Class_11_pt2

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```
library(bio3d)
pdb <- read.pdb("1hel")
```

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

```
pdb
```

```
##
##  Call:  read.pdb(file = "1hel")
##
##    Total Models#: 1
##      Total Atoms#: 1186,  XYZs#: 3558  Chains#: 1  (values: A)
##
##      Protein Atoms#: 1001  (residues/Calpha atoms#: 129)
##      Nucleic acid Atoms#: 0  (residues/phosphate atoms#: 0)
##
##      Non-protein/nucleic Atoms#: 185  (residues: 185)
##      Non-protein/nucleic resid values: [ HOH (185) ]
##
##    Protein sequence:
##       KVFGRCELAAAMKRHGLDNYRGYSLGNWVCAAKFESNFNTQATNRNTDGSTDYGILQINS
##       RWWCNDGRTPGSRNLCNIPCSALLSSDITASVNCAKKIVSDGNGMNAWVAWRNRCKGTDV
##       QAWIRGCRL
##
## + attr: atom, xyz, seqres, helix, sheet,
##         calpha, remark, call
```

```
#print out:
head(pdb$atom)
```

```
##   type eleno elety  alt resid chain resno insert      x      y      z o     b
## 1 ATOM     1     N <NA>   LYS     A     1  <NA>  3.294 10.164 10.266 1 11.18
## 2 ATOM     2    CA <NA>   LYS     A     1  <NA>  2.388 10.533  9.168 1  9.68
## 3 ATOM     3     C <NA>   LYS     A     1  <NA>  2.438 12.049  8.889 1 14.00
## 4 ATOM     4     O <NA>   LYS     A     1  <NA>  2.406 12.898  9.815 1 14.00
## 5 ATOM     5    CB <NA>   LYS     A     1  <NA>  0.949 10.101  9.559 1 13.29
## 6 ATOM     6    CG <NA>   LYS     A     1  <NA> -0.050 10.621  8.573 1 13.52
##   segid elesy charge
## 1  <NA>     N   <NA>
## 2  <NA>     C   <NA>
```
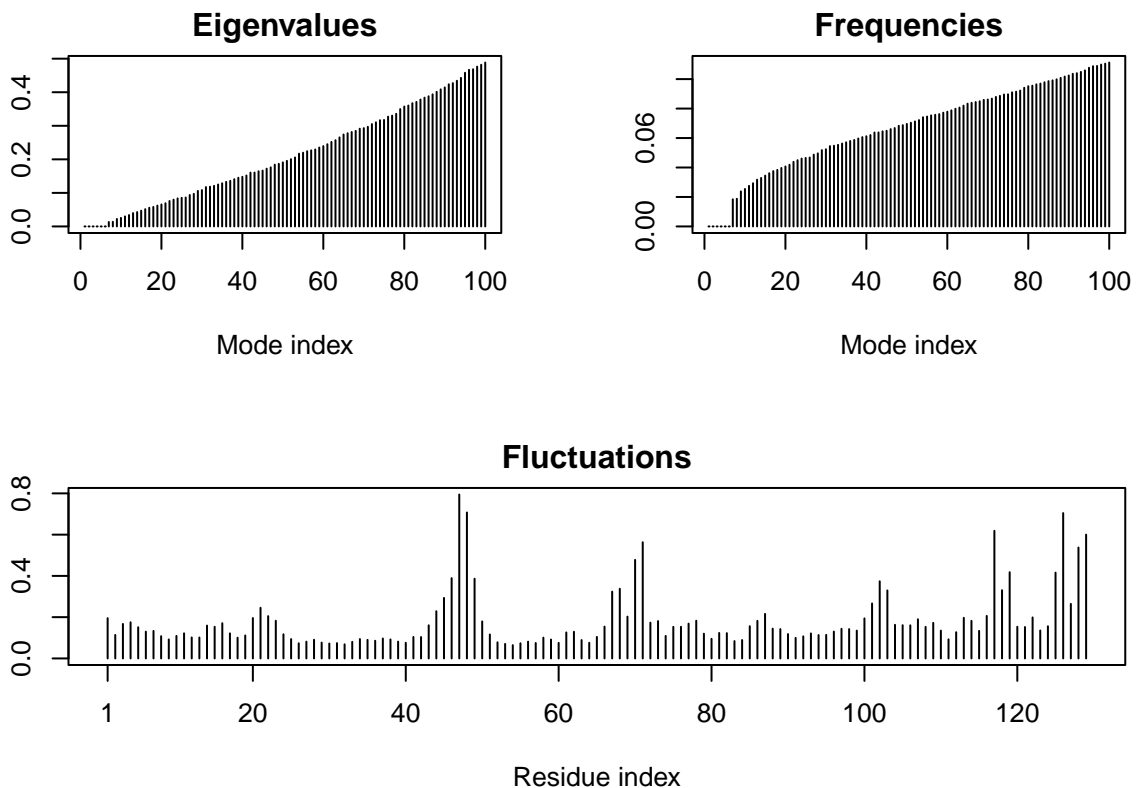
```
## 3  <NA>    C   <NA>
## 4  <NA>    O   <NA>
## 5  <NA>    C   <NA>
## 6  <NA>    C   <NA>
```

Lets do a quick bioinformatic prediction of protein dynamics (aka flexibility). We will use the 'nma()' function, which does Normal Mode Anlysis.

```
modes <- nma(pdb)
```

```
##  Building Hessian...     Done in 0.033 seconds.
##  Diagonalizing Hessian...    Done in 0.299 seconds.
```
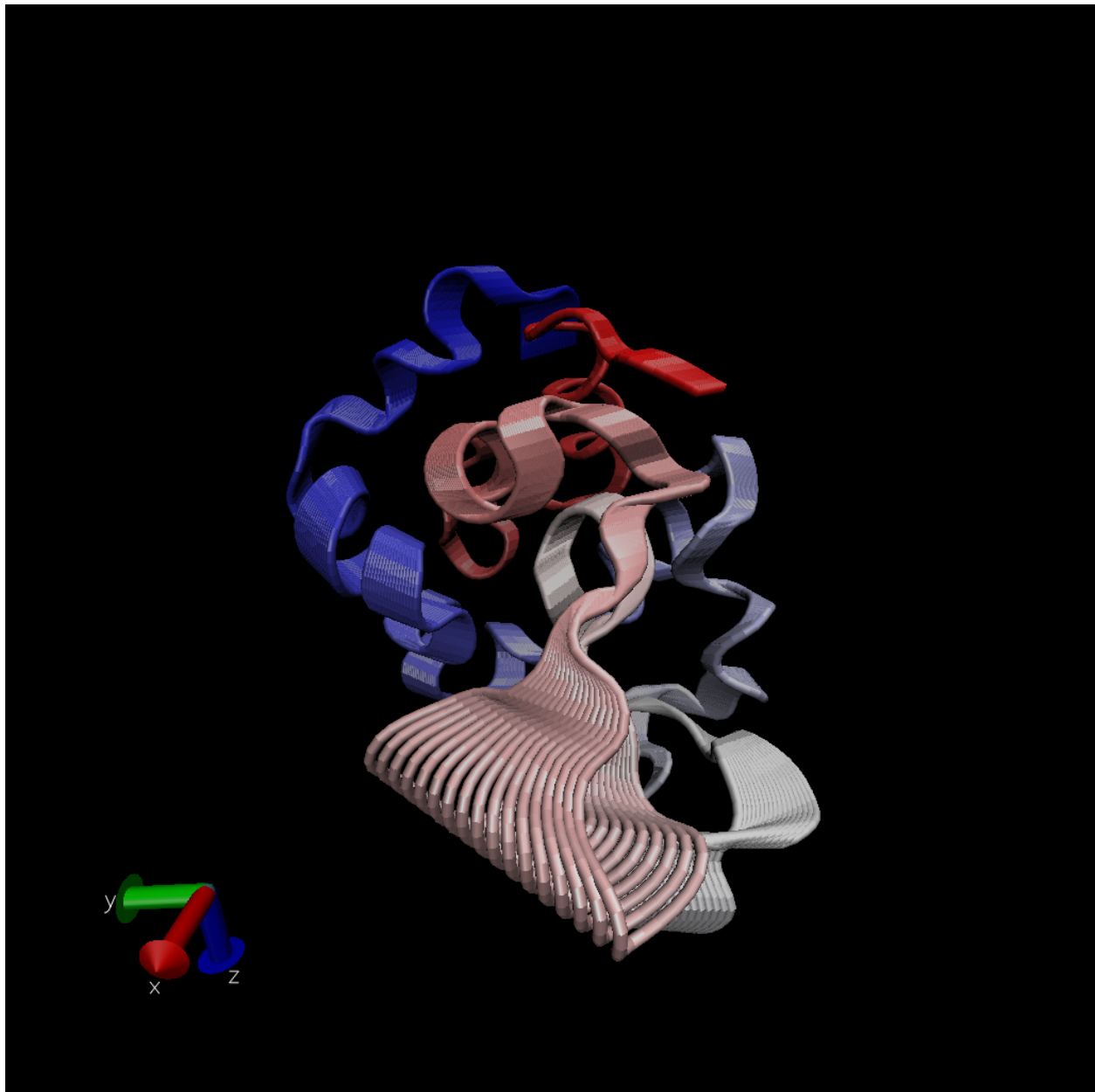
```
#now plot
plot(modes)
```


Make a trajectory of this prediction with the 'mktrj()'

```
mktrj(modes, file= "nma.pdb")
```

And the image from VMD

2

Comparative Structure Analysis

Start by getting a sequence of interest

```
aa <- get.seq("1AKE_A")
```

```
## Warning in get.seq("1AKE_A"): 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
```

I want to search the PDB database (the main db for exp structures) for sequences like this aa sequence.
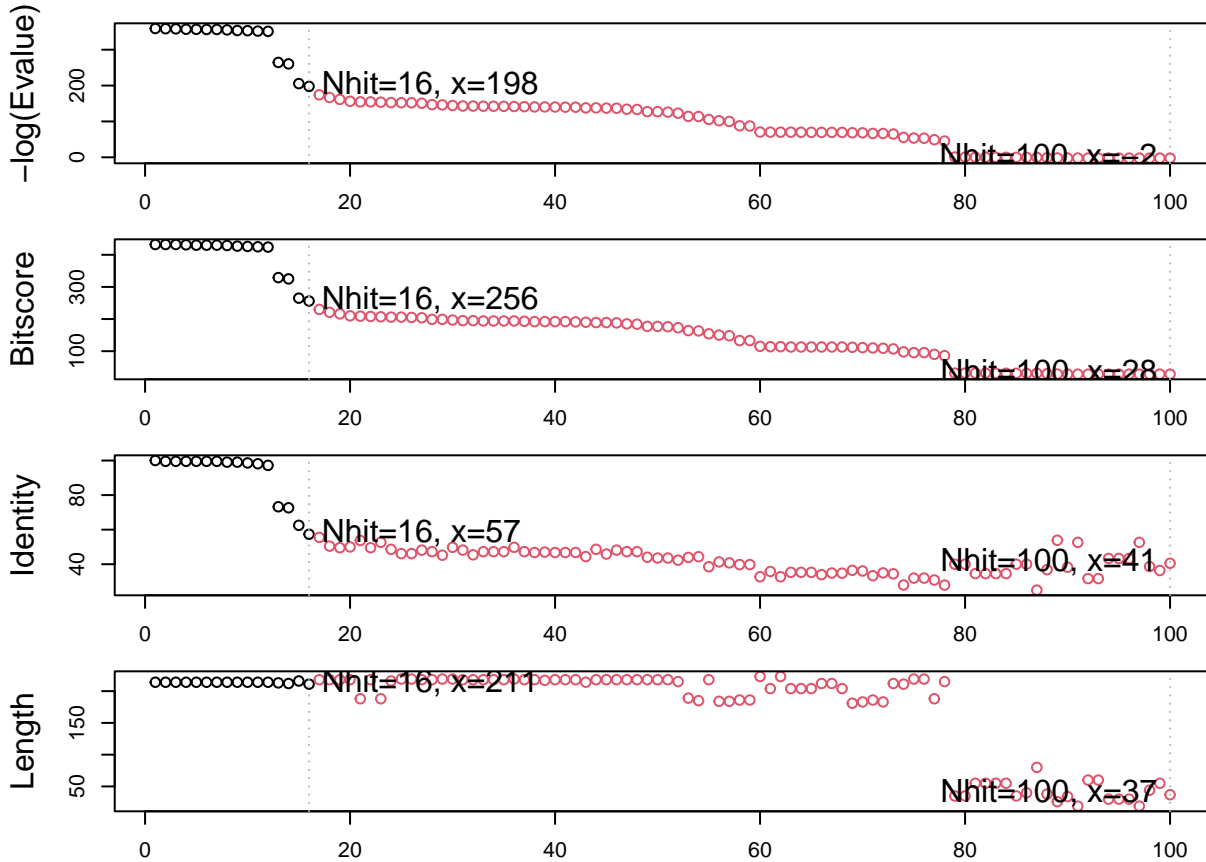
```
blast <- blast.pdb(aa)
```

```
##  Searching ... please wait (updates every 5 seconds) RID = SETCT2BA016
##  .
##  Reporting 100 hits
```

plot the blast

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

```
##    * Possible cutoff values:    197 -3
##            Yielding Nhits:    16 100
##
##    * Chosen cutoff value of:    197
##            Yielding Nhits:    16
```

Now I have my top hits from the search of the PDB

```
hits$pdb.id
```

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

Here we download all these similar structures in the PDB and store them on our computer

```
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/
## 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/
## 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

##    |                                                                      |
```

Now we want to align all thes structures. We will use the function 'pdbaln()'

```
#Align related PDBs
pdbs <- pdbaln(files, fit = T)
```

```
## Reading PDB files:
## pdbs/split_chain/1AKE_A.pdb
## pdbs/split_chain/4X8M_A.pdb
## pdbs/split_chain/6S36_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
## ....
##
## 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/4X8M_A.pdb
## pdb/seq: 3   name: pdbs/split_chain/6S36_A.pdb
##     PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 4   name: pdbs/split_chain/6RZE_A.pdb
##     PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 5   name: pdbs/split_chain/4X8H_A.pdb
## pdb/seq: 6   name: pdbs/split_chain/3HPR_A.pdb
##     PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 7   name: pdbs/split_chain/1E4V_A.pdb
## pdb/seq: 8   name: pdbs/split_chain/5EJE_A.pdb
##     PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 9   name: pdbs/split_chain/1E4Y_A.pdb
## pdb/seq: 10   name: pdbs/split_chain/3X2S_A.pdb
## pdb/seq: 11   name: pdbs/split_chain/6HAP_A.pdb
## pdb/seq: 12   name: pdbs/split_chain/6HAM_A.pdb
##     PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 13   name: pdbs/split_chain/4K46_A.pdb
##     PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 14   name: pdbs/split_chain/4NP6_A.pdb
## pdb/seq: 15   name: pdbs/split_chain/3GMT_A.pdb
## pdb/seq: 16   name: pdbs/split_chain/4PZL_A.pdb
```

pdbs

```
##                                    1         .         .         .        40
## [Truncated_Name:1]1AKE_A.pdb    ----------MRIILLGAPGAGKGTQAQFIMEKYGIPQIS
## [Truncated_Name:2]4X8M_A.pdb    ----------MRIILLGAPGAGKGTQAQFIMEKYGIPQIS
## [Truncated_Name:3]6S36_A.pdb    ----------MRIILLGAPGAGKGTQAQFIMEKYGIPQIS
## [Truncated_Name:4]6RZE_A.pdb    ----------MRIILLGAPGAGKGTQAQFIMEKYGIPQIS
## [Truncated_Name:5]4X8H_A.pdb    ----------MRIILLGAPGAGKGTQAQFIMEKYGIPQIS
## [Truncated_Name:6]3HPR_A.pdb    ----------MRIILLGAPGAGKGTQAQFIMEKYGIPQIS
## [Truncated_Name:7]1E4V_A.pdb    ----------MRIILLGAPVAGKGTQAQFIMEKYGIPQIS
## [Truncated_Name:8]5EJE_A.pdb    ----------MRIILLGAPGAGKGTQAQFIMEKYGIPQIS
## [Truncated_Name:9]1E4Y_A.pdb    ----------MRIILLGALVAGKGTQAQFIMEKYGIPQIS
```

```
## [Truncated_Name:10]3X2S_A.pdb    ----------MRIILLGAPGAGKGTQAQFIMEKYGIPQIS
## [Truncated_Name:11]6HAP_A.pdb    ----------MRIILLGAPGAGKGTQAQFIMEKYGIPQIS
## [Truncated_Name:12]6HAM_A.pdb    ----------MRIILLGAPGAGKGTQAQFIMEKYGIPQIS
## [Truncated_Name:13]4K46_A.pdb    ----------MRIILLGAPGAGKGTQAQFIMAKFGIPQIS
## [Truncated_Name:14]4NP6_A.pdb    --------NAMRIILLGAPGAGKGTQAQFIMEKFGIPQIS
## [Truncated_Name:15]3GMT_A.pdb    ----------MRLILLGAPGAGKGTQANFIKEKFGIPQIS
## [Truncated_Name:16]4PZL_A.pdb    TENLYFQSNAMRIILLGAPGAGKGTQAKIIEQKYNIAHIS
##                                            **^***** ******* * *^ *  **
##                                   1         .         .         .        40
##
## 
##                                   41        .         .         .        80
## [Truncated_Name:1]1AKE_A.pdb      TGDMLRAAVKSGSELGKQAKDIMDAGKLVTDELVIALVKE
## [Truncated_Name:2]4X8M_A.pdb      TGDMLRAAVKSGSELGKQAKDIMDAGKLVTDELVIALVKE
## [Truncated_Name:3]6S36_A.pdb      TGDMLRAAVKSGSELGKQAKDIMDAGKLVTDELVIALVKE
## [Truncated_Name:4]6RZE_A.pdb      TGDMLRAAVKSGSELGKQAKDIMDAGKLVTDELVIALVKE
## [Truncated_Name:5]4X8H_A.pdb      TGDMLRAAVKSGSELGKQAKDIMDAGKLVTDELVIALVKE
## [Truncated_Name:6]3HPR_A.pdb      TGDMLRAAVKSGSELGKQAKDIMDAGKLVTDELVIALVKE
## [Truncated_Name:7]1E4V_A.pdb      TGDMLRAAVKSGSELGKQAKDIMDAGKLVTDELVIALVKE
## [Truncated_Name:8]5EJE_A.pdb      TGDMLRAAVKSGSELGKQAKDIMDACKLVTDELVIALVKE
## [Truncated_Name:9]1E4Y_A.pdb      TGDMLRAAVKSGSELGKQAKDIMDAGKLVTDELVIALVKE
## [Truncated_Name:10]3X2S_A.pdb     TGDMLRAAVKSGSELGKQAKDIMDCGKLVTDELVIALVKE
## [Truncated_Name:11]6HAP_A.pdb     TGDMLRAAVKSGSELGKQAKDIMDAGKLVTDELVIALVRE
## [Truncated_Name:12]6HAM_A.pdb     TGDMLRAAIKSGSELGKQAKDIMDAGKLVTDEIIIALVKE
## [Truncated_Name:13]4K46_A.pdb     TGDMLRAAIKAGTELGKQAKSVIDAGQLVSDDIILGLVKE
## [Truncated_Name:14]4NP6_A.pdb     TGDMLRAAIKAGTELGKQAKAVIDAGQLVSDDIILGLIKE
## [Truncated_Name:15]3GMT_A.pdb     TGDMLRAAVKAGTPLGVEAKTYMDEGKLVPDSLIIGLVKE
## [Truncated_Name:16]4PZL_A.pdb     TGDMIRETIKSGSALGQELKKVLDAGELVSDEFIIKIVKD
##                                   ****^*  ^* *^ **    *  ^*   ** *   ^^ ^^^^
##                                   41        .         .         .        80
##
##                                   81        .         .         .       120
## [Truncated_Name:1]1AKE_A.pdb      RIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:2]4X8M_A.pdb      RIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:3]6S36_A.pdb      RIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:4]6RZE_A.pdb      RIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:5]4X8H_A.pdb      RIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:6]3HPR_A.pdb      RIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:7]1E4V_A.pdb      RIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:8]5EJE_A.pdb      RIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:9]1E4Y_A.pdb      RIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:10]3X2S_A.pdb     RIAQEDSRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:11]6HAP_A.pdb     RICQEDSRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:12]6HAM_A.pdb     RICQEDSRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:13]4K46_A.pdb     RIAQDDCAKGFLLDGFPRTIPQADGLKEVGVVVDYVIEFD
## [Truncated_Name:14]4NP6_A.pdb     RIAQADCEKGFLLDGFPRTIPQADGLKEMGINVDYVIEFD
## [Truncated_Name:15]3GMT_A.pdb     RLKEADCANGYLFDGFPRTIAQADAMKEAGVAIDYVLEID
## [Truncated_Name:16]4PZL_A.pdb     RISKNDCNNGFLLDGVPRTIPQAQELDKLGVNIDYIVEVD
##                                   *^    *   *^* ** **** **  ^    *^ ^**^^* *
##                                   81        .         .         .       120
##
##                                   121       .         .         .       160
## [Truncated_Name:1]1AKE_A.pdb      VPDELIVDRIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTG
## [Truncated_Name:2]4X8M_A.pdb      VPDELIVDRIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTG
## [Truncated_Name:3]6S36_A.pdb      VPDELIVDKIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTG
```

8

```
## [Truncated_Name:4]6RZE_A.pdb       VPDELIVDAIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTG
## [Truncated_Name:5]4X8H_A.pdb       VPDELIVDRIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTG
## [Truncated_Name:6]3HPR_A.pdb       VPDELIVDRIVGRRVHAPSGRVYHVKFNPPKVEGKDDGTG
## [Truncated_Name:7]1E4V_A.pdb       VPDELIVDRIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTG
## [Truncated_Name:8]5EJE_A.pdb       VPDELIVDRIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTG
## [Truncated_Name:9]1E4Y_A.pdb       VPDELIVDRIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTG
## [Truncated_Name:10]3X2S_A.pdb      VPDELIVDRIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTG
## [Truncated_Name:11]6HAP_A.pdb      VPDELIVDRIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTG
## [Truncated_Name:12]6HAM_A.pdb      VPDELIVDRIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTG
## [Truncated_Name:13]4K46_A.pdb      VADSVIVERMAGRRAHLASGRTYHNVYNPPKVEGKDDVTG
## [Truncated_Name:14]4NP6_A.pdb      VADDVIVERMAGRRAHLPSGRTYHVVYNPPKVEGKDDVTG
## [Truncated_Name:15]3GMT_A.pdb      VPFSEIIERMSGRRTHPASGRTYHVKFNPPKVEGKDDVTG
## [Truncated_Name:16]4PZL_A.pdb      VADNLLIERITGRRIHPASGRTYHTKFNPPKVADKDDVTG
##                                     *    ^ ^^ ^ *** *  *** **  ^*****  *** **
##                                   121         .         .         .        160
##
##                                   161         .         .         .        200
## [Truncated_Name:1]1AKE_A.pdb       EELTTRKDDQEETVRKRLVEYHQMTAPLIGYYSKEAEAGN
## [Truncated_Name:2]4X8M_A.pdb       EELTTRKDDQEETVRKRLVEWHQMTAPLIGYYSKEAEAGN
## [Truncated_Name:3]6S36_A.pdb       EELTTRKDDQEETVRKRLVEYHQMTAPLIGYYSKEAEAGN
## [Truncated_Name:4]6RZE_A.pdb       EELTTRKDDQEETVRKRLVEYHQMTAPLIGYYSKEAEAGN
## [Truncated_Name:5]4X8H_A.pdb       EELTTRKDDQEETVRKRLVEYHQMTAALIGYYSKEAEAGN
## [Truncated_Name:6]3HPR_A.pdb       EELTTRKDDQEETVRKRLVEYHQMTAPLIGYYSKEAEAGN
## [Truncated_Name:7]1E4V_A.pdb       EELTTRKDDQEETVRKRLVEYHQMTAPLIGYYSKEAEAGN
## [Truncated_Name:8]5EJE_A.pdb       EELTTRKDDQEECVRKRLVEYHQMTAPLIGYYSKEAEAGN
## [Truncated_Name:9]1E4Y_A.pdb       EELTTRKDDQEETVRKRLVEYHQMTAPLIGYYSKEAEAGN
## [Truncated_Name:10]3X2S_A.pdb      EELTTRKDDQEETVRKRLCEYHQMTAPLIGYYSKEAEAGN
## [Truncated_Name:11]6HAP_A.pdb      EELTTRKDDQEETVRKRLVEYHQMTAPLIGYYSKEAEAGN
## [Truncated_Name:12]6HAM_A.pdb      EELTTRKDDQEETVRKRLVEYHQMTAPLIGYYSKEAEAGN
## [Truncated_Name:13]4K46_A.pdb      EDLVIREDDKEETVLARLGVYHNQTAPLIAYYGKEAEAGN
## [Truncated_Name:14]4NP6_A.pdb      EDLVIREDDKEETVRARLNVYHTQTAPLIEYYGKEAAAGK
## [Truncated_Name:15]3GMT_A.pdb      EPLVQRDDDKEETVKKRLDVYEAQTKPLITYYGDWARRGA
## [Truncated_Name:16]4PZL_A.pdb      EPLITRTDDNEDTVKQRLSVYHAQTAKLIDFYRNFSSTNT
##                                     * *  * ** *^ *  **   ^   *  ** ^*
##                                   161         .         .         .        200
##
##                                   201         .         .      227
## [Truncated_Name:1]1AKE_A.pdb        T--KYAKVDGTKPVAEVRADLEKILG-
## [Truncated_Name:2]4X8M_A.pdb        T--KYAKVDGTKPVAEVRADLEKILG-
## [Truncated_Name:3]6S36_A.pdb        T--KYAKVDGTKPVAEVRADLEKILG-
## [Truncated_Name:4]6RZE_A.pdb        T--KYAKVDGTKPVAEVRADLEKILG-
## [Truncated_Name:5]4X8H_A.pdb        T--KYAKVDGTKPVAEVRADLEKILG-
## [Truncated_Name:6]3HPR_A.pdb        T--KYAKVDGTKPVAEVRADLEKILG-
## [Truncated_Name:7]1E4V_A.pdb        T--KYAKVDGTKPVAEVRADLEKILG-
## [Truncated_Name:8]5EJE_A.pdb        T--KYAKVDGTKPVAEVRADLEKILG-
## [Truncated_Name:9]1E4Y_A.pdb        T--KYAKVDGTKPVAEVRADLEKILG-
## [Truncated_Name:10]3X2S_A.pdb       T--KYAKVDGTKPVAEVRADLEKILG-
## [Truncated_Name:11]6HAP_A.pdb       T--KYAKVDGTKPVCEVRADLEKILG-
## [Truncated_Name:12]6HAM_A.pdb       T--KYAKVDGTKPVCEVRADLEKILG-
## [Truncated_Name:13]4K46_A.pdb       T--QYLKFDGTKAVAEVSAELEKALA-
## [Truncated_Name:14]4NP6_A.pdb       T--QYLKFDGTKQVSEVSADIAKALA-
## [Truncated_Name:15]3GMT_A.pdb       E-------NGLKAPA-----YRKISG-
## [Truncated_Name:16]4PZL_A.pdb       KIPKYIKINGDQAVEKVSQDIFDQLNK
##                                                    *
```

```
##                              201           .           .           227
##
## Call:
##   pdbaln(files = files, fit = T)
##
## Class:
##   pdbs, fasta
##
## Alignment dimensions:
##   16 sequence rows; 227 position columns (204 non-gap, 23 gap)
##
## + attr: xyz, resno, b, chain, id, ali, resid, sse, call
```
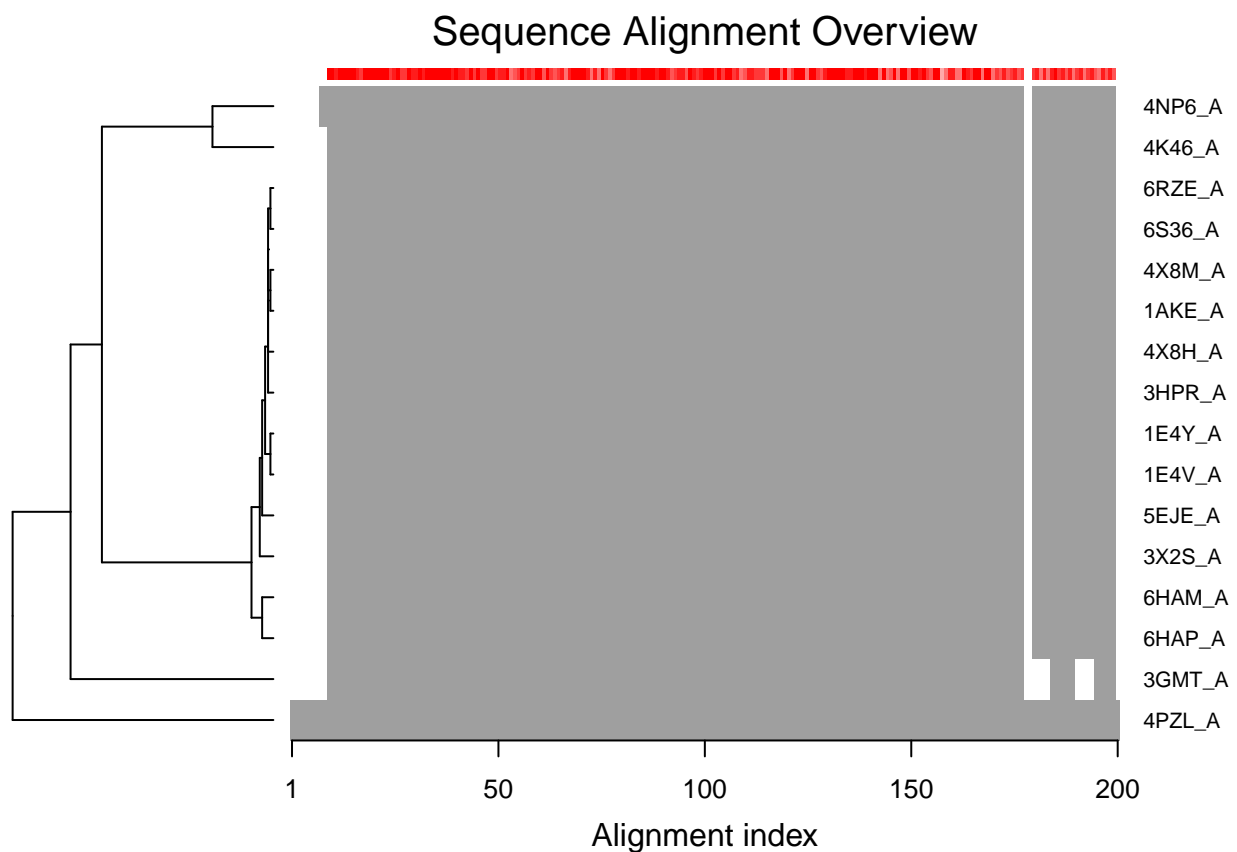
Let's have a look

```
# bector containing PDB codes for figure axis
ids <- basename.pdb(pdbs$id)

#Draw schematic alignment
plot(pdbs, labels=ids)
```
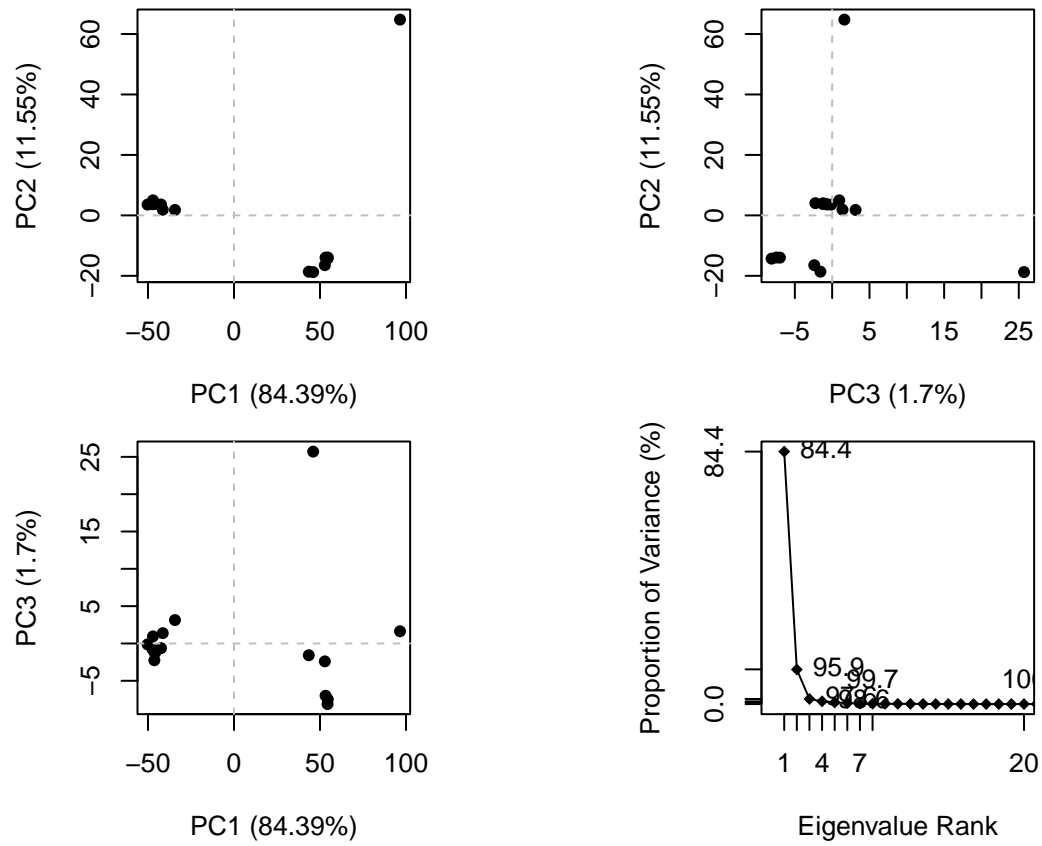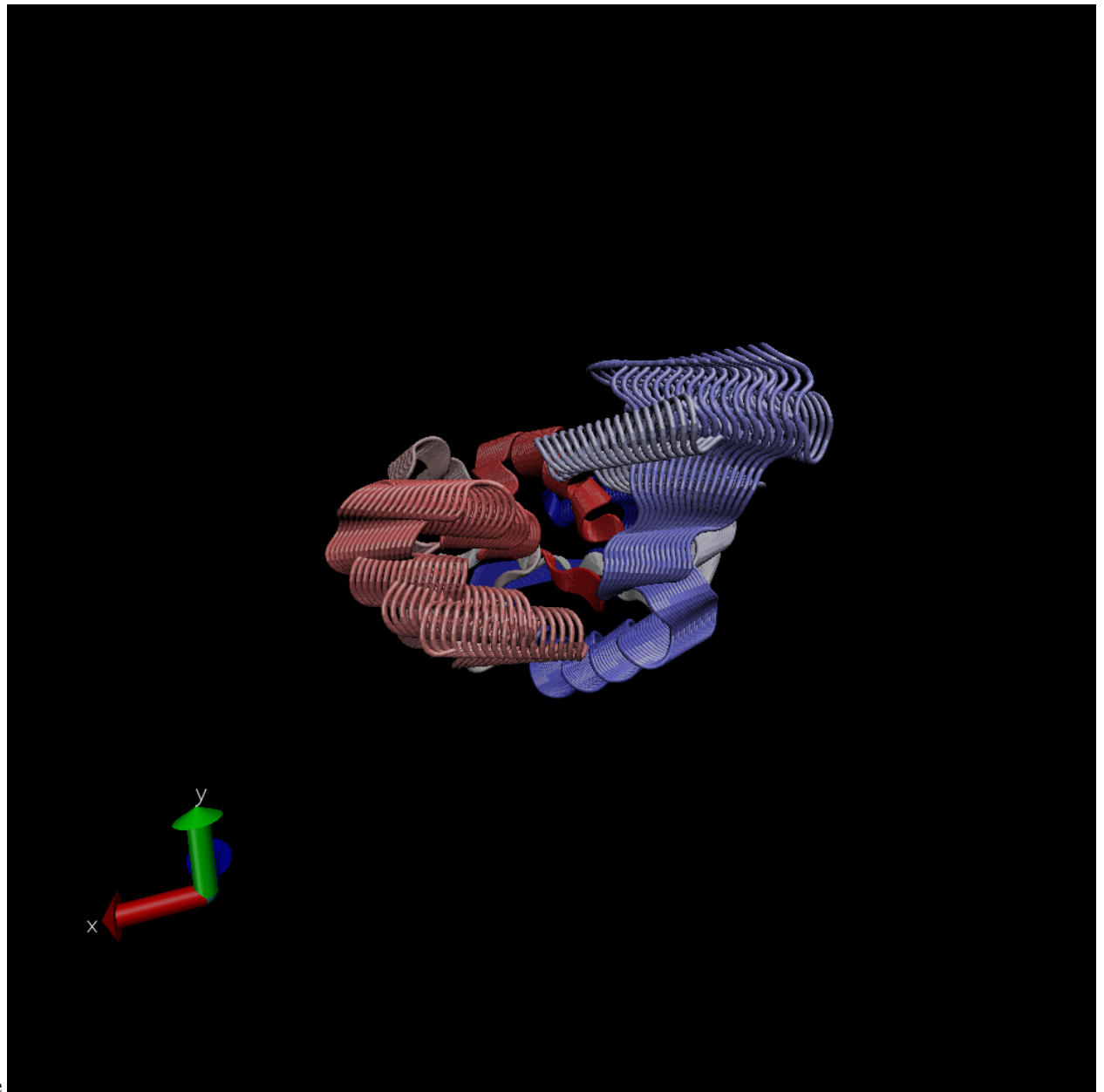

Principal Component Analysis (PCA)

Now do a PCA on the xyz coordinate data of all these structures with the 'pca()' function in bio3d.

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


Let's visualize the displacements (ie: movements of the structe) that are captured by PC1

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

VMD Image

Save our important results

```
save(blast, hits, pca, pdbs, file = "myresults.RData")
```

Alpha folding

VMD of find a gene sequence