Class 11: AlphaFold

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

```
library(bio3d)

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

Align and superimpose all these models

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

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

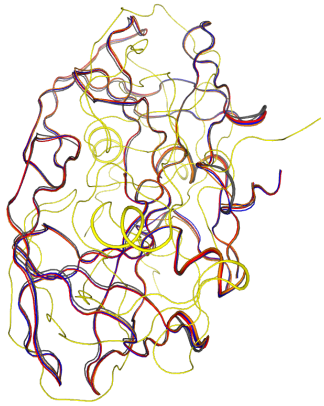
```
pdbs <- pdbaln(pdb.files, fit = TRUE, exefile="msa")
```

```
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
pdb/seq: 2   name: dimer_23119//dimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5
pdb/seq: 3   name: dimer_23119//dimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4
pdb/seq: 4   name: dimer_23119//dimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_1
pdb/seq: 5   name: dimer_23119//dimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3
```

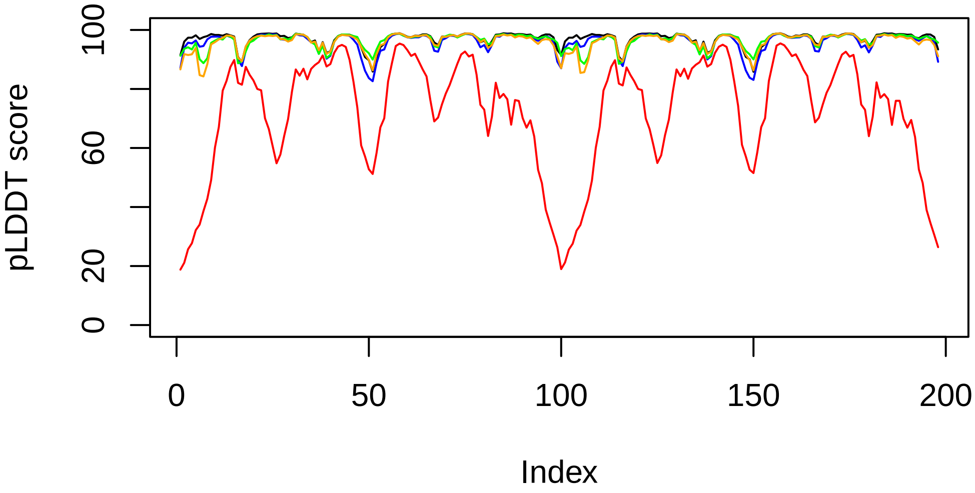
```r
library(bio3dview)

view.pdbs(pdbs)
```

```
PhantomJS not found. You can install it with webshot::install_phantomjs(). If it is installe
```

```
file:////private/var/folders/6n/3sr7q3vj2dg6y_wms7y6bxvh0000gn/T/RtmpWTJCyv/file13c7c5d65cc9
```



```
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")
```



```
# File names for all PDB models
pdb_files <- list.files(path=pth,
                        pattern="*.pdb",
                        full.names = TRUE)

# Print our PDB file names
basename(pdb_files)
```

```
[1] "dimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_2_seed_000.pdb"
[2] "dimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000.pdb"
[3] "dimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000.pdb"
[4] "dimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_1_seed_000.pdb"
[5] "dimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000.pdb"
```

```r
library(bio3d)

# Read all data from Models
#  and superpose/fit coords
pdbs <- 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_
pdb/seq: 2   name: dimer_23119//dimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_
pdb/seq: 3   name: dimer_23119//dimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_
pdb/seq: 4   name: dimer_23119//dimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_
pdb/seq: 5   name: dimer_23119//dimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_
```

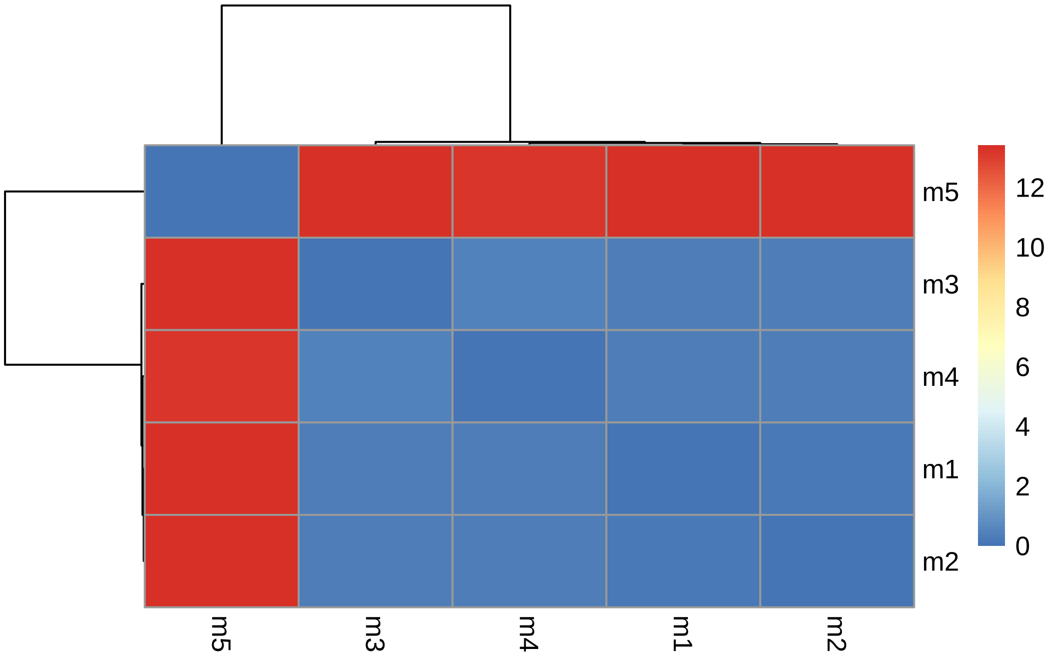
```r
rd <- rmsd(pdbs, fit=T)
```

```
Warning in rmsd(pdbs, fit = T): No indices provided, using the 198 non NA positions
```

```r
range(rd)
```

```
[1]  0.000 13.406
```

```r
library(pheatmap)

colnames(rd) <- paste0("m",1:5)
rownames(rd) <- paste0("m",1:5)
pheatmap(rd)
```



```
# Read a reference PDB structure
pdb <- read.pdb("1hsg")
```

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

```
core <- core.find(pdbs)
```

```
 core size 197 of 198  vol = 32.323
 core size 196 of 198  vol = 28.916
 core size 195 of 198  vol = 27.276
 core size 194 of 198  vol = 25.733
 core size 193 of 198  vol = 24.724
 core size 192 of 198  vol = 23.805
 core size 191 of 198  vol = 23.128
 core size 190 of 198  vol = 22.502
 core size 189 of 198  vol = 21.867
 core size 188 of 198  vol = 21.293
 core size 187 of 198  vol = 20.774
 core size 186 of 198  vol = 20.305
 core size 185 of 198  vol = 19.783
 core size 184 of 198  vol = 19.353
```

```
core size 183 of 198  vol = 18.94
core size 182 of 198  vol = 18.539
core size 181 of 198  vol = 18.097
core size 180 of 198  vol = 17.694
core size 179 of 198  vol = 17.257
core size 178 of 198  vol = 16.867
core size 177 of 198  vol = 16.519
core size 176 of 198  vol = 16.237
core size 175 of 198  vol = 15.978
core size 174 of 198  vol = 15.693
core size 173 of 198  vol = 15.412
core size 172 of 198  vol = 15.174
core size 171 of 198  vol = 14.957
core size 170 of 198  vol = 14.733
core size 169 of 198  vol = 14.532
core size 168 of 198  vol = 14.363
core size 167 of 198  vol = 14.222
core size 166 of 198  vol = 13.981
core size 165 of 198  vol = 13.885
core size 164 of 198  vol = 13.822
core size 163 of 198  vol = 13.736
core size 162 of 198  vol = 13.646
core size 161 of 198  vol = 13.58
core size 160 of 198  vol = 13.46
core size 159 of 198  vol = 13.261
core size 158 of 198  vol = 13.076
core size 157 of 198  vol = 12.91
core size 156 of 198  vol = 12.971
core size 155 of 198  vol = 12.926
core size 154 of 198  vol = 12.892
core size 153 of 198  vol = 12.769
core size 152 of 198  vol = 12.648
core size 151 of 198  vol = 12.53
core size 150 of 198  vol = 12.326
core size 149 of 198  vol = 12.104
core size 148 of 198  vol = 11.905
core size 147 of 198  vol = 11.473
core size 146 of 198  vol = 11.155
core size 145 of 198  vol = 10.956
core size 144 of 198  vol = 10.755
core size 143 of 198  vol = 10.546
core size 142 of 198  vol = 10.276
core size 141 of 198  vol = 10.066
core size 140 of 198  vol = 9.835
core size 139 of 198  vol = 9.619
core size 138 of 198  vol = 9.405
core size 137 of 198  vol = 9.142
core size 136 of 198  vol = 8.863
core size 135 of 198  vol = 8.526
core size 134 of 198  vol = 8.229
core size 133 of 198  vol = 7.998
core size 132 of 198  vol = 7.809
core size 131 of 198  vol = 7.509
core size 130 of 198  vol = 7.288
core size 129 of 198  vol = 7.084
core size 128 of 198  vol = 6.88
core size 127 of 198  vol = 6.59
core size 126 of 198  vol = 6.38
core size 125 of 198  vol = 6.197
core size 124 of 198  vol = 5.976
core size 123 of 198  vol = 5.764
core size 122 of 198  vol = 5.568
core size 121 of 198  vol = 5.312
core size 120 of 198  vol = 5.021
core size 119 of 198  vol = 4.758
core size 118 of 198  vol = 4.501
core size 117 of 198  vol = 4.218
core size 116 of 198  vol = 4.031
core size 115 of 198  vol = 3.801
core size 114 of 198  vol = 3.604
core size 113 of 198  vol = 3.379
core size 112 of 198  vol = 3.183
core size 111 of 198  vol = 3.002
core size 110 of 198  vol = 2.79
core size 109 of 198  vol = 2.603
core size 108 of 198  vol = 2.508
core size 107 of 198  vol = 2.421
core size 106 of 198  vol = 2.24
core size 105 of 198  vol = 2.084
core size 104 of 198  vol = 1.945
core size 103 of 198  vol = 1.832
core size 102 of 198  vol = 1.659
core size 101 of 198  vol = 1.582
core size 100 of 198  vol = 1.483
core size 99 of 198  vol = 1.382
core size 98 of 198  vol = 1.331
```

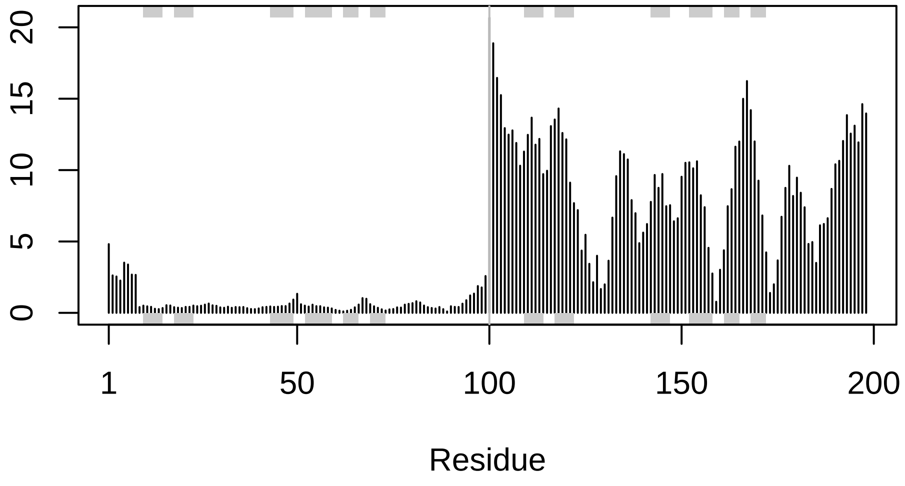
```
 core size 97 of 198  vol = 1.264
 core size 96 of 198  vol = 1.137
 core size 95 of 198  vol = 1.043
 core size 94 of 198  vol = 0.957
 core size 93 of 198  vol = 0.885
 core size 92 of 198  vol = 0.803
 core size 91 of 198  vol = 0.73
 core size 90 of 198  vol = 0.637
 core size 89 of 198  vol = 0.56
 core size 88 of 198  vol = 0.489
 FINISHED: Min vol ( 0.5 ) reached
```

```
core.inds <- print(core, vol=0.5)
```

```
# 89 positions (cumulative volume <= 0.5 Angstrom^3)
  start end length
1    10  42     33
2    44  50      7
3    52  66     15
4    69  77      9
5    80  98     19
```

```
xyz <- pdbfit(pdbs, core.inds, outpath="corefit_structures")
```

```
rf <- rmsf(xyz)

plotb3(rf, sse=pdb)
abline(v=100, col="gray", ylab="RMSF")
```



```
library(jsonlite)

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

```
pae1 <- read_json(pae_files[1],simplifyVector = TRUE)
pae5 <- read_json(pae_files[5],simplifyVector = TRUE)

attributes(pae1)
```

```
$names
[1] "plddt"   "max_pae" "pae"     "ptm"     "iptm"
```

```
# Per-residue pLDDT scores
#  same as B-factor of PDB..
head(pae1$plddt)
```

```
[1] 91.44 96.06 97.38 97.38 98.19 96.94
```

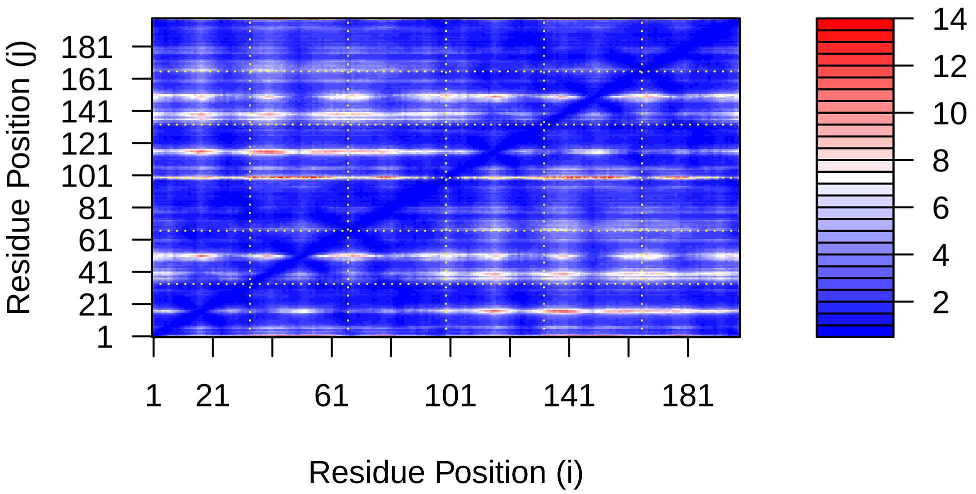
```
pae1$max_pae
```

```
[1] 13.57812
```

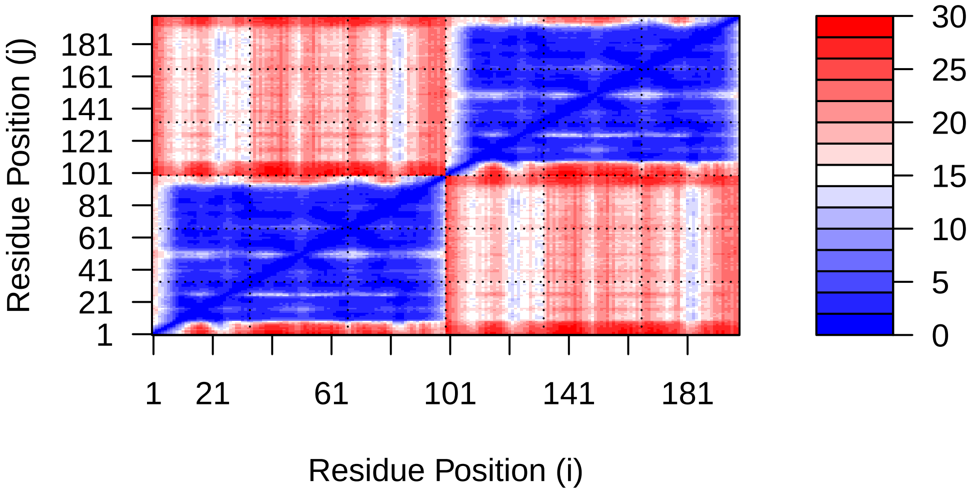
```
pae5$max_pae
```

```
[1] 29.85938
```

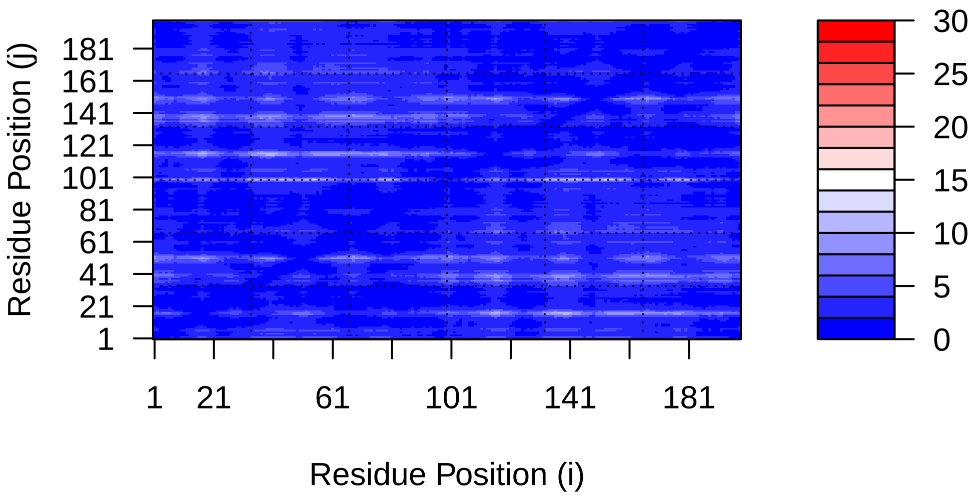
```
plot.dmat(pae1$pae,
          xlab="Residue Position (i)",
          ylab="Residue Position (j)")
```



```
plot.dmat(pae5$pae,
          xlab="Residue Position (i)",
          ylab="Residue Position (j)",
          grid.col = "black",
          zlim=c(0,30))
```



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



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

```
[1] "dimer_23119//dimer_23119.a3m"
```

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

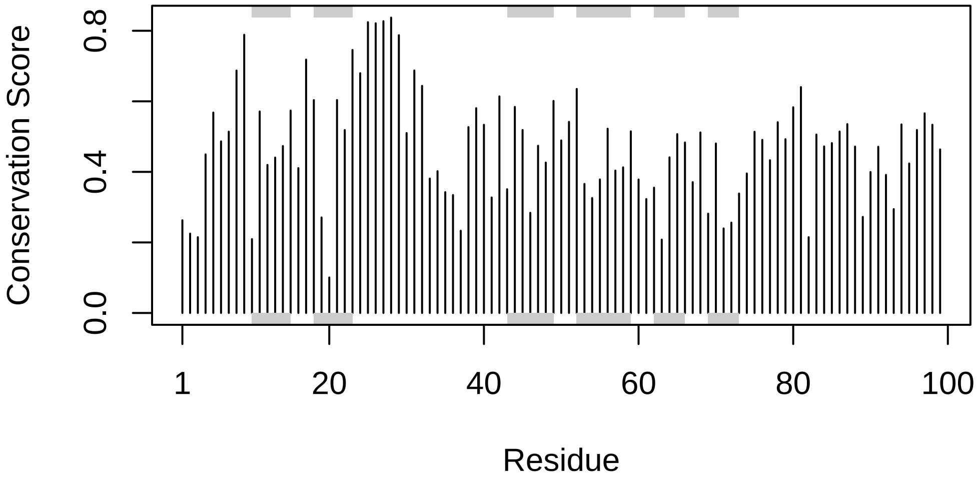
```
[1] " ** Duplicated sequence id's: 101 **"
[2] " ** Duplicated sequence id's: 101 **"
```

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

```
[1] 5378  132
```

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

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



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

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

```r
m1.pdb <- read.pdb(pdb_files[1])
occ <- vec2resno(c(sim[1:99], sim[1:99]), m1.pdb$atom$resno)
write.pdb(m1.pdb, o=occ, file="m1_conserv.pdb")
```