# Class 11: Structural Bioinformatics Pt. 2

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Today, before delving into structure prediction with AlphaFold, we will finish off our previous
lab10 "compariative structure analysis" section.

```
library(bio3d)

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 = JTKYMKAE013
 ..........
 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_6579943     1AKE_A  100.000             214          0        0       1
2 Query_6579943     8BQF_A   99.533             214          1        0       1
3 Query_6579943     4X8M_A   99.533             214          1        0       1
4 Query_6579943     6S36_A   99.533             214          1        0       1
5 Query_6579943     8Q2B_A   99.533             214          1        0       1
6 Query_6579943     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
```
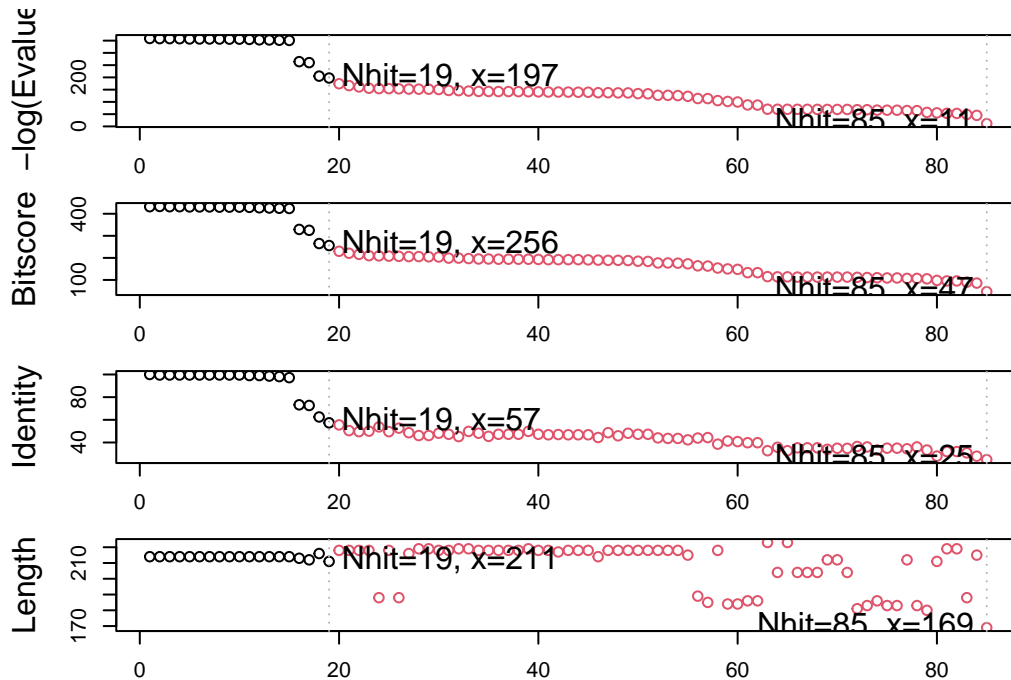
```
plot(b)
```

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

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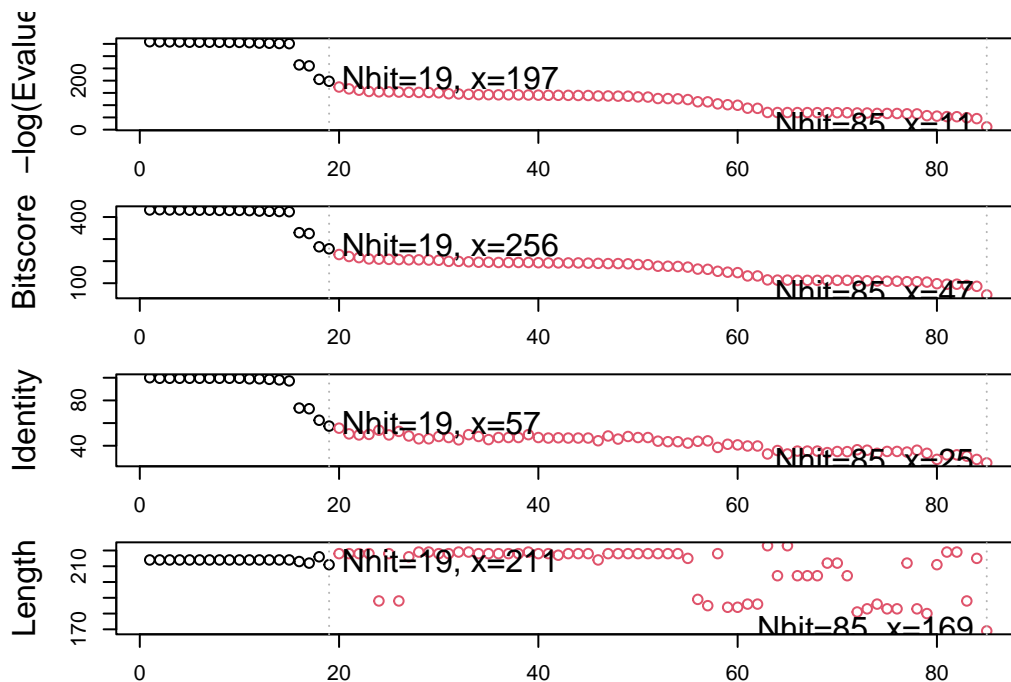


```
hits<-plot(b)
```

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

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

```r
attributes(hits)
```

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

$class
[1] "blast"
```

```r
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"
```

```r
#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
```
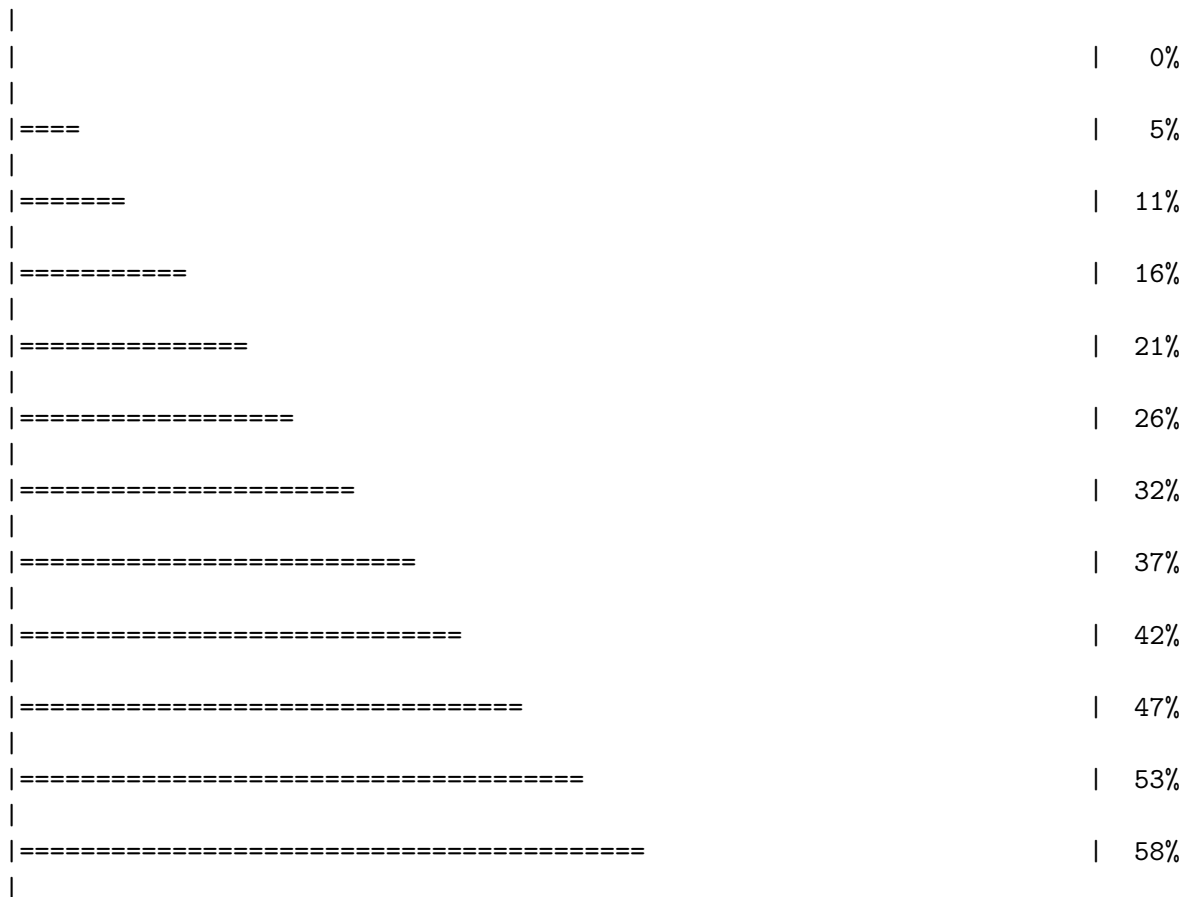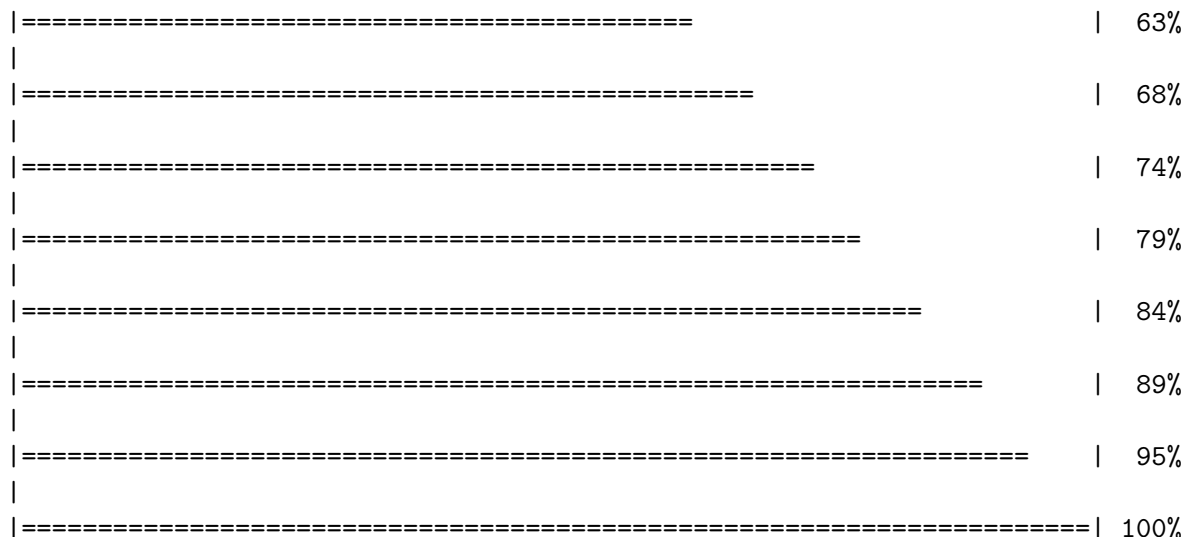
```
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```

I have now found and downloaded all 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. Here we installed `"msa"`

```r
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
```

10

```
[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
```
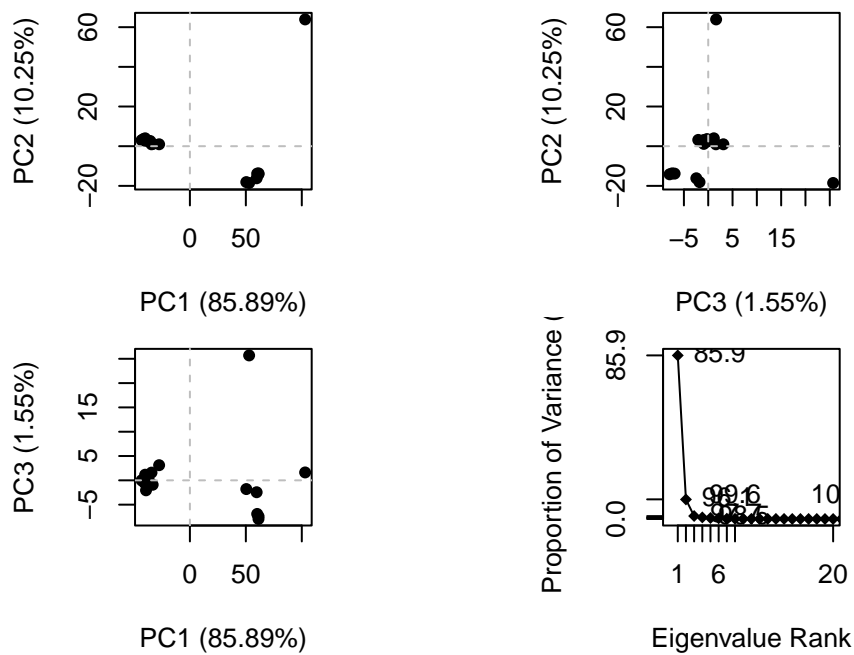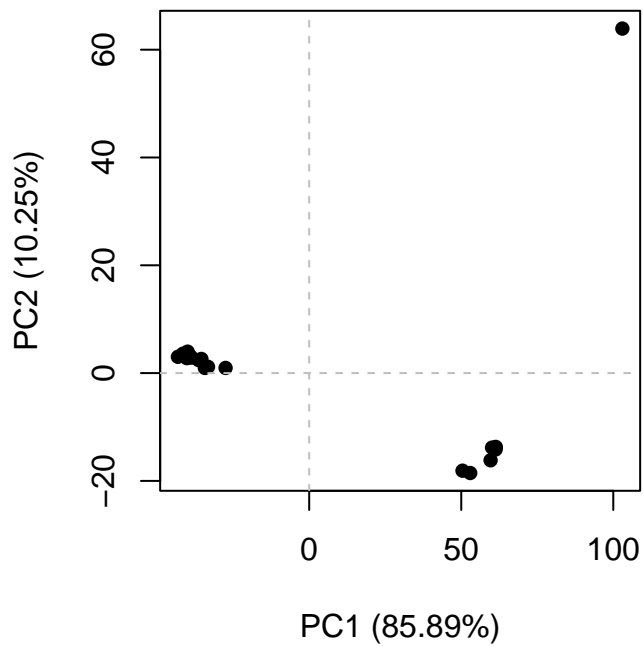
#Principal Component Analysis

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

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```
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")
```