Class09_lab

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

PDB statistics

We are moving the CSV file into RStudio and reading it using `read.csv`.

```
url <- "Data Export Summary.csv"
pdb.data <- read.csv(url, row.names = 1)
pdb.data
```

```
                         X.ray     EM    NMR Multiple.methods Neutron Other
Protein (only)         154,766 10,155 12,187              191      72    32
Protein/Oligosaccharide  9,083  1,802     32                7       1     0
Protein/NA               8,110  3,176    283                6       0     0
Nucleic acid (only)      2,664     94  1,450               12       2     1
Other                      163      9     32                0       0     0
Oligosaccharide (only)      11      0      6                1       0     4
                          Total
Protein (only)          177,403
Protein/Oligosaccharide  10,925
Protein/NA               11,575
Nucleic acid (only)       4,223
Other                       204
Oligosaccharide (only)       22
```

> **Q1:** What percentage of structures in the PDB are solved by X-Ray and Electron Microscopy.
>
> I need to sum all the elements of the X.ray column.

```
# R is understanding that these are letters because there are commas
pdb.data$X.ray
```

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

We are going to use `gsub` to remove the commas. Then we can convert to numbers.

```
#replace the commas with nothing (empty string)
xray.n <- as.numeric(gsub(",", '', pdb.data$X.ray))

em.n <- as.numeric(gsub(",", '', pdb.data$EM))

total.n <- as.numeric(gsub(",", '', pdb.data$Total))
```

Now we can get the sums of each row to find the percentage.

```
(sum(xray.n) + sum(em.n))/sum(total.n) * 100
```

```
[1] 92.99297
```

93% of the structures in the PDB are solved by X-ray and Electron Microscopy.

> **Q2:** What proportion of structures in the PDB are protein

```
as.numeric(gsub(",", '', pdb.data[1,7]))/sum(total.n)
```

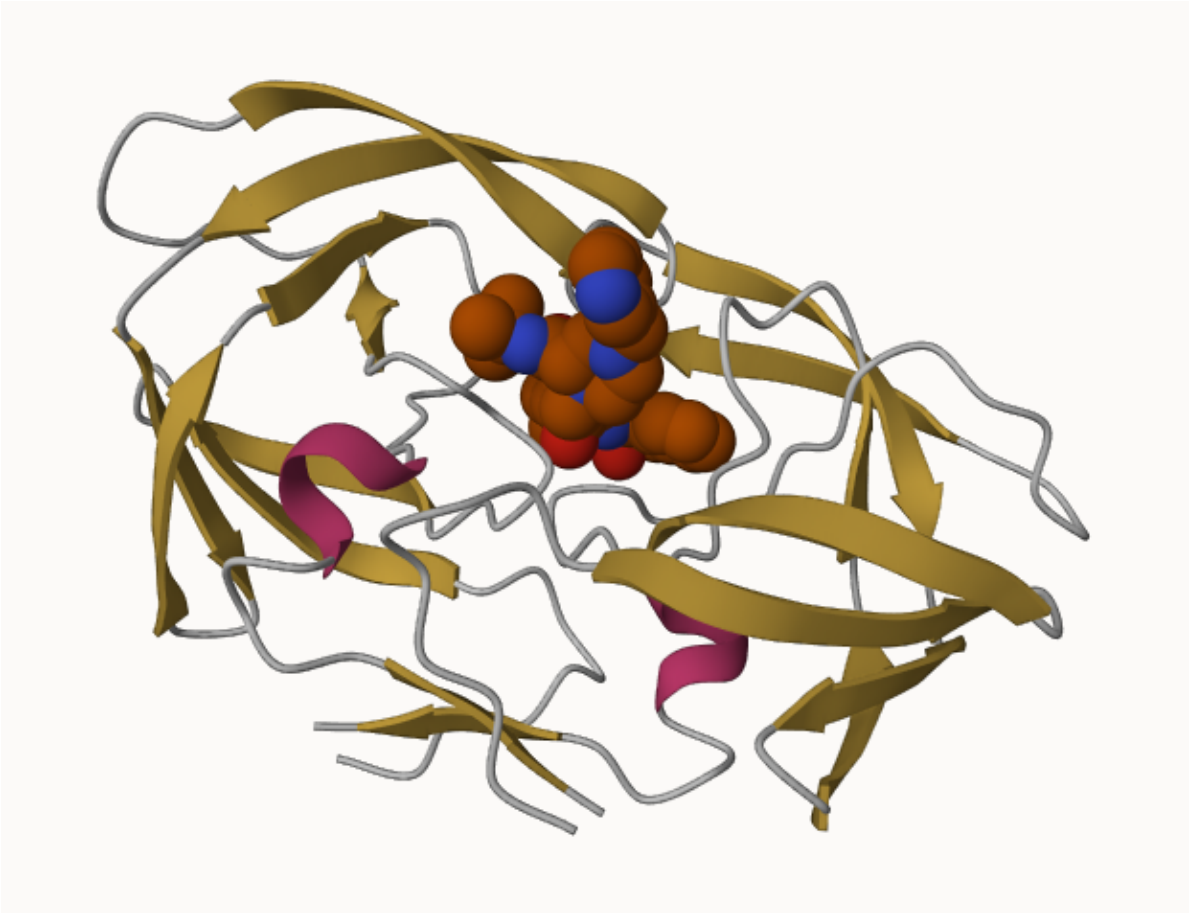
```
[1] 0.8681246
```

87% of the structures in the PDB are protein.

> **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?
>
> Maybe, there are 2003 HIV-1 protease structures in the PDB.

2. Visualizing the HIV-1 protease structure

Using Mol*



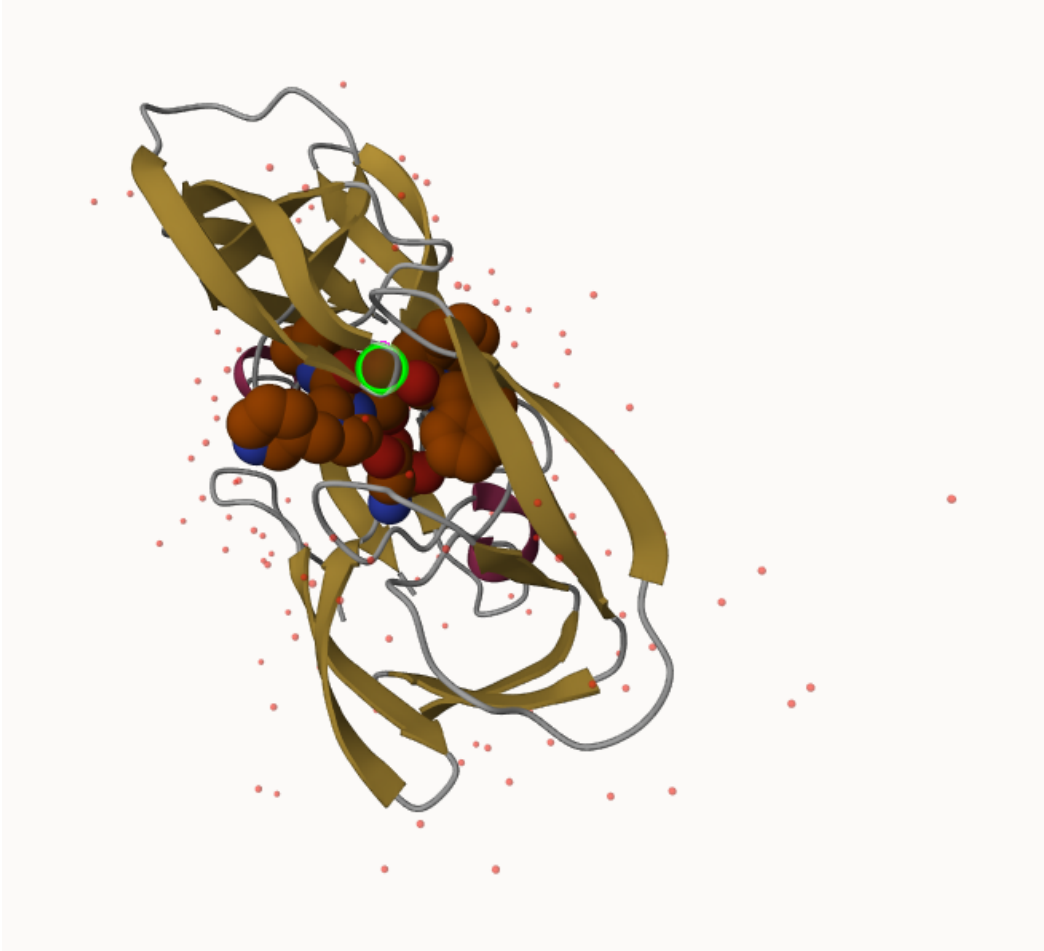
Q4: Water molecules normally have 3 atoms. Why do we see just one atom per water molecule in this structure?

The PDB viewer only shows the main atom in a molecule which is oxygen for water.

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

The critical water molecule that binds to the ligand is number 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 (we recommend *"Ball & Stick"* for these side-chains). 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
```

```
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?

There are 198.

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

One of them is HOH 127.

Q9: How many protein chains are in this structure?

There are 2.

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
```

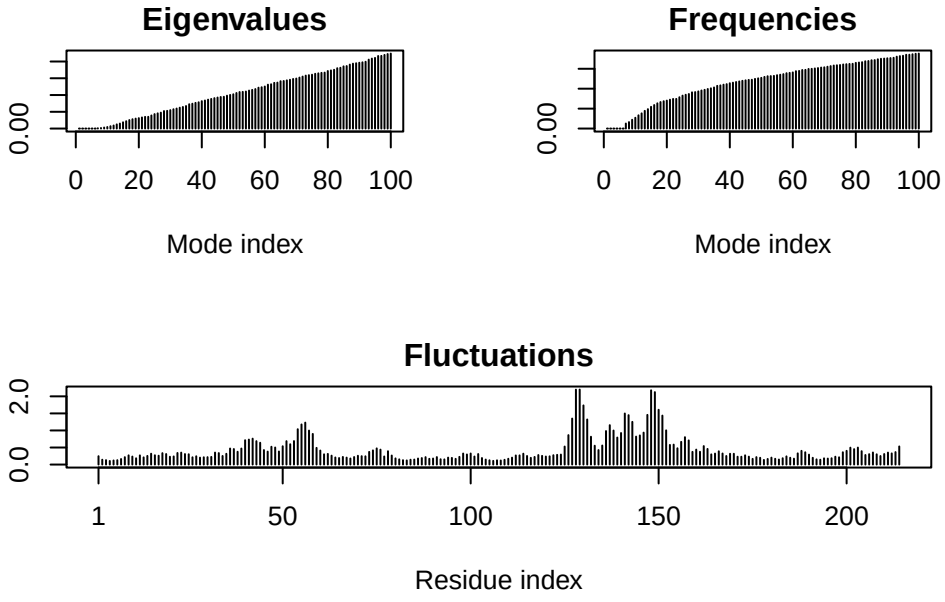
```
#normal mode analysis to see the flexibility of the protein
m <- nma(adk)
```

```
 Building Hessian...        Done in 0.03 seconds.
 Diagonalizing Hessian...   Done in 0.3 seconds.
```

```
#check what type of class m is
class(m)
```

```
[1] "VibrationalModes" "nma"
```

```
#class nma objects have their own type of plot
#fluctuations tells us the flexibility of each amino acid
plot(m)
```



It would be nice to see this in 3D...

```
#this will create a new file
mktrj(m, file = "adk_m7.pdb")
```