Class 11: Protein Structure Prediction with AlphaFold

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Generating your own structure predictions

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

```
# Call bio3d
library(bio3d)

# Read in the files
pth <- "HIV_Pr_Dimer_23119/"
pdbfiles <- list.files(path = pth, full.names=TRUE, pattern = "
```

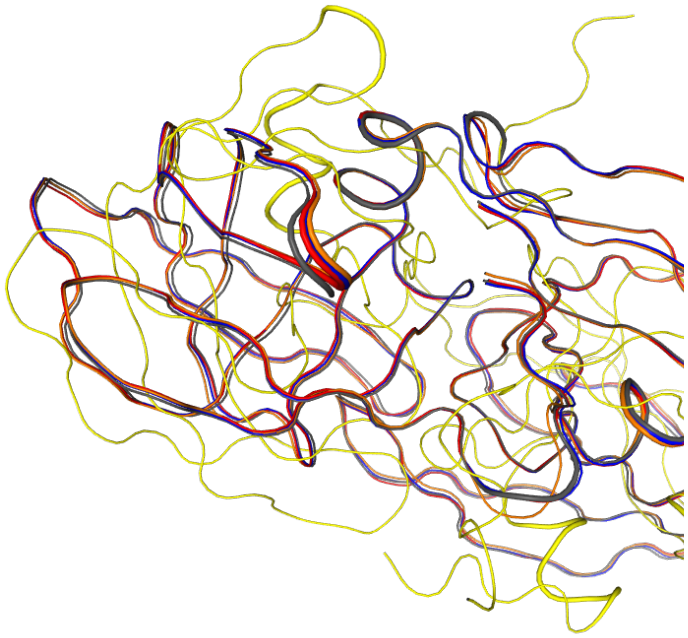
Let's align and superpose all of these models:

```
# Adding the models
pdbs <- pdbaln(pdbfiles, fit=TRUE, exefile="msa")
```

```
Reading PDB files:
HIV_Pr_Dimer_23119//HIV_Pr_Dimer_23119_unrelaxed_rank_001_alpha
fold2_multimer_v3_model_2_seed_000.pdb
HIV_Pr_Dimer_23119//HIV_Pr_Dimer_23119_unrelaxed_rank_002_alpha
fold2_multimer_v3_model_5_seed_000.pdb
HIV_Pr_Dimer_23119//HIV_Pr_Dimer_23119_unrelaxed_rank_003_alpha
fold2_multimer_v3_model_4_seed_000.pdb
HIV_Pr_Dimer_23119//HIV_Pr_Dimer_23119_unrelaxed_rank_004_alpha
fold2_multimer_v3_model_1_seed_000.pdb
HIV_Pr_Dimer_23119//HIV_Pr_Dimer_23119_unrelaxed_rank_005_alpha
fold2_multimer_v3_model_3_seed_000.pdb
.....

Extracting sequences

pdb/seq: 1   name:
HIV_Pr_Dimer_23119//HIV_Pr_Dimer_23119_unrelaxed_rank_001_alpha
fold2_multimer_v3_model_2_seed_000.pdb
pdb/seq: 2   name:
HIV_Pr_Dimer_23119//HIV_Pr_Dimer_23119_unrelaxed_rank_002_alpha
fold2_multimer_v3_model_5_seed_000.pdb
```

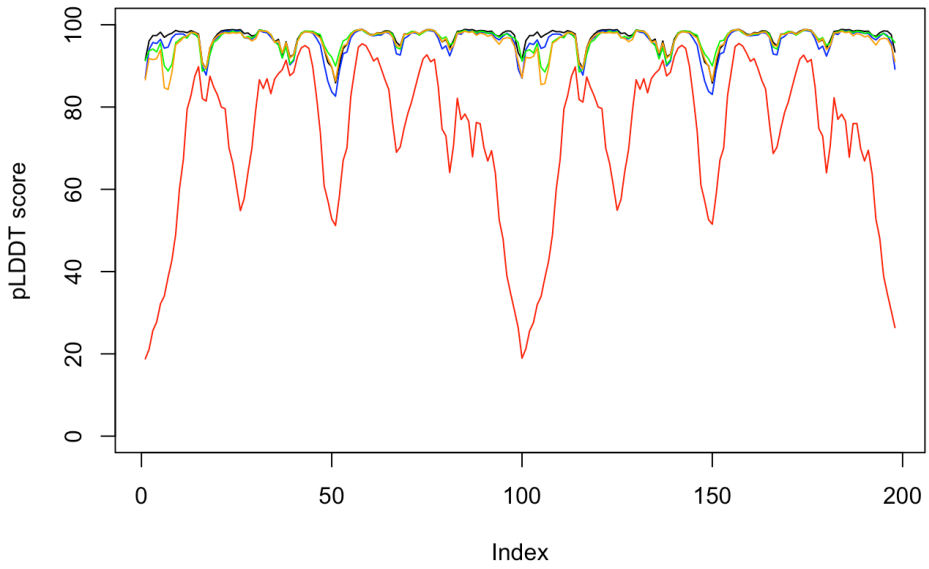
```
pdb/seq: 3   name:
HIV_Pr_Dimer_23119//HIV_Pr_Dimer_23119_unrelaxed_rank_003_alpha
fold2_multimer_v3_model_4_seed_000.pdb
pdb/seq: 4   name:
HIV_Pr_Dimer_23119//HIV_Pr_Dimer_23119_unrelaxed_rank_004_alpha
fold2_multimer_v3_model_1_seed_000.pdb
pdb/seq: 5   name:
HIV_Pr_Dimer_23119//HIV_Pr_Dimer_23119_unrelaxed_rank_005_alpha
fold2_multimer_v3_model_3_seed_000.pdb
```

```r
# Viewing the superposition
library(bio3dview)
view.pdbs(pdbs)
```



pLDDT Plot

```r
plot(pdbs$b[1,], typ="l", ylim=c(0,100), ylab="pLDDT score")
lines(pdbs$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")
```

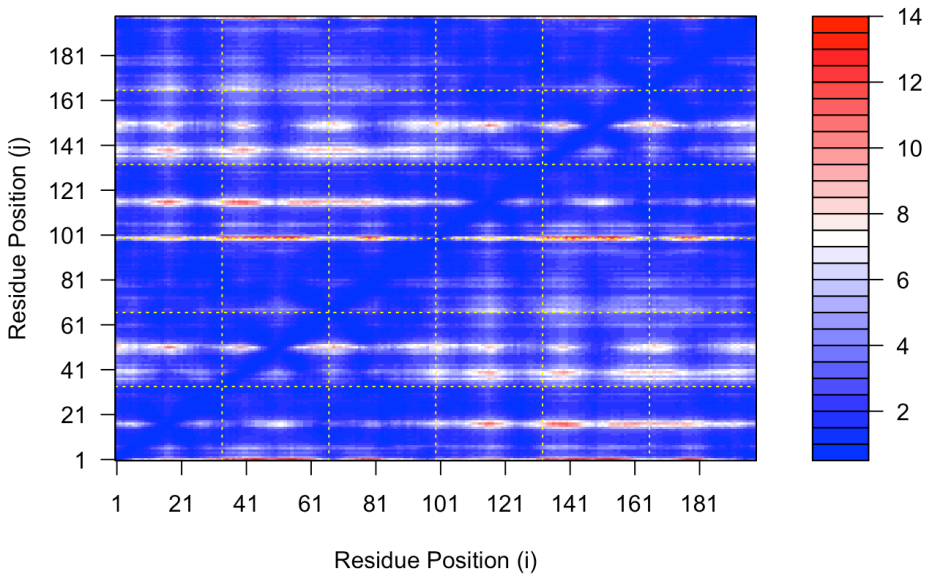


PAE Plot

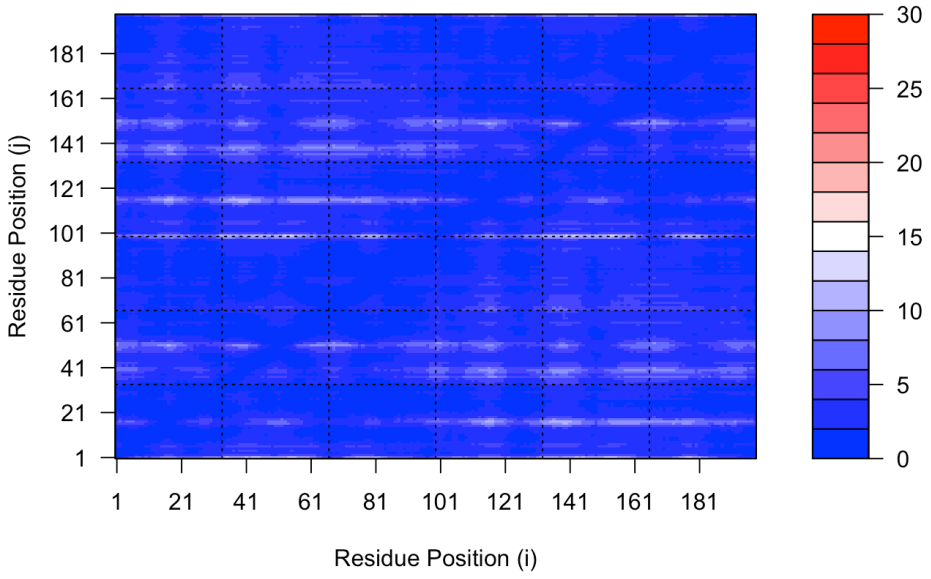
```
# Calling jsonlite
library(jsonlite)

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

# Creating objects
pae1 <- read_json(pae_files[1],simplifyVector = TRUE)
pae2 <- read_json(pae_files[2],simplifyVector = TRUE)
pae3 <- read_json(pae_files[3],simplifyVector = TRUE)
pae4 <- read_json(pae_files[4],simplifyVector = TRUE)
pae5 <- read_json(pae_files[5],simplifyVector = TRUE)
```

And now for our plots:

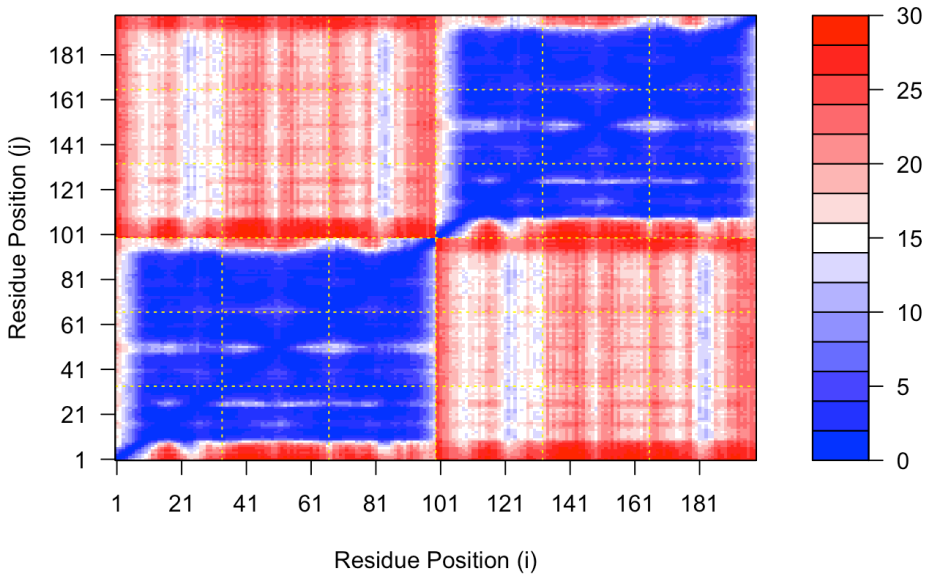
```
# Plotting PAE1
plot.dmat(pae1$pae, xlab="Residue Position (i)", ylab="Residue I
```



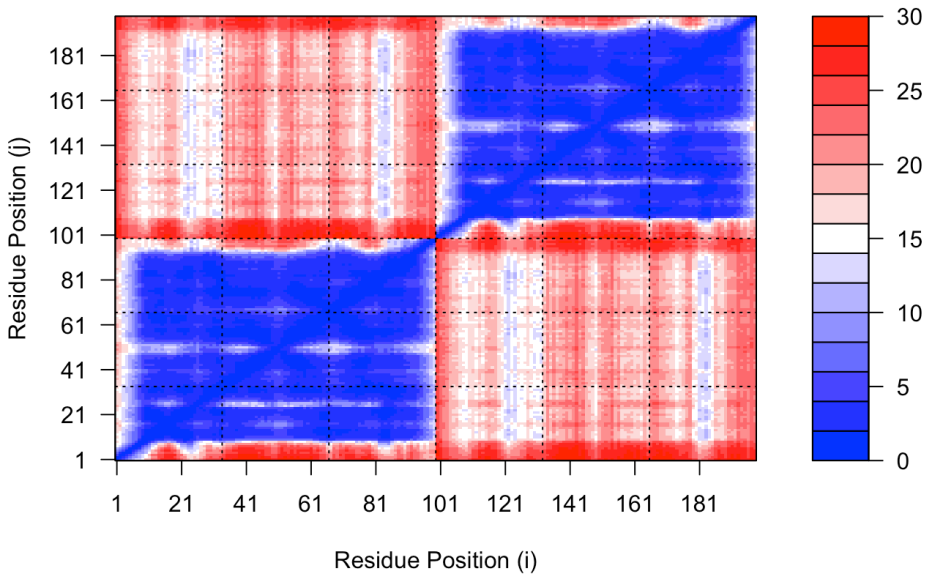

```
plot.dmat(pae1$pae,
          xlab="Residue Position (i)",
          ylab="Residue Position (j)",
          grid.col = "black",
          zlim=c(0,30))
```



```
# Plotting PAE5
plot.dmat(pae5$pae, xlab="Residue Position (i)", ylab="Residue P
```




```
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=pth,
                       pattern=".a3m$",
                        full.names = TRUE)
aln_file
```

```
[1] "HIV_Pr_Dimer_23119//HIV_Pr_Dimer_23119.a3m"
```

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

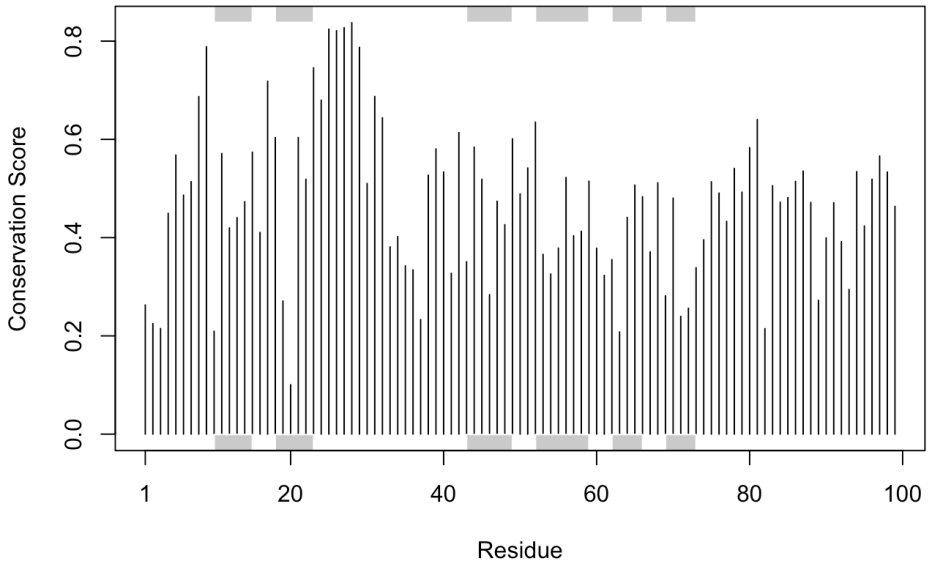
```
[1] " ** Duplicated sequence id's: 101 **"
[2] " ** Duplicated sequence id's: 101 **"
```

Let's plot:

```
sim <- conserv(aln)

# Here we can use a sample pdb file:
pdb <- read.pdb("1hsg")
```

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

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


Conservation Score
0.0
0.2
0.4
0.6
0.8
1
20
40
60
80
100
Residue