class 9 : structural

Mia Fava

```
library(readr)
pdbdata <- read_csv("Data Export Summary.csv")
```

```
Rows: 6 Columns: 8
-- Column specification --------------------------------------------------------
Delimiter: ","
chr (1): Molecular Type
dbl (3): 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.
```

```
head(pdbdata)
```

```
# A tibble: 6 x 8
  `Molecular Type`   `X-ray`    EM   NMR `Multiple methods` Neutron Other  Total
  <chr>                <dbl> <dbl> <dbl>              <dbl>   <dbl> <dbl>  <dbl>
1 Protein (only)      167317 15698 12534                208      77    32 195866
2 Protein/Oligosacc~    9645  2639    34                  8       2     0  12328
3 Protein/NA            8735  4718   286                  7       0     0  13746
4 Nucleic acid (onl~    2869   138  1507                 14       3     1   4532
5 Other                  170    10    33                  0       0     0    213
6 Oligosaccharide (~      11     0     6                  1       0     4     22
```

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

```
sum(pdbdata$`X-ray`)/sum(pdbdata$Total) *100
```

```
[1] 83.25592
```

Percentage of Xray is 83.3%

```
sum(pdbdata$EM)/sum(pdbdata$Total) *100
```

```
[1] 10.2348
```

Percentage of EM is 10.2%

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

```
pdbdata$Total[1]/sum(pdbdata$Total) *100
```

```
[1] 86.3961
```

> 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?

According to the search data base, there are 226,707 structures of HIV-1 protease.

##Mol*

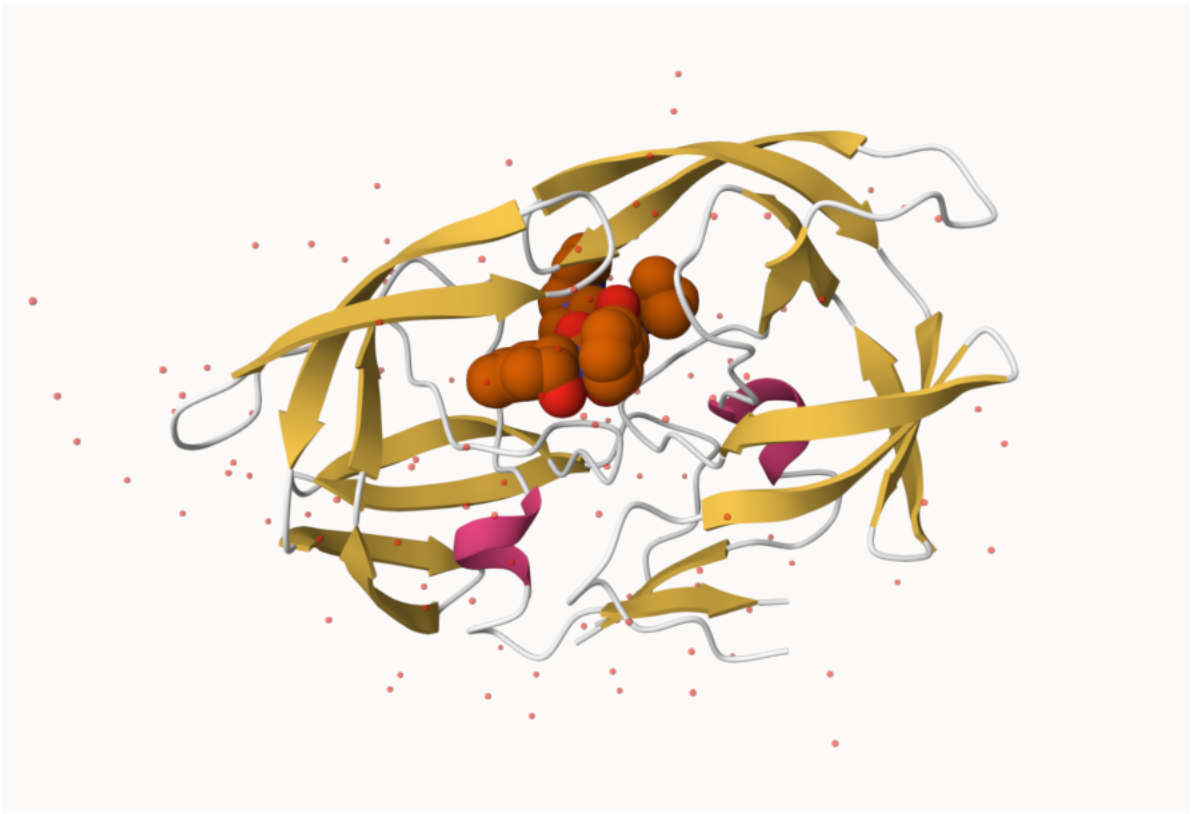


Figure 1: beginning strand

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

There is only one atom per water molecule in this structure due to how the single atom represents only the oxygen. Oxygen is more electron-dense than hydrogen atoms, resulting in them being easier to detect in comparison to hydrogen atoms.

> 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

The critical conserved water molecule for 1HSG residue number was seen to be 301.

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

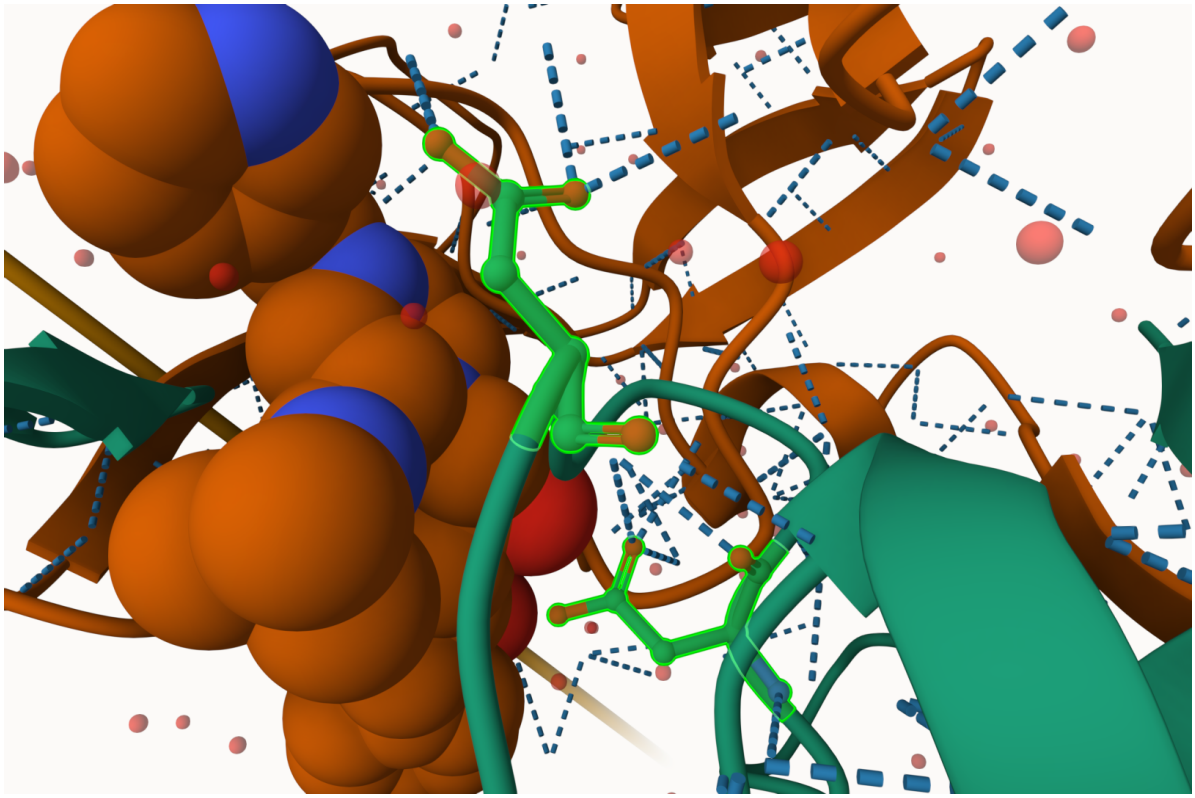


Figure 2: Ligand Strand

> Q7: [Optional] As you have hopefully observed HIV protease is a homodimer (i.e. it is composed of two identical chains). With the aid of the graphic display can you identify secondary structure elements that are likely to only form in the dimer rather than the monomer?

The Beta sheets is an example of secondary structures that would form in the dimer rather than the monomer. Another example would be the residue arrangements of Asp25, as they are positioned where dimerization is necessary for them to interact with each other.

##Introduction to BIO3D

```
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
```

```
attributes(pdb)
```

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

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

```
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
```

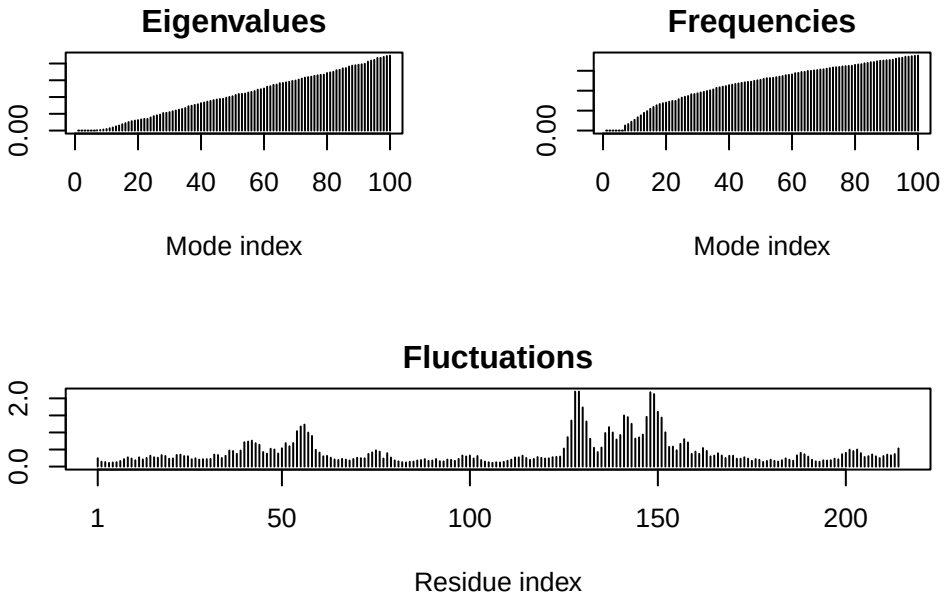
```
adk
```

```
 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
```

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

```
 Building Hessian...        Done in 0.014 seconds.
 Diagonalizing Hessian...   Done in 0.281 seconds.
```

```
plot(m)
```




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

##Comparative analysis of Adenylate Kinase

```
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
```

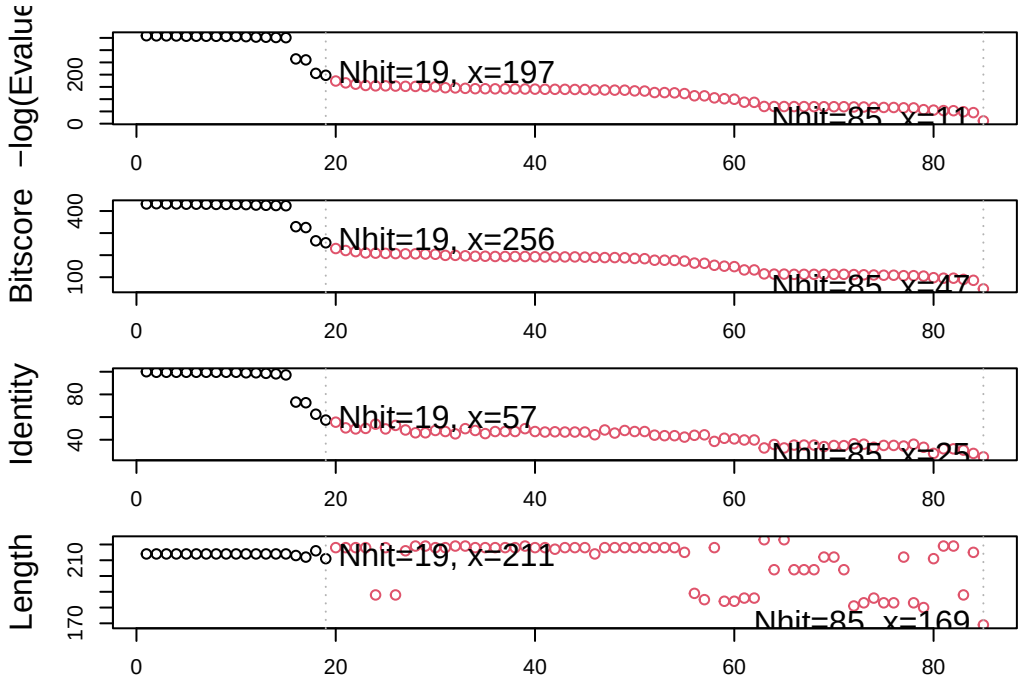
```
# Blast or hmmer search
b <- blast.pdb(aa)
```

```
 Searching ... please wait (updates every 5 seconds) RID = JMYWUN7K016
 ....
 Reporting 85 hits
```

Plot a summary of search results

```
hits <- plot(b)
```

```
  * Possible cutoff values:    197 11
            Yielding Nhits:    19 85

  * Chosen cutoff value of:    197
            Yielding Nhits:    19
```




```
head(hits$pdb.id)
```

```
[1] "1AKE_A" "8BQF_A" "4X8M_A" "6S36_A" "8Q2B_A" "8RJ9_A"
```

```
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/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/4K46.pdb.gz exists. Skipping download

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

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

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


  |
  |                                                                      |   0%
  |
  |====                                                                  |   5%
  |
  |=======                                                               |  11%
  |
  |===========                                                           |  16%
  |
  |===============                                                       |  21%
  |
  |==================                                                    |  26%
  |
  |======================                                                |  32%
  |
  |==========================                                            |  37%
  |
  |==============================                                        |  42%
  |
  |==================================                                    |  47%
  |
  |======================================                                |  53%
  |
  |==========================================                            |  58%
  |
  |==============================================                        |  63%
  |
  |==================================================                    |  68%
  |
  |======================================================                |  74%
  |
  |==========================================================            |  79%
  |
  |==============================================================        |  84%
  |
  |==================================================================    |  89%
  |
  |======================================================================|  95%
```

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

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

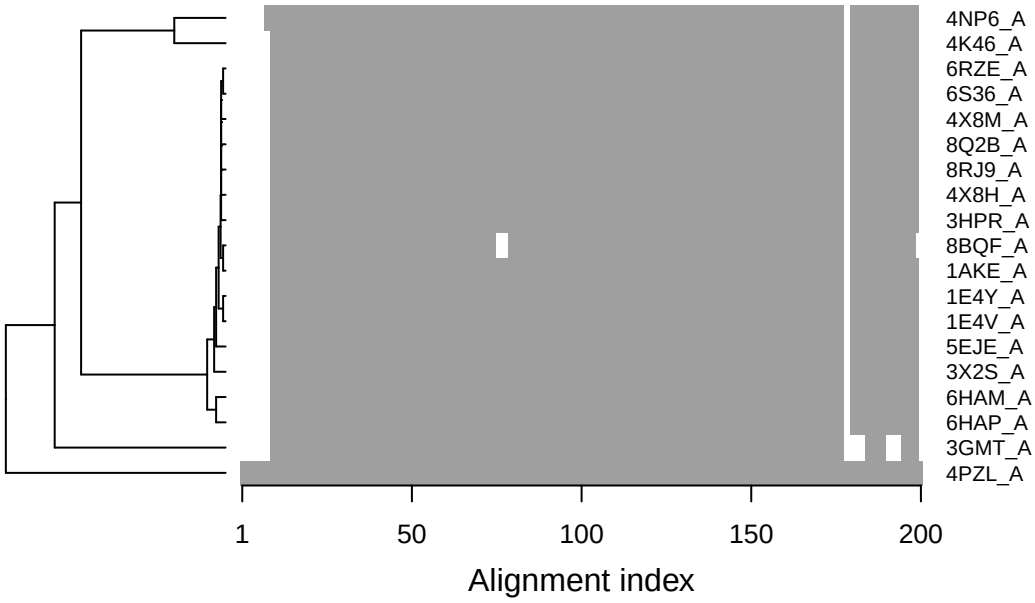
```
Reading PDB files:
pdbs/split_chain/1AKE_A.pdb
pdbs/split_chain/8BQF_A.pdb
pdbs/split_chain/4X8M_A.pdb
pdbs/split_chain/6S36_A.pdb
pdbs/split_chain/8Q2B_A.pdb
pdbs/split_chain/8RJ9_A.pdb
pdbs/split_chain/6RZE_A.pdb
pdbs/split_chain/4X8H_A.pdb
pdbs/split_chain/3HPR_A.pdb
pdbs/split_chain/1E4V_A.pdb
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/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
..   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/8Q2B_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 6   name: pdbs/split_chain/8RJ9_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 7   name: pdbs/split_chain/6RZE_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 8   name: pdbs/split_chain/4X8H_A.pdb
pdb/seq: 9   name: pdbs/split_chain/3HPR_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 10   name: pdbs/split_chain/1E4V_A.pdb
pdb/seq: 11   name: pdbs/split_chain/5EJE_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 12   name: pdbs/split_chain/1E4Y_A.pdb
pdb/seq: 13   name: pdbs/split_chain/3X2S_A.pdb
pdb/seq: 14   name: pdbs/split_chain/6HAP_A.pdb
pdb/seq: 15   name: pdbs/split_chain/6HAM_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 16   name: pdbs/split_chain/4K46_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 17   name: pdbs/split_chain/4NP6_A.pdb
pdb/seq: 18   name: pdbs/split_chain/3GMT_A.pdb
pdb/seq: 19   name: pdbs/split_chain/4PZL_A.pdb
```

```
library(bio3d)
# vector containing PDB codes for figure axis
ids <- basename.pdb(pdbs$id)

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

```
Error in plot.new(): figure margins too large
```

```
str(pdbs)
```




```
List of 9
 $ xyz  : 'xyz' num [1:19, 1:681] NA NA NA NA NA NA NA NA NA NA ...
  ..- attr(*, "dimnames")=List of 2
  .. ..$ : chr [1:19] "pdbs/split_chain/1AKE_A.pdb" "pdbs/split_chain/8BQF_A.pdb" "pdbs/split
  .. ..$ : NULL
 $ resno: int [1:19, 1:227] NA NA NA NA NA NA NA NA NA NA ...
  ..- attr(*, "dimnames")=List of 2
  .. ..$ : chr [1:19] "pdbs/split_chain/1AKE_A.pdb" "pdbs/split_chain/8BQF_A.pdb" "pdbs/split
  .. ..$ : NULL
 $ b    : num [1:19, 1:227] NA NA NA NA NA NA NA NA NA NA ...
  ..- attr(*, "dimnames")=List of 2
  .. ..$ : chr [1:19] "pdbs/split_chain/1AKE_A.pdb" "pdbs/split_chain/8BQF_A.pdb" "pdbs/split
  .. ..$ : NULL
 $ chain: chr [1:19, 1:227] NA NA NA NA ...
  ..- attr(*, "dimnames")=List of 2
  .. ..$ : chr [1:19] "pdbs/split_chain/1AKE_A.pdb" "pdbs/split_chain/8BQF_A.pdb" "pdbs/split
  .. ..$ : NULL
 $ id   : chr [1:19] "pdbs/split_chain/1AKE_A.pdb" "pdbs/split_chain/8BQF_A.pdb" "pdbs/split_
 $ ali  : chr [1:19, 1:227] "-" "-" "-" "-" ...
  ..- attr(*, "dimnames")=List of 2
  .. ..$ : chr [1:19] "pdbs/split_chain/1AKE_A.pdb" "pdbs/split_chain/8BQF_A.pdb" "pdbs/split
  .. ..$ : NULL
 $ resid: chr [1:19, 1:227] NA NA NA NA ...
  ..- attr(*, "dimnames")=List of 2
  .. ..$ : chr [1:19] "pdbs/split_chain/1AKE_A.pdb" "pdbs/split_chain/8BQF_A.pdb" "pdbs/split
```

```
  .. ..$ : NULL
 $ sse  : chr [1:19, 1:227] NA NA NA NA ...
  ..- attr(*, "dimnames")=List of 2
  .. ..$ : chr [1:19] "pdbs/split_chain/1AKE_A.pdb" "pdbs/split_chain/8BQF_A.pdb" "pdbs/split
  .. ..$ : NULL
 $ call : language pdbaln(files = files, fit = TRUE, exefile = "msa")
 - attr(*, "class")= chr [1:2] "pdbs" "fasta"
```

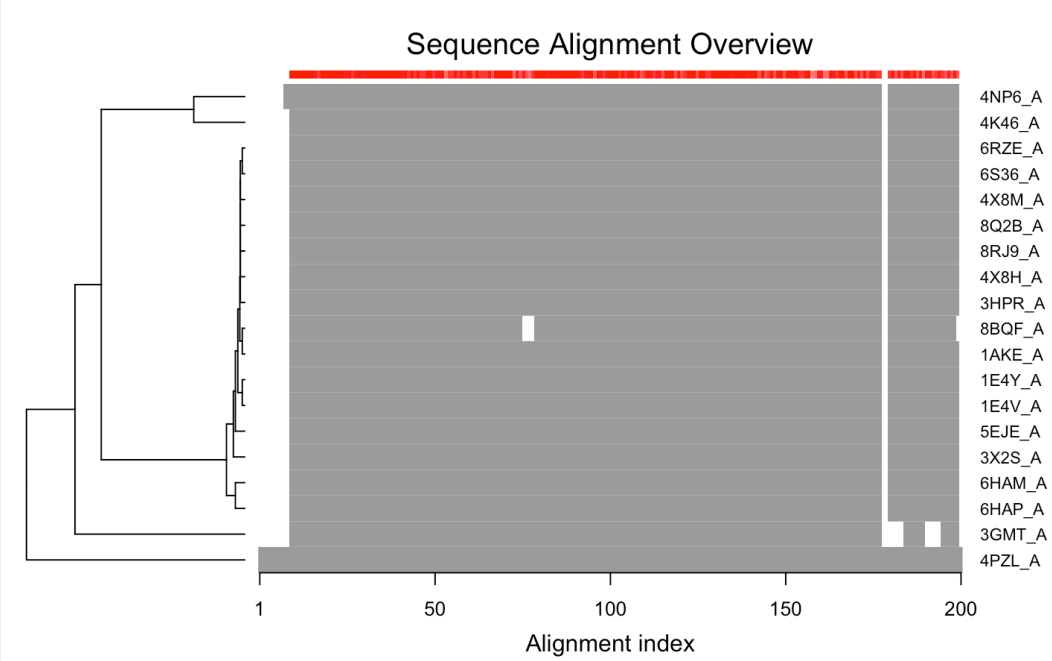


Figure 3: Alignment index because margins too big

```
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] "Vibrio cholerae O1 biovar El Tor str. N16961"
[7] "Burkholderia pseudomallei 1710b"
[8] "Francisella tularensis subsp. tularensis SCHU S4"
```

```
anno
```

	structureId	chainId	macromoleculeType	chainLength	experimentalTechnique
1AKE_A	1AKE	A	Protein	214	X-ray
8BQF_A	8BQF	A	Protein	234	X-ray
4X8M_A	4X8M	A	Protein	214	X-ray
6S36_A	6S36	A	Protein	214	X-ray
8Q2B_A	8Q2B	A	Protein	214	X-ray
8RJ9_A	8RJ9	A	Protein	214	X-ray
6RZE_A	6RZE	A	Protein	214	X-ray
4X8H_A	4X8H	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
4NP6_A	4NP6	A	Protein	217	X-ray
3GMT_A	3GMT	A	Protein	230	X-ray
4PZL_A	4PZL	A	Protein	242	X-ray

	resolution	scopDomain	pfam
1AKE_A	2.000	Adenylate kinase	Adenylate kinase, active site lid (ADK_lid)
8BQF_A	2.050	<NA>	Adenylate kinase, active site lid (ADK_lid)
4X8M_A	2.600	<NA>	Adenylate kinase, active site lid (ADK_lid)
6S36_A	1.600	<NA>	Adenylate kinase, active site lid (ADK_lid)
8Q2B_A	1.760	<NA>	Adenylate kinase (ADK)
8RJ9_A	1.590	<NA>	Adenylate kinase, active site lid (ADK_lid)
6RZE_A	1.690	<NA>	Adenylate kinase (ADK)
4X8H_A	2.500	<NA>	Adenylate kinase, active site lid (ADK_lid)
3HPR_A	2.000	<NA>	Adenylate kinase, active site lid (ADK_lid)
1E4V_A	1.850	Adenylate kinase	Adenylate kinase (ADK)
5EJE_A	1.900	<NA>	Adenylate kinase, active site lid (ADK_lid)
1E4Y_A	1.850	Adenylate kinase	Adenylate kinase, active site lid (ADK_lid)
3X2S_A	2.800	<NA>	Adenylate kinase (ADK)
6HAP_A	2.700	<NA>	Adenylate kinase (ADK)
6HAM_A	2.550	<NA>	Adenylate kinase, active site lid (ADK_lid)
4K46_A	2.010	<NA>	Adenylate kinase, active site lid (ADK_lid)
4NP6_A	2.004	<NA>	Adenylate kinase (ADK)
3GMT_A	2.100	<NA>	Adenylate kinase, active site lid (ADK_lid)
4PZL_A	2.100	<NA>	Adenylate kinase (ADK)

	ligandId	ligandName	source
1AKE_A	AP5	BIS(ADENOSINE)-5'-PENTAPHOSPHATE	Escherichia coli
8BQF_A	AP5	BIS(ADENOSINE)-5'-PENTAPHOSPHATE	Escherichia coli
4X8M_A	<NA>	<NA>	
6S36_A	CL (3),NA,MG (2)	CHLORIDE ION (3),SODIUM ION,MAGNESIUM ION (2)	
8Q2B_A	AP5,SO4,MPO	BIS(ADENOSINE)-5'-PENTAPHOSPHATE,SULFATE ION,3[N-MORPHOLINO]PROPANE SULFONIC ACID	
8RJ9_A	ADP (2)	ADENOSINE-5'-DIPHOSPHATE (2)	
6RZE_A	NA (3),CL (2)	SODIUM ION (3),CHLORIDE ION (2)	
4X8H_A	<NA>	<NA>	
3HPR_A	AP5	BIS(ADENOSINE)-5'-PENTAPHOSPHATE	
1E4V_A	AP5	BIS(ADENOSINE)-5'-PENTAPHOSPHATE	
5EJE_A	AP5,CO	BIS(ADENOSINE)-5'-PENTAPHOSPHATE,COBALT (II) ION	
1E4Y_A	AP5	BIS(ADENOSINE)-5'-PENTAPHOSPHATE	
3X2S_A	JPY (2),AP5,MG	N-(pyren-1-ylmethyl)acetamide (2),BIS(ADENOSINE)-5'-PENTAPHOSPHATE,MAGNESIUM ION	
6HAP_A	AP5	BIS(ADENOSINE)-5'-PENTAPHOSPHATE	
6HAM_A	AP5	BIS(ADENOSINE)-5'-PENTAPHOSPHATE	
4K46_A	ADP,AMP,PO4	ADENOSINE-5'-DIPHOSPHATE,ADENOSINE MONOPHOSPHATE,PHOSPHATE ION	
4NP6_A	<NA>	<NA>	
3GMT_A	SO4 (2)	SULFATE ION (2)	
4PZL_A	CA,FMT,GOL	CALCIUM ION,FORMIC ACID,GLYCEROL	

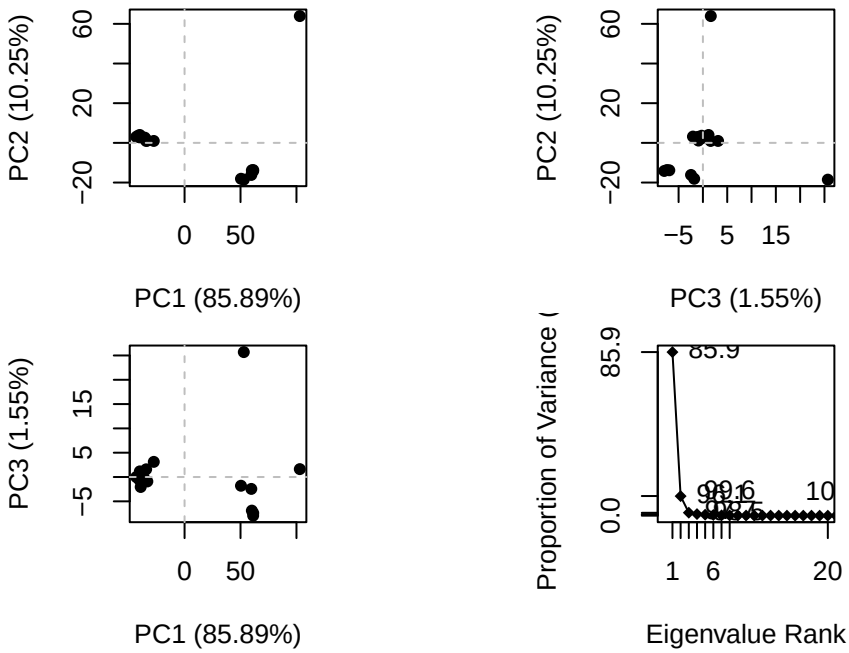
4X8M_A	Escherichia coli	
6S36_A	Escherichia coli	
8Q2B_A	Escherichia coli	
8RJ9_A	Escherichia coli	
6RZE_A	Escherichia coli	
4X8H_A	Escherichia coli	
3HPR_A	Escherichia coli K-12	
1E4V_A	Escherichia coli	
5EJE_A	Escherichia coli O139:H28 str. E24377A	
1E4Y_A	Escherichia coli	
3X2S_A	Escherichia coli str. K-12 substr. MDS42	
6HAP_A	Escherichia coli O139:H28 str. E24377A	
6HAM_A	Escherichia coli K-12	
4K46_A	Photobacterium profundum	
4NP6_A	Vibrio cholerae O1 biovar El Tor str. N16961	
3GMT_A	Burkholderia pseudomallei 1710b	
4PZL_A	Francisella tularensis subsp. tularensis SCHU S4	

1AKE_A	STRUCTURE OF THE COMPLEX BETWEEN ADENYLATE KINASE FROM ESCHERICHIA COLI AND THE INHIBI
8BQF_A	
4X8M_A	
6S36_A	
8Q2B_A	E. coli Adenylate Kinase variant D158A (
8RJ9_A	E. coli adenylate kinase Asp84
6RZE_A	
4X8H_A	
3HPR_A	
1E4V_A	
5EJE_A	Cryst
1E4Y_A	
3X2S_A	
6HAP_A	
6HAM_A	
4K46_A	
4NP6_A	
3GMT_A	
4PZL_A	The cryst

	citation	rObserved	rFree
1AKE_A	Muller, C.W., et al. J Mol Biol (1992)	0.19600	NA
8BQF_A	Scheerer, D., et al. Proc Natl Acad Sci U S A (2023)	0.22073	0.25789
4X8M_A	Kovermann, M., et al. Nat Commun (2015)	0.24910	0.30890
6S36_A	Rogne, P., et al. Biochemistry (2019)	0.16320	0.23560
8Q2B_A	Nam, K., et al. J Chem Inf Model (2024)	0.18320	0.22440

```
8RJ9_A                         Nam, K., et al. Sci Adv (2024)   0.15190 0.20290
6RZE_A                   Rogne, P., et al. Biochemistry (2019)   0.18650 0.23500
4X8H_A                 Kovermann, M., et al. Nat Commun (2015)   0.19610 0.28950
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
4NP6_A                        Kim, Y., et al. To be published   0.18800 0.22200
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
8BQF_A 0.21882  P 2 21 21
4X8M_A 0.24630    C 1 2 1
6S36_A 0.15940    C 1 2 1
8Q2B_A 0.18100   P 1 21 1
8RJ9_A 0.15010  P 21 21 2
6RZE_A 0.18190    C 1 2 1
4X8H_A 0.19140    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
4NP6_A 0.18600       P 43
3GMT_A 0.23500   P 1 21 1
4PZL_A 0.19130       P 32
```

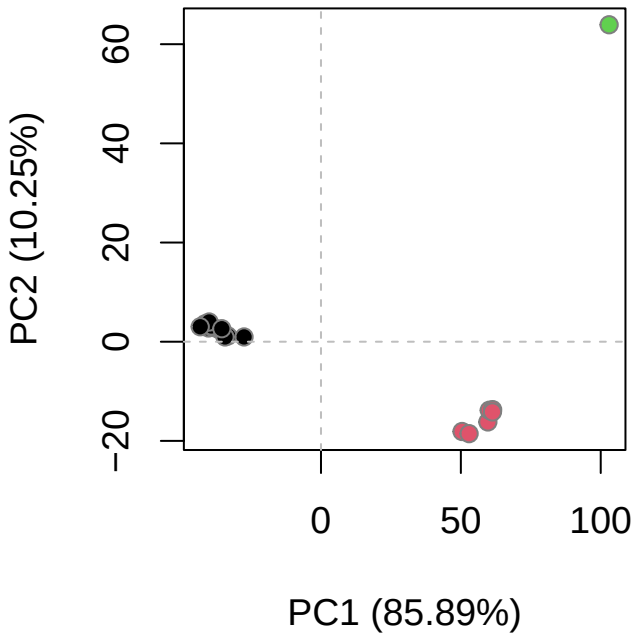
```
# Perform PCA
pc.xray <- pca(pdbs)
plot(pc.xray)
```




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

```
Warning in rmsd(pdbs): No indices provided, using the 199 non NA positions
```

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

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




```
                                  [,1]        [,2]
pdbs/split_chain/1AKE_A.pdb -39.03740   3.0421850
pdbs/split_chain/8BQF_A.pdb -36.37905   2.4249533
pdbs/split_chain/4X8M_A.pdb  59.65065 -16.1779052
pdbs/split_chain/6S36_A.pdb  60.14366 -13.8206057
pdbs/split_chain/8Q2B_A.pdb -33.27350   1.1612328
pdbs/split_chain/8RJ9_A.pdb -41.51263   3.5939187
pdbs/split_chain/6RZE_A.pdb  61.36041 -13.6961278
pdbs/split_chain/4X8H_A.pdb  61.29688 -14.1643852
pdbs/split_chain/3HPR_A.pdb -40.24653   2.7785289
pdbs/split_chain/1E4V_A.pdb -38.73611   2.8738870
pdbs/split_chain/5EJE_A.pdb -39.20371   3.1681058
pdbs/split_chain/1E4Y_A.pdb -34.30994   0.9572993
pdbs/split_chain/3X2S_A.pdb -39.98943   3.9793904
pdbs/split_chain/6HAP_A.pdb -27.50232   0.9631241
pdbs/split_chain/6HAM_A.pdb -35.45248   2.6237571
pdbs/split_chain/4K46_A.pdb -43.17271   3.0175923
pdbs/split_chain/4NP6_A.pdb  50.42370 -18.1043626
pdbs/split_chain/3GMT_A.pdb 102.99489  63.9179475
pdbs/split_chain/4PZL_A.pdb  52.94564 -18.5385358
```

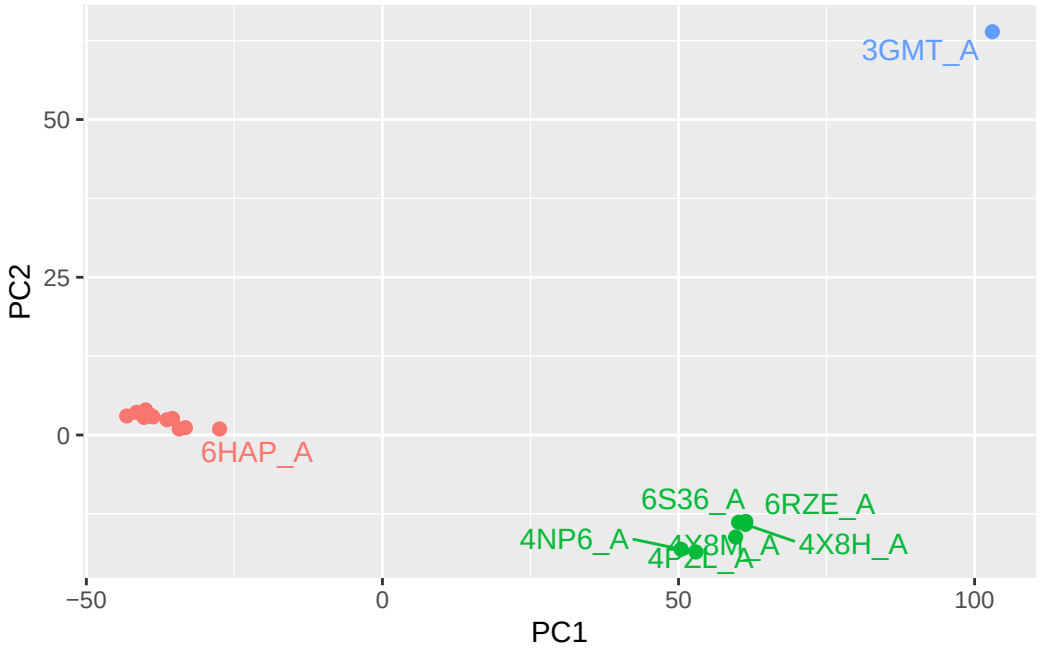
##Optional Further Investigation

```
# Visualize first principal component
pc1 <- mktrj(pc.xray, pc=1, file="pc_1.pdb")
```

```
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
```

```
Warning: ggrepel: 11 unlabeled data points (too many overlaps). Consider
increasing max.overlaps
```



Optional futher visualization

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

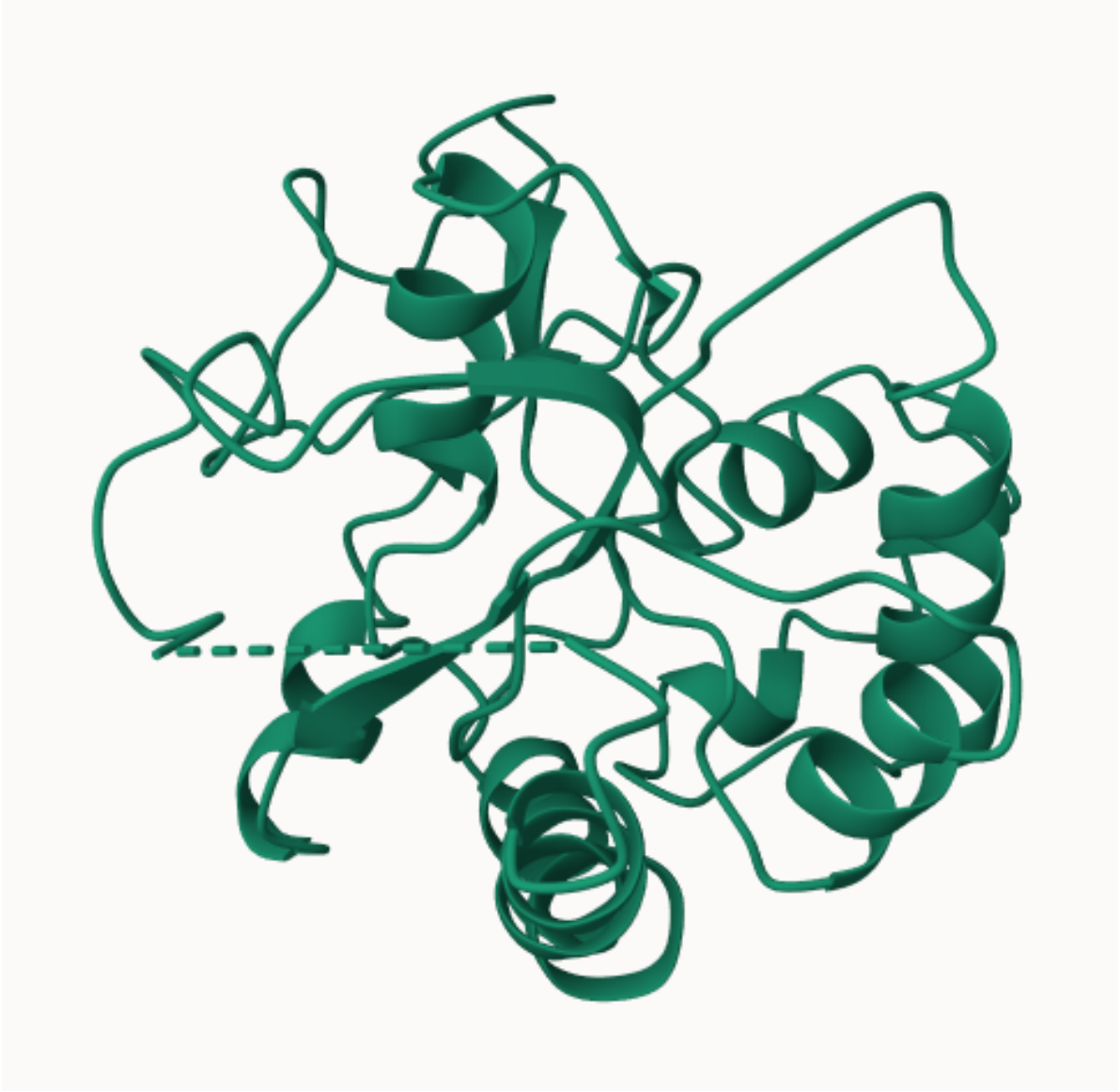


Figure 4: MolStar of pc1

```
uniprot <-248838887
pdb <- 195610

pdb/uniprot * 100
```

```
[1] 0.0786091
```