA <NA>   LEU     B    76   <NA> 16.390  13.196  -4.575 1
## 1339   ATOM  1340     C <NA>   LEU     B    76   <NA> 14.972  13.423  -5.073 1
## 1340   ATOM  1341     O <NA>   LEU     B    76   <NA> 14.652  14.514  -5.518 1
## 1341   ATOM  1342    CB <NA>   LEU     B    76   <NA> 16.450  13.476  -3.067 1
## 1342   ATOM  1343    CG <NA>   LEU     B    76   <NA> 17.787  13.595  -2.330 1
## 1343   ATOM  1344   CD1 <NA>   LEU     B    76   <NA> 17.591  13.640  -0.845 1
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## 1350   ATOM  1351   CG1 <NA>   VAL     B    77   <NA> 11.065  12.148  -7.398 1
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## 1353   ATOM  1354    CA <NA>   GLY     B    78   <NA> 10.004  12.229  -2.965 1
## 1354   ATOM  1355     C <NA>   GLY     B    78   <NA>  8.832  13.128  -2.672 1
## 1355   ATOM  1356     O <NA>   GLY     B    78   <NA>  8.614  14.117  -3.393 1
## 1356   ATOM  1357     N <NA>   PRO     B    79   <NA>  8.032  12.814  -1.646 1
## 1357   ATOM  1358    CA <NA>   PRO     B    79   <NA>  6.887  13.664  -1.350 1
## 1358   ATOM  1359     C <NA>   PRO     B    79   <NA>  7.292  14.915  -0.550 1
## 1359   ATOM  1360     O <NA>   PRO     B    79   <NA>  7.007  15.036   0.638 1
## 1360   ATOM  1361    CB <NA>   PRO     B    79   <NA>  5.951  12.742  -0.594 1
## 1361   ATOM  1362    CG <NA>   PRO     B    79   <NA>  6.838  11.781   0.040 1
## 1362   ATOM  1363    CD <NA>   PRO     B    79   <NA>  8.096  11.665  -0.739 1
## 1363   ATOM  1364     N <NA>   THR     B    80   <NA>  7.997  15.816  -1.220 1
## 1364   ATOM  1365    CA <NA>   THR     B    80   <NA>  8.324  17.137  -0.702 1
## 1365   ATOM  1366     C <NA>   THR     B    80   <NA>  7.227  18.114  -1.090 1
## 1366   ATOM  1367     O <NA>   THR     B    80   <NA>  6.528  17.896  -2.080 1
## 1367   ATOM  1368    CB <NA>   THR     B    80   <NA>  9.677  17.594  -1.299 1
## 1368   ATOM  1369   OG1 <NA>   THR     B    80   <NA>  9.952  18.951  -0.924 1
## 1369   ATOM  1370   CG2 <NA>   THR     B    80   <NA>  9.688  17.449  -2.825 1
## 1370   ATOM  1371     N <NA>   PRO     B    81   <NA>  6.922  19.074  -0.214 1
## 1371   ATOM  1372    CA <NA>   PRO     B    81   <NA>  5.896  20.066  -0.556 1
## 1372   ATOM  1373     C <NA>   PRO     B    81   <NA>  6.244  20.969  -1.727 1
## 1373   ATOM  1374     O <NA>   PRO     B    81   <NA>  5.343  21.294  -2.509 1
## 1374   ATOM  1375    CB <NA>   PRO     B    81   <NA>  5.694  20.874   0.729 1
## 1375   ATOM  1376    CG <NA>   PRO     B    81   <NA>  6.274  19.954   1.831 1
## 1376   ATOM  1377    CD <NA>   PRO     B    81   <NA>  7.387  19.243   1.190 1
## 1377   ATOM  1378     N <NA>   VAL     B    82   <NA>  7.520  21.355  -1.868 1
## 1378   ATOM  1379    CA <NA>   VAL     B    82   <NA>  7.990  22.207  -2.983 1
## 1379   ATOM  1380     C <NA>   VAL     B    82   <NA>  9.255  21.636  -3.581 1
## 1380   ATOM  1381     O <NA>   VAL     B    82   <NA>  9.973  20.911  -2.929 1
## 1381   ATOM  1382    CB <NA>   VAL     B    82   <NA>  8.375  23.616  -2.484 1
## 1382   ATOM  1383   CG1 <NA>   VAL     B    82   <NA>  7.122  24.513  -2.361 1
## 1383   ATOM  1384   CG2 <NA>   VAL     B    82   <NA>  9.101  23.485  -1.163 1
## 1384   ATOM  1385     N <NA>   ASN     B    83   <NA>  9.588  21.960  -4.812 1
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## 1386   ATOM  1387     C <NA>   ASN     B    83   <NA> 11.922  22.373  -4.576 1
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## 1388   ATOM  1389    CB <NA>   ASN     B    83   <NA> 11.068  21.763  -6.823 1
## 1389   ATOM  1390    CG <NA>   ASN     B    83   <NA> 10.096  20.950  -7.647 1
## 1390   ATOM  1391   OD1 <NA>   ASN     B    83   <NA> 10.013  19.733  -7.494 1
## 1391   ATOM  1392   ND2 <NA>   ASN     B    83   <NA>  9.305  21.627  -8.498 1
## 1392   ATOM  1393     N <NA>   ILE     B    84   <NA> 12.983  21.755  -4.066 1
## 1393   ATOM  1394    CA <NA>   ILE     B    84   <NA> 13.979  22.449  -3.233 1
## 1394   ATOM  1395     C <NA>   ILE     B    84   <NA> 15.345  22.255  -3.870 1
## 1395   ATOM  1396     O <NA>   ILE     B    84   <NA> 15.779  21.111  -4.072 1
## 1396   ATOM  1397    CB <NA>   ILE     B    84   <NA> 14.041  21.833  -1.837 1
## 1397   ATOM  1398   CG1 <NA>   ILE     B    84   <NA> 12.754  22.151  -1.088 1
## 1398   ATOM  1399   CG2 <NA>   ILE     B    84   <NA> 15.323  22.264  -1.122 1
## 1399   ATOM  1400   CD1 <NA>   ILE     B    84   <NA> 12.438  21.217   0.060 1
## 1400   ATOM  1401     N <NA>   ILE     B    85   <NA> 16.044  23.346  -4.167 1
## 1401   ATOM  1402    CA <NA>   ILE     B    85   <NA> 17.441  23.243  -4.575 1
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## 1402   ATOM  1403     C <NA>   ILE     B    85   <NA> 18.305  23.504  -3.345 1
## 1403   ATOM  1404     O <NA>   ILE     B    85   <NA> 18.262  24.613  -2.802 1
## 1404   ATOM  1405    CB <NA>   ILE     B    85   <NA> 17.805  24.332  -5.644 1
## 1405   ATOM  1406   CG1 <NA>   ILE     B    85   <NA> 16.809  24.299  -6.827 1
## 1406   ATOM  1407   CG2 <NA>   ILE     B    85   <NA> 19.271  24.191  -6.067 1
## 1407   ATOM  1408   CD1 <NA>   ILE     B    85   <NA> 16.672  22.956  -7.581 1
## 1408   ATOM  1409     N <NA>   GLY     B    86   <NA> 19.121  22.530  -2.936 1
## 1409   ATOM  1410    CA <NA>   GLY     B    86   <NA> 19.857  22.642  -1.690 1
## 1410   ATOM  1411     C <NA>   GLY     B    86   <NA> 21.324  22.800  -1.940 1
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## 1412   ATOM  1413     N <NA>   ARG     B    87   <NA> 22.117  22.755  -0.887 1
## 1413   ATOM  1414    CA <NA>   ARG     B    87   <NA> 23.533  23.126  -0.985 1
## 1414   ATOM  1415     C <NA>   ARG     B    87   <NA> 24.413  22.356  -1.973 1
## 1415   ATOM  1416     O <NA>   ARG     B    87   <NA> 25.398  22.903  -2.461 1
## 1416   ATOM  1417    CB <NA>   ARG     B    87   <NA> 24.171  23.147   0.403 1
## 1417   ATOM  1418    CG <NA>   ARG     B    87   <NA> 23.646  24.256   1.283 1
## 1418   ATOM  1419    CD <NA>   ARG     B    87   <NA> 24.429  24.306   2.576 1
## 1419   ATOM  1420    NE <NA>   ARG     B    87   <NA> 24.362  23.068   3.371 1
## 1420   ATOM  1421    CZ <NA>   ARG     B    87   <NA> 25.357  22.185   3.495 1
## 1421   ATOM  1422   NH1 <NA>   ARG     B    87   <NA> 26.467  22.303   2.795 1
## 1422   ATOM  1423   NH2 <NA>   ARG     B    87   <NA> 25.255  21.190   4.368 1
## 1423   ATOM  1424     N <NA>   ASN     B    88   <NA> 24.074  21.101  -2.275 1
## 1424   ATOM  1425    CA <NA>   ASN     B    88   <NA> 24.950  20.312  -3.132 1
## 1425   ATOM  1426     C <NA>   ASN     B    88   <NA> 24.980  20.893  -4.527 1
## 1426   ATOM  1427     O <NA>   ASN     B    88   <NA> 26.015  20.853  -5.202 1
## 1427   ATOM  1428    CB <NA>   ASN     B    88   <NA> 24.512  18.849  -3.197 1
## 1428   ATOM  1429    CG <NA>   ASN     B    88   <NA> 23.126  18.649  -3.777 1
## 1429   ATOM  1430   OD1 <NA>   ASN     B    88   <NA> 22.167  19.280  -3.351 1
## 1430   ATOM  1431   ND2 <NA>   ASN     B    88   <NA> 23.020  17.775  -4.767 1
## 1431   ATOM  1432     N <NA>   LEU     B    89   <NA> 23.863  21.490  -4.949 1
## 1432   ATOM  1433    CA <NA>   LEU     B    89   <NA> 23.811  22.125  -6.273 1
## 1433   ATOM  1434     C <NA>   LEU     B    89   <NA> 24.018  23.645  -6.231 1
## 1434   ATOM  1435     O <NA>   LEU     B    89   <NA> 24.321  24.242  -7.236 1

## 1435   ATOM  1436    CB <NA>   LEU     B    89   <NA> 22.457  21.815  -6.962 1
## 1436   ATOM  1437    CG <NA>   LEU     B    89   <NA> 22.219  20.372  -7.436 1
## 1437   ATOM  1438   CD1 <NA>   LEU     B    89   <NA> 20.937  20.300  -8.243 1
## 1438   ATOM  1439   CD2 <NA>   LEU     B    89   <NA> 23.408  19.901  -8.273 1
## 1439   ATOM  1440     N <NA>   LEU     B    90   <NA> 23.819  24.255  -5.075 1
## 1440   ATOM  1441    CA <NA>   LEU     B    90   <NA> 24.020  25.701  -4.954 1
## 1441   ATOM  1442     C <NA>   LEU     B    90   <NA> 25.511  26.005  -5.072 1
## 1442   ATOM  1443     O <NA>   LEU     B    90   <NA> 25.907  26.959  -5.732 1
## 1443   ATOM  1444    CB <NA>   LEU     B    90   <NA> 23.430  26.234  -3.624 1
## 1444   ATOM  1445    CG <NA>   LEU     B    90   <NA> 21.900  26.309  -3.475 1
## 1445   ATOM  1446   CD1 <NA>   LEU     B    90   <NA> 21.487  26.779  -2.081 1
## 1446   ATOM  1447   CD2 <NA>   LEU     B    90   <NA> 21.358  27.241  -4.506 1
## 1447   ATOM  1448     N <NA>   THR     B    91   <NA> 26.336  25.143  -4.491 1
## 1448   ATOM  1449    CA <NA>   THR     B    91   <NA> 27.785  25.304  -4.546 1
## 1449   ATOM  1450     C <NA>   THR     B    91   <NA> 28.270  25.184  -5.969 1
## 1450   ATOM  1451     O <NA>   THR     B    91   <NA> 29.168  25.903  -6.378 1
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## 1451   ATOM  1452    CB <NA>   THR     B    91   <NA> 28.501  24.261  -3.669 1
## 1452   ATOM  1453   OG1 <NA>   THR     B    91   <NA> 27.898  22.990  -3.894 1
## 1453   ATOM  1454   CG2 <NA>   THR     B    91   <NA> 28.366  24.579  -2.208 1
## 1454   ATOM  1455     N <NA>   GLN     B    92   <NA> 27.619  24.323  -6.741 1
## 1455   ATOM  1456    CA <NA>   GLN     B    92   <NA> 28.009  24.110  -8.150 1
## 1456   ATOM  1457     C <NA>   GLN     B    92   <NA> 27.823  25.361  -8.999 1
## 1457   ATOM  1458     O <NA>   GLN     B    92   <NA> 28.719  25.701  -9.794 1
## 1458   ATOM  1459    CB <NA>   GLN     B    92   <NA> 27.226  22.956  -8.793 1
## 1459   ATOM  1460    CG <NA>   GLN     B    92   <NA> 27.720  21.588  -8.406 1
## 1460   ATOM  1461    CD <NA>   GLN     B    92   <NA> 27.313  20.496  -9.421 1
## 1461   ATOM  1462   OE1 <NA>   GLN     B    92   <NA> 27.138  20.746 -10.620 1
## 1462   ATOM  1463   NE2 <NA>   GLN     B    92   <NA> 27.230  19.281  -8.941 1
## 1463   ATOM  1464     N <NA>   ILE     B    93   <NA> 26.683  26.043  -8.820 1
## 1464   ATOM  1465    CA <NA>   ILE     B    93   <NA> 26.362  27.233  -9.606 1
## 1465   ATOM  1466     C <NA>   ILE     B    93   <NA> 26.904  28.524  -8.963 1
## 1466   ATOM  1467     O <NA>   ILE     B    93   <NA> 26.574  29.627  -9.385 1
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## 1468   ATOM  1469   CG1 <NA>   ILE     B    93   <NA> 24.103  27.648  -8.559 1
## 1469   ATOM  1470   CG2 <NA>   ILE     B    93   <NA> 24.300  26.092 -10.460 1
## 1470   ATOM  1471   CD1 <NA>   ILE     B    93   <NA> 22.672  28.017  -8.785 1
## 1471   ATOM  1472     N <NA>   GLY     B    94   <NA> 27.741  28.369  -7.949 1
## 1472   ATOM  1473    CA <NA>   GLY     B    94   <NA> 28.481  29.498  -7.421 1
## 1473   ATOM  1474     C <NA>   GLY     B    94   <NA> 27.749  30.439  -6.488 1
## 1474   ATOM  1475     O <NA>   GLY     B    94   <NA> 28.177  31.555  -6.261 1
## 1475   ATOM  1476     N <NA>   CYS     B    95   <NA> 26.808  29.899  -5.748 1
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## 1477   ATOM  1478     C <NA>   CYS     B    95   <NA> 26.408  30.993  -3.598 1
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## 1480   ATOM  1481    SG <NA>   CYS     B    95   <NA> 23.221  30.929  -4.410 1
## 1481   ATOM  1482     N <NA>   THR     B    96   <NA> 26.473  32.277  -3.244 1
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## 1484   ATOM  1485     O <NA>   THR     B    96   <NA> 24.760  34.079  -1.852 1
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## 1486   ATOM  1487   OG1 <NA>   THR     B    96   <NA> 27.888  34.689  -2.857 1
## 1487   ATOM  1488   CG2 <NA>   THR     B    96   <NA> 29.316  32.870  -2.141 1
## 1488   ATOM  1489     N <NA>   LEU     B    97   <NA> 25.759  33.617   0.119 1
## 1489   ATOM  1490    CA <NA>   LEU     B    97   <NA> 24.902  34.468   0.963 1
## 1490   ATOM  1491     C <NA>   LEU     B    97   <NA> 25.714  35.689   1.398 1
## 1491   ATOM  1492     O <NA>   LEU     B    97   <NA> 26.854  35.558   1.870 1
## 1492   ATOM  1493    CB <NA>   LEU     B    97   <NA> 24.489  33.718   2.236 1
## 1493   ATOM  1494    CG <NA>   LEU     B    97   <NA> 23.211  32.901   2.344 1
## 1494   ATOM  1495   CD1 <NA>   LEU     B    97   <NA> 23.114  32.358   3.719 1
## 1495   ATOM  1496   CD2 <NA>   LEU     B    97   <NA> 22.037  33.773   2.076 1
## 1496   ATOM  1497     N <NA>   ASN     B    98   <NA> 25.121  36.868   1.264 1
## 1497   ATOM  1498    CA <NA>   ASN     B    98   <NA> 25.870  38.101   1.449 1
## 1498   ATOM  1499     C <NA>   ASN     B    98   <NA> 25.102  39.038   2.370 1
## 1499   ATOM  1500     O <NA>   ASN     B    98   <NA> 23.889  39.124   2.261 1
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## 1500   ATOM  1501    CB <NA>   ASN     B    98   <NA> 26.140  38.756   0.086 1
## 1501   ATOM  1502    CG <NA>   ASN     B    98   <NA> 27.048  37.921  -0.814 1
## 1502   ATOM  1503   OD1 <NA>   ASN     B    98   <NA> 28.268  37.895  -0.630 1
## 1503   ATOM  1504   ND2 <NA>   ASN     B    98   <NA> 26.455  37.192  -1.754 1
## 1504   ATOM  1505     N <NA>   PHE     B    99   <NA> 25.809  39.706   3.283 1
## 1505   ATOM  1506    CA <NA>   PHE     B    99   <NA> 25.267  40.855   4.034 1
## 1506   ATOM  1507     C <NA>   PHE     B    99   <NA> 26.351  41.742   4.659 1
## 1507   ATOM  1508     O <NA>   PHE     B    99   <NA> 27.448  41.208   5.013 1
## 1508   ATOM  1509    CB <NA>   PHE     B    99   <NA> 24.284  40.418   5.127 1
## 1509   ATOM  1510    CG <NA>   PHE     B    99   <NA> 24.859  39.479   6.130 1
## 1510   ATOM  1511   CD1 <NA>   PHE     B    99   <NA> 25.061  38.150   5.808 1
## 1511   ATOM  1512   CD2 <NA>   PHE     B    99   <NA> 25.071  39.890   7.436 1
## 1512   ATOM  1513   CE1 <NA>   PHE     B    99   <NA> 25.450  37.240   6.756 1
## 1513   ATOM  1514   CE2 <NA>   PHE     B    99   <NA> 25.473  38.988   8.409 1
## 1514   ATOM  1515    CZ <NA>   PHE     B    99   <NA> 25.658  37.663   8.073 1
## 1515 HETATM  1517    N1 <NA>   MK1     B   902   <NA>  9.280  23.763   3.004 1
## 1516 HETATM  1518    C1 <NA>   MK1     B   902   <NA>  9.498  23.983   4.459 1
## 1517 HETATM  1519    C2 <NA>   MK1     B   902   <NA> 10.591  24.905   4.962 1
## 1518 HETATM  1520    C3 <NA>   MK1     B   902   <NA> 10.591  24.864   6.466 1
## 1519 HETATM  1521    O1 <NA>   MK1     B   902   <NA> 10.937  23.849   7.057 1
## 1520 HETATM  1522    N2 <NA>   MK1     B   902   <NA> 10.193  25.953   7.094 1
## 1521 HETATM  1523    C4 <NA>   MK1     B   902   <NA> 10.145  26.250   8.490 1
## 1522 HETATM  1524    C5 <NA>   MK1     B   902   <NA>  9.379  27.577   8.641 1
## 1523 HETATM  1525    C6 <NA>   MK1     B   902   <NA> 11.398  26.347   9.074 1
## 1524 HETATM  1526    C7 <NA>   MK1     B   902   <NA>  9.364  25.283   9.268 1
## 1525 HETATM  1527    N3 <NA>   MK1     B   902   <NA> 11.819  24.282   4.355 1
## 1526 HETATM  1528    C8 <NA>   MK1     B   902   <NA> 11.753  23.776   2.961 1
## 1527 HETATM  1529    C9 <NA>   MK1     B   902   <NA> 10.440  23.182   2.493 1
## 1528 HETATM  1530   C10 <NA>   MK1     B   902   <NA> 13.083  24.963   4.552 1
## 1529 HETATM  1531   C11 <NA>   MK1     B   902   <NA> 14.203  24.064   5.078 1
## 1530 HETATM  1532    O2 <NA>   MK1     B   902   <NA> 15.242  24.884   4.634 1
## 1531 HETATM  1533   C12 <NA>   MK1     B   902   <NA> 14.440  23.761   6.569 1
## 1532 HETATM  1534   C13 <NA>   MK1     B   902   <NA> 15.573  22.821   7.005 1

## 1533 HETATM  1535   C14 <NA>   MK1     B   902   <NA> 15.644  22.664   8.534 1
## 1534 HETATM  1536   C15 <NA>   MK1     B   902   <NA> 16.733  21.750   8.961 1
## 1535 HETATM  1537   C16 <NA>   MK1     B   902   <NA> 18.058  21.916   8.553 1
## 1536 HETATM  1538   C17 <NA>   MK1     B   902   <NA> 19.037  21.016   8.947 1
## 1537 HETATM  1539   C18 <NA>   MK1     B   902   <NA> 18.673  19.939   9.758 1
## 1538 HETATM  1540   C19 <NA>   MK1     B   902   <NA> 17.347  19.773  10.176 1
## 1539 HETATM  1541   C20 <NA>   MK1     B   902   <NA> 16.374  20.687   9.772 1
## 1540 HETATM  1542   C21 <NA>   MK1     B   902   <NA> 15.447  21.440   6.373 1
## 1541 HETATM  1543    O3 <NA>   MK1     B   902   <NA> 14.367  20.831   6.397 1
## 1542 HETATM  1544    N4 <NA>   MK1     B   902   <NA> 16.583  20.913   5.924 1
## 1543 HETATM  1545   C22 <NA>   MK1     B   902   <NA> 16.692  19.500   5.604 1
## 1544 HETATM  1546   C23 <NA>   MK1     B   902   <NA> 18.067  18.945   5.936 1
## 1545 HETATM  1547    O4 <NA>   MK1     B   902   <NA> 19.061  19.938   5.729 1
## 1546 HETATM  1548   C24 <NA>   MK1     B   902   <NA> 18.226  17.726   5.057 1
## 1547 HETATM  1549   C25 <NA>   MK1     B   902   <NA> 17.476  17.904   3.760 1
## 1548 HETATM  1550   C26 <NA>   MK1     B   902   <NA> 17.500  17.363   2.496 1
```

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## 1549 HETATM  1551   C27 <NA>   MK1     B   902   <NA> 16.613  17.872   1.541 1
## 1550 HETATM  1552   C28 <NA>   MK1     B   902   <NA> 15.722  18.906   1.865 1
## 1551 HETATM  1553   C29 <NA>   MK1     B   902   <NA> 15.683  19.479   3.129 1
## 1552 HETATM  1554   C30 <NA>   MK1     B   902   <NA> 16.504  19.061   4.128 1
## 1553 HETATM  1555   C31 <NA>   MK1     B   902   <NA>  8.033  23.100   2.604 1
## 1554 HETATM  1556   C32 <NA>   MK1     B   902   <NA>  6.666  23.739   2.876 1
## 1555 HETATM  1557   C33 <NA>   MK1     B   902   <NA>  6.158  24.808   2.124 1
## 1556 HETATM  1558    N5 <NA>   MK1     B   902   <NA>  4.911  25.430   2.300 1
## 1557 HETATM  1559   C34 <NA>   MK1     B   902   <NA>  4.207  24.839   3.348 1
## 1558 HETATM  1560   C35 <NA>   MK1     B   902   <NA>  4.654  23.774   4.136 1
## 1559 HETATM  1561   C36 <NA>   MK1     B   902   <NA>  5.905  23.211   3.897 1
## 1560 HETATM  1562     O <NA>   HOH     A   305   <NA> 20.857  43.192  21.450 1
## 1561 HETATM  1563     O <NA>   HOH     A   307   <NA> 14.076  19.789  19.440 1
## 1562 HETATM  1564     O <NA>   HOH     A   309   <NA> 28.075  21.177   7.222 1
## 1563 HETATM  1565     O <NA>   HOH     A   314   <NA> 16.759  40.274   1.287 1
## 1564 HETATM  1566     O <NA>   HOH     A   315   <NA> 13.997  22.233  21.468 1
## 1565 HETATM  1567     O <NA>   HOH     A   324   <NA> 11.282  30.738   1.625 1
## 1566 HETATM  1568     O <NA>   HOH     A   325   <NA> 16.774  42.740   2.296 1
## 1567 HETATM  1569     O <NA>   HOH     A   327   <NA> 14.623  29.552  28.235 1
## 1568 HETATM  1570     O <NA>   HOH     A   328   <NA>  1.651  36.463  19.459 1
## 1569 HETATM  1571     O <NA>   HOH     A   329   <NA> 14.435  44.966  11.913 1
## 1570 HETATM  1572     O <NA>   HOH     A   330   <NA> 19.877  40.160  21.917 1
## 1571 HETATM  1573     O <NA>   HOH     A   331   <NA> 17.126  45.934  10.801 1
## 1572 HETATM  1574     O <NA>   HOH     A   332   <NA>  8.840  28.026   4.860 1
## 1573 HETATM  1575     O <NA>   HOH     A   335   <NA> 10.341  18.480  14.477 1
## 1574 HETATM  1576     O <NA>   HOH     A   341   <NA> 19.233  16.711   9.027 1
## 1575 HETATM  1577     O <NA>   HOH     A   342   <NA> 23.799  21.928  12.391 1
## 1576 HETATM  1578     O <NA>   HOH     A   344   <NA>  9.953  37.934   4.548 1
## 1577 HETATM  1579     O <NA>   HOH     A   345   <NA>  8.478  35.995   5.789 1
## 1578 HETATM  1580     O <NA>   HOH     A   357   <NA>  3.960  19.389  17.384 1
## 1579 HETATM  1581     O <NA>   HOH     A   373   <NA> 27.561  43.155  19.015 1
## 1580 HETATM  1582     O <NA>   HOH     A   384   <NA>  1.245  19.292  18.124 1
## 1581 HETATM  1583     O <NA>   HOH     A   386   <NA> 31.402  27.051   3.335 1

## 1582 HETATM  1584     O <NA>   HOH     A   389   <NA> 32.446  31.200   4.417 1
## 1583 HETATM  1585     O <NA>   HOH     A   391   <NA> 25.480  38.468  17.938 1
## 1584 HETATM  1586     O <NA>   HOH     A   394   <NA> 23.940  41.721   0.346 1
## 1585 HETATM  1587     O <NA>   HOH     A   401   <NA>  5.912  15.727   3.369 1
## 1586 HETATM  1588     O <NA>   HOH     A   406   <NA>  9.272  33.891  12.681 1
## 1587 HETATM  1589     O <NA>   HOH     A   408   <NA> 21.185  25.233  16.048 1
## 1588 HETATM  1590     O <NA>   HOH     A   416   <NA> 18.474  26.012  21.664 1
## 1589 HETATM  1591     O <NA>   HOH     A   420   <NA>  9.469  16.910  17.371 1
## 1590 HETATM  1592     O <NA>   HOH     A   422   <NA> 13.074  17.786  16.615 1
## 1591 HETATM  1593     O <NA>   HOH     A   439   <NA> 28.821  29.338   7.342 1
## 1592 HETATM  1594     O <NA>   HOH     A   457   <NA> 23.284  23.107  15.132 1
## 1593 HETATM  1595     O <NA>   HOH     A   468   <NA>  3.114  26.260   6.773 1
## 1594 HETATM  1596     O <NA>   HOH     A   501   <NA>  6.382  26.424   5.893 1
## 1595 HETATM  1597     O <NA>   HOH     A   503   <NA> 35.293  43.006   5.212 1
## 1596 HETATM  1598     O <NA>   HOH     A   510   <NA> 21.891  49.715   7.192 1
## 1597 HETATM  1599     O <NA>   HOH     A   524   <NA> 34.085  32.735   2.849 1
```

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## 1598 HETATM  1600     O <NA>   HOH     A   529   <NA> 31.491  41.524   6.678 1
## 1599 HETATM  1601     O <NA>   HOH     A   553   <NA>  5.943  34.223   6.748 1
## 1600 HETATM  1602     O <NA>   HOH     A   561   <NA>  0.934  40.259  19.405 1
## 1601 HETATM  1603     O <NA>   HOH     A   567   <NA> 29.539  25.486  13.281 1
## 1602 HETATM  1604     O <NA>   HOH     A   572   <NA> 24.552  17.352  10.295 1
## 1603 HETATM  1605     O <NA>   HOH     A   575   <NA> 23.112  15.510   8.776 1
## 1604 HETATM  1606     O <NA>   HOH     B   301   <NA> 20.445   8.036 -12.631 1
## 1605 HETATM  1607     O <NA>   HOH     B   303   <NA> 20.044  14.822   4.638 1
## 1606 HETATM  1608     O <NA>   HOH     B   304   <NA> 21.538   6.875 -10.099 1
## 1607 HETATM  1609     O <NA>   HOH     B   306   <NA> 22.449  23.958   5.252 1
## 1608 HETATM  1610     O <NA>   HOH     B   308   <NA> 11.720  21.289   7.190 1
## 1609 HETATM  1611     O <NA>   HOH     B   312   <NA> 14.097   5.111 -11.638 1
## 1610 HETATM  1612     O <NA>   HOH     B   313   <NA> 20.998  21.834   6.561 1
## 1611 HETATM  1613     O <NA>   HOH     B   316   <NA> 22.659  14.583  -2.196 1
## 1612 HETATM  1614     O <NA>   HOH     B   317   <NA> 28.724  15.629 -11.660 1
## 1613 HETATM  1615     O <NA>   HOH     B   318   <NA> 16.539  45.207   0.079 1
## 1614 HETATM  1616     O <NA>   HOH     B   319   <NA> 23.678  14.931   2.680 1
## 1615 HETATM  1617     O <NA>   HOH     B   321   <NA> 20.718  15.976  -3.657 1
## 1616 HETATM  1618     O <NA>   HOH     B   323   <NA> 31.249  26.796  -9.595 1
## 1617 HETATM  1619     O <NA>   HOH     B   326   <NA> 28.813  28.445  -2.106 1
## 1618 HETATM  1620     O <NA>   HOH     B   333   <NA> 12.251  39.551  -2.672 1
## 1619 HETATM  1621     O <NA>   HOH     B   334   <NA> 25.465  12.592  -8.670 1
## 1620 HETATM  1622     O <NA>   HOH     B   338   <NA> 12.998  36.205  -3.972 1
## 1621 HETATM  1623     O <NA>   HOH     B   339   <NA> 17.541  17.060 -17.194 1
## 1622 HETATM  1624     O <NA>   HOH     B   340   <NA>  5.321  14.325  -4.866 1
## 1623 HETATM  1625     O <NA>   HOH     B   346   <NA>  9.314  17.330  -9.801 1
## 1624 HETATM  1626     O <NA>   HOH     B   347   <NA>  7.435  26.652 -14.854 1
## 1625 HETATM  1627     O <NA>   HOH     B   348   <NA>  4.405  16.704  -3.635 1
## 1626 HETATM  1628     O <NA>   HOH     B   349   <NA> 19.414   7.026   4.428 1
## 1627 HETATM  1629     O <NA>   HOH     B   350   <NA>  6.718  34.538  -1.322 1
## 1628 HETATM  1630     O <NA>   HOH     B   354   <NA> 15.041  31.743 -13.235 1
## 1629 HETATM  1631     O <NA>   HOH     B   355   <NA> 27.404  32.078 -10.860 1
## 1630 HETATM  1632     O <NA>   HOH     B   356   <NA> 27.673  18.789  -6.155 1

## 1631 HETATM  1633     O <NA>   HOH     B   358   <NA> 21.289  -1.161  -5.102 1
## 1632 HETATM  1634     O <NA>   HOH     B   359   <NA>  6.973  36.523   1.489 1
## 1633 HETATM  1635     O <NA>   HOH     B   360   <NA> 27.602  21.234  -0.635 1
## 1634 HETATM  1636     O <NA>   HOH     B   362   <NA>  3.902   9.376  -0.027 1
## 1635 HETATM  1637     O <NA>   HOH     B   364   <NA> 28.498  36.632  -7.529 1
## 1636 HETATM  1638     O <NA>   HOH     B   366   <NA> 18.572  40.567 -10.042 1
## 1637 HETATM  1639     O <NA>   HOH     B   367   <NA> 25.658  18.970   0.428 1
## 1638 HETATM  1640     O <NA>   HOH     B   369   <NA> 20.843   1.263  -7.014 1
## 1639 HETATM  1641     O <NA>   HOH     B   370   <NA> 13.975  15.741  12.070 1
## 1640 HETATM  1642     O <NA>   HOH     B   374   <NA>  7.661  23.876  -6.324 1
## 1641 HETATM  1643     O <NA>   HOH     B   375   <NA> 10.125   5.706  -1.458 1
## 1642 HETATM  1644     O <NA>   HOH     B   376   <NA> 18.450  20.497 -18.728 1
## 1643 HETATM  1645     O <NA>   HOH     B   377   <NA> 29.267  20.487  -3.497 1
## 1644 HETATM  1646     O <NA>   HOH     B   379   <NA>  6.685  26.541  -5.608 1
## 1645 HETATM  1647     O <NA>   HOH     B   381   <NA> 25.810  26.789 -19.106 1
## 1646 HETATM  1648     O <NA>   HOH     B   383   <NA> 21.144  -4.428 -11.331 1
```

```
## 1647 HETATM  1649     O <NA>   HOH     B   387   <NA> 16.904  27.594 -15.938 1
## 1648 HETATM  1650     O <NA>   HOH     B   388   <NA> 23.926  45.612  -4.998 1
## 1649 HETATM  1651     O <NA>   HOH     B   390   <NA> 25.300  17.493   3.076 1
## 1650 HETATM  1652     O <NA>   HOH     B   392   <NA>  6.618  28.079  -3.427 1
## 1651 HETATM  1653     O <NA>   HOH     B   393   <NA> 19.795  13.651 -16.606 1
## 1652 HETATM  1654     O <NA>   HOH     B   395   <NA>  7.202   9.982  -4.103 1
## 1653 HETATM  1655     O <NA>   HOH     B   400   <NA>  8.474  34.203  -4.893 1
## 1654 HETATM  1656     O <NA>   HOH     B   405   <NA> 16.659  15.866  11.446 1
## 1655 HETATM  1657     O <NA>   HOH     B   410   <NA> 26.400  10.057  -3.287 1
## 1656 HETATM  1658     O <NA>   HOH     B   414   <NA>  9.503   3.489  -4.419 1
## 1657 HETATM  1659     O <NA>   HOH     B   419   <NA> 15.438  12.973 -18.484 1
## 1658 HETATM  1660     O <NA>   HOH     B   425   <NA> 11.428  19.956 -24.551 1
## 1659 HETATM  1661     O <NA>   HOH     B   430   <NA> 18.725  43.171  -5.575 1
## 1660 HETATM  1662     O <NA>   HOH     B   436   <NA> 32.141  29.620  -8.580 1
## 1661 HETATM  1663     O <NA>   HOH     B   443   <NA>  8.811  13.667 -20.256 1
## 1662 HETATM  1664     O <NA>   HOH     B   444   <NA>  4.071  26.169  -0.230 1
## 1663 HETATM  1665     O <NA>   HOH     B   461   <NA> 11.425  44.636  -3.033 1
## 1664 HETATM  1666     O <NA>   HOH     B   469   <NA>  6.902  23.686 -10.066 1
## 1665 HETATM  1667     O <NA>   HOH     B   471   <NA>  5.749  25.785 -19.792 1
## 1666 HETATM  1668     O <NA>   HOH     B   500   <NA> 25.592  16.404  -5.805 1
## 1667 HETATM  1669     O <NA>   HOH     B   502   <NA>  4.040  15.516  -7.200 1
## 1668 HETATM  1670     O <NA>   HOH     B   505   <NA> 28.640  34.232  -5.637 1
## 1669 HETATM  1671     O <NA>   HOH     B   506   <NA>  8.979  11.173  11.112 1
## 1670 HETATM  1672     O <NA>   HOH     B   509   <NA> 19.882   3.986 -18.136 1
## 1671 HETATM  1673     O <NA>   HOH     B   514   <NA> 27.409  15.355   2.200 1
## 1672 HETATM  1674     O <NA>   HOH     B   515   <NA> 17.222  39.766 -23.774 1
## 1673 HETATM  1675     O <NA>   HOH     B   517   <NA> 28.742  24.158 -16.641 1
## 1674 HETATM  1676     O <NA>   HOH     B   525   <NA> 22.694  -2.192 -12.589 1
## 1675 HETATM  1677     O <NA>   HOH     B   526   <NA> 17.901  43.157 -14.082 1
## 1676 HETATM  1678     O <NA>   HOH     B   531   <NA> 18.192   8.914  11.344 1
## 1677 HETATM  1679     O <NA>   HOH     B   532   <NA> 19.507  45.215   1.709 1
## 1678 HETATM  1680     O <NA>   HOH     B   548   <NA>  1.442  14.700  -6.128 1
## 1679 HETATM  1681     O <NA>   HOH     B   549   <NA> 19.908   8.718 -19.215 1

## 1680 HETATM  1682     O <NA>   HOH     B   556   <NA> 21.499  44.884  -1.280 1
## 1681 HETATM  1683     O <NA>   HOH     B   564   <NA> 10.031   8.593 -22.052 1
## 1682 HETATM  1684     O <NA>   HOH     B   568   <NA>  2.817  28.133   2.191 1
## 1683 HETATM  1685     O <NA>   HOH     B   591   <NA> 15.835  40.105  -5.971 1
## 1684 HETATM  1686     O <NA>   HOH     B   595   <NA>  4.515  36.451  -4.499 1
## 1685 HETATM  1687     O <NA>   HOH     B   613   <NA> 24.127 -10.994  -0.982 1
## 1686 HETATM  1688     O <NA>   HOH     B   617   <NA> 30.112  17.912  -4.791 1
##          b segid elesy charge
## 1    38.10  <NA>     N   <NA>
## 2    40.62  <NA>     C   <NA>
## 3    42.64  <NA>     C   <NA>
## 4    43.40  <NA>     O   <NA>
## 5    37.87  <NA>     C   <NA>
## 6    38.40  <NA>     C   <NA>
## 7    38.74  <NA>     C   <NA>
## 8    41.76  <NA>     N   <NA>
```

```
## 9    41.30  <NA>     C   <NA>
## 10   41.38  <NA>     C   <NA>
## 11   43.09  <NA>     O   <NA>
## 12   40.81  <NA>     C   <NA>
## 13   46.61  <NA>     C   <NA>
## 14   50.36  <NA>     C   <NA>
## 15   53.89  <NA>     O   <NA>
## 16   51.46  <NA>     N   <NA>
## 17   37.80  <NA>     N   <NA>
## 18   34.13  <NA>     C   <NA>
## 19   33.19  <NA>     C   <NA>
## 20   32.74  <NA>     O   <NA>
## 21   34.34  <NA>     C   <NA>
## 22   33.95  <NA>     C   <NA>
## 23   33.06  <NA>     C   <NA>
## 24   32.50  <NA>     C   <NA>
## 25   31.65  <NA>     N   <NA>
## 26   30.14  <NA>     C   <NA>
## 27   29.74  <NA>     C   <NA>
## 28   27.88  <NA>     O   <NA>
## 29   29.24  <NA>     C   <NA>
## 30   27.60  <NA>     O   <NA>
## 31   26.26  <NA>     C   <NA>
## 32   29.27  <NA>     N   <NA>
## 33   30.12  <NA>     C   <NA>
## 34   32.98  <NA>     C   <NA>
## 35   32.32  <NA>     O   <NA>
## 36   26.21  <NA>     C   <NA>
## 37   24.56  <NA>     C   <NA>
## 38   20.74  <NA>     C   <NA>
## 39   21.87  <NA>     C   <NA>
## 40   31.52  <NA>     N   <NA>
## 41   30.82  <NA>     C   <NA>

## 42   31.90  <NA>     C   <NA>
## 43   33.26  <NA>     O   <NA>
## 44   28.66  <NA>     C   <NA>
## 45   26.42  <NA>     C   <NA>
## 46   28.49  <NA>     C   <NA>
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## 48   29.88  <NA>     N   <NA>
## 49   28.86  <NA>     C   <NA>
## 50   25.06  <NA>     C   <NA>
## 51   32.14  <NA>     C   <NA>
## 52   27.41  <NA>     C   <NA>
## 53   30.03  <NA>     C   <NA>
## 54   33.01  <NA>     N   <NA>
## 55   32.37  <NA>     C   <NA>
## 56   29.95  <NA>     C   <NA>
## 57   26.55  <NA>     O   <NA>
```

```
## 58   38.12  <NA>     C   <NA>
## 59   48.91  <NA>     C   <NA>
## 60   59.75  <NA>     C   <NA>
## 61   61.83  <NA>     O   <NA>
## 62   59.99  <NA>     N   <NA>
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## 72   30.95  <NA>     N   <NA>
## 73   26.02  <NA>     N   <NA>
## 74   30.21  <NA>     N   <NA>
## 75   29.48  <NA>     C   <NA>
## 76   29.45  <NA>     C   <NA>
## 77   28.45  <NA>     O   <NA>
## 78   27.88  <NA>     C   <NA>
## 79   28.12  <NA>     C   <NA>
## 80   31.64  <NA>     C   <NA>
## 81   28.83  <NA>     N   <NA>
## 82   31.57  <NA>     C   <NA>
## 83   30.48  <NA>     C   <NA>
## 84   31.00  <NA>     O   <NA>
## 85   31.09  <NA>     C   <NA>
## 86   35.91  <NA>     C   <NA>
## 87   40.15  <NA>     C   <NA>
## 88   40.51  <NA>     C   <NA>
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## 90   30.14  <NA>     C   <NA>

## 91   33.13  <NA>     C   <NA>
## 92   34.48  <NA>     O   <NA>
## 93   27.12  <NA>     C   <NA>
## 94   28.48  <NA>     C   <NA>
## 95   26.29  <NA>     C   <NA>
## 96   32.34  <NA>     N   <NA>
## 97   32.56  <NA>     C   <NA>
## 98   33.07  <NA>     C   <NA>
## 99   33.62  <NA>     O   <NA>
## 100  33.81  <NA>     C   <NA>
## 101  40.47  <NA>     O   <NA>
## 102  34.22  <NA>     C   <NA>
## 103  31.84  <NA>     N   <NA>
## 104  32.26  <NA>     C   <NA>
## 105  33.69  <NA>     C   <NA>
## 106  30.43  <NA>     O   <NA>
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```
## 107  32.80  <NA>     C   <NA>
## 108  31.81  <NA>     C   <NA>
## 109  27.69  <NA>     C   <NA>
## 110  32.46  <NA>     C   <NA>
## 111  36.78  <NA>     N   <NA>
## 112  38.20  <NA>     C   <NA>
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## 126  47.78  <NA>     C   <NA>
## 127  50.24  <NA>     C   <NA>
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## 133  59.71  <NA>     C   <NA>
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## 135  63.20  <NA>     O   <NA>
## 136  59.37  <NA>     N   <NA>
## 137  58.98  <NA>     C   <NA>
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## 139  56.84  <NA>     O   <NA>

## 140  63.37  <NA>     C   <NA>
## 141  67.60  <NA>     C   <NA>
## 142  72.39  <NA>     C   <NA>
## 143  76.16  <NA>     O   <NA>
## 144  74.55  <NA>     N   <NA>
## 145  53.88  <NA>     N   <NA>
## 146  49.32  <NA>     C   <NA>
## 147  46.38  <NA>     C   <NA>
## 148  43.18  <NA>     O   <NA>
## 149  47.14  <NA>     C   <NA>
## 150  46.02  <NA>     C   <NA>
## 151  46.45  <NA>     C   <NA>
## 152  46.45  <NA>     C   <NA>
## 153  44.76  <NA>     N   <NA>
## 154  44.52  <NA>     C   <NA>
## 155  42.87  <NA>     C   <NA>
```

```
## 156  41.39  <NA>     O   <NA>
## 157  43.50  <NA>     C   <NA>
## 158  46.90  <NA>     C   <NA>
## 159  49.38  <NA>     C   <NA>
## 160  54.07  <NA>     C   <NA>
## 161  60.37  <NA>     N   <NA>
## 162  41.75  <NA>     N   <NA>
## 163  40.02  <NA>     C   <NA>
## 164  35.18  <NA>     C   <NA>
## 165  30.96  <NA>     O   <NA>
## 166  45.21  <NA>     C   <NA>
## 167  55.20  <NA>     C   <NA>
## 168  63.88  <NA>     C   <NA>
## 169  67.73  <NA>     O   <NA>
## 170  60.14  <NA>     O   <NA>
## 171  30.04  <NA>     N   <NA>
## 172  26.79  <NA>     C   <NA>
## 173  26.36  <NA>     C   <NA>
## 174  24.88  <NA>     O   <NA>
## 175  22.80  <NA>     C   <NA>
## 176  25.58  <NA>     N   <NA>
## 177  25.08  <NA>     C   <NA>
## 178  23.67  <NA>     C   <NA>
## 179  25.94  <NA>     O   <NA>
## 180  27.31  <NA>     C   <NA>
## 181  27.99  <NA>     C   <NA>
## 182  29.29  <NA>     C   <NA>
## 183  31.05  <NA>     C   <NA>
## 184  21.67  <NA>     N   <NA>
## 185  18.03  <NA>     C   <NA>
## 186  19.77  <NA>     C   <NA>
## 187  20.40  <NA>     O   <NA>
## 188  15.36  <NA>     C   <NA>

## 189  18.86  <NA>     C   <NA>
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## 192  18.83  <NA>     N   <NA>
## 193  18.91  <NA>     C   <NA>
## 194  16.83  <NA>     C   <NA>
## 195  17.64  <NA>     O   <NA>
## 196  16.55  <NA>     C   <NA>
## 197  21.74  <NA>     C   <NA>
## 198  22.87  <NA>     O   <NA>
## 199  24.00  <NA>     O   <NA>
## 200  15.44  <NA>     N   <NA>
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## 202  15.12  <NA>     C   <NA>
## 203  12.07  <NA>     O   <NA>
## 204  17.69  <NA>     C   <NA>
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```
## 205  16.60  <NA>     O   <NA>
## 206  13.90  <NA>     C   <NA>
## 207  17.61  <NA>     N   <NA>
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## 209  13.84  <NA>     C   <NA>
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## 212  13.20  <NA>     C   <NA>
## 213  17.23  <NA>     C   <NA>
## 214  15.43  <NA>     O   <NA>
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## 225  22.55  <NA>     C   <NA>
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## 227  22.98  <NA>     O   <NA>
## 228  24.31  <NA>     C   <NA>
## 229  25.77  <NA>     C   <NA>
## 230  37.03  <NA>     O   <NA>
## 231  33.64  <NA>     O   <NA>
## 232  21.65  <NA>     N   <NA>
## 233  19.28  <NA>     C   <NA>
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## 236  21.21  <NA>     C   <NA>
## 237  17.85  <NA>     O   <NA>

## 238  20.08  <NA>     C   <NA>
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## 242  21.86  <NA>     O   <NA>
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## 248  25.37  <NA>     C   <NA>
## 249  25.11  <NA>     O   <NA>
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## 252  31.03  <NA>     C   <NA>
## 253  30.18  <NA>     C   <NA>
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```
## 254  29.09  <NA>     N   <NA>
## 255  32.79  <NA>     C   <NA>
## 256  33.96  <NA>     C   <NA>
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## 258  36.48  <NA>     C   <NA>
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## 270  50.36  <NA>     O   <NA>
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## 273  32.08  <NA>     C   <NA>
## 274  33.50  <NA>     C   <NA>
## 275  33.82  <NA>     O   <NA>
## 276  31.77  <NA>     C   <NA>
## 277  33.78  <NA>     C   <NA>
## 278  38.76  <NA>     S   <NA>
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## 281  33.81  <NA>     C   <NA>
## 282  32.96  <NA>     C   <NA>
## 283  32.62  <NA>     O   <NA>
## 284  34.02  <NA>     C   <NA>
## 285  38.20  <NA>     O   <NA>
## 286  35.12  <NA>     N   <NA>

## 287  38.10  <NA>     C   <NA>
## 288  42.61  <NA>     C   <NA>
## 289  41.25  <NA>     O   <NA>
## 290  35.60  <NA>     C   <NA>
## 291  33.68  <NA>     C   <NA>
## 292  33.91  <NA>     C   <NA>
## 293  34.05  <NA>     C   <NA>
## 294  45.17  <NA>     N   <NA>
## 295  45.32  <NA>     C   <NA>
## 296  44.13  <NA>     C   <NA>
## 297  44.57  <NA>     O   <NA>
## 298  48.51  <NA>     C   <NA>
## 299  47.48  <NA>     C   <NA>
## 300  48.21  <NA>     C   <NA>
## 301  43.26  <NA>     N   <NA>
## 302  44.04  <NA>     C   <NA>
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## 303  46.02  <NA>     C   <NA>
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## 305  47.22  <NA>     N   <NA>
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## 307  45.12  <NA>     C   <NA>
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## 332  38.09  <NA>     C   <NA>
## 333  37.97  <NA>     O   <NA>
## 334  40.22  <NA>     C   <NA>
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## 1665 63.96  <NA>     0   <NA>
## 1666 23.98  <NA>     0   <NA>
## 1667 52.93  <NA>     0   <NA>
## 1668 58.06  <NA>     0   <NA>
## 1669 64.79  <NA>     0   <NA>
## 1670 55.54  <NA>     0   <NA>
## 1671 61.69  <NA>     0   <NA>
## 1672 69.12  <NA>     0   <NA>
## 1673 78.93  <NA>     0   <NA>
## 1674 71.37  <NA>     0   <NA>
```

```
## 1675 78.14  <NA>     O   <NA>
## 1676 54.05  <NA>     O   <NA>
## 1677 72.78  <NA>     O   <NA>
## 1678 58.40  <NA>     O   <NA>
## 1679 58.78  <NA>     O   <NA>
## 1680 68.40  <NA>     O   <NA>
## 1681 64.90  <NA>     O   <NA>
## 1682 67.95  <NA>     O   <NA>
## 1683 53.68  <NA>     O   <NA>
## 1684 49.41  <NA>     O   <NA>
## 1685 64.49  <NA>     O   <NA>
## 1686 54.09  <NA>     O   <NA>
```

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

Due to the limitations of x-ray diffraction, the resolution of the structures are limited and only the oxygen atom can be seen from a water molecule.

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)?

HOH308:0.

Q6. As you have hopefully observed HIV protease is a homodimer (i.e. it is composed of two identical chains). With the aid of the graphic display and the sequence viewer extension can you identify secondary structure elements that are likely to only form in the dimer rather than the monomer?

The hollow space in the center of the homodimer where the ligand is found.

3. Introduction to Bio3D in R

Q7: How many amino acid residues are there in this pdb object?

There are 198.

Q8: Name one of the two non-protein residues?

MK1

Q9: How many protein chains are in this structure?

There are 2.

4. Comparative structure analysis of Adenylate Kinase

Q10. Which of the packages above is found only on BioConductor and not CRAN?

msa

Q11. Which of the above packages is not found on BioConductor or CRAN?:

bio3d-view

Q12. True or False? Functions from the devtools package can be used to install packages from GitHub and BitBucket?

TRUE

```
# install.packages("httr")
aa <- get.seq("1ake_A")
```

```
## Warning in get.seq("1ake_A"): Removing existing file: seqs.fasta

## Fetching... Please wait. Done.
```

```
aa
```

```
##              1        .         .         .         .         .         60
## pdb|1AKE|A   MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAAVKSGSELGKQAKDIMDAGKLVT
##              1        .         .         .         .         .         60
##
##             61        .         .         .         .         .         120
## pdb|1AKE|A   DELVIALVKERIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVDRI

##             61        .         .         .         .         .         120
##
##            121        .         .         .         .         .         180
## pdb|1AKE|A   VGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKDDQEETVRKRLVEYHQMTAPLIG
##            121        .         .         .         .         .         180
##
##            181        .         .         .   214
## pdb|1AKE|A   YYSKEAEAGNTKYAKVDGTKPVAEVRADLEKILG
##            181        .         .         .   214
##
## Call:
##   read.fasta(file = outfile)
##
## Class:
##   fasta
##
## Alignment dimensions:
##   1 sequence rows; 214 position columns (214 non-gap, 0 gap)
##
## + attr: id, ali, call
```

Q13. How many amino acids are in this sequence, i.e. how long is this sequence?

There are 214 amino acids.

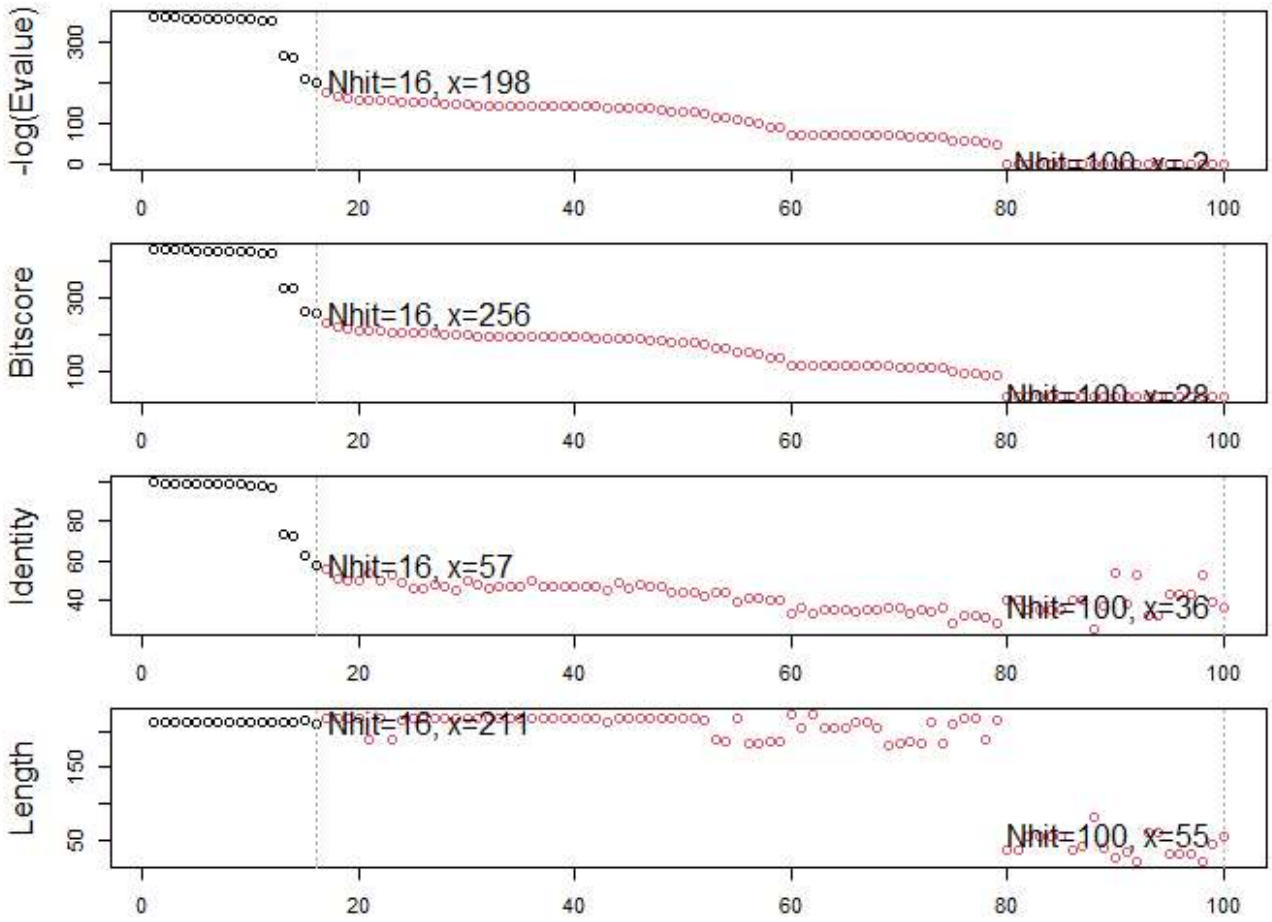
```
# Blast or hmmer search
b <- blast.pdb(aa)
```

```
##  Searching ... please wait (updates every 5 seconds) RID = 0V6VMPSJ013
##  .............
##  Reporting 100 hits
```

```
# Plot a summary of search results
hits <- plot(b)
```

```
##   * Possible cutoff values:    197 -3
##             Yielding Nhits:    16 100
##

##   * Chosen cutoff value of:    197
##             Yielding Nhits:    16
```




```
# List out some 'top hits'
head(hits$pdb.id)
```

```
## [1] "1AKE_A" "4X8M_A" "6S36_A" "6RZE_A" "4X8H_A" "3HPR_A"
```

```
hits$pdb.id
```

```
##  [1] "1AKE_A" "4X8M_A" "6S36_A" "6RZE_A" "4X8H_A" "3HPR_A" "1E4V_A" "5EJE_A"
##  [9] "1E4Y_A" "3X2S_A" "6HAP_A" "6HAM_A" "4K46_A" "4NP6_A" "3GMT_A" "4PZL_A"
```

```
# Download releated PDB files
files <- get.pdb(hits$pdb.id, path="pdbs", split=TRUE, gzip=TRUE)
```

```
## Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE): pdbs/
## 1AKE.pdb exists. Skipping download
```

```
## Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE): pdbs/
## 4X8M.pdb exists. Skipping download

## Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE): pdbs/
## 6S36.pdb exists. Skipping download

## Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE): pdbs/
## 6RZE.pdb exists. Skipping download

## Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE): pdbs/
## 4X8H.pdb exists. Skipping download

## Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE): pdbs/
## 3HPR.pdb exists. Skipping download

## Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE): pdbs/
## 1E4V.pdb exists. Skipping download

## Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE): pdbs/
## 5EJE.pdb exists. Skipping download

## Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE): pdbs/
## 1E4Y.pdb exists. Skipping download

## Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE): pdbs/
## 3X2S.pdb exists. Skipping download

## Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE): pdbs/
## 6HAP.pdb exists. Skipping download

## Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE): pdbs/
## 6HAM.pdb exists. Skipping download

## Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE): pdbs/
## 4K46.pdb exists. Skipping download

## Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE): pdbs/
## 4NP6.pdb exists. Skipping download

## Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE): pdbs/
## 3GMT.pdb exists. Skipping download

## Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE): pdbs/
## 4PZL.pdb exists. Skipping download

##   |                                                                      |
```

Align and superpose structures

```
# Align releated PDBs
pdbs <- pdbaln(files, fit = TRUE)#, exefile="msa")
```

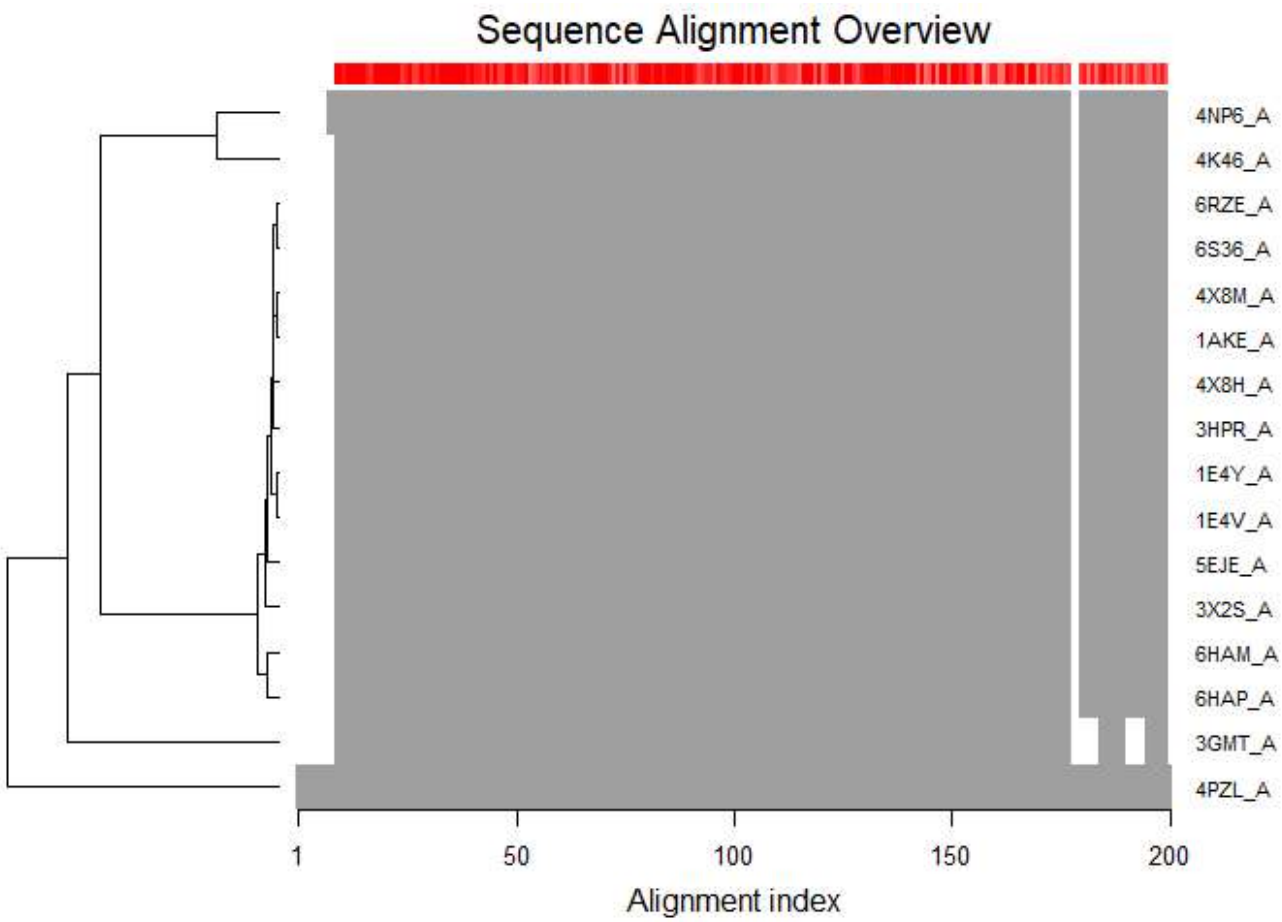
```
## Reading PDB files:
## pdbs/split_chain/1AKE_A.pdb
## pdbs/split_chain/4X8M_A.pdb
## pdbs/split_chain/6S36_A.pdb
## pdbs/split_chain/6RZE_A.pdb
## pdbs/split_chain/4X8H_A.pdb
## pdbs/split_chain/3HPR_A.pdb
## pdbs/split_chain/1E4V_A.pdb
## pdbs/split_chain/5EJE_A.pdb
## pdbs/split_chain/1E4Y_A.pdb
## pdbs/split_chain/3X2S_A.pdb
## pdbs/split_chain/6HAP_A.pdb
## pdbs/split_chain/6HAM_A.pdb
## pdbs/split_chain/4K46_A.pdb
## pdbs/split_chain/4NP6_A.pdb
## pdbs/split_chain/3GMT_A.pdb
## pdbs/split_chain/4PZL_A.pdb
##    PDB has ALT records, taking A only, rm.alt=TRUE
## ..   PDB has ALT records, taking A only, rm.alt=TRUE
## .   PDB has ALT records, taking A only, rm.alt=TRUE
## ..   PDB has ALT records, taking A only, rm.alt=TRUE
## ..   PDB has ALT records, taking A only, rm.alt=TRUE
## ....   PDB has ALT records, taking A only, rm.alt=TRUE
## .   PDB has ALT records, taking A only, rm.alt=TRUE
## ....
##
## Extracting sequences
##
## pdb/seq: 1   name: pdbs/split_chain/1AKE_A.pdb
##    PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 2   name: pdbs/split_chain/4X8M_A.pdb
## pdb/seq: 3   name: pdbs/split_chain/6S36_A.pdb
##    PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 4   name: pdbs/split_chain/6RZE_A.pdb

##    PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 5   name: pdbs/split_chain/4X8H_A.pdb
## pdb/seq: 6   name: pdbs/split_chain/3HPR_A.pdb
##    PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 7   name: pdbs/split_chain/1E4V_A.pdb
## pdb/seq: 8   name: pdbs/split_chain/5EJE_A.pdb
```

```
##    PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 9   name: pdbs/split_chain/1E4Y_A.pdb
## pdb/seq: 10   name: pdbs/split_chain/3X2S_A.pdb
## pdb/seq: 11   name: pdbs/split_chain/6HAP_A.pdb
## pdb/seq: 12   name: pdbs/split_chain/6HAM_A.pdb
##    PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 13   name: pdbs/split_chain/4K46_A.pdb
##    PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 14   name: pdbs/split_chain/4NP6_A.pdb
## pdb/seq: 15   name: pdbs/split_chain/3GMT_A.pdb
## pdb/seq: 16   name: pdbs/split_chain/4PZL_A.pdb
```

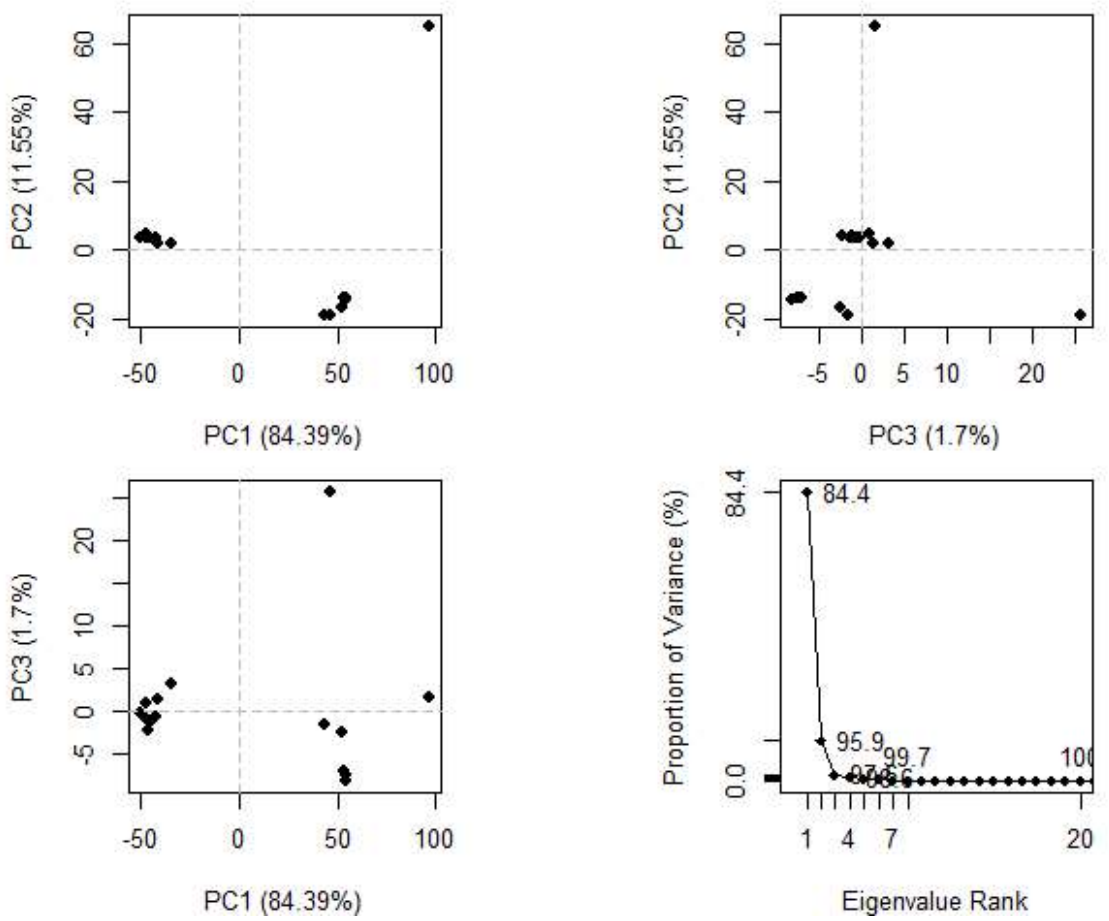
```
# Vector containing PDB codes for figure axis
ids <- basename.pdb(pdbs$id)

# Draw schematic alignment
plot(pdbs, labels=ids)
```



PCA

```
# Perform PCA
pc.xray <- pca(pdbs)
plot(pc.xray)
```

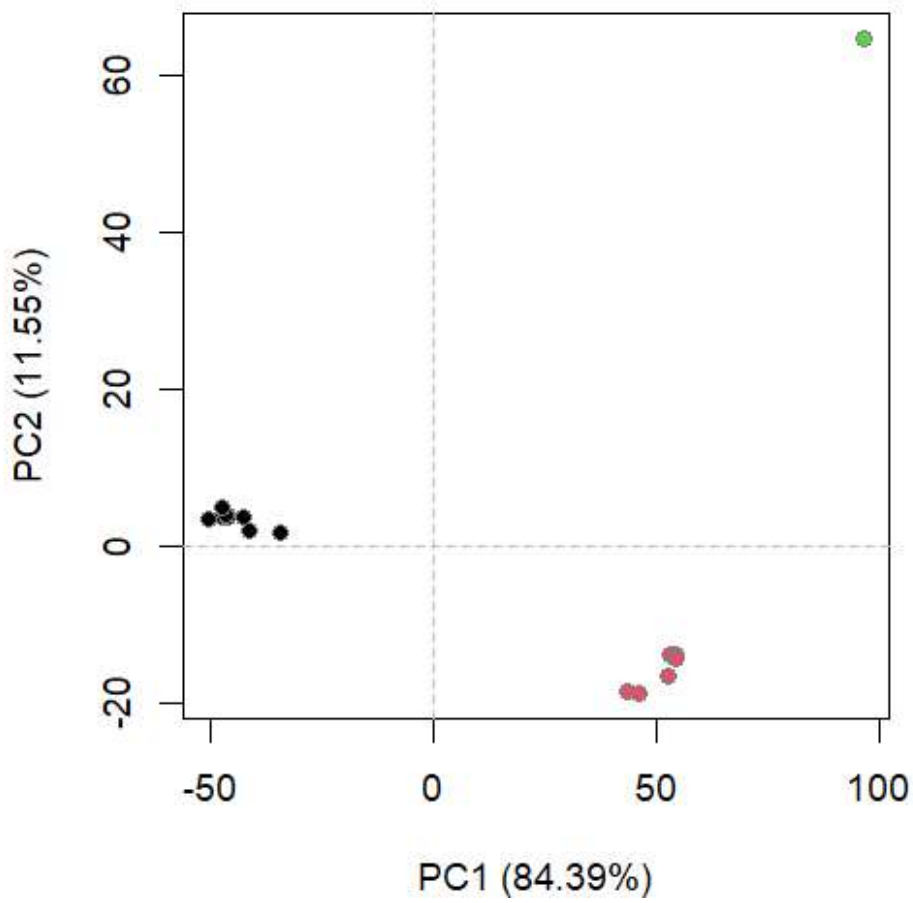



```
# Calculate RMSD
rd <- rmsd(pdbs)
```

```
## Warning in rmsd(pdbs): No indices provided, using the 204 non NA positions
```

```
# Structure-based clustering
hc.rd <- hclust(dist(rd))
grps.rd <- cutree(hc.rd, k=3)

plot(pc.xray, 1:2, col="grey50", bg=grps.rd, pch=21, cex=1)
```



6. Normal mode analysis

```
pdb <- read.pdb("1ake")
```

```
##   Note: Accessing on-line PDB file
##    PDB has ALT records, taking A only, rm.alt=TRUE
```

```
pdb
```

```
##
##  Call:  read.pdb(file = "1ake")
##
##    Total Models#: 1
##      Total Atoms#: 3804,  XYZs#: 11412  Chains#: 2  (values: A B)
##
##      Protein Atoms#: 3312  (residues/Calpha atoms#: 428)
##      Nucleic acid Atoms#: 0  (residues/phosphate atoms#: 0)
```

```
##
##      Non-protein/nucleic Atoms#: 492  (residues: 380)
##      Non-protein/nucleic resid values: [ AP5 (2), HOH (378) ]
##
##    Protein sequence:
##       MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAAVKSGSELGKQAKDIMDAGKLVT
##       DELVIALVKERIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVDRI
##       VGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKDDQEETVRKRLVEYHQMTAPLIG
##       YYSKEAEAGNTKYAKVDGTKPVAEVRADLEKILGMRIILLGAPGA...<cut>...KILG
##

## + attr: atom, xyz, seqres, helix, sheet,
##         calpha, remark, call
```

```
# trim to chain A only
chain <- trim.pdb(pdb, chain = "A")
chain
```

```
##
##  Call:  trim.pdb(pdb = pdb, chain = "A")
##
##    Total Models#: 1
##      Total Atoms#: 1954,  XYZs#: 5862  Chains#: 1  (values: A)
##
##      Protein Atoms#: 1656  (residues/Calpha atoms#: 214)
##      Nucleic acid Atoms#: 0  (residues/phosphate atoms#: 0)
##
##      Non-protein/nucleic Atoms#: 298  (residues: 242)

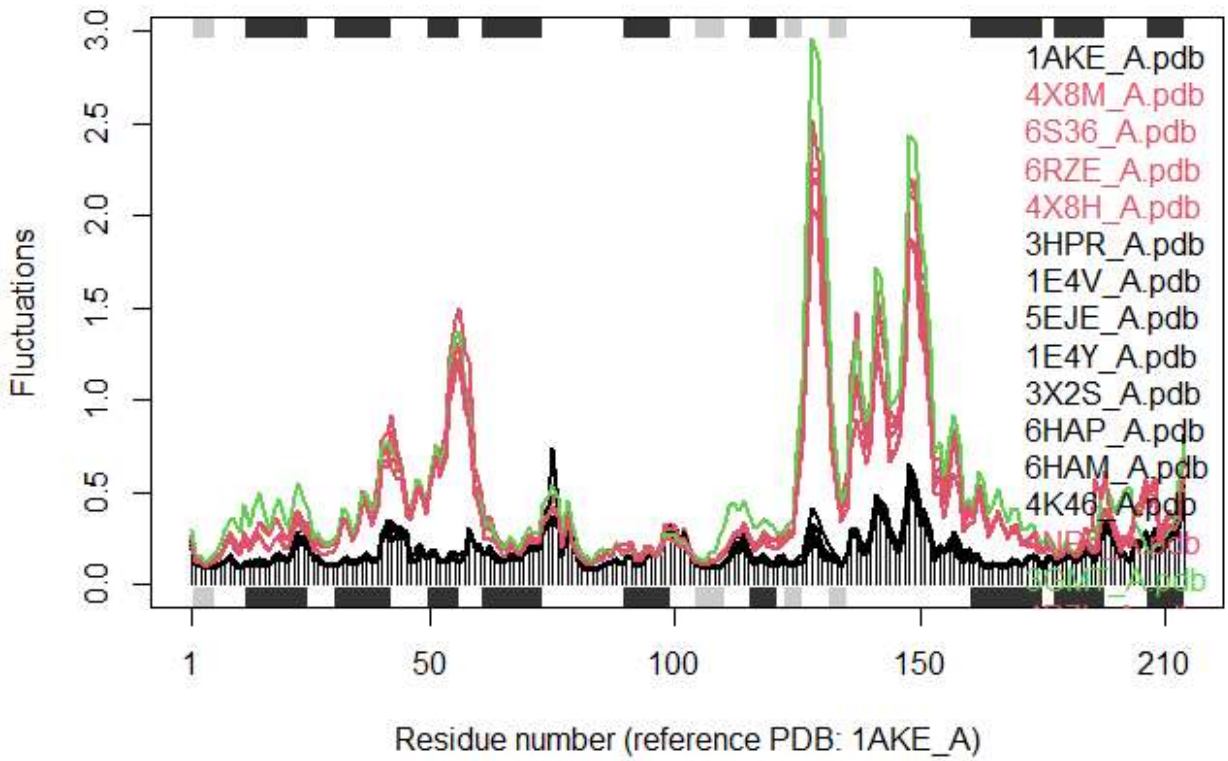
##      Non-protein/nucleic resid values: [ AP5 (1), HOH (241) ]
##
##    Protein sequence:
##       MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAAVKSGSELGKQAKDIMDAGKLVT
##       DELVIALVKERIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVDRI
##       VGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKDDQEETVRKRLVEYHQMTAPLIG
##       YYSKEAEAGNTKYAKVDGTKPVAEVRADLEKILG
##
## + attr: atom, helix, sheet, seqres, xyz,
##         calpha, call
```

```
# NMA of all structures
modes <- nma(pdbs)
```

```
##
## Details of Scheduled Calculation:
##   ... 16 input structures
##   ... storing 606 eigenvectors for each structure
##   ... dimension of x$U.subspace: ( 612x606x16 )
##   ... coordinate superposition prior to NM calculation
##   ... aligned eigenvectors (gap containing positions removed)
##   ... estimated memory usage of final 'eNMA' object: 45.4 Mb
##
##   |                                                                    |
```

```
plot(modes, pdbs, col=grps.rd)
```

```
## Extracting SSE from pdbs$sse attribute
```

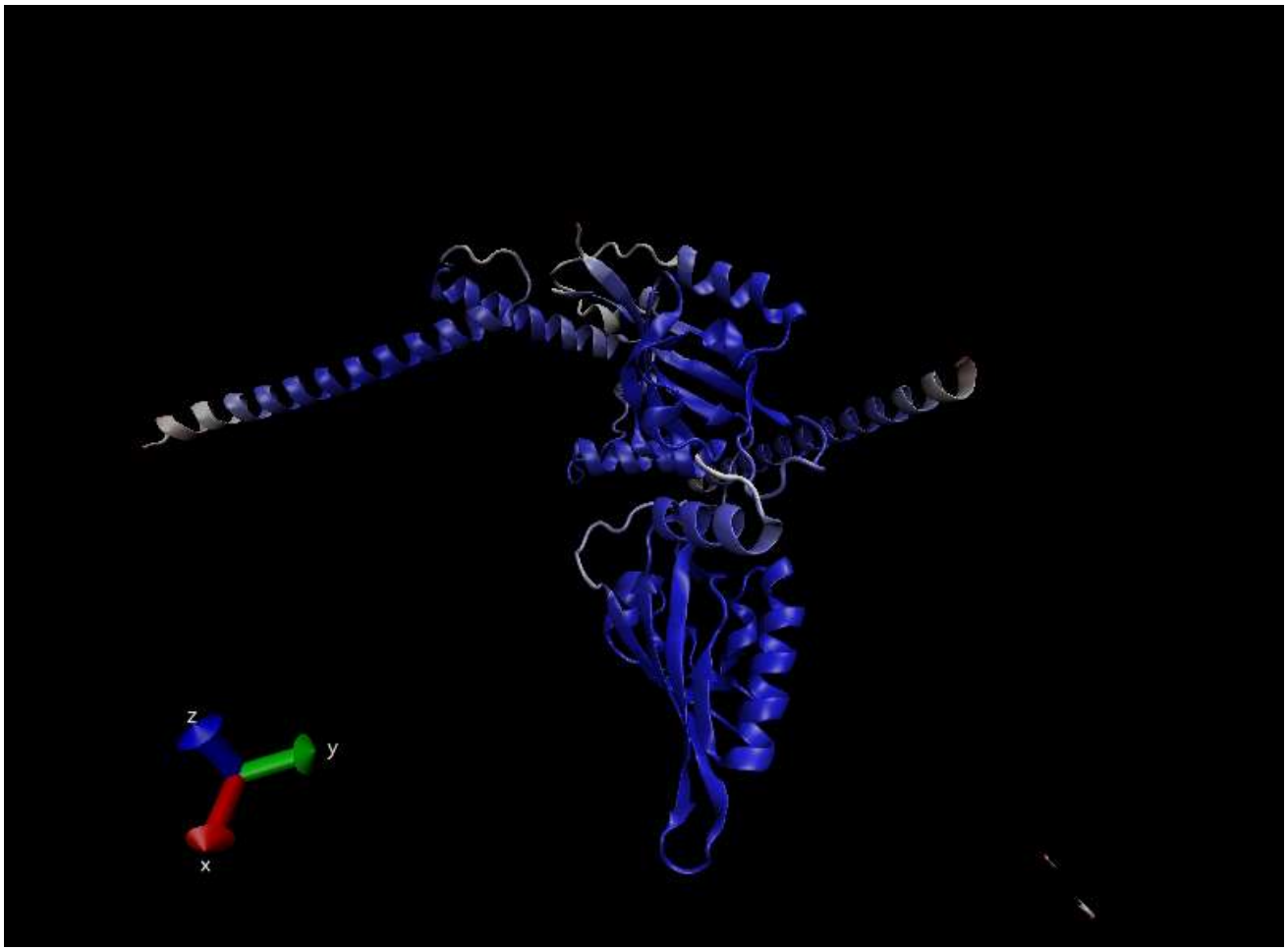



```
# NMA of a chain
modes <- nma(chain)
```

```
##  Building Hessian...     Done in 0.02 seconds.
##  Diagonalizing Hessian...    Done in 0.36 seconds.
```

```
mktrj.nma(modes, mode = 7, file = "mode_7.pdb")
```

AlphaFold structure of protein of interest (from project)



Only parts where beta > 50 are shown.

Q14. What do you note about this plot? Are the black and colored lines similar or different? Where do you think they differ most and why?

The black lines are noticeably lower than the colored lines at residues 50-60 and 130-150. This means that the protein structures represented by the colored lines are significantly more flexible at those positions compared to the proteins represented by the black lines.