Class 9 Structural Bioinformatics (Pt.1)

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Introduction to the RCSB PDB

Download a CSV file from the PDB site

```
Data_Export_Summary <- read.csv("Data Export Summary.csv")
des <- Data_Export_Summary
```

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

```
# I kept getting error messages for this part so I manually calculated the
sum for total structures, xray structures, and em structures. At first the
sum function worked but I had problems when knitting.

# Calculate the total number of structures
total_structures <- 215908

# Calculate the number of structures solved by X-Ray and Electron Microscopy
xray_structures <- 182491
em_structures <- 18889

# Calculate the percentage of structures solved by X-Ray and Electron
Microscopy
percentage_xray <- (xray_structures / total_structures) * 100
percentage_em <- (em_structures / total_structures) * 100

# Display percentages
percentage_xray
```

```
## [1] 84.52257
```

```
percentage_em
```

```
## [1] 8.748634
```

```
# Add the two percentages
sum(percentage_xray,percentage_em)
```

```
## [1] 93.27121
```

Answer: For X-ray 84.52%, and for electron microscopy 8.75%. Together this is 93.27%.

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

```
# Again I had issues with the sum function when knitting.

# Calculate the amount of protein
protein <- 211299

#Display amount of protein
protein
```

```
## [1] 211299
```

```
# Find proportion or percent of structures that are proteins
percentage_protein <- (protein/total_structures)*100

#Display percentage of proteins
percentage_protein
```

```
## [1] 97.86529
```

I included protein only, protein/oligosaccharide, and protein/NA and found that 97.9% of the structures are proteins.

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?

The search for HIV displays 4,412 structures.

Visualizing the HIV-1 Protease Structure

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

This simplification is done to reduce visual clutter and make it easier to interpret the structure since water molecules are so abundant.

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, the residue number is 313.

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?

Ligands and substrates can enter the binding site by inducing conformational changes.

Introduction to Bio3D in R

```
# Load the Bio3D package
library(bio3d)

# Read PDB file
pdb <- read.pdb("1hsg")
```

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

```
# Quick summary of the contents of the pdb
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?

There are 198 amino acid residues.

Q8 Name one of the two non-protein residues?

HOH is one of the non-protein residues.

Q9 How many protein chains are in this structure?

There are 2 protein chains.

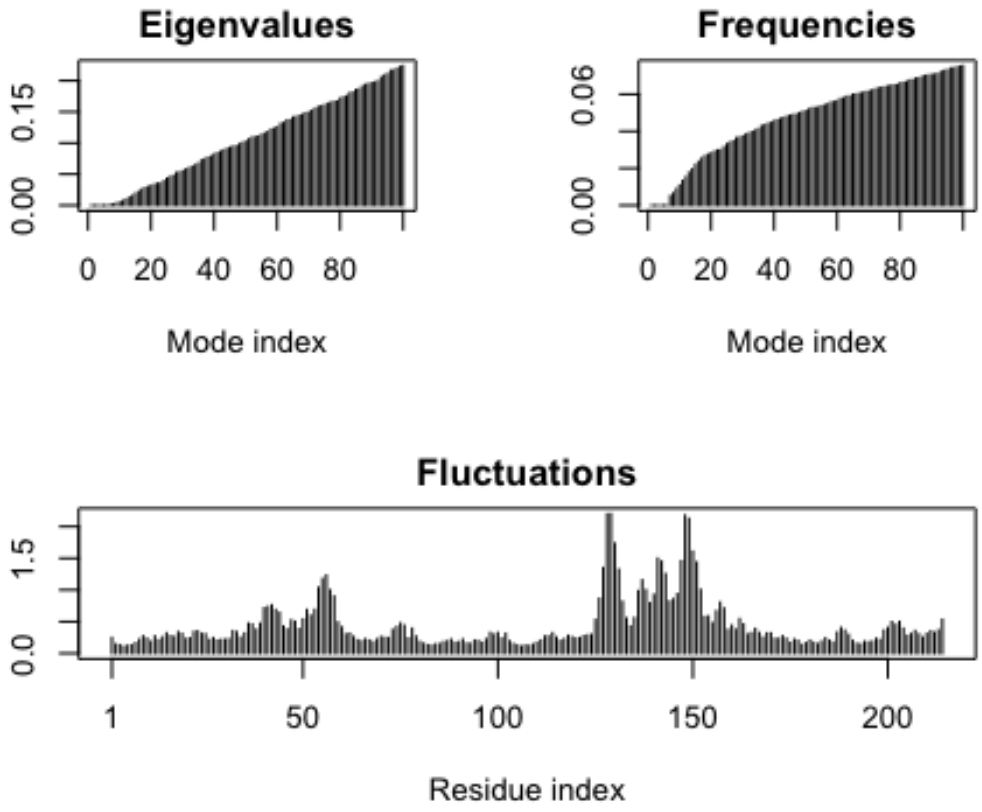
```
# Find the attributes
attributes(pdb)

## $names
## [1] "atom"   "xyz"    "seqres" "helix"  "sheet"  "calpha" "remark" "call"
##
## $class
## [1] "pdb" "sse"

# Acess the atom attribute
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>

# Read a new PDB structure of Adenylate Kinase and perform Normal mode
analysis
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 0.017 seconds.
##  Diagonalizing Hessian...    Done in 0.278 seconds.
```

```
plot(m)
```




```
# View a "movie" of these predicted motions/generate a molecular "trajectory"
with the mktrj() function.
mktrj(m, file="adk_m7.pdb")
```

Comparative structure analysis of Adenylate Kinase

```
# Install packages in the R console NOT your Rmd/Quarto file
```

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

msa is found only on BioConductor.

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

bio3d-view is not found on BioConductor or CRAN.

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

True.

Search and retrieve ADK structures

```
# Search and retrieve ADK structures
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
```

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

There are 214 amino acids in this sequence.

```
# Use this sequence as a query to BLAST search the PDB to find similar
sequences and structures.

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

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

Visualize and filter blast results

```
# List out some 'top hits'
#head(hits$pdb.id)

hits <- NULL
hits$pdb.id <-
c('1AKE_A','6S36_A','6RZE_A','3HPR_A','1E4V_A','5EJE_A','1E4Y_A','3X2S_A','6H
AP_A','6HAM_A','4K46_A','3GMT_A','4PZL_A')

# Download releated 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/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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```

Align and superpose structures

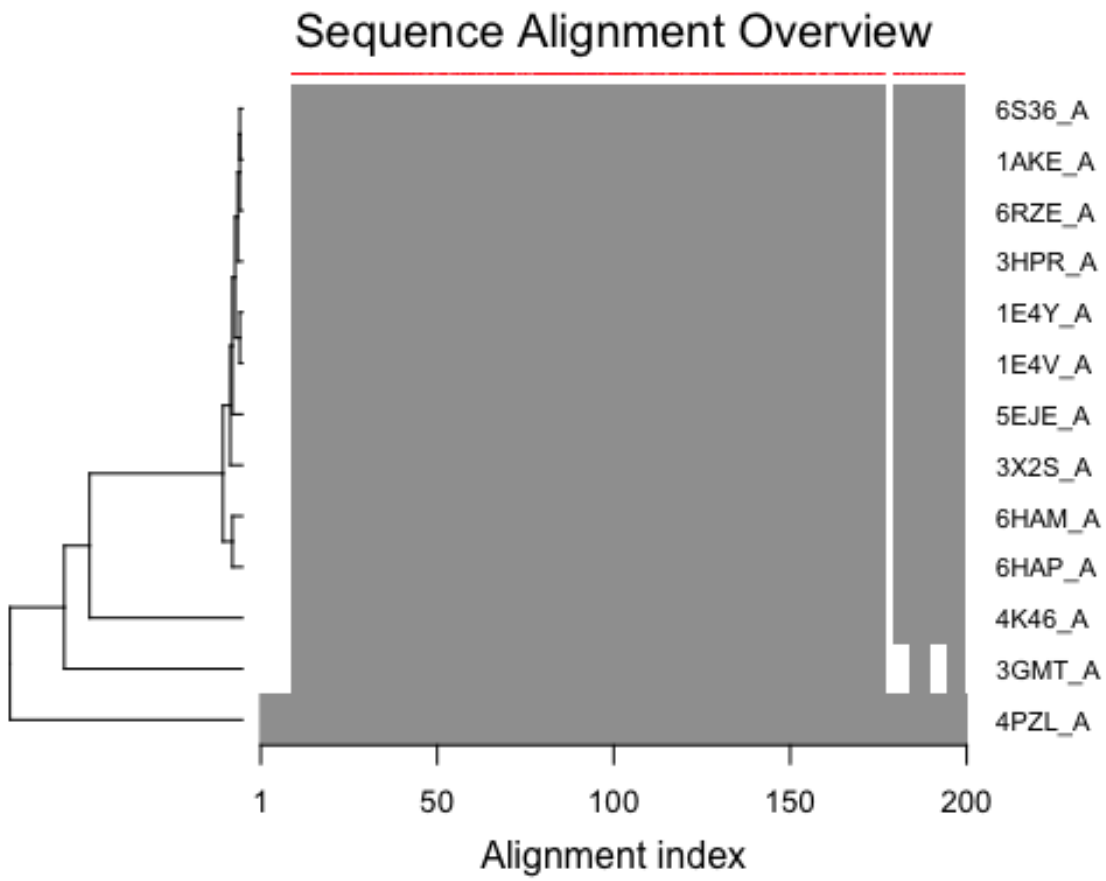
```
# Align releated PDBs
pdbs <- pdbaln(files, fit = TRUE, exefile="msa")

## 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

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

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



Annotate collected PDB structures

```
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"

# View all available annotation data
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
(ADK)
## 1E4V_A       1.85 Adenylate kinase                      Adenylate kinase
(ADK)
## 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
(ADK)
## 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
```

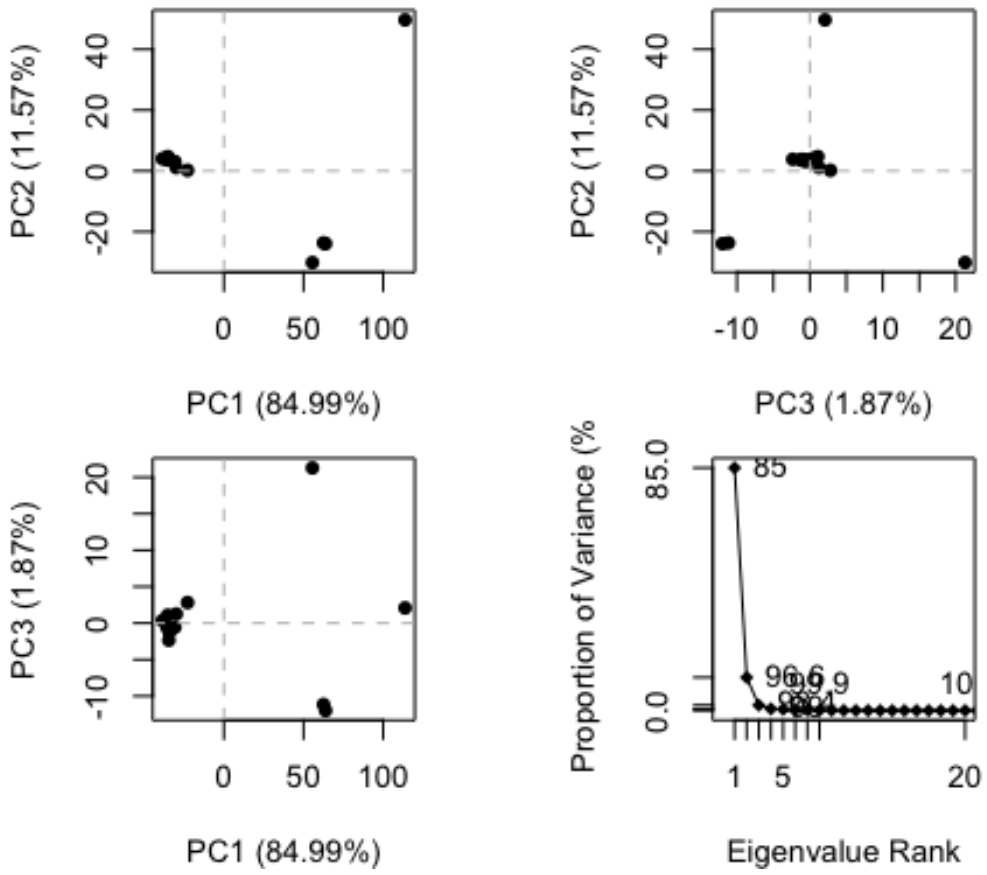
```
## 6S36_A CL (3),NA,MG (2)
## 6RZE_A    NA (3),CL (2)
## 3HPR_A              AP5
## 1E4V_A              AP5
## 5EJE_A           AP5,CO
## 1E4Y_A              AP5
## 3X2S_A   JPY (2),AP5,MG
## 6HAP_A              AP5
## 6HAM_A              AP5
## 4K46_A      ADP,AMP,PO4
## 3GMT_A          SO4 (2)
## 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
```

Principal component analysis

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



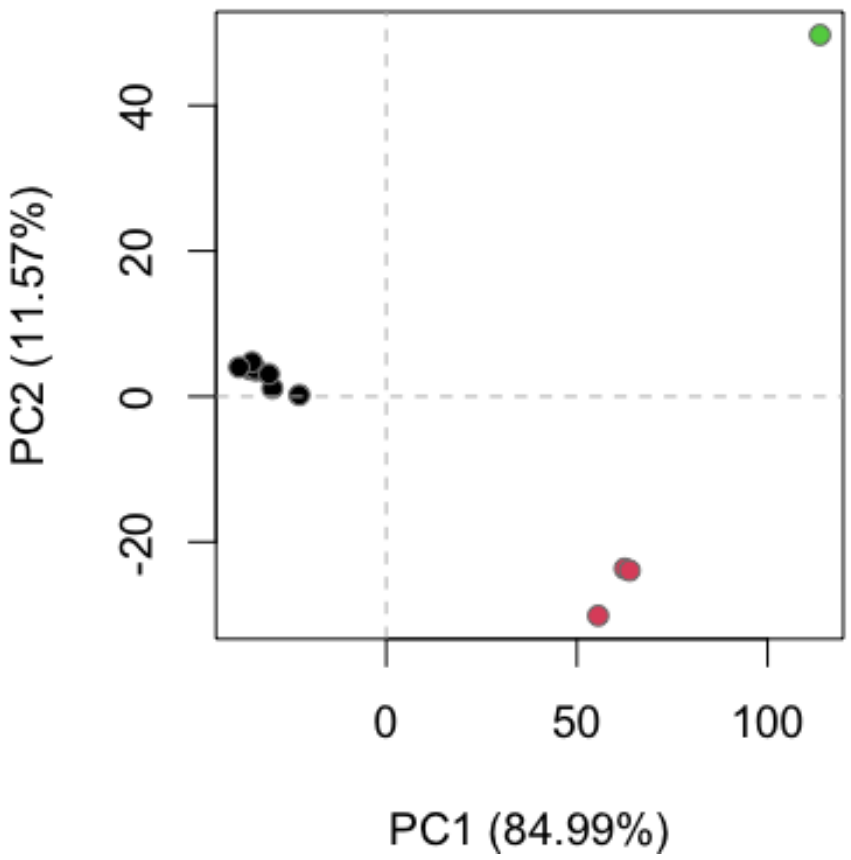
Calculate all pairwise RMSD values of the structural ensemble

```
# 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)
```


PC2 (11.57%)
40
20
0
-20
0
50
100
PC1 (84.99%)