class10 (cont.)

Bayah Essayem (A17303992)

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Here we run through a complete "pipeline" of structure analysis that begins with a single sequence identifier and ends in a PCA analysis.

```
library(bio3d)
```

Step 1. Retrieve a sequence for the protein we are interested in. We will take ADK "1ake_A

```
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
```

Step 2.

Run a BLAST search of the PDB for all related sequences to our input 'aa'

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

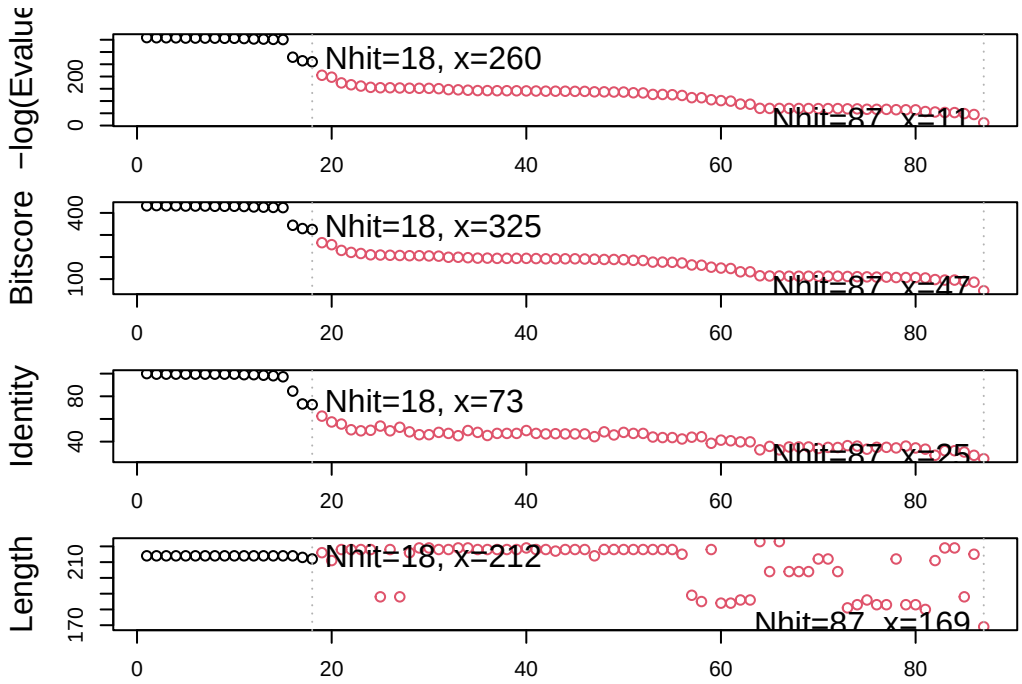
```
 Searching ... please wait (updates every 5 seconds) RID = UU1W16VK013
 ...
 Reporting 87 hits
```

```
hits <- plot(blast)
```

```
  * Possible cutoff values:    260 11
```

```
          Yielding Nhits:    18 87

 * Chosen cutoff value of:    260
          Yielding Nhits:    18
```



Step 3. Download all structures

These are our "top hits" i.e. all the structures in the PDB database related to our input sequence.

```
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" "8PVW_A"
[17] "4K46_A" "4NP6_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 exists. Skipping download

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Step 4. Align and superpose

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/8PVW_A.pdb
```

```
pdbs/split_chain/4K46_A.pdb
pdbs/split_chain/4NP6_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
.   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/8PVW_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
```

```
pdb/seq: 17   name: pdbs/split_chain/4K46_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 18   name: pdbs/split_chain/4NP6_A.pdb
```

```
pdbs
```

```
                                 1        .         .         .         40
[Truncated_Name:1]1AKE_A.pdb    --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAA
[Truncated_Name:2]8BQF_A.pdb    --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAA
[Truncated_Name:3]4X8M_A.pdb    --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAA
[Truncated_Name:4]6S36_A.pdb    --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAA
[Truncated_Name:5]8Q2B_A.pdb    --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAA
[Truncated_Name:6]8RJ9_A.pdb    --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAA
[Truncated_Name:7]6RZE_A.pdb    --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAA
[Truncated_Name:8]4X8H_A.pdb    --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAA
[Truncated_Name:9]3HPR_A.pdb    --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAA
[Truncated_Name:10]1E4V_A.pdb   --MRIILLGAPVAGKGTQAQFIMEKYGIPQISTGDMLRAA
[Truncated_Name:11]5EJE_A.pdb   --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAA
[Truncated_Name:12]1E4Y_A.pdb   --MRIILLGALVAGKGTQAQFIMEKYGIPQISTGDMLRAA
[Truncated_Name:13]3X2S_A.pdb   --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAA
[Truncated_Name:14]6HAP_A.pdb   --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAA
[Truncated_Name:15]6HAM_A.pdb   --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAA
[Truncated_Name:16]8PVW_A.pdb   --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAA
[Truncated_Name:17]4K46_A.pdb   --MRIILLGAPGAGKGTQAQFIMAKFGIPQISTGDMLRAA
[Truncated_Name:18]4NP6_A.pdb   NAMRIILLGAPGAGKGTQAQFIMEKFGIPQISTGDMLRAA
                                  ********  *********** *^***************
                                 1        .         .         .         40

                                41        .         .         .         80
[Truncated_Name:1]1AKE_A.pdb    VKSGSELGKQAKDIMDAGKLVTDELVIALVKERIAQEDCR
[Truncated_Name:2]8BQF_A.pdb    VKSGSELGKQAKDIMDAGKLVTDELVIALVKERIAQE---
[Truncated_Name:3]4X8M_A.pdb    VKSGSELGKQAKDIMDAGKLVTDELVIALVKERIAQEDCR
[Truncated_Name:4]6S36_A.pdb    VKSGSELGKQAKDIMDAGKLVTDELVIALVKERIAQEDCR
[Truncated_Name:5]8Q2B_A.pdb    VKSGSELGKQAKDIMDAGKLVTDELVIALVKERIAQEDCR
[Truncated_Name:6]8RJ9_A.pdb    VKSGSELGKQAKDIMDAGKLVTDELVIALVKERIAQEDCR
[Truncated_Name:7]6RZE_A.pdb    VKSGSELGKQAKDIMDAGKLVTDELVIALVKERIAQEDCR
[Truncated_Name:8]4X8H_A.pdb    VKSGSELGKQAKDIMDAGKLVTDELVIALVKERIAQEDCR
[Truncated_Name:9]3HPR_A.pdb    VKSGSELGKQAKDIMDAGKLVTDELVIALVKERIAQEDCR
[Truncated_Name:10]1E4V_A.pdb   VKSGSELGKQAKDIMDAGKLVTDELVIALVKERIAQEDCR
[Truncated_Name:11]5EJE_A.pdb   VKSGSELGKQAKDIMDACKLVTDELVIALVKERIAQEDCR
[Truncated_Name:12]1E4Y_A.pdb   VKSGSELGKQAKDIMDAGKLVTDELVIALVKERIAQEDCR
[Truncated_Name:13]3X2S_A.pdb   VKSGSELGKQAKDIMDCGKLVTDELVIALVKERIAQEDSR
```

```
[Truncated_Name:14]6HAP_A.pdb   VKSGSELGKQAKDIMDAGKLVTDELVIALVRERICQEDSR
[Truncated_Name:15]6HAM_A.pdb   IKSGSELGKQAKDIMDAGKLVTDEIIIALVKERICQEDSR
[Truncated_Name:16]8PVW_A.pdb   VKSGSELGKQAKDIMDAGKLVTDELVIALVKERIAQEDCR
[Truncated_Name:17]4K46_A.pdb   IKAGTELGKQAKSVIDAGQLVSDDIILGLVKERIAQDDCA
[Truncated_Name:18]4NP6_A.pdb   IKAGTELGKQAKAVIDAGQLVSDDIILGLIKERIAQADCE
                                ^* *^******* ^^*   **^*^^^^^*^^*** *
                               41        .         .         .        80

                               81        .         .         .        120
[Truncated_Name:1]1AKE_A.pdb    NGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:2]8BQF_A.pdb    -GFLLDGFPRTIPQADAMKEAGINVDYVIEFDVPDELIVD
[Truncated_Name:3]4X8M_A.pdb    NGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:4]6S36_A.pdb    NGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:5]8Q2B_A.pdb    NGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:6]8RJ9_A.pdb    NGFLLAGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:7]6RZE_A.pdb    NGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:8]4X8H_A.pdb    NGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:9]3HPR_A.pdb    NGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:10]1E4V_A.pdb   NGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:11]5EJE_A.pdb   NGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:12]1E4Y_A.pdb   NGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:13]3X2S_A.pdb   NGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:14]6HAP_A.pdb   NGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:15]6HAM_A.pdb   NGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:16]8PVW_A.pdb   NGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:17]4K46_A.pdb   KGFLLDGFPRTIPQADGLKEVGVVVDYVIEFDVADSVIVE
[Truncated_Name:18]4NP6_A.pdb   KGFLLDGFPRTIPQADGLKEMGINVDYVIEFDVADDVIVE
                                 **** **********^^** *^ ****^**** * ^**^
                               81        .         .         .        120

                              121        .         .         .        160
[Truncated_Name:1]1AKE_A.pdb    RIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:2]8BQF_A.pdb    RIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:3]4X8M_A.pdb    RIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:4]6S36_A.pdb    KIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:5]8Q2B_A.pdb    RIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKA
[Truncated_Name:6]8RJ9_A.pdb    RIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:7]6RZE_A.pdb    AIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:8]4X8H_A.pdb    RIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:9]3HPR_A.pdb    RIVGRRVHAPSGRVYHVKFNPPKVEGKDDGTGEELTTRKD
[Truncated_Name:10]1E4V_A.pdb   RIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:11]5EJE_A.pdb   RIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:12]1E4Y_A.pdb   RIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKD
```

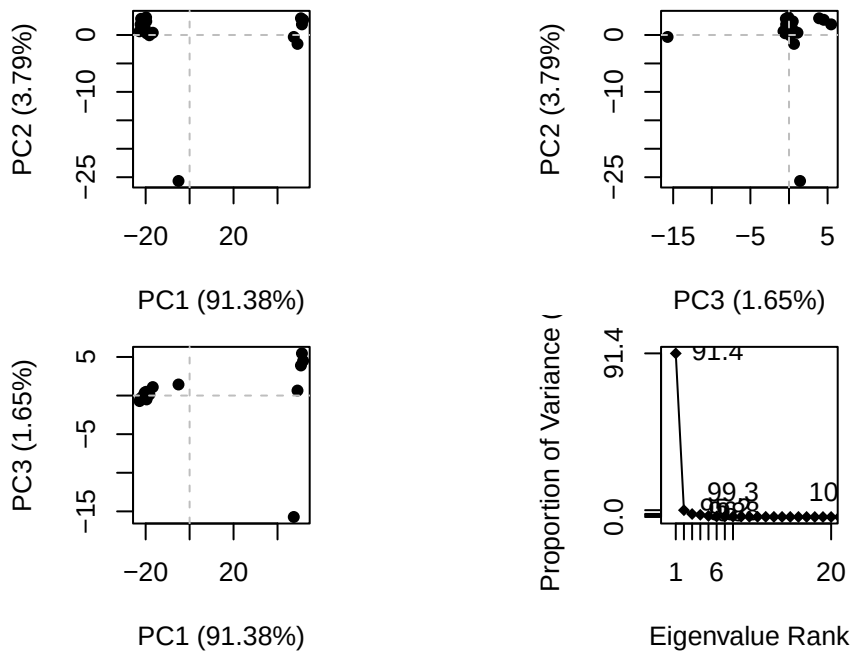
```
[Truncated_Name:13]3X2S_A.pdb   RIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:14]6HAP_A.pdb   RIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:15]6HAM_A.pdb   RIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:16]8PVW_A.pdb   RILKRGE--TSGRV------------------------D
[Truncated_Name:17]4K46_A.pdb   RMAGRRAHLASGRTYHNVYNPPKVEGKDDVTGEDLVIRED
[Truncated_Name:18]4NP6_A.pdb   RMAGRRAHLPSGRTYHVVYNPPKVEGKDDVTGEDLVIRED
                                 ^  *     ***
                               121        .         .         .         160

                               161        .         .         .         200
[Truncated_Name:1]1AKE_A.pdb    DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:2]8BQF_A.pdb    DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:3]4X8M_A.pdb    DQEETVRKRLVEWHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:4]6S36_A.pdb    DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:5]8Q2B_A.pdb    DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:6]8RJ9_A.pdb    DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:7]6RZE_A.pdb    DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:8]4X8H_A.pdb    DQEETVRKRLVEYHQMTAALIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:9]3HPR_A.pdb    DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:10]1E4V_A.pdb   DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:11]5EJE_A.pdb   DQEECVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:12]1E4Y_A.pdb   DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:13]3X2S_A.pdb   DQEETVRKRLCEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:14]6HAP_A.pdb   DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:15]6HAM_A.pdb   DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:16]8PVW_A.pdb   DNEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:17]4K46_A.pdb   DKEETVLARLGVYHNQTAPLIAYYGKEAEAGNTQYLKFDG
[Truncated_Name:18]4NP6_A.pdb   DKEETVRARLNVYHTQTAPLIEYYGKEAAAGKTQYLKFDG
                                 * ** *  **  ^*  ** ** ** *** ** * * * **
                               161        .         .         .         200

                               201        .     216
[Truncated_Name:1]1AKE_A.pdb    TKPVAEVRADLEKILG
[Truncated_Name:2]8BQF_A.pdb    TKPVAEVRADLEKIL-
[Truncated_Name:3]4X8M_A.pdb    TKPVAEVRADLEKILG
[Truncated_Name:4]6S36_A.pdb    TKPVAEVRADLEKILG
[Truncated_Name:5]8Q2B_A.pdb    TKPVAEVRADLEKILG
[Truncated_Name:6]8RJ9_A.pdb    TKPVAEVRADLEKILG
[Truncated_Name:7]6RZE_A.pdb    TKPVAEVRADLEKILG
[Truncated_Name:8]4X8H_A.pdb    TKPVAEVRADLEKILG
[Truncated_Name:9]3HPR_A.pdb    TKPVAEVRADLEKILG
[Truncated_Name:10]1E4V_A.pdb   TKPVAEVRADLEKILG
[Truncated_Name:11]5EJE_A.pdb   TKPVAEVRADLEKILG
```

```
[Truncated_Name:12]1E4Y_A.pdb   TKPVAEVRADLEKILG
[Truncated_Name:13]3X2S_A.pdb   TKPVAEVRADLEKILG
[Truncated_Name:14]6HAP_A.pdb   TKPVCEVRADLEKILG
[Truncated_Name:15]6HAM_A.pdb   TKPVCEVRADLEKILG
[Truncated_Name:16]8PVW_A.pdb   TKPVAEVRADLEKILG
[Truncated_Name:17]4K46_A.pdb   TKAVAEVSAELEKALA
[Truncated_Name:18]4NP6_A.pdb   TKQVSEVSADIAKALA
                                ** * ** *^^ * *
                              201        .     216

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

Class:
  pdbs, fasta

Alignment dimensions:
  18 sequence rows; 216 position columns (182 non-gap, 34 gap)

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

Step 5. PCA

Let's use our old friend PCA to make sense of these confusing, complicated structure relationships.

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



Let's make a trajectory (or movie) of the main conformational changes captured by PC1. We will use the 'mktrj()' function for this…

```
mktrj(pc, file = "pca_result.pdb")
```

Back of the envelope comparison of the PDB size to UniProt PDB: 231029, UniProt size: 2531029

```
uniprot <- 253206171
pdb <- 231029
pdb/uniprot * 100
```

```
[1] 0.09124146
```

Calculate RMSD

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

```
Warning in rmsd(pdbs): No indices provided, using the 182 non NA positions
```

```
# Structure-based clustering
hc.rd <- hclust(dist(rd))
grps.rd <- cutree(hc.rd, k=3)

plot(pc, 1:2, col="grey50", bg=grps.rd, pch=21, cex=1)
```