Lab 11: Structural Bioinformatics 2

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Lab 10 Completion

Lab 10, including PCA, was submitted in full in the Lab 10 gradescope assignment

Alpha Fold

6. Generating your own structure predictions

Colabfold plots:

7. Interpreting Results

8.1 Custom analysis of resulting models

```
results_dir <- "hivprdimer_23119/"


# File names for all PDB models
pdb_files <- list.files(path=results_dir, pattern="*.pdb", full.names = TRUE)

# Print our PDB file names
basename(pdb_files)
```

```
[1] "hivprdimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_5_seed_000.pdb"
[2] "hivprdimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_1_seed_000.pdb"
[3] "hivprdimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000.pdb"
[4] "hivprdimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_seed_000.pdb"
[5] "hivprdimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000.pdb"
```

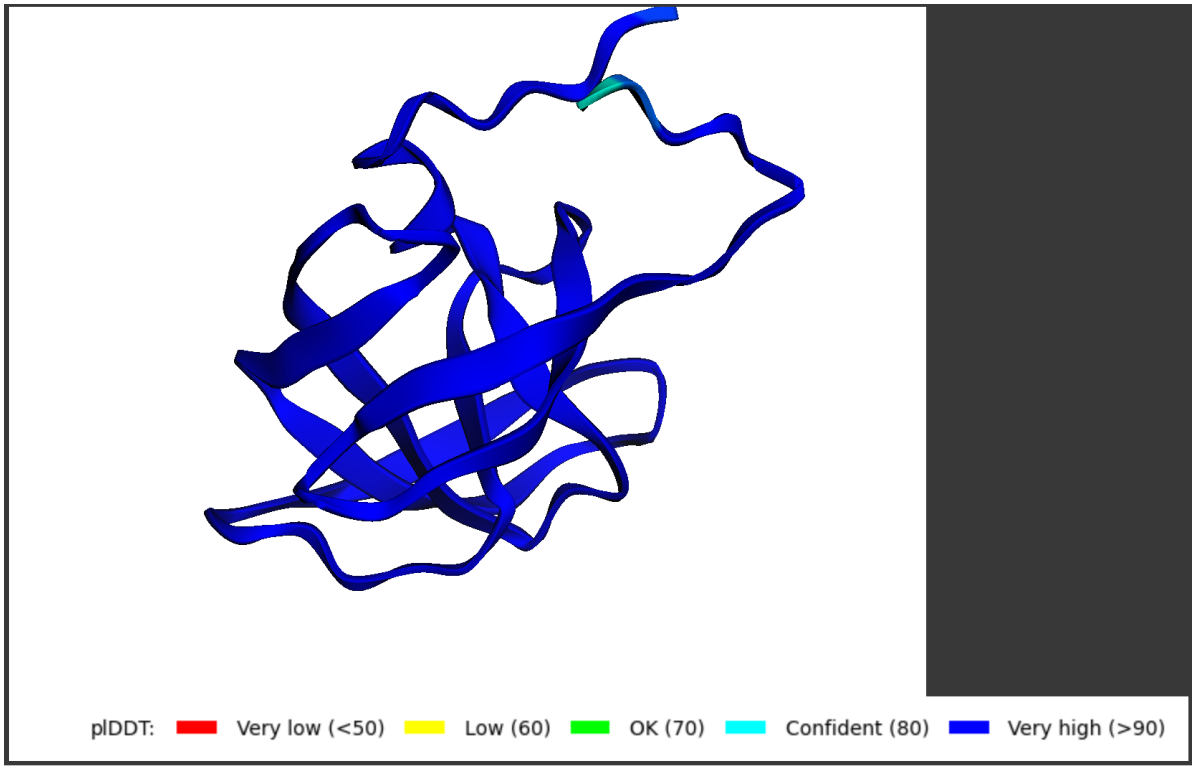


Figure 1: colabfold plot 1

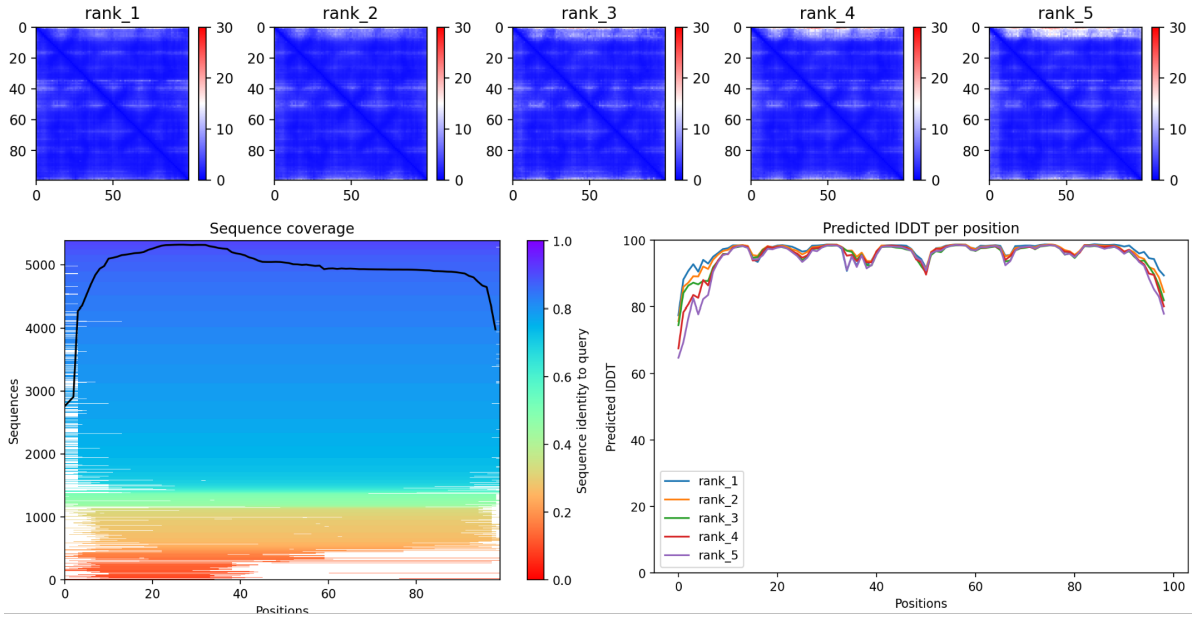


Figure 2: colabfold plot 2

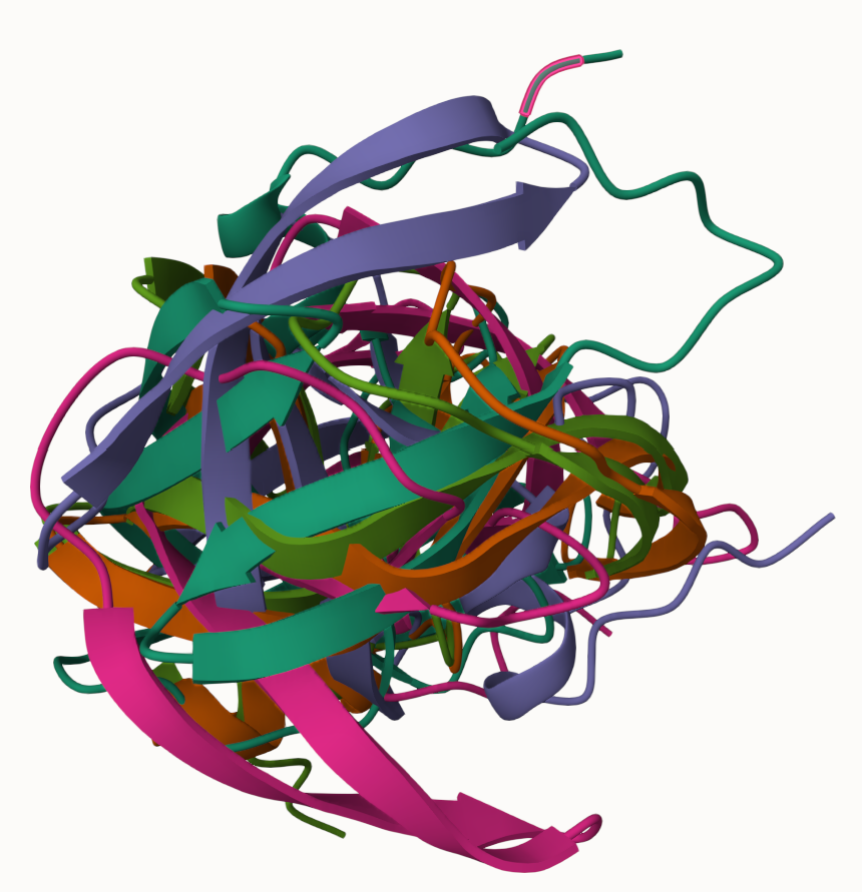


Figure 3: molstar plot 1

Figure 4: molstar plot 2

```
library(bio3d)

# Read all data from Models
#  and superpose/fit coords
pdbs <- pdbaln(pdb_files, fit=TRUE, exefile="msa")
```

```
Reading PDB files:
hivprdimer_23119/hivprdimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_5_seed_000
hivprdimer_23119/hivprdimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_1_seed_000
hivprdimer_23119/hivprdimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000
hivprdimer_23119/hivprdimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_seed_000
hivprdimer_23119/hivprdimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000
.....

Extracting sequences

pdb/seq: 1   name: hivprdimer_23119/hivprdimer_23119_unrelaxed_rank_001_alphafold2_multimer_v
pdb/seq: 2   name: hivprdimer_23119/hivprdimer_23119_unrelaxed_rank_002_alphafold2_multimer_v
pdb/seq: 3   name: hivprdimer_23119/hivprdimer_23119_unrelaxed_rank_003_alphafold2_multimer_v
pdb/seq: 4   name: hivprdimer_23119/hivprdimer_23119_unrelaxed_rank_004_alphafold2_multimer_v
pdb/seq: 5   name: hivprdimer_23119/hivprdimer_23119_unrelaxed_rank_005_alphafold2_multimer_v
```

```
pdbs
```

```
                                1        .        .        .        .        50
[Truncated_Name:1]hivprdimer   PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGI
[Truncated_Name:2]hivprdimer   PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGI
[Truncated_Name:3]hivprdimer   PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGI
[Truncated_Name:4]hivprdimer   PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGI
[Truncated_Name:5]hivprdimer   PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGI
                               **************************************************
                               1        .        .        .        .        50

                              51        .        .        .        .        100
[Truncated_Name:1]hivprdimer   GGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFP
[Truncated_Name:2]hivprdimer   GGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFP
[Truncated_Name:3]hivprdimer   GGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFP
[Truncated_Name:4]hivprdimer   GGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFP
[Truncated_Name:5]hivprdimer   GGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFP
                               **************************************************
```

```
                            51        .         .         .         .         100

                           101        .         .         .         .         150
[Truncated_Name:1]hivprdimer   QITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGIG
[Truncated_Name:2]hivprdimer   QITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGIG
[Truncated_Name:3]hivprdimer   QITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGIG
[Truncated_Name:4]hivprdimer   QITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGIG
[Truncated_Name:5]hivprdimer   QITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGIG
                               **************************************************
                           101        .         .         .         .         150

                           151        .         .         .         .       198
[Truncated_Name:1]hivprdimer   GFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNF
[Truncated_Name:2]hivprdimer   GFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNF
[Truncated_Name:3]hivprdimer   GFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNF
[Truncated_Name:4]hivprdimer   GFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNF
[Truncated_Name:5]hivprdimer   GFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNF
                               **************************************************
                           151        .         .         .         .       198

Call:
  pdbaln(files = pdb_files, fit = TRUE, exefile = "msa")

Class:
  pdbs, fasta

Alignment dimensions:
  5 sequence rows; 198 position columns (198 non-gap, 0 gap)

+ attr: xyz, resno, b, chain, id, ali, resid, sse, call
```

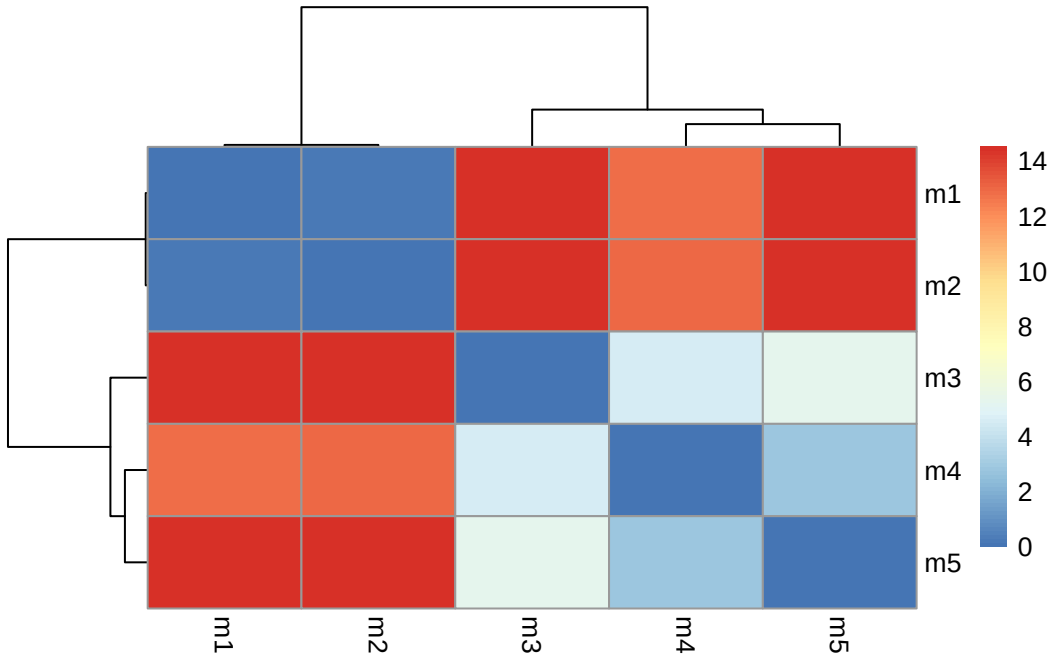
```
rd <- rmsd(pdbs, fit=T)
```

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

```
range(rd)
```

```
[1]  0.000 14.507
```

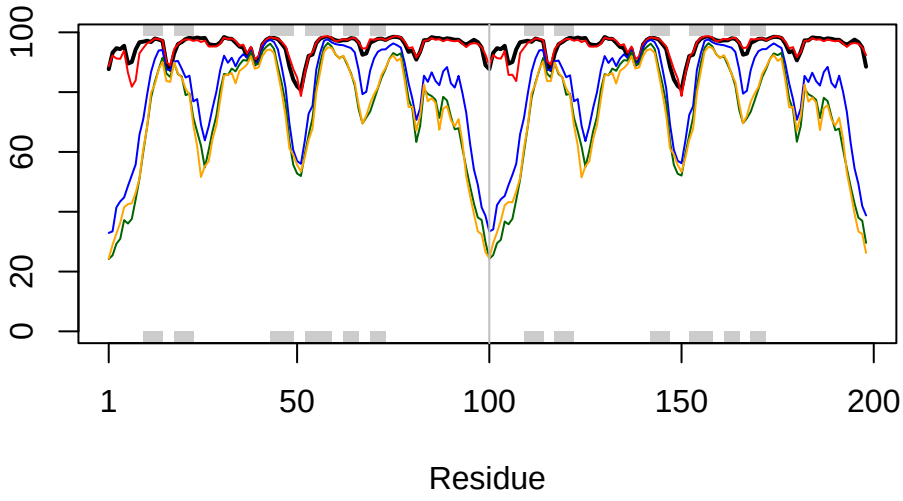
```
#install.packages("pheatmap")
library(pheatmap)

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




```
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")
```




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

```
core size 197 of 198  vol = 5017.583
core size 196 of 198  vol = 4299.462
core size 195 of 198  vol = 4030.786
core size 194 of 198  vol = 3797.241
core size 193 of 198  vol = 3567.126
core size 192 of 198  vol = 3378.469
core size 191 of 198  vol = 3249.342
core size 190 of 198  vol = 3149.254
core size 189 of 198  vol = 3070.29
core size 188 of 198  vol = 2993.999
core size 187 of 198  vol = 2917.618
core size 186 of 198  vol = 2865.321
core size 185 of 198  vol = 2835.031
core size 184 of 198  vol = 2825.584
core size 183 of 198  vol = 2833.979
core size 182 of 198  vol = 2894.691
core size 181 of 198  vol = 2975.843
core size 180 of 198  vol = 3026.495
core size 179 of 198  vol = 3070.895
core size 178 of 198  vol = 3121.204
```

```
core size 177 of 198  vol = 3127.656
core size 176 of 198  vol = 3102.311
core size 175 of 198  vol = 3060.45
core size 174 of 198  vol = 2993.84
core size 173 of 198  vol = 2902.747
core size 172 of 198  vol = 2841.824
core size 171 of 198  vol = 2771.39
core size 170 of 198  vol = 2708.164
core size 169 of 198  vol = 2616.115
core size 168 of 198  vol = 2540.663
core size 167 of 198  vol = 2471.823
core size 166 of 198  vol = 2396.567
core size 165 of 198  vol = 2324.756
core size 164 of 198  vol = 2258.532
core size 163 of 198  vol = 2189.811
core size 162 of 198  vol = 2118.531
core size 161 of 198  vol = 2048.541
core size 160 of 198  vol = 1964.22
core size 159 of 198  vol = 1878.019
core size 158 of 198  vol = 1802.026
core size 157 of 198  vol = 1719.543
core size 156 of 198  vol = 1640.479
core size 155 of 198  vol = 1561.746
core size 154 of 198  vol = 1490.107
core size 153 of 198  vol = 1416.211
core size 152 of 198  vol = 1345.494
core size 151 of 198  vol = 1287.606
core size 150 of 198  vol = 1225.523
core size 149 of 198  vol = 1168.6
core size 148 of 198  vol = 1123.809
core size 147 of 198  vol = 1069.607
core size 146 of 198  vol = 1028.33
core size 145 of 198  vol = 986.295
core size 144 of 198  vol = 947.191
core size 143 of 198  vol = 910.624
core size 142 of 198  vol = 868.922
core size 141 of 198  vol = 829.982
core size 140 of 198  vol = 788.548
core size 139 of 198  vol = 749.234
core size 138 of 198  vol = 713.554
core size 137 of 198  vol = 679.035
core size 136 of 198  vol = 639.012
core size 135 of 198  vol = 599.236
```

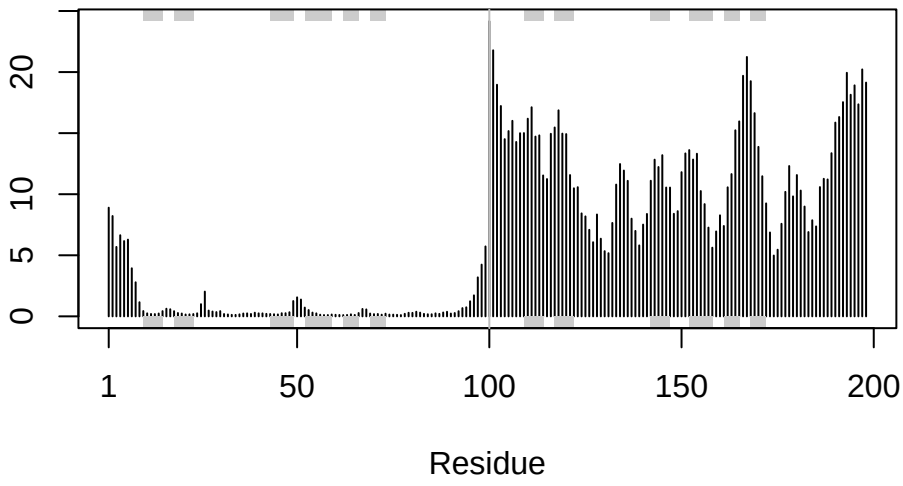
```
core size 134 of 198  vol = 556.226
core size 133 of 198  vol = 521.307
core size 132 of 198  vol = 484.526
core size 131 of 198  vol = 453.614
core size 130 of 198  vol = 422.947
core size 129 of 198  vol = 404.641
core size 128 of 198  vol = 397.064
core size 127 of 198  vol = 371.629
core size 126 of 198  vol = 355.609
core size 125 of 198  vol = 334.859
core size 124 of 198  vol = 313.691
core size 123 of 198  vol = 291.489
core size 122 of 198  vol = 268.734
core size 121 of 198  vol = 245.865
core size 120 of 198  vol = 236.559
core size 119 of 198  vol = 218.641
core size 118 of 198  vol = 201.313
core size 117 of 198  vol = 183.861
core size 116 of 198  vol = 167.249
core size 115 of 198  vol = 151.276
core size 114 of 198  vol = 137.843
core size 113 of 198  vol = 124.983
core size 112 of 198  vol = 112.07
core size 111 of 198  vol = 101.394
core size 110 of 198  vol = 91.994
core size 109 of 198  vol = 82.201
core size 108 of 198  vol = 74.644
core size 107 of 198  vol = 70.256
core size 106 of 198  vol = 64.859
core size 105 of 198  vol = 58.745
core size 104 of 198  vol = 54.966
core size 103 of 198  vol = 49.885
core size 102 of 198  vol = 45.389
core size 101 of 198  vol = 41.648
core size 100 of 198  vol = 38.714
core size 99 of 198  vol = 36.289
core size 98 of 198  vol = 33.698
core size 97 of 198  vol = 28.156
core size 96 of 198  vol = 23.583
core size 95 of 198  vol = 19.899
core size 94 of 198  vol = 16.637
core size 93 of 198  vol = 12.448
core size 92 of 198  vol = 9.42
```

```
 core size 91 of 198  vol = 8.296
 core size 90 of 198  vol = 5.783
 core size 89 of 198  vol = 4.006
 core size 88 of 198  vol = 2.903
 core size 87 of 198  vol = 2.24
 core size 86 of 198  vol = 1.765
 core size 85 of 198  vol = 1.408
 core size 84 of 198  vol = 1.164
 core size 83 of 198  vol = 0.969
 core size 82 of 198  vol = 0.833
 core size 81 of 198  vol = 0.675
 core size 80 of 198  vol = 0.579
 core size 79 of 198  vol = 0.529
 core size 78 of 198  vol = 0.456
 FINISHED: Min vol ( 0.5 ) reached
```

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

```
# 79 positions (cumulative volume <= 0.5 Angstrom^3)
  start end length
1    10  24     15
2    27  48     22
3    53  94     42
```

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

rf <- rmsf(xyz)

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



8.2 Predicted Alignment Error for domains

```
#install.packages("jsonlite")

library(jsonlite)

# Listing of all PAE JSON files
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"
```

```
# Per-residue pLDDT scores
#  same as B-factor of PDB..
head(pae1$plddt)
```

```
[1] 87.69 93.19 94.69 94.38 95.50 89.56
```

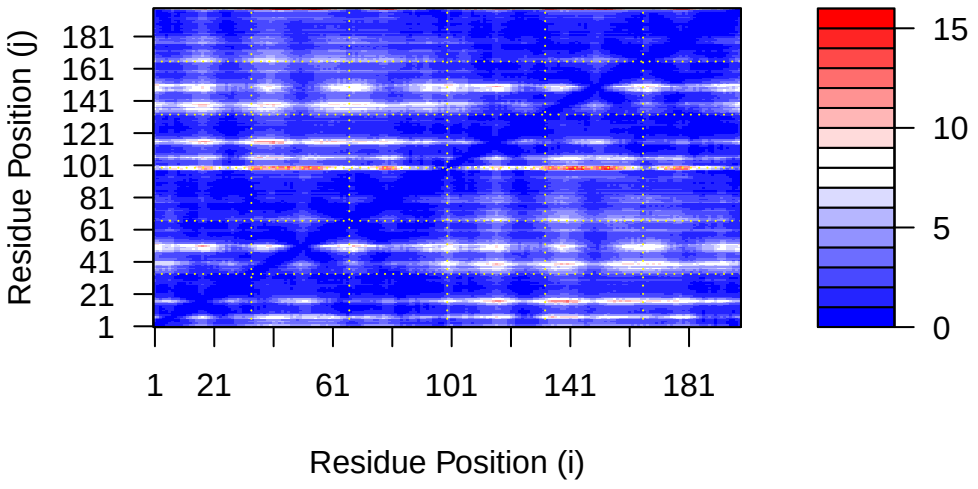
```
pae1$max_pae
```

```
[1] 15.89844
```

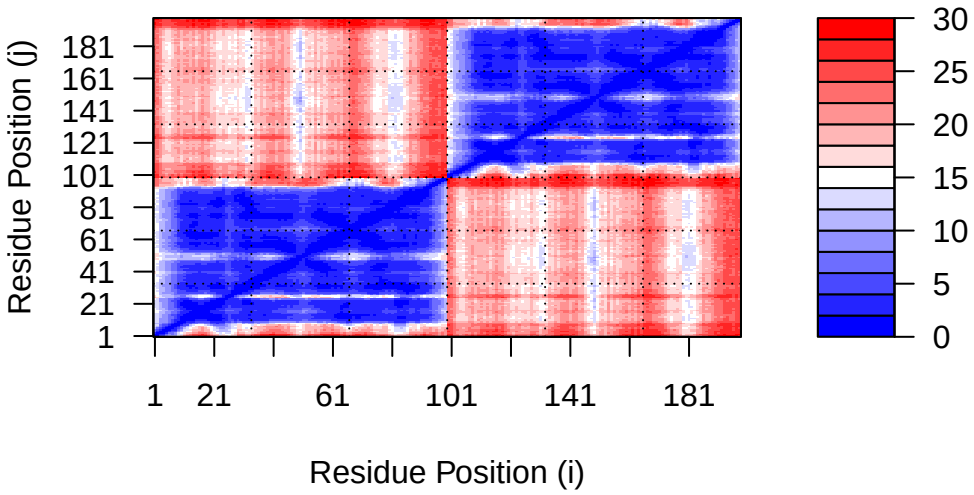
```
pae5$max_pae
```

```
[1] 29.25
```

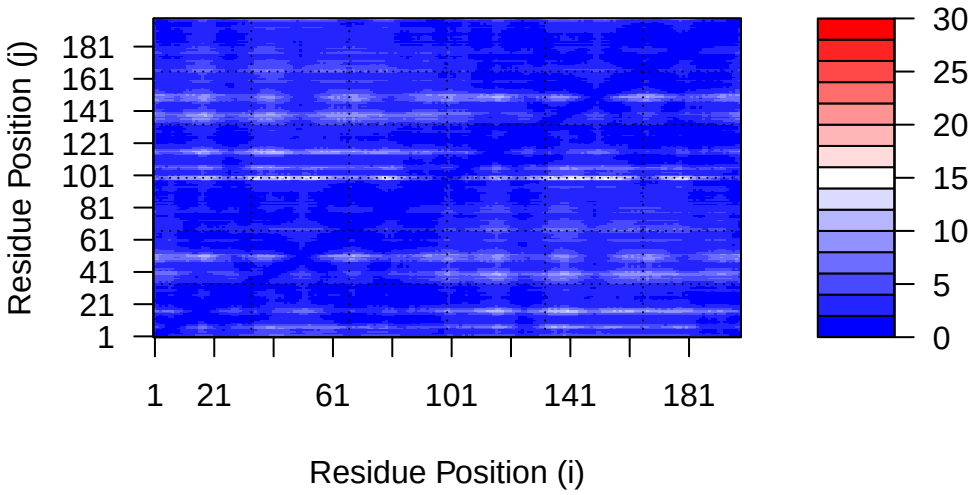
```
plot.dmat(pae1$pae,
          xlab="Residue Position (i)",
          ylab="Residue Position (j)")
```



```
plot.dmat(pae5$pae,
          xlab="Residue Position (i)",
          ylab="Residue Position (j)",
          grid.col = "black",
          zlim=c(0,30))
```




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



8.3 Residue conservation from alignment file

```
aln_file <- list.files(path=results_dir,
                       pattern=".a3m$",
                        full.names = TRUE)
aln_file
```

```
[1] "hivprdimer_23119/hivprdimer_23119.a3m"
```

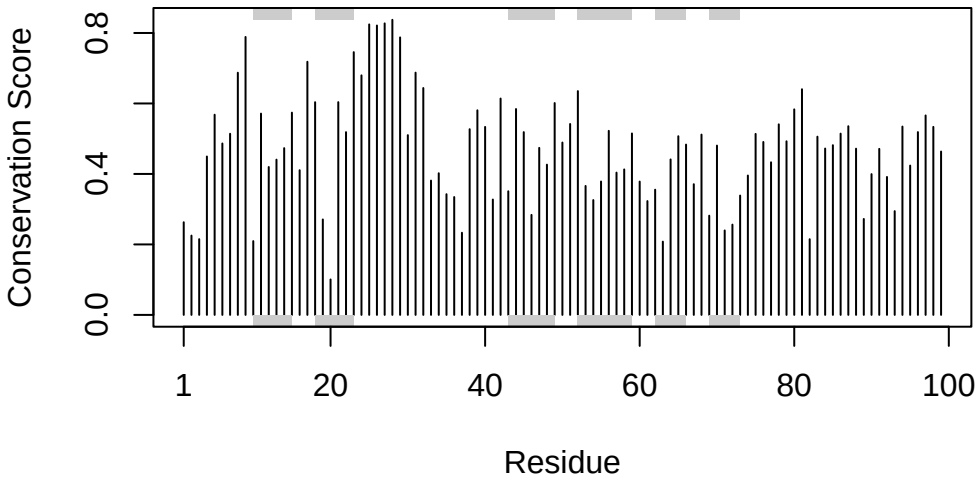
```
aln <- read.fasta(aln_file[1], to.upper = TRUE)
```

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

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

```
[1] 5378  132
```

```
sim <- conserv(aln)

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




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

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

```
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")
```