lab10

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```
pdb_data <- read.csv("Data Export Summary.csv")
pdb_data$X.ray <- as.numeric(gsub(",", "", pdb_data$X.ray))
pdb_data$EM <- as.numeric(gsub(",", "", pdb_data$EM))
pdb_data$Total <- as.numeric(gsub(",", "", pdb_data$Total))
```

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

```
xray_em_total <- sum(pdb_data$X.ray, pdb_data$EM, na.rm = TRUE)
total_structures <- sum(pdb_data$Total, na.rm = TRUE)
xray_em_percentage <- (xray_em_total / total_structures) * 100

xray_em_percentage
```

```
## [1] 93.49072
```

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

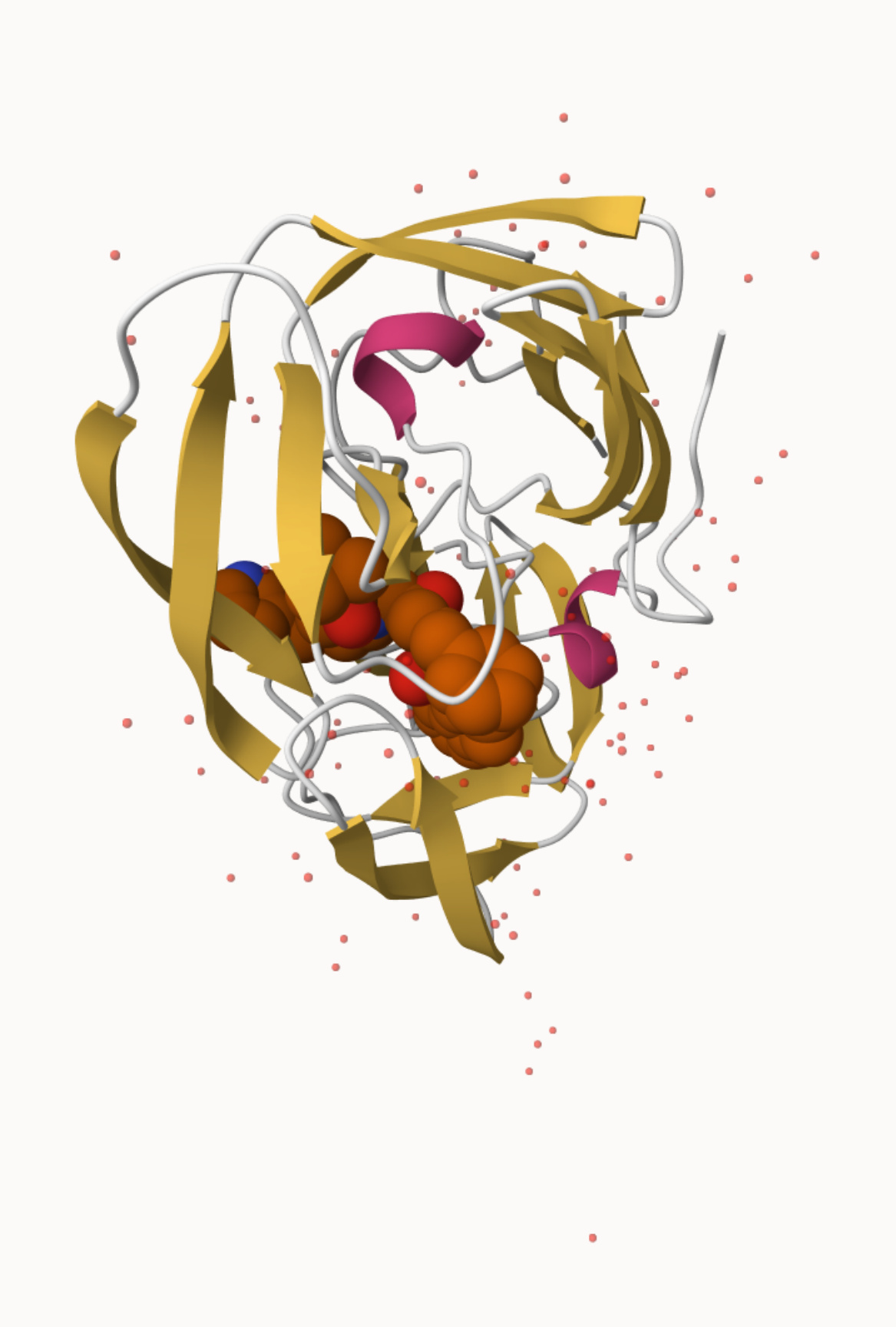
```
protein_data <- pdb_data[grepl("Protein", pdb_data$Molecular.Type), ]
protein_total <- sum(protein_data$Total, na.rm = TRUE)
protein_proportion <- protein_total / total_structures
protein_proportion
```

```
## [1] 0.9789729
```

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?

226,707 structures are in the current PDB.

```
HSG <- "https://files.rcsb.org/view/1HSG.pdb"
```



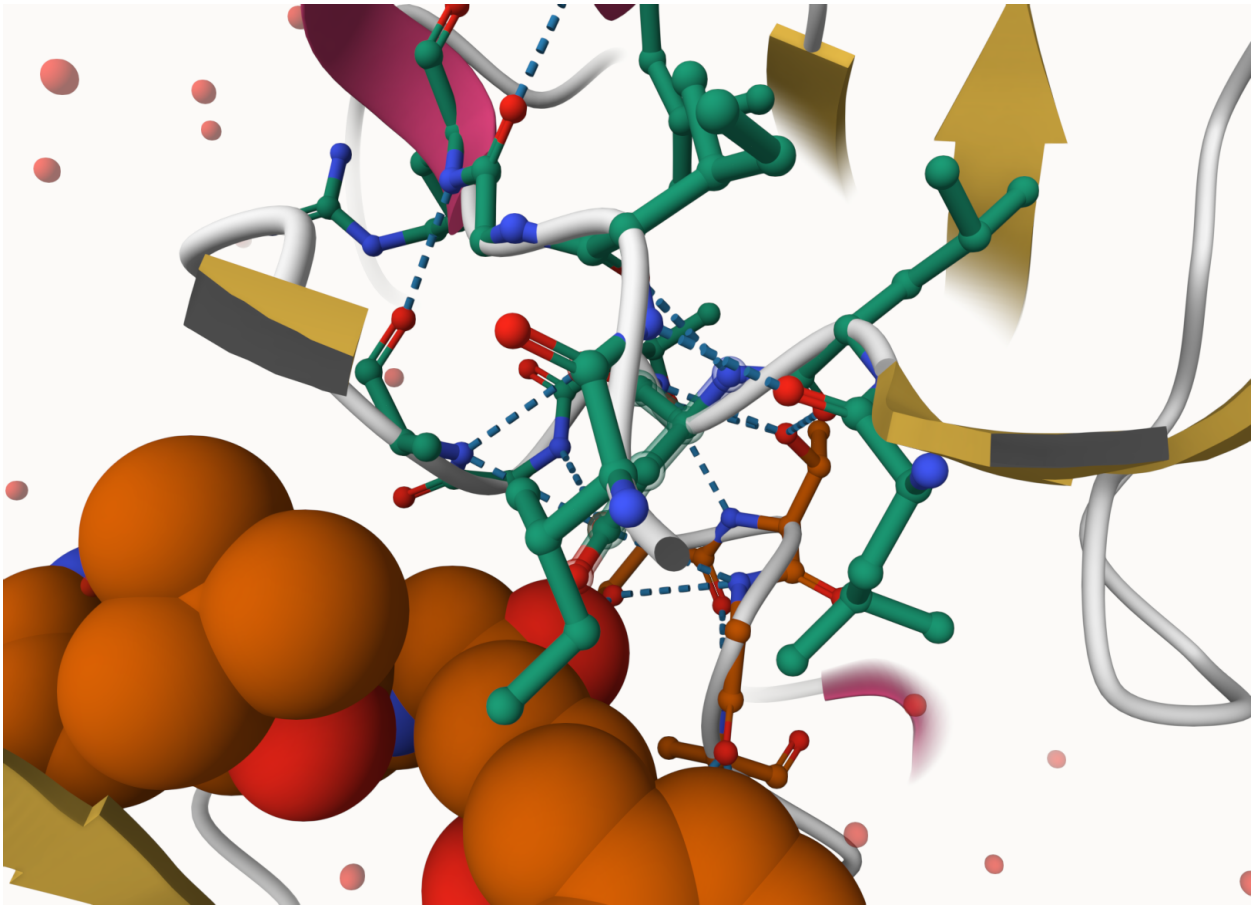
> Q4: Water molecules normally have 3 atoms. Why do we see just one atom per water molecule in this structure?

We see just one atom per water molecule in this structure as water molecules are represented by only the oxygen atom to simplify the structure.

> 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, I can identify this water molecule and the residue number is 301.

> 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.



```
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
```

Q7: How many amino acid residues are there in this pdb object?

```
sum(pdb$calpha)
```

```
## [1] 198
```

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

```
non_protein_residues <- unique(pdb$atom$resid[!(pdb$atom$resid %in% c("ALA", "ARG", "ASN", "ASP", "CYS"
non_protein_residues
```

```
## [1] "MK1" "HOH"
```

Q9: How Many Protein Chains Are in This Structure?

```
num_chains <- length(unique(pdb$atom$chain))
num_chains
```

```
## [1] 2
```

```
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
```

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

```
##  Building Hessian...     Done in 0.047 seconds.
##  Diagonalizing Hessian...    Done in 0.484 seconds.
```

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

```
options(repos = c(CRAN = "https://cran.rstudio.com/"))
```

options(repos = c(CRAN = “https://cran.rstudio.com/”))

```
library(bio3d)
install.packages("devtools")
```

```
##
## The downloaded binary packages are in
##  /var/folders/7c/m9tcwy_x5_g5gth0cn3j9j3w0000gn/T//RtmpXJK7aO/downloaded_packages
```

```
install.packages("BiocManager")
```

```
##
## The downloaded binary packages are in
##  /var/folders/7c/m9tcwy_x5_g5gth0cn3j9j3w0000gn/T//RtmpXJK7aO/downloaded_packages
```

```
BiocManager::install("msa")
```

```
## 'getOption("repos")' replaces Bioconductor standard repositories, see
## 'help("repositories", package = "BiocManager")' for details.
## Replacement repositories:
##     CRAN: https://cran.rstudio.com/
```

```
## Bioconductor version 3.20 (BiocManager 1.30.25), R 4.4.1 (2024-06-14)

## Warning: package(s) not installed when version(s) same as or greater than current; use
##   `force = TRUE` to re-install: 'msa'
```

```
devtools::install_bitbucket("Grantlab/bio3d-view")
```

```
## Skipping install of 'bio3d.view' from a bitbucket remote, the SHA1 (dd153987) has not changed since l
##   Use `force = TRUE` to force installation
```

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

msa is found only on BioConductor and not CRAN.

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

bio3d-view is not found on BioConductor or CRAN.

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?

```
sequence_length <- length(aa$ali)
sequence_length
```

```
## [1] 214
```

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','6HAP_A','6HAM
```

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

##   |                                                                      |
```

Align releated PDBs

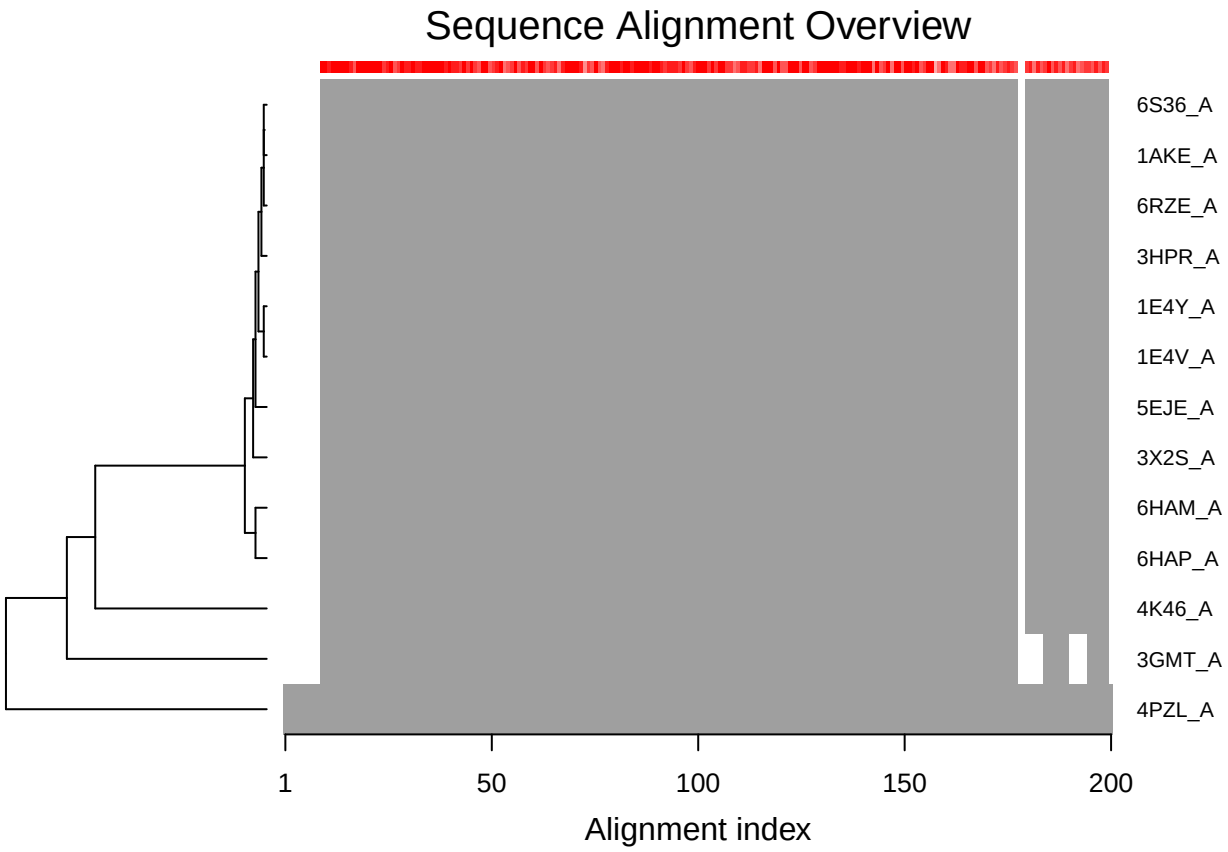
```
pdbs <- pdbaln(files, fit = TRUE, exefile="msa")
```

```
## 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)
```




```
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
```

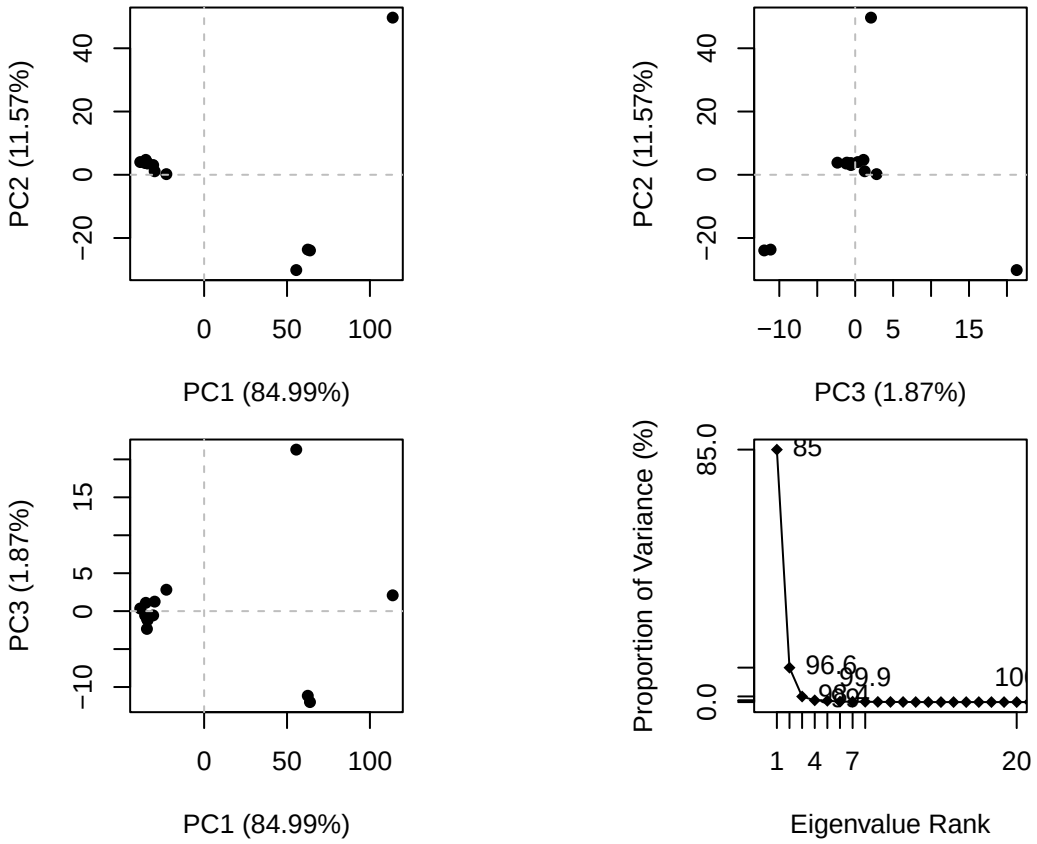
```
##        structureId chainId macromoleculeType chainLength experimentalTechnique
## 1AKE_A        1AKE       A           Protein         214                X-ray
## 6S36_A        6S36       A           Protein         214                X-ray
## 6RZE_A        6RZE       A           Protein         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 (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, 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 (ADK)
## 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 (ADK)
##                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
##
## 1AKE_A STRUCTURE OF THE COMPLEX BETWEEN ADENYLATE KINASE FROM ESCHERICHIA COLI AND THE INHIBITOR AP5
## 6S36_A
## 6RZE_A
## 3HPR_A
## 1E4V_A
## 5EJE_A                                                                                  Crystal stru
## 1E4Y_A
## 3X2S_A
## 6HAP_A
## 6HAM_A
## 4K46_A
## 3GMT_A
## 4PZL_A                                                                                The crystal stru
##                                                      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
```

Perform PCA

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

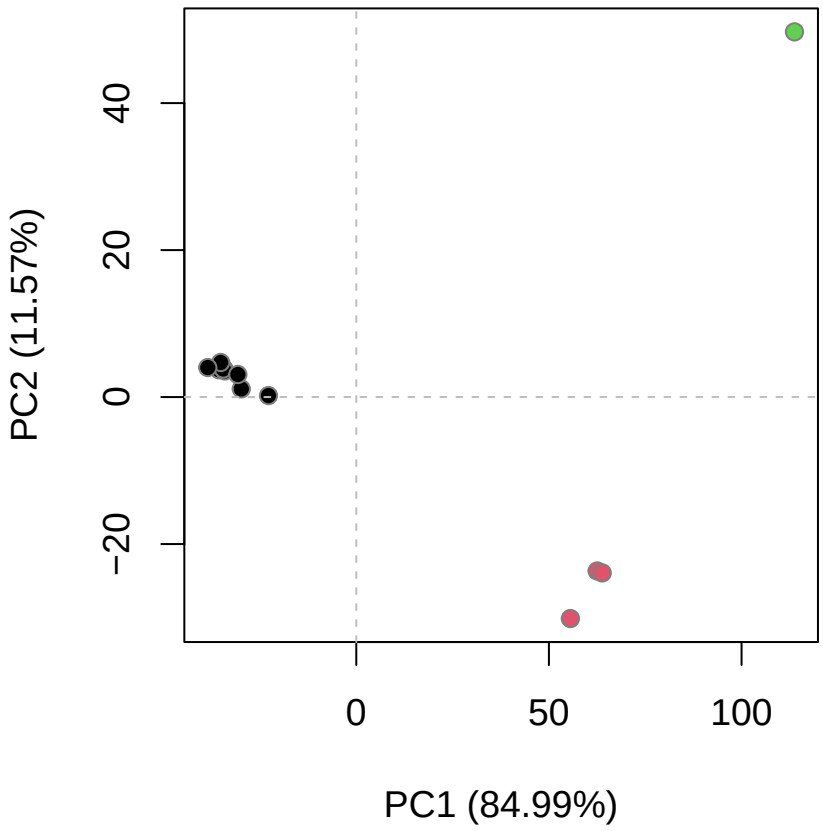



```
# Calculate RMSD
rd <- rmsd(pdbs)
```

```
## 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)
```


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