

class12:structural bioinformatics

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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
## QAWIRGCR L
##
## + 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

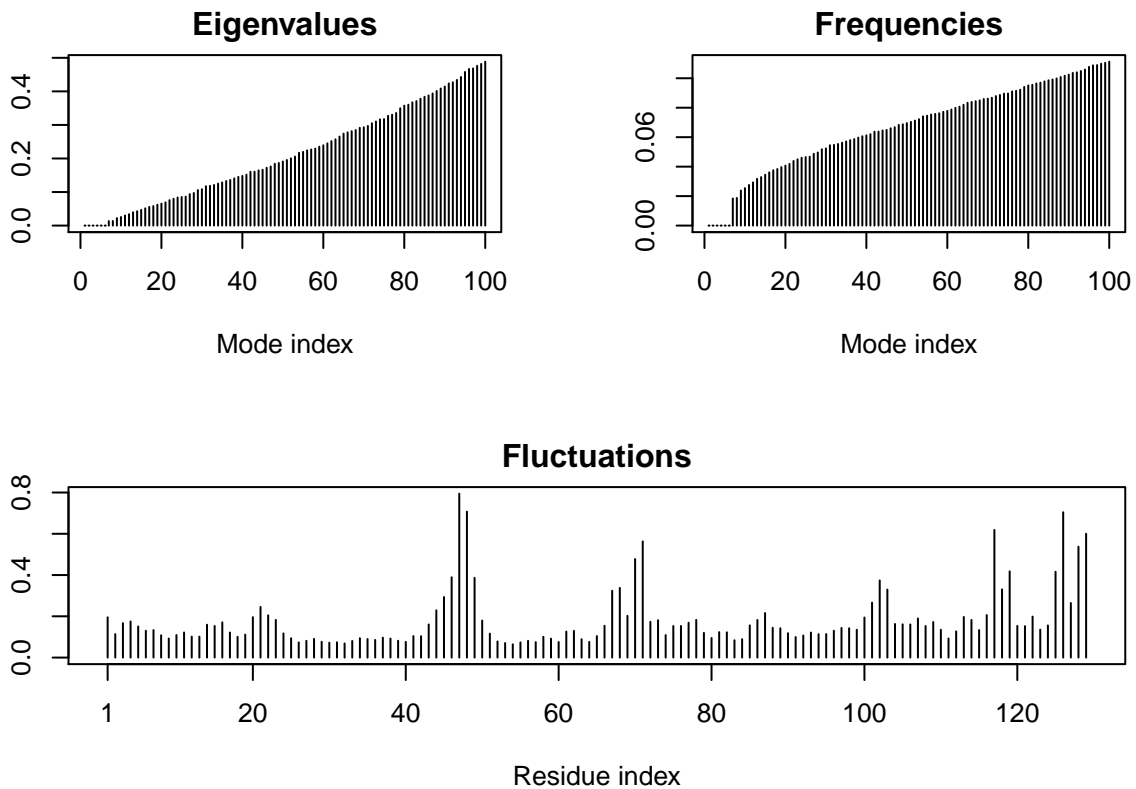
```
##      segid elesy charge
## 1  <NA>      N  <NA>
## 2  <NA>      C  <NA>
## 3  <NA>      C  <NA>
## 4  <NA>      O  <NA>
## 5  <NA>      C  <NA>
## 6  <NA>      C  <NA>
```

#a quick bioinformatics prediction of protein dynamics (flexibility). we use the `nma()` function, which does normal mode analysis

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

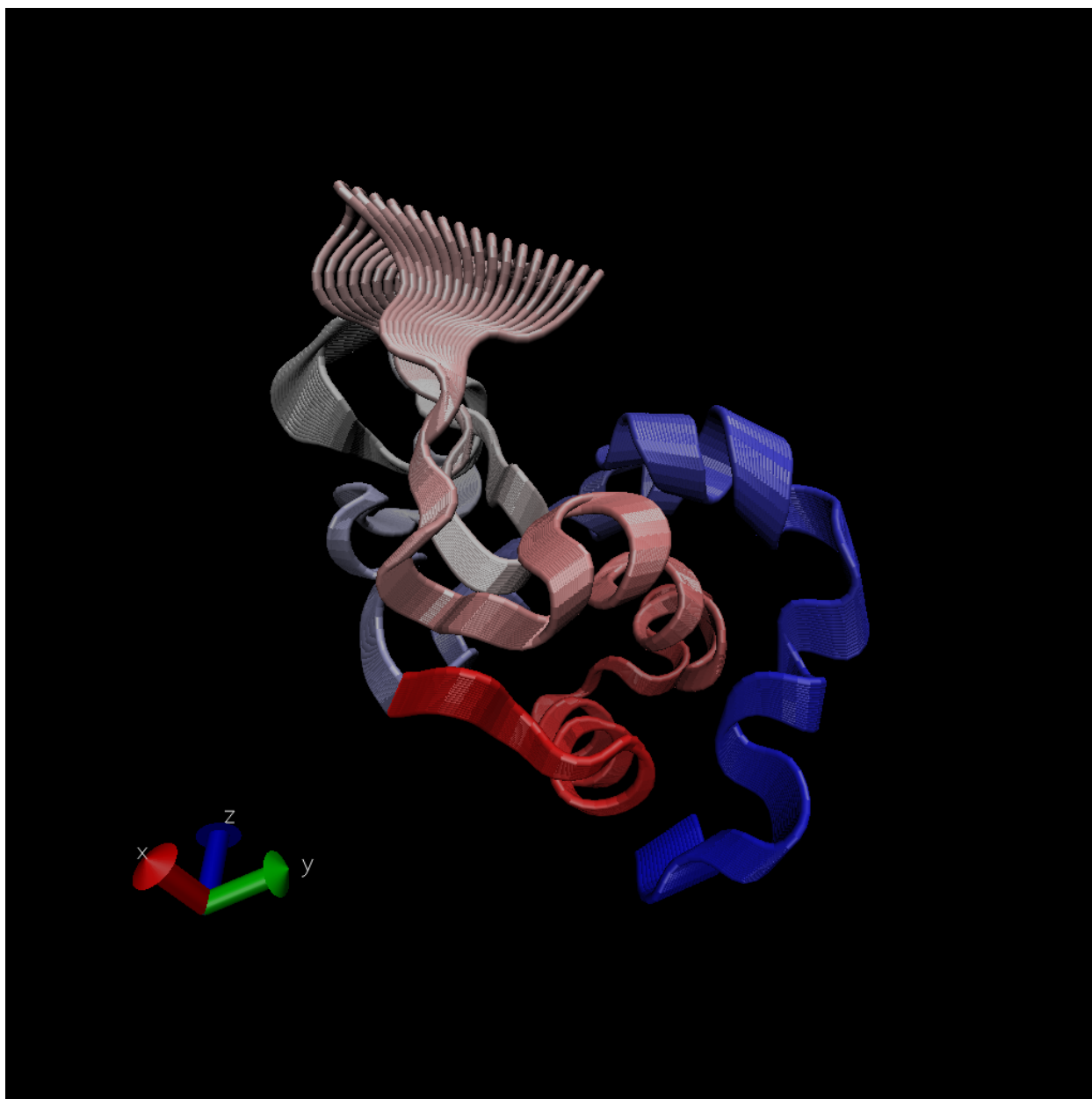
```
## Building Hessian...      Done in 0.021 seconds.
## Diagonalizing Hessian... Done in 0.062 seconds.
```

```
plot(modes)
```



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

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



```
#Comparative structural analysis
```

```
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  MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAAVKSGSELGKQAKDIMDAGKLV
##          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
##
```

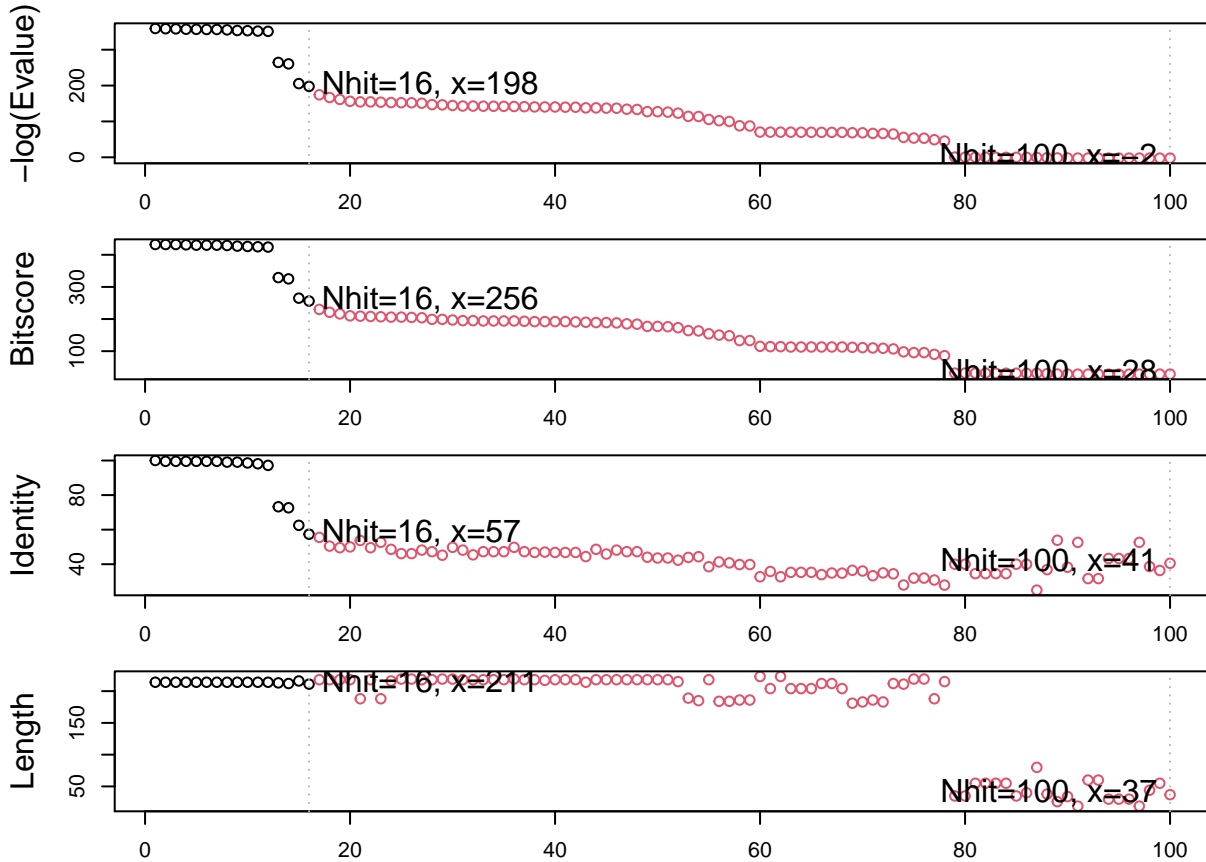
```
## Call:
##   read.fasta(file = outfile)
##
## Class:
##   fasta
##
## Alignment dimensions:
##   1 sequence rows; 214 position columns (214 non-gap, 0 gap)
##
## + attr: id, ali, call
```

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

```
## Searching ... please wait (updates every 5 seconds) RID = SBCPBNEP01R
## .
## Reporting 100 hits
```

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

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



```
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"
```

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

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

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

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

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

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

```
## Warning in get.pdb(hits$ pdb.id, path = "pdbc", split = TRUE, gzip = TRUE): pdbc/
## 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
```

```
## |
```

```
#align all the structures
```

```
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
## pdbs/split_chain/6HAP_A.pdb
## pdbs/split_chain/6HAM_A.pdb
## pdbs/split_chain/4K46_A.pdb
## pdbs/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

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 TGDMLRAAIKAGTELGKQAKSVIDAGQLVSDDIILGLVKE
## [Truncated_Name:14] 4NP6_A.pdb TGDMLRAAIKAGTELGKQAKAVIDAGQLVSDDIILGLIKE
## [Truncated_Name:15] 3GMT_A.pdb TGDMLRAAVKAGTPLGVEAKTYMDEGKLVPSLSIIGLVKE
## [Truncated_Name:16] 4PZL_A.pdb TGDMIRETIKSGSALGQELKKVLDAGELVSDEFI I KIVKD
##
##          ****~*  ^*  ^*  **  *  ^*  **  *  ^^  ~~~~
##          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 RLKEADCANGYLFDDGFPRTIAQADAMKEAGVAIDYVLEID
## [Truncated_Name:16] 4PZL_A.pdb RISKNCNNGFLLDGVPRTIPQAQELDKLGVNIDYIVEVD
##
##          *~  *  *~*  **  *****  **  ^  *~  ^~~~*  *
##          81          .          .          .          120
##
##          121         .          .          .          160
## [Truncated_Name:1] 1AKE_A.pdb VPDELIVDRIVGRRVHAPSGRVYHVKFNPVKVEGKDDVTG
## [Truncated_Name:2] 4X8M_A.pdb VPDELIVDRIVGRRVHAPSGRVYHVKFNPVKVEGKDDVTG
## [Truncated_Name:3] 6S36_A.pdb VPDELIVDKIVGRRVHAPSGRVYHVKFNPVKVEGKDDVTG
## [Truncated_Name:4] 6RZE_A.pdb VPDELIVDAIVGRRVHAPSGRVYHVKFNPVKVEGKDDVTG
## [Truncated_Name:5] 4X8H_A.pdb VPDELIVDRIVGRRVHAPSGRVYHVKFNPVKVEGKDDVTG

```



```

## [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 VADSVIVERMAGRAHLASGRTYHNVYNPPKVEGKDDVTG
## [Truncated_Name:14] 4NP6_A.pdb VADDVIVERMAGRAHLPSGRTYHVVYNPPKVEGKDDVTG
## [Truncated_Name:15] 3GMT_A.pdb VPFSEIIERMSGRRTHPASGRTYHVKNPPKVEGKDDVTG
## [Truncated_Name:16] 4PZL_A.pdb VADNLLIERITGRIHPASGRTYHTKFNPPKVADKDDVTG
## * ~~~ ^ *** * *** * ~***** ** **
## 121 . . . 160
##
## 161 . . 200
## [Truncated_Name:1] 1AKE_A.pdb EELTTRKDDQEETVRKRLVEYHQM TAPLIGYYSKEAEAGN
## [Truncated_Name:2] 4X8M_A.pdb EELTTRKDDQEETVRKRLVEWHQM TAPLIGYYSKEAEAGN
## [Truncated_Name:3] 6S36_A.pdb EELTTRKDDQEETVRKRLVEYHQM TAPLIGYYSKEAEAGN
## [Truncated_Name:4] 6RZE_A.pdb EELTTRKDDQEETVRKRLVEYHQM TAPLIGYYSKEAEAGN
## [Truncated_Name:5] 4X8H_A.pdb EELTTRKDDQEETVRKRLVEYHQM TAA LIGYYSKEAEAGN
## [Truncated_Name:6] 3HPR_A.pdb EELTTRKDDQEETVRKRLVEYHQM TAPLIGYYSKEAEAGN
## [Truncated_Name:7] 1E4V_A.pdb EELTTRKDDQEETVRKRLVEYHQM TAPLIGYYSKEAEAGN
## [Truncated_Name:8] 5EJE_A.pdb EELTTRKDDQEECVRKRLVEYHQM TAPLIGYYSKEAEAGN
## [Truncated_Name:9] 1E4Y_A.pdb EELTTRKDDQEETVRKRLVEYHQM TAPLIGYYSKEAEAGN
## [Truncated_Name:10] 3X2S_A.pdb EELTTRKDDQEETVRKRLCEYHQM TAPLIGYYSKEAEAGN
## [Truncated_Name:11] 6HAP_A.pdb EELTTRKDDQEETVRKRLVEYHQM TAPLIGYYSKEAEAGN
## [Truncated_Name:12] 6HAM_A.pdb EELTTRKDDQEETVRKRLVEYHQM TAPLIGYYSKEAEAGN
## [Truncated_Name:13] 4K46_A.pdb EDLVIREDDKEETVLARLGVYHNQTAPLIAYYGKEAEAGN
## [Truncated_Name:14] 4NP6_A.pdb EDLVIREDDKEETVRARLNVYHTQTAPLIEYYGKEAAAGK
## [Truncated_Name:15] 3GMT_A.pdb EPLVQRDDDKKEETVKKRLDVYEAQTKPLITYYGDWARRGA
## [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
##

```

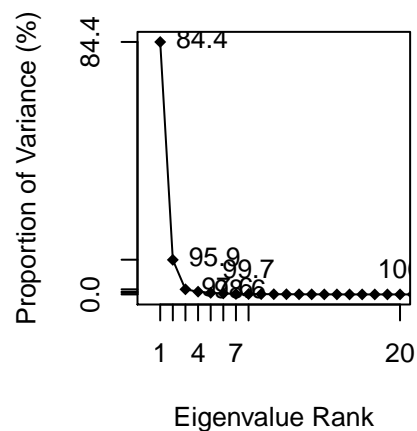
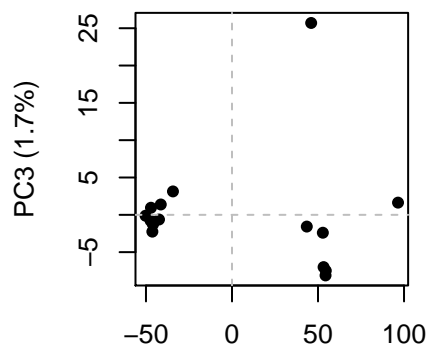
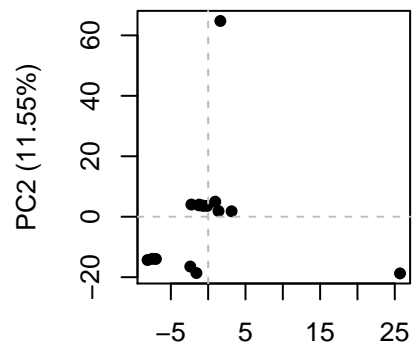
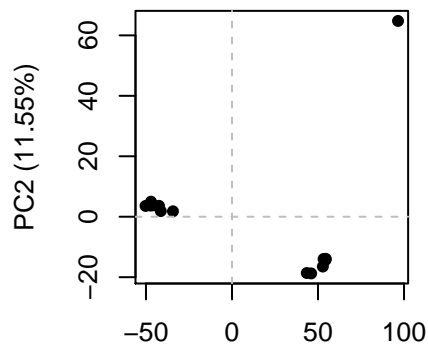
```
## Call:
##   pdbaln(files = files, fit = TRUE)
##
## Class:
##   pdba, fasta
##
## Alignment dimensions:
##   16 sequence rows; 227 position columns (204 non-gap, 23 gap)
##
## + attr: xyz, resno, b, chain, id, ali, resid, sse, call
```

```
pdba$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
```

```
#PCA analysis
```

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



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