# AlphaFold analysis

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

```
library(bio3d)
```

```
Warning: package 'bio3d' was built under R version 4.3.3
```

PDB file names of my models

```
files <- list.files("hiv_monomer_94b5b_1/",
           pattern = ".pdb",
           full.names = T)
```

Align and superpose

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

```
Reading PDB files:
hiv_monomer_94b5b_1//hiv_monomer_94b5b_1_unrelaxed_rank_001_alphafold2_ptm_model_5_seed_0
00.pdb
hiv_monomer_94b5b_1//hiv_monomer_94b5b_1_unrelaxed_rank_002_alphafold2_ptm_model_4_seed_0
00.pdb
hiv_monomer_94b5b_1//hiv_monomer_94b5b_1_unrelaxed_rank_003_alphafold2_ptm_model_1_seed_0
00.pdb
hiv_monomer_94b5b_1//hiv_monomer_94b5b_1_unrelaxed_rank_004_alphafold2_ptm_model_3_seed_0
00.pdb
hiv_monomer_94b5b_1//hiv_monomer_94b5b_1_unrelaxed_rank_005_alphafold2_ptm_model_2_seed_0
00.pdb
.....

Extracting sequences

pdb/seq: 1   name:
hiv_monomer_94b5b_1//hiv_monomer_94b5b_1_unrelaxed_rank_001_alphafold2_ptm_model_5_seed_0
00.pdb
pdb/seq: 2   name:
hiv_monomer_94b5b_1//hiv_monomer_94b5b_1_unrelaxed_rank_002_alphafold2_ptm_model_4_seed_0
00.pdb
pdb/seq: 3   name:
hiv_monomer_94b5b_1//hiv_monomer_94b5b_1_unrelaxed_rank_003_alphafold2_ptm_model_1_seed_0
00.pdb
pdb/seq: 4   name:
hiv_monomer_94b5b_1//hiv_monomer_94b5b_1_unrelaxed_rank_004_alphafold2_ptm_model_3_seed_0
```

```
00.pdb
pdb/seq: 5   name:
hiv_monomer_94b5b_1//hiv_monomer_94b5b_1_unrelaxed_rank_005_alphafold2_ptm_model_2_seed_0
00.pdb
```

RMSD analysis

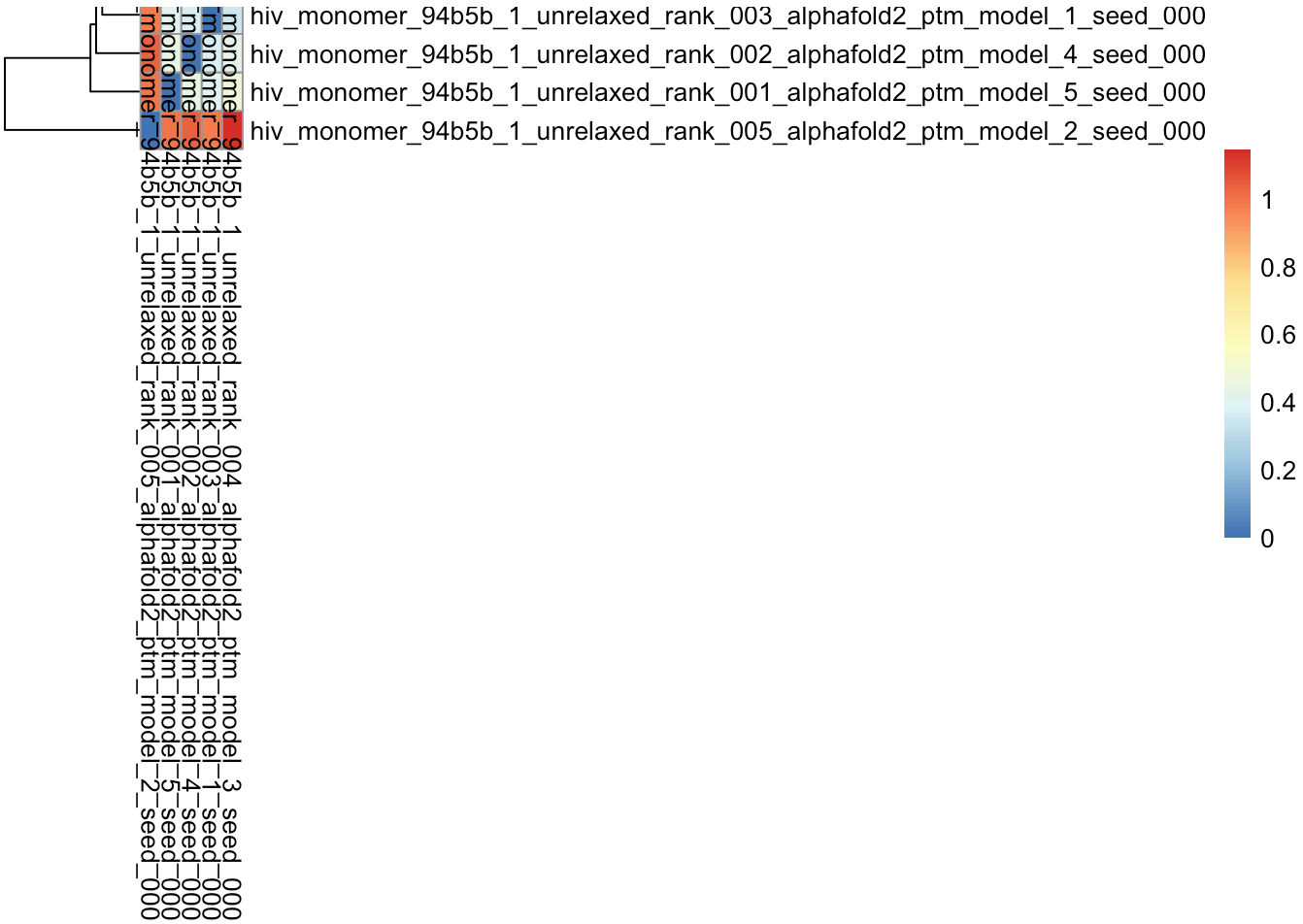
```
rd <- rmsd(pdbs)
```

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

```
mean(rd)
```

```
[1] 0.53248
```

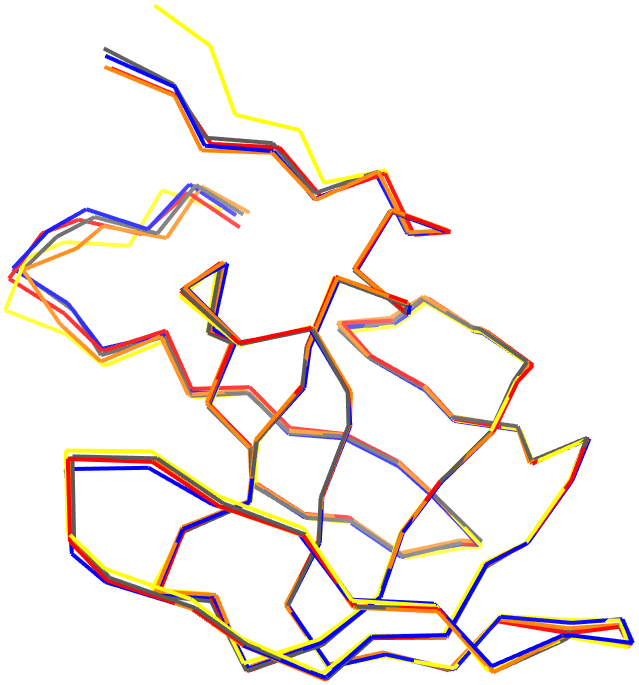
```
library(pheatmap)
pheatmap(rd)
```




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

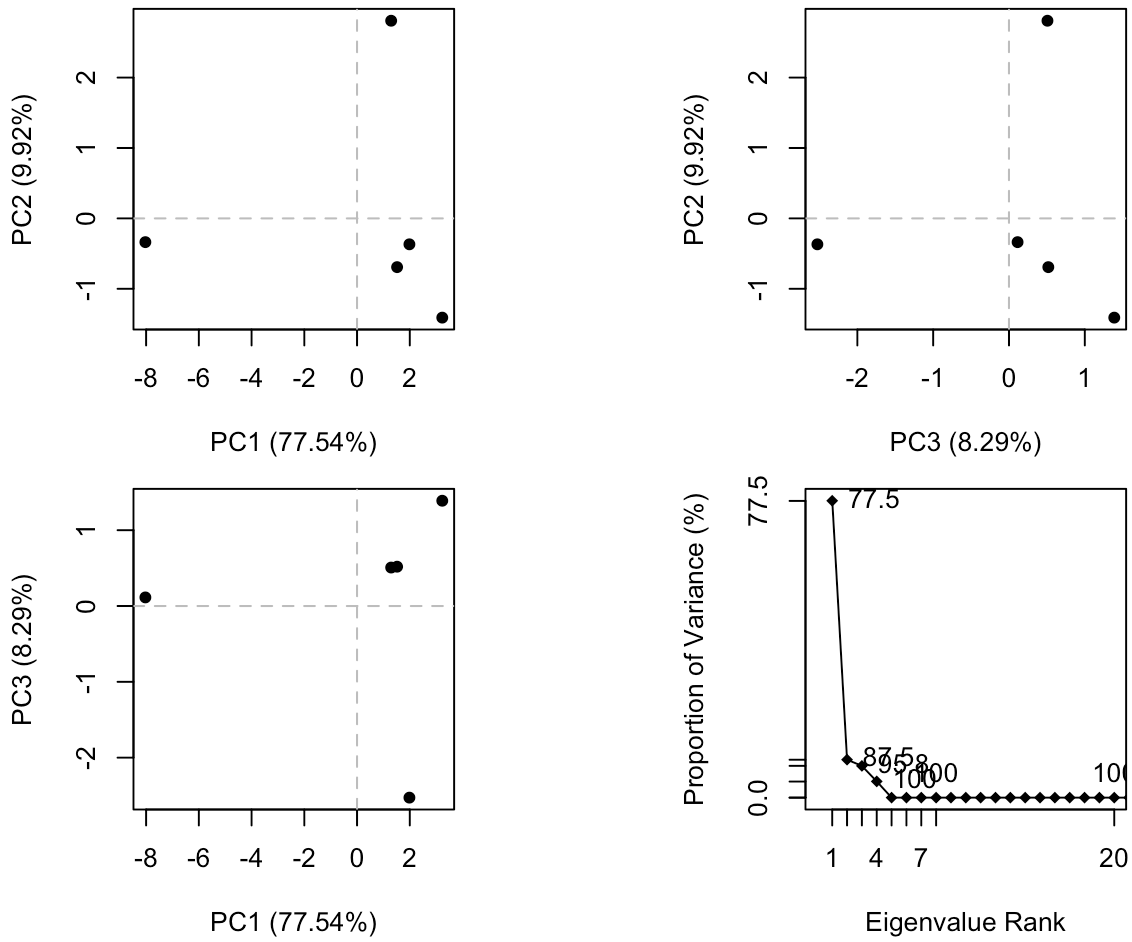
```
Warning: package 'NGLVieweR' was built under R version 4.3.3
```

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



## PCA

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




# Redidue conservation from alignment file

AlphaFold writes out the MSA it calculated and used for structure prediction to A3M.

```
aln_file <- list.files(path="hiv_monomer_94b5b_1/",
                       pattern=".a3m$",
                        full.names = TRUE)
aln_file
```

```
[1] "hiv_monomer_94b5b_1//hiv_monomer_94b5b_1.a3m"
```

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

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

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

```
[1] 5378  132
```

Score residue consevation:

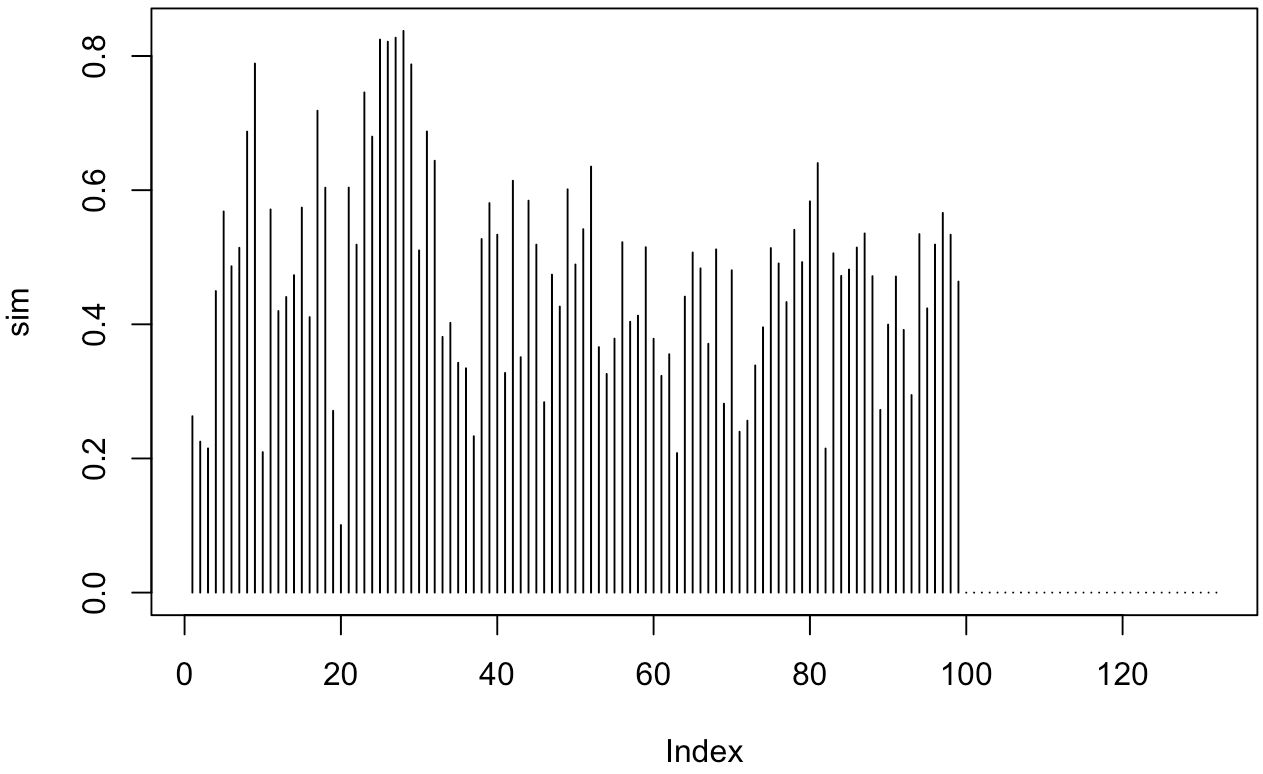
```
sim <- conserv(aln)
```

```
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, typ="h")
```




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

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

view.pdb(pdb, backgroundColor = "pink",
```

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