

class12:Structural Bioinformatics 2

Jose Chacon (PID A59010515)

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```
#working with biod3d
```

```
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:
## KVFGRCELAAMKRHGLDNYRGYSLGNWVCAAKFESNFNTQATNRNTDGSTDYGILQINS
## RWWCNDGRTPGSRNLCNIPCSALLSSDITASVNC AKKIVSDGNGMNAWVAWRNRCKGTDV
## QAWIRGCRL
##
## + attr: atom, xyz, seqres, helix, sheet,
## calpha, remark, call
```

```
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
```

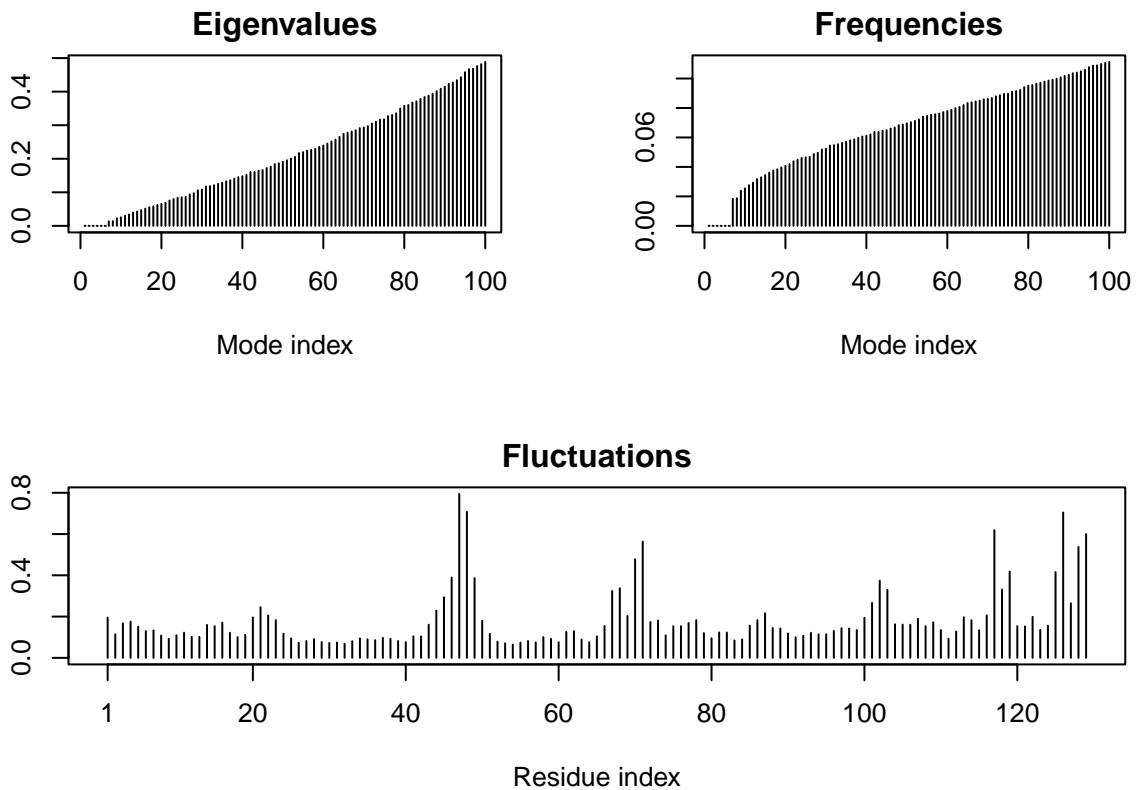
```
## 1 <NA>      N <NA>
## 2 <NA>      C <NA>
## 3 <NA>      C <NA>
## 4 <NA>      O <NA>
## 5 <NA>      C <NA>
## 6 <NA>      C <NA>
```

Let's do a quick bioinformatics prediction of protein dynamics (flexibility). We use the `nma()` function, which does Normal Mode Analysis.

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

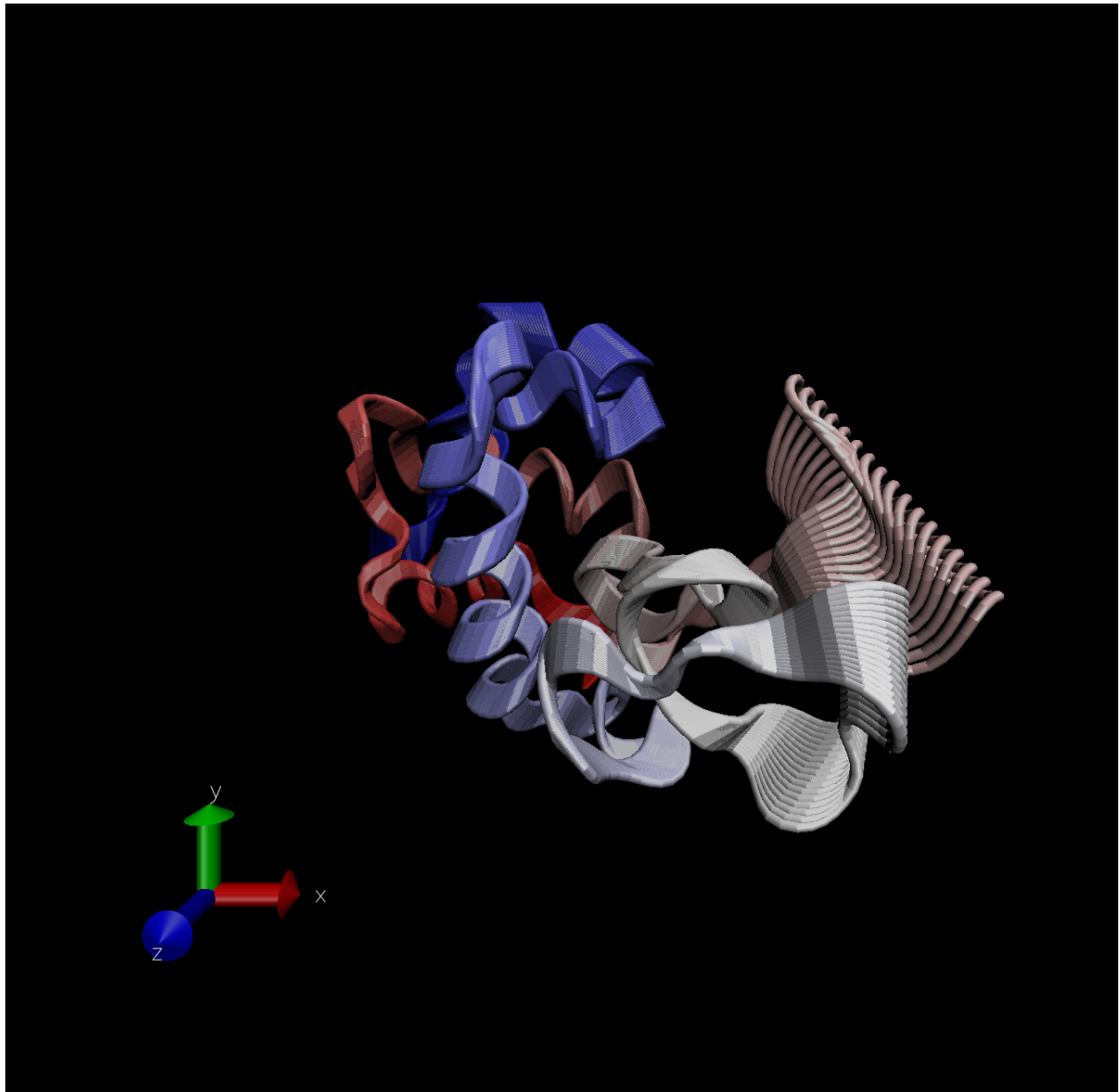
```
## Building Hessian...      Done in 0.078 seconds.
## Diagonalizing Hessian... Done in 0.317 seconds.
```

```
plot(modes)
```



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

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



```
##Comparitive Strucutre 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   VGRRVHAPSGRVYHVKFNPVKVEGKDDVTGEELTRKDDQEETVRKRLVEYHQMTPALIG
##              121     .      .      .      .      .      .      180
##
##              181     .      .      .      214
## pdb|1AKE|A   YYSKEAEAGNTKYAKVDGTPVAEVRADLEKILG
##              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 my aa sequence.

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

```

## Searching ... please wait (updates every 5 seconds) RID = SHCW85KW013
## .
## Reporting 100 hits

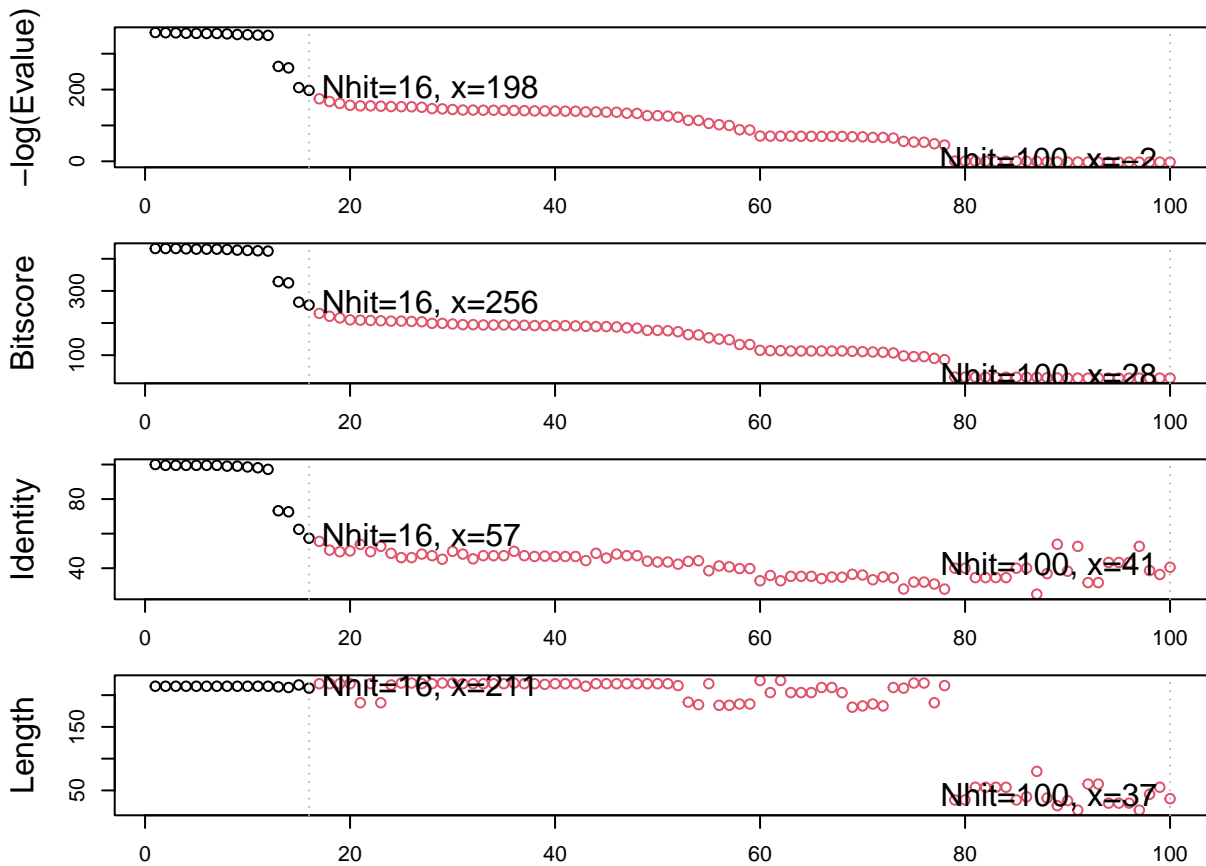
```

```
plot(blast)
```

```

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

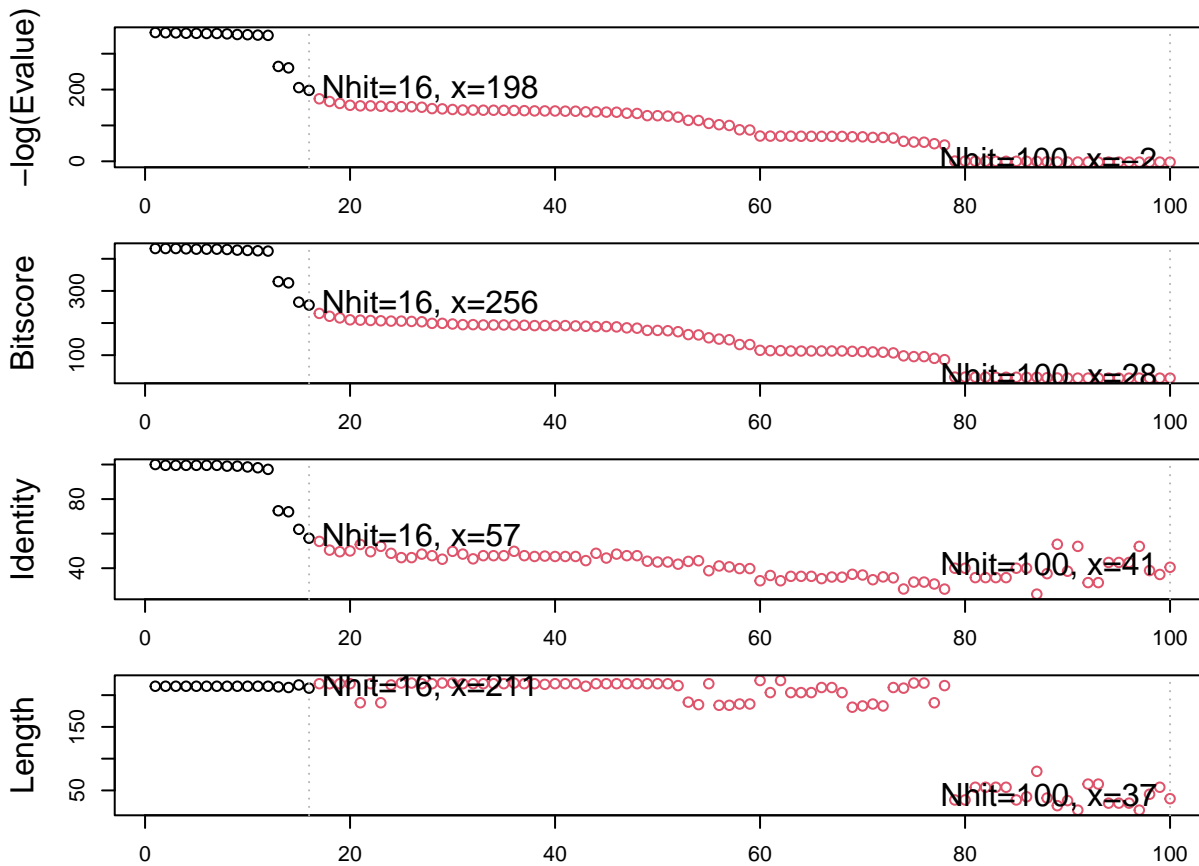
```



Code here??

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

```
#Download related PDB files
```

```
files <- get.pdb(hits$pdb.id, path="pdb", split=TRUE, gzip=TRUE)
```

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

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

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

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

```
## Warning in get.pdb(hits$pdb.id, path = "pdb", split = TRUE, gzip = TRUE): pdb/
## 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 these structures. We will use the function `pdbaln()`

```
pdbs <- pdbaln(files, fit = TRUE)
```

```
## 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
```

```

## pdb/split_chain/6HAP_A.pdb
## pdb/split_chain/6HAM_A.pdb
## pdb/split_chain/4K46_A.pdb
## pdb/split_chain/4NP6_A.pdb
## pdb/split_chain/3GMT_A.pdb
## pdb/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: pdb/split_chain/1AKE_A.pdb
##   PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 2   name: pdb/split_chain/4X8M_A.pdb
## pdb/seq: 3   name: pdb/split_chain/6S36_A.pdb
##   PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 4   name: pdb/split_chain/6RZE_A.pdb
##   PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 5   name: pdb/split_chain/4X8H_A.pdb
## pdb/seq: 6   name: pdb/split_chain/3HPR_A.pdb
##   PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 7   name: pdb/split_chain/1E4V_A.pdb
## pdb/seq: 8   name: pdb/split_chain/5EJE_A.pdb
##   PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 9   name: pdb/split_chain/1E4Y_A.pdb
## pdb/seq: 10  name: pdb/split_chain/3X2S_A.pdb
## pdb/seq: 11  name: pdb/split_chain/6HAP_A.pdb
## pdb/seq: 12  name: pdb/split_chain/6HAM_A.pdb
##   PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 13  name: pdb/split_chain/4K46_A.pdb
##   PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 14  name: pdb/split_chain/4NP6_A.pdb
## pdb/seq: 15  name: pdb/split_chain/3GMT_A.pdb
## pdb/seq: 16  name: pdb/split_chain/4PZL_A.pdb

```

Let's have a wee look see

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 TGDMLRAAVKSGSELGKQAKDIMDAGKLVDELVIALVKE
## [Truncated_Name:2] 4X8M_A.pdb TGDMLRAAVKSGSELGKQAKDIMDAGKLVDELVIALVKE
## [Truncated_Name:3] 6S36_A.pdb TGDMLRAAVKSGSELGKQAKDIMDAGKLVDELVIALVKE
## [Truncated_Name:4] 6RZE_A.pdb TGDMLRAAVKSGSELGKQAKDIMDAGKLVDELVIALVKE
## [Truncated_Name:5] 4X8H_A.pdb TGDMLRAAVKSGSELGKQAKDIMDAGKLVDELVIALVKE
## [Truncated_Name:6] 3HPR_A.pdb TGDMLRAAVKSGSELGKQAKDIMDAGKLVDELVIALVKE
## [Truncated_Name:7] 1E4V_A.pdb TGDMLRAAVKSGSELGKQAKDIMDAGKLVDELVIALVKE
## [Truncated_Name:8] 5EJE_A.pdb TGDMLRAAVKSGSELGKQAKDIMDACKLVDELVIALVKE
## [Truncated_Name:9] 1E4Y_A.pdb TGDMLRAAVKSGSELGKQAKDIMDAGKLVDELVIALVKE
## [Truncated_Name:10] 3X2S_A.pdb TGDMLRAAVKSGSELGKQAKDIMDCGKLVDELVIALVKE
## [Truncated_Name:11] 6HAP_A.pdb TGDMLRAAVKSGSELGKQAKDIMDAGKLVDELVIALVRE
## [Truncated_Name:12] 6HAM_A.pdb TGDMLRAAIKSGSELGKQAKDIMDAGKLVDEIIIALVKE
## [Truncated_Name:13] 4K46_A.pdb TGDMLRAAIKAGTELKGQAKSVIDAGQLVSDDIILGLVKE
## [Truncated_Name:14] 4NP6_A.pdb TGDMLRAAIKAGTELKGQAKAVIDAGQLVSDDIILGLIKE
## [Truncated_Name:15] 3GMT_A.pdb TGDMLRAAVKAGTPLGVEAKTYMDEGKLPDSLIIIGLVKE
## [Truncated_Name:16] 4PZL_A.pdb TGDMIRETIKSGSALGQELKKVLDAGELVSDEFI IKIVKD
##          *****  ~*  ~*  **  *  ~*  **  *  ~  ~~~~
##          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 RLKEADCANGYLFDFGFPRTIAQADAMKEAGVAIDYVLEID
## [Truncated_Name:16] 4PZL_A.pdb RISKNCNNGFLLDGVPRTIPQAQELDKLGVNIDYIVEVD
##          *~  *  ~*  **  *****  **  ~  *  ~***~*  *
##          81          .          .          .          120
##
##          121          .          .          .          160
## [Truncated_Name:1] 1AKE_A.pdb VPDELIVDRIVGRRVHAPSGRVYHVKFNPVKVEGKDDVTG

```

```

## [Truncated_Name:2] 4X8M_A.pdb      VPDELIVDRIVGRRVHAPSGRVYHVKNPPKVEGKDDVTG
## [Truncated_Name:3] 6S36_A.pdb      VPDELIVDKIVGRRVHAPSGRVYHVKNPPKVEGKDDVTG
## [Truncated_Name:4] 6RZE_A.pdb      VPDELIVDAIVGRRVHAPSGRVYHVKNPPKVEGKDDVTG
## [Truncated_Name:5] 4X8H_A.pdb      VPDELIVDRIVGRRVHAPSGRVYHVKNPPKVEGKDDVTG
## [Truncated_Name:6] 3HPR_A.pdb      VPDELIVDRIVGRRVHAPSGRVYHVKNPPKVEGKDDGTG
## [Truncated_Name:7] 1E4V_A.pdb      VPDELIVDRIVGRRVHAPSGRVYHVKNPPKVEGKDDVTG
## [Truncated_Name:8] 5EJE_A.pdb      VPDELIVDRIVGRRVHAPSGRVYHVKNPPKVEGKDDVTG
## [Truncated_Name:9] 1E4Y_A.pdb      VPDELIVDRIVGRRVHAPSGRVYHVKNPPKVEGKDDVTG
## [Truncated_Name:10] 3X2S_A.pdb      VPDELIVDRIVGRRVHAPSGRVYHVKNPPKVEGKDDVTG
## [Truncated_Name:11] 6HAP_A.pdb      VPDELIVDRIVGRRVHAPSGRVYHVKNPPKVEGKDDVTG
## [Truncated_Name:12] 6HAM_A.pdb      VPDELIVDRIVGRRVHAPSGRVYHVKNPPKVEGKDDVTG
## [Truncated_Name:13] 4K46_A.pdb      VADSVIVERMAGRRRAHLASGRTYHNVYNPPKVEGKDDVTG
## [Truncated_Name:14] 4NP6_A.pdb      VADDVIVERMAGRRRAHLPSGRTYHVYVYNPPKVEGKDDVTG
## [Truncated_Name:15] 3GMT_A.pdb      VPFSEIIERMSGRRTHPASGRTYHVKNPPKVEGKDDVTG
## [Truncated_Name:16] 4PZL_A.pdb      VADNLLIERITGRR.IHPASGRTYHTKFNPPKVADKDDVTG
##                                     *   ^^^ ^ *** * *** ** ^***** ** **
##                                     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      EPLVQRDDDDKEETVKKRLDVYEAQTKPLITYYGDWARRGA
## [Truncated_Name:16] 4PZL_A.pdb      EPLITRTDDNEDTVKQRLSVYHAQTAKLIDFYRNFSSNT
##                                     * * * ** *^ * ** ^ * ** ^*
##                                     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--QYLKFDGTKQVSEVSADIKALA-
## [Truncated_Name:15] 3GMT_A.pdb      E-----NGLKAPA-----YRKISG-

```

```
## [Truncated_Name:16]4PZL_A.pdb    KIPKYIKINGDQAVEKVSQDIFDQLNK
##                                     *
##                               201      .      .      227
##
## Call:
##   pdbaln(files = files, fit = TRUE)
##
## Class:
##   pdba, fasta
##
## Alignment dimensions:
##   16 sequence rows; 227 position columns (204 non-gap, 23 gap)
##
## + attr: xyz, resno, b, chain, id, ali, resid, sse, call
```

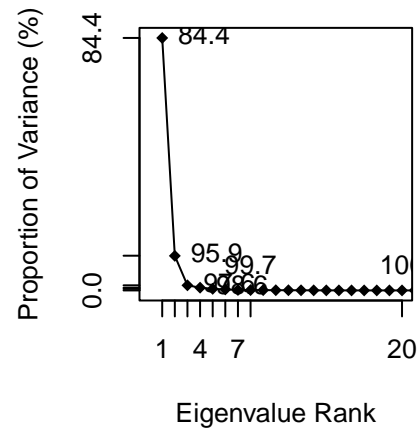
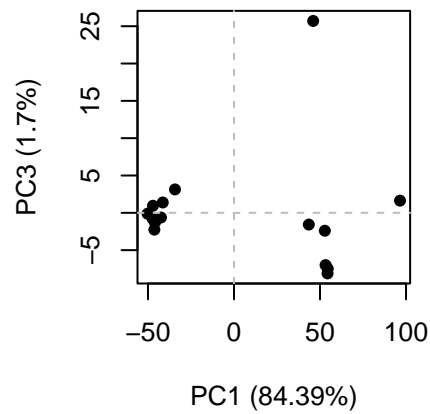
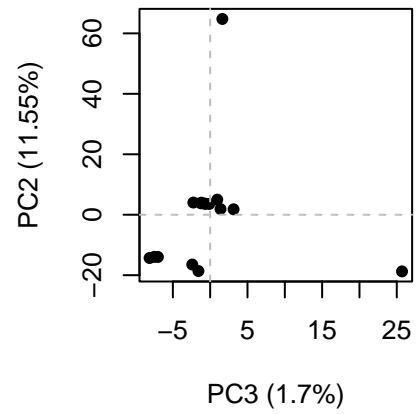
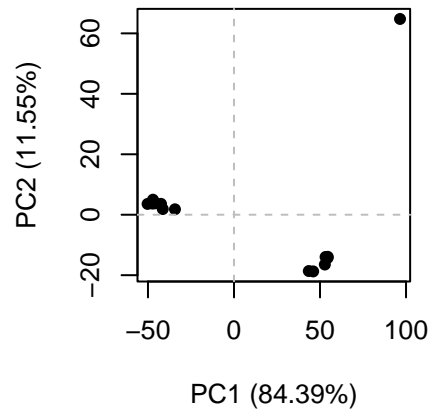
```
pdbs$xyz
```

```
##
##   Total Frames#: 16
##   Total XYZs#:   681, (Atoms#:  227)
##
##   [1] NA NA NA <...> 15.818 46.771 47.7 [10896]
##
## + attr: Matrix DIM = 16 x 681
```

Principle Component Analysis (PCA)

Here we will do PCA on the xyz coordinate data of all these structures with the `pca()` function in `biod3d`.

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



Let's visualize the displacements (i.e. movements of the structure) that are captured by PC1

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

Let's save our important results

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

Protein ELAV alphafold

