class11

james woolley A16440072

##CLASS 10 CONTENT BELOW (finishing up class 10)

Before we finish the lab, we need to install some important packages, including `bio3d`, and `msa`.

The `msa` package is from BioConductor and focuses on genomics. It is managed by `BiocManager`

```
library(bio3d)

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
```

Now we can search the PDB database for related sequences:

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

```
#hits <- plot(b) #the black dots in the graph are the close sequences
```

```
#attributes(b)
#head(b$hit.tbl) #we can see that all the information displayed here is the same as from t
```

```
#hits$pdb.id #this command shows the best/closest matches
```

Below we're collecting all the similar sequences and downloading them using the `get.pdb` function.

```
hits <- NULL
hits$pdb.id <- c('1AKE_A','6S36_A','6RZE_A','3HPR_A','1E4V_A','5EJE_A','1E4Y_A','3X2S_A','
```

```
files <- get.pdb(hits$pdb.id, path="pdbs", split=TRUE, gzip=TRUE) #lets go through and dow
```

```
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/6S36.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/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/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


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```

```
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```

Also lets annotate the structures to find out what they are and what species they're from and stuff like that. You can think of it as adding the convenient links that can be found on the blast website. We can do this by running the `pdb.annotate()` function.

```
anno <- pdb.annotate(ids = hits$pdb.id) #this is giving the function the list of closest m
```

```
attributes (anno) #this shows all the information we got usign `pdb.annotate`
```

```
$names
 [1] "structureId"           "chainId"               "macromoleculeType"
 [4] "chainLength"           "experimentalTechnique" "resolution"
 [7] "scopDomain"            "pfam"                  "ligandId"
[10] "ligandName"            "source"                "structureTitle"
[13] "citation"              "rObserved"             "rFree"
[16] "rWork"                 "spaceGroup"

$class
[1] "data.frame"
```

```
$row.names
 [1] "1AKE_A" "6S36_A" "6RZE_A" "3HPR_A" "1E4V_A" "5EJE_A" "1E4Y_A" "3X2S_A"
 [9] "6HAP_A" "6HAM_A" "4K46_A" "3GMT_A" "4PZL_A"
```

```
head(anno)
```

```
       structureId chainId macromoleculeType chainLength experimentalTechnique
1AKE_A        1AKE       A           Protein         214                 X-ray
6S36_A        6S36       A           Protein         214                 X-ray
6RZE_A        6RZE       A           Protein         214                 X-ray
3HPR_A        3HPR       A           Protein         214                 X-ray
1E4V_A        1E4V       A           Protein         214                 X-ray
5EJE_A        5EJE       A           Protein         214                 X-ray
       resolution       scopDomain                    pfam         ligandId
1AKE_A       2.00 Adenylate kinase Adenylate kinase (ADK)              AP5
6S36_A       1.60             <NA> Adenylate kinase (ADK) CL (3),NA,MG (2)
6RZE_A       1.69             <NA> Adenylate kinase (ADK)    NA (3),CL (2)
3HPR_A       2.00             <NA> Adenylate kinase (ADK)              AP5
1E4V_A       1.85 Adenylate kinase Adenylate kinase (ADK)              AP5
5EJE_A       1.90             <NA> Adenylate kinase (ADK)           AP5,CO
                                                ligandName
1AKE_A                 BIS(ADENOSINE)-5'-PENTAPHOSPHATE
6S36_A    CHLORIDE ION (3),SODIUM ION,MAGNESIUM ION (2)
6RZE_A                  SODIUM ION (3),CHLORIDE ION (2)
3HPR_A                 BIS(ADENOSINE)-5'-PENTAPHOSPHATE
1E4V_A                 BIS(ADENOSINE)-5'-PENTAPHOSPHATE
5EJE_A BIS(ADENOSINE)-5'-PENTAPHOSPHATE,COBALT (II) ION
                                      source
1AKE_A                       Escherichia coli
6S36_A                       Escherichia coli
6RZE_A                       Escherichia coli
3HPR_A                  Escherichia coli K-12
1E4V_A                       Escherichia coli
5EJE_A Escherichia coli O139:H28 str. E24377A

1AKE_A STRUCTURE OF THE COMPLEX BETWEEN ADENYLATE KINASE FROM ESCHERICHIA COLI AND THE INHIBI
6S36_A
6RZE_A
3HPR_A
1E4V_A
```

```
5EJE_A                                                                                       Crys
                                                      citation rObserved  rFree
1AKE_A               Muller, C.W., et al. J Mol Biol (1992)    0.1960     NA
6S36_A                Rogne, P., et al. Biochemistry (2019)    0.1632 0.2356
6RZE_A                Rogne, P., et al. Biochemistry (2019)    0.1865 0.2350
3HPR_A Schrank, T.P., et al. Proc Natl Acad Sci U S A (2009)    0.2100 0.2432
1E4V_A                  Muller, C.W., et al. Proteins (1993)    0.1960     NA
5EJE_A Kovermann, M., et al. Proc Natl Acad Sci U S A (2017)    0.1889 0.2358
        rWork spaceGroup
1AKE_A 0.1960  P 21 2 21
6S36_A 0.1594    C 1 2 1
6RZE_A 0.1819    C 1 2 1
3HPR_A 0.2062  P 21 21 2
1E4V_A 0.1960  P 21 2 21
5EJE_A 0.1863  P 21 2 21
```

Now that we have all the files, we can use the `pdbaln()` function to align and fit the structures, then plot it out to visually see the alignment.

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

```
Reading PDB files:
pdbs/split_chain/1AKE_A.pdb
pdbs/split_chain/6S36_A.pdb
pdbs/split_chain/6RZE_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/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/6S36_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 3   name: pdbs/split_chain/6RZE_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 4   name: pdbs/split_chain/3HPR_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 5   name: pdbs/split_chain/1E4V_A.pdb
pdb/seq: 6   name: pdbs/split_chain/5EJE_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 7   name: pdbs/split_chain/1E4Y_A.pdb
pdb/seq: 8   name: pdbs/split_chain/3X2S_A.pdb
pdb/seq: 9   name: pdbs/split_chain/6HAP_A.pdb
pdb/seq: 10   name: pdbs/split_chain/6HAM_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 11   name: pdbs/split_chain/4K46_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 12   name: pdbs/split_chain/3GMT_A.pdb
pdb/seq: 13   name: pdbs/split_chain/4PZL_A.pdb
```

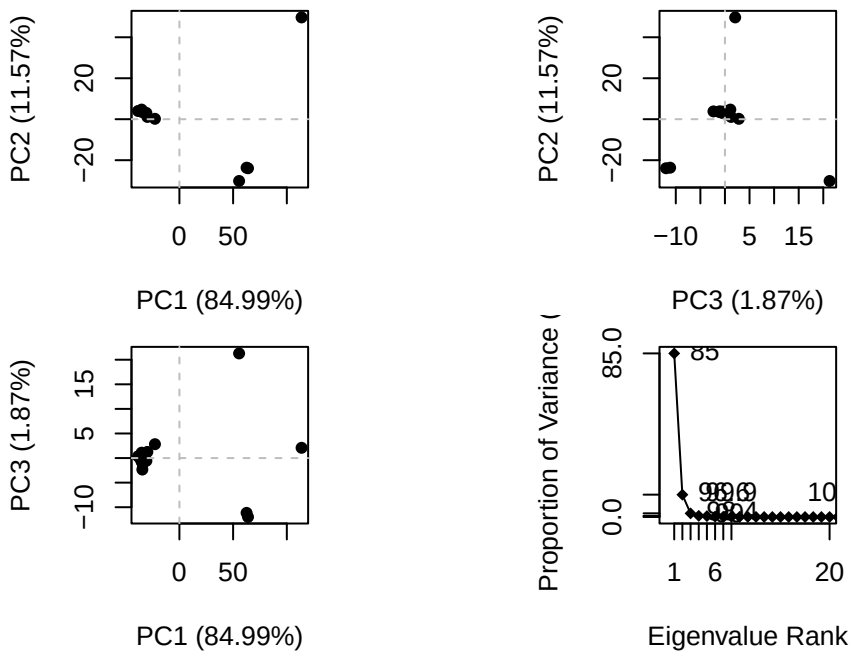
The following code was commented out becuase it broke the PDF when trying to render. Cannot figure out why.

```
# this creates a vector with all the pdb names
#ids <- basename.pdb(pdbs$id)

# this will plot the sequence alignment, where the grey areas indicate a match and the whi
#plot(pdbs, labels=ids)
```

Now we can perform PCA to look at the areas that have the highest variance. This will show us where the proteins are the most different from each other. This is much easier than using a visualiser and slowly comparing all the proteins by hand.

```
pc.xray <- pca(pdbs)
plot(pc.xray)
```



We can make a pdb file that lets us visualise the major structure variations with mol*. Loading it into a visualiser shows all of the different active and inactive structures.

```
pc1 <- mktrj(pc.xray, pc=1, file="pc_1.pdb")
```

##CLASS 11 STUFF

This im-

age shows the monomers all "stacked up" against eachother so we can visualise how different they are.

We're going to try visualising information from AlphaFold2 with `bio3d` First lets make sure our files are all available for us to read.

```
results_dir <- "HIVpr_homodimer_23119_0"
pdb_files <- list.files(path=results_dir,
                        pattern="*.pdb",
                        full.names = TRUE)
pdb_files
```

```
[1] "HIVpr_homodimer_23119_0/HIVpr_homodimer_23119_0_unrelaxed_rank_001_alphafold2_multimer_v
[2] "HIVpr_homodimer_23119_0/HIVpr_homodimer_23119_0_unrelaxed_rank_002_alphafold2_multimer_v
[3] "HIVpr_homodimer_23119_0/HIVpr_homodimer_23119_0_unrelaxed_rank_003_alphafold2_multimer_v
[4] "HIVpr_homodimer_23119_0/HIVpr_homodimer_23119_0_unrelaxed_rank_004_alphafold2_multimer_v
[5] "HIVpr_homodimer_23119_0/HIVpr_homodimer_23119_0_unrelaxed_rank_005_alphafold2_multimer_v
```

Now we can extract the sequences, making sure we have muscle downloaded first.

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

```
Reading PDB files:
HIVpr_homodimer_23119_0/HIVpr_homodimer_23119_0_unrelaxed_rank_001_alphafold2_multimer_v3_mod
HIVpr_homodimer_23119_0/HIVpr_homodimer_23119_0_unrelaxed_rank_002_alphafold2_multimer_v3_mod
HIVpr_homodimer_23119_0/HIVpr_homodimer_23119_0_unrelaxed_rank_003_alphafold2_multimer_v3_mod
HIVpr_homodimer_23119_0/HIVpr_homodimer_23119_0_unrelaxed_rank_004_alphafold2_multimer_v3_mod
HIVpr_homodimer_23119_0/HIVpr_homodimer_23119_0_unrelaxed_rank_005_alphafold2_multimer_v3_mod
.....

Extracting sequences

pdb/seq: 1   name: HIVpr_homodimer_23119_0/HIVpr_homodimer_23119_0_unrelaxed_rank_001_alphafo
pdb/seq: 2   name: HIVpr_homodimer_23119_0/HIVpr_homodimer_23119_0_unrelaxed_rank_002_alphafo
pdb/seq: 3   name: HIVpr_homodimer_23119_0/HIVpr_homodimer_23119_0_unrelaxed_rank_003_alphafo
pdb/seq: 4   name: HIVpr_homodimer_23119_0/HIVpr_homodimer_23119_0_unrelaxed_rank_004_alphafo
pdb/seq: 5   name: HIVpr_homodimer_23119_0/HIVpr_homodimer_23119_0_unrelaxed_rank_005_alphafo
```

Now we can calculate the RMSD between all the models and generate a heat map

```
rd <- rmsd(pdbs)
```

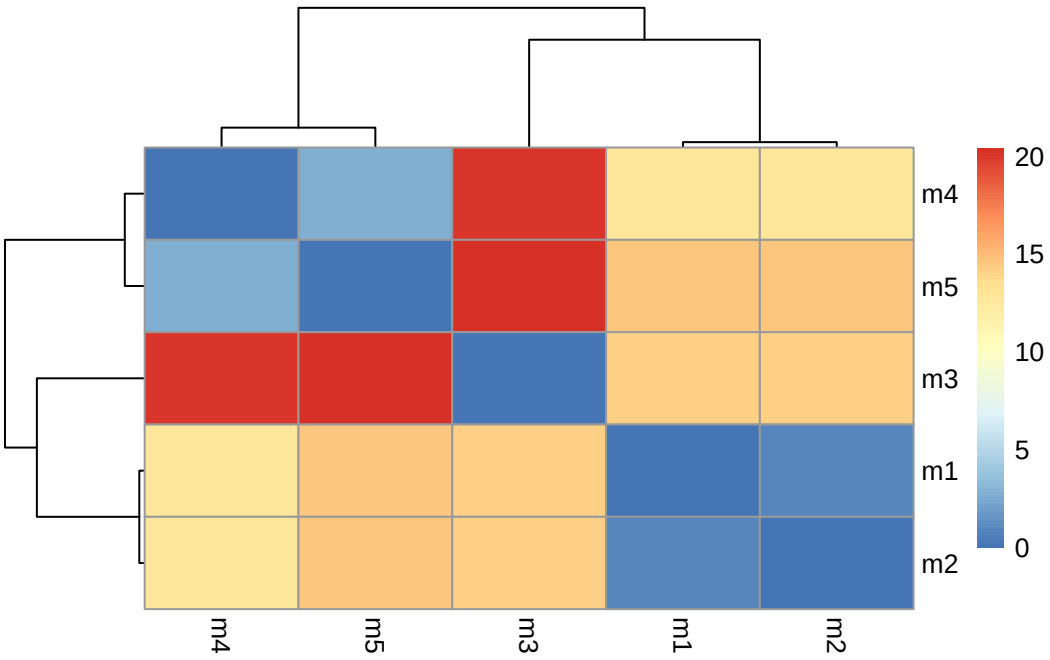
```
Warning in rmsd(pdbs): No indices provided, using the 198 non NA positions
```

```
range(rd)
```

```
[1]  0.000 20.431
```

```
#remember to `install.packages("pheatmap")` first
library(pheatmap)

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



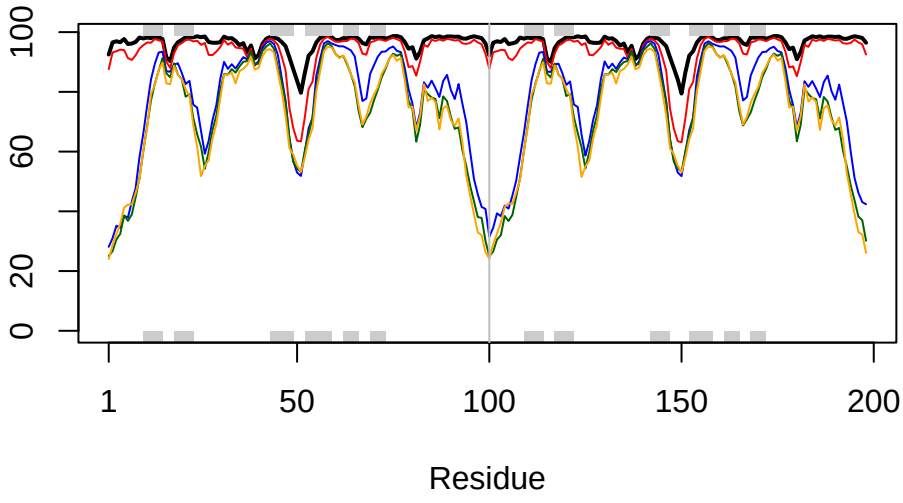
This shows a beautiful heat map of all the RMSD matrix values

Next we can plot all the plDDT values

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

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

```
plotb3(pdbs$b, typ="l", lwd=2, sse=pdb)
points(pdbs$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")
```



This graph shows how "good" our predicted structures are/how confident AlphaFold2 is that the predicted structures are correct. The fitting of the model can be additionally improved with the following commands

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

```
core size 197 of 198  vol = 6154.839
core size 196 of 198  vol = 5399.676
```

```
core size 195 of 198  vol = 5074.795
core size 194 of 198  vol = 4802.518
core size 193 of 198  vol = 4520.256
core size 192 of 198  vol = 4305.362
core size 191 of 198  vol = 4089.792
core size 190 of 198  vol = 3886.145
core size 189 of 198  vol = 3758.321
core size 188 of 198  vol = 3620.18
core size 187 of 198  vol = 3496.698
core size 186 of 198  vol = 3389.985
core size 185 of 198  vol = 3320.114
core size 184 of 198  vol = 3258.683
core size 183 of 198  vol = 3208.591
core size 182 of 198  vol = 3156.736
core size 181 of 198  vol = 3141.668
core size 180 of 198  vol = 3136.574
core size 179 of 198  vol = 3155.52
core size 178 of 198  vol = 3185.362
core size 177 of 198  vol = 3204.487
core size 176 of 198  vol = 3211.978
core size 175 of 198  vol = 3234.993
core size 174 of 198  vol = 3244.062
core size 173 of 198  vol = 3237.845
core size 172 of 198  vol = 3218.77
core size 171 of 198  vol = 3180.743
core size 170 of 198  vol = 3130.369
core size 169 of 198  vol = 3067.881
core size 168 of 198  vol = 2989.546
core size 167 of 198  vol = 2928.272
core size 166 of 198  vol = 2851.193
core size 165 of 198  vol = 2780.877
core size 164 of 198  vol = 2708.433
core size 163 of 198  vol = 2636.516
core size 162 of 198  vol = 2563.25
core size 161 of 198  vol = 2478.024
core size 160 of 198  vol = 2404.793
core size 159 of 198  vol = 2330.997
core size 158 of 198  vol = 2250.477
core size 157 of 198  vol = 2159.432
core size 156 of 198  vol = 2070.759
core size 155 of 198  vol = 1983.579
core size 154 of 198  vol = 1917.913
core size 153 of 198  vol = 1842.556
```

```
core size 152 of 198  vol = 1775.398
core size 151 of 198  vol = 1695.133
core size 150 of 198  vol = 1632.173
core size 149 of 198  vol = 1570.391
core size 148 of 198  vol = 1497.238
core size 147 of 198  vol = 1434.802
core size 146 of 198  vol = 1367.706
core size 145 of 198  vol = 1302.596
core size 144 of 198  vol = 1251.985
core size 143 of 198  vol = 1207.976
core size 142 of 198  vol = 1167.112
core size 141 of 198  vol = 1118.27
core size 140 of 198  vol = 1081.664
core size 139 of 198  vol = 1029.75
core size 138 of 198  vol = 981.766
core size 137 of 198  vol = 944.446
core size 136 of 198  vol = 899.224
core size 135 of 198  vol = 859.402
core size 134 of 198  vol = 814.694
core size 133 of 198  vol = 771.862
core size 132 of 198  vol = 733.807
core size 131 of 198  vol = 702.053
core size 130 of 198  vol = 658.757
core size 129 of 198  vol = 622.574
core size 128 of 198  vol = 578.29
core size 127 of 198  vol = 543.07
core size 126 of 198  vol = 510.934
core size 125 of 198  vol = 481.595
core size 124 of 198  vol = 464.672
core size 123 of 198  vol = 451.721
core size 122 of 198  vol = 430.417
core size 121 of 198  vol = 409.141
core size 120 of 198  vol = 378.942
core size 119 of 198  vol = 348.325
core size 118 of 198  vol = 324.738
core size 117 of 198  vol = 312.394
core size 116 of 198  vol = 300.89
core size 115 of 198  vol = 279.976
core size 114 of 198  vol = 263.434
core size 113 of 198  vol = 250.263
core size 112 of 198  vol = 229.592
core size 111 of 198  vol = 209.929
core size 110 of 198  vol = 196.379
```

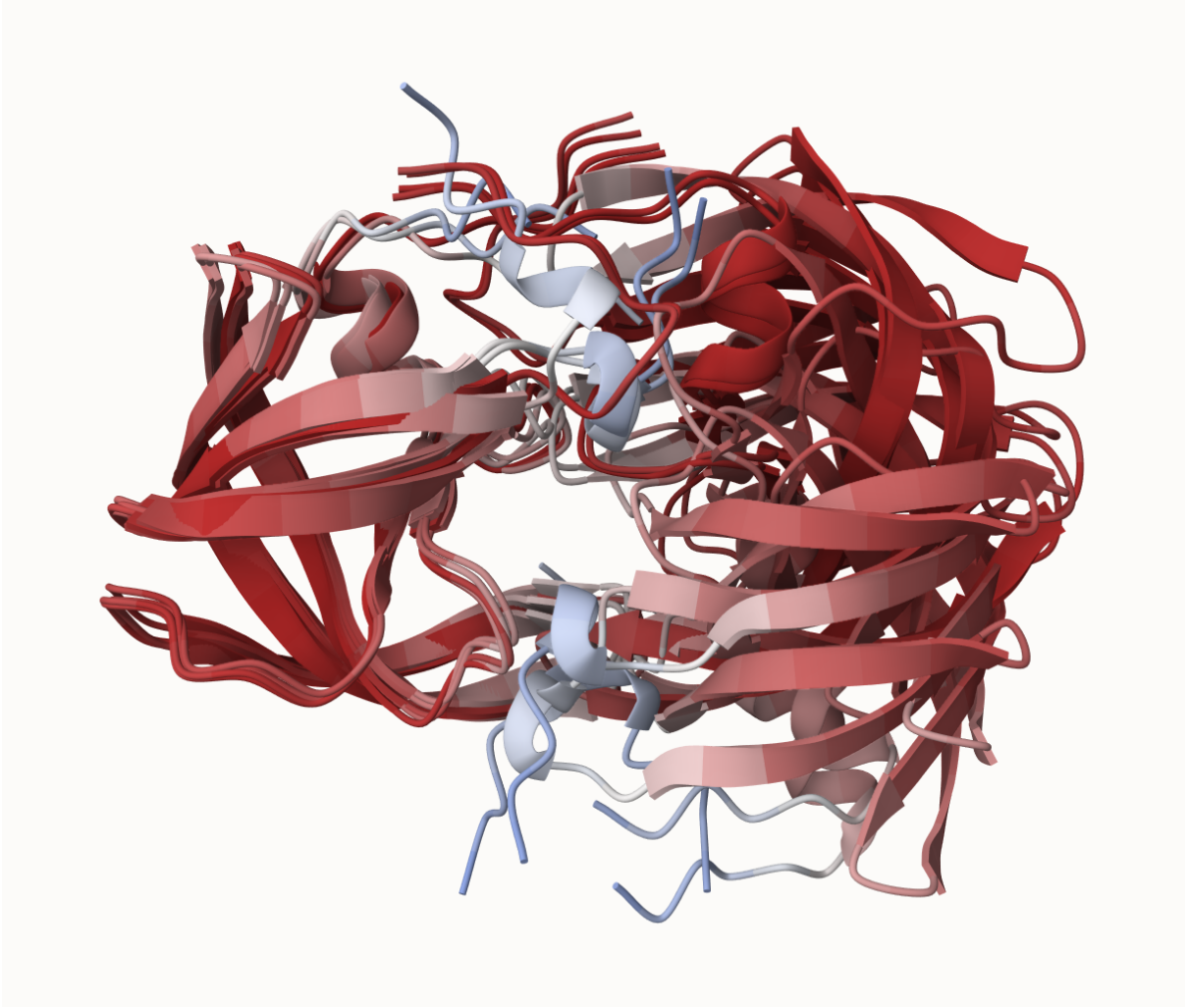
```
 core size 109 of 198  vol = 180.628
 core size 108 of 198  vol = 167.088
 core size 107 of 198  vol = 155.875
 core size 106 of 198  vol = 142.595
 core size 105 of 198  vol = 128.924
 core size 104 of 198  vol = 114.054
 core size 103 of 198  vol = 100.936
 core size 102 of 198  vol = 90.431
 core size 101 of 198  vol = 81.972
 core size 100 of 198  vol = 74.017
 core size 99 of 198  vol = 66.855
 core size 98 of 198  vol = 59.525
 core size 97 of 198  vol = 52.263
 core size 96 of 198  vol = 43.699
 core size 95 of 198  vol = 35.813
 core size 94 of 198  vol = 28.888
 core size 93 of 198  vol = 20.692
 core size 92 of 198  vol = 14.975
 core size 91 of 198  vol = 9.146
 core size 90 of 198  vol = 5.232
 core size 89 of 198  vol = 3.53
 core size 88 of 198  vol = 2.657
 core size 87 of 198  vol = 1.998
 core size 86 of 198  vol = 1.333
 core size 85 of 198  vol = 1.141
 core size 84 of 198  vol = 1.012
 core size 83 of 198  vol = 0.891
 core size 82 of 198  vol = 0.749
 core size 81 of 198  vol = 0.618
 core size 80 of 198  vol = 0.538
 core size 79 of 198  vol = 0.479
 FINISHED: Min vol ( 0.5 ) reached
```

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

```
# 80 positions (cumulative volume <= 0.5 Angstrom^3)
  start end length
1    10  25     16
2    27  48     22
3    53  94     42
```

```
xyz <- pdbfit(pdbs, core.inds, outpath="corefit_structures")
```

This should spit out a file that can be read by mol*, and we can then colour it by uncertainty/disorder to see how "good" the predicted structure is.



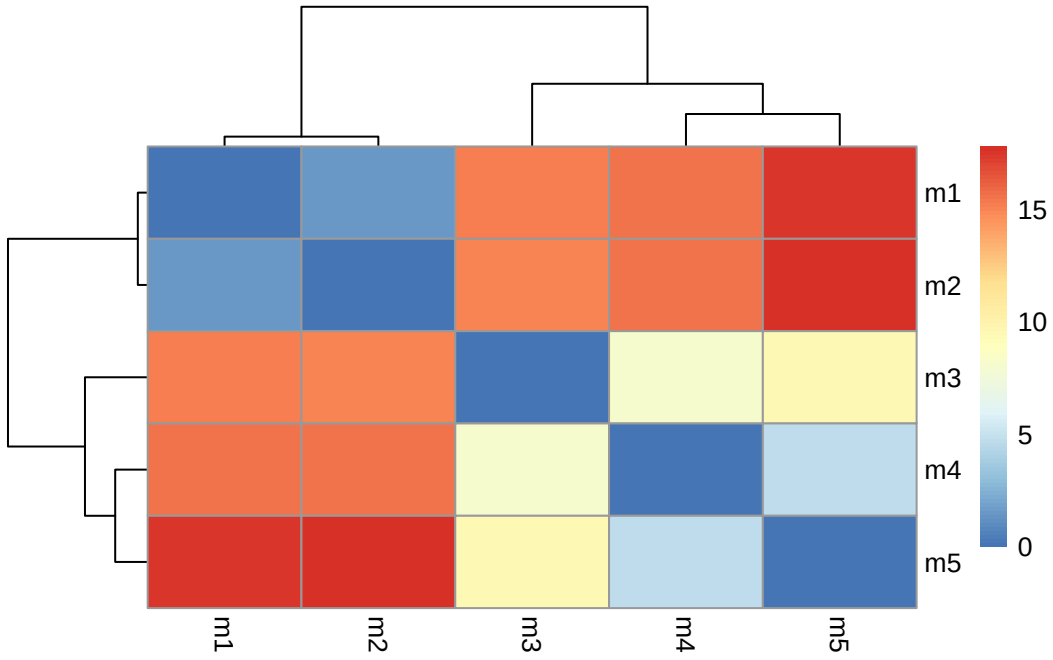
This shows the superposed structures coloured by uncertainty.

Now we can update the RMSD and examine the RMSF of the positions of the structure

```
rd <- rmsd(xyz)
```

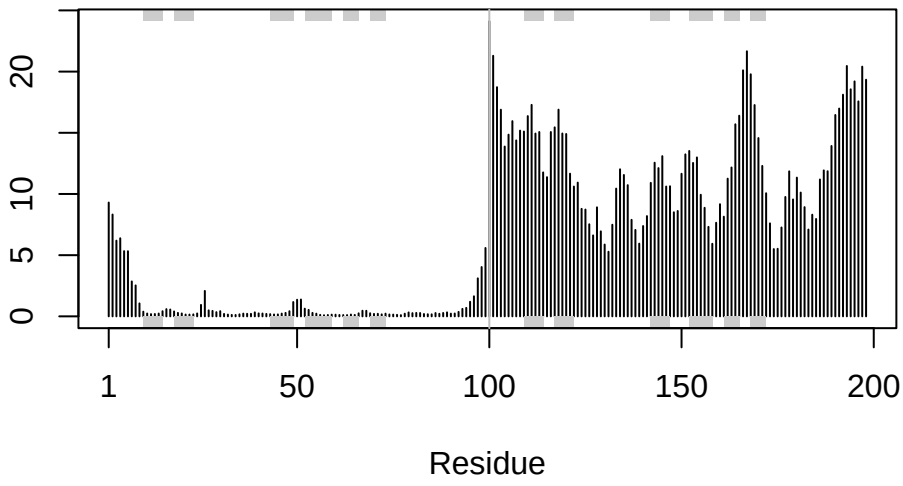
```
Warning in rmsd(xyz): No indices provided, using the 198 non NA positions
```

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




```
rf <- rmsf(xyz)

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



#predicted alignment errors for domains

```
library(jsonlite)

pae_files <- list.files(path=results_dir,
                        pattern=".*model.*\\.json",
                        full.names = TRUE)
pae1 <- read_json(pae_files[1],simplifyVector = TRUE)
pae5 <- read_json(pae_files[5],simplifyVector = TRUE)

attributes(pae1)
```

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

```
head(pae1$plddt)
```

```
[1] 92.50 96.56 96.94 96.62 97.69 96.00
```

This shows the maximum PAE values, and we can see in the vector that model 1 is the best, because it has the lowest score.

```
pae1$max_pae
```

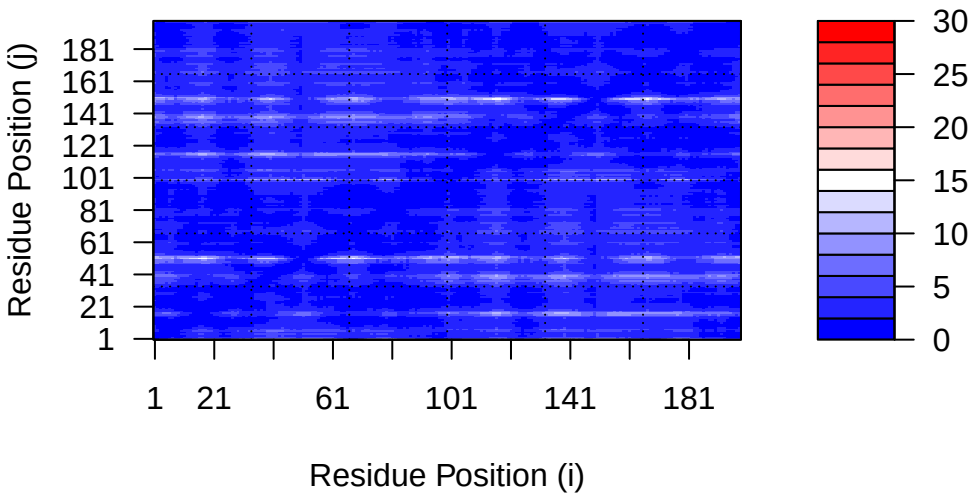
```
[1] 15.54688
```

```
pae5$max_pae
```

```
[1] 29.29688
```

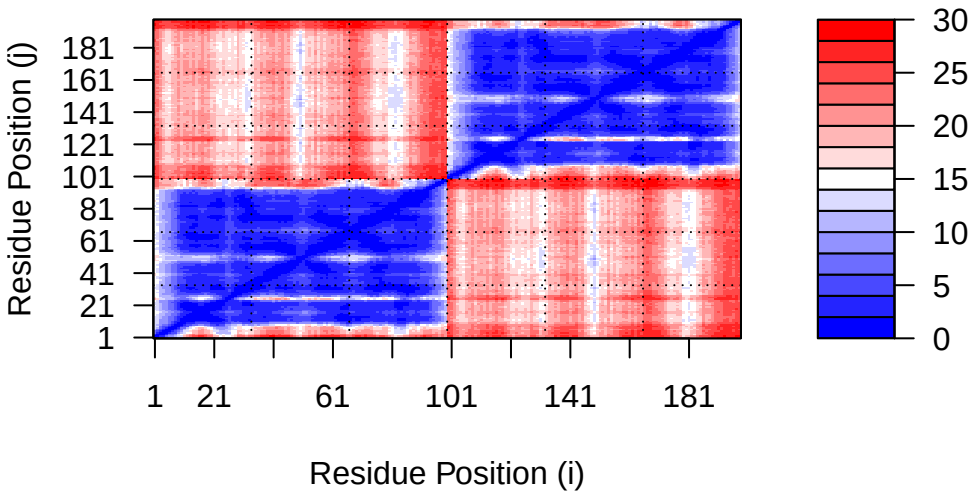
We can plot these together like so

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




```
plot.dmat(pae5$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=results_dir,
                       pattern=".a3m$",
                        full.names = TRUE)
aln <- read.fasta(aln_file[1], to.upper = TRUE)
```

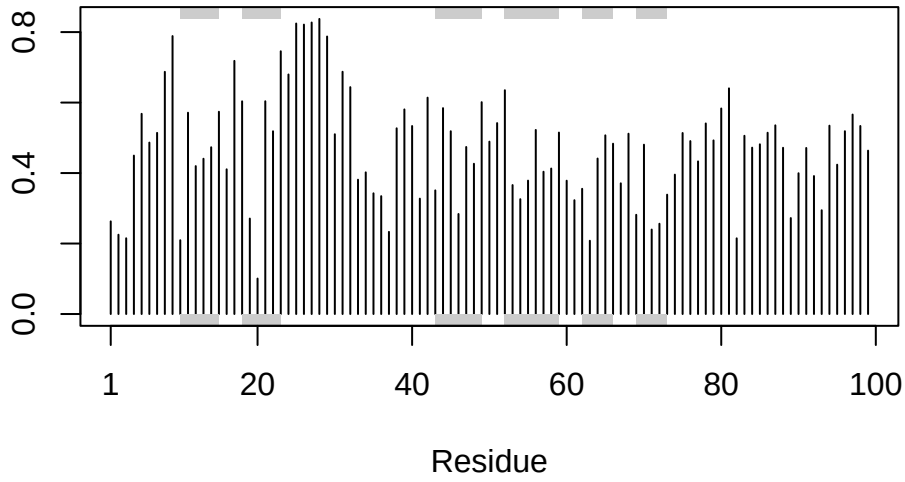
```
[1] " ** Duplicated sequence id's: 101 **"
[2] " ** Duplicated sequence id's: 101 **"
```

```
dim(aln$ali)
```

```
[1] 5378  132
```

Now we can see how conserved the residues are

```
sim <- conserv(aln)
plotb3(sim[1:99], sse=trim.pdb(pdb, chain="A"))
```



This graph shows that there are highly conserved active sites at D25, T26, G27, A28.

```
con <- consensus(aln, cutoff = 0.9)
con$seq
```

```
  [1] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
 [19] "-" "-" "-" "-" "-" "-" "D" "T" "G" "A" "-" "-" "-" "-" "-" "-" "-" "-"
 [37] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
 [55] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
 [73] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
 [91] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
[109] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
[127] "-" "-" "-" "-" "-" "-"
```

Finally, we can map the conservation score to visualise the highly conserved areas using programs like mol*

```
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")
```