

Class 11: AlphaFold

Allen (A16897142)

Here are the results from AlphaFold to try to interpret the models and quality of the score metrics from PDB:

```
library(bio3d)

pth <- "dimer_23119/"
pdb.files <- list.files(path = pth, full.names = TRUE, pattern = ".pdb")
```

Now to align and superimpose the models

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

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

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

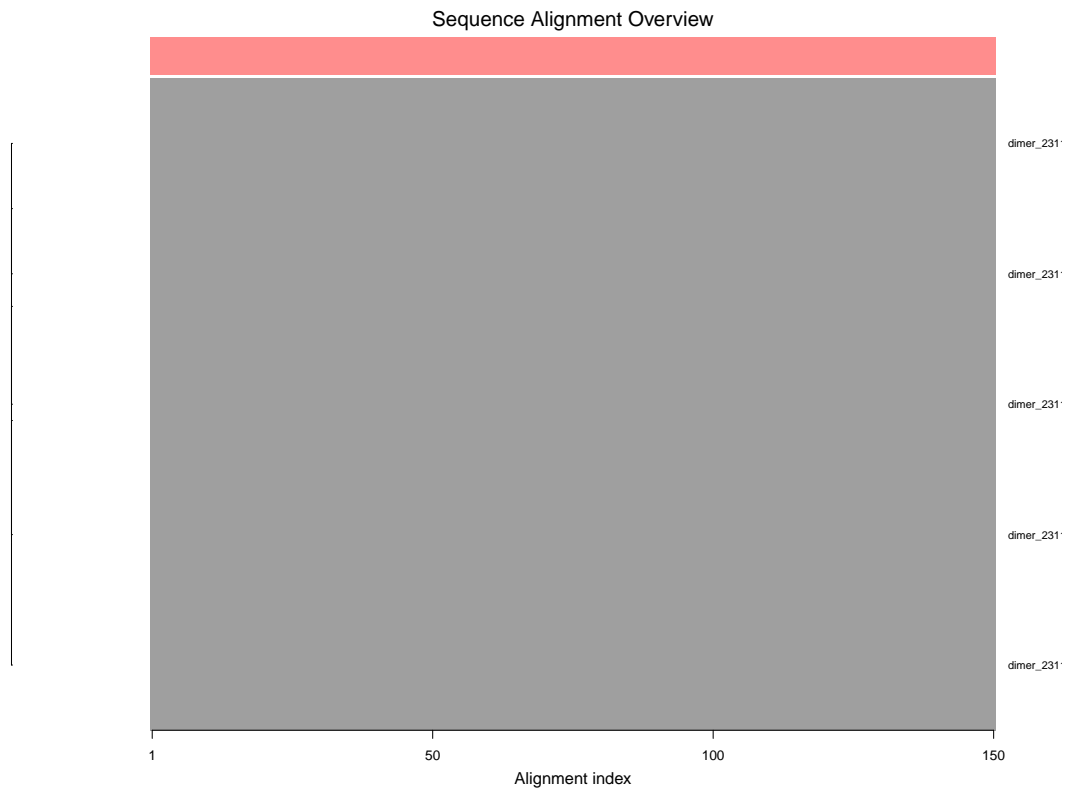
Reading PDB files:

```
dimer_23119//dimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_2_seed_000.pdb
dimer_23119//dimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000.pdb
dimer_23119//dimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000.pdb
dimer_23119//dimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_1_seed_000.pdb
dimer_23119//dimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000.pdb
.....
```

Extracting sequences

```
pdb/seq: 1   name: dimer_23119//dimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_2_seed_000.pdb
pdb/seq: 2   name: dimer_23119//dimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000.pdb
pdb/seq: 3   name: dimer_23119//dimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000.pdb
pdb/seq: 4   name: dimer_23119//dimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_1_seed_000.pdb
pdb/seq: 5   name: dimer_23119//dimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000.pdb
```

```
library(bio3d)
plot(pdbb)
```



```
plot(pdbb$b[1,],type="l", ylim=c(0,100), ylab="pLDDR score")
lines(pdbb$b[2,], type = "l",col="lightblue")
lines(pdbb$b[3,], type = "l",col="lightgreen")
lines(pdbb$b[4,], type = "l",col="yellow")
lines(pdbb$b[5,], type = "l",col="pink")
```

