# Class 9: Structural Bioinformatics 1

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To analyze PDB file, can download csv and use read.csv() to analyze the data. Protein structures by X-ray crystalography dominate this database. We are skipping Q1-3 as the website was too slow for us.

```
d <- read.csv("Data Export Summary.csv")
head(d)
```

```
           Molecular.Type   X.ray    NMR    EM
Multiple.methods Neutron Other
1          Protein (only) 150,342 12,053 8,534
188      72    32
2 Protein/Oligosaccharide   8,866     32 1,540
6       0     0
3              Protein/NA   7,911    278 2,681
6       0     0
4     Nucleic acid (only)   2,510  1,425    74
13       2     1
5                   Other     154     31     6
0       0     0
6  Oligosaccharide (only)      11      6     0
1       0     4
    Total
1 171,221
2  10,444
3  10,876
4   4,025
5     191
6      22
```

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

```
(169794 + 13825)/196779
```

```
[1] 0.9331229
```

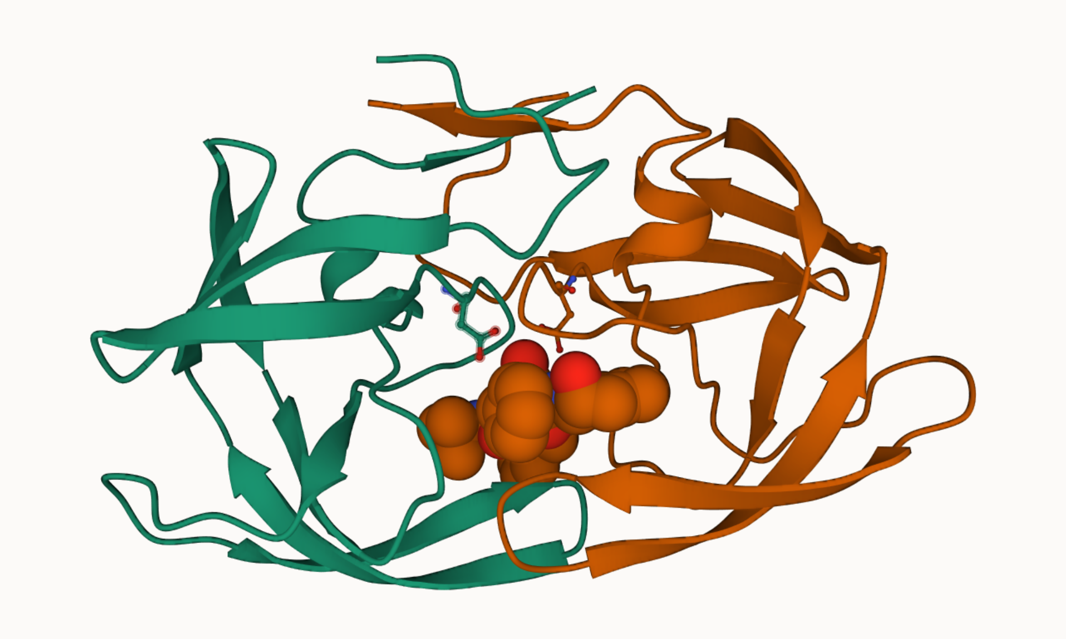
> Q2: What proportion of structures in the PDB are protein?

```
(171221 + 10444 + 10876)/196779
```

```
[1] 0.9784631
```

> 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?

2,545 Structures



HIV-Pr structure from 1hsg

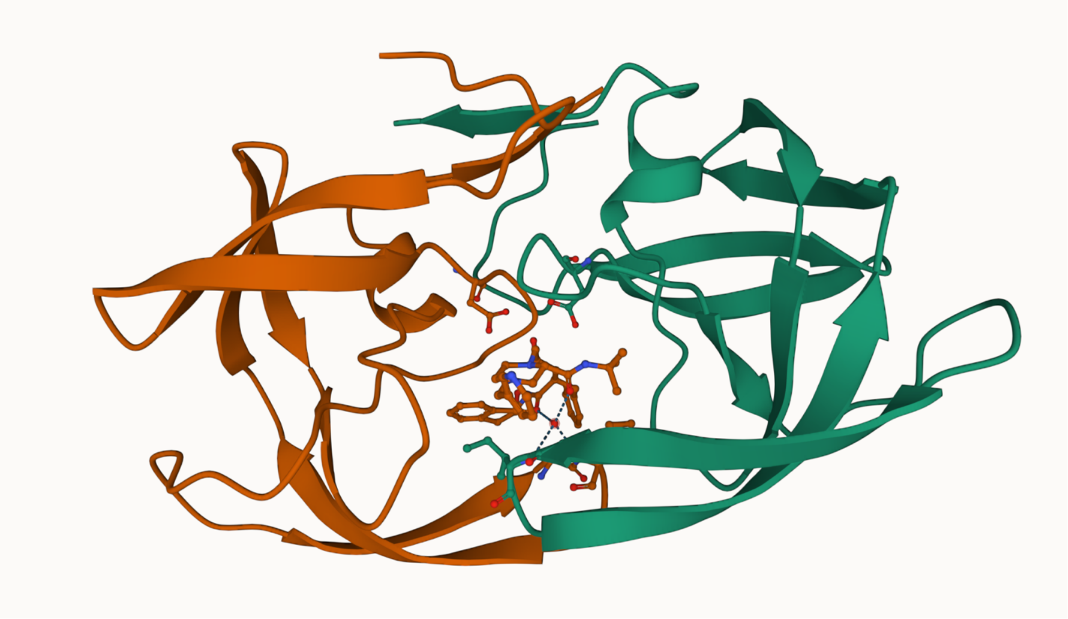
> Q4: Water molecules normally have 3 atoms. Why do we see just one atom per water molecule in this structure?

Because the resolution is not high enough/hydrogen molecules are too small so only oxygen atom is displayed per water molecule.

> 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

Yes, 308

> 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 (we recommend "Ball & Stick" for these side-chains). Add this figure to your Quarto document. Discussion Topic: Can you think of a way in which indinavir, or even larger ligands and substrates, could enter the binding site?



HIV-Pr structure from 1hsg

# 3. Introduction to Bio3D in R

Bio3D is an R packaged for structural bioinformatcis. To use it we ned to call it up with the `library` function (just like any package)

```
library(bio3d)
```

To read PDF file we can use `read.pdb()`

```
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?

198

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

MK1

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

2

```
attributes(pdb)
```

```
$names
[1] "atom"   "xyz"    "seqres" "helix"  "sheet"  "calpha"
"remark" "call"

$class
[1] "pdb" "sse"
```

The ATOM records of a PDB file are stored in `pdb$atom`

```
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>
```

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

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

```
adk
```

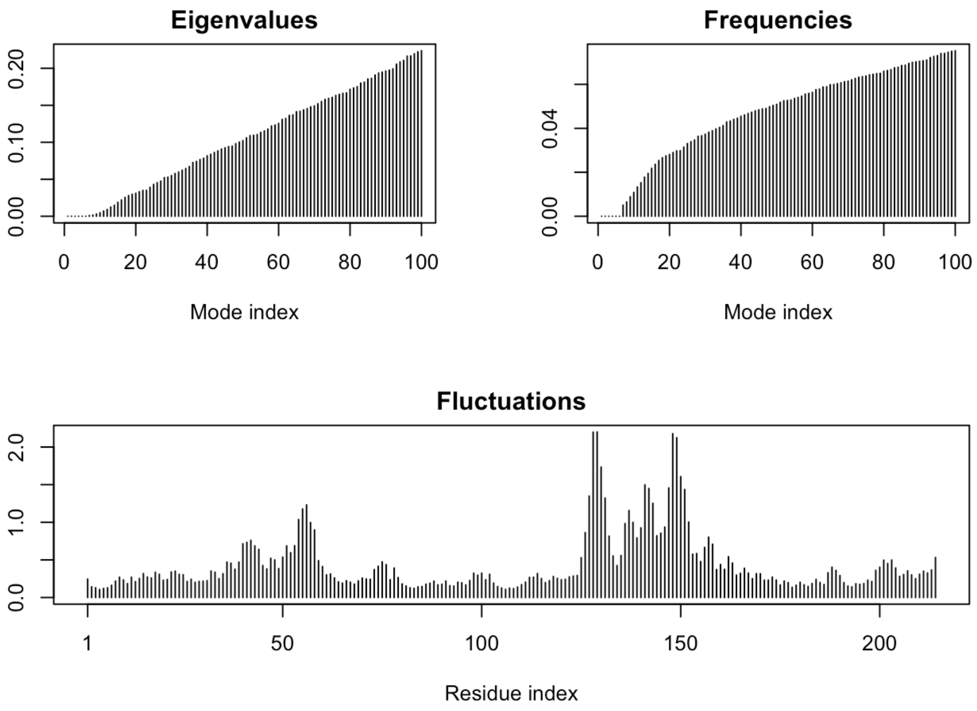
```
 Call:  read.pdb(file = "6s36")
```

```
   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
```

```
m <- nma(adk)
```

```
 Building Hessian...        Done in 0.111 seconds.
 Diagonalizing Hessian...   Done in 0.344 seconds.
```

```
plot(m)
```



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

# 4. Comparative analysis of Adenylate kinase (ADK)

We will start our analysis with a single PDB id (code from the PDB database): 1AKE

First we get its primary sequence:

```r
#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

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

bio3d-view

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

TRUE

```r
aa <- get.seq("1ake_a")
```

```
Warning in get.seq("1ake_a"): Removing existing file:
seqs.fasta

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

```r
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?

214

```
# Blast or hmmer search
#b <- blast.pdb(aa)
```

```
# Plot a summary of search results
#hits <- plot(b)
```

```
# List out some 'top hits'
hits <- NULL
hits$pdb.id <- c('1AKE_A','6S36_A','6RZE_A','3HPR_A','1E4V_A','
head(hits$pdb.id)
```

```
[1] "1AKE_A" "6S36_A" "6RZE_A" "3HPR_A" "1E4V_A" "5EJE_A"
```

```
# Download releated PDB files
files <- get.pdb(hits$pdb.id, path="pdbs", split=TRUE, gzip=TRU
```

```
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/
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/
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/
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


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```
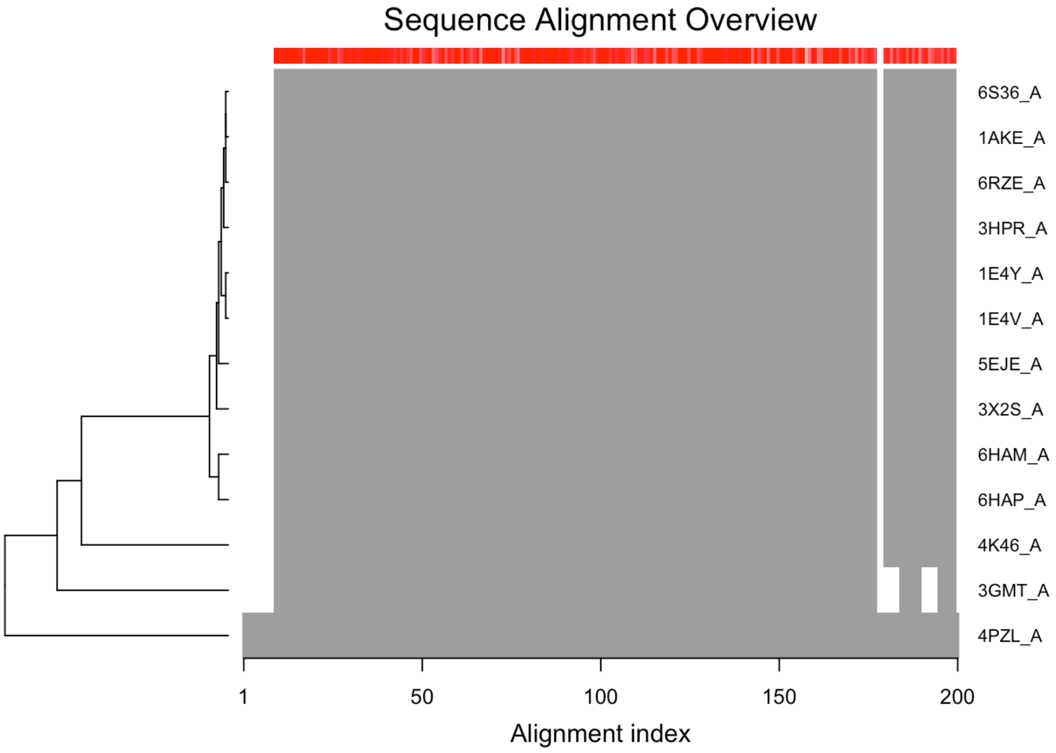

```r
# Align releated PDBs
pdbs <- pdbaln(files, fit = TRUE, exefile="msa")
```

```
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
```

```r
# Vector containing PDB codes for figure axis
ids <- basename.pdb(pdbs$id)

# Draw schematic alignment
plot(pdbs, labels=ids)
```



```r
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, active
site lid (ADK_lid)
6RZE_A       1.69             <NA> Adenylate kinase, active
site lid (ADK_lid)
3HPR_A       2.00             <NA> Adenylate kinase, active
site lid (ADK_lid)
1E4V_A       1.85 Adenylate kinase Adenylate kinase, active
```

```
site lid (ADK_lid)
5EJE_A       1.90             <NA> Adenylate kinase, active
site lid (ADK_lid)
1E4Y_A       1.85 Adenylate kinase Adenylate kinase, active
site lid (ADK_lid)
3X2S_A       2.80             <NA> Adenylate kinase, active
site lid (ADK_lid)
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, active
site lid (ADK_lid)
4PZL_A       2.10             <NA> Adenylate kinase, active
site lid (ADK_lid)
               ligandId
1AKE_A              AP5
6S36_A CL (3),NA,MG (2)
6RZE_A    NA (3),CL (2)
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,FMT,GOL

ligandName
1AKE_A
BIS(ADENOSINE)-5'-PENTAPHOSPHATE
6S36_A                                    CHLORIDE ION
(3),SODIUM ION,MAGNESIUM ION (2)
6RZE_A                                                  SODIUM
ION (3),CHLORIDE ION (2)
3HPR_A
BIS(ADENOSINE)-5'-PENTAPHOSPHATE
1E4V_A
BIS(ADENOSINE)-5'-PENTAPHOSPHATE
5EJE_A                                 BIS(ADENOSINE)-5'-
PENTAPHOSPHATE,COBALT (II) ION
```

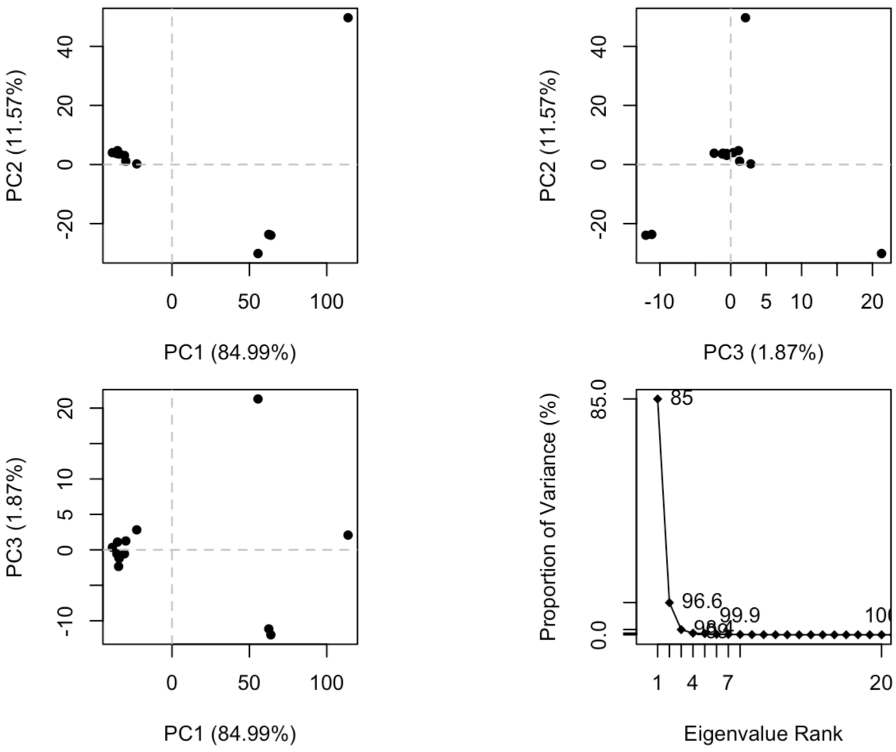
```
1E4Y_A
BIS(ADENOSINE)-5'-PENTAPHOSPHATE
3X2S_A N-(pyren-1-ylmethyl)acetamide (2),BIS(ADENOSINE)-5'-
PENTAPHOSPHATE,MAGNESIUM ION
6HAP_A
BIS(ADENOSINE)-5'-PENTAPHOSPHATE
6HAM_A
BIS(ADENOSINE)-5'-PENTAPHOSPHATE
4K46_A                   ADENOSINE-5'-DIPHOSPHATE,ADENOSINE
MONOPHOSPHATE,PHOSPHATE ION
3GMT_A
SULFATE ION (2)
4PZL_A                                                 CALCIUM
ION,FORMIC ACID,GLYCEROL
                                                 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
```

# Jump to PCA

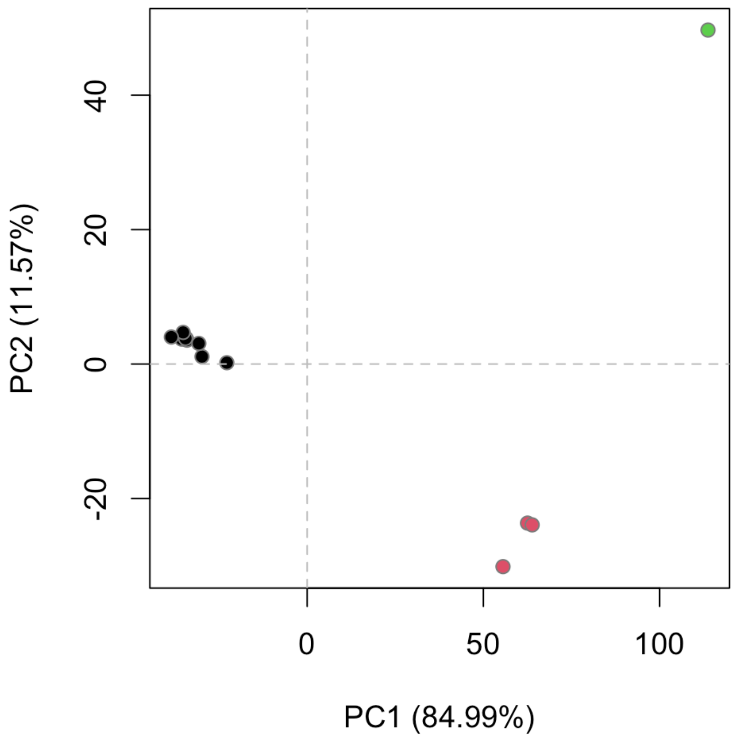
```
# Perform PCA
pc.xray <- pca(pdbs)
plot(pc.xray)
```



```
# Calculate RMSD
rd <- rmsd(pdbs)
```

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

```
# Structure-based clustering
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)
```



## 6. Normal mode analysis [optional]

```
# NMA of all structures
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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|  85%
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  |

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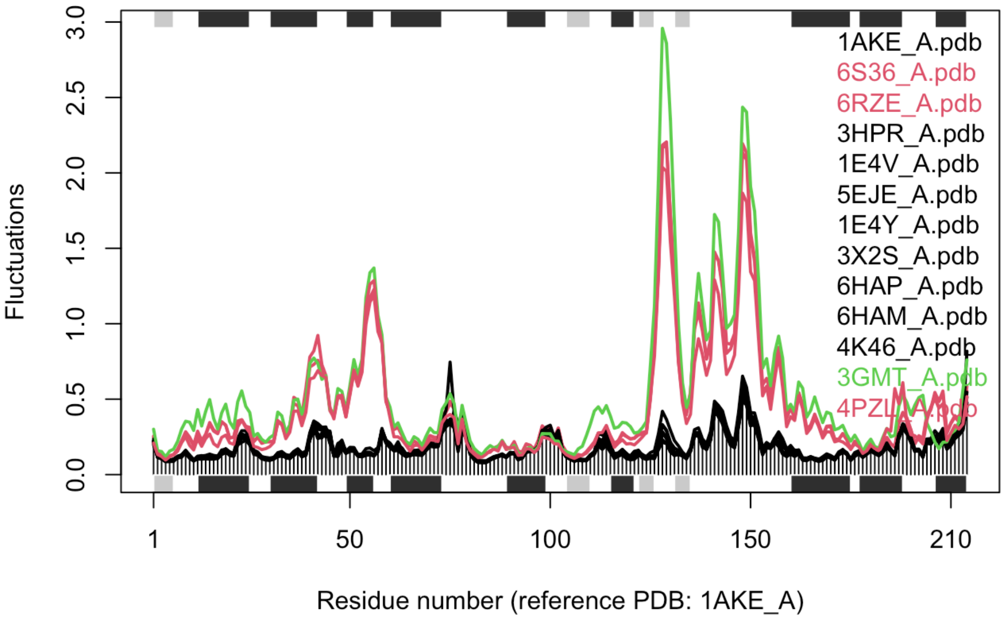

```
plot(modes, pdbs, col=grps.rd)
```

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


Fluctuations
Residue number (reference PDB: 1AKE_A)
1AKE_A.pdb
6S36_A.pdb
6RZE_A.pdb
3HPR_A.pdb
1E4V_A.pdb
5EJE_A.pdb
1E4Y_A.pdb
3X2S_A.pdb
6HAP_A.pdb
6HAM_A.pdb
4K46_A.pdb
3GMT_A.pdb
4PZL_A.pdb