Class 9

Nicole Chang

5/3/23

1. Introduction to the RCSB Protein Data Bank (PDB)

PDB statistics

To read the file we are going to use the command `read.csv`.

```
pdb_stats <- read.csv('Data Export Summary.csv', row.names = 1)
View(pdb_stats)
```

I need to sum all the elements of the X.ray column.

```
pdb_stats$X.ray
```

```
[1] "154,766" "9,083"   "8,110"   "2,664"   "163"     "11"
```

We are gonna use `gsub` to remove the commas

```
xray_without_commas <- gsub(',', '', pdb_stats$X.ray)
as.numeric( xray_without_commas )
```

```
[1] 154766   9083   8110   2664    163     11
```

I use the `sum` command to get the sum

```
n_xray <- sum( as.numeric( xray_without_commas ) )
n_em <- sum( as.numeric( gsub(',', '', pdb_stats$EM) ) )
n_total <- sum( as.numeric( gsub(',', '', pdb_stats$Total) ) )
```

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

```
p_xray <- (n_xray) / n_total
p_em <- (n_em) / n_total
p_xray
```

```
[1] 0.8553721
```

```
p_em
```

```
[1] 0.07455763
```

```
p_total <- (p_xray + p_em) *100
p_total
```

```
[1] 92.99297
```

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

```
total_protein <- as.numeric( gsub(',', '', pdb_stats[1, 7]) )
```

Proportion

```
total_protein/n_total
```

```
[1] 0.8681246
```

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?

Too difficult to determine.

2. Visualizing the HIV-1 protease structure

Using Mol*

The important role of water

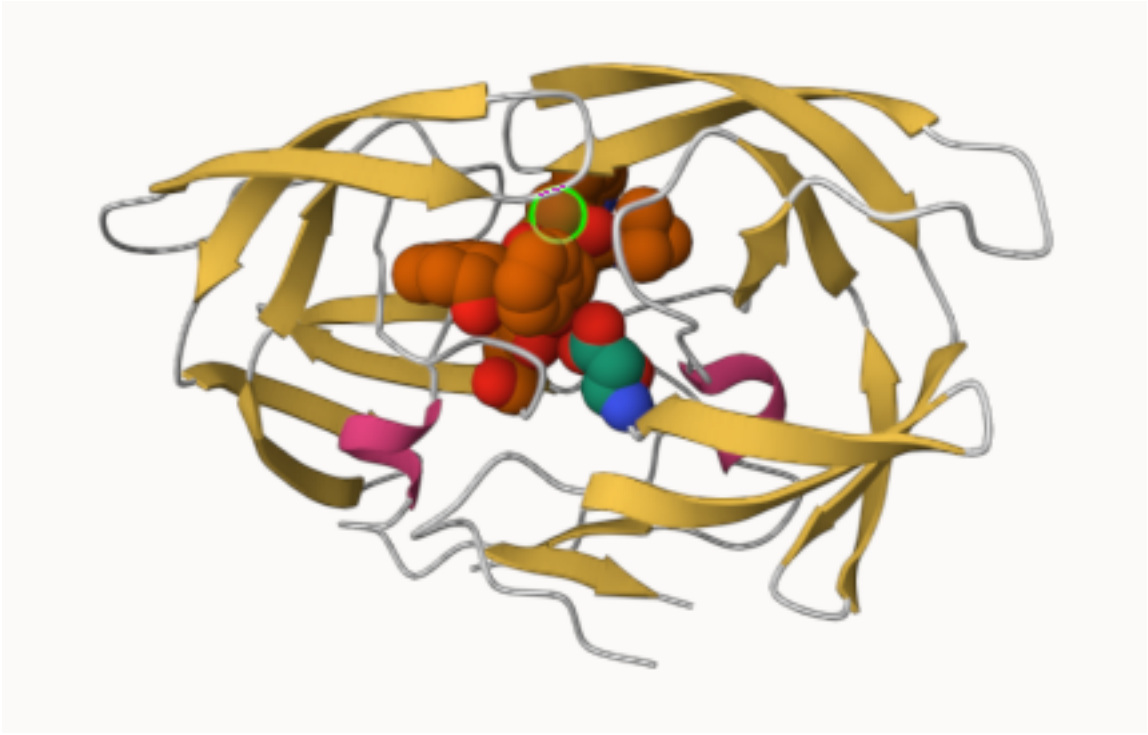
Q4. Water molecules normally have 3 atoms. Why do we see just one atom per water molecule in this structure?

Including the hydrogens would make the image too cluttered and not show the interaction.

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?

308

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. Add this figure to your Quarto document.



3. Introduction to Bio3D in R

```
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?

198

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

HOH

Q9. How many protein chains are in this structure?

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>
```

Predicting functional motions of a single structure by NMA

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

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

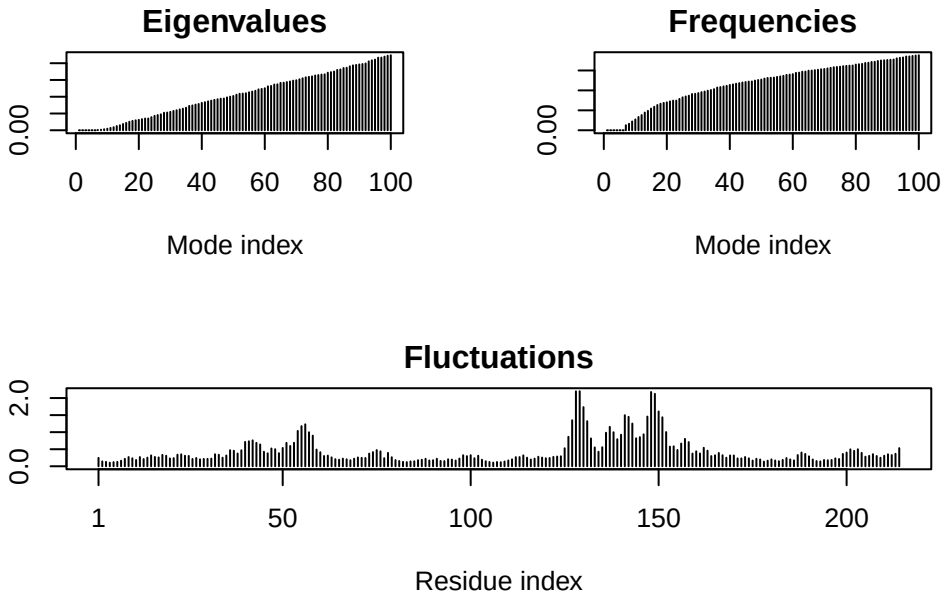
```
adk
```

```
 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 0.066 seconds.
Diagonalizing Hessian...    Done in 0.545 seconds.
```

```
plot(m)
```




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