AlphaFold analysis

Here we demonstrate how to analyze and make sense of models from AlphaFold. We begin by reading all the model PDB files….

```
library(bio3d)
```

PDB file names of my models

```
files <- list.files("hiv_monomer_94b5b_0/",
           pattern = ".pdb",
           full.names = T)
```

Align and superimpose

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

```
Reading PDB files:
hiv_monomer_94b5b_0/hiv_monomer_94b5b_0_unrelaxed_rank_001_alphafold2_ptm_model_5_seed_000.pd
hiv_monomer_94b5b_0/hiv_monomer_94b5b_0_unrelaxed_rank_002_alphafold2_ptm_model_4_seed_000.pd
hiv_monomer_94b5b_0/hiv_monomer_94b5b_0_unrelaxed_rank_003_alphafold2_ptm_model_1_seed_000.pd
hiv_monomer_94b5b_0/hiv_monomer_94b5b_0_unrelaxed_rank_004_alphafold2_ptm_model_3_seed_000.pd
hiv_monomer_94b5b_0/hiv_monomer_94b5b_0_unrelaxed_rank_005_alphafold2_ptm_model_2_seed_000.pd
.....

Extracting sequences

pdb/seq: 1   name: hiv_monomer_94b5b_0/hiv_monomer_94b5b_0_unrelaxed_rank_001_alphafold2_ptm_
pdb/seq: 2   name: hiv_monomer_94b5b_0/hiv_monomer_94b5b_0_unrelaxed_rank_002_alphafold2_ptm_
pdb/seq: 3   name: hiv_monomer_94b5b_0/hiv_monomer_94b5b_0_unrelaxed_rank_003_alphafold2_ptm_
pdb/seq: 4   name: hiv_monomer_94b5b_0/hiv_monomer_94b5b_0_unrelaxed_rank_004_alphafold2_ptm_
pdb/seq: 5   name: hiv_monomer_94b5b_0/hiv_monomer_94b5b_0_unrelaxed_rank_005_alphafold2_ptm_
```

RMSD analysis

```
rd <- rmsd(pdbs)
```

```
Warning in rmsd(pdbs): No indices provided, using the 99 non NA positions
```

```
mean(rd)
```

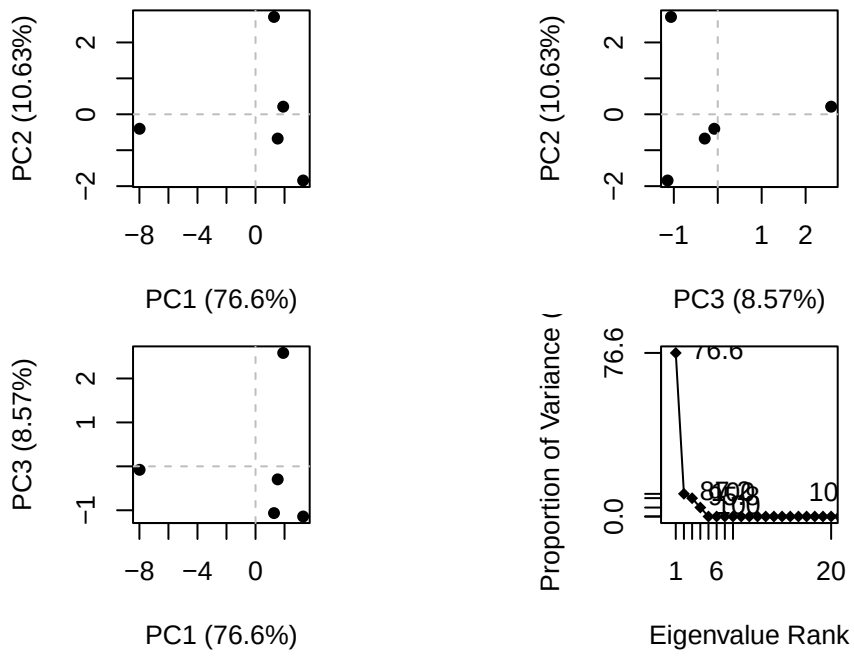
```
[1] 0.536
```

```
source("https://tinyurl.com/newviewngl")
library(NGLVieweR)
```

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

#PCA

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



#Residue conservation from alignment file

AlphaFold writes out the MSA it calculated and used for structure prediction to a A3M format file that we can read into R for further analysis:

```
aln_file <- list.files(path="hiv_monomer_94b5b_0/",
                       pattern=".a3m$",
                        full.names = TRUE)
aln_file
```

```
[1] "hiv_monomer_94b5b_0/hiv_monomer_94b5b_0.a3m"
```

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

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

```
dim(aln$ali)
```

```
[1] 5378  132
```

We can score residue conservation:

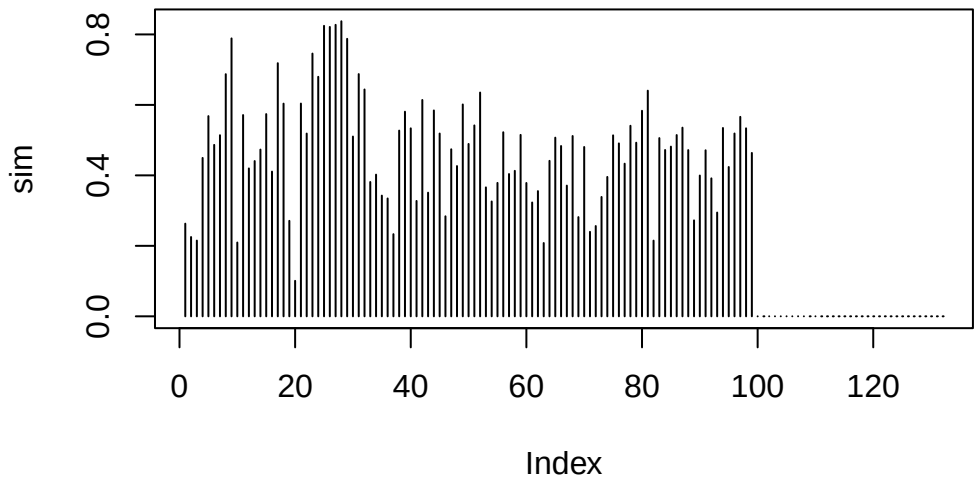
```
sim <- conserv(aln)
```

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

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

Plot the conservation along the sequence/structure

```
plot(sim, type = "h")
```



Let's look at these conversved positions in the structure:

```
pdb <- read.pdb( files[1] )

#view.pdb(pdb,  backgroundColor ="pink",
 #        highlight = atom.select(pdb,resno=25:28),
  #       highlight.style = "spacefill")
```