class10

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The PDB database

Here we examine the size and composition of the main database of biomolecular structures - the PDB.

Get a CSV file from the PDB database and read it into R.

```
stat_summary <- read.csv("pdb stat summary.csv", row.names = 1)
stat_summary
```

	X.ray	EM	NMR	Multiple.methods	Neutron	Other
Protein (only)	161,663	12,592	12,337	200	74	32
Protein/Oligosaccharide	9,348	2,167	34	8	2	0
Protein/NA	8,404	3,924	286	7	0	0
Nucleic acid (only)	2,758	125	1,477	14	3	1
Other	164	9	33	0	0	0
Oligosaccharide (only)	11	0	6	1	0	4

	Total
Protein (only)	186,898
Protein/Oligosaccharide	11,559
Protein/NA	12,621
Nucleic acid (only)	4,378
Other	206
Oligosaccharide (only)	22

My pdbstats data frame has numbers with commas in them. This may cause us problems. Let's see

```
stat_summary$X.ray #chr with numbers
```

```
[1] "161,663" "9,348"   "8,404"   "2,758"   "164"     "11"
```

I can turn this snipet into a function that I can use for every column in the table

```
commasum <- function (x) {
  sum(as.numeric(gsub(",", "", x)))
}

commasum(stat_summary$X.ray)
```

```
[1] 182348
```

Apply accross all columns

```
totals <- apply(stat_summary, 2, commasum)
totals
```

```
          X.ray             EM            NMR Multiple.methods
         182348          18817          14173            230
        Neutron          Other          Total
             79             37         215684
```

```
(totals/totals["Total"])*100
```

```
          X.ray             EM            NMR Multiple.methods
    84.54405519     8.72433746     6.57118748     0.10663749
        Neutron          Other          Total
     0.03662766     0.01715473   100.00000000
```

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

From the code above, 84.544% of structures are solved by X-ray and 8.724% by EM.

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

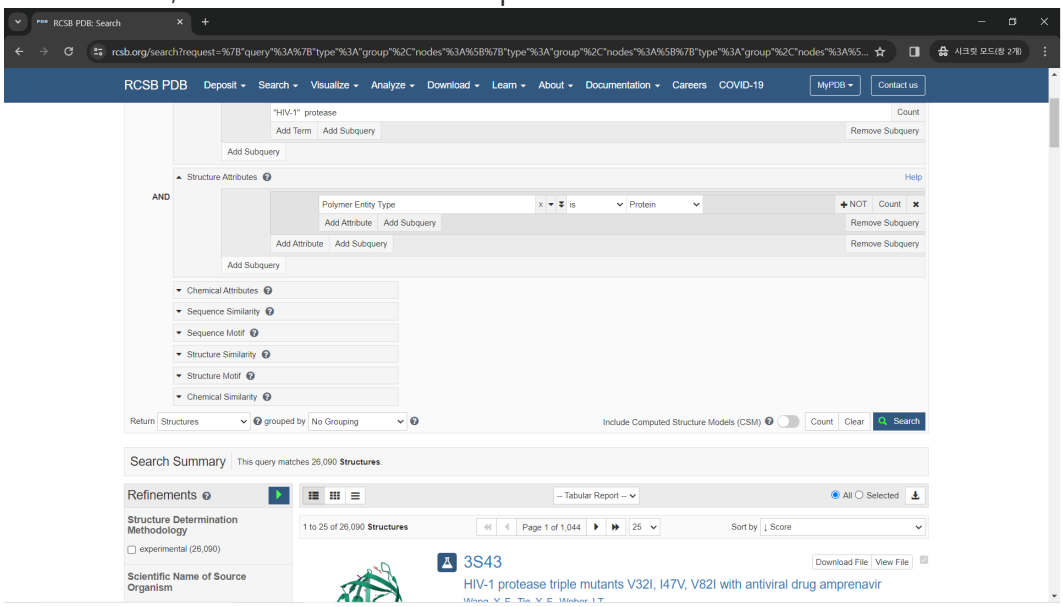
```
total.row <- apply(stat_summary, 1, commasum)
(total.row/sum(total.row))*100
```

```
      Protein (only) Protein/Oligosaccharide              Protein/NA
         86.65362289             5.35922924             5.85161625
Nucleic acid (only)                  Other Oligosaccharide (only)
          2.02982141             0.09551010             0.01020011
```

Therefore, 86.654% of structures in PDB are protein.

Q3: Type HIV in the PDB website search box on the home page and determine how many HIV-1 protease structures are in the current PDB?

There are 26,090 structures of HIV-1 protease in current PDB.



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

Oxygen atoms is larger than hydrogen atoms that size of hydrogen atoms are insignificant compared to oxygen and rest of protein structure (Also prof. said hydrogen are too small to be

visible in size during lecture?). Therefore, only oxygen molecule is displayed.

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

HOH308 is forming bond with both ligand and I50 in protein.

Visualizing Protein Structure

We will learn the basics of Mol* (mol-star) homepage: https://molstar.org/viewer/

We will play with PDB code 1HSG

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.

HIV-Pr with a bound inhibitor showing the two important ASP 25

Discussion Topic: Can you think of a way in which indinavir, or even larger ligands and substrates, could enter the binding site?

If question is asking "How do ligans enter binding site" : Two chains rotates (like twist) that binding site opens up, making larger space for ligand to enter. As ligand form bond with protein, two chains untwist and closes its binding site.

If question is asking "is there way to modify protein so that larger ligand can bind" : Maybe modify protein usign bump and hole method so that larger ligands have a space to bind.

Back to R and working with PDB structure

Predict the dynmics (flexibility) of an important protein:

```
library(bio3d)

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

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

```
hiv
```

```

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?

There are 198 aa residues.

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

There are 128 non-protein residues, where their types are HOH (water) and MK1 (inhibitor)

Q9: How many protein chains are in this structure?

There are two chains, chain A and B.

```
head(hiv$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>
```

```
pdbseq(hiv)
```

```
  1   2   3   4   5   6   7   8   9  10  11  12  13  14  15  16  17  18  19  20
"P" "Q" "I" "T" "L" "W" "Q" "R" "P" "L" "V" "T" "I" "K" "I" "G" "G" "Q" "L" "K"
 21  22  23  24  25  26  27  28  29  30  31  32  33  34  35  36  37  38  39  40
"E" "A" "L" "L" "D" "T" "G" "A" "D" "D" "T" "V" "L" "E" "E" "M" "S" "L" "P" "G"
 41  42  43  44  45  46  47  48  49  50  51  52  53  54  55  56  57  58  59  60
"R" "W" "K" "P" "K" "M" "I" "G" "G" "I" "G" "G" "F" "I" "K" "V" "R" "Q" "Y" "D"
 61  62  63  64  65  66  67  68  69  70  71  72  73  74  75  76  77  78  79  80
```

```
"Q" "I" "L" "I" "E" "I" "C" "G" "H" "K" "A" "I" "G" "T" "V" "L" "V" "G" "P" "T"
 81  82  83  84  85  86  87  88  89  90  91  92  93  94  95  96  97  98  99   1
"P" "V" "N" "I" "I" "G" "R" "N" "L" "L" "T" "Q" "I" "G" "C" "T" "L" "N" "F" "P"
  2   3   4   5   6   7   8   9  10  11  12  13  14  15  16  17  18  19  20  21
"Q" "I" "T" "L" "W" "Q" "R" "P" "L" "V" "T" "I" "K" "I" "G" "G" "Q" "L" "K" "E"
 22  23  24  25  26  27  28  29  30  31  32  33  34  35  36  37  38  39  40  41
"A" "L" "L" "D" "T" "G" "A" "D" "D" "T" "V" "L" "E" "E" "M" "S" "L" "P" "G" "R"
 42  43  44  45  46  47  48  49  50  51  52  53  54  55  56  57  58  59  60  61
"W" "K" "P" "K" "M" "I" "G" "G" "I" "G" "G" "F" "I" "K" "V" "R" "Q" "Y" "D" "Q"
 62  63  64  65  66  67  68  69  70  71  72  73  74  75  76  77  78  79  80  81
"I" "L" "I" "E" "I" "C" "G" "H" "K" "A" "I" "G" "T" "V" "L" "V" "G" "P" "T" "P"
 82  83  84  85  86  87  88  89  90  91  92  93  94  95  96  97  98  99
"V" "N" "I" "I" "G" "R" "N" "L" "L" "T" "Q" "I" "G" "C" "T" "L" "N" "F"
```

Here we will do a normal mode analysis (nma) to predict functional motion of a kinase

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

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

```
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) ]

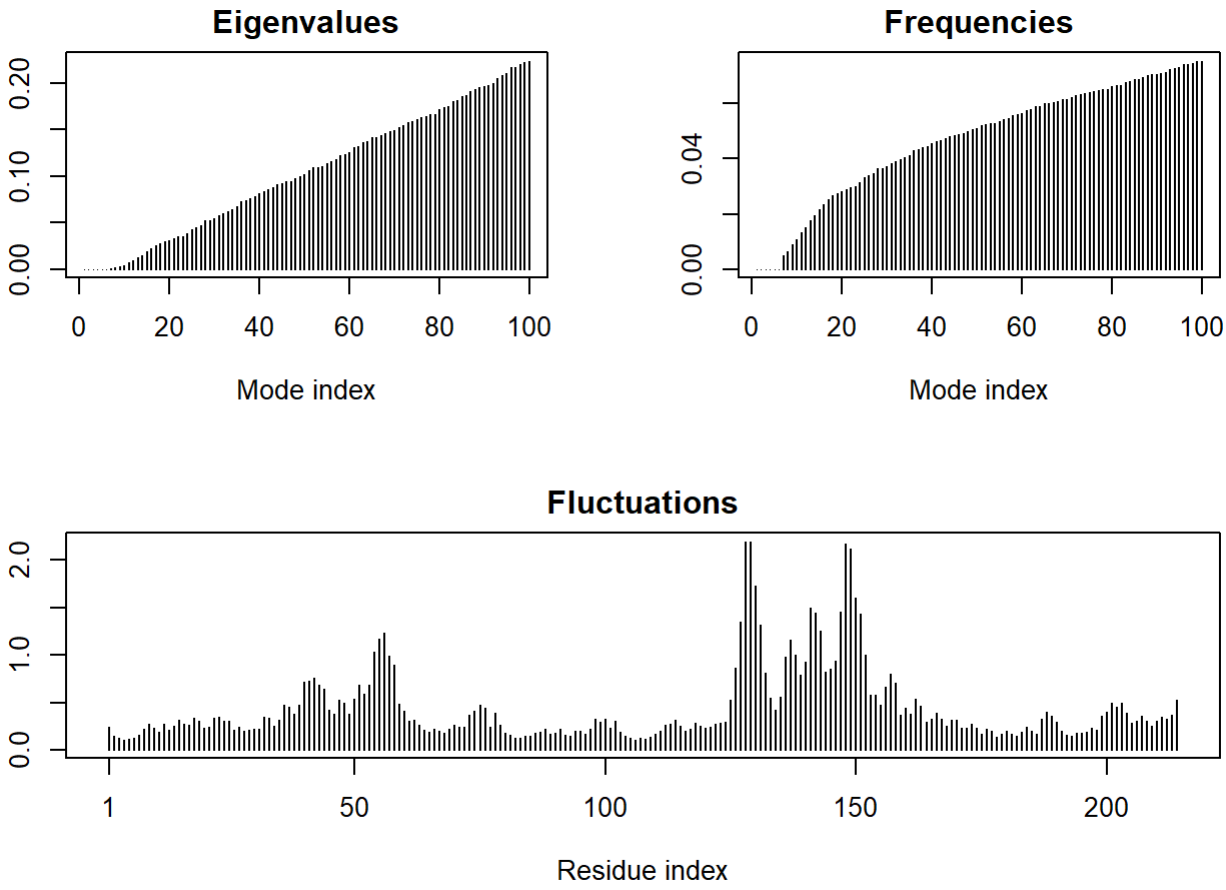
   Protein sequence:
      MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAAVKSGSELGKQAKDIMDAGKLVT
      DELVIALVKERIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVDKI
      VGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKDDQEETVRKRLVEYHQMTAPLIG
      YYSKEAEAGNTKYAKVDGTKPVAEVRADLEKILG

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

```
modes <- nma(adk)
```

```
 Building Hessian...        Done in 0.01 seconds.
 Diagonalizing Hessian...   Done in 0.23 seconds.
```

```
plot(modes)
```



Make a "movie" called a trajectory of the predicted motions:

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

Then I can open this file in Mol*...

```
modes1 <- nma(read.pdb("1hsg"))
```

```
  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\louis\AppData\Local\Temp\RtmpEtEyMb/1hsg.pdb exists. Skipping download

Warning in nma.pdb(read.pdb("1hsg")): Possible multi-chain structure or missing in-structure
residue(s) present
  Fluctuations at neighboring positions may be affected.

 Building Hessian...        Done in 0.02 seconds.
 Diagonalizing Hessian...   Done in 0.18 seconds.
```

```
mktrj(modes1, file = "1hsg_m7.pdb")
```

install.packages("bio3d") install.packages("devtools") install.packages("BiocManager") BiocManager::install("msa") devtools::install_bitbucket("Grantlab/bio3d-view")

Q10. Which of the packages above is found only on BioConductor and not CRAN?

msa package is found only on BioConductor.

Q11. Which of the above packages is not found on BioConductor or CRAN?

bio3d-view (Grantlab/bio3d-view) is found only on bitbucket.

Q12. True or False? Functions from the devtools package can be used to install packages from GitHub and BitBucket?

True.

```
library(bio3d)
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   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
```

Q13. How many amino acids are in this sequence, i.e. how long is this sequence?

There are 214 aa in this sequence.

```
#b <- blast.pdb(aa)
#hits <- plot(b)
```

```
#head(hits$pdb.id)
#Takes to long

hits <- NULL
hits$pdb.id <- c('1AKE_A','6S36_A','6RZE_A','3HPR_A','1E4V_A','5EJE_A','1E4Y_A','3X2S_A','6HAP
```

```
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 exists. Skipping download

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

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

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

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

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

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

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

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

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

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

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

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

```
  |
  |                                                                      |   0%
  |
  |=====                                                                 |   8%
  |
```

```
  |===========                                                     |  15%
  |
  |================                                                |  23%
  |
  |======================                                          |  31%
  |
  |============================                                    |  38%
  |
  |================================                                |  46%
  |
  |====================================                            |  54%
  |
  |========================================                        |  62%
  |
  |============================================                    |  69%
  |
  |================================================                |  77%
  |
  |========================================================        |  85%
  |
  |============================================================    |  92%
  |
  |================================================================| 100%
```

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

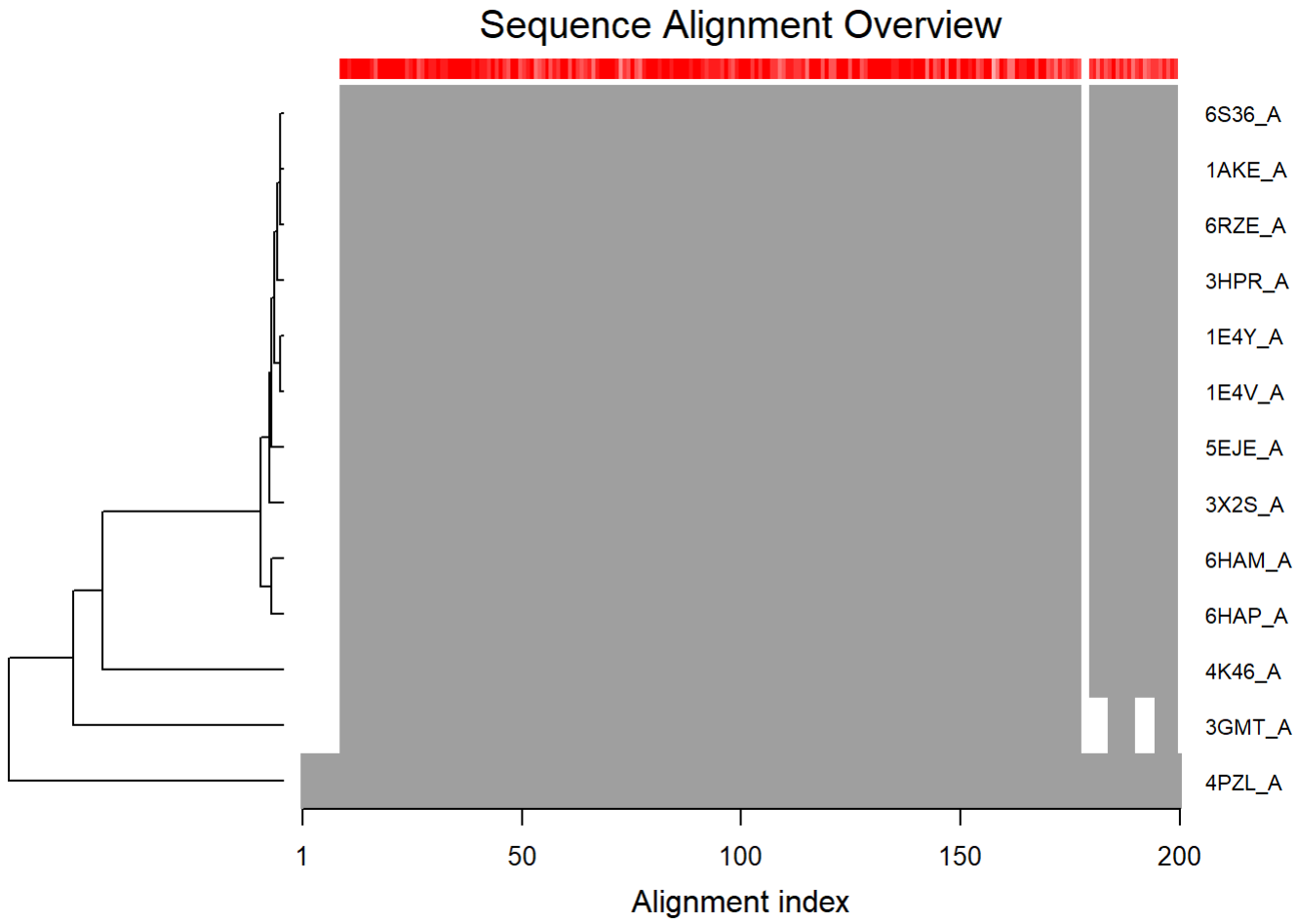
```
Reading PDB files:
pdbs/split_chain/1AKE_A.pdb
pdbs/split_chain/6S36_A.pdb
pdbs/split_chain/6RZE_A.pdb
pdbs/split_chain/3HPR_A.pdb
pdbs/split_chain/1E4V_A.pdb
pdbs/split_chain/5EJE_A.pdb
pdbs/split_chain/1E4Y_A.pdb
pdbs/split_chain/3X2S_A.pdb
pdbs/split_chain/6HAP_A.pdb
pdbs/split_chain/6HAM_A.pdb
pdbs/split_chain/4K46_A.pdb
pdbs/split_chain/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/6S36_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 3   name: pdbs/split_chain/6RZE_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 4   name: pdbs/split_chain/3HPR_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 5   name: pdbs/split_chain/1E4V_A.pdb
pdb/seq: 6   name: pdbs/split_chain/5EJE_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 7   name: pdbs/split_chain/1E4Y_A.pdb
pdb/seq: 8   name: pdbs/split_chain/3X2S_A.pdb
pdb/seq: 9   name: pdbs/split_chain/6HAP_A.pdb
pdb/seq: 10   name: pdbs/split_chain/6HAM_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 11   name: pdbs/split_chain/4K46_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 12   name: pdbs/split_chain/3GMT_A.pdb
pdb/seq: 13   name: pdbs/split_chain/4PZL_A.pdb
```

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




```
#Why is this not working? Please commentttt
library(bio3d.view)
library(rgl)
```

```
view.pdbs(pdbs)
```

```
anno <- pdb.annotate(ids)
unique(anno$source)
```

```
[1] "Escherichia coli"
[2] "Escherichia coli K-12"
[3] "Escherichia coli O139:H28 str. E24377A"
[4] "Escherichia coli str. K-12 substr. MDS42"
[5] "Photobacterium profundum"
[6] "Burkholderia pseudomallei 1710b"
[7] "Francisella tularensis subsp. tularensis SCHU S4"
```

```
anno
```

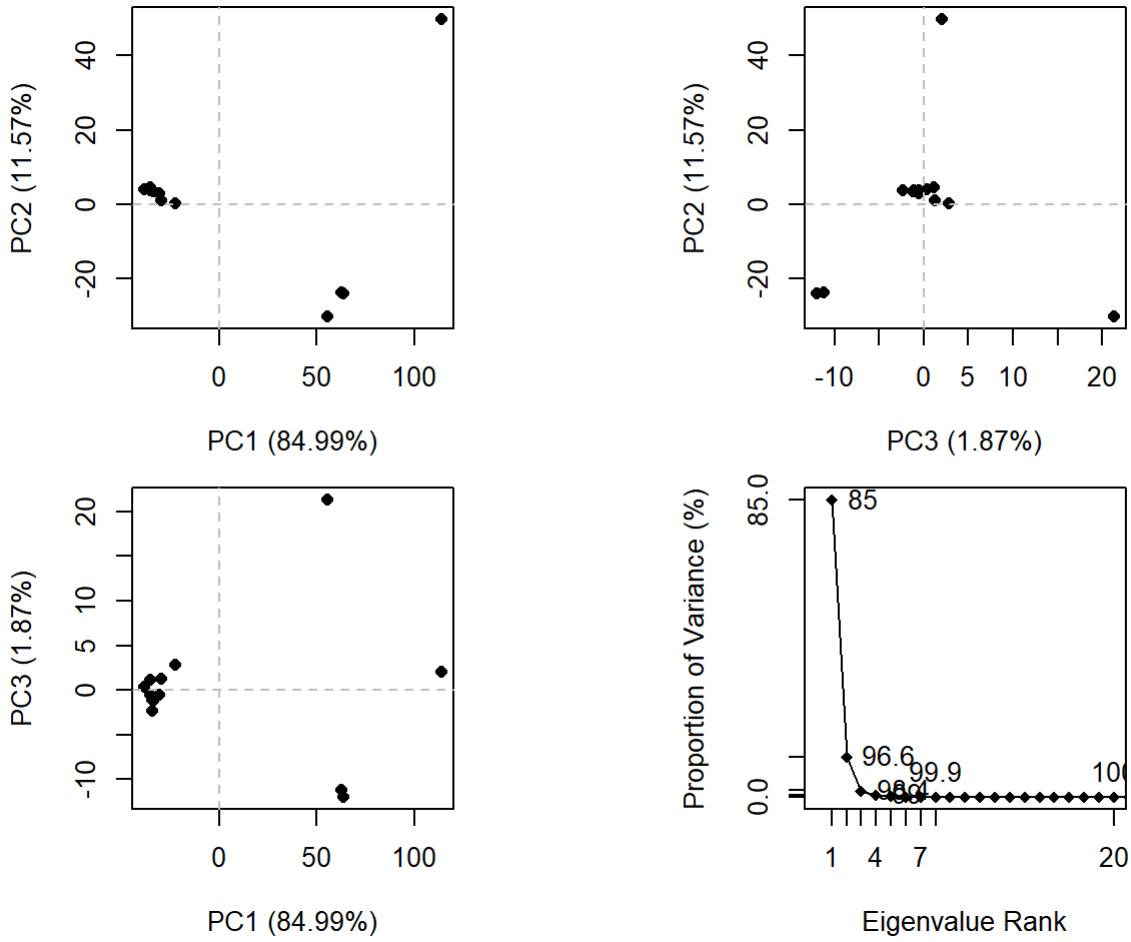
```
       structureId chainId macromoleculeType chainLength experimentalTechnique
1AKE_A        1AKE       A           Protein         214                X-ray
6S36_A        6S36       A           Protein         214                X-ray
6RZE_A        6RZE       A           Protein         214                X-ray
3HPR_A        3HPR       A           Protein         214                X-ray
1E4V_A        1E4V       A           Protein         214                X-ray
5EJE_A        5EJE       A           Protein         214                X-ray
1E4Y_A        1E4Y       A           Protein         214                X-ray
3X2S_A        3X2S       A           Protein         214                X-ray
6HAP_A        6HAP       A           Protein         214                X-ray
6HAM_A        6HAM       A           Protein         214                X-ray
4K46_A        4K46       A           Protein         214                X-ray
3GMT_A        3GMT       A           Protein         230                X-ray
4PZL_A        4PZL       A           Protein         242                X-ray
       resolution       scopDomain                                      pfam
1AKE_A       2.00 Adenylate kinase Adenylate kinase, active site lid (ADK_lid)
6S36_A       1.60             <NA>                     Adenylate kinase (ADK)
6RZE_A       1.69             <NA>                     Adenylate kinase (ADK)
3HPR_A       2.00             <NA> Adenylate kinase, active site lid (ADK_lid)
1E4V_A       1.85 Adenylate kinase                     Adenylate kinase (ADK)
5EJE_A       1.90             <NA>                     Adenylate kinase (ADK)
1E4Y_A       1.85 Adenylate kinase                     Adenylate kinase (ADK)
3X2S_A       2.80             <NA>                     Adenylate kinase (ADK)
6HAP_A       2.70             <NA> Adenylate kinase, active site lid (ADK_lid)
6HAM_A       2.55             <NA> Adenylate kinase, active site lid (ADK_lid)
4K46_A       2.01             <NA> Adenylate kinase, active site lid (ADK_lid)
3GMT_A       2.10             <NA>                     Adenylate kinase (ADK)
4PZL_A       2.10             <NA>                     Adenylate kinase (ADK)
              ligandId
1AKE_A             AP5
6S36_A NA,MG (2),CL (3)
6RZE_A    CL (2),NA (3)
3HPR_A             AP5
1E4V_A             AP5
5EJE_A          AP5,CO
1E4Y_A             AP5
3X2S_A   JPY (2),AP5,MG
```

```
6HAP_A              AP5
6HAM_A              AP5
4K46_A      ADP,AMP,PO4
3GMT_A          SO4 (2)
4PZL_A       CA,GOL,FMT
                                                                                ligandName
1AKE_A                                                  BIS(ADENOSINE)-5'-PENTAPHOSPHATE
6S36_A                                  SODIUM ION,MAGNESIUM ION (2),CHLORIDE ION (3)
6RZE_A                                                   CHLORIDE ION (2),SODIUM ION (3)
3HPR_A                                                  BIS(ADENOSINE)-5'-PENTAPHOSPHATE
1E4V_A                                                  BIS(ADENOSINE)-5'-PENTAPHOSPHATE
5EJE_A                                BIS(ADENOSINE)-5'-PENTAPHOSPHATE,COBALT (II) ION
1E4Y_A                                                  BIS(ADENOSINE)-5'-PENTAPHOSPHATE
3X2S_A N-(pyren-1-ylmethyl)acetamide (2),BIS(ADENOSINE)-5'-PENTAPHOSPHATE,MAGNESIUM ION
6HAP_A                                                  BIS(ADENOSINE)-5'-PENTAPHOSPHATE
6HAM_A                                                  BIS(ADENOSINE)-5'-PENTAPHOSPHATE
4K46_A                   ADENOSINE-5'-DIPHOSPHATE,ADENOSINE MONOPHOSPHATE,PHOSPHATE ION
3GMT_A                                                                  SULFATE ION (2)
4PZL_A                                                  CALCIUM ION,GLYCEROL,FORMIC ACID
                                                 source
1AKE_A                                 Escherichia coli
6S36_A                                 Escherichia coli
6RZE_A                                 Escherichia coli
3HPR_A                             Escherichia coli K-12
1E4V_A                                 Escherichia coli
5EJE_A           Escherichia coli O139:H28 str. E24377A
1E4Y_A                                 Escherichia coli
3X2S_A         Escherichia coli str. K-12 substr. MDS42
6HAP_A           Escherichia coli O139:H28 str. E24377A
6HAM_A                             Escherichia coli K-12
4K46_A                          Photobacterium profundum
3GMT_A                  Burkholderia pseudomallei 1710b
4PZL_A Francisella tularensis subsp. tularensis SCHU S4

structureTitle
1AKE_A STRUCTURE OF THE COMPLEX BETWEEN ADENYLATE KINASE FROM ESCHERICHIA COLI AND THE
INHIBITOR AP5A REFINED AT 1.9 ANGSTROMS RESOLUTION: A MODEL FOR A CATALYTIC TRANSITION STATE
6S36_A
Crystal structure of E. coli Adenylate kinase R119K mutant
6RZE_A
Crystal structure of E. coli Adenylate kinase R119A mutant
3HPR_A
Crystal structure of V148G adenylate kinase from E. coli, in complex with Ap5A
1E4V_A
Mutant G10V of adenylate kinase from E. coli, modified in the Gly-loop
5EJE_A
Crystal structure of E. coli Adenylate kinase G56C/T163C double mutant in complex with Ap5a
1E4Y_A
Mutant P9L of adenylate kinase from E. coli, modified in the Gly-loop
3X2S_A
Crystal structure of pyrene-conjugated adenylate kinase
6HAP_A
Adenylate kinase
6HAM_A
```

```
Adenylate kinase
4K46_A
Crystal Structure of Adenylate Kinase from Photobacterium profundum
3GMT_A
Crystal structure of adenylate kinase from burkholderia pseudomallei
4PZL_A                                                                    The
crystal structure of adenylate kinase from Francisella tularensis subsp. tularensis SCHU S4
                                                  citation rObserved   rFree
1AKE_A                Muller, C.W., et al. J Mol Biol (1992)   0.19600      NA
6S36_A                 Rogne, P., et al. Biochemistry (2019)   0.16320 0.23560
6RZE_A                 Rogne, P., et al. Biochemistry (2019)   0.18650 0.23500
3HPR_A  Schrank, T.P., et al. Proc Natl Acad Sci U S A (2009)   0.21000 0.24320
1E4V_A                  Muller, C.W., et al. Proteins (1993)   0.19600      NA
5EJE_A  Kovermann, M., et al. Proc Natl Acad Sci U S A (2017)   0.18890 0.23580
1E4Y_A                  Muller, C.W., et al. Proteins (1993)   0.17800      NA
3X2S_A               Fujii, A., et al. Bioconjug Chem (2015)   0.20700 0.25600
6HAP_A              Kantaev, R., et al. J Phys Chem B (2018)   0.22630 0.27760
6HAM_A              Kantaev, R., et al. J Phys Chem B (2018)   0.20511 0.24325
4K46_A                   Cho, Y.-J., et al. To be published    0.17000 0.22290
3GMT_A Buchko, G.W., et al. Biochem Biophys Res Commun (2010)   0.23800 0.29500
4PZL_A                       Tan, K., et al. To be published    0.19360 0.23680
         rWork spaceGroup
1AKE_A 0.19600  P 21 2 21
6S36_A 0.15940    C 1 2 1
6RZE_A 0.18190    C 1 2 1
3HPR_A 0.20620  P 21 21 2
1E4V_A 0.19600  P 21 2 21
5EJE_A 0.18630  P 21 2 21
1E4Y_A 0.17800   P 1 21 1
3X2S_A 0.20700 P 21 21 21
6HAP_A 0.22370    I 2 2 2
6HAM_A 0.20311       P 43
4K46_A 0.16730 P 21 21 21
3GMT_A 0.23500   P 1 21 1
4PZL_A 0.19130       P 32
```

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

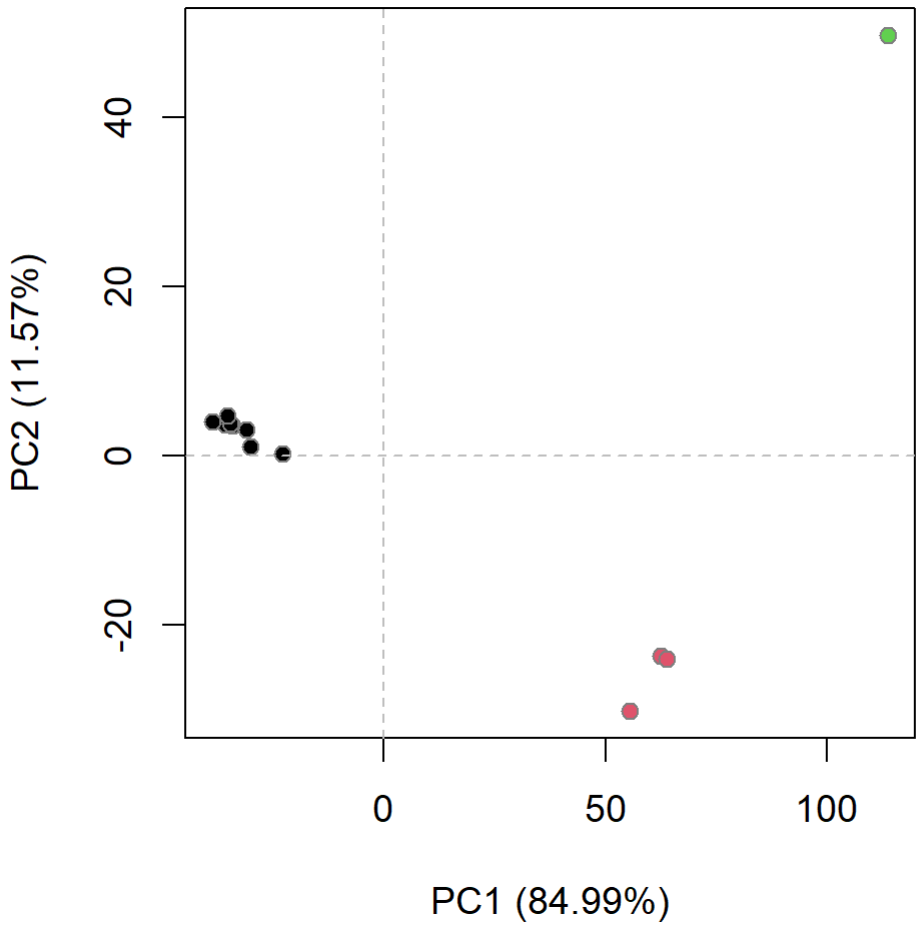



```
rd <- rmsd(pdbs)
```

```
Warning in rmsd(pdbs): No indices provided, using the 204 non NA positions
```

```
hc.rd <- hclust(dist(rd))
grps.rd <- cutree(hc.rd, k=3)

plot(pc.xray, 1:2, col="grey50", bg=grps.rd, pch=21, cex=1)
```




```
library(ggplot2)
library(ggrepel)

df <- data.frame(PC1=pc.xray$z[,1],
                 PC2=pc.xray$z[,2],
                 col=as.factor(grps.rd),
                 ids=ids)

p <- ggplot(df) +
  aes(PC1, PC2, col=col, label=ids) +
  geom_point(size=2) +
  geom_text_repel(max.overlaps = 20) +
  theme(legend.position = "none")
p
```


```
modes <- nma(pdbs)
```

```
Details of Scheduled Calculation:
  ... 13 input structures
  ... storing 606 eigenvectors for each structure
  ... dimension of x$U.subspace: ( 612x606x13 )
  ... coordinate superposition prior to NM calculation
  ... aligned eigenvectors (gap containing positions removed)
  ... estimated memory usage of final 'eNMA' object: 36.9 Mb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```

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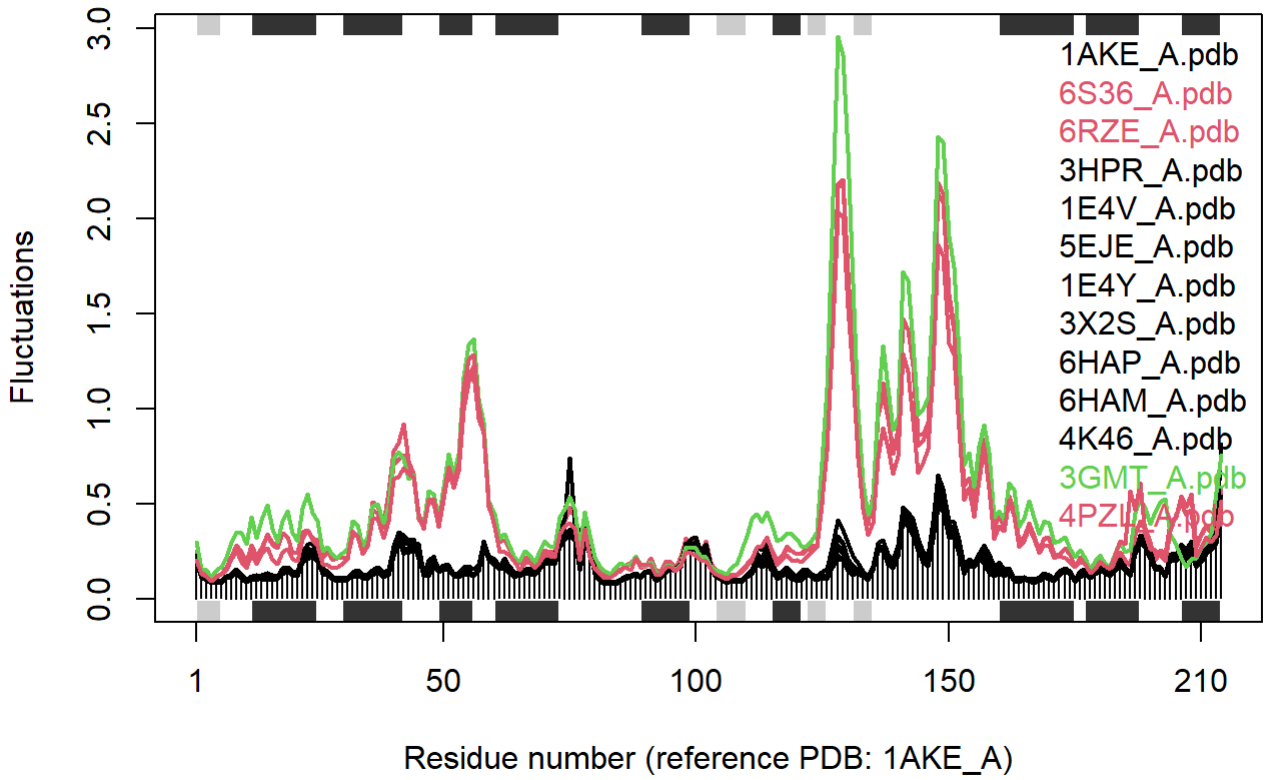
  |=====================================================================| 100%
```

```
plot(modes, pdbs, col=grps.rd)
```

```
Extracting SSE from pdbs$sse attribute
```



Q14. What do you note about this plot? Are the black and colored lines similar or different? Where do you think they differ most and why?

Colored line and black lines are different in flucuations around residue 1~50 and 120~170. Fluctuation differs the most around residue 130. This is because corresponding area is where protein moves (open and close activation site) to enable substrate binding.