AlphaFold Analysis

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2025-02-11

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Here we analyze our AlphaFold structure prediction models. The input direcotry/folder comers from the ColabFold server:

```
results_dir <- "test_23119/"
```

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

basename(pdb_files)
```

```
[1] "test_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_1_seed_000.pdb"
[2] "test_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000.pdb"
[3] "test_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000.pdb"
[4] "test_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_seed_000.pdb"
[5] "test_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000.pdb"
```

```
library(bio3d)
```

```
Warning: package 'bio3d' was built under R version 4.4.1
```

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

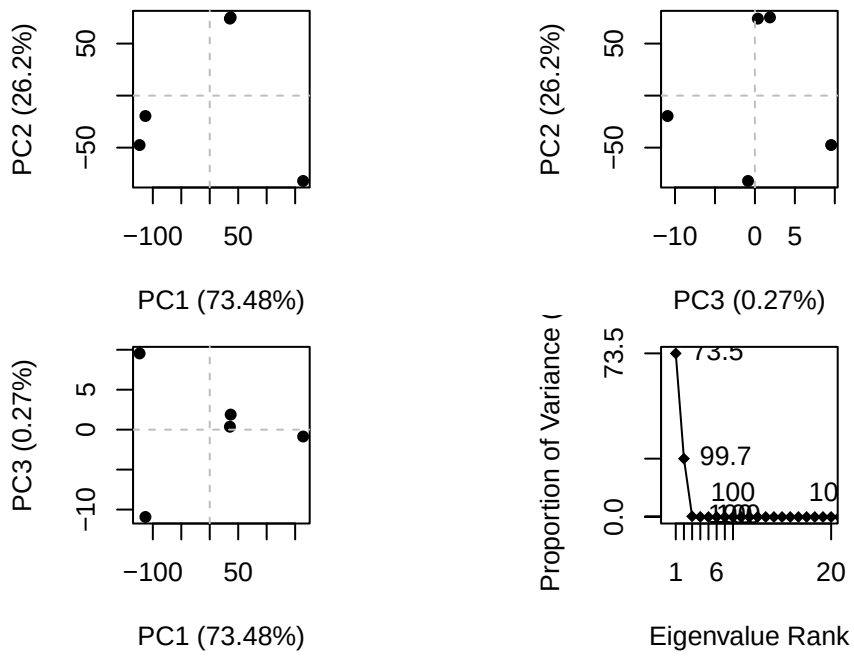
```
Reading PDB files:
test_23119//test_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_1_seed_000.pdb
test_23119//test_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000.pdb
test_23119//test_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000.pdb
test_23119//test_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_seed_000.pdb
test_23119//test_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000.pdb
.....

Extracting sequences

pdb/seq: 1   name: test_23119//test_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_1_s
pdb/seq: 2   name: test_23119//test_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_s
pdb/seq: 3   name: test_23119//test_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_s
pdb/seq: 4   name: test_23119//test_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_s
pdb/seq: 5   name: test_23119//test_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_s
```

```
pdbs
```

```
                              1        .         .         .         .         50
[Truncated_Name:1]test_23119   PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGI
[Truncated_Name:2]test_23119   PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGI
[Truncated_Name:3]test_23119   PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGI
[Truncated_Name:4]test_23119   PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGI
[Truncated_Name:5]test_23119   PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGI
                               **************************************************
                              1        .         .         .         .         50

                             51        .         .         .         .         100
[Truncated_Name:1]test_23119   GGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFP
[Truncated_Name:2]test_23119   GGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFP
[Truncated_Name:3]test_23119   GGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFP
[Truncated_Name:4]test_23119   GGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFP
[Truncated_Name:5]test_23119   GGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFP
                               **************************************************
                             51        .         .         .         .         100

                            101        .         .         .         .         150
[Truncated_Name:1]test_23119   QITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGIG
[Truncated_Name:2]test_23119   QITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGIG
[Truncated_Name:3]test_23119   QITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGIG
[Truncated_Name:4]test_23119   QITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGIG
[Truncated_Name:5]test_23119   QITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGIG
```

```
                                 **************************************************
                               101        .         .         .         .         150

                               151        .         .         .         .       198
[Truncated_Name:1]test_23119   GFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNF
[Truncated_Name:2]test_23119   GFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNF
[Truncated_Name:3]test_23119   GFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNF
[Truncated_Name:4]test_23119   GFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNF
[Truncated_Name:5]test_23119   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
```

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



RMSD analysis

RMSD is a common measure of structural distance used in structural biology.

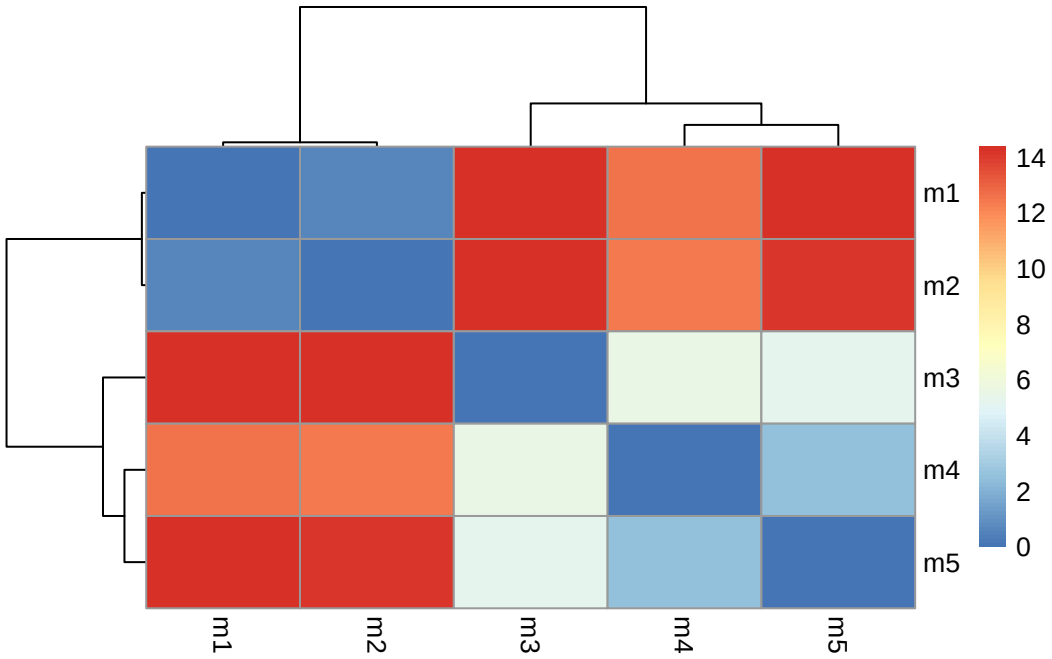
```
rd <- rmsd(pdbs, fit=T)
```

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

```
range(rd)
```

```
[1]  0.000 14.376
```

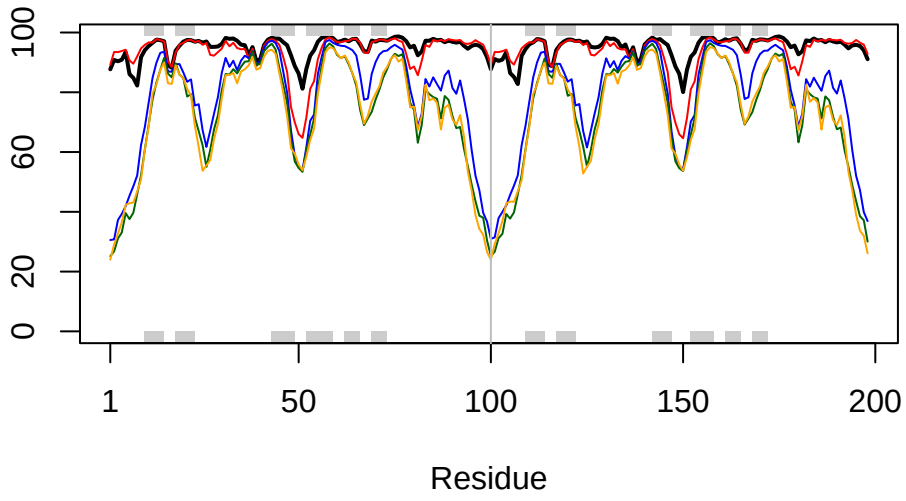
```
library(pheatmap)

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




```
# 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")
```




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

```
 core size 197 of 198  vol = 4916.702
 core size 196 of 198  vol = 4311.481
 core size 195 of 198  vol = 4101.445
 core size 194 of 198  vol = 3907.124
 core size 193 of 198  vol = 3711.925
 core size 192 of 198  vol = 3546.511
 core size 191 of 198  vol = 3440.437
 core size 190 of 198  vol = 3317.571
 core size 189 of 198  vol = 3220.079
 core size 188 of 198  vol = 3142.057
 core size 187 of 198  vol = 3066.79
 core size 186 of 198  vol = 3015.892
 core size 185 of 198  vol = 2959.969
 core size 184 of 198  vol = 2913.74
 core size 183 of 198  vol = 2880.923
 core size 182 of 198  vol = 2848.081
 core size 181 of 198  vol = 2857.001
 core size 180 of 198  vol = 2871.24
 core size 179 of 198  vol = 2905.696
 core size 178 of 198  vol = 2953.776
```

```
core size 177 of 198  vol = 3020.847
core size 176 of 198  vol = 3087.22
core size 175 of 198  vol = 3109.99
core size 174 of 198  vol = 3129.601
core size 173 of 198  vol = 3135.085
core size 172 of 198  vol = 3092.283
core size 171 of 198  vol = 3036.012
core size 170 of 198  vol = 2947.995
core size 169 of 198  vol = 2886.897
core size 168 of 198  vol = 2829.355
core size 167 of 198  vol = 2746.377
core size 166 of 198  vol = 2671.189
core size 165 of 198  vol = 2600.848
core size 164 of 198  vol = 2534.651
core size 163 of 198  vol = 2464.3
core size 162 of 198  vol = 2390.171
core size 161 of 198  vol = 2322.47
core size 160 of 198  vol = 2236.698
core size 159 of 198  vol = 2160.475
core size 158 of 198  vol = 2077.281
core size 157 of 198  vol = 2003.596
core size 156 of 198  vol = 1939.94
core size 155 of 198  vol = 1859.188
core size 154 of 198  vol = 1781.083
core size 153 of 198  vol = 1699.1
core size 152 of 198  vol = 1622.558
core size 151 of 198  vol = 1546.319
core size 150 of 198  vol = 1473.01
core size 149 of 198  vol = 1414.087
core size 148 of 198  vol = 1352.547
core size 147 of 198  vol = 1295.278
core size 146 of 198  vol = 1246.999
core size 145 of 198  vol = 1203.962
core size 144 of 198  vol = 1163.009
core size 143 of 198  vol = 1110.955
core size 142 of 198  vol = 1064.672
core size 141 of 198  vol = 1028.458
core size 140 of 198  vol = 986.121
core size 139 of 198  vol = 944.003
core size 138 of 198  vol = 895.914
core size 137 of 198  vol = 853.508
core size 136 of 198  vol = 827.977
core size 135 of 198  vol = 796.874
```

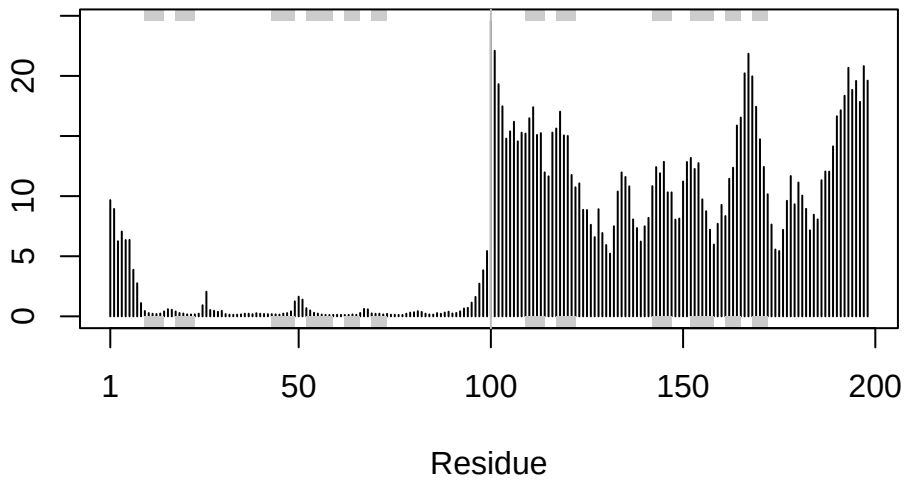
```
core size 134 of 198  vol = 772.763
core size 133 of 198  vol = 743.108
core size 132 of 198  vol = 707.65
core size 131 of 198  vol = 669.172
core size 130 of 198  vol = 634.655
core size 129 of 198  vol = 594.035
core size 128 of 198  vol = 559.154
core size 127 of 198  vol = 525.971
core size 126 of 198  vol = 493.19
core size 125 of 198  vol = 466.473
core size 124 of 198  vol = 438.433
core size 123 of 198  vol = 410.725
core size 122 of 198  vol = 401.38
core size 121 of 198  vol = 391.76
core size 120 of 198  vol = 362.084
core size 119 of 198  vol = 338.183
core size 118 of 198  vol = 312.338
core size 117 of 198  vol = 282.176
core size 116 of 198  vol = 262.215
core size 115 of 198  vol = 241.577
core size 114 of 198  vol = 225.151
core size 113 of 198  vol = 204.137
core size 112 of 198  vol = 185.038
core size 111 of 198  vol = 162.728
core size 110 of 198  vol = 146.181
core size 109 of 198  vol = 133.352
core size 108 of 198  vol = 123.207
core size 107 of 198  vol = 109.228
core size 106 of 198  vol = 98.824
core size 105 of 198  vol = 89.735
core size 104 of 198  vol = 81.206
core size 103 of 198  vol = 74.188
core size 102 of 198  vol = 67.042
core size 101 of 198  vol = 62.043
core size 100 of 198  vol = 58.432
core size 99 of 198  vol = 55.149
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 = 29.784
core size 93 of 198  vol = 23.233
core size 92 of 198  vol = 16.669
```

```
 core size 91 of 198  vol = 9.459
 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 = 1.935
 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
xyz <- pdbfit(pdbs, core.inds, outpath="corefit_structures")

rf <- rmsf(xyz)

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


0
5
10
20
1
50
100
150
200
Residue