class10 structural bioinf pt1

Sylvia ho a18482382

pdb database

prothein data bank is main repo of biomol structure data >q1 81, 13 % in pdb solved by x ray and em

q2 1

```
stats<- read.csv(url("https://tinyurl.com/pdbstats26"))
stat<- data.frame(stats)
```

```
df <- stat[, -1]

n.sums<-colSums(df)
n<- n.sums/n.sums["Total"]
round(n, digits = 2)
```

```
           X.ray               EM              NMR      Integrative
            0.81             0.13             0.06             0.00
Multiple.methods          Neutron            Other            Total
            0.00             0.00             0.00             1.00
```

q3 1,173

molstar

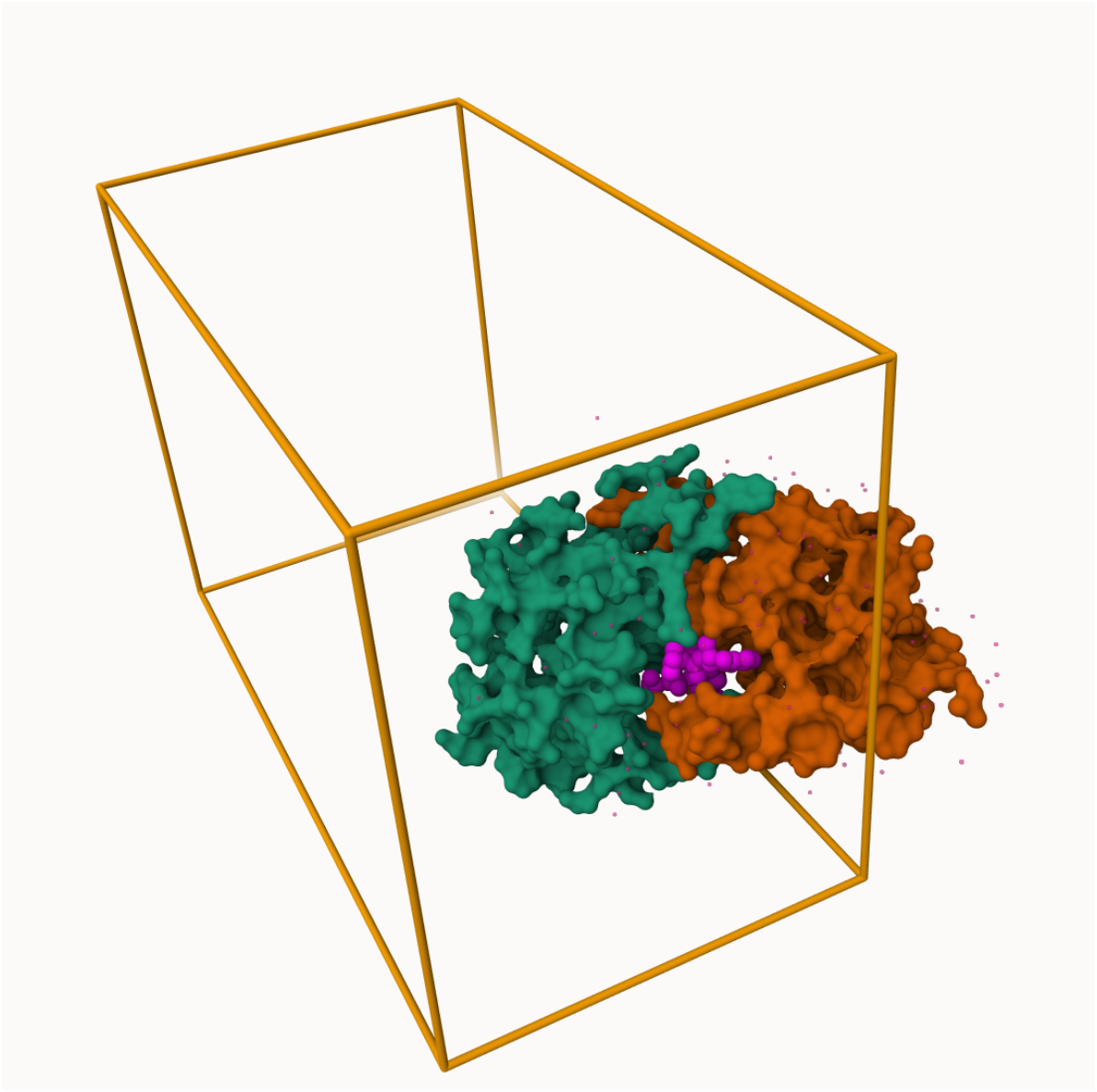


Figure 1: olstar 1hsb

Q4: Water molecules normally have 3 atoms. Why do we see just one atom per water molecule in this structure? microscopy detected es not full nuclei

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

1552

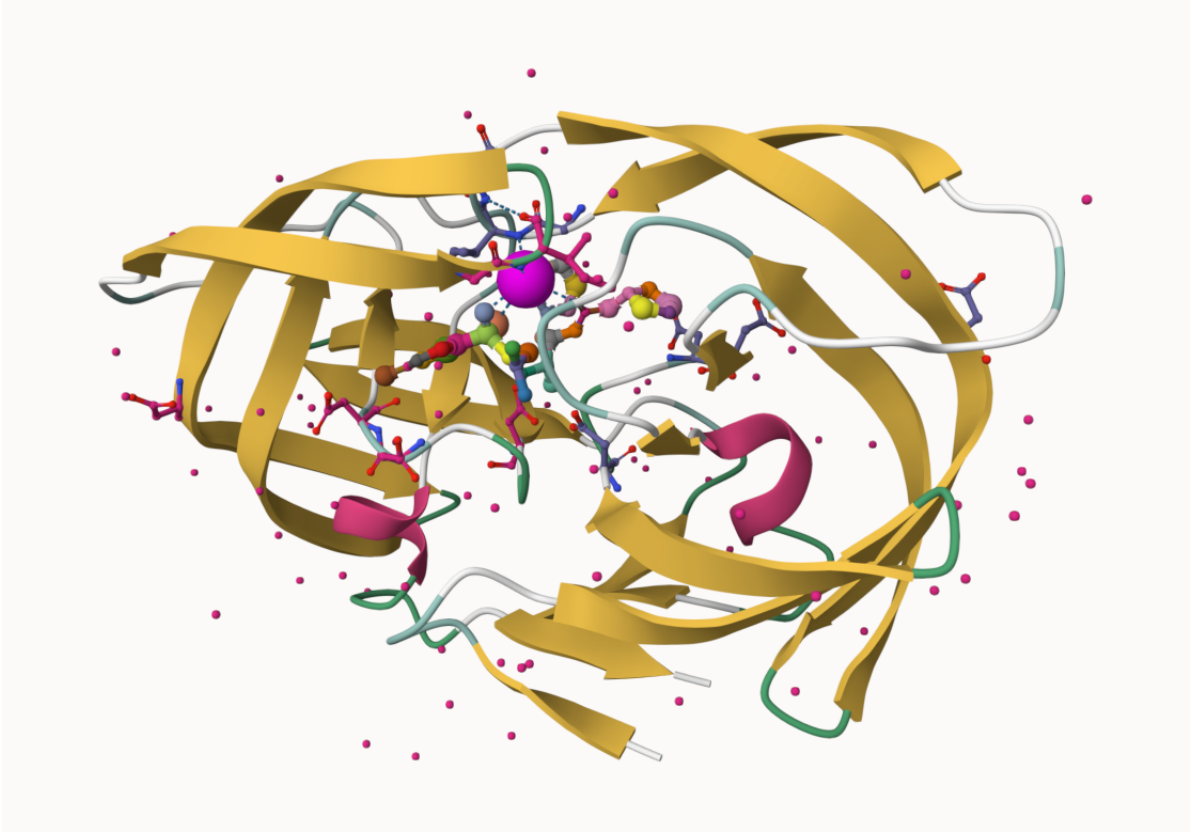


Figure 2: olstar hpv pr

q6 gen img hiv pr cartoon colored by secondary strcuture, showing inhibitor (lignad) ball and stick

q7 the asps at the secondary site, the loops on both sides

##bio3d

```
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? - 128

Q8: Name one of the two non-protein residues? - h2o, mk1

Q9: How many protein chains are in this structure? - 2

```
hide<- pdbseq(hiv)
attributes(hiv)
```

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

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

bio3dview pkg not yet on cran. can use **remotes** pkg ot install

```
library(bio3dview)
library(NGLVieweR)

hid<- view.pdb(hiv) |>
  setSpin()
```

```
# Select the important ASP 25 residue
sele <- atom.select(hiv, resno=25)

# and highlight them in spacefill representation
hides<- view.pdb(hiv, cols=c("navy","pink"),
         highlight = sele,
         highlight.style = "spacefill") |>
  setRock()
```

predict protein flex

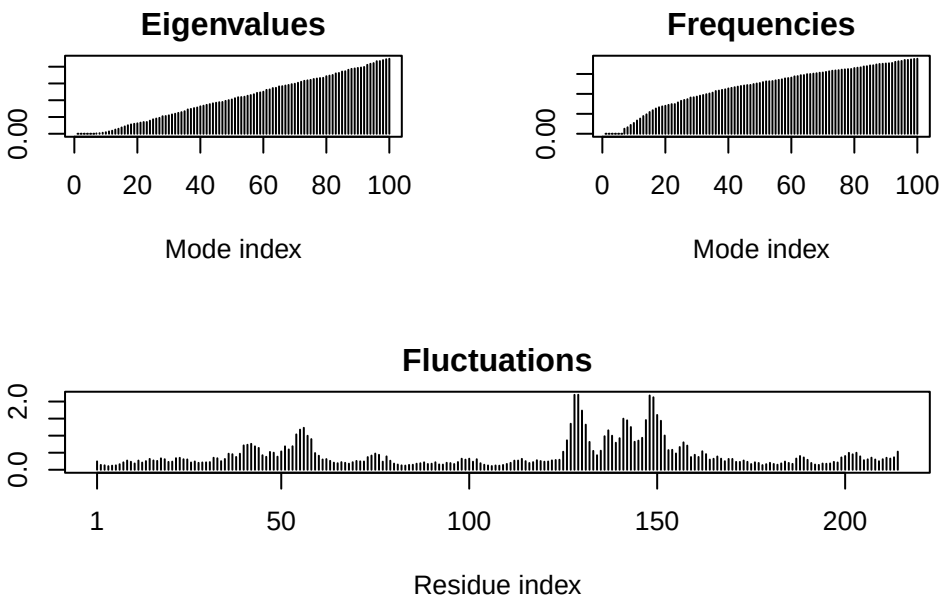
```
adk <- read.pdb("6s36")
```

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

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

```
 Building Hessian...        Done in 0.029 seconds.
 Diagonalizing Hessian...   Done in 0.39 seconds.
```

```
plot (m)
```




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

```
hide3<- view.nma(m, pdb=adk)
```

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

Q11. bio3dview Which of the above packages is not found on BioConductor or CRAN?:

Q12. TRUE Functions from the pak package can be used to install packages from GitHub and BitBucket?

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

```
# Blast or hmmer search
#b <- blast.pdb(aa)
# Plot a summary of search results
#hits <- plot(b)
# 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
```

```
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
```

```
  |
  |                                                                      |   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
```

##annotate

```
# Vector containing PDB database codes
ids <- basename.pdb(pdbs$id)

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)
```

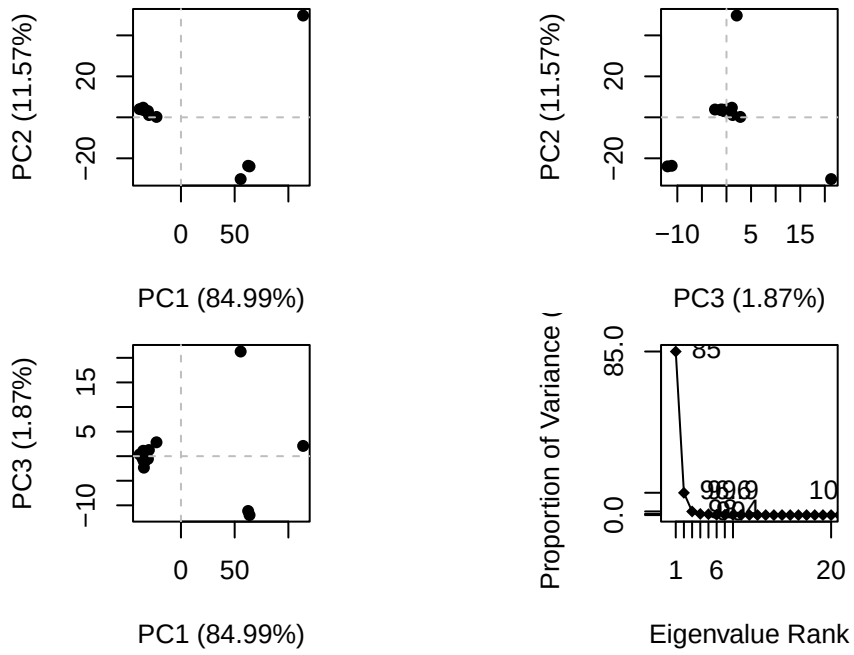
```
6RZE_A       1.69             <NA> Adenylate kinase, active site lid (ADK_lid)
3HPR_A       2.00             <NA>                       Adenylate kinase (ADK)
1E4V_A       1.85 Adenylate kinase                       Adenylate kinase (ADK)
5EJE_A       1.90             <NA> Adenylate kinase, active site lid (ADK_lid)
1E4Y_A       1.85 Adenylate kinase                       Adenylate kinase (ADK)
3X2S_A       2.80             <NA>                                        <NA>
6HAP_A       2.70             <NA> Adenylate kinase, active site lid (ADK_lid)
6HAM_A       2.55             <NA>                       Adenylate kinase (ADK)
4K46_A       2.01             <NA> Adenylate kinase, active site lid (ADK_lid)
3GMT_A       2.10             <NA>                                        <NA>
4PZL_A       2.10             <NA> Adenylate kinase, active site lid (ADK_lid)
               ligandId
1AKE_A              AP5
6S36_A NA,MG (2),CL (3)
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                                  SODIUM ION,MAGNESIUM ION (2),CHLORIDE ION (3)
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

1AKE_A STRUCTURE OF THE COMPLEX BETWEEN ADENYLATE KINASE FROM ESCHERICHIA COLI AND THE INHIBI
6S36_A
6RZE_A
3HPR_A
1E4V_A
loop
5EJE_A                                                                          Cryst
1E4Y_A
loop
3X2S_A
conjugated adenylate kinase
6HAP_A
6HAM_A
4K46_A
3GMT_A
4PZL_A                                                                  The cryst
                                                    citation rObserved   rFree
1AKE_A              Muller, C.W., et al. J Mol Biology (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
```

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

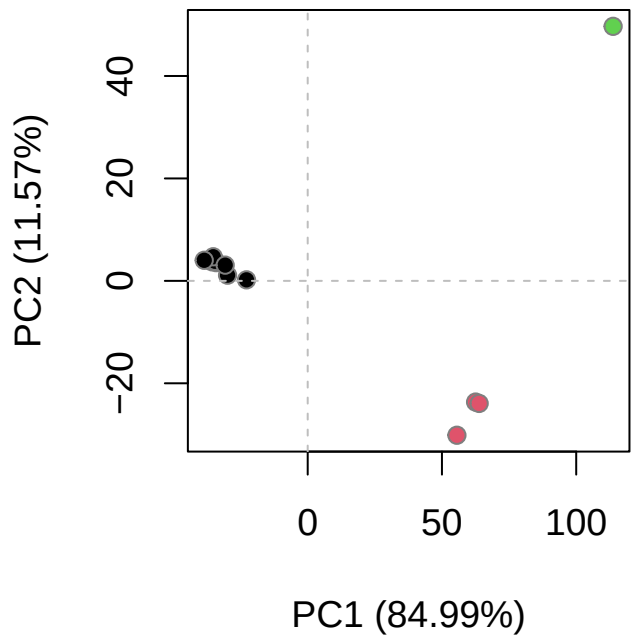


```
# Calculate RMSD
rd <- rmsd(pdbs)
```

```
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)
```

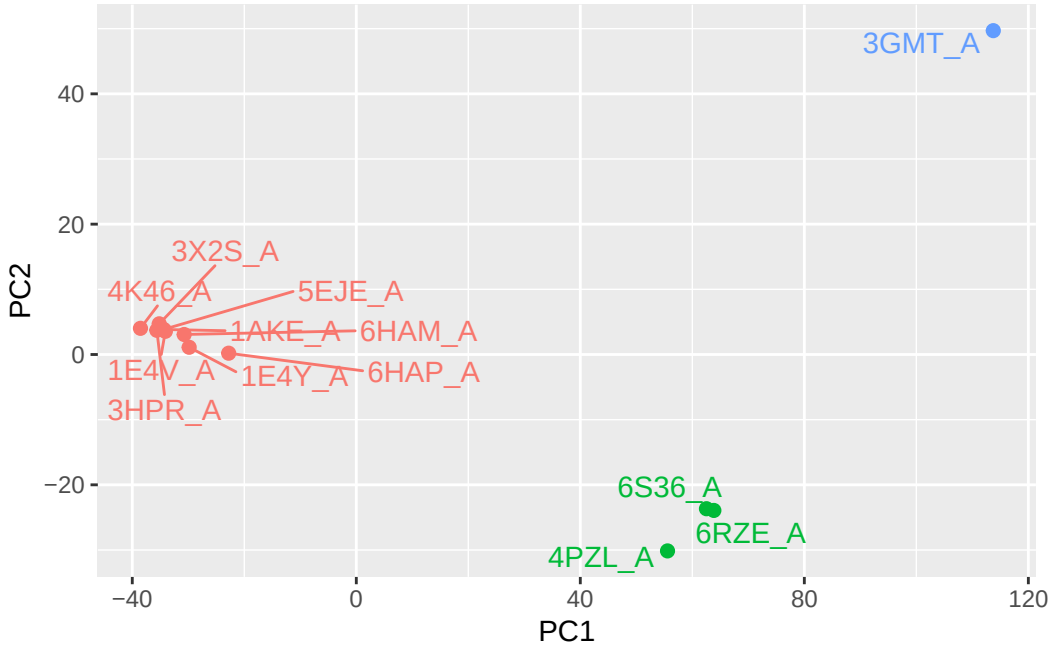



```
#Plotting results with ggplot2
library(ggplot2)
library(ggrepel)

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 = 50) +
  theme(legend.position = "none")
p
```



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? - they are similar in pattern, the colored lines are taller and differ most in the 50-70 region. i think they might differ because they are more flexible.