

# Class11: Alphafold2 Analysis

Brian Wells (PID: A69026838)

Here we post process and inspect our modeling results from AlphaFold2

```
library(bio3d)
results_dir <- "HIVprdimer_23119_0/"
pdb_files <- list.files(results_dir, pattern = ".pdb", full.names = T)
```

We first need to align and superpose these PDB models we can use the `pdbaln()` function for this:

```
pdbbs <- pdbaln(pdb_files, fit=T, exefile="msa")
```

Reading PDB files:

```
HIVprdimer_23119_0//HIVprdimer_23119_0_unrelaxed_rank_001_alphafold2_multimer_v3_model_1_seed.pdb
HIVprdimer_23119_0//HIVprdimer_23119_0_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed.pdb
HIVprdimer_23119_0//HIVprdimer_23119_0_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed.pdb
HIVprdimer_23119_0//HIVprdimer_23119_0_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_seed.pdb
HIVprdimer_23119_0//HIVprdimer_23119_0_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed.pdb
.....
```

Extracting sequences

```
pdb/seq: 1  name: HIVprdimer_23119_0//HIVprdimer_23119_0_unrelaxed_rank_001_alphafold2_multimer_v3_model_1_seed.pdb
pdb/seq: 2  name: HIVprdimer_23119_0//HIVprdimer_23119_0_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed.pdb
pdb/seq: 3  name: HIVprdimer_23119_0//HIVprdimer_23119_0_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed.pdb
pdb/seq: 4  name: HIVprdimer_23119_0//HIVprdimer_23119_0_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_seed.pdb
pdb/seq: 5  name: HIVprdimer_23119_0//HIVprdimer_23119_0_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed.pdb
```

## the RMSD matrix

A common measure of structural dis-similarity is called RMSD (root mean square distance)

```
rd <- rmsd(pdbbs)
```

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

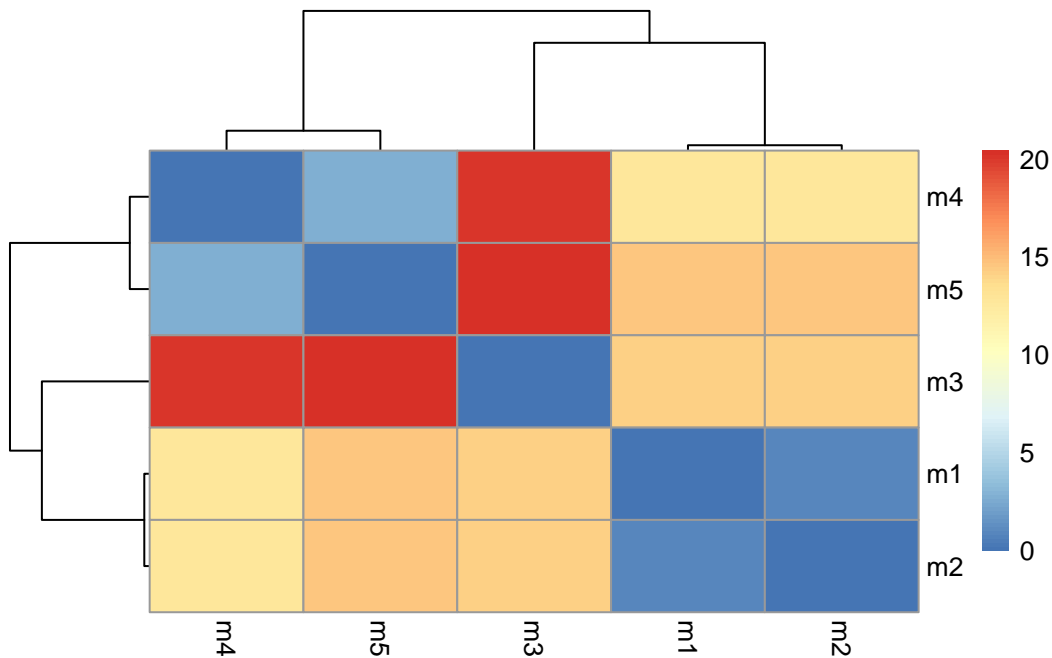
```
rd
```

```
HIVprdimer_23119_0_unrelaxed_rank_001_alphafold2_multimer_v3_model_1_seed_000
HIVprdimer_23119_0_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000
HIVprdimer_23119_0_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000
HIVprdimer_23119_0_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_seed_000
HIVprdimer_23119_0_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000
HIVprdimer_23119_0_unrelaxed_rank_001_alphafold2_multimer_v3_model_1_seed_000
HIVprdimer_23119_0_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000
HIVprdimer_23119_0_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000
HIVprdimer_23119_0_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_seed_000
HIVprdimer_23119_0_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000
HIVprdimer_23119_0_unrelaxed_rank_001_alphafold2_multimer_v3_model_1_seed_000
HIVprdimer_23119_0_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000
HIVprdimer_23119_0_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000
HIVprdimer_23119_0_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_seed_000
HIVprdimer_23119_0_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000
HIVprdimer_23119_0_unrelaxed_rank_001_alphafold2_multimer_v3_model_1_seed_000
HIVprdimer_23119_0_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000
HIVprdimer_23119_0_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000
HIVprdimer_23119_0_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_seed_000
HIVprdimer_23119_0_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000
HIVprdimer_23119_0_unrelaxed_rank_001_alphafold2_multimer_v3_model_1_seed_000
HIVprdimer_23119_0_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000
HIVprdimer_23119_0_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000
HIVprdimer_23119_0_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_seed_000
HIVprdimer_23119_0_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000
```

```
library(pheatmap)
```

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

pheatmap(rd)
```



let's view these in mol\*. Here we want the fitted coords.

```
xyz <- pdbfit(pdb, outpath = "fitted")
```

A full atom based fitting or superposition did not work very well because we have multiple chains that are in different conformations

I want to focus our superposition on the most invariant part (the rigid “core”)

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

```
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 <- core
```

```
xyz <- pdbfit(pdb, inds=core.inds, outpath = "core_fitted")
```

To evaluate how good multichain or multidomain models are, we need to look at the PAE scores (Predicted aligned error)

There are output as JSON format files.

```

pae_files <- list.files(results_dir, pattern = "0.json", full.names = T)
pae_files

```

```
[1] "HIVprdimer_23119_0//HIVprdimer_23119_0_scores_rank_001_alphafold2_multimer_v3_model_1_s
[2] "HIVprdimer_23119_0//HIVprdimer_23119_0_scores_rank_002_alphafold2_multimer_v3_model_5_s
[3] "HIVprdimer_23119_0//HIVprdimer_23119_0_scores_rank_003_alphafold2_multimer_v3_model_4_s
[4] "HIVprdimer_23119_0//HIVprdimer_23119_0_scores_rank_004_alphafold2_multimer_v3_model_2_s
[5] "HIVprdimer_23119_0//HIVprdimer_23119_0_scores_rank_005_alphafold2_multimer_v3_model_3_s
```

```
library(jsonlite)
```

```
pae1 <- read_json(pae_files[1], simplifyVector = T)
pae5 <- read_json(pae_files[5], simplifyVector = T)
```

```
attributes(pae1)
```

```
$names
```

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

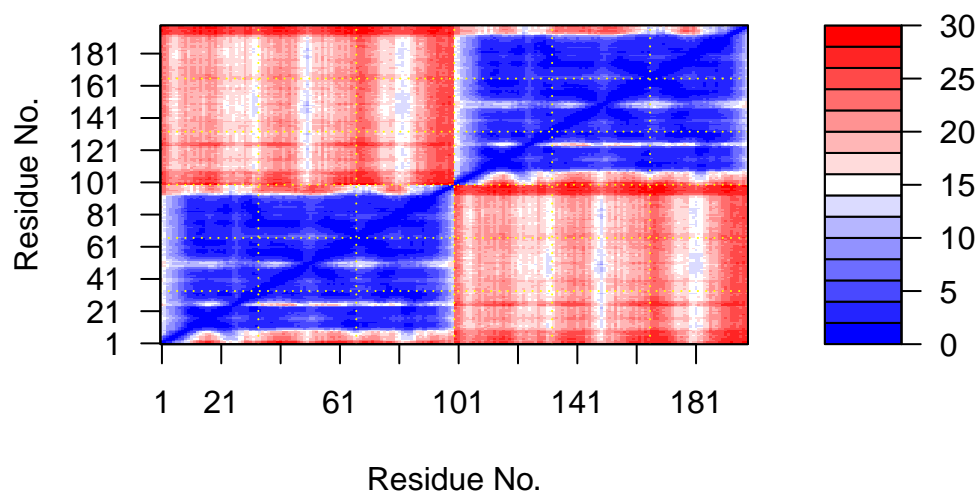
```
pae1$max_pae
```

```
[1] 15.54688
```

```
pae5$max_pae
```

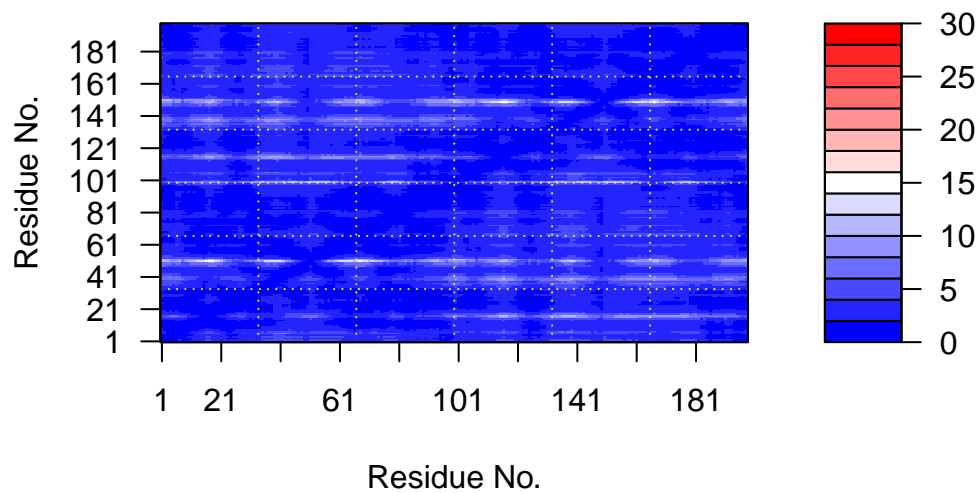
```
[1] 29.29688
```

```
plot.dmat(pae5$pae,
          xlab="Residue No.",
          ylab="Residue No.",
          zlim=c(0,30))
```



```
plot.dmat(pae1$pae,
          xlab="Residue No.",
          ylab="Residue No.",
          zlim=c(0,30))
```





#main points

We can run AlphaFold on google compute infrastructure :) We can read these results into R and process to help us make sense of these models and their PAE and pLDDT scores