Class 10: Structural Bioinformatics pt1

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What is the PDB database

The main repository of biomolecular structure info is the PDB <www.rcsd.org>.

Let's see what this data base contains:

```
stats <- read.csv("pdb_stats.csv", row.names = 1)
stats
```

```
                         X.ray     EM    NMR Multiple.methods Neutron Other
Protein (only)         161,663 12,592 12,337              200      74    32
Protein/Oligosaccharide  9,348  2,167     34                8       2     0
Protein/NA               8,404  3,924    286                7       0     0
Nucleic acid (only)      2,758    125  1,477               14       3     1
Other                      164      9     33                0       0     0
Oligosaccharide (only)      11      0      6                1       0     4
                         Total
Protein (only)         186,898
Protein/Oligosaccharide  11,559
Protein/NA               12,621
Nucleic acid (only)       4,378
Other                       206
Oligosaccharide (only)       22
```

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

84% are solved by xray and EM solves 8.7%

```
as.numeric(stats$X.ray)
```

```
Warning: NAs introduced by coercion
```

```
[1]  NA  NA  NA  NA 164  11
```

We got to get rid of the commas. Can you find a function to get rid of the commas?

```
x <- stats$X.ray
sum(as.numeric(gsub(",", "", x)))
```

```
[1] 182348
```

I am going to turn this into a function and then use `apply()` to work on the entire table of data

```
sumcomma <- function(x) {
  sum(as.numeric(gsub(",", "", x)))
}

sumcomma(stats$X.ray)
```

```
[1] 182348
```

```
sumcomma(stats$Total)
```

```
[1] 215684
```

```
n.total <- sumcomma(stats$Total)
n.total
```

```
[1] 215684
```

```
sumcomma(stats$EM)
```

```
[1] 18817
```

```
apply(stats,2, sumcomma)
```

```
          X.ray              EM             NMR Multiple.methods
         182348           18817           14173             230
        Neutron           Other           Total
             79              37          215684
```

```
apply(stats,2, sumcomma) / sumcomma(stats$Total)
```

```
       X.ray               EM              NMR Multiple.methods
0.8454405519     0.0872433746     0.0657118748     0.0010663749
     Neutron            Other            Total
0.0003662766     0.0001715473     1.0000000000
```

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

In UniProt there are 248,805,733 entries which compared to PDB protein entries (186898) means there are only 7% of known sequences with a known structure

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?

5

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

the hydrogen is too small to be shown

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

D25

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.

Visualizing the HIV-1 protease structure

Mol* (mol-star) viewer is now everywhere. The homepage is here: https://molstar.org/viewer/.

I want to insert my image from Mol* here.

Working iwht ht ebio3d package

```
library(bio3d)
```

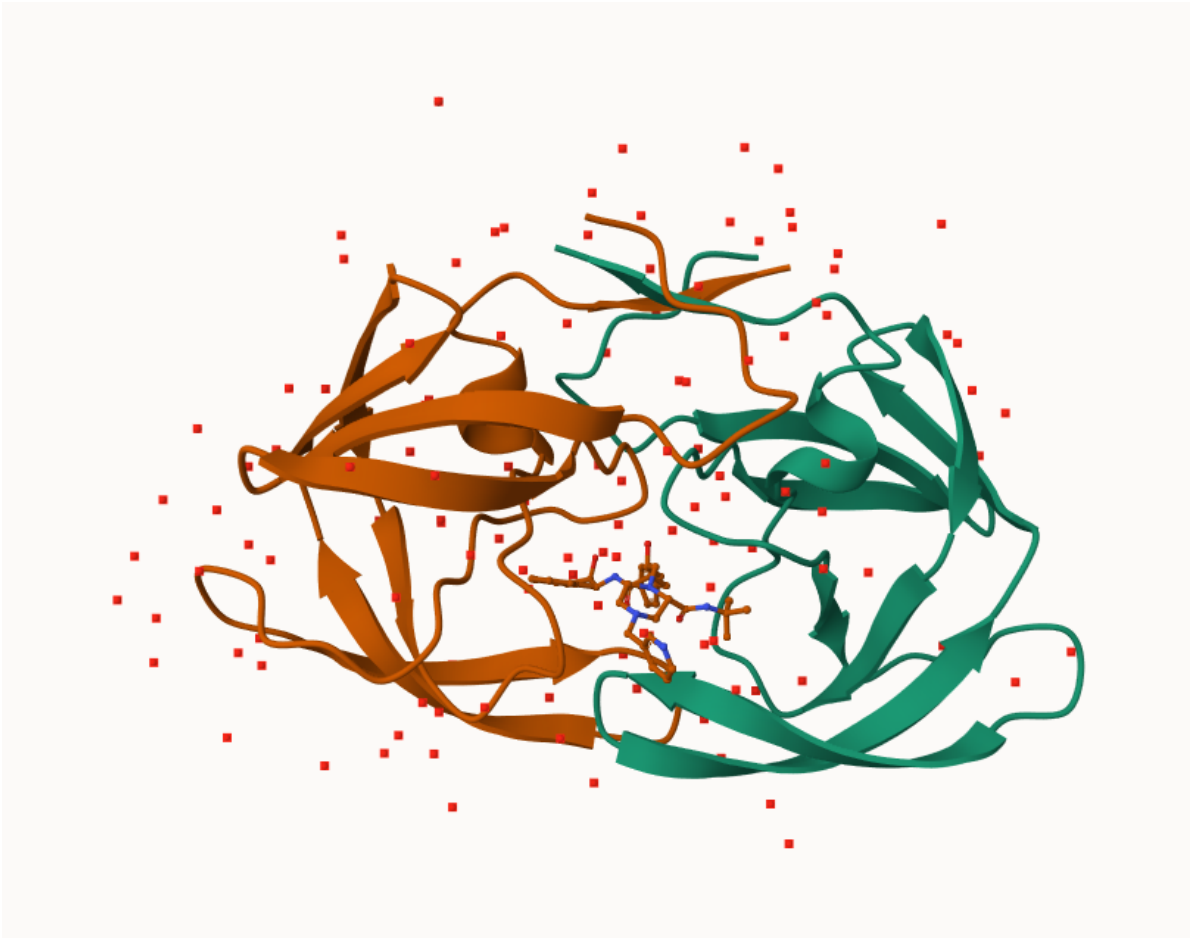


Figure 1: My first molecular image

```
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
```

```
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>
```

```
pdbseq(pdb)[25]
```

```
 25
"D"
```

Predicting functional motions of a single structure

We can do bioinformatics prediction of functional motions (i.e. flexibility/dynamics)

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

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

```
pdb
```

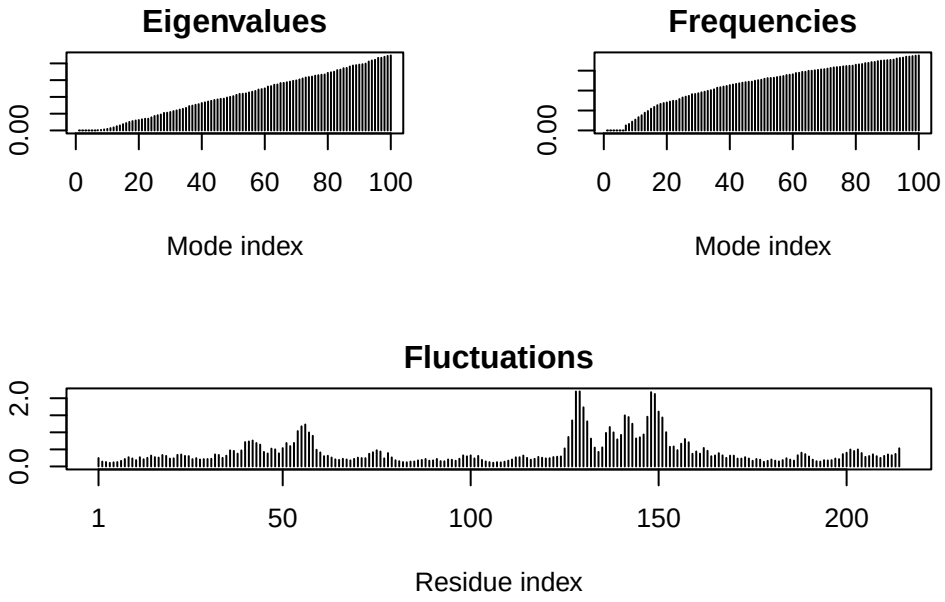
```
 Call:  read.pdb(file = "6s36")

   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(pdb)
```

```
 Building Hessian...        Done in 0.013 seconds.
 Diagonalizing Hessian...   Done in 0.273 seconds.
```

```
plot(m)
```



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

214

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

CL (3)

Q9: How many protein chains are in this structure?

1

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