Class 11: Structural Bioinformatics pt 2

Morgan Black (PID: A14904860)

Before looking at AlphaFold, we'll finish the rest of Section 4 from last class' lab. (I've already done this in my previous Class 10 Quarto document I submitted on Gradescope, but I'll repeat it again here with the class)

```r
library(bio3d)
id <- "1ake_A"
aa <- get.seq(id)
```

```
Warning in get.seq(id): Removing existing file: seqs.fasta
```

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

```r
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
```

```
b <- blast.pdb(aa)
```

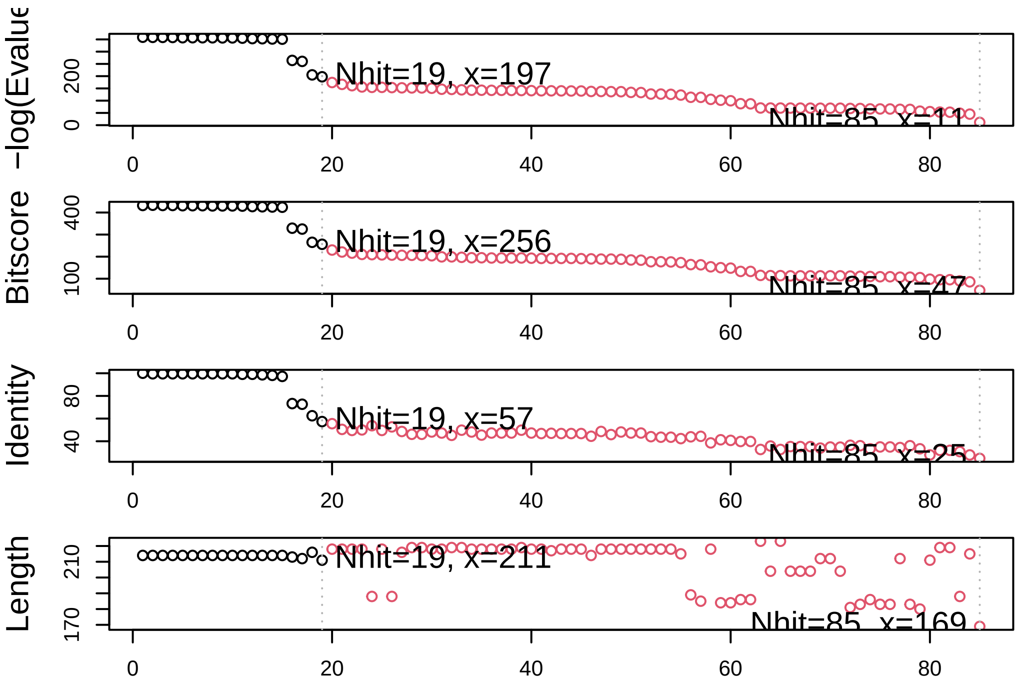
```
 Searching ... please wait (updates every 5 seconds) RID = JXEGUWX9013
 .
 Reporting 85 hits
```

```
head(b$hit.tbl)
```

```
        queryid subjectids identity alignmentlength mismatches gapopens q.start
1 Query_7228653     1AKE_A  100.000             214          0        0       1
2 Query_7228653     8BQF_A   99.533             214          1        0       1
3 Query_7228653     4X8M_A   99.533             214          1        0       1
4 Query_7228653     6S36_A   99.533             214          1        0       1
5 Query_7228653     8Q2B_A   99.533             214          1        0       1
6 Query_7228653     8RJ9_A   99.533             214          1        0       1
  q.end s.start s.end    evalue bitscore positives mlog.evalue pdb.id    acc
1   214       1   214 1.58e-156      432    100.00    358.7458 1AKE_A 1AKE_A
2   214      21   234 2.58e-156      433    100.00    358.2555 8BQF_A 8BQF_A
3   214       1   214 2.82e-156      432    100.00    358.1665 4X8M_A 4X8M_A
4   214       1   214 4.14e-156      432    100.00    357.7826 6S36_A 6S36_A
5   214       1   214 1.10e-155      431     99.53    356.8054 8Q2B_A 8Q2B_A
6   214       1   214 1.10e-155      431     99.53    356.8054 8RJ9_A 8RJ9_A
```

```
hits <- plot(b)
```

```
  * Possible cutoff values:    197 11
            Yielding Nhits:    19 85

  * Chosen cutoff value of:    197
            Yielding Nhits:    19
```



Top hits that we like from the blast results (find the identifiers):

```
hits$pdb.id
```

```
 [1] "1AKE_A" "8BQF_A" "4X8M_A" "6S36_A" "8Q2B_A" "8RJ9_A" "6RZE_A" "4X8H_A"
 [9] "3HPR_A" "1E4V_A" "5EJE_A" "1E4Y_A" "3X2S_A" "6HAP_A" "6HAM_A" "4K46_A"
[17] "4NP6_A" "3GMT_A" "4PZL_A"
```

```
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.gz exists. Skipping download
```

```
Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE):
pdbs/8BQF.pdb.gz exists. Skipping download
```

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

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

```
Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE):
pdbs/8Q2B.pdb.gz exists. Skipping download

Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE):
pdbs/8RJ9.pdb.gz exists. Skipping download

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

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

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

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

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

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

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

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

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

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

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

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

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

```
  |
  |                                                                      |   0%
  |
  |====                                                                  |   5%
  |
  |=======                                                               |  11%
  |
  |===========                                                           |  16%
  |
  |===============                                                       |  21%
  |
  |==================                                                    |  26%
  |
  |======================                                                |  32%
  |
  |==========================                                            |  37%
  |
  |=============================                                         |  42%
  |
  |=================================                                     |  47%
  |
  |=====================================                                 |  53%
  |
  |=========================================                             |  58%
  |
  |============================================                          |  63%
  |
  |================================================                      |  68%
  |
  |====================================================                  |  74%
  |
  |=======================================================               |  79%
  |
  |===========================================================           |  84%
  |
  |==============================================================        |  89%
  |
  |==================================================================    |  95%
  |
  |======================================================================| 100%
```

Above, we've downloaded the ADK structures but viewing all of them is messy. They need to be aligned and superimposed.

Align and fit (superimpose) the structures:

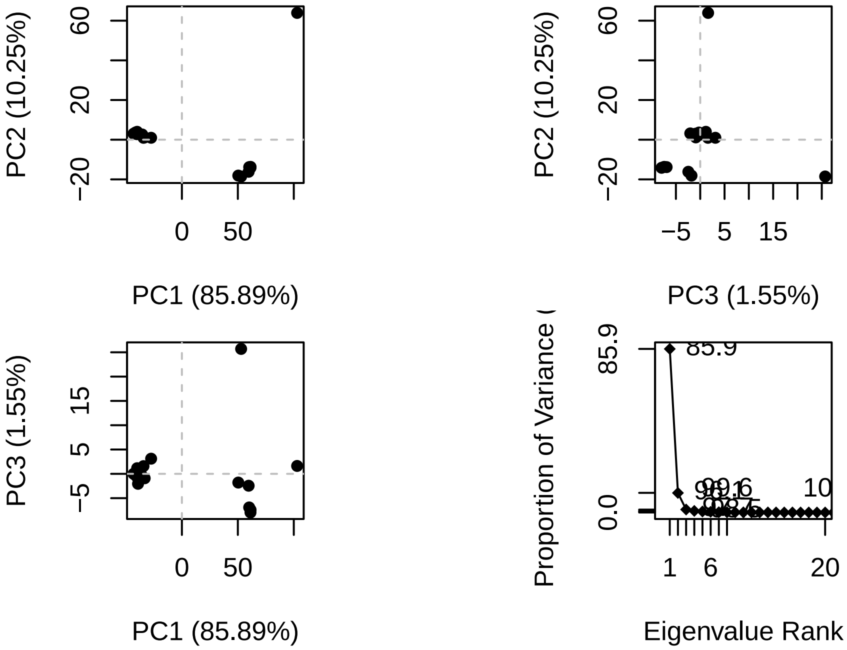
```r
pdbs <- pdbaln(files, fit = TRUE, exefile="msa")
```

```
Reading PDB files:
pdbs/split_chain/1AKE_A.pdb
pdbs/split_chain/8BQF_A.pdb
pdbs/split_chain/4X8M_A.pdb
pdbs/split_chain/6S36_A.pdb
pdbs/split_chain/8Q2B_A.pdb
pdbs/split_chain/8RJ9_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
..   PDB has ALT records, taking A only, rm.alt=TRUE
....   PDB has ALT records, taking A only, rm.alt=TRUE
```

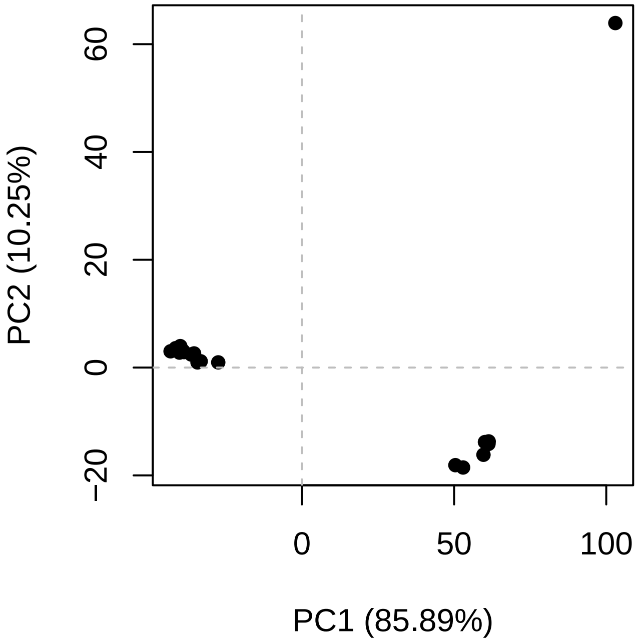
```
.   PDB has ALT records, taking A only, rm.alt=TRUE
....

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/8BQF_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 3   name: pdbs/split_chain/4X8M_A.pdb
pdb/seq: 4   name: pdbs/split_chain/6S36_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 5   name: pdbs/split_chain/8Q2B_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 6   name: pdbs/split_chain/8RJ9_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 7   name: pdbs/split_chain/6RZE_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 8   name: pdbs/split_chain/4X8H_A.pdb
pdb/seq: 9   name: pdbs/split_chain/3HPR_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 10   name: pdbs/split_chain/1E4V_A.pdb
pdb/seq: 11   name: pdbs/split_chain/5EJE_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 12   name: pdbs/split_chain/1E4Y_A.pdb
pdb/seq: 13   name: pdbs/split_chain/3X2S_A.pdb
pdb/seq: 14   name: pdbs/split_chain/6HAP_A.pdb
pdb/seq: 15   name: pdbs/split_chain/6HAM_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 16   name: pdbs/split_chain/4K46_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 17   name: pdbs/split_chain/4NP6_A.pdb
pdb/seq: 18   name: pdbs/split_chain/3GMT_A.pdb
pdb/seq: 19   name: pdbs/split_chain/4PZL_A.pdb
```

PCA

```r
pc <- pca(pdbs)
plot(pc)
```



```
#To just plot PC1. vs PC2
plot(pc, pc.axes=c(1:2))
```



To examine in more detail what PC1 is capturing, we'll plot the loadings or make a movie of moving along PC1.

```
mktrj(pc, pc=1, file="pc1.pdb")
```

Now we'll move on to the Class 11 lab sheet after working through how to use Alphafold and Mol* together to look at different models of the HIV-Pr dimer.

```
pdb_files <- list.files(path='/Users/mobla1/Documents/Graduate/Fall 2024/BGGN213/Class 11/di
                        pattern="*.pdb",
                        full.names = TRUE)

basename(pdb_files)
```

```
[1] "dimer_test_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_1_seed_000.pdb"
[2] "dimer_test_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000.pdb"
[3] "dimer_test_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000.pdb"
[4] "dimer_test_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_seed_000.pdb"
[5] "dimer_test_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000.pdb"
```

```
library(bio3d)
pdbs <- pdbaln(pdb_files, fit=TRUE, exefile="msa")
```

```
Reading PDB files:
/Users/mobla1/Documents/Graduate/Fall 2024/BGGN213/Class 11/dimer_test_23119/dimer_test_2311
/Users/mobla1/Documents/Graduate/Fall 2024/BGGN213/Class 11/dimer_test_23119/dimer_test_2311
/Users/mobla1/Documents/Graduate/Fall 2024/BGGN213/Class 11/dimer_test_23119/dimer_test_2311
/Users/mobla1/Documents/Graduate/Fall 2024/BGGN213/Class 11/dimer_test_23119/dimer_test_2311
/Users/mobla1/Documents/Graduate/Fall 2024/BGGN213/Class 11/dimer_test_23119/dimer_test_2311
.....

Extracting sequences

pdb/seq: 1   name: /Users/mobla1/Documents/Graduate/Fall 2024/BGGN213/Class 11/dimer_test_23
pdb/seq: 2   name: /Users/mobla1/Documents/Graduate/Fall 2024/BGGN213/Class 11/dimer_test_23
pdb/seq: 3   name: /Users/mobla1/Documents/Graduate/Fall 2024/BGGN213/Class 11/dimer_test_23
pdb/seq: 4   name: /Users/mobla1/Documents/Graduate/Fall 2024/BGGN213/Class 11/dimer_test_23
pdb/seq: 5   name: /Users/mobla1/Documents/Graduate/Fall 2024/BGGN213/Class 11/dimer_test_23
```

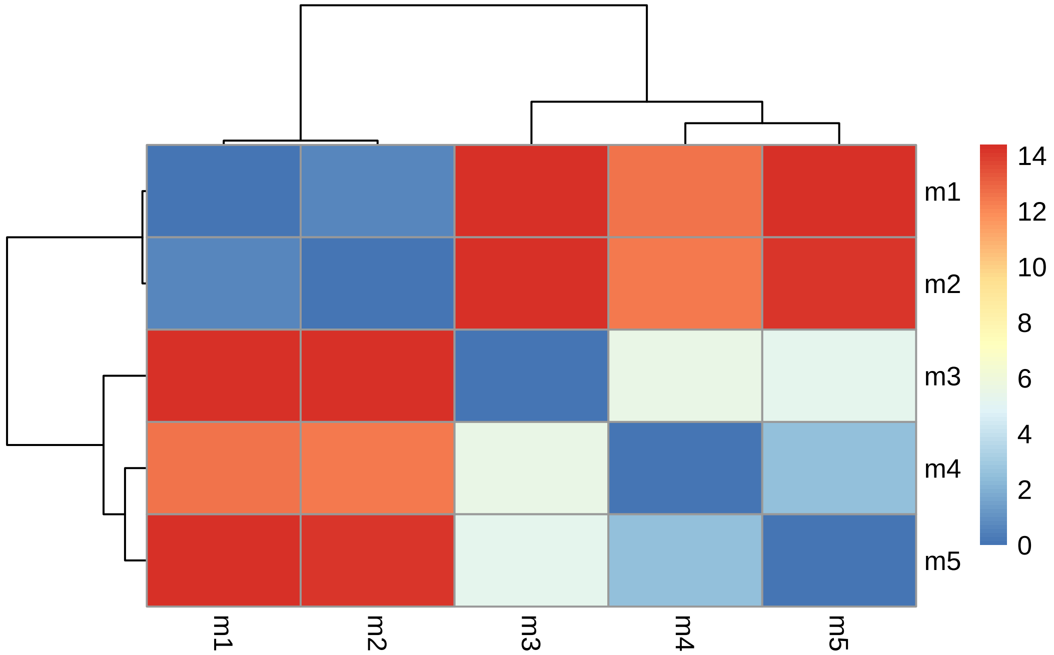
```r
rd <- rmsd(pdbs, fit=T)
```

```
Warning in rmsd(pdbs, fit = T): No indices provided, using the 198 non NA positions
```

```r
range(rd)
```

```
[1]  0.000 14.376
```

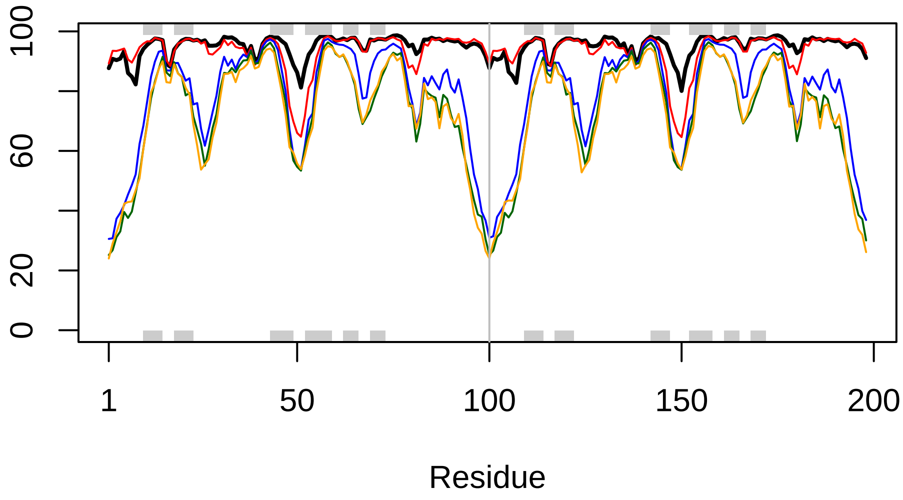
```r
#install.packages("pheatmap")
library(pheatmap)

colnames(rd) <- paste0("m", 1:5)
rownames(rd) <- paste0("m", 1:5)
pheatmap(rd)
```



```r
# Read a reference PDB structure
pdb <- read.pdb("1hsg")
```

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

```
plotb3(pdbs$b[1,], typ="l", lwd=2, sse=pdb)
points(pdbs$b[2,], typ="l", col="red")
points(pdbs$b[3,], typ="l", col="blue")
points(pdbs$b[4,], typ="l", col="darkgreen")
points(pdbs$b[5,], typ="l", col="orange")
abline(v=100, col="gray")
```



Improve the superposition of the models (find the most consistent core across all models):

```
core <- core.find(pdbs)
```

```
 core size 197 of 198  vol = 4916.723
 core size 196 of 198  vol = 4311.504
 core size 195 of 198  vol = 4101.471
 core size 194 of 198  vol = 3907.146
 core size 193 of 198  vol = 3711.949
 core size 192 of 198  vol = 3546.534
 core size 191 of 198  vol = 3440.459
 core size 190 of 198  vol = 3317.592
 core size 189 of 198  vol = 3220.101
 core size 188 of 198  vol = 3142.08
 core size 187 of 198  vol = 3066.812
```

```
core size 186 of 198  vol = 3015.913
core size 185 of 198  vol = 2959.991
core size 184 of 198  vol = 2913.761
core size 183 of 198  vol = 2880.945
core size 182 of 198  vol = 2848.102
core size 181 of 198  vol = 2857.022
core size 180 of 198  vol = 2871.261
core size 179 of 198  vol = 2905.713
core size 178 of 198  vol = 2953.792
core size 177 of 198  vol = 3020.862
core size 176 of 198  vol = 3087.233
core size 175 of 198  vol = 3110.003
core size 174 of 198  vol = 3129.613
core size 173 of 198  vol = 3135.096
core size 172 of 198  vol = 3092.292
core size 171 of 198  vol = 3036.019
core size 170 of 198  vol = 2948.003
core size 169 of 198  vol = 2886.906
core size 168 of 198  vol = 2829.363
core size 167 of 198  vol = 2746.384
core size 166 of 198  vol = 2671.196
core size 165 of 198  vol = 2600.855
core size 164 of 198  vol = 2534.66
core size 163 of 198  vol = 2464.308
core size 162 of 198  vol = 2390.178
core size 161 of 198  vol = 2322.478
core size 160 of 198  vol = 2236.706
core size 159 of 198  vol = 2160.483
core size 158 of 198  vol = 2077.288
core size 157 of 198  vol = 2003.604
core size 156 of 198  vol = 1939.947
core size 155 of 198  vol = 1859.195
core size 154 of 198  vol = 1781.09
core size 153 of 198  vol = 1699.107
core size 152 of 198  vol = 1622.565
core size 151 of 198  vol = 1546.326
core size 150 of 198  vol = 1473.016
core size 149 of 198  vol = 1414.092
core size 148 of 198  vol = 1352.553
core size 147 of 198  vol = 1295.283
core size 146 of 198  vol = 1247.006
core size 145 of 198  vol = 1203.967
core size 144 of 198  vol = 1163.014
core size 143 of 198  vol = 1110.959
core size 142 of 198  vol = 1064.676
core size 141 of 198  vol = 1028.462
core size 140 of 198  vol = 986.124
core size 139 of 198  vol = 944.007
core size 138 of 198  vol = 895.918
core size 137 of 198  vol = 853.511
core size 136 of 198  vol = 827.98
core size 135 of 198  vol = 796.876
core size 134 of 198  vol = 772.766
core size 133 of 198  vol = 743.11
core size 132 of 198  vol = 707.652
core size 131 of 198  vol = 669.174
core size 130 of 198  vol = 634.657
core size 129 of 198  vol = 594.036
core size 128 of 198  vol = 559.156
core size 127 of 198  vol = 525.972
core size 126 of 198  vol = 493.192
core size 125 of 198  vol = 466.475
core size 124 of 198  vol = 438.434
core size 123 of 198  vol = 410.726
core size 122 of 198  vol = 401.382
core size 121 of 198  vol = 391.762
core size 120 of 198  vol = 362.085
core size 119 of 198  vol = 338.185
core size 118 of 198  vol = 312.34
core size 117 of 198  vol = 282.177
core size 116 of 198  vol = 262.216
core size 115 of 198  vol = 241.578
core size 114 of 198  vol = 225.153
core size 113 of 198  vol = 204.138
core size 112 of 198  vol = 185.039
core size 111 of 198  vol = 162.729
core size 110 of 198  vol = 146.182
core size 109 of 198  vol = 133.353
core size 108 of 198  vol = 123.208
core size 107 of 198  vol = 109.228
core size 106 of 198  vol = 98.824
core size 105 of 198  vol = 89.736
core size 104 of 198  vol = 81.207
core size 103 of 198  vol = 74.188
core size 102 of 198  vol = 67.043
core size 101 of 198  vol = 62.044
```

```
 core size 100 of 198  vol = 58.433 
 core size 99 of 198  vol = 55.151 
 core size 98 of 198  vol = 51.114 
 core size 97 of 198  vol = 45.798 
 core size 96 of 198  vol = 41.161 
 core size 95 of 198  vol = 35.619 
 core size 94 of 198  vol = 29.785 
 core size 93 of 198  vol = 23.234 
 core size 92 of 198  vol = 16.67 
 core size 91 of 198  vol = 9.46 
 core size 90 of 198  vol = 4.595 
 core size 89 of 198  vol = 3.161 
 core size 88 of 198  vol = 2.678 
 core size 87 of 198  vol = 2.293 
 core size 86 of 198  vol = 1.936 
 core size 85 of 198  vol = 1.619 
 core size 84 of 198  vol = 1.367 
 core size 83 of 198  vol = 1.09 
 core size 82 of 198  vol = 0.906 
 core size 81 of 198  vol = 0.764 
 core size 80 of 198  vol = 0.649 
 core size 79 of 198  vol = 0.596 
 core size 78 of 198  vol = 0.53 
 core size 77 of 198  vol = 0.486 
 FINISHED: Min vol ( 0.5 ) reached
```

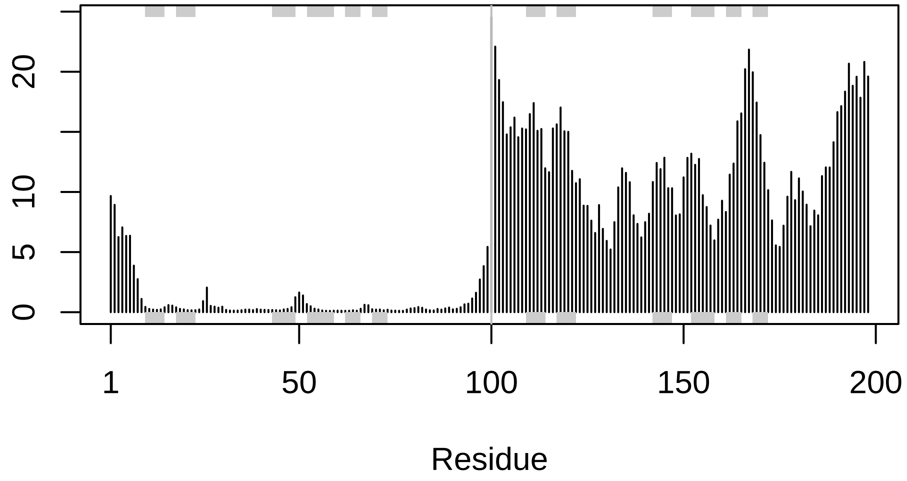
```r
core.inds <- print(core, vol=0.5)
```

```
# 78 positions (cumulative volume <= 0.5 Angstrom^3) 
  start end length
1    10  25     16
2    28  48     21
3    53  93     41
```

```r
#New directory in Class 11 folder with the new superposed coordinates, can view in Mol*
xyz <- pdbfit(pdbs, core.inds, outpath="corefit_structures")
```

```r
#Look at the RMSF between positions

rf <- rmsf(xyz)
```

```r
plotb3(rf, sse=pdb)
abline(v=100, col="gray", ylab="RMSF")
```



```r
library(jsonlite)

# Listing of all PAE JSON files
pae_files <- list.files(path='/Users/mobla1/Documents/Graduate/Fall 2024/BGGN213/Class 11/di
                        pattern=".*model.*\\.json",
                        full.names = TRUE)
```

```r
pae1 <- read_json(pae_files[1],simplifyVector = TRUE)
pae2 <- read_json(pae_files[2],simplifyVector = TRUE)
pae3 <- read_json(pae_files[3],simplifyVector = TRUE)
pae4 <- read_json(pae_files[4],simplifyVector = TRUE)
pae5 <- read_json(pae_files[5],simplifyVector = TRUE)

attributes(pae1)
```

```
$names
[1] "plddt"   "max_pae" "pae"     "ptm"     "iptm"
```

```
#Maximum PAE values for each model (lower score is better!)
pae1$max_pae
```

```
[1] 15.47656
```

```
pae2$max_pae
```

```
[1] 16.125
```

```
pae3$max_pae
```

```
[1] 29.07812
```

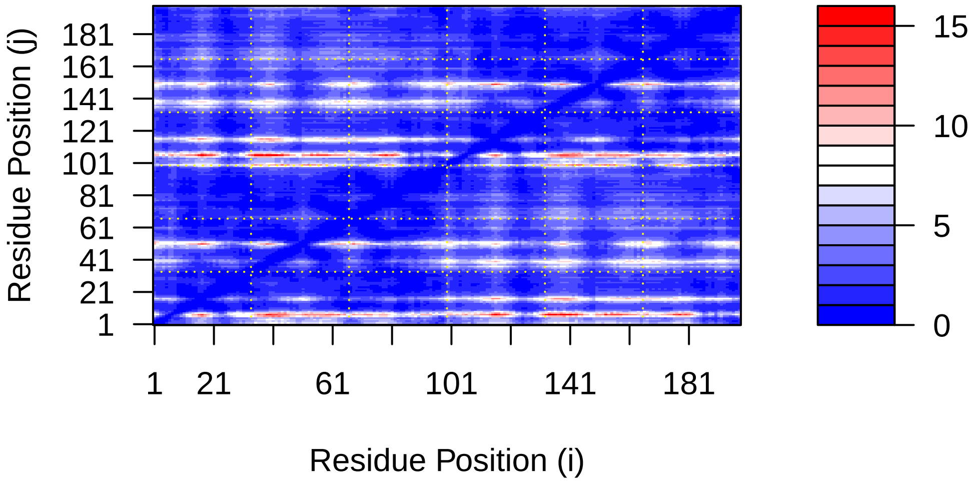
```
pae4$max_pae
```

```
[1] 28.89062
```

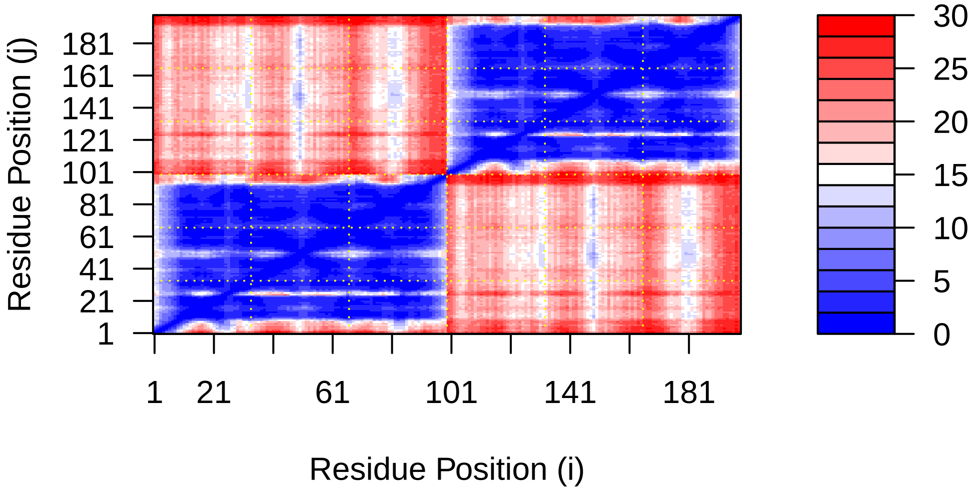
```
pae5$max_pae
```

```
[1] 29.32812
```

```
plot.dmat(pae1$pae,
          xlab="Residue Position (i)",
          ylab="Residue Position (j)")
```

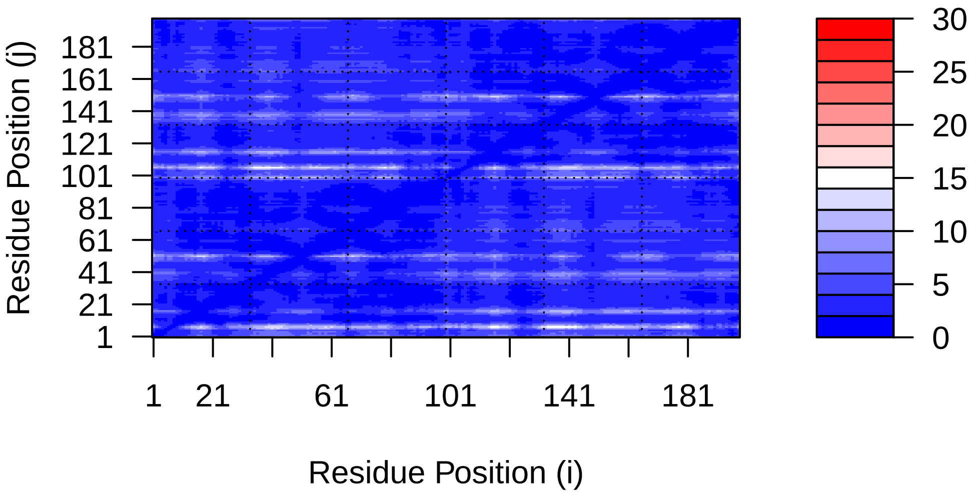


```
plot.dmat(pae5$pae,
          xlab="Residue Position (i)",
          ylab="Residue Position (j)")
```



Re-do the plot for model 1 but with the same data range as the plot for model 5:

```
plot.dmat(pae1$pae,
          xlab="Residue Position (i)",
          ylab="Residue Position (j)",
          grid.col = "black",
          zlim=c(0,30))
```



Residue conservation from alignment file:

```
aln_file <- list.files(path='/Users/mobla1/Documents/Graduate/Fall 2024/BGGN213/Class 11/dim
                       pattern=".a3m$",
                        full.names = TRUE)
aln_file
```

```
[1] "/Users/mobla1/Documents/Graduate/Fall 2024/BGGN213/Class 11/dimer_test_23119/dimer_test
```

```
aln <- read.fasta(aln_file[1], to.upper = TRUE)
```

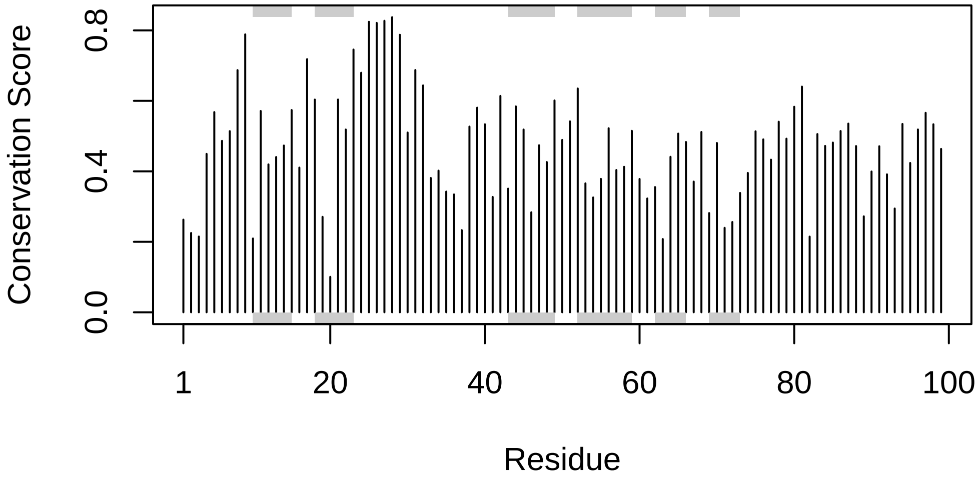
```
[1] " ** Duplicated sequence id's: 101 **"
[2] " ** Duplicated sequence id's: 101 **"
```

```
#How many sequences are in this alignment?
dim(aln$ali)
```

```
[1] 5378  132
```

```
#Score residue conservation
sim <- conserv(aln)
```

```
plotb3(sim[1:99], sse=trim.pdb(pdb, chain="A"),
       ylab="Conservation Score")
```



```
#Generate consensus sequence with high cutoff value to see conserved residues
con <- consensus(aln, cutoff = 0.9)
con$seq
```

```
 [1] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
[19] "-" "-" "-" "-" "-" "-" "D" "T" "G" "A" "-" "-" "-" "-" "-" "-" "-" "-"
[37] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
[55] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
[73] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
[91] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
```

```
[109] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
[127] "-" "-" "-" "-" "-" "-"
```

```
#Visualize these functionally important residue sites
m1.pdb <- read.pdb(pdb_files[1])
occ <- vec2resno(c(sim[1:99], sim[1:99]), m1.pdb$atom$resno)
write.pdb(m1.pdb, o=occ, file="m1_conserv.pdb")
```

```
knitr::include_graphics("M1_CONSERV.PDB.png")
```