# class10

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## What's in 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("Data Export Summary.csv",row.names=1)
stats
```

| | X.ray | EM | NMR | Multiple.methods | Neutron | Other |
|---|---|---|---|---|---|---|
| Protein (only) | 163,468 | 13,582 | 12,390 | 204 | 74 | 32 |
| Protein/Oligosaccharide | 9,437 | 2,287 | 34 | 8 | 2 | 0 |
| Protein/NA | 8,482 | 4,181 | 286 | 7 | 0 | 0 |
| Nucleic acid (only) | 2,800 | 132 | 1,488 | 14 | 3 | 1 |
| Other | 164 | 9 | 33 | 0 | 0 | 0 |
| Oligosaccharide (only) | 11 | 0 | 6 | 1 | 0 | 4 |

| | Total |
|---|---|
| Protein (only) | 189,750 |
| Protein/Oligosaccharide | 11,768 |
| Protein/NA | 12,956 |
| Nucleic acid (only) | 4,438 |
| Other | 206 |
| Oligosaccharide (only) | 22 |

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

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

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

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

```
as.numeric(stats$EM)
```

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

```
[1]  NA  NA  NA 132   9   0
```

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

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

```
[1] 184362
```

I'm 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] 184362
```

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

```
[1] 219140
```

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

```
[1] 20191
```

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

```
          X.ray              EM             NMR Multiple.methods
         184362           20191           14237             234
        Neutron           Other           Total
             79              37          219140
```

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

```
       X.ray               EM              NMR Multiple.methods
0.8412978005     0.0921374464     0.0649676006     0.0010678105
     Neutron            Other            Total
0.0003605001     0.0001688418     1.0000000000
```

A: 84.13% percent of structures in the PDB are solved by X-Ray and 9.2% solved by Electron Microscopy.

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

```
apply(stats[,-ncol(stats)], 1, sumcomma)
```

```
     Protein (only) Protein/Oligosaccharide              Protein/NA
             189750                    11768                   12956
Nucleic acid (only)                    Other  Oligosaccharide (only)
               4438                      206                      22
```

```
apply(stats[,-ncol(stats)], 1, sumcomma)/(sumcomma(stats$Total))
```

```
     Protein (only) Protein/Oligosaccharide              Protein/NA
       0.8658848225            0.0537008305           0.0591220225
Nucleic acid (only)                    Other  Oligosaccharide (only)
       0.0202518938            0.0009400383           0.0001003924
```

A: 86.6% 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?

A: 26812 HIV-1 protease structures in the current PDB.

In Uniprot there are 248,805,733 entries, which, compared to PDB protein entries (186,898), means there are only 0.07% of known sequences with a known structure.

```
186898/248805733*100
```

```
[1] 0.07511804
```

## Visualizing the HIV-1 protease structure

Mol* ("mol-star") viewer is now everywhere. The Mol* homepage at https://molstar.org/viewer/. I want to insert my image from Mol* here.

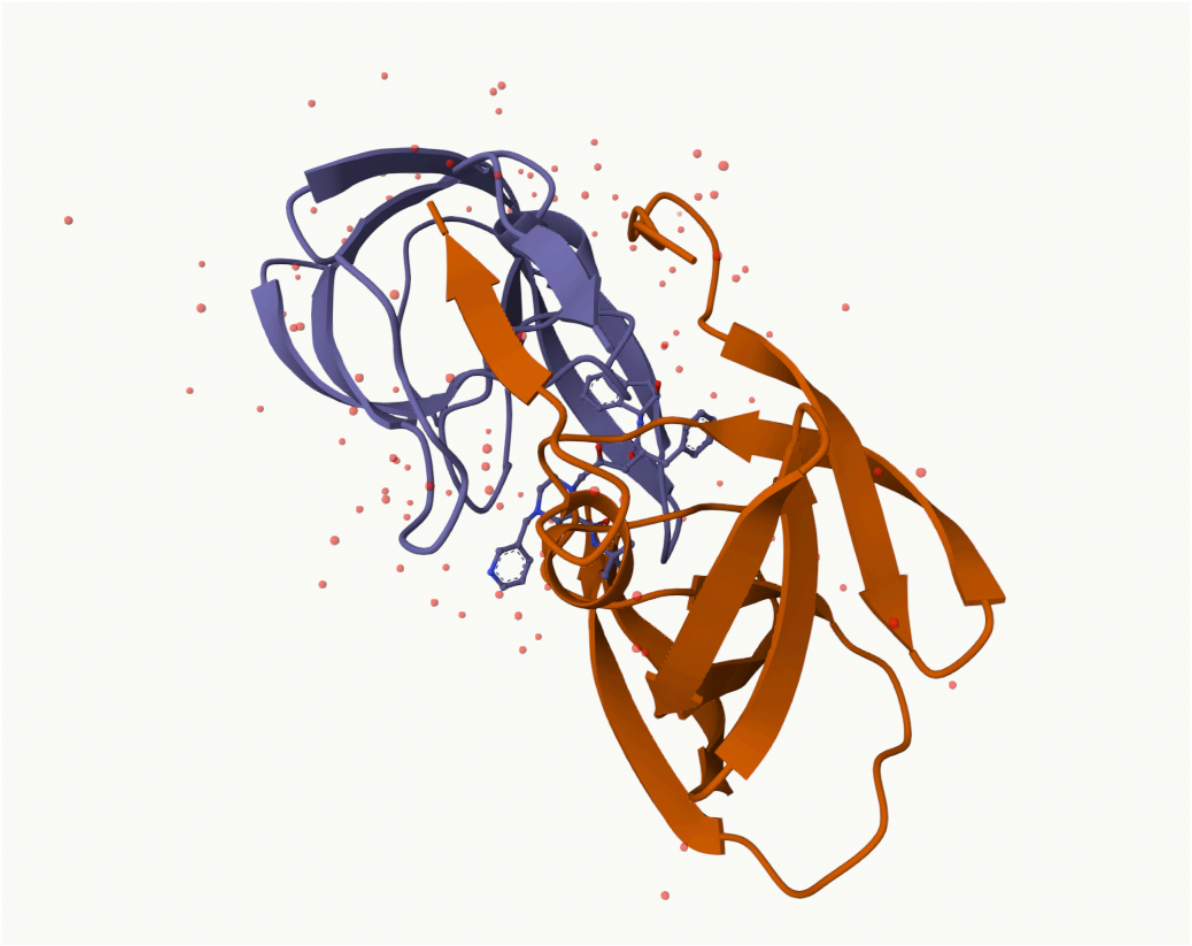


Figure 1: My first molecular image

## 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 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
```

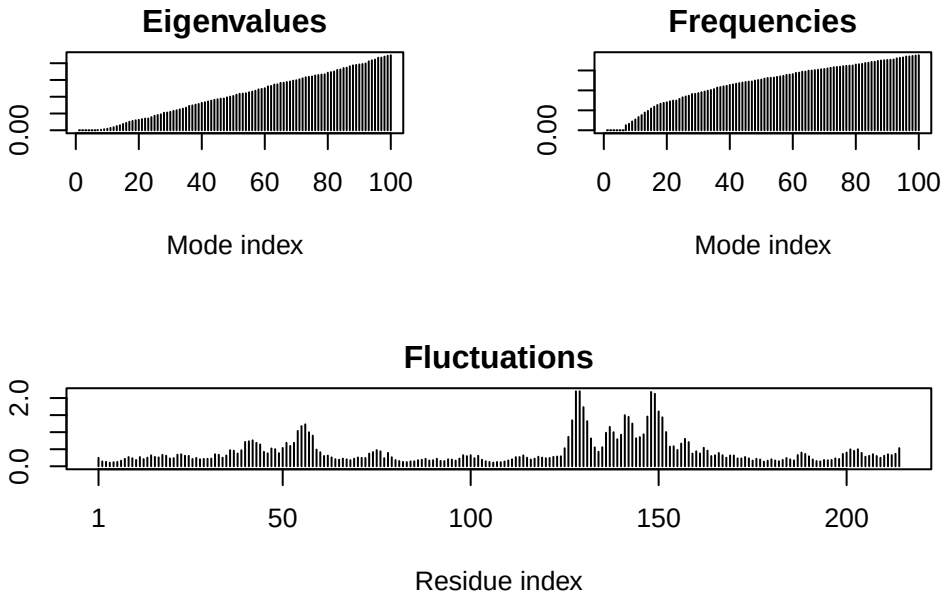
```
pdb
```

```

 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 0.014 seconds.
Diagonalizing Hessian...    Done in 0.277 seconds.
```

```
plot(m)
```




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