class09

Phoebe LI

2/13/2022

```
# import the csv file
db <- read.csv("Data Export Summary.csv", row.names = 1)
db
```

```
##                           X.ray   NMR   EM Multiple.methods Neutron Other  Total
## Protein (only)           144433 11881 6732              182      70    32 163330
## Protein/Oligosaccharide    8543    31 1125                5       0     0   9704
## Protein/NA                 7621   274 2165                3       0     0  10063
## Nucleic acid (only)        2396  1399   61                8       2     1   3867
## Other                       150    31    3                0       0     0    184
## Oligosaccharide (only)       11     6    0                1       0     4     22
```

```
# Xray structure percent
xray.percent <- sum(db$X.ray)/sum(db$Total)*100
round(xray.percent, 2)
```

```
## [1] 87.17
```

```
# EM structure percent
EM.percent <- sum(db$EM)/sum(db$Total)*100
round(EM.percent, 2)
```

```
## [1] 5.39
```

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

x-ray:87.2% EM:5.39%

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

```
percent.protein <- (db$Total[1])/sum(db$Total)
round(percent.protein*100, 2)
```

```
## [1] 87.26
```

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?

4486 Structures

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

Because It does not show the H atom in this structure. The resolution is too low that they can not detect H atom.

> Q5: There is a conserved water molecule in the binding site. Can you identify this water molecule? What residue number does this water molecule have (see note below)?

OH308O

```
install.packages("bio3d", repos="http://cran.us.r-project.org")
```

Introduction to Bio3D in R

```
##
## The downloaded binary packages are in
##  /var/folders/9d/xssg21015fq5rb8769f22wfw0000gn/T//RtmpOMLiWy/downloaded_packages
```

```
library(bio3d)
```

Reading PDB file data into R

```
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>
```

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

PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGIGGFIKVRQYD QILIE-
ICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFPQITLWQRPLVTIKIGGQLKE ALLDTGAD-
DTVLEEMSLPGRWKPKMIGGIGGFIKVRQYDQILIEICGHKAIGTVLVGPTP VNIIGRNLLTQIGCTLNF

```
  198 amino acid residues
```

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

HOH

Q9: How many protein chains are in this structure?

2 chains

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

Q13

```
options(repos = list(CRAN="http://cran.rstudio.com/"))
install.packages("bio3d")
```

```
##
## The downloaded binary packages are in
##  /var/folders/9d/xssg21015fq5rb8769f22wfw0000gn/T//RtmpOMLiWy/downloaded_packages
```

```
install.packages("ggplot2")
```

```
##
## The downloaded binary packages are in
##  /var/folders/9d/xssg21015fq5rb8769f22wfw0000gn/T//RtmpOMLiWy/downloaded_packages
```

```
install.packages("ggrepel")
```

```
##
## The downloaded binary packages are in
##  /var/folders/9d/xssg21015fq5rb8769f22wfw0000gn/T//RtmpOMLiWy/downloaded_packages
```

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

```
##
## The downloaded binary packages are in
##  /var/folders/9d/xssg21015fq5rb8769f22wfw0000gn/T//RtmpOMLiWy/downloaded_packages
```

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

```
##
## The downloaded binary packages are in
##  /var/folders/9d/xssg21015fq5rb8769f22wfw0000gn/T//RtmpOMLiWy/downloaded_packages
```

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

```
## 'getOption("repos")' replaces Bioconductor standard repositories, see
## '?repositories' for details
##
## replacement repositories:
##     CRAN: http://cran.rstudio.com/
```

```
## Bioconductor version 3.14 (BiocManager 1.30.16), R 4.1.2 (2021-11-01)

## Warning: package(s) not installed when version(s) same as 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
```

```
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? 214

```
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
```

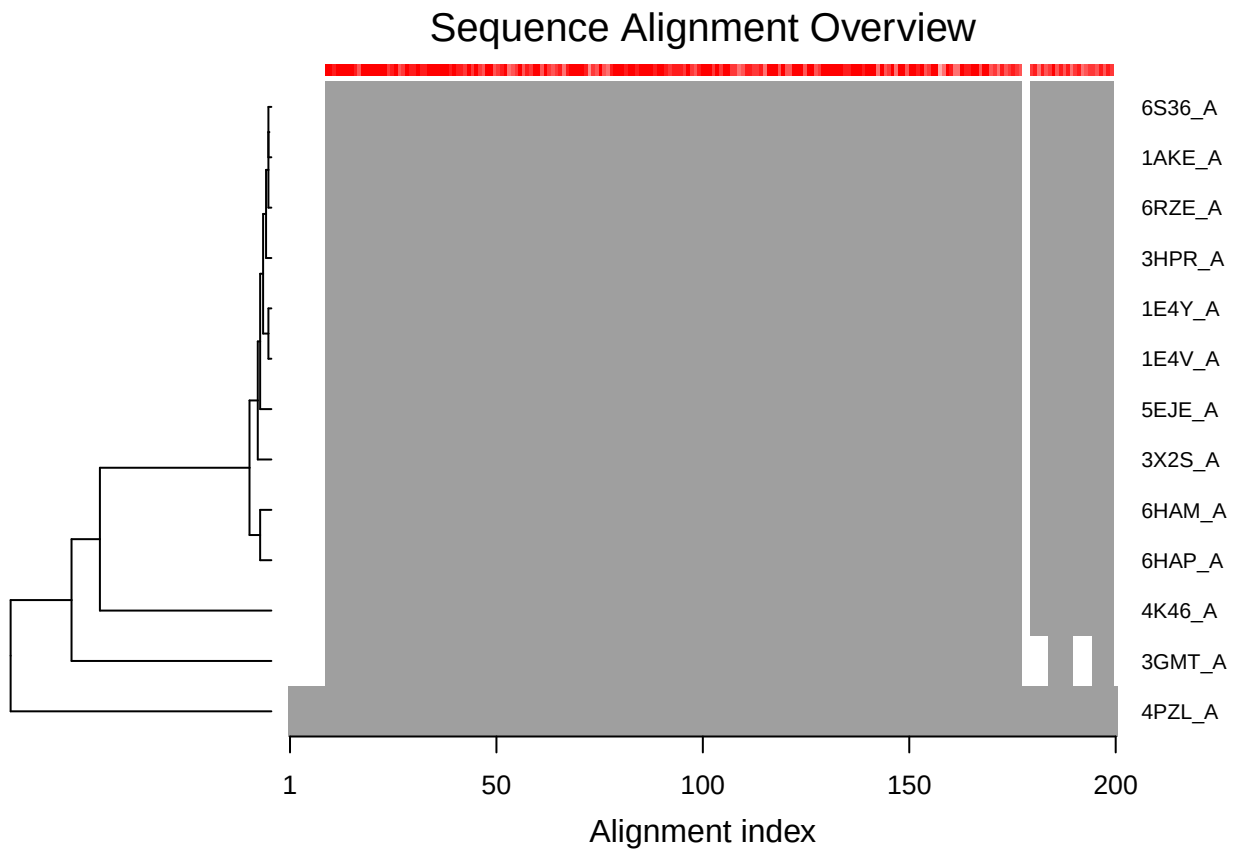
```
files <- get.pdb(hits$pdb.id, path="pdbs", split=TRUE, gzip=TRUE)
```

```
## 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

##   |                                                                              |
```

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

```
## 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)
```



Viewing our superposed structures

```
install.packages("rgl")
```

```
##
## The downloaded binary packages are in
##  /var/folders/9d/xssg21015fq5rb8769f22wfw0000gn/T//RtmpOMLiWy/downloaded_packages
```

```
library(bio3d.view)
library(rgl)

view.pdbs(pdbs)
```