Class 10: Structural Bioinformatics 1

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PDB statistics

The Protein Data Bank (PDB) is a main repository of biomolecular structures. Let's see what it contains:

```
stats <- read.csv("~/Downloads/Data Export Summary.csv")
head(stats)
```

```
           Molecular.Type   X.ray     EM    NMR Integrative Multiple.methods
1          Protein (only) 178,795 21,825 12,773         343              226
2 Protein/Oligosaccharide  10,363  3,564     34           8               11
3              Protein/NA   9,106  6,335    287          24                7
4     Nucleic acid (only)   3,132    221  1,566           3               15
5                   Other     175     25     33           4                0
6  Oligosaccharide (only)      11      0      6           0                1
  Neutron Other   Total
1      84    32 214,078
2       1     0  13,981
3       0     0  15,759
4       3     1   4,941
5       0     0     237
6       0     4      22
```

```
stats$X.ray
```

```
[1] "178,795" "10,363"  "9,106"   "3,132"   "175"     "11"
```

```
sum(stats$Neutron)
```

```
[1] 88
```

The comma in these numbers leads to the numbers here being read as characters.

```r
c(100,10, "barry")
```

```
[1] "100"   "10"    "barry"
```

```r
library(readr)
stats <- read_csv("~/Downloads/Data Export Summary.csv")
```

```
Rows: 6 Columns: 9
-- Column specification --------------------------------------------------------
Delimiter: ","
chr (1): Molecular Type
dbl (4): Integrative, Multiple methods, Neutron, Other
num (4): X-ray, EM, NMR, Total

i Use `spec()` to retrieve the full column specification for this data.
i Specify the column types or set `show_col_types = FALSE` to quiet this message.
```

```r
head(stats)
```

```
# A tibble: 6 x 9
  `Molecular Type`     `X-ray`    EM   NMR Integrative `Multiple methods` Neutron
  <chr>                  <dbl> <dbl> <dbl>       <dbl>              <dbl>   <dbl>
1 Protein (only)        178795 21825 12773         343                226      84
2 Protein/Oligosacch~    10363  3564    34           8                 11       1
3 Protein/NA              9106  6335   287          24                  7       0
4 Nucleic acid (only)     3132   221  1566           3                 15       3
5 Other                    175    25    33           4                  0       0
6 Oligosaccharide (o~       11     0     6           0                  1       0
# i 2 more variables: Other <dbl>, Total <dbl>
```

> Q1: What percentage of structures in the PDB are solved by X-Ray and Electron Microscopy.

```r
n.xray <- sum(stats$`X-ray`)
#n.em <-
n.total <- sum(stats$Total)

n.xray/n.total
```

```
[1] 0.8095077
```

```
n.em <- sum(stats$EM)
(n.xray/n.total)+(n.em/n.total)
```

```
[1] 0.937892
```

93.7892% percent of structures are solved by x-ray and EM.

> Q2: What proportion of structures in the PDB are protein?

```
n.protein <- c(214078)
n.protein/n.total
```

```
[1] 0.8596889
```

85.96889%

> Q3: SKIP…

> Q4: Water molecules normally have 3 atoms. Why do we see just one atom per water molecule in this structure?

One molecule is show to make it easier to see and it shows the interactions between water and the protein.

> Q5: There is a critical "conserved" water molecule in the binding site. Can you identify this water molecule? What residue number does this water molecule have

residue number is 301

Visualizing the HIV-1 protease structure

> Q6: Generate and save a figure clearly showing the two distinct chains of HIV-protease along with the ligand. You might also consider showing the catalytic residues ASP 25 in each chain and the critical water (we recommend "Ball & Stick" for these side-chains). Add this figure to your Quarto document.

We can use the Molecular viewer online: https://molstar.org/viewer/

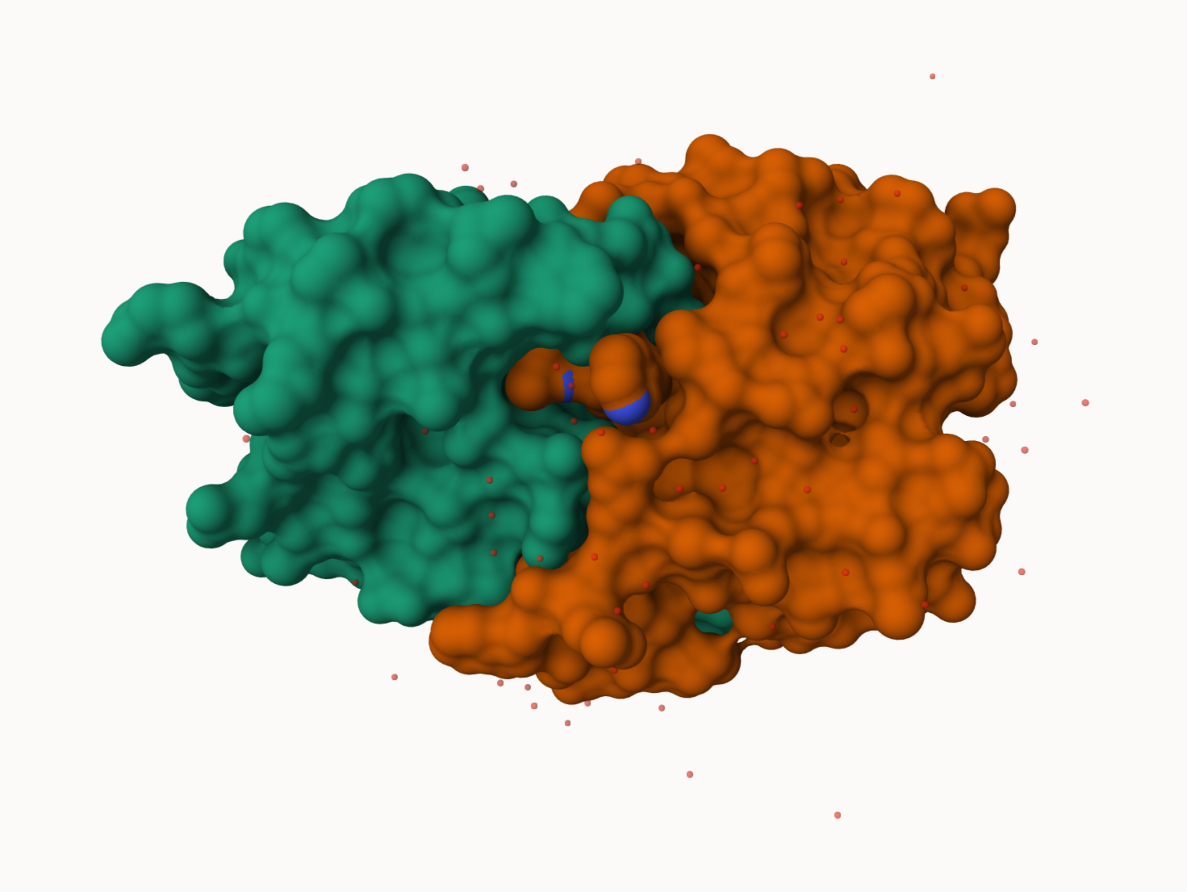
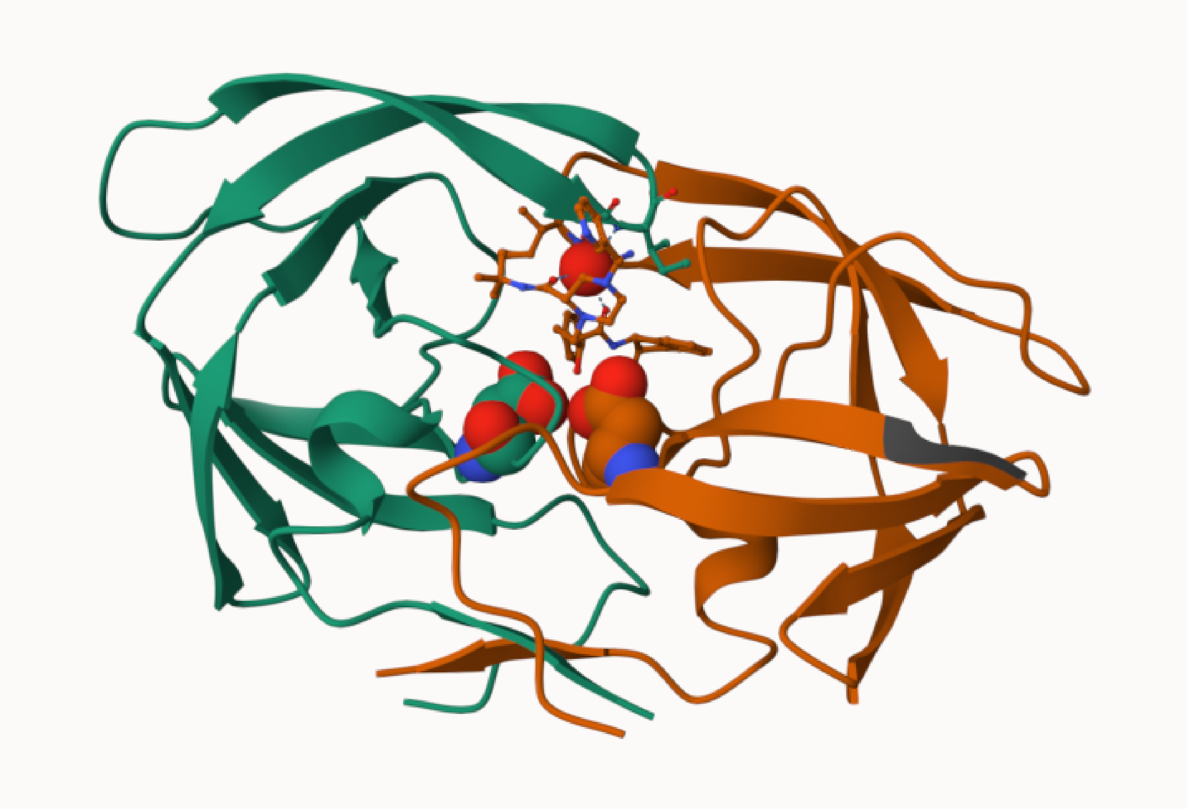


Figure 1: My First image of HIV-Pr with surface display shoing ligand binding

A new clean image showing the catalytic ASP25 amino acids in both chains of the HIV-PR dimer along with the inhibitor and the all important active site water.



Bio3D package for structual bioinformatics

```
library(bio3d)

pdb <- read.pdb("1hsg")
```

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

```
pdb
```

```


 Call:  read.pdb(file = "1hsg")

   Total Models#: 1
     Total Atoms#: 1686,  XYZs#: 5058  Chains#: 2  (values: A B)
     Protein Atoms#: 1514  (residues/Calpha atoms#: 198)
     Nucleic acid Atoms#: 0  (residues/phosphate atoms#: 0)

     Non-protein/nucleic Atoms#: 172  (residues: 128)
     Non-protein/nucleic resid values: [ HOH (127), MK1 (1) ]

   Protein sequence:
      PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGIGGFIKVRQYD
      QILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFPQITLWQRPLVTIKIGGQLKE
      ALLDTGADDTVLEEMSLPGRWKPKMIGGIGGFIKVRQYDQILIEICGHKAIGTVLVGPTP
      VNIIGRNLLTQIGCTLNF

+ attr: atom, xyz, seqres, helix, sheet,
        calpha, remark, call
```

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

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

MK1 > Q9: How many protein chains are in this structure?

2

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

```
  type eleno elety  alt resid chain resno insert      x      y     z o     b
1 ATOM     1     N <NA>   PRO     A     1   <NA> 29.361 39.686 5.862 1 38.10
2 ATOM     2    CA <NA>   PRO     A     1   <NA> 30.307 38.663 5.319 1 40.62
3 ATOM     3     C <NA>   PRO     A     1   <NA> 29.760 38.071 4.022 1 42.64
4 ATOM     4     O <NA>   PRO     A     1   <NA> 28.600 38.302 3.676 1 43.40
5 ATOM     5    CB <NA>   PRO     A     1   <NA> 30.508 37.541 6.342 1 37.87
6 ATOM     6    CG <NA>   PRO     A     1   <NA> 29.296 37.591 7.162 1 38.40
  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>
```

Predicting fuctional motions of a single structure

Read an ADK structure from the PDB database

```r
adk <- read.pdb("6s36")
```

```
  Note: Accessing on-line PDB file
   PDB has ALT records, taking A only, rm.alt=TRUE
```

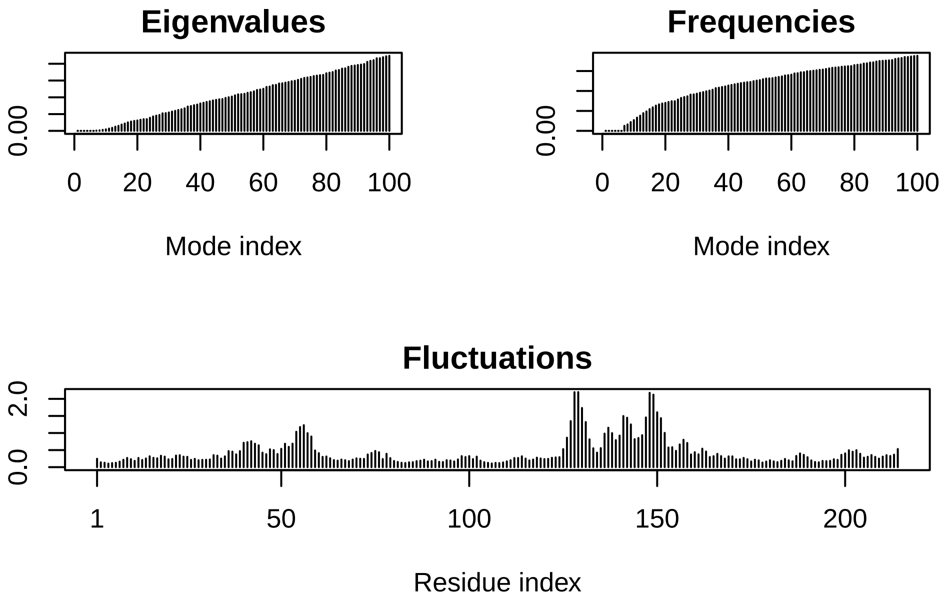
```r
adk
```

```

 Call:  read.pdb(file = "6s36")

   Total Models#: 1
     Total Atoms#: 1898,  XYZs#: 5694  Chains#: 1  (values: A)

     Protein Atoms#: 1654  (residues/Calpha atoms#: 214)
     Nucleic acid Atoms#: 0  (residues/phosphate atoms#: 0)

     Non-protein/nucleic Atoms#: 244  (residues: 244)
     Non-protein/nucleic resid values: [ CL (3), HOH (238), MG (2), NA (1) ]

   Protein sequence:
      MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAAVKSGSELGKQAKDIMDAGKLVT
      DELVIALVKERIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVDKI
      VGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKDDQEETVRKRLVEYHQMTAPLIG
      YYSKEAEAGNTKYAKVDGTKPVAEVRADLEKILG

+ attr: atom, xyz, seqres, helix, sheet,
        calpha, remark, call
```

```r
# Perform protein flexiblity prediction
m <- nma(adk)
```

```
 Building Hessian...        Done in 0.034 seconds.
 Diagonalizing Hessian...   Done in 0.394 seconds.
```

```r
plot(m)
```



write out our results as a wee trajectory/movie of predicted motions:

```
mktrj(m, file="adk_m7.pdb")
```

Comparative analysis with PCA

First step find an ADK sequence:

```
library(bio3d)
id <- "1ake_A" ## Change this to run a different analysis
aa <- get.seq( id)
```

```
Warning in get.seq(id): 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
```

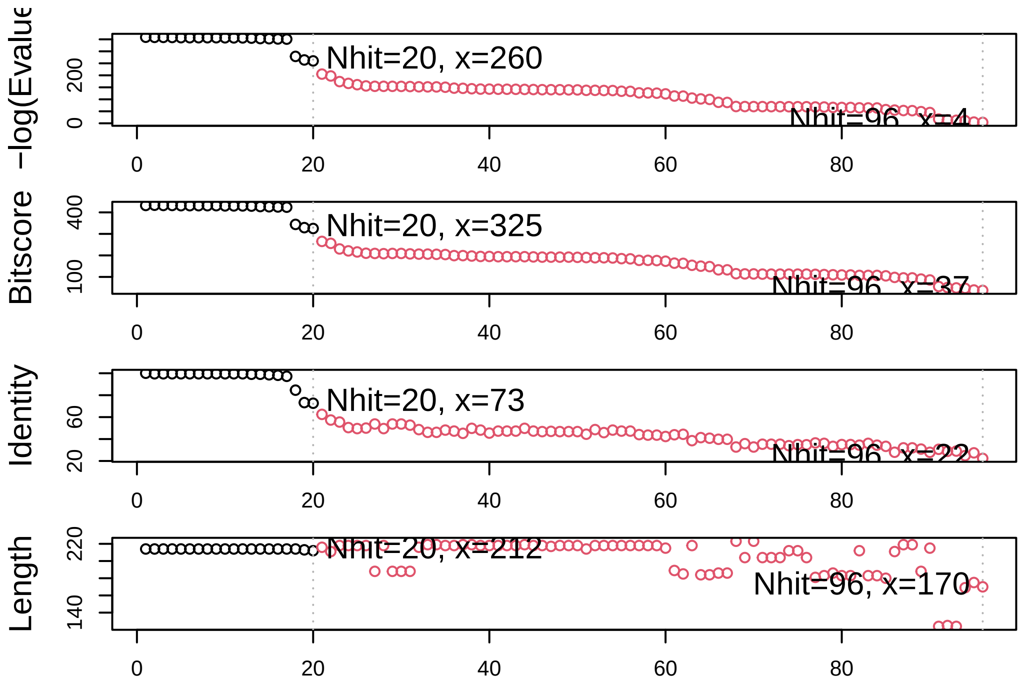
DB database for all related entries:

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

```
 Searching ... please wait (updates every 5 seconds) RID = SPYKXYWE014
 .....
 Reporting 96 hits
```

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

```
  * Possible cutoff values:    260 3
            Yielding Nhits:    20 96

  * Chosen cutoff value of:    260
            Yielding Nhits:    20
```



```
head(blast$hit.tbl)
```

```
        queryid subjectids identity alignmentlength mismatches gapopens q.start
1 Query_6403663     1AKE_A  100.000             214          0        0       1
2 Query_6403663     8BQF_A   99.533             214          1        0       1
3 Query_6403663     4X8M_A   99.533             214          1        0       1
4 Query_6403663     6S36_A   99.533             214          1        0       1
5 Query_6403663     9R6U_A   99.533             214          1        0       1
6 Query_6403663     9R71_A   99.533             214          1        0       1
  q.end s.start s.end    evalue bitscore positives mlog.evalue pdb.id    acc
1   214       1   214 1.78e-156      432    100.00    358.6267 1AKE_A 1AKE_A
2   214      21   234 2.91e-156      433    100.00    358.1351 8BQF_A 8BQF_A
3   214       1   214 3.18e-156      432    100.00    358.0464 4X8M_A 4X8M_A
4   214       1   214 4.67e-156      432    100.00    357.6621 6S36_A 6S36_A
5   214       1   214 1.04e-155      431     99.53    356.8615 9R6U_A 9R6U_A
6   214       1   214 1.23e-155      431     99.53    356.6937 9R71_A 9R71_A
```

The "top hits" are in the `hits` object. Now we can download these to our computer. Put these in a sub-folder (directory) called pdbs

```r
## Download related PDB files
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/8BQF.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/9R6U.pdb.gz exists. Skipping download
```

```
Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE):
pdbs/9R71.pdb.gz exists. Skipping download
```

```
Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE):
pdbs/8Q2B.pdb.gz exists. Skipping download
```

```
Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE):
pdbs/8RJ9.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/8PVW.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
```

```
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```
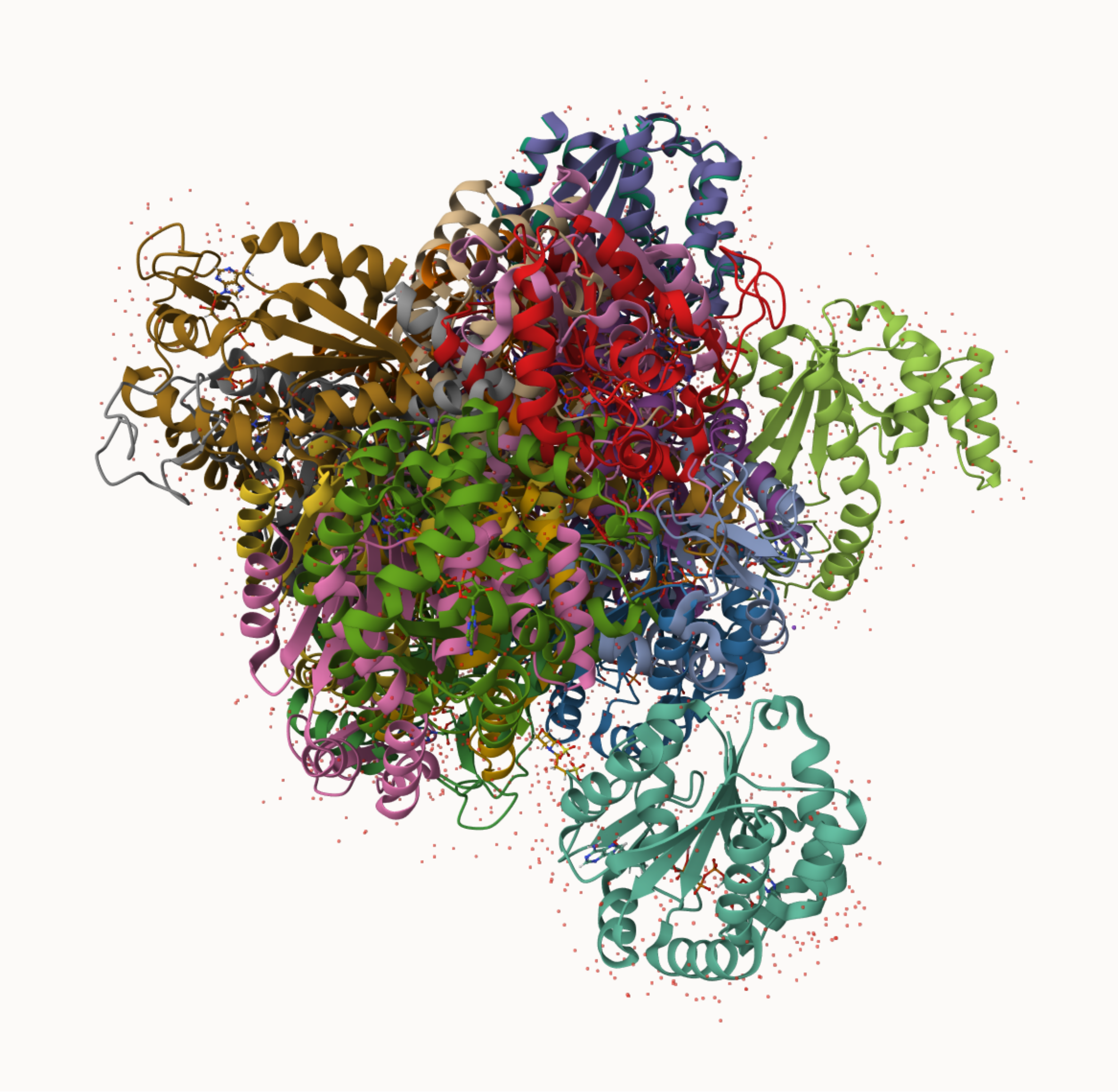

These look like a hot mess



Next we will use thepdbaln() function to align and also superpose the PDB structure.

This requires a BioConductor package called “msa” that we need to install. First we install BiocManager. Then we use `BiocManager::install("msa")`

```
# Align related PDBs
pdbs <- pdbaln(files, fit = TRUE, exefile="msa")
```

```
Reading PDB files:
pdbs/split_chain/1AKE_A.pdb
```

```
pdbs/split_chain/8BQF_A.pdb
pdbs/split_chain/4X8M_A.pdb
pdbs/split_chain/6S36_A.pdb
pdbs/split_chain/9R6U_A.pdb
pdbs/split_chain/9R71_A.pdb
pdbs/split_chain/8Q2B_A.pdb
pdbs/split_chain/8RJ9_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/8PVW_A.pdb
pdbs/split_chain/4K46_A.pdb
pdbs/split_chain/4NP6_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
.   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/8BQF_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 3   name: pdbs/split_chain/4X8M_A.pdb
pdb/seq: 4   name: pdbs/split_chain/6S36_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
```

```
pdb/seq: 5   name: pdbs/split_chain/9R6U_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 6   name: pdbs/split_chain/9R71_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 7   name: pdbs/split_chain/8Q2B_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 8   name: pdbs/split_chain/8RJ9_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 9   name: pdbs/split_chain/6RZE_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 10   name: pdbs/split_chain/4X8H_A.pdb
pdb/seq: 11   name: pdbs/split_chain/3HPR_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 12   name: pdbs/split_chain/1E4V_A.pdb
pdb/seq: 13   name: pdbs/split_chain/5EJE_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 14   name: pdbs/split_chain/1E4Y_A.pdb
pdb/seq: 15   name: pdbs/split_chain/3X2S_A.pdb
pdb/seq: 16   name: pdbs/split_chain/6HAP_A.pdb
pdb/seq: 17   name: pdbs/split_chain/6HAM_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 18   name: pdbs/split_chain/8PVW_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 19   name: pdbs/split_chain/4K46_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 20   name: pdbs/split_chain/4NP6_A.pdb
```

Have a look at this new "alignment object" `pdbs`

```
pdbs
```

```
                                1        .         .         .         40 
[Truncated_Name:1]1AKE_A.pdb    --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAA
[Truncated_Name:2]8BQF_A.pdb    --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAA
[Truncated_Name:3]4X8M_A.pdb    --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAA
[Truncated_Name:4]6S36_A.pdb    --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAA
[Truncated_Name:5]9R6U_A.pdb    --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAA
[Truncated_Name:6]9R71_A.pdb    --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAA
[Truncated_Name:7]8Q2B_A.pdb    --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAA
[Truncated_Name:8]8RJ9_A.pdb    --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAA
[Truncated_Name:9]6RZE_A.pdb    --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAA
[Truncated_Name:10]4X8H_A.pdb   --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAA
```

```
[Truncated_Name:11]3HPR_A.pdb   --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAA
[Truncated_Name:12]1E4V_A.pdb   --MRIILLGAPVAGKGTQAQFIMEKYGIPQISTGDMLRAA
[Truncated_Name:13]5EJE_A.pdb   --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAA
[Truncated_Name:14]1E4Y_A.pdb   --MRIILLGALVAGKGTQAQFIMEKYGIPQISTGDMLRAA
[Truncated_Name:15]3X2S_A.pdb   --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAA
[Truncated_Name:16]6HAP_A.pdb   --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAA
[Truncated_Name:17]6HAM_A.pdb   --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAA
[Truncated_Name:18]8PVW_A.pdb   --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAA
[Truncated_Name:19]4K46_A.pdb   --MRIILLGAPGAGKGTQAQFIMAKFGIPQISTGDMLRAA
[Truncated_Name:20]4NP6_A.pdb   NAMRIILLGAPGAGKGTQAQFIMEKFGIPQISTGDMLRAA
                                  ********  *********** *^**************
                                1        .         .         .         40

                               41        .         .         .         80
[Truncated_Name:1]1AKE_A.pdb    VKSGSELGKQAKDIMDAGKLVTDELVIALVKERIAQEDCR
[Truncated_Name:2]8BQF_A.pdb    VKSGSELGKQAKDIMDAGKLVTDELVIALVKERIAQE---
[Truncated_Name:3]4X8M_A.pdb    VKSGSELGKQAKDIMDAGKLVTDELVIALVKERIAQEDCR
[Truncated_Name:4]6S36_A.pdb    VKSGSELGKQAKDIMDAGKLVTDELVIALVKERIAQEDCR
[Truncated_Name:5]9R6U_A.pdb    VKSGSELGAQAKDIMDAGKLVTDELVIALVKERIAQEDCR
[Truncated_Name:6]9R71_A.pdb    VKSGSELGKQAKDIMDAGKLVTDELVIALVKERIAQEDCR
[Truncated_Name:7]8Q2B_A.pdb    VKSGSELGKQAKDIMDAGKLVTDELVIALVKERIAQEDCR
[Truncated_Name:8]8RJ9_A.pdb    VKSGSELGKQAKDIMDAGKLVTDELVIALVKERIAQEDCR
[Truncated_Name:9]6RZE_A.pdb    VKSGSELGKQAKDIMDAGKLVTDELVIALVKERIAQEDCR
[Truncated_Name:10]4X8H_A.pdb   VKSGSELGKQAKDIMDAGKLVTDELVIALVKERIAQEDCR
[Truncated_Name:11]3HPR_A.pdb   VKSGSELGKQAKDIMDAGKLVTDELVIALVKERIAQEDCR
[Truncated_Name:12]1E4V_A.pdb   VKSGSELGKQAKDIMDAGKLVTDELVIALVKERIAQEDCR
[Truncated_Name:13]5EJE_A.pdb   VKSGSELGKQAKDIMDACKLVTDELVIALVKERIAQEDCR
[Truncated_Name:14]1E4Y_A.pdb   VKSGSELGKQAKDIMDAGKLVTDELVIALVKERIAQEDCR
[Truncated_Name:15]3X2S_A.pdb   VKSGSELGKQAKDIMDCGKLVTDELVIALVKERIAQEDSR
[Truncated_Name:16]6HAP_A.pdb   VKSGSELGKQAKDIMDAGKLVTDELVIALVRERICQEDSR
[Truncated_Name:17]6HAM_A.pdb   IKSGSELGKQAKDIMDAGKLVTDEIIIALVKERICQEDSR
[Truncated_Name:18]8PVW_A.pdb   VKSGSELGKQAKDIMDAGKLVTDELVIALVKERIAQEDCR
[Truncated_Name:19]4K46_A.pdb   IKAGTELGKQAKSVIDAGQLVSDDIILGLVKERIAQDDCA
[Truncated_Name:20]4NP6_A.pdb   IKAGTELGKQAKAVIDAGQLVSDDIILGLIKERIAQADCE
                                ^* *^*** *** ^^*   **^*^^^^^*^^*** *
                               41        .         .         .         80

                               81        .         .         .         120
[Truncated_Name:1]1AKE_A.pdb    NGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:2]8BQF_A.pdb    -GFLLDGFPRTIPQADAMKEAGINVDYVIEFDVPDELIVD
[Truncated_Name:3]4X8M_A.pdb    NGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:4]6S36_A.pdb    NGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:5]9R6U_A.pdb    NGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
```

```
[Truncated_Name:6]9R71_A.pdb    NGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDALIVD
[Truncated_Name:7]8Q2B_A.pdb    NGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:8]8RJ9_A.pdb    NGFLLAGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:9]6RZE_A.pdb    NGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:10]4X8H_A.pdb   NGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:11]3HPR_A.pdb   NGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:12]1E4V_A.pdb   NGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:13]5EJE_A.pdb   NGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:14]1E4Y_A.pdb   NGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:15]3X2S_A.pdb   NGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:16]6HAP_A.pdb   NGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:17]6HAM_A.pdb   NGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:18]8PVW_A.pdb   NGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:19]4K46_A.pdb   KGFLLDGFPRTIPQADGLKEVGVVVDYVIEFDVADSVIVE
[Truncated_Name:20]4NP6_A.pdb   KGFLLDGFPRTIPQADGLKEMGINVDYVIEFDVADDVIVE
                                 **** **********^^** *^ ****^**** * ^**^
                               81        .         .         .         120

                              121        .         .         .         160
[Truncated_Name:1]1AKE_A.pdb    RIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:2]8BQF_A.pdb    RIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:3]4X8M_A.pdb    RIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:4]6S36_A.pdb    KIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:5]9R6U_A.pdb    RIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:6]9R71_A.pdb    RIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:7]8Q2B_A.pdb    RIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKA
[Truncated_Name:8]8RJ9_A.pdb    RIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:9]6RZE_A.pdb    AIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:10]4X8H_A.pdb   RIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:11]3HPR_A.pdb   RIVGRRVHAPSGRVYHVKFNPPKVEGKDDGTGEELTTRKD
[Truncated_Name:12]1E4V_A.pdb   RIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:13]5EJE_A.pdb   RIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:14]1E4Y_A.pdb   RIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:15]3X2S_A.pdb   RIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:16]6HAP_A.pdb   RIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:17]6HAM_A.pdb   RIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:18]8PVW_A.pdb   RILKR--GETSGRV-------------------------D
[Truncated_Name:19]4K46_A.pdb   RMAGRRAHLASGRTYHNVYNPPKVEGKDDVTGEDLVIRED
[Truncated_Name:20]4NP6_A.pdb   RMAGRRAHLPSGRTYHVVYNPPKVEGKDDVTGEDLVIRED
                                 ^  *     ***
                              121        .         .         .         160

                              161        .         .         .         200
```

```
[Truncated_Name:1]1AKE_A.pdb    DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:2]8BQF_A.pdb    DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:3]4X8M_A.pdb    DQEETVRKRLVEWHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:4]6S36_A.pdb    DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:5]9R6U_A.pdb    DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:6]9R71_A.pdb    DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:7]8Q2B_A.pdb    DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:8]8RJ9_A.pdb    DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:9]6RZE_A.pdb    DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:10]4X8H_A.pdb   DQEETVRKRLVEYHQMTAALIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:11]3HPR_A.pdb   DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:12]1E4V_A.pdb   DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:13]5EJE_A.pdb   DQEECVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:14]1E4Y_A.pdb   DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:15]3X2S_A.pdb   DQEETVRKRLCEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:16]6HAP_A.pdb   DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:17]6HAM_A.pdb   DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:18]8PVW_A.pdb   DNEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:19]4K46_A.pdb   DKEETVLARLGVYHNQTAPLIAYYGKEAEAGNTQYLKFDG
[Truncated_Name:20]4NP6_A.pdb   DKEETVRARLNVYHTQTAPLIEYYGKEAAAGKTQYLKFDG
                                * ** *  **  ^*  ** ** ** *** ** * * * **
                              161        .         .         .         200

                              201        .     216
[Truncated_Name:1]1AKE_A.pdb    TKPVAEVRADLEKILG
[Truncated_Name:2]8BQF_A.pdb    TKPVAEVRADLEKIL-
[Truncated_Name:3]4X8M_A.pdb    TKPVAEVRADLEKILG
[Truncated_Name:4]6S36_A.pdb    TKPVAEVRADLEKILG
[Truncated_Name:5]9R6U_A.pdb    TKPVAEVRADLEKILG
[Truncated_Name:6]9R71_A.pdb    TKPVAEVRADLEKILG
[Truncated_Name:7]8Q2B_A.pdb    TKPVAEVRADLEKILG
[Truncated_Name:8]8RJ9_A.pdb    TKPVAEVRADLEKILG
[Truncated_Name:9]6RZE_A.pdb    TKPVAEVRADLEKILG
[Truncated_Name:10]4X8H_A.pdb   TKPVAEVRADLEKILG
[Truncated_Name:11]3HPR_A.pdb   TKPVAEVRADLEKILG
[Truncated_Name:12]1E4V_A.pdb   TKPVAEVRADLEKILG
[Truncated_Name:13]5EJE_A.pdb   TKPVAEVRADLEKILG
[Truncated_Name:14]1E4Y_A.pdb   TKPVAEVRADLEKILG
[Truncated_Name:15]3X2S_A.pdb   TKPVAEVRADLEKILG
[Truncated_Name:16]6HAP_A.pdb   TKPVCEVRADLEKILG
[Truncated_Name:17]6HAM_A.pdb   TKPVCEVRADLEKILG
[Truncated_Name:18]8PVW_A.pdb   TKPVAEVRADLEKILG
[Truncated_Name:19]4K46_A.pdb   TKAVAEVSAELEKALA
```

```
[Truncated_Name:20]4NP6_A.pdb   TKQVSEVSADIAKALA
                                ** * ** *^^ * *
                              201         .     216

Call:
  pdbaln(files = files, fit = TRUE, exefile = "msa")

Class:
  pdbs, fasta

Alignment dimensions:
  20 sequence rows; 216 position columns (182 non-gap, 34 gap)

+ attr: xyz, resno, b, chain, id, ali, resid, sse, call
```

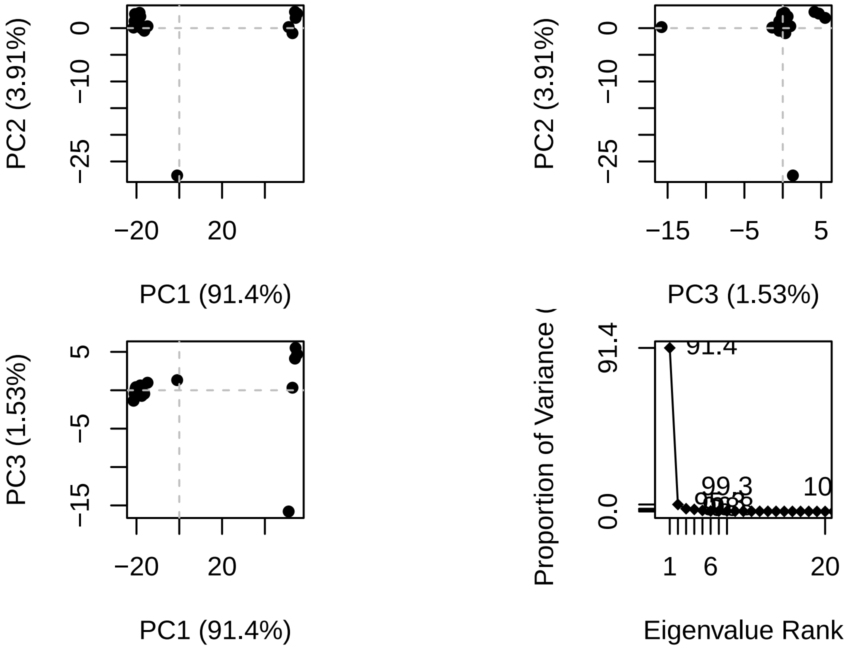
We could view these in R with **bio3dview** `view.pdbs()`function.

```
# library(bio3dview)
# view.pdbs(pdbs, colorScheme = "residue")
```

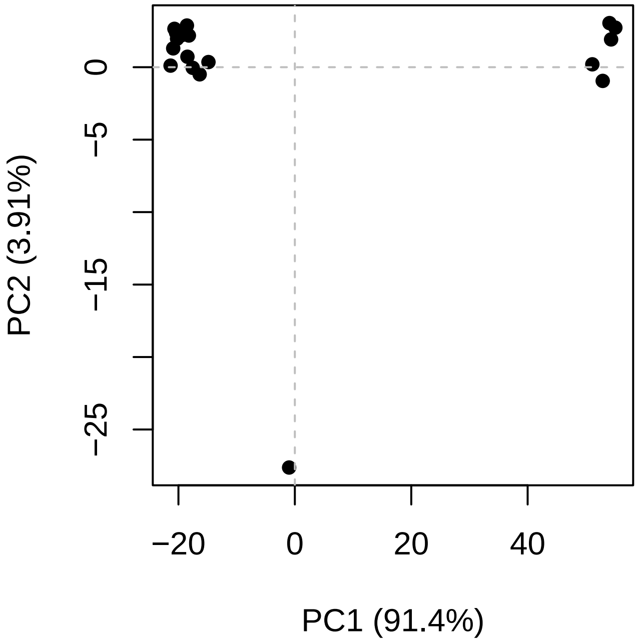
PCA

We can run PCA on our `pdbs` object using the `pca()` function from **bio3d**

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



```r
plot(pc.xray,1:2)
```



We can make a visualization of the major conformational difference (i.e. large scale structure change) captured by our PCA analysis with `mktrj()` function.

```r
pc1 <- mktrj(pc.xray, pc=1, file="pc_1.pdb")
```

Let’s see in Molstar