class11

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Here we read the results from AlphaFold and try to interpret all the models and quality score metrics:

```
library(bio3d)

pth <- "dimmer_23119/"
pdb.files <- list.files(path=pth, full.names = TRUE, pattern = ".pdb")
```

Align and superpose all these models

```
file.exists(pdb.files)
```

```
[1] TRUE TRUE TRUE TRUE TRUE
```

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

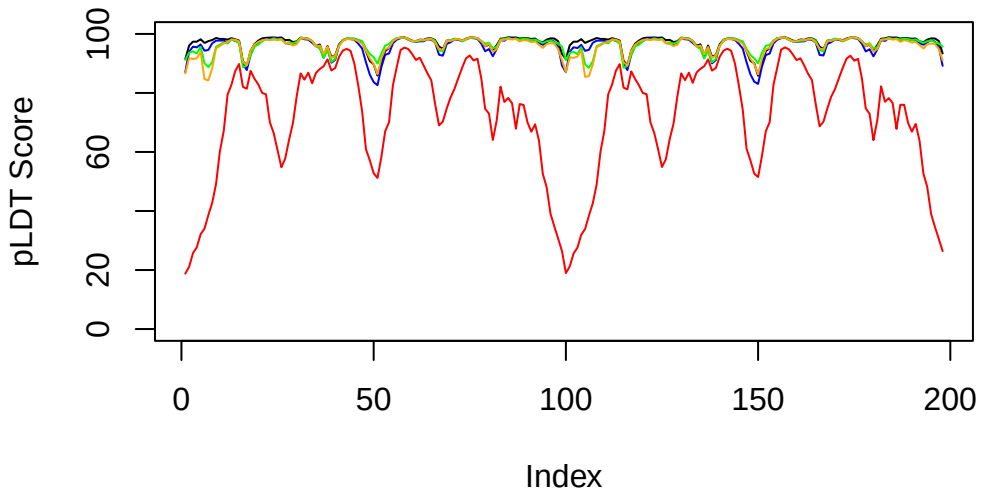
```
Reading PDB files:
dimmer_23119//dimmer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_2_seed_000.pdb
dimmer_23119//dimmer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000.pdb
dimmer_23119//dimmer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000.pdb
dimmer_23119//dimmer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_1_seed_000.pdb
dimmer_23119//dimmer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000.pdb
.....
```

```
Extracting sequences

pdb/seq: 1   name: dimmer_23119//dimmer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model
pdb/seq: 2   name: dimmer_23119//dimmer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model
pdb/seq: 3   name: dimmer_23119//dimmer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model
pdb/seq: 4   name: dimmer_23119//dimmer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model
pdb/seq: 5   name: dimmer_23119//dimmer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model
```

```
#view.pdbs(pdbs)
```

```
plot(pdbs$b[1,], typ="l", ylim=c(0, 100), ylab="pLDT Score")
lines(pdbs$b[2,], typ="l", col="blue")
lines(pdbs$b[3,], typ="l", col="green")
lines(pdbs$b[4,], typ="l", col="orange")
lines(pdbs$b[5,], typ="l", col="red")
```

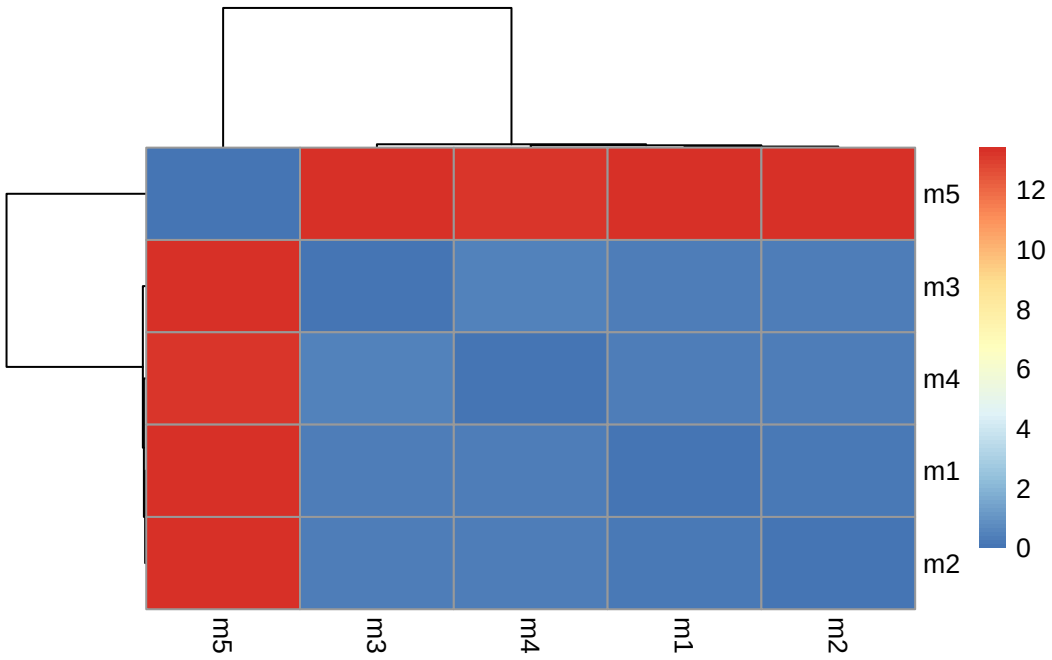



```
rd <- rmsd(pdbs, fit=T)
```

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

```
library(pheatmap)

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



Predicted Alignment Error for domains

```
library(jsonlite)

# Listing of all PAE JSON files
pae_files <- list.files(path=pth,
                        pattern=".*model.*\\.json",
                        full.names = TRUE)
```

Score Residue Conservation from alignment file

AlphaFold returns its's large alignment file used for analysis. Here we read this file and score conservation per position

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

```
[1] "dimmer_23119//dimmer_23119.a3m"
```

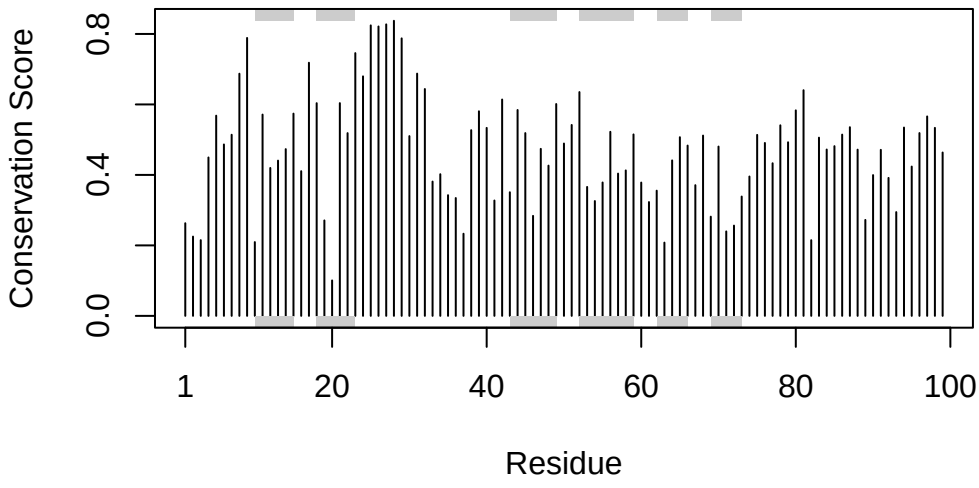
```
pdb <- read.pdb("1hsg")
```

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

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

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

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



Find the consensus sequence at a very high cut-off to find invariant residues

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

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