class11-pt2

Quarto

```
library(bio3d)
results_dir<- "HIVPrDimer_23119/"
pdb_files<-list.files(results_dir,pattern=".pdb", full.names=T)
pdbs <-pdbaln(pdb_files, fit=TRUE, exefile="msa")
```

```
Reading PDB files:
HIVPrDimer_23119//HIVPrDimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_1_seed_000
HIVPrDimer_23119//HIVPrDimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000
HIVPrDimer_23119//HIVPrDimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000
HIVPrDimer_23119//HIVPrDimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_seed_000
HIVPrDimer_23119//HIVPrDimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000
.....

Extracting sequences

pdb/seq: 1   name: HIVPrDimer_23119//HIVPrDimer_23119_unrelaxed_rank_001_alphafold2_multimer_
pdb/seq: 2   name: HIVPrDimer_23119//HIVPrDimer_23119_unrelaxed_rank_002_alphafold2_multimer_
pdb/seq: 3   name: HIVPrDimer_23119//HIVPrDimer_23119_unrelaxed_rank_003_alphafold2_multimer_
pdb/seq: 4   name: HIVPrDimer_23119//HIVPrDimer_23119_unrelaxed_rank_004_alphafold2_multimer_
pdb/seq: 5   name: HIVPrDimer_23119//HIVPrDimer_23119_unrelaxed_rank_005_alphafold2_multimer_
```

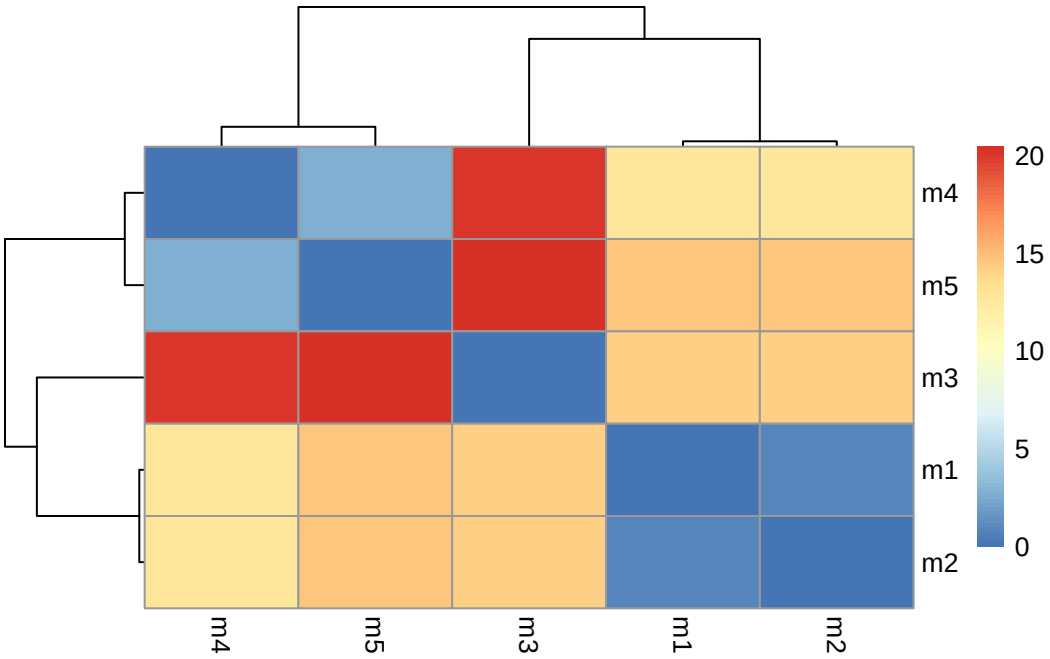
```
rd<- rmsd(pdbs)
```

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

```
rd
```

```
                                                                         HIVPrDimer_23119_
HIVPrDimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_1_seed_000
HIVPrDimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000
HIVPrDimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000
HIVPrDimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_seed_000
HIVPrDimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000
                                                                         HIVPrDimer_23119_
HIVPrDimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_1_seed_000
HIVPrDimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000
HIVPrDimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000
HIVPrDimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_seed_000
HIVPrDimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000
                                                                         HIVPrDimer_23119_
HIVPrDimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_1_seed_000
HIVPrDimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000
HIVPrDimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000
HIVPrDimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_seed_000
HIVPrDimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000
                                                                         HIVPrDimer_23119_
HIVPrDimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_1_seed_000
HIVPrDimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000
HIVPrDimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000
HIVPrDimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_seed_000
HIVPrDimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000
                                                                         HIVPrDimer_23119_
HIVPrDimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_1_seed_000
HIVPrDimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000
HIVPrDimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000
HIVPrDimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_seed_000
HIVPrDimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000
```

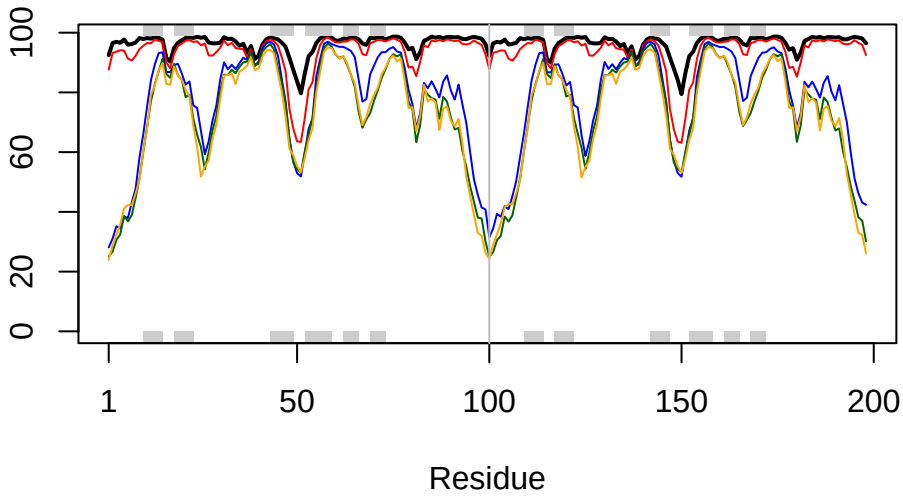
```r
library(pheatmap)
rownames(rd)<-paste0("m",1:5)
colnames(rd)<-paste0("m",1:5)
pheatmap(rd)
```




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

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

```
#Note: Accessing on-line PDB file
plotb3(pdbs$b[1,], typ="l", lwd=2, sse=pdb)
points(pdbs$b[2,], typ="l", col="red")
points(pdbs$b[3,], typ="l", col="blue")
points(pdbs$b[4,], typ="l", col="darkgreen")
points(pdbs$b[5,], typ="l", col="orange")
abline(v=100, col="gray")
```




```
# Find a rigid core amongst the structures
core <- core.find(pdbs)
```

```
core size 197 of 198  vol = 6154.839
core size 196 of 198  vol = 5399.676
core size 195 of 198  vol = 5074.795
core size 194 of 198  vol = 4802.518
core size 193 of 198  vol = 4520.256
core size 192 of 198  vol = 4305.362
core size 191 of 198  vol = 4089.792
core size 190 of 198  vol = 3886.145
core size 189 of 198  vol = 3758.321
core size 188 of 198  vol = 3620.18
core size 187 of 198  vol = 3496.698
core size 186 of 198  vol = 3389.985
core size 185 of 198  vol = 3320.114
core size 184 of 198  vol = 3258.683
core size 183 of 198  vol = 3208.591
core size 182 of 198  vol = 3156.736
core size 181 of 198  vol = 3141.668
core size 180 of 198  vol = 3136.574
core size 179 of 198  vol = 3155.52
```

```
core size 178 of 198  vol = 3185.362
core size 177 of 198  vol = 3204.487
core size 176 of 198  vol = 3211.978
core size 175 of 198  vol = 3234.993
core size 174 of 198  vol = 3244.062
core size 173 of 198  vol = 3237.845
core size 172 of 198  vol = 3218.77
core size 171 of 198  vol = 3180.743
core size 170 of 198  vol = 3130.369
core size 169 of 198  vol = 3067.881
core size 168 of 198  vol = 2989.546
core size 167 of 198  vol = 2928.272
core size 166 of 198  vol = 2851.193
core size 165 of 198  vol = 2780.877
core size 164 of 198  vol = 2708.433
core size 163 of 198  vol = 2636.516
core size 162 of 198  vol = 2563.25
core size 161 of 198  vol = 2478.024
core size 160 of 198  vol = 2404.793
core size 159 of 198  vol = 2330.997
core size 158 of 198  vol = 2250.477
core size 157 of 198  vol = 2159.432
core size 156 of 198  vol = 2070.759
core size 155 of 198  vol = 1983.579
core size 154 of 198  vol = 1917.913
core size 153 of 198  vol = 1842.556
core size 152 of 198  vol = 1775.398
core size 151 of 198  vol = 1695.133
core size 150 of 198  vol = 1632.173
core size 149 of 198  vol = 1570.391
core size 148 of 198  vol = 1497.238
core size 147 of 198  vol = 1434.802
core size 146 of 198  vol = 1367.706
core size 145 of 198  vol = 1302.596
core size 144 of 198  vol = 1251.985
core size 143 of 198  vol = 1207.976
core size 142 of 198  vol = 1167.112
core size 141 of 198  vol = 1118.27
core size 140 of 198  vol = 1081.664
core size 139 of 198  vol = 1029.75
core size 138 of 198  vol = 981.766
core size 137 of 198  vol = 944.446
core size 136 of 198  vol = 899.224
```

```
core size 135 of 198  vol = 859.402
core size 134 of 198  vol = 814.694
core size 133 of 198  vol = 771.862
core size 132 of 198  vol = 733.807
core size 131 of 198  vol = 702.053
core size 130 of 198  vol = 658.757
core size 129 of 198  vol = 622.574
core size 128 of 198  vol = 578.29
core size 127 of 198  vol = 543.07
core size 126 of 198  vol = 510.934
core size 125 of 198  vol = 481.595
core size 124 of 198  vol = 464.672
core size 123 of 198  vol = 451.721
core size 122 of 198  vol = 430.417
core size 121 of 198  vol = 409.141
core size 120 of 198  vol = 378.942
core size 119 of 198  vol = 348.325
core size 118 of 198  vol = 324.738
core size 117 of 198  vol = 312.394
core size 116 of 198  vol = 300.89
core size 115 of 198  vol = 279.976
core size 114 of 198  vol = 263.434
core size 113 of 198  vol = 250.263
core size 112 of 198  vol = 229.592
core size 111 of 198  vol = 209.929
core size 110 of 198  vol = 196.379
core size 109 of 198  vol = 180.628
core size 108 of 198  vol = 167.088
core size 107 of 198  vol = 155.875
core size 106 of 198  vol = 142.595
core size 105 of 198  vol = 128.924
core size 104 of 198  vol = 114.054
core size 103 of 198  vol = 100.936
core size 102 of 198  vol = 90.431
core size 101 of 198  vol = 81.972
core size 100 of 198  vol = 74.017
core size 99 of 198  vol = 66.855
core size 98 of 198  vol = 59.525
core size 97 of 198  vol = 52.263
core size 96 of 198  vol = 43.699
core size 95 of 198  vol = 35.813
core size 94 of 198  vol = 28.888
core size 93 of 198  vol = 20.692
```

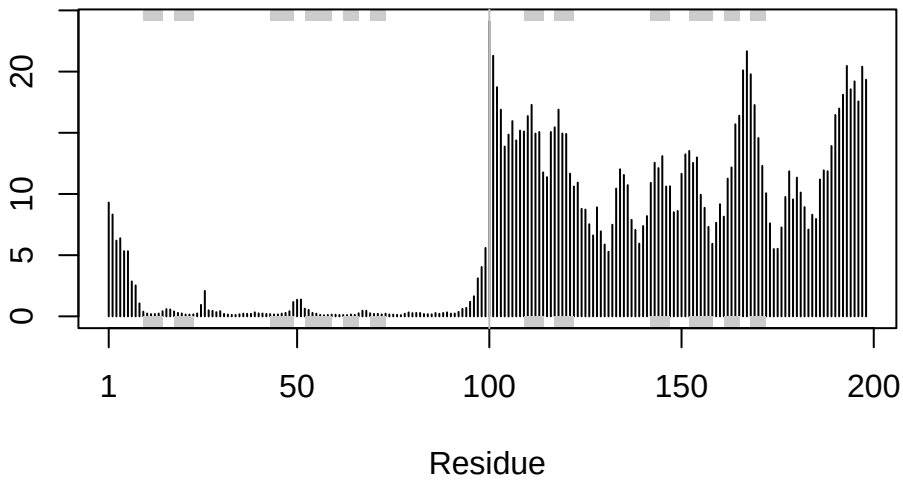
```
 core size 92 of 198  vol = 14.975
 core size 91 of 198  vol = 9.146
 core size 90 of 198  vol = 5.232
 core size 89 of 198  vol = 3.53
 core size 88 of 198  vol = 2.657
 core size 87 of 198  vol = 1.998
 core size 86 of 198  vol = 1.333
 core size 85 of 198  vol = 1.141
 core size 84 of 198  vol = 1.012
 core size 83 of 198  vol = 0.891
 core size 82 of 198  vol = 0.749
 core size 81 of 198  vol = 0.618
 core size 80 of 198  vol = 0.538
 core size 79 of 198  vol = 0.479
 FINISHED: Min vol ( 0.5 ) reached
```

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

```
# 80 positions (cumulative volume <= 0.5 Angstrom^3)
  start end length
1    10  25     16
2    27  48     22
3    53  94     42
```

view in molstar

```
xyz <- pdbfit(pdbs, core.inds, outpath="corefit_structures")
# Examine RMSDs
rf <- rmsf(xyz)
plotb3(rf, sse=pdb)
abline(v=100, col="gray", ylab="RMSF")
```




```
# Examine PAE
library(jsonlite)
# Listing of all PAE JSON files
pae_files <- list.files(path=results_dir,

pattern=".*model.*\\.json",
full.names = TRUE)

# Look at json files 1 and 5
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"
```

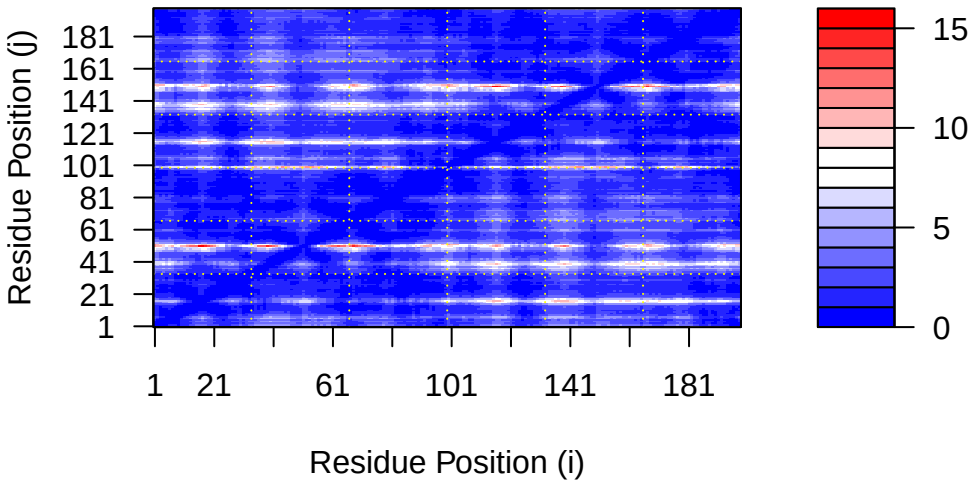
```
# Per-residue pLDDT scores
# same as B-factor of PDB..
head(pae1$plddt)
```

```
[1] 92.50 96.56 96.94 96.62 97.69 96.00
```

```
#PAE is prdicted aligned error- looks like model 1 has the lowest=good
```

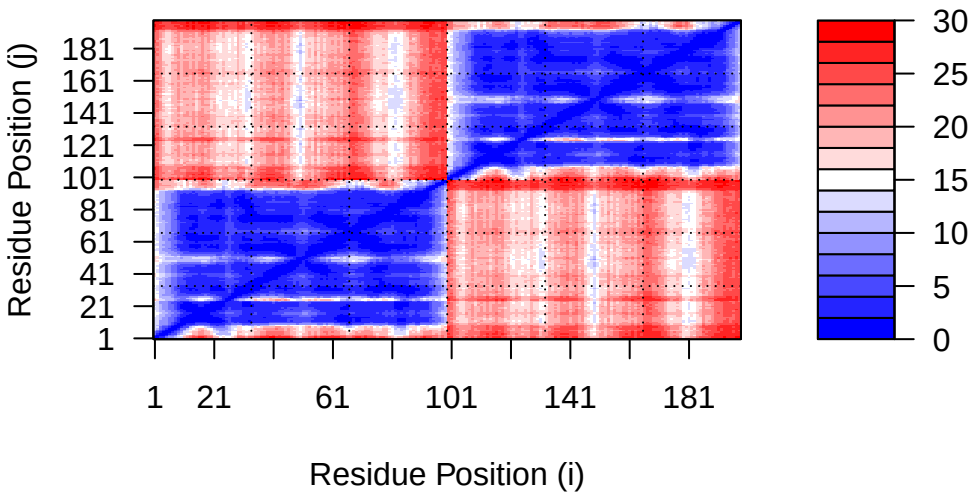
```
# plot model 1
plot.dmat(pae1$pae,

xlab="Residue Position (i)",
ylab="Residue Position (j)")
```



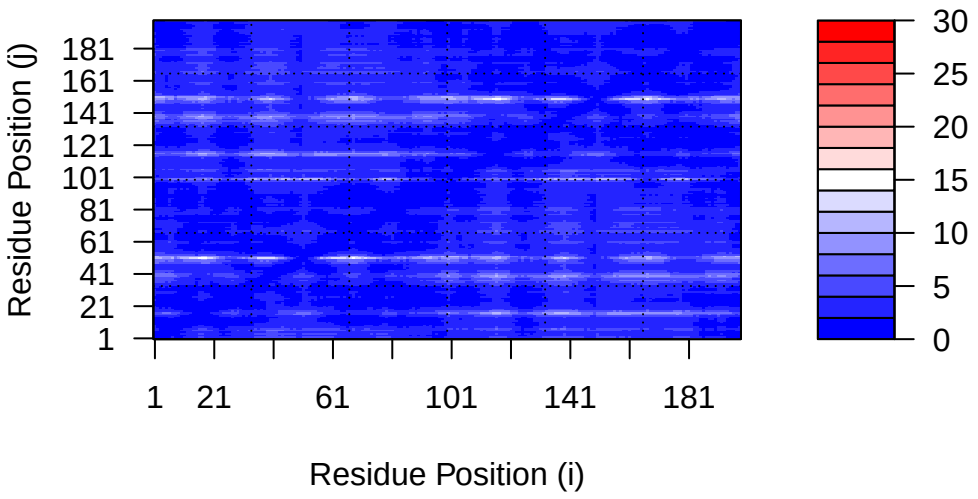

```
# plot model 5
plot.dmat(pae5$pae,

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




```
# Re-plot model 1 using same scale as model 5
plot.dmat(pae1$pae,

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




```
# Look at alignment
aln_file <- list.files(path=results_dir,pattern=".a3m$",full.names = TRUE)
```

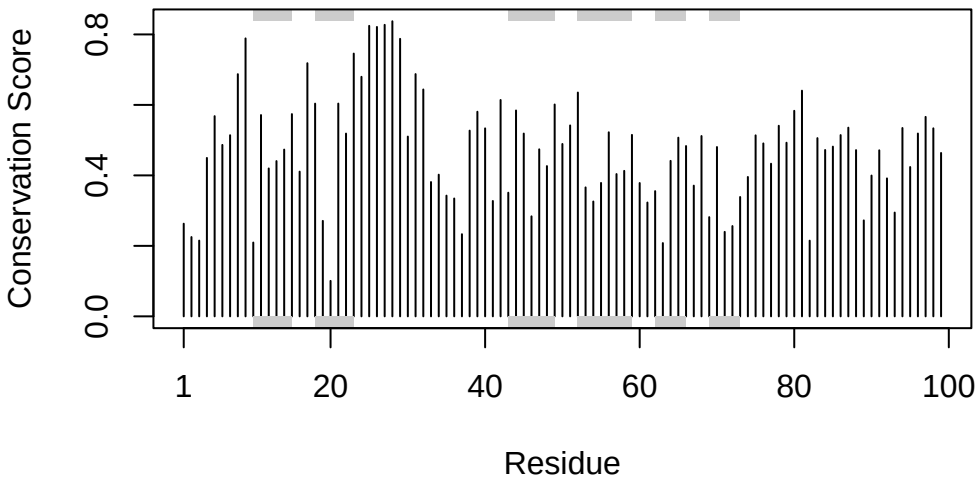
```
aln <- read.fasta(aln_file[1], to.upper = TRUE)
```

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

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

```
[1] 5378  132
```

```
# Look at conservation
sim <- conserv(aln)
plotb3(sim[1:99], sse=trim.pdb(pdb, chain="A"),
ylab="Conservation Score")
```




```
# Look at conserved residues by sequence
con <- consensus(aln, cutoff = 0.9)
con$seq
```

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

```
# Generate pdb file for mol*
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")
```