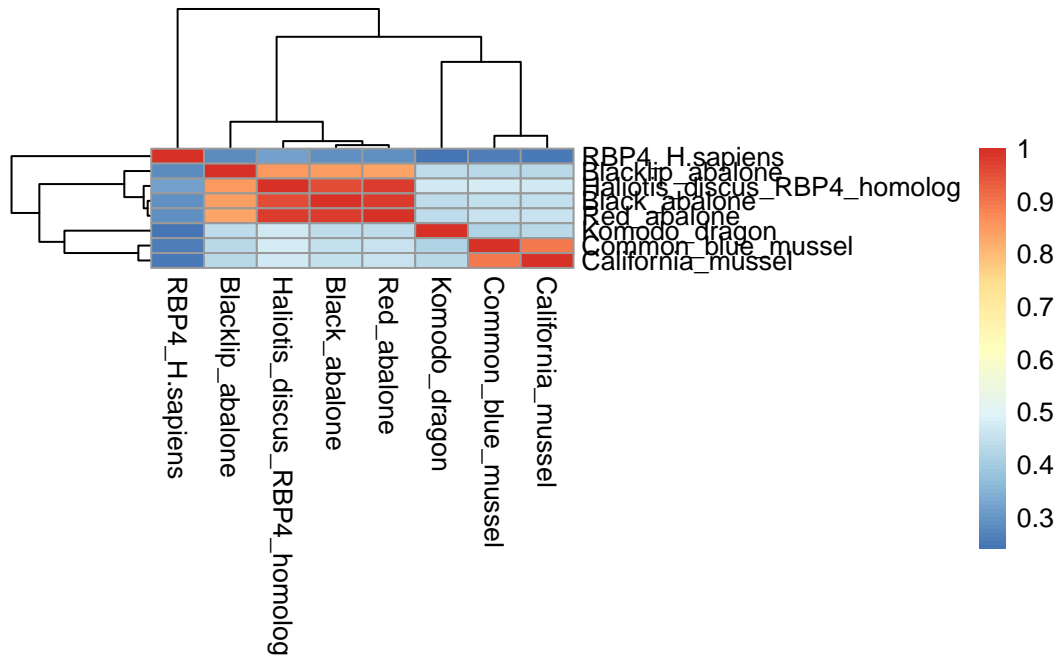# AlphaFold Analysis

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Here we analyze our AlphaFold structure prediction models. The input directory/folder comes from the ColabFold server:

7.

```r
library("bio3d")
library(pheatmap)
alignment <- read.fasta("muscle-I20250304-204254-0769-79950964-p1m.fa")

identity_matrix <- seqidentity(alignment)

p <- pheatmap(identity_matrix)
```

8. Custom analysis of resulting models

```r
results_dir <- "test_a8676"
```

```r
pdb_files <-list.files(path=results_dir,
                       pattern="*.pdb",
                       full.names = TRUE)
basename(pdb_files)
```

```
[1] "test_a8676_unrelaxed_rank_001_alphafold2_ptm_model_4_seed_000.pdb"
[2] "test_a8676_unrelaxed_rank_002_alphafold2_ptm_model_1_seed_000.pdb"
[3] "test_a8676_unrelaxed_rank_003_alphafold2_ptm_model_2_seed_000.pdb"
[4] "test_a8676_unrelaxed_rank_004_alphafold2_ptm_model_3_seed_000.pdb"
[5] "test_a8676_unrelaxed_rank_005_alphafold2_ptm_model_5_seed_000.pdb"
```

```r
alignment$id
```

```
[1] "RBP4_H.sapiens"              "Common_blue_mussel"
[3] "California_mussel"           "Komodo_dragon"
[5] "Blacklip_abalone"           "Black_abalone"
[7] "Haliotis_discus_RBP4_homolog" "Red_abalone"
```

```r
library(bio3d)

pdb_inputseq <- paste0(alignment$ali[7,], collapse ="") #Row 7 is the Haliotis_discus_RBP4_h

blast_pdb_res <- blast.pdb(pdb_inputseq)
```

```
 Searching ... please wait (updates every 5 seconds) RID = X98MJ7K6013
 .....................
 Reporting 37 hits
```

```r
hits <- blast_pdb_res$hit.tbl

pdb_annot <- pdb.annotate(c("2HZQ_A", "7YX1_A", "1Z24_A"))

pdb_annot_res <- pdb_annot[,c(1,5,6,11)]

hits_stats <- hits[hits$subjectids %in% c("2HZQ_A", "7YX1_A", "1Z24_A"), c("identity", "evalu

q8_res <- cbind(pdb_annot_res, hits_stats)

q8_res <- q8_res[, c(3,1,2,4,5)]

write.csv(q8_res, "Q8_top3_res.csv", row.names = F)
```