

Class 12: Structural Bioinformatics II

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Working with bio3d

```
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
## 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

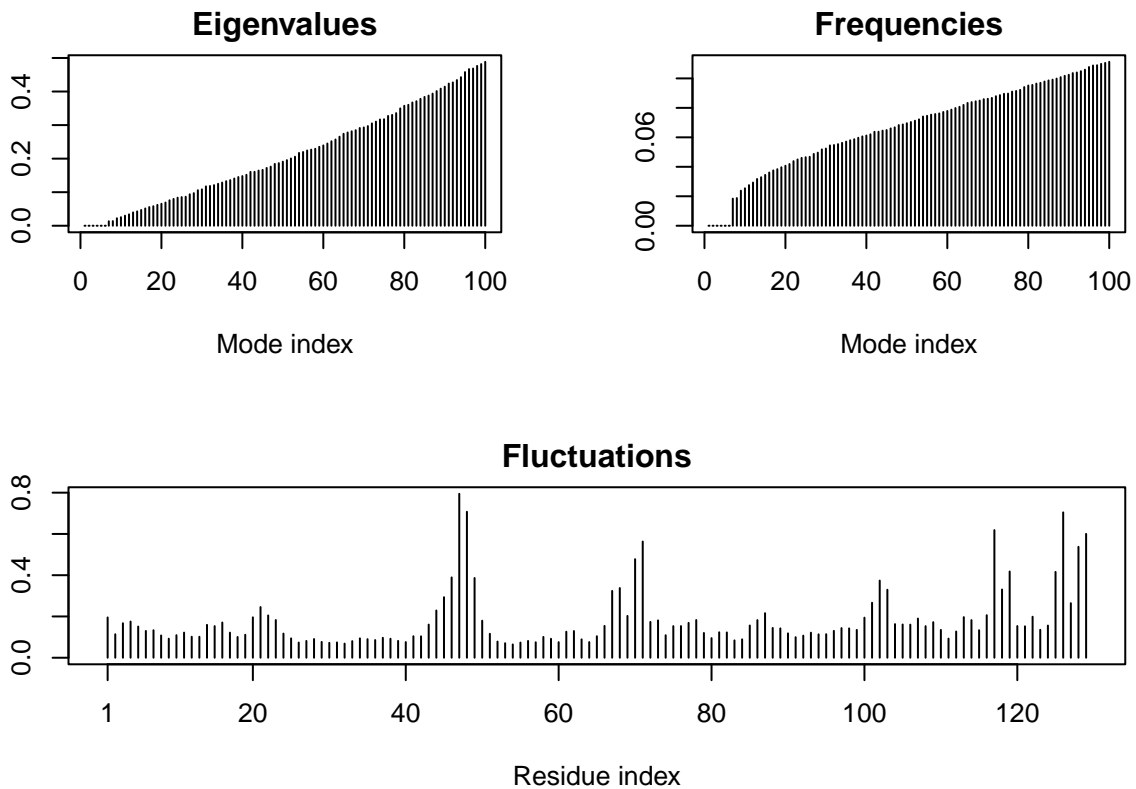
```
##      segid elesy charge
## 1  <NA>      N  <NA>
## 2  <NA>      C  <NA>
## 3  <NA>      C  <NA>
## 4  <NA>      O  <NA>
## 5  <NA>      C  <NA>
## 6  <NA>      C  <NA>
```

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

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

```
## Building Hessian...      Done in 0.023 seconds.
## Diagonalizing Hessian... Done in 0.121 seconds.
```

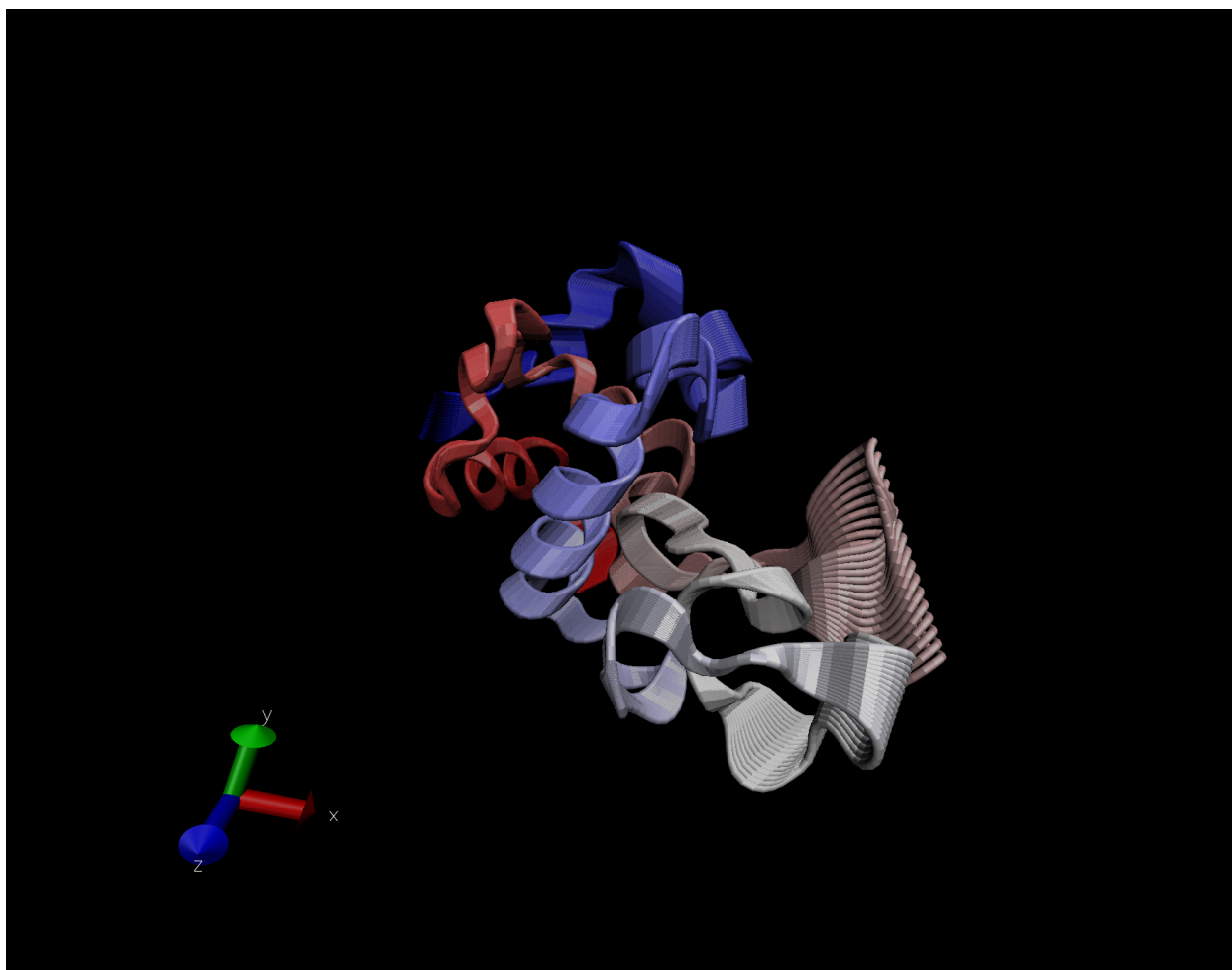
```
plot(modes)
```



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

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

And the image from VMD



4. Comparative Structure Analysis

Start by getting a sequence of interest

```
aa <- get.seq("lake_A")
```

```
## Warning in get.seq("lake_A"): Removing existing file: seqs.fasta
```

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

```
aa
```

```
##          1          .          .          .          .          .          60
## pdb|1AKE|A  MRIILLGAPGACKGTQAQFIMEKYGIPQISTGDMLRAAVKSGSELGKQAKDIMDAGKLV
##          1          .          .          .          .          .          60
##
##          61          .          .          .          .          .          120
## pdb|1AKE|A  DELVIALVKERIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVDRI
##          61          .          .          .          .          .          120
##
```

```
##          121          .          .          .          .          180
## pdb|1AKE|A  VGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTRKDDQEETVRKRLVEYHQMTAPLIG
##          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
```

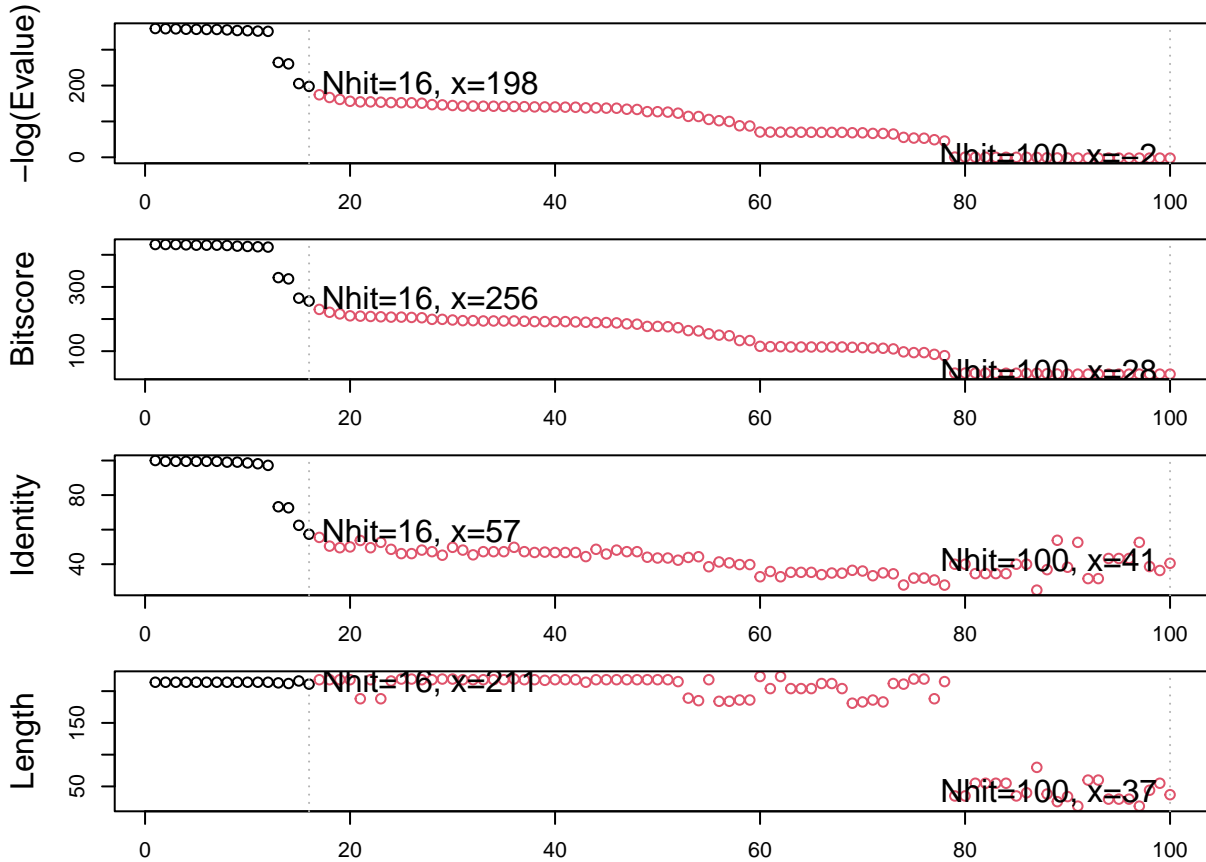
I want to search the PDB database (the main db for exp structures) for sequences like my aa sequence

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

```
## Searching ... please wait (updates every 5 seconds) RID = SBCXK41401R
## .
## Reporting 100 hits
```

```
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 (structures in the db more like mine).

```
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.

```
# Download related PDB files
# If we open this directly on VMD it'll show all the structures as they are, not overlapped or aligned
```

```
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 these structures... We'll use the function 'pdbaln()'

```
# Takes the files as input and then aligns related PDBs
pdbs <- pdbaln(files, fit = TRUE)#, exefile="msa")
```

```
## 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

```

Let's have a look:

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 TENLYFQSNAMEIILLGAPGAGKGTQAKIIQKYNIAHIS
## **~***** ***** * ~* **
## 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 TGDMLRAAVKSGSELGKQAKDIMDACKLVDELVIALVKE
## [Truncated_Name:9] 1E4Y_A.pdb TGDMLRAAVKSGSELGKQAKDIMDAGKLVTDELVIALVKE
## [Truncated_Name:10] 3X2S_A.pdb TGDMLRAAVKSGSELGKQAKDIMDCGKLVDELVIALVKE
## [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 TGDMLRAAVKAGTPLGVEAKTYMDEGKLPVDSLIIIGLVKE
## [Truncated_Name:16] 4PZL_A.pdb TGMIRETIKSGSALGQELKKVLDADELVSDEFIIKIVKD
## ****~* ~* *~** * ~* *** * ~~~~~~
## 41 . . . 80
##
## 81 . . . 120
## [Truncated_Name:1] 1AKE_A.pdb RIAQEDCRNGFLLDGFRTIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:2] 4X8M_A.pdb RIAQEDCRNGFLLDGFRTIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:3] 6S36_A.pdb RIAQEDCRNGFLLDGFRTIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:4] 6RZE_A.pdb RIAQEDCRNGFLLDGFRTIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:5] 4X8H_A.pdb RIAQEDCRNGFLLDGFRTIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:6] 3HPR_A.pdb RIAQEDCRNGFLLDGFRTIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:7] 1E4V_A.pdb RIAQEDCRNGFLLDGFRTIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:8] 5EJE_A.pdb RIAQEDCRNGFLLDGFRTIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:9] 1E4Y_A.pdb RIAQEDCRNGFLLDGFRTIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:10] 3X2S_A.pdb RIAQEDSRNGFLLDGFRTIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:11] 6HAP_A.pdb RICQEDSRNGFLLDGFRTIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:12] 6HAM_A.pdb RICQEDSRNGFLLDGFRTIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:13] 4K46_A.pdb RIAQDDCAKGFLLDGFRTIPQADGLKEVGVVVDYVIEFD
## [Truncated_Name:14] 4NP6_A.pdb RLAEADCEKGYFLDGFPRTIPQADGLKEMGINVDYVIEFD
## [Truncated_Name:15] 3GMT_A.pdb RLKEADCANGYLFDGFPRTIAQADAMEAGVAIDYVLEID
## [Truncated_Name:16] 4PZL_A.pdb RISKNDCNNGFLLDGVPTIPQAQELDKLGVNIDYIVEVD
## *~ * *~* ** ***** * ~* *~****~*
```



```

##                                     81          .          .          .          120
##
##                                     121          .          .          .          160
## [Truncated_Name:1] 1AKE_A.pdb      VPDELIVDRIVGRRVHAPSGRVYHVKNPPKVEGKDDVTG
## [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      VADSVIVERMAGRRAHLASGRTYHNVYNPPKVEGKDDVTG
## [Truncated_Name:14] 4NP6_A.pdb      VADDVIVERMAGRRAHLPSGRTYHVYNPPKVEGKDDVTG
## [Truncated_Name:15] 3GMT_A.pdb      VPFSEIIERMSGRRTHPASGRTYHVKNPPKVEGKDDVTG
## [Truncated_Name:16] 4PZL_A.pdb      VADNLLIERITGRRIHPSGRTYHTKFNPPKVADKDDVTG
##                                     *   ^^^ ^ *** * *** * ^***** *** **
##                                     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-

```



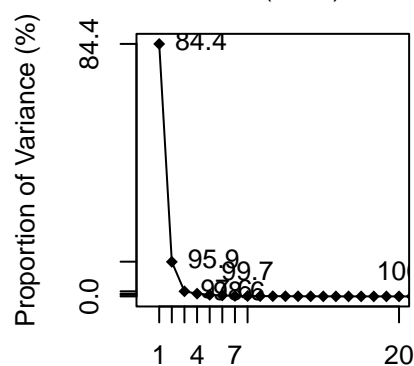
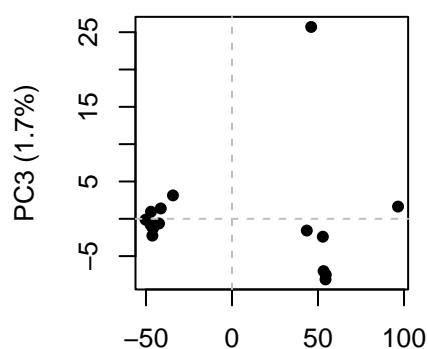
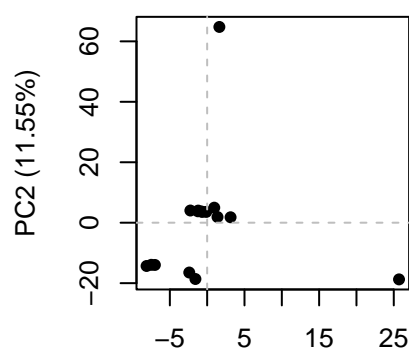
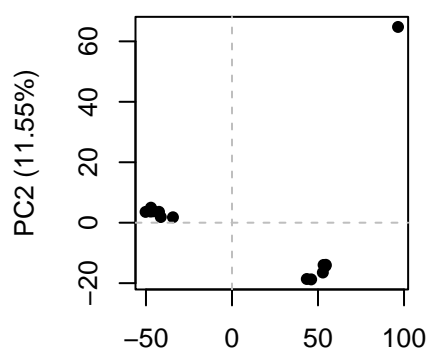
```
pdb$xyz
```

```
##
##   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
```

Principal Component Analysis

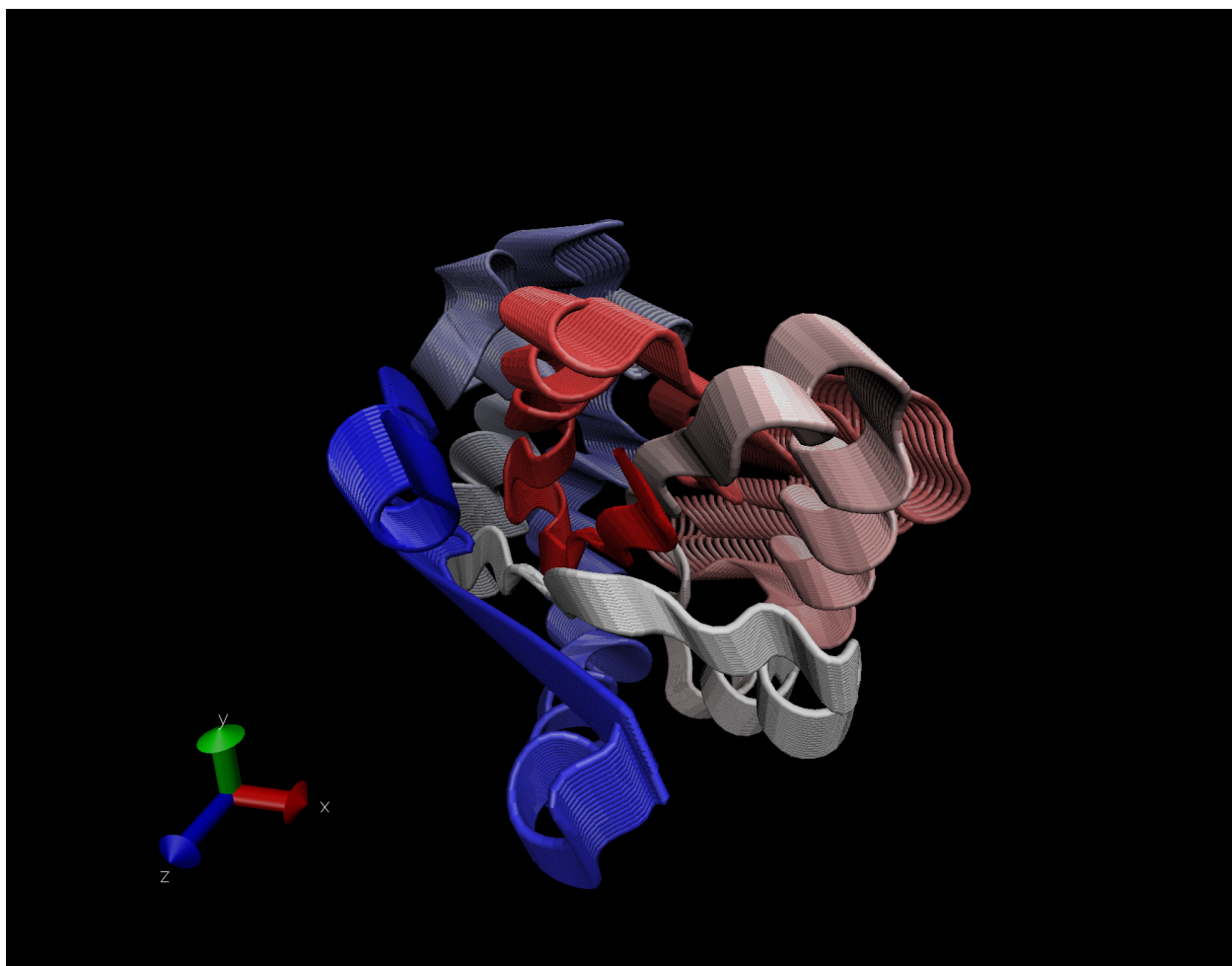
Here we will do PCA on the xyz coordinates data of all these structures with the 'pca()' function in bio3d

```
pc <- pca(pdb$xyz)
plot(pc)
```



Let's visualize the displacements/movements of the structure that are captured by PC1

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



My protein:

