# Class 10: Structural Bioinformatics Pt 1

## What is the PDB database

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

Let's see what this database contains:

```
stats <- read.csv(url("https://raw.githubusercontent.com/bioboot/bggn213_W24/gh-pages/class-material/p
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?

We have to get rid of the commas

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

```
[1] 182348
```

I am going to turn this unto 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
```

```
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?

> 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?

248,805,733 - 186,898

```
186898/248805733 * 100
```

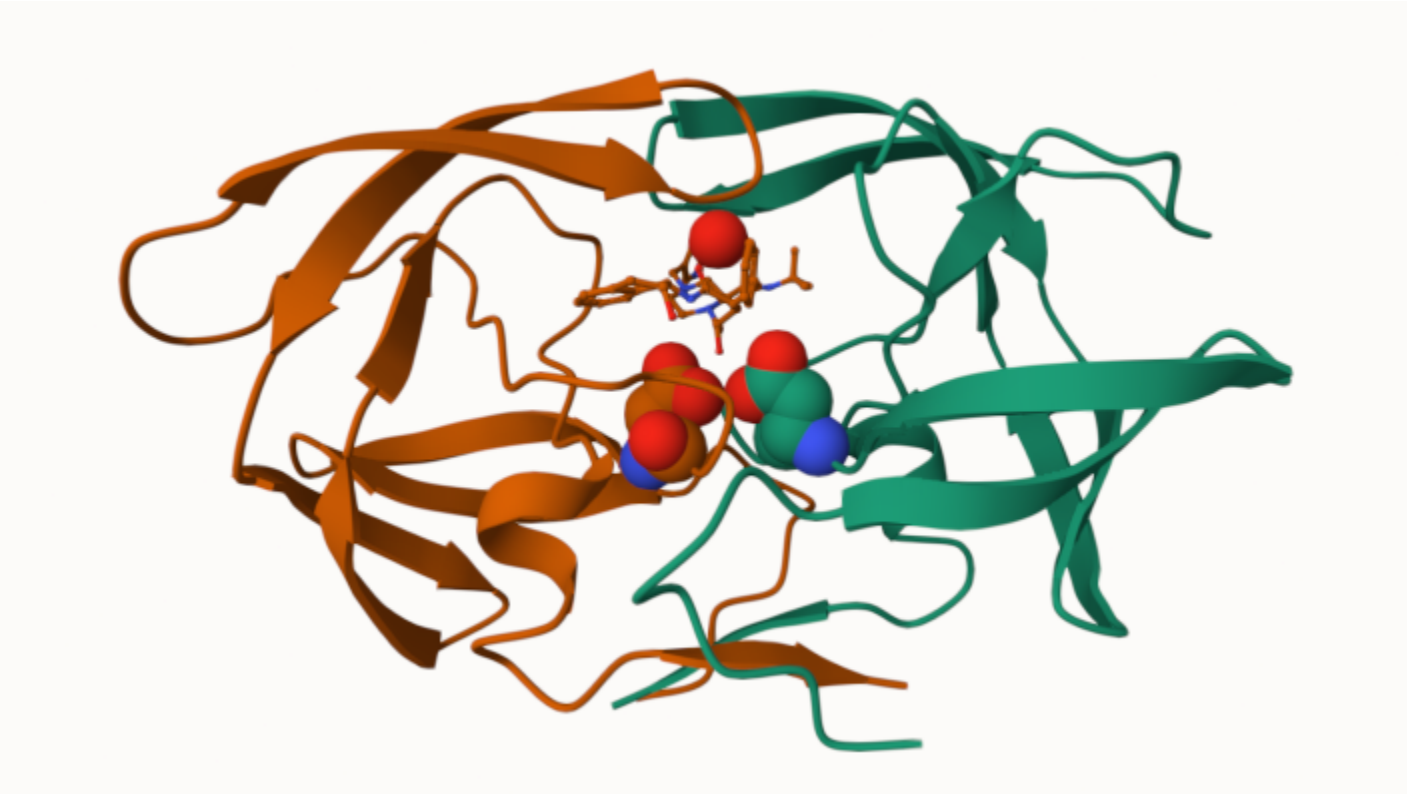
```
[1] 0.07511804
```

## 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.

My first molecular image



A version that's easier to look at

## Working with the bio3d package

```
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
```

```
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 a bioinformatucs prediction of functional motions

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

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

```
adk
```

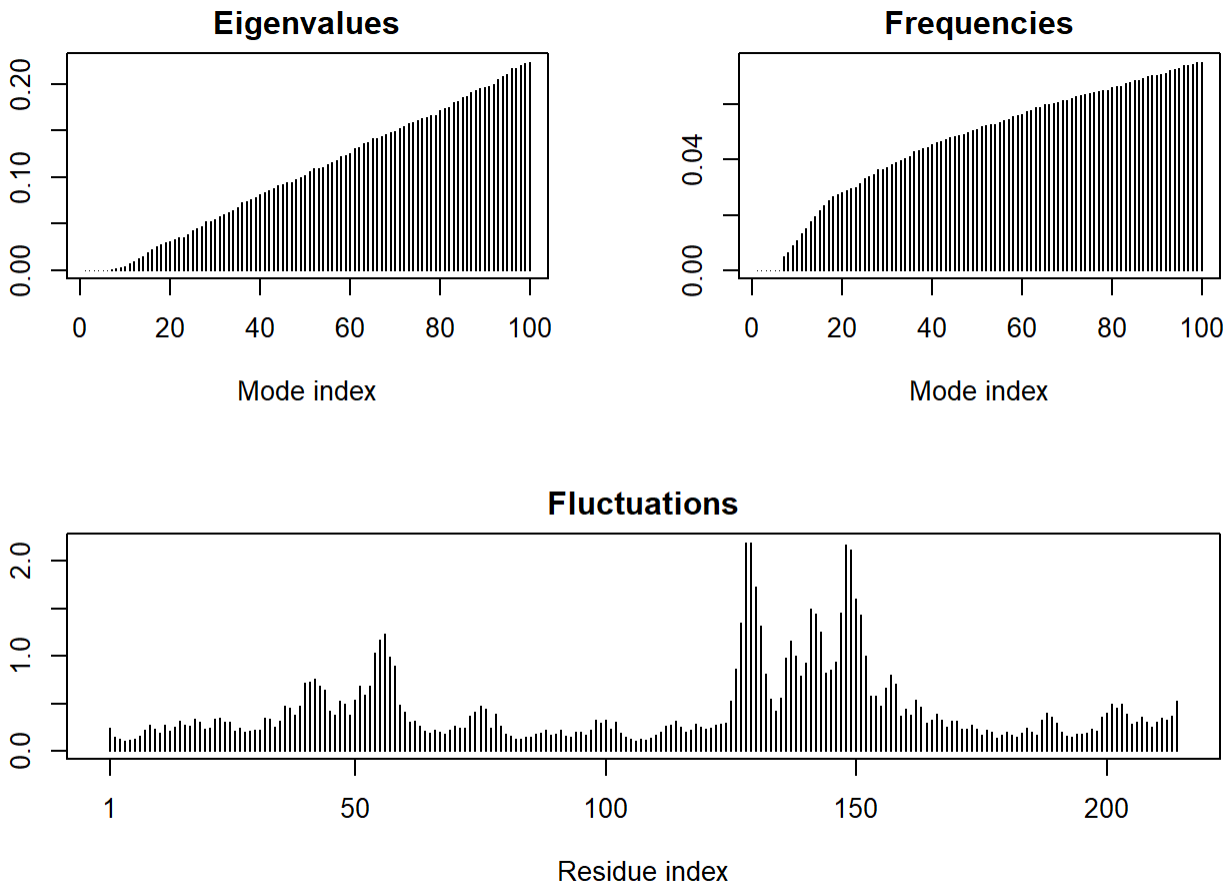
```

 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 0.03 seconds.
 Diagonalizing Hessian...   Done in 0.38 seconds.
```

```
plot(m)
```




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