

Class12: Structural Bioinformatics pt. 2

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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
```

Q7: How many amino acid residues are there in this pdb object?

129 amino acids

Q8: Name one of the two non-protein residues?

A non-protein residue example is water

How many protein chains are in this structure?

There is 1 chain

```
head(pdb$atom)
```

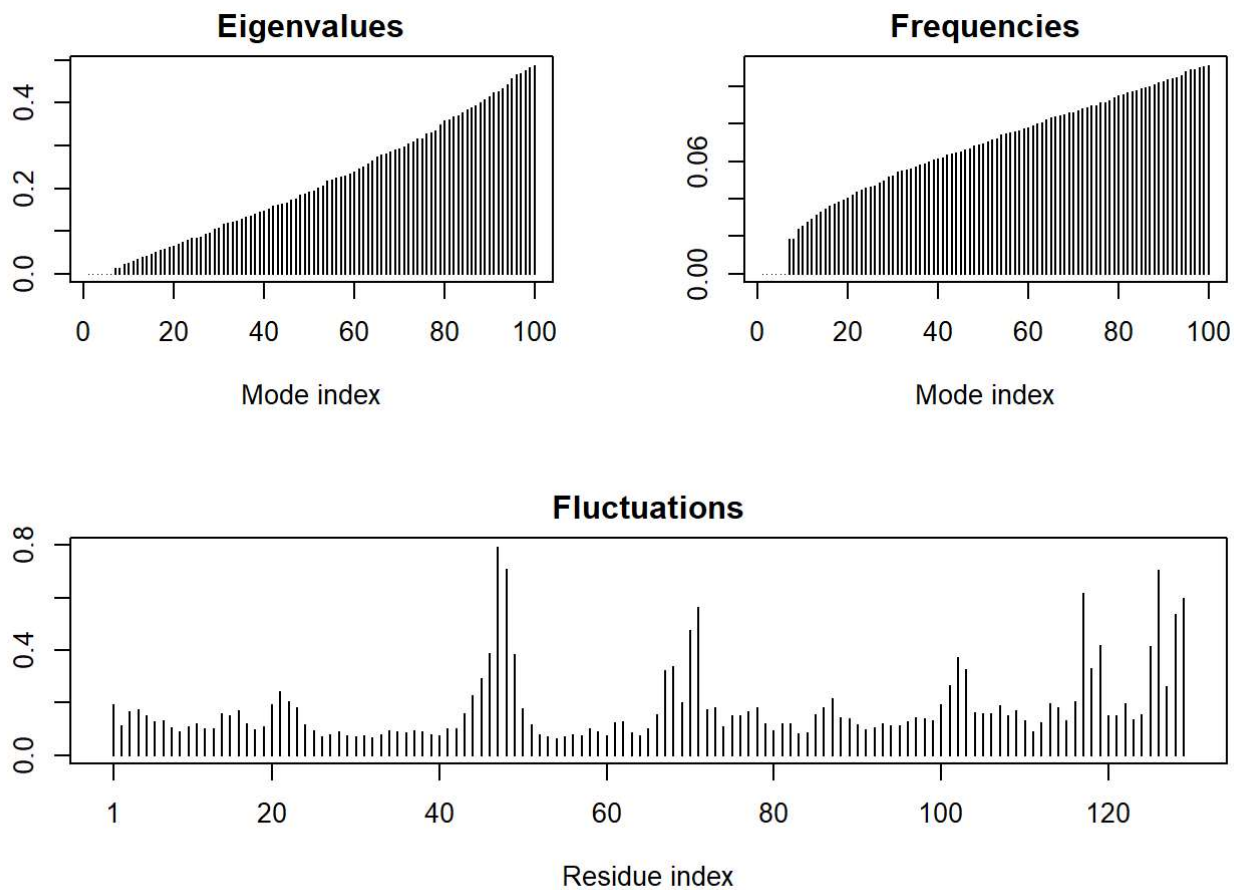
```
##   type eleno elety  alt resid chain resno insert      x      y      z o      b
## 1 ATOM     1     N <NA>  LYS   A     1   <NA>  3.294 10.164 10.266 1 11.18
## 2 ATOM     2     CA <NA>  LYS   A     1   <NA>  2.388 10.533  9.168 1  9.68
## 3 ATOM     3     C <NA>  LYS   A     1   <NA>  2.438 12.049  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)
```

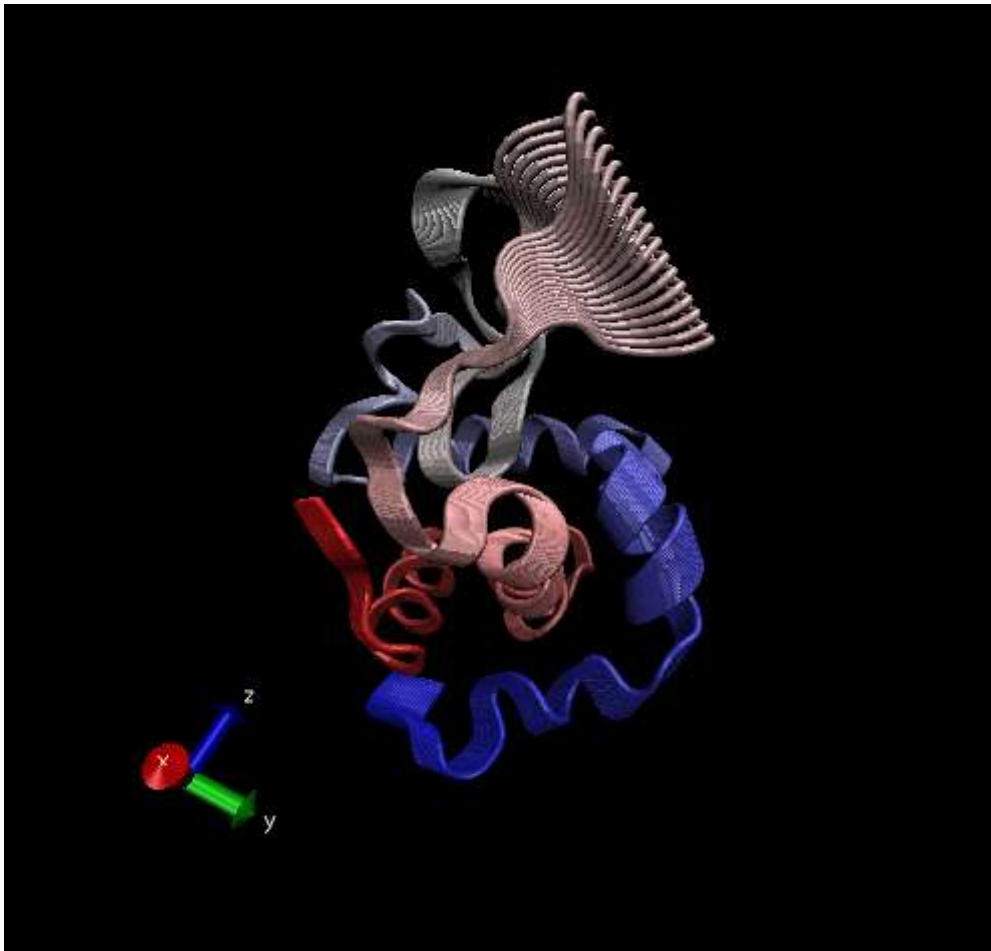
```
## Building Hessian...      Done in 0.03 seconds.
## Diagonalizing Hessian... Done in 0.15 seconds.
```

```
plot(modes)
```



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

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



Workflow: Sequence -> PDB -> Structures -> MSA -> PCA

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.
```

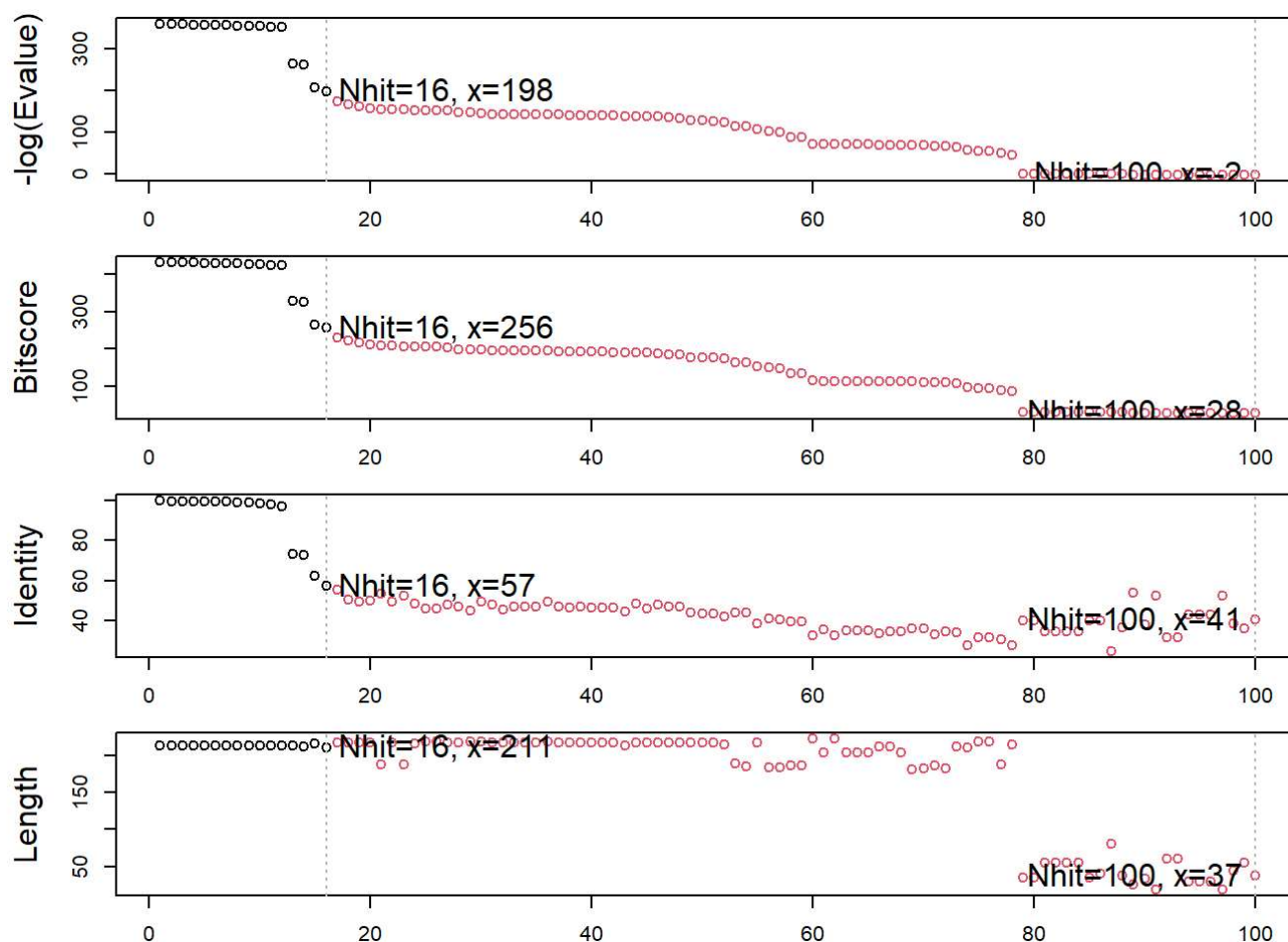
To search the **PDB database** (main database for exp structures) for sequences like aa. Looking for intersection of all values (E, coverage, query ...)

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

```
## Searching ... please wait (updates every 5 seconds) RID = SDNG6Z1D016  
## ...  
## Reporting 100 hits
```

```
tophits <- plot(blast)
```

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



We will use the 16 top hits (chosen by the plot function) from the search of PDB

```
tophits$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"
```

Now to download all these similar structures in the PDB and store them on our computer

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

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

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

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

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

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

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

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

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

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

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

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

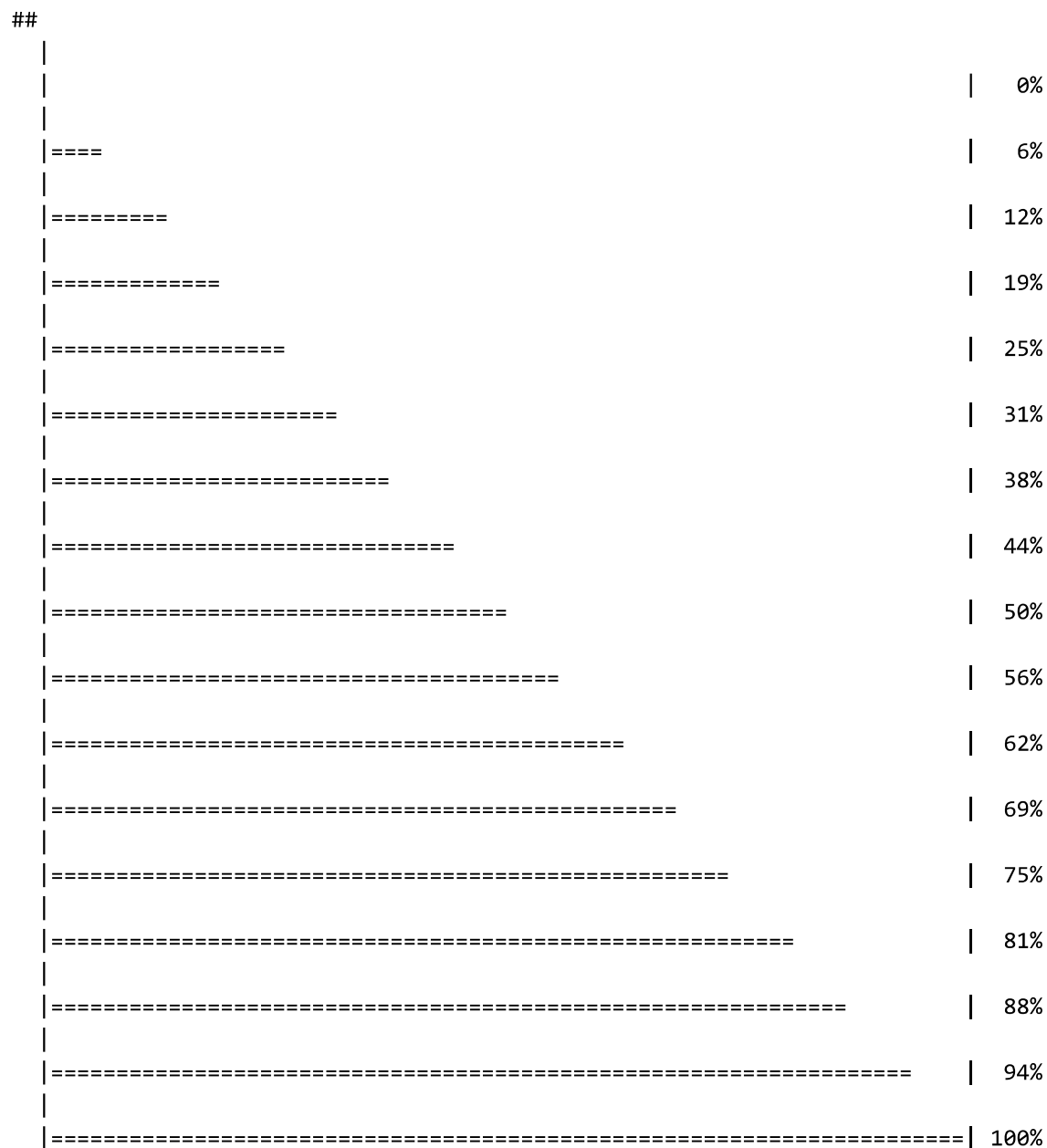
```
## Warning in get.pdb(tophits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE):  
## pdbs/6HAM.pdb exists. Skipping download
```

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

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

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

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



Want to align/superimpose all the structures now. Use the function **pdbaln()**

```
pdbbs <- 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
## 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 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 TGDMLRAAVKAGTPLGVEAKTYMDEGKLPDLSLIIGLVKE
## [Truncated_Name:16]4PZL_A.pdb TGDMIRETIKSGSALGQELKKVLDA GELVSDEFI IKIVKD
## ***** ^* *^ ** * ^* ** * ^^ ^^ ^^
## 41 . . 80
##
## 81 . . 120
## [Truncated_Name:1]1AKE_A.pdb RIAQEDCRNGFLLDGFPR TIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:2]4X8M_A.pdb RIAQEDCRNGFLLDGFPR TIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:3]6S36_A.pdb RIAQEDCRNGFLLDGFPR TIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:4]6RZE_A.pdb RIAQEDCRNGFLLDGFPR TIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:5]4X8H_A.pdb RIAQEDCRNGFLLDGFPR TIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:6]3HPR_A.pdb RIAQEDCRNGFLLDGFPR TIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:7]1E4V_A.pdb RIAQEDCRNGFLLDGFPR TIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:8]5EJE_A.pdb RIAQEDCRNGFLLDGFPR TIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:9]1E4Y_A.pdb RIAQEDCRNGFLLDGFPR TIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:10]3X2S_A.pdb RIAQEDSRNGFLLDGFPR TIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:11]6HAP_A.pdb RICQEDSRNGFLLDGFPR TIPQADAMKEAGINVDYVLEFD
## [Truncated_Name:12]6HAM_A.pdb RICQEDSRNGFLLDGFPR TIPQADAMKEAGINVDYVLEFD

```

```

## [Truncated_Name:13]4K46_A.pdb  RIAQDDCAKGFLLDGFPRTIPQADGLKEVGWVVDYVIEFD
## [Truncated_Name:14]4NP6_A.pdb  RIAQADCEKGFLLDGFRTIPQADGLKEMGINVDYVIEFD
## [Truncated_Name:15]3GMT_A.pdb  RLKEADCANGYLFDFGFPRTIAQADAMKEAGVAIDYVLEID
## [Truncated_Name:16]4PZL_A.pdb  RISKNCDCNNGFLLDGVPRITPQAQELDKLGVNIDYIVEVD
##                                *^  *  ^*^ **  ****  **  ^  *^  ^**^*^ *
##                                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    VADSVIVERMAGRRRAHLASGRTYHNVNPPKVEGKDDVTG
## [Truncated_Name:14]4NP6_A.pdb    VADSVIVERMAGRRRAHLPASGRTYHVYNPPKVEGKDDVTG
## [Truncated_Name:15]3GMT_A.pdb    VPFSEIIERMSGRRTHPASGRTYHVKNPPKVEGKDDVTG
## [Truncated_Name:16]4PZL_A.pdb    VADNLLIERITGRRIHAPASGRTYHTKNPPKVADKDDVTG
##                                *  ^^^ ^  *** *  *** **  ^*****  *** **
##                                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 TAPLIGYYSKEAEAGN
## [Truncated_Name:6]3HPR_A.pdb    EELTTRKDDQEETVRKRLVEYHQM TAPLIGYYSKEAEAGN
## [Truncated_Name:7]1E4V_A.pdb    EELTTRKDDQEETVRKRLVEYHQM TAPLIGYYSKEAEAGN
## [Truncated_Name:8]5EJE_A.pdb    EELTTRKDDQEECVKRLVEYHQM 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    EDLVIREDDKEETVRLARLGVYHNQTAPLIAYYGKEAEAGN
## [Truncated_Name:14]4NP6_A.pdb    EDLVIREDDKEETVRARLNVTYHTQTAPLIEYYGKEAAAGK
## [Truncated_Name:15]3GMT_A.pdb    EPLVQRDDKEETVKKRLDVYEAQTKPLITYYGDWARRGA
## [Truncated_Name:16]4PZL_A.pdb    EPLITRTDDNEDTVKQRLSVYHAQTAKLIDFYRNFSSTNT
##                                *  *  *  **  ^*  *  **  ^  *  **  ^*
##                                161      .      .      .      200
##
##                                201      .      .      227
## [Truncated_Name:1]1AKE_A.pdb    T--KYAKVDGTPVAEVRADLEKILG-
## [Truncated_Name:2]4X8M_A.pdb    T--KYAKVDGTPVAEVRADLEKILG-
## [Truncated_Name:3]6S36_A.pdb    T--KYAKVDGTPVAEVRADLEKILG-
## [Truncated_Name:4]6RZE_A.pdb    T--KYAKVDGTPVAEVRADLEKILG-
## [Truncated_Name:5]4X8H_A.pdb    T--KYAKVDGTPVAEVRADLEKILG-
## [Truncated_Name:6]3HPR_A.pdb    T--KYAKVDGTPVAEVRADLEKILG-

```

```

## [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

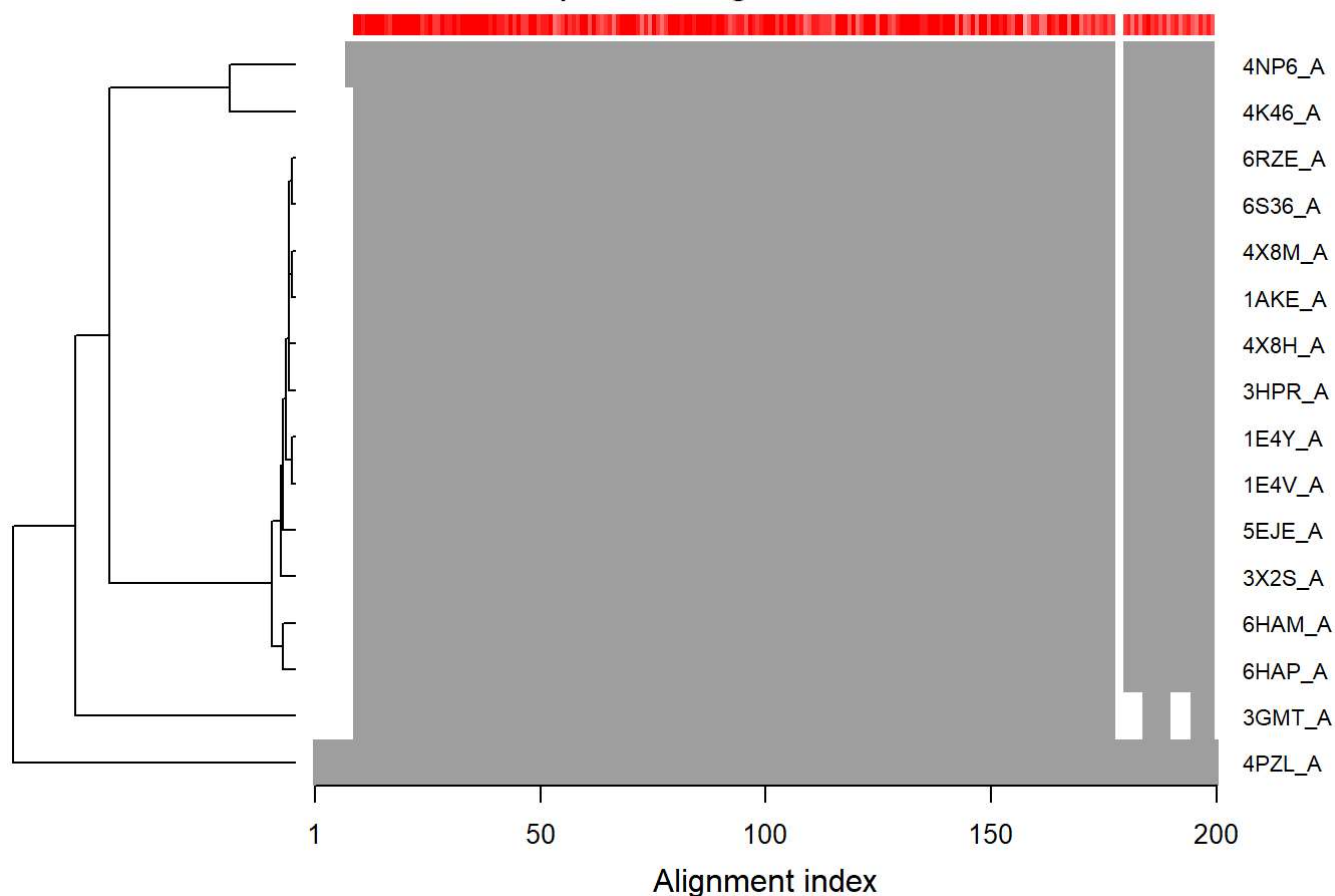
```

```

ids <- basename.pdb(pdba$id)
plot(pdba, labels=ids)

```

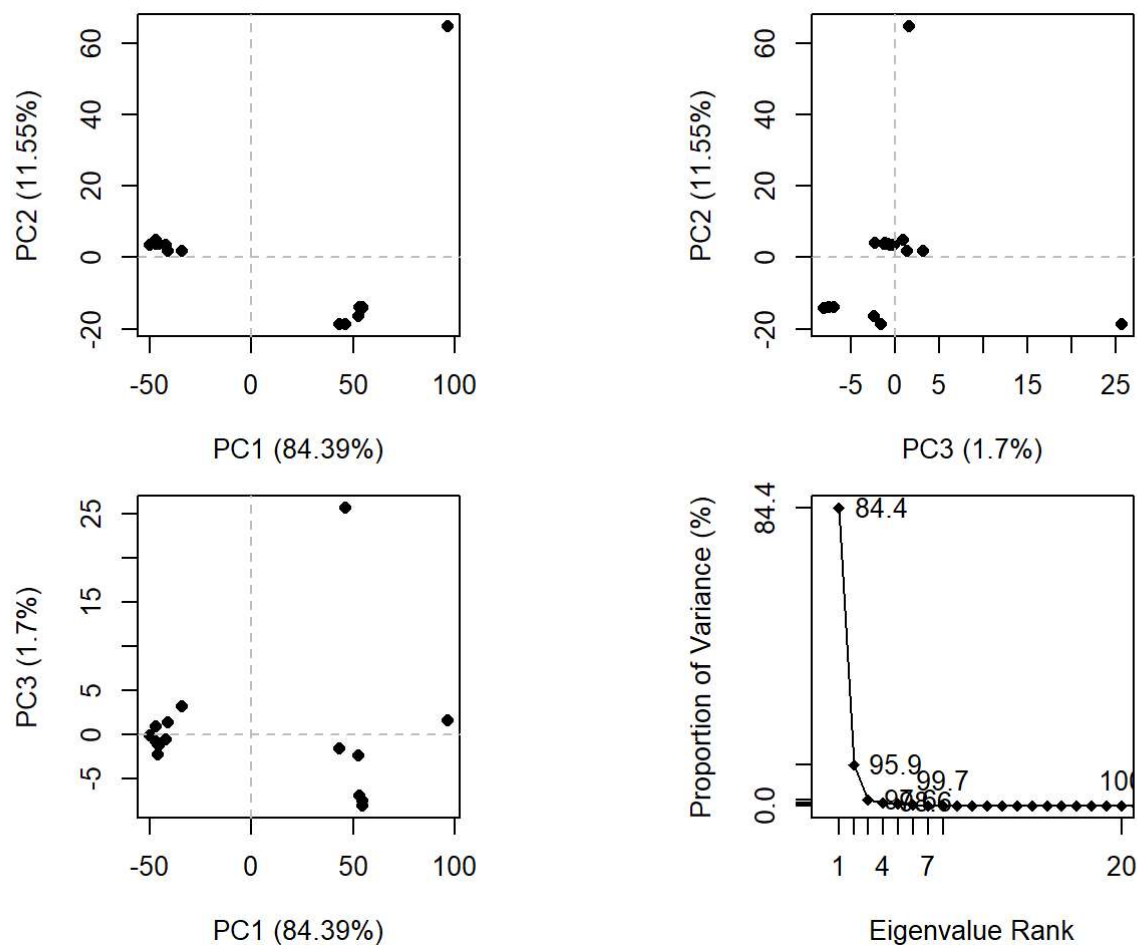
Sequence Alignment Overview



Principal Component Analysis

Time to do PCA on the xyz coordinate data of all these structures with the **pca()** function in bio3d.

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



Let's visualize the displacements/movements of the structure that are captured by PC1 (because it captures the most variance)

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

Open in VMD to see the movie

Now, let's save our important results

```
#save(blast, files, pids, tophits, pc, file = "myPDBresults.RData")
```

Next time, use

```
#Load("myPDBresults.RData")
```