

11: Structural Bioinformatics (pt2. Focus on new AlphaFold2)

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

```
#Change this for your results dir name
results_dir <- "hivpr_dimer_23119/"
```

```
#File names for all PDB models
pdb_files <- list.files(path = "/Users/Mason/Desktop/BIMM143/Class11/hivpr_dimer_23119",
                        pattern = ".pdb",
                        full.names = TRUE)
```

```
#printing PDB file names
basename(pdb_files)
```

```
[1] "hivpr_dimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_1_seed_000.pdb"
[2] "hivpr_dimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000.pdb"
[3] "hivpr_dimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000.pdb"
[4] "hivpr_dimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_seed_000.pdb"
[5] "hivpr_dimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000.pdb"
```

I will now be using BIO3D for further analysis

```
library(bio3d)
```

Align and superpose

```
pdbbs <- pdbaln(pdb_files, fit = TRUE, exefile = "msa")
```

Reading PDB files:

```
/Users/Mason/Desktop/BIMM143/Class11/hivpr_dimer_23119/hivpr_dimer_23119_unrelaxed_rank_001_
/Users/Mason/Desktop/BIMM143/Class11/hivpr_dimer_23119/hivpr_dimer_23119_unrelaxed_rank_002_
/Users/Mason/Desktop/BIMM143/Class11/hivpr_dimer_23119/hivpr_dimer_23119_unrelaxed_rank_003_
/Users/Mason/Desktop/BIMM143/Class11/hivpr_dimer_23119/hivpr_dimer_23119_unrelaxed_rank_004_
/Users/Mason/Desktop/BIMM143/Class11/hivpr_dimer_23119/hivpr_dimer_23119_unrelaxed_rank_005_
.....
```

Extracting sequences

```
pdb/seq: 1   name: /Users/Mason/Desktop/BIMM143/Class11/hivpr_dimer_23119/hivpr_dimer_23119_
pdb/seq: 2   name: /Users/Mason/Desktop/BIMM143/Class11/hivpr_dimer_23119/hivpr_dimer_23119_
pdb/seq: 3   name: /Users/Mason/Desktop/BIMM143/Class11/hivpr_dimer_23119/hivpr_dimer_23119_
pdb/seq: 4   name: /Users/Mason/Desktop/BIMM143/Class11/hivpr_dimer_23119/hivpr_dimer_23119_
pdb/seq: 5   name: /Users/Mason/Desktop/BIMM143/Class11/hivpr_dimer_23119/hivpr_dimer_23119_
```

pdbbs

```

1               .               .               .               .               50
[Truncated_Name:1]hivpr_dime PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWPKPMIGGI
[Truncated_Name:2]hivpr_dime PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWPKPMIGGI
[Truncated_Name:3]hivpr_dime PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWPKPMIGGI
[Truncated_Name:4]hivpr_dime PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWPKPMIGGI
[Truncated_Name:5]hivpr_dime PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWPKPMIGGI
*****
1               .               .               .               .               50
51              .               .               .               .               100
[Truncated_Name:1]hivpr_dime GGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFP
[Truncated_Name:2]hivpr_dime GGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFP
[Truncated_Name:3]hivpr_dime GGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFP
[Truncated_Name:4]hivpr_dime GGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFP
[Truncated_Name:5]hivpr_dime GGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFP
*****
51              .               .               .               .               100
101             .               .               .               .               150
```

```

[Truncated_Name:1]hivpr_dime  QITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWPKPMIGGIG
[Truncated_Name:2]hivpr_dime  QITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWPKPMIGGIG
[Truncated_Name:3]hivpr_dime  QITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWPKPMIGGIG
[Truncated_Name:4]hivpr_dime  QITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWPKPMIGGIG
[Truncated_Name:5]hivpr_dime  QITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWPKPMIGGIG
                                *****
                                101          .          .          .          .          150

                                151          .          .          .          .          198
[Truncated_Name:1]hivpr_dime  GFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNF
[Truncated_Name:2]hivpr_dime  GFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNF
[Truncated_Name:3]hivpr_dime  GFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNF
[Truncated_Name:4]hivpr_dime  GFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNF
[Truncated_Name:5]hivpr_dime  GFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNF
                                *****
                                151          .          .          .          .          198

```

Call:

```
pdbaln(files = pdb_files, fit = TRUE, exefile = "msa")
```

Class:

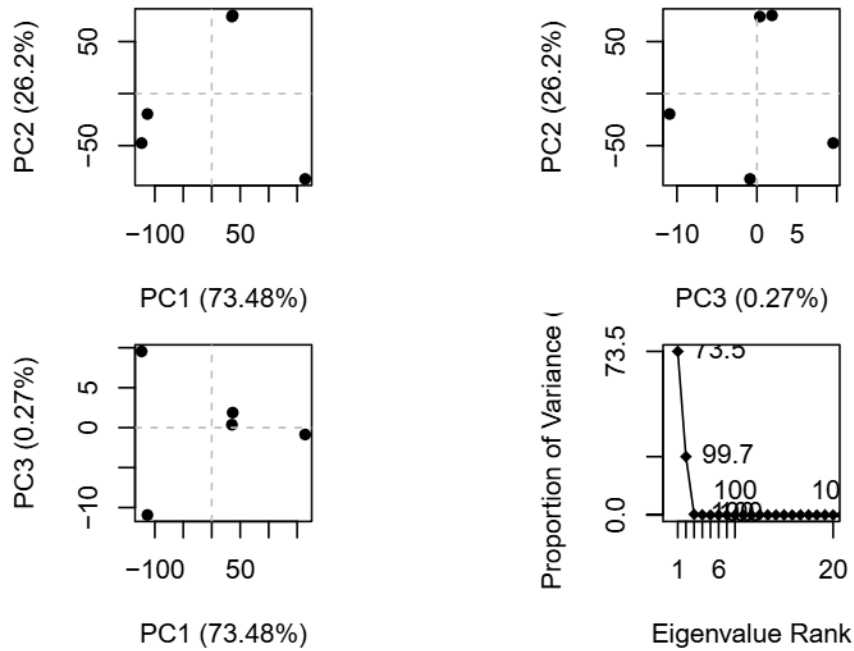
```
pdb, fasta
```

Alignment dimensions:

```
5 sequence rows; 198 position columns (198 non-gap, 0 gap)
```

```
+ attr: xyz, resno, b, chain, id, ali, resid, sse, call
```

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



##RMSD Analysis

RMSD is a common measure of structural distance

```
rd <- rmsd(pdbbs, fit=T)
```

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

```
rd
```

```

hivpr_dimer_231
hivpr_dimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_1_seed_000
hivpr_dimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000
hivpr_dimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000
hivpr_dimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_seed_000
hivpr_dimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000
hivpr_dimer_231
hivpr_dimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_1_seed_000
hivpr_dimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000
hivpr_dimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000
hivpr_dimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_seed_000
hivpr_dimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000
hivpr_dimer_231

```

```

hivpr_dimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_1_seed_000
hivpr_dimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000
hivpr_dimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000
hivpr_dimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_seed_000
hivpr_dimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000

```

hivpr_dimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_1_seed_000

```

hivpr_dimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_1_seed_000
hivpr_dimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000
hivpr_dimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000
hivpr_dimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_seed_000
hivpr_dimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000

```

hivpr_dimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_1_seed_000

```

hivpr_dimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_1_seed_000
hivpr_dimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000
hivpr_dimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000
hivpr_dimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_seed_000
hivpr_dimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000

```

```
range(rd)
```

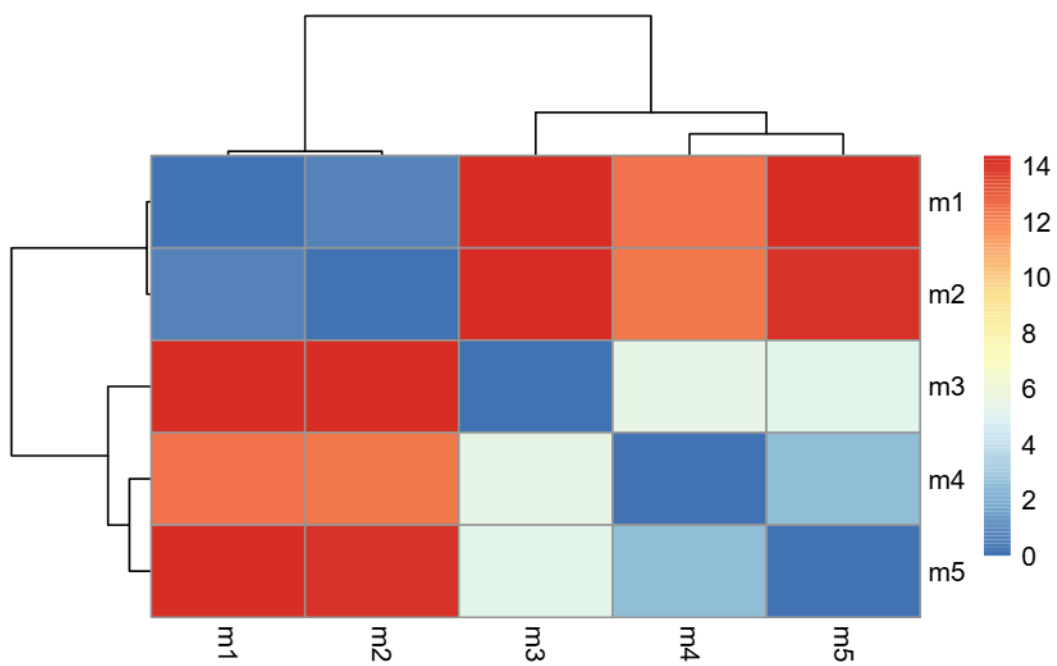
```
[1] 0.000 14.376
```

```
library(pheatmap)
```

```

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

```



Mol* superposed dimers structure:

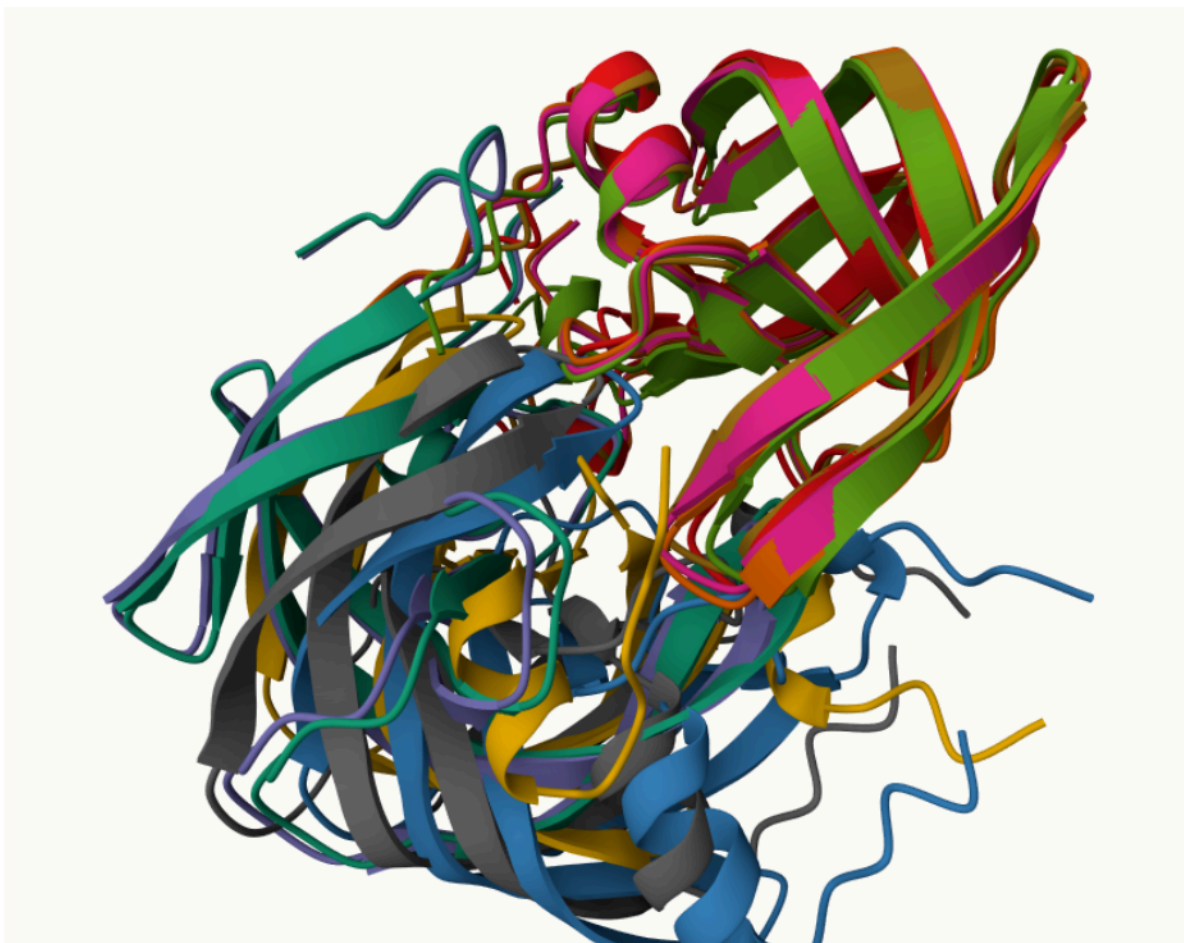
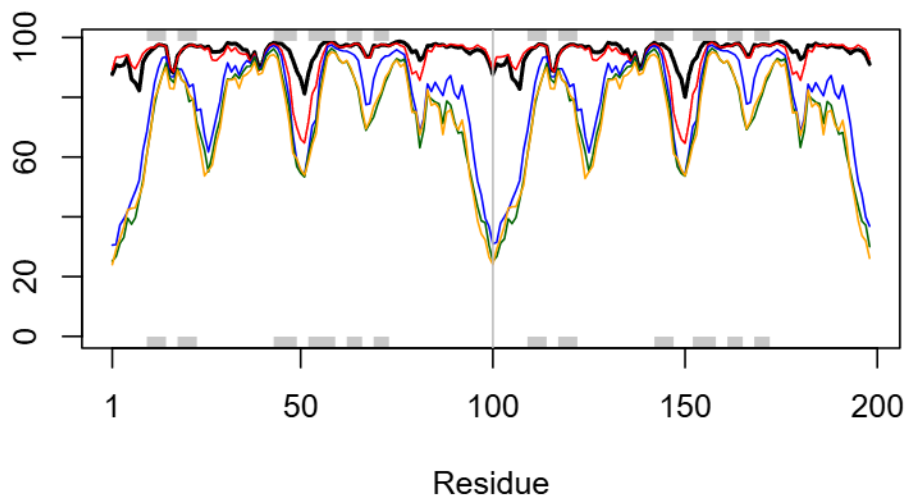


Figure 1: Figure 1: Superposed dimer

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

Note: Accessing on-line PDB file

```
plotb3(pdb$b[1,], typ="l", lwd=2, sse=pdb)
points(pdb$b[2,], typ="l", col="red")
points(pdb$b[3,], typ="l", col="blue")
points(pdb$b[4,], typ="l", col="darkgreen")
points(pdb$b[5,], typ="l", col="orange")
abline(v=100, col="gray")
```



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

```
core size 197 of 198 vol = 4916.702
core size 196 of 198 vol = 4311.481
core size 195 of 198 vol = 4101.445
core size 194 of 198 vol = 3907.124
core size 193 of 198 vol = 3711.925
core size 192 of 198 vol = 3546.511
core size 191 of 198 vol = 3440.437
core size 190 of 198 vol = 3317.571
core size 189 of 198 vol = 3220.079
core size 188 of 198 vol = 3142.057
core size 187 of 198 vol = 3066.79
core size 186 of 198 vol = 3015.892
core size 185 of 198 vol = 2959.969
core size 184 of 198 vol = 2913.74
core size 183 of 198 vol = 2880.923
core size 182 of 198 vol = 2848.081
core size 181 of 198 vol = 2857.001
core size 180 of 198 vol = 2871.24
core size 179 of 198 vol = 2905.696
core size 178 of 198 vol = 2953.776
```


core size 177 of 198	vol = 3020.847
core size 176 of 198	vol = 3087.22
core size 175 of 198	vol = 3109.99
core size 174 of 198	vol = 3129.601
core size 173 of 198	vol = 3135.085
core size 172 of 198	vol = 3092.283
core size 171 of 198	vol = 3036.012
core size 170 of 198	vol = 2947.995
core size 169 of 198	vol = 2886.897
core size 168 of 198	vol = 2829.355
core size 167 of 198	vol = 2746.377
core size 166 of 198	vol = 2671.189
core size 165 of 198	vol = 2600.848
core size 164 of 198	vol = 2534.651
core size 163 of 198	vol = 2464.3
core size 162 of 198	vol = 2390.171
core size 161 of 198	vol = 2322.47
core size 160 of 198	vol = 2236.698
core size 159 of 198	vol = 2160.475
core size 158 of 198	vol = 2077.281
core size 157 of 198	vol = 2003.596
core size 156 of 198	vol = 1939.94
core size 155 of 198	vol = 1859.188
core size 154 of 198	vol = 1781.083
core size 153 of 198	vol = 1699.1
core size 152 of 198	vol = 1622.558
core size 151 of 198	vol = 1546.319
core size 150 of 198	vol = 1473.01
core size 149 of 198	vol = 1414.087
core size 148 of 198	vol = 1352.547
core size 147 of 198	vol = 1295.278
core size 146 of 198	vol = 1246.999
core size 145 of 198	vol = 1203.962
core size 144 of 198	vol = 1163.009
core size 143 of 198	vol = 1110.955
core size 142 of 198	vol = 1064.672
core size 141 of 198	vol = 1028.458
core size 140 of 198	vol = 986.121
core size 139 of 198	vol = 944.003
core size 138 of 198	vol = 895.914
core size 137 of 198	vol = 853.508
core size 136 of 198	vol = 827.977
core size 135 of 198	vol = 796.874

core size 134 of 198	vol = 772.763
core size 133 of 198	vol = 743.108
core size 132 of 198	vol = 707.65
core size 131 of 198	vol = 669.172
core size 130 of 198	vol = 634.655
core size 129 of 198	vol = 594.035
core size 128 of 198	vol = 559.154
core size 127 of 198	vol = 525.971
core size 126 of 198	vol = 493.19
core size 125 of 198	vol = 466.473
core size 124 of 198	vol = 438.433
core size 123 of 198	vol = 410.725
core size 122 of 198	vol = 401.38
core size 121 of 198	vol = 391.76
core size 120 of 198	vol = 362.084
core size 119 of 198	vol = 338.183
core size 118 of 198	vol = 312.338
core size 117 of 198	vol = 282.176
core size 116 of 198	vol = 262.215
core size 115 of 198	vol = 241.577
core size 114 of 198	vol = 225.151
core size 113 of 198	vol = 204.137
core size 112 of 198	vol = 185.038
core size 111 of 198	vol = 162.728
core size 110 of 198	vol = 146.181
core size 109 of 198	vol = 133.352
core size 108 of 198	vol = 123.207
core size 107 of 198	vol = 109.228
core size 106 of 198	vol = 98.824
core size 105 of 198	vol = 89.735
core size 104 of 198	vol = 81.206
core size 103 of 198	vol = 74.188
core size 102 of 198	vol = 67.042
core size 101 of 198	vol = 62.043
core size 100 of 198	vol = 58.432
core size 99 of 198	vol = 55.149
core size 98 of 198	vol = 51.114
core size 97 of 198	vol = 45.798
core size 96 of 198	vol = 41.161
core size 95 of 198	vol = 35.619
core size 94 of 198	vol = 29.784
core size 93 of 198	vol = 23.233
core size 92 of 198	vol = 16.669

```

core size 91 of 198  vol = 9.459
core size 90 of 198  vol = 4.595
core size 89 of 198  vol = 3.161
core size 88 of 198  vol = 2.678
core size 87 of 198  vol = 2.293
core size 86 of 198  vol = 1.935
core size 85 of 198  vol = 1.619
core size 84 of 198  vol = 1.367
core size 83 of 198  vol = 1.09
core size 82 of 198  vol = 0.906
core size 81 of 198  vol = 0.764
core size 80 of 198  vol = 0.649
core size 79 of 198  vol = 0.596
core size 78 of 198  vol = 0.53
core size 77 of 198  vol = 0.486
FINISHED: Min vol ( 0.5 ) reached

```

```
core.inds <- print(core, vol=0.51)
```

```
# 78 positions (cumulative volume <= 0.51 Angstrom^3)
```

```

start end length
1    10  25    16
2    28  48    21
3    53  93    41

```

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

```
rf <- rmsf(xyz)
```

```
plotb3(rf, sse=pdb)
```

```
abline(v=100, col="gray", ylab="RMSF")
```

