Class 11: Structural Bioinformatics Pt2

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Today we are delving into structure predictin with Alphafold, we will finish of previous lab 10 "comparative structure analysis" section.

```
library(bio3d)
```

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

```
id <- "1ake_A"

aa <- get.seq(id)
```

```
Warning in get.seq(id): Removing existing file: seqs.fasta
```

```
Fetching... Please wait. Done.
```

```
aa
```

```
              1        .         .         .         .         .         60
pdb|1AKE|A    MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAAVKSGSELGKQAKDIMDAGKLVT
              1        .         .         .         .         .         60

             61        .         .         .         .         .         120
pdb|1AKE|A    DELVIALVKERIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVDRI
             61        .         .         .         .         .         120

            121        .         .         .         .         .         180
pdb|1AKE|A    VGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKDDQEETVRKRLVEYHQMTAPLIG
            121        .         .         .         .         .         180

            181        .         .         .   214
```

```
pdb|1AKE|A   YYSKEAEAGNTKYAKVDGTKPVAEVRADLEKILG
           181        .         .         .   214

Call:
  read.fasta(file = outfile)

Class:
  fasta

Alignment dimensions:
  1 sequence rows; 214 position columns (214 non-gap, 0 gap)

+ attr: id, ali, call
```

```
b <- blast.pdb(aa)
```

```
 Searching ... please wait (updates every 5 seconds) RID = JWK5YRCF013
 .............
 Reporting 85 hits
```

```
attributes(b)
```

```
$names
[1] "hit.tbl" "raw"     "url"

$class
[1] "blast"
```

```
head(b$hit.tbl)
```

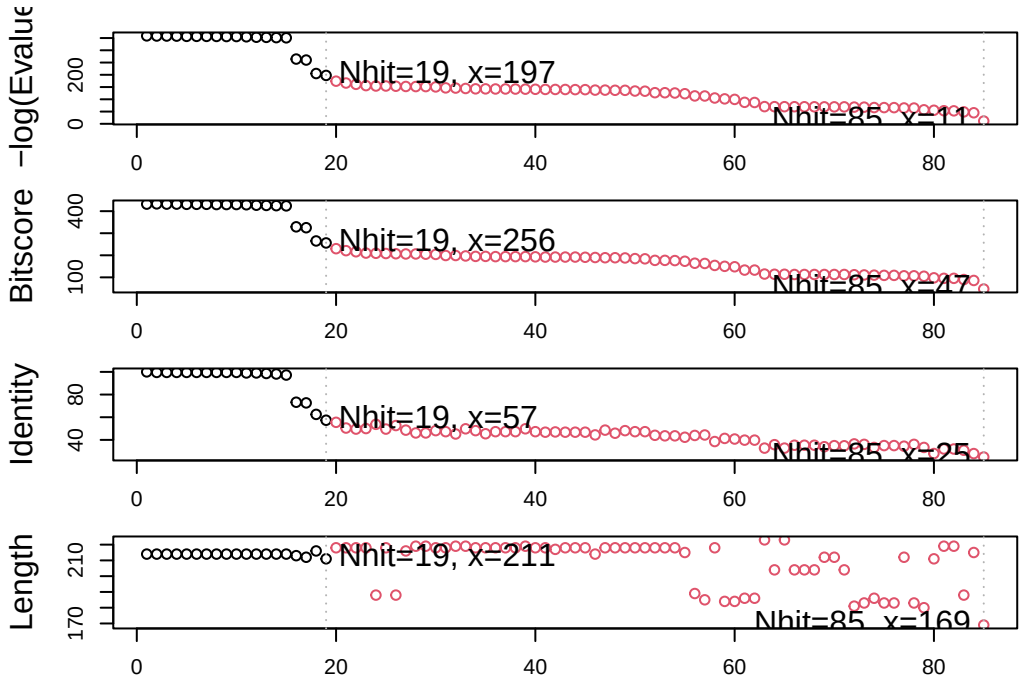
```
        queryid subjectids identity alignmentlength mismatches gapopens q.start
1 Query_7246153     1AKE_A  100.000             214          0        0       1
2 Query_7246153     8BQF_A   99.533             214          1        0       1
3 Query_7246153     4X8M_A   99.533             214          1        0       1
4 Query_7246153     6S36_A   99.533             214          1        0       1
5 Query_7246153     8Q2B_A   99.533             214          1        0       1
6 Query_7246153     8RJ9_A   99.533             214          1        0       1
  q.end s.start s.end    evalue bitscore positives mlog.evalue pdb.id    acc
1   214       1   214 1.58e-156      432    100.00    358.7458 1AKE_A 1AKE_A
2   214      21   234 2.58e-156      433    100.00    358.2555 8BQF_A 8BQF_A
```

```
3   214       1   214 2.82e-156      432    100.00    358.1665 4X8M_A 4X8M_A
4   214       1   214 4.14e-156      432    100.00    357.7826 6S36_A 6S36_A
5   214       1   214 1.10e-155      431     99.53    356.8054 8Q2B_A 8Q2B_A
6   214       1   214 1.10e-155      431     99.53    356.8054 8RJ9_A 8RJ9_A
```

```
hits <- plot(b)
```

```
  * Possible cutoff values:    197 11
           Yielding Nhits:     19 85

  * Chosen cutoff value of:    197
           Yielding Nhits:     19
```




```
attributes(hits)
```

```
$names
[1] "hits"   "pdb.id" "acc"    "inds"

$class
[1] "blast"
```

Top hits that we like from Blast results:

```
hits$pdb.id
```

```
 [1] "1AKE_A" "8BQF_A" "4X8M_A" "6S36_A" "8Q2B_A" "8RJ9_A" "6RZE_A" "4X8H_A"
 [9] "3HPR_A" "1E4V_A" "5EJE_A" "1E4Y_A" "3X2S_A" "6HAP_A" "6HAM_A" "4K46_A"
[17] "4NP6_A" "3GMT_A" "4PZL_A"
```

```
# Download related PDB files
files <- get.pdb(hits$pdb.id, path="pdbs", split=TRUE, gzip=TRUE)
```

```
Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE):
pdbs/1AKE.pdb.gz exists. Skipping download
```

```
Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE):
pdbs/8BQF.pdb.gz exists. Skipping download
```

```
Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE):
pdbs/4X8M.pdb.gz exists. Skipping download
```

```
Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE):
pdbs/6S36.pdb.gz exists. Skipping download
```

```
Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE):
pdbs/8Q2B.pdb.gz exists. Skipping download
```

```
Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE):
pdbs/8RJ9.pdb.gz exists. Skipping download
```

```
Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE):
pdbs/6RZE.pdb.gz exists. Skipping download
```

```
Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE):
pdbs/4X8H.pdb.gz exists. Skipping download
```

```
Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE):
pdbs/3HPR.pdb.gz exists. Skipping download
```

```
Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE):
pdbs/1E4V.pdb.gz exists. Skipping download

Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE):
pdbs/5EJE.pdb.gz exists. Skipping download

Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE):
pdbs/1E4Y.pdb.gz exists. Skipping download

Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE):
pdbs/3X2S.pdb.gz exists. Skipping download

Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE):
pdbs/6HAP.pdb.gz exists. Skipping download

Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE):
pdbs/6HAM.pdb.gz exists. Skipping download

Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE):
pdbs/4K46.pdb.gz exists. Skipping download

Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE):
pdbs/4NP6.pdb.gz exists. Skipping download

Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE):
pdbs/3GMT.pdb.gz exists. Skipping download

Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE):
pdbs/4PZL.pdb.gz exists. Skipping download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```

I have now downloaded all the ADK structures in the PDB database but viewing them is difficult as they need to be aligned and superposed.

I am going to install BiocManager package from CRAN. Then I can use `BiocManager::install()` to install any bioconductor package.

```
# Align releated PDBs
pdbs <- pdbaln(files, fit = TRUE, exefile="msa")
```

```
Reading PDB files:
```

```
pdbs/split_chain/1AKE_A.pdb
pdbs/split_chain/8BQF_A.pdb
pdbs/split_chain/4X8M_A.pdb
pdbs/split_chain/6S36_A.pdb
pdbs/split_chain/8Q2B_A.pdb
pdbs/split_chain/8RJ9_A.pdb
pdbs/split_chain/6RZE_A.pdb
pdbs/split_chain/4X8H_A.pdb
pdbs/split_chain/3HPR_A.pdb
pdbs/split_chain/1E4V_A.pdb
pdbs/split_chain/5EJE_A.pdb
pdbs/split_chain/1E4Y_A.pdb
pdbs/split_chain/3X2S_A.pdb
pdbs/split_chain/6HAP_A.pdb
pdbs/split_chain/6HAM_A.pdb
pdbs/split_chain/4K46_A.pdb
pdbs/split_chain/4NP6_A.pdb
pdbs/split_chain/3GMT_A.pdb
pdbs/split_chain/4PZL_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
.   PDB has ALT records, taking A only, rm.alt=TRUE
..   PDB has ALT records, taking A only, rm.alt=TRUE
.   PDB has ALT records, taking A only, rm.alt=TRUE
.   PDB has ALT records, taking A only, rm.alt=TRUE
.   PDB has ALT records, taking A only, rm.alt=TRUE
..   PDB has ALT records, taking A only, rm.alt=TRUE
..   PDB has ALT records, taking A only, rm.alt=TRUE
....   PDB has ALT records, taking A only, rm.alt=TRUE
.   PDB has ALT records, taking A only, rm.alt=TRUE
....

Extracting sequences

pdb/seq: 1   name: pdbs/split_chain/1AKE_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 2   name: pdbs/split_chain/8BQF_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 3   name: pdbs/split_chain/4X8M_A.pdb
pdb/seq: 4   name: pdbs/split_chain/6S36_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 5   name: pdbs/split_chain/8Q2B_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 6   name: pdbs/split_chain/8RJ9_A.pdb
```

```
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 7   name: pdbs/split_chain/6RZE_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 8   name: pdbs/split_chain/4X8H_A.pdb
pdb/seq: 9   name: pdbs/split_chain/3HPR_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 10   name: pdbs/split_chain/1E4V_A.pdb
pdb/seq: 11   name: pdbs/split_chain/5EJE_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 12   name: pdbs/split_chain/1E4Y_A.pdb
pdb/seq: 13   name: pdbs/split_chain/3X2S_A.pdb
pdb/seq: 14   name: pdbs/split_chain/6HAP_A.pdb
pdb/seq: 15   name: pdbs/split_chain/6HAM_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 16   name: pdbs/split_chain/4K46_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 17   name: pdbs/split_chain/4NP6_A.pdb
pdb/seq: 18   name: pdbs/split_chain/3GMT_A.pdb
pdb/seq: 19   name: pdbs/split_chain/4PZL_A.pdb
```

```
pdbs
```

```
                                 1        .         .         .         40
[Truncated_Name:1]1AKE_A.pdb    ----------MRIILLGAPGAGKGTQAQFIMEKYGIPQIS
[Truncated_Name:2]8BQF_A.pdb    ----------MRIILLGAPGAGKGTQAQFIMEKYGIPQIS
[Truncated_Name:3]4X8M_A.pdb    ----------MRIILLGAPGAGKGTQAQFIMEKYGIPQIS
[Truncated_Name:4]6S36_A.pdb    ----------MRIILLGAPGAGKGTQAQFIMEKYGIPQIS
[Truncated_Name:5]8Q2B_A.pdb    ----------MRIILLGAPGAGKGTQAQFIMEKYGIPQIS
[Truncated_Name:6]8RJ9_A.pdb    ----------MRIILLGAPGAGKGTQAQFIMEKYGIPQIS
[Truncated_Name:7]6RZE_A.pdb    ----------MRIILLGAPGAGKGTQAQFIMEKYGIPQIS
[Truncated_Name:8]4X8H_A.pdb    ----------MRIILLGAPGAGKGTQAQFIMEKYGIPQIS
[Truncated_Name:9]3HPR_A.pdb    ----------MRIILLGAPGAGKGTQAQFIMEKYGIPQIS
[Truncated_Name:10]1E4V_A.pdb   ----------MRIILLGAPVAGKGTQAQFIMEKYGIPQIS
[Truncated_Name:11]5EJE_A.pdb   ----------MRIILLGAPGAGKGTQAQFIMEKYGIPQIS
[Truncated_Name:12]1E4Y_A.pdb   ----------MRIILLGALVAGKGTQAQFIMEKYGIPQIS
[Truncated_Name:13]3X2S_A.pdb   ----------MRIILLGAPGAGKGTQAQFIMEKYGIPQIS
[Truncated_Name:14]6HAP_A.pdb   ----------MRIILLGAPGAGKGTQAQFIMEKYGIPQIS
[Truncated_Name:15]6HAM_A.pdb   ----------MRIILLGAPGAGKGTQAQFIMEKYGIPQIS
[Truncated_Name:16]4K46_A.pdb   ----------MRIILLGAPGAGKGTQAQFIMAKFGIPQIS
[Truncated_Name:17]4NP6_A.pdb   --------NAMRIILLGAPGAGKGTQAQFIMEKFGIPQIS
[Truncated_Name:18]3GMT_A.pdb   ----------MRLILLGAPGAGKGTQANFIKEKFGIPQIS
[Truncated_Name:19]4PZL_A.pdb   TENLYFQSNAMRIILLGAPGAGKGTQAKIIEQKYNIAHIS
```

```
                                  **^*****  *******  *  *^ *  **
                                1         .         .         .        40

                               41         .         .         .        80
[Truncated_Name:1]1AKE_A.pdb    TGDMLRAAVKSGSELGKQAKDIMDAGKLVTDELVIALVKE
[Truncated_Name:2]8BQF_A.pdb    TGDMLRAAVKSGSELGKQAKDIMDAGKLVTDELVIALVKE
[Truncated_Name:3]4X8M_A.pdb    TGDMLRAAVKSGSELGKQAKDIMDAGKLVTDELVIALVKE
[Truncated_Name:4]6S36_A.pdb    TGDMLRAAVKSGSELGKQAKDIMDAGKLVTDELVIALVKE
[Truncated_Name:5]8Q2B_A.pdb    TGDMLRAAVKSGSELGKQAKDIMDAGKLVTDELVIALVKE
[Truncated_Name:6]8RJ9_A.pdb    TGDMLRAAVKSGSELGKQAKDIMDAGKLVTDELVIALVKE
[Truncated_Name:7]6RZE_A.pdb    TGDMLRAAVKSGSELGKQAKDIMDAGKLVTDELVIALVKE
[Truncated_Name:8]4X8H_A.pdb    TGDMLRAAVKSGSELGKQAKDIMDAGKLVTDELVIALVKE
[Truncated_Name:9]3HPR_A.pdb    TGDMLRAAVKSGSELGKQAKDIMDAGKLVTDELVIALVKE
[Truncated_Name:10]1E4V_A.pdb   TGDMLRAAVKSGSELGKQAKDIMDAGKLVTDELVIALVKE
[Truncated_Name:11]5EJE_A.pdb   TGDMLRAAVKSGSELGKQAKDIMDACKLVTDELVIALVKE
[Truncated_Name:12]1E4Y_A.pdb   TGDMLRAAVKSGSELGKQAKDIMDAGKLVTDELVIALVKE
[Truncated_Name:13]3X2S_A.pdb   TGDMLRAAVKSGSELGKQAKDIMDCGKLVTDELVIALVKE
[Truncated_Name:14]6HAP_A.pdb   TGDMLRAAVKSGSELGKQAKDIMDAGKLVTDELVIALVRE
[Truncated_Name:15]6HAM_A.pdb   TGDMLRAAIKSGSELGKQAKDIMDAGKLVTDEIIIALVKE
[Truncated_Name:16]4K46_A.pdb   TGDMLRAAIKAGTELGKQAKSVIDAGQLVSDDIILGLVKE
[Truncated_Name:17]4NP6_A.pdb   TGDMLRAAIKAGTELGKQAKAVIDAGQLVSDDIILGLIKE
[Truncated_Name:18]3GMT_A.pdb   TGDMLRAAVKAGTPLGVEAKTYMDEGKLVPDSLIIGLVKE
[Truncated_Name:19]4PZL_A.pdb   TGDMIRETIKSGSALGQELKKVLDAGELVSDEFIIKIVKD
                                ****^*  ^* *^ **   *  ^*   ** *  ^^ ^^^^
                               41         .         .         .        80

                               81         .         .         .        120
[Truncated_Name:1]1AKE_A.pdb    RIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFD
[Truncated_Name:2]8BQF_A.pdb    RIAQE----GFLLDGFPRTIPQADAMKEAGINVDYVIEFD
[Truncated_Name:3]4X8M_A.pdb    RIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFD
[Truncated_Name:4]6S36_A.pdb    RIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFD
[Truncated_Name:5]8Q2B_A.pdb    RIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFD
[Truncated_Name:6]8RJ9_A.pdb    RIAQEDCRNGFLLAGFPRTIPQADAMKEAGINVDYVLEFD
[Truncated_Name:7]6RZE_A.pdb    RIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFD
[Truncated_Name:8]4X8H_A.pdb    RIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFD
[Truncated_Name:9]3HPR_A.pdb    RIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFD
[Truncated_Name:10]1E4V_A.pdb   RIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFD
[Truncated_Name:11]5EJE_A.pdb   RIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFD
[Truncated_Name:12]1E4Y_A.pdb   RIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFD
[Truncated_Name:13]3X2S_A.pdb   RIAQEDSRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFD
[Truncated_Name:14]6HAP_A.pdb   RICQEDSRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFD
[Truncated_Name:15]6HAM_A.pdb   RICQEDSRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFD
[Truncated_Name:16]4K46_A.pdb   RIAQDDCAKGFLLDGFPRTIPQADGLKEVGVVVDYVIEFD
```

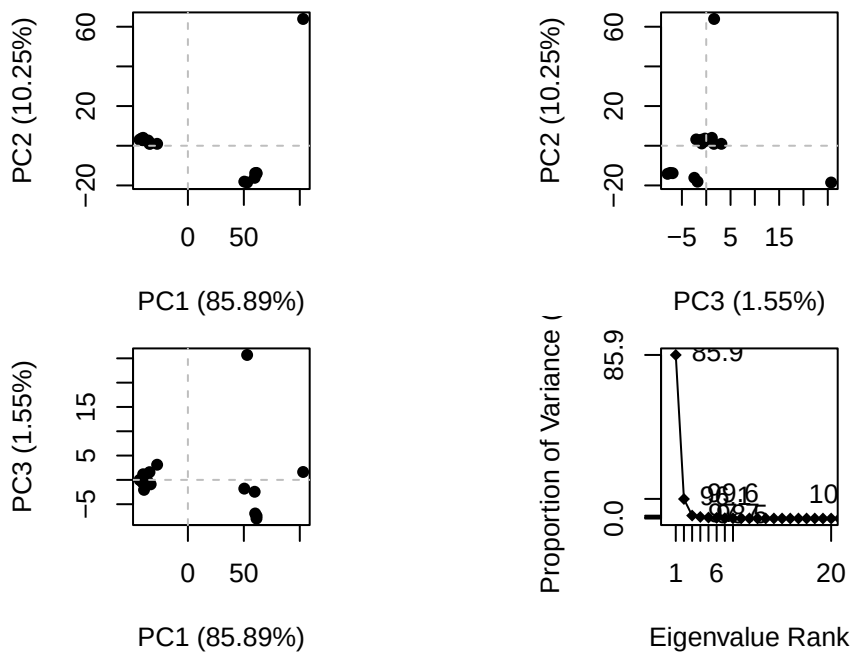
```
[Truncated_Name:17]4NP6_A.pdb   RIAQADCEKGFLLDGFPRTIPQADGLKEMGINVDYVIEFD
[Truncated_Name:18]3GMT_A.pdb   RLKEADCANGYLFDGFPRTIAQADAMKEAGVAIDYVLEID
[Truncated_Name:19]4PZL_A.pdb   RISKNDCNNGFLLDGVPRTIPQAQELDKLGVNIDYIVEVD
                                *^       *^*  * **** **  ^   *^ ^**^^* *
                               81        .         .         .        120

                              121        .         .         .        160
[Truncated_Name:1]1AKE_A.pdb    VPDELIVDRIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTG
[Truncated_Name:2]8BQF_A.pdb    VPDELIVDRIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTG
[Truncated_Name:3]4X8M_A.pdb    VPDELIVDRIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTG
[Truncated_Name:4]6S36_A.pdb    VPDELIVDKIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTG
[Truncated_Name:5]8Q2B_A.pdb    VPDELIVDRIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTG
[Truncated_Name:6]8RJ9_A.pdb    VPDELIVDRIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTG
[Truncated_Name:7]6RZE_A.pdb    VPDELIVDAIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTG
[Truncated_Name:8]4X8H_A.pdb    VPDELIVDRIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTG
[Truncated_Name:9]3HPR_A.pdb    VPDELIVDRIVGRRVHAPSGRVYHVKFNPPKVEGKDDGTG
[Truncated_Name:10]1E4V_A.pdb   VPDELIVDRIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTG
[Truncated_Name:11]5EJE_A.pdb   VPDELIVDRIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTG
[Truncated_Name:12]1E4Y_A.pdb   VPDELIVDRIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTG
[Truncated_Name:13]3X2S_A.pdb   VPDELIVDRIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTG
[Truncated_Name:14]6HAP_A.pdb   VPDELIVDRIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTG
[Truncated_Name:15]6HAM_A.pdb   VPDELIVDRIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTG
[Truncated_Name:16]4K46_A.pdb   VADSVIVERMAGRRAHLASGRTYHNVYNPPKVEGKDDVTG
[Truncated_Name:17]4NP6_A.pdb   VADDVIVERMAGRRAHLPSGRTYHVVYNPPKVEGKDDVTG
[Truncated_Name:18]3GMT_A.pdb   VPFSEIIERMSGRRTHPASGRTYHVKFNPPKVEGKDDVTG
[Truncated_Name:19]4PZL_A.pdb   VADNLLIERITGRRIHPASGRTYHTKFNPPKVADKDDVTG
                                *    ^^^ ^ *** *  *** **  ^*****  *** **
                               121        .         .         .        160

                              161        .         .         .        200
[Truncated_Name:1]1AKE_A.pdb    EELTTRKDDQEETVRKRLVEYHQMTAPLIGYYSKEAEAGN
[Truncated_Name:2]8BQF_A.pdb    EELTTRKDDQEETVRKRLVEYHQMTAPLIGYYSKEAEAGN
[Truncated_Name:3]4X8M_A.pdb    EELTTRKDDQEETVRKRLVEWHQMTAPLIGYYSKEAEAGN
[Truncated_Name:4]6S36_A.pdb    EELTTRKDDQEETVRKRLVEYHQMTAPLIGYYSKEAEAGN
[Truncated_Name:5]8Q2B_A.pdb    EELTTRKADQEETVRKRLVEYHQMTAPLIGYYSKEAEAGN
[Truncated_Name:6]8RJ9_A.pdb    EELTTRKDDQEETVRKRLVEYHQMTAPLIGYYSKEAEAGN
[Truncated_Name:7]6RZE_A.pdb    EELTTRKDDQEETVRKRLVEYHQMTAPLIGYYSKEAEAGN
[Truncated_Name:8]4X8H_A.pdb    EELTTRKDDQEETVRKRLVEYHQMTAALIGYYSKEAEAGN
[Truncated_Name:9]3HPR_A.pdb    EELTTRKDDQEETVRKRLVEYHQMTAPLIGYYSKEAEAGN
[Truncated_Name:10]1E4V_A.pdb   EELTTRKDDQEETVRKRLVEYHQMTAPLIGYYSKEAEAGN
[Truncated_Name:11]5EJE_A.pdb   EELTTRKDDQEECVRKRLVEYHQMTAPLIGYYSKEAEAGN
[Truncated_Name:12]1E4Y_A.pdb   EELTTRKDDQEETVRKRLVEYHQMTAPLIGYYSKEAEAGN
[Truncated_Name:13]3X2S_A.pdb   EELTTRKDDQEETVRKRLCEYHQMTAPLIGYYSKEAEAGN
```

```
[Truncated_Name:14]6HAP_A.pdb   EELTTRKDDQEETVRKRLVEYHQMTAPLIGYYSKEAEAGN
[Truncated_Name:15]6HAM_A.pdb   EELTTRKDDQEETVRKRLVEYHQMTAPLIGYYSKEAEAGN
[Truncated_Name:16]4K46_A.pdb   EDLVIREDDKEETVLARLGVYHNQTAPLIAYYGKEAEAGN
[Truncated_Name:17]4NP6_A.pdb   EDLVIREDDKEETVRARLNVYHTQTAPLIEYYGKEAAAGK
[Truncated_Name:18]3GMT_A.pdb   EPLVQRDDDKEETVKKRLDVYEAQTKPLITYYGDWARRGA
[Truncated_Name:19]4PZL_A.pdb   EPLITRTDDNEDTVKQRLSVYHAQTAKLIDFYRNFSSTNT
                                * *  *  * *^ *  **  ^   *  ** ^*
                               161        .         .         .         200

                               201        .         .      227
[Truncated_Name:1]1AKE_A.pdb     T--KYAKVDGTKPVAEVRADLEKILG-
[Truncated_Name:2]8BQF_A.pdb     T--KYAKVDGTKPVAEVRADLEKIL--
[Truncated_Name:3]4X8M_A.pdb     T--KYAKVDGTKPVAEVRADLEKILG-
[Truncated_Name:4]6S36_A.pdb     T--KYAKVDGTKPVAEVRADLEKILG-
[Truncated_Name:5]8Q2B_A.pdb     T--KYAKVDGTKPVAEVRADLEKILG-
[Truncated_Name:6]8RJ9_A.pdb     T--KYAKVDGTKPVAEVRADLEKILG-
[Truncated_Name:7]6RZE_A.pdb     T--KYAKVDGTKPVAEVRADLEKILG-
[Truncated_Name:8]4X8H_A.pdb     T--KYAKVDGTKPVAEVRADLEKILG-
[Truncated_Name:9]3HPR_A.pdb     T--KYAKVDGTKPVAEVRADLEKILG-
[Truncated_Name:10]1E4V_A.pdb    T--KYAKVDGTKPVAEVRADLEKILG-
[Truncated_Name:11]5EJE_A.pdb    T--KYAKVDGTKPVAEVRADLEKILG-
[Truncated_Name:12]1E4Y_A.pdb    T--KYAKVDGTKPVAEVRADLEKILG-
[Truncated_Name:13]3X2S_A.pdb    T--KYAKVDGTKPVAEVRADLEKILG-
[Truncated_Name:14]6HAP_A.pdb    T--KYAKVDGTKPVCEVRADLEKILG-
[Truncated_Name:15]6HAM_A.pdb    T--KYAKVDGTKPVCEVRADLEKILG-
[Truncated_Name:16]4K46_A.pdb    T--QYLKFDGTKAVAEVSAELEKALA-
[Truncated_Name:17]4NP6_A.pdb    T--QYLKFDGTKQVSEVSADIAKALA-
[Truncated_Name:18]3GMT_A.pdb    E-------NGLKAPA-----YRKISG-
[Truncated_Name:19]4PZL_A.pdb    KIPKYIKINGDQAVEKVSQDIFDQLNK
                                          *
                               201        .         .      227
```

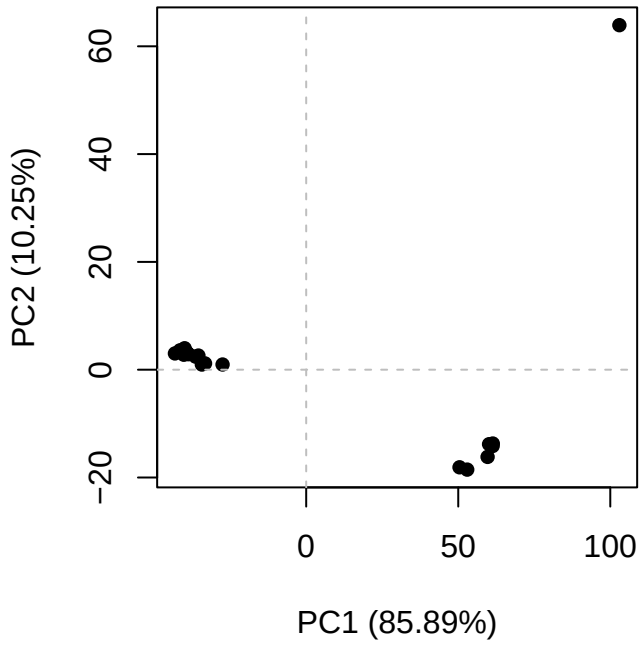
```
Call:
  pdbaln(files = files, fit = TRUE, exefile = "msa")

Class:
  pdbs, fasta

Alignment dimensions:
  19 sequence rows; 227 position columns (199 non-gap, 28 gap)

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

Principal Component Analysis

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




```
plot(pc, pc.axes = c(1:2))
```



To examine in more detail what PC1 (or any PC) is capturing here we can plot the loadings or make a wee movie (trajectory) of moving along PC1.

```
mktrj(pc, pc = 1, file = "pc1.pdb")
```

8. Custom Analysis of resulting models

```
results_dir <- "dimer_test_23119"
```

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

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

```
[1] "dimer_test_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_1_seed_000.pdb"
[2] "dimer_test_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000.pdb"
[3] "dimer_test_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000.pdb"
[4] "dimer_test_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_seed_000.pdb"
```

```
[5] "dimer_test_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000.pdb"
```

```
library(bio3d)

# Read all data from Models
#  and superpose/fit coords
pdbs <- pdbaln(pdb_files, fit=TRUE, exefile="msa")
```

```
Reading PDB files:
dimer_test_23119/dimer_test_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_1_seed_000
dimer_test_23119/dimer_test_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000
dimer_test_23119/dimer_test_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000
dimer_test_23119/dimer_test_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_seed_000
dimer_test_23119/dimer_test_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000
.....

Extracting sequences

pdb/seq: 1   name: dimer_test_23119/dimer_test_23119_unrelaxed_rank_001_alphafold2_multimer_v
pdb/seq: 2   name: dimer_test_23119/dimer_test_23119_unrelaxed_rank_002_alphafold2_multimer_v
pdb/seq: 3   name: dimer_test_23119/dimer_test_23119_unrelaxed_rank_003_alphafold2_multimer_v
pdb/seq: 4   name: dimer_test_23119/dimer_test_23119_unrelaxed_rank_004_alphafold2_multimer_v
pdb/seq: 5   name: dimer_test_23119/dimer_test_23119_unrelaxed_rank_005_alphafold2_multimer_v
```

```
pdbs
```

```
                                1        .        .        .        .         50
[Truncated_Name:1]dimer_test   PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGI
[Truncated_Name:2]dimer_test   PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGI
[Truncated_Name:3]dimer_test   PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGI
[Truncated_Name:4]dimer_test   PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGI
[Truncated_Name:5]dimer_test   PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGI
                               **************************************************
                               1        .        .        .        .         50

                              51        .        .        .        .         100
[Truncated_Name:1]dimer_test   GGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFP
[Truncated_Name:2]dimer_test   GGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFP
[Truncated_Name:3]dimer_test   GGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFP
[Truncated_Name:4]dimer_test   GGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFP
[Truncated_Name:5]dimer_test   GGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFP
```

```
                              **************************************************
                             51        .         .         .         .         100

                            101        .         .         .         .         150
[Truncated_Name:1]dimer_test   QITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGIG
[Truncated_Name:2]dimer_test   QITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGIG
[Truncated_Name:3]dimer_test   QITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGIG
[Truncated_Name:4]dimer_test   QITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGIG
[Truncated_Name:5]dimer_test   QITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGIG
                              **************************************************
                            101        .         .         .         .         150

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

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

Class:
  pdbs, fasta

Alignment dimensions:
  5 sequence rows; 198 position columns (198 non-gap, 0 gap)

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

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

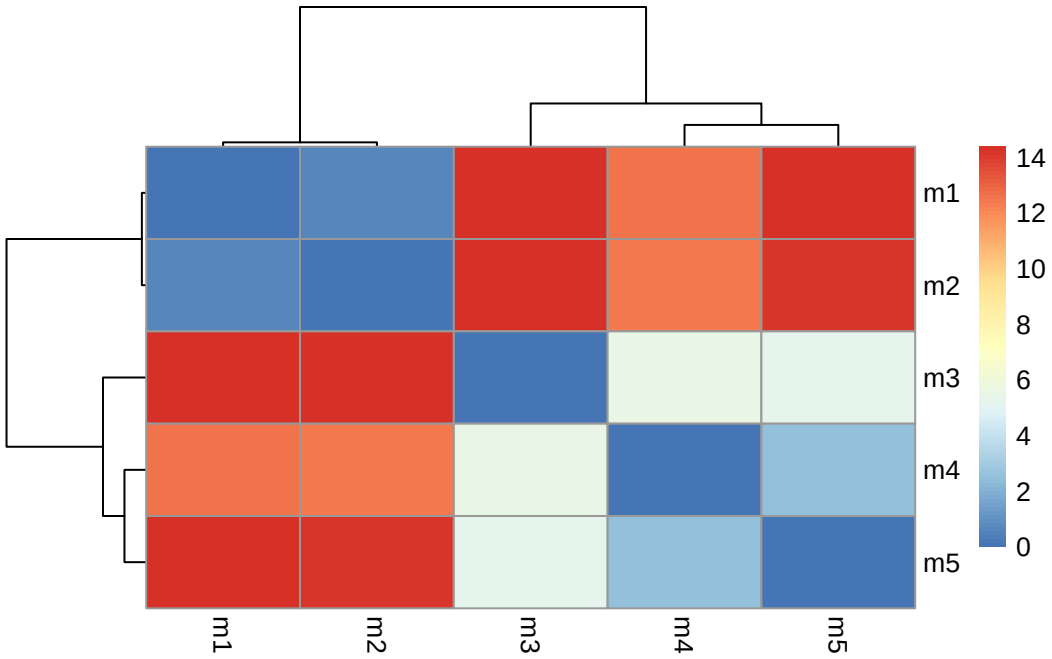
```
Warning in rmsd(pdbs, fit = T): No indices provided, using the 198 non NA positions
```

```
range(rd)
```

```
[1]  0.000 14.376
```

Draw a heatmap of the RMSD Matrix values

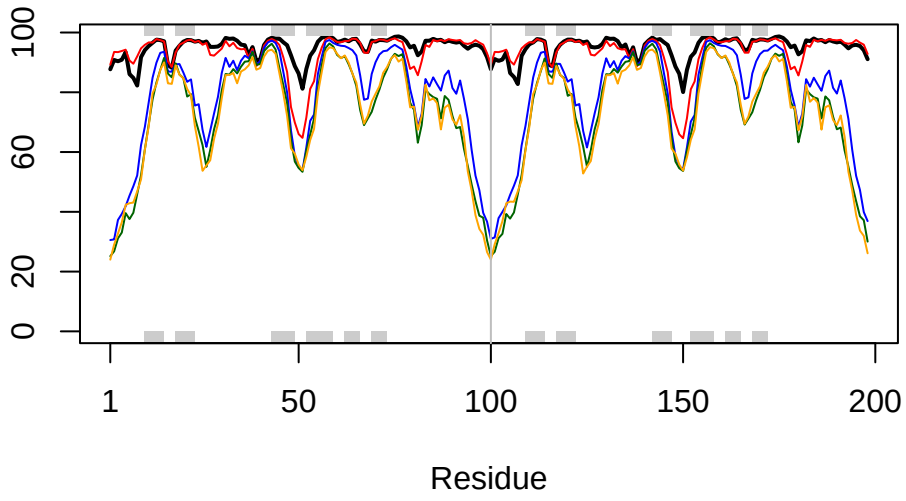
```
library(pheatmap)

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
```

```
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")
```




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

```
 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
```

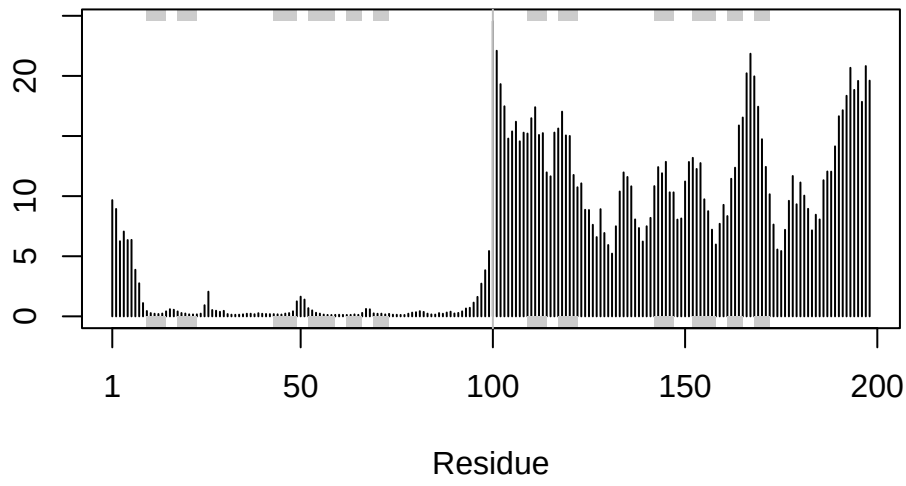
```
core size 134 of 198  vol = 772.763
core size 133 of 198  vol = 743.108
core size 132 of 198  vol = 707.65
core size 131 of 198  vol = 669.172
core size 130 of 198  vol = 634.655
core size 129 of 198  vol = 594.035
core size 128 of 198  vol = 559.154
core size 127 of 198  vol = 525.971
core size 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=0.5)
```

```
# 78 positions (cumulative volume <= 0.5 Angstrom^3)
  start end length
1    10  25     16
2    28  48     21
3    53  93     41
```

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

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



Predicted Alignment Error

```
library(jsonlite)

# Listing of all PAE JSON files
pae_files <- list.files(path=results_dir,
                        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] 87.69 90.81 90.38 90.88 93.44 86.06
```

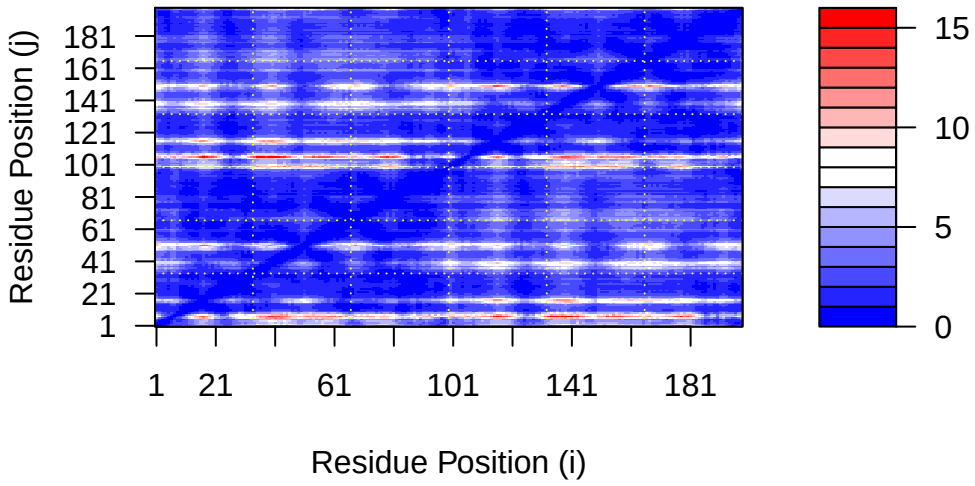
```
pae1$max_pae
```

```
[1] 15.47656
```

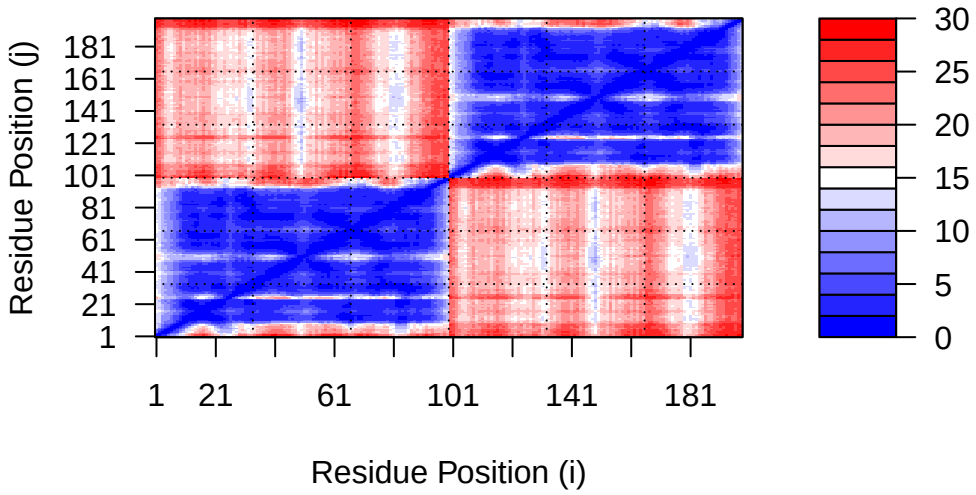
```
pae5$max_pae
```

```
[1] 29.32812
```

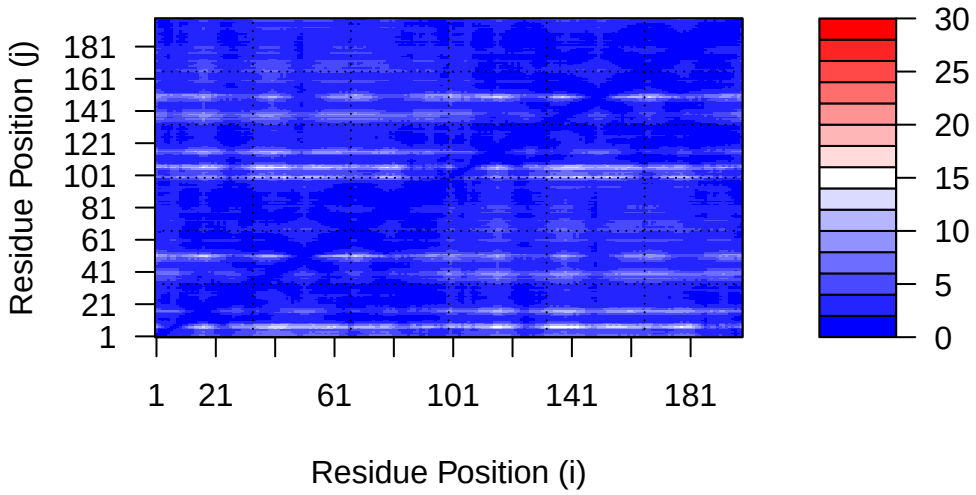
```
plot.dmat(pae1$pae,
          xlab="Residue Position (i)",
          ylab="Residue Position (j)")
```




```
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))
```



Residue Conservation from Alignment File

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

```
[1] "dimer_test_23119/dimer_test_23119.a3m"
```

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

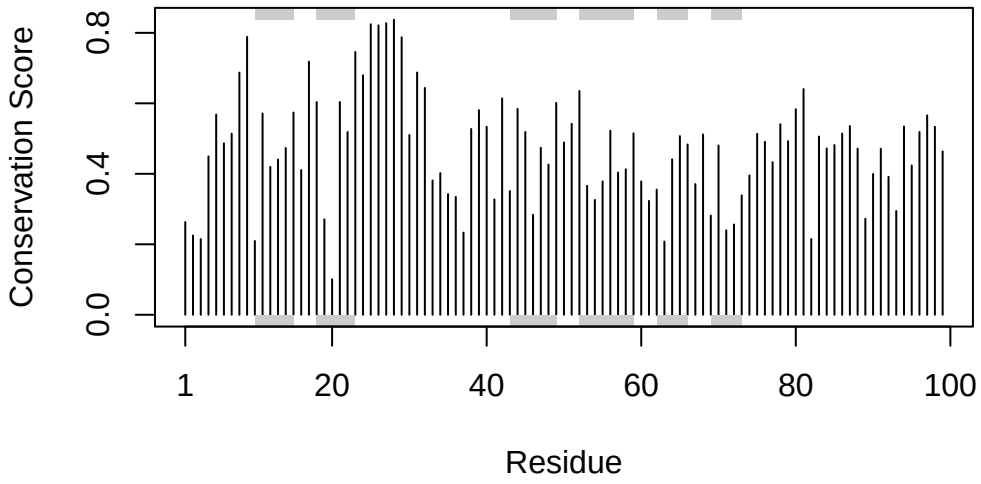
```
[1] " ** Duplicated sequence id's: 101 **"
[2] " ** Duplicated sequence id's: 101 **"
```

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

```
[1] 5378  132
```

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

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




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

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

```
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")
```