class10

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The PDB database

Here we examine the size and composition of the main databse of biomolecular structures - the PDB.

```
pdbstats <- read.csv("Data Export Summary.csv", row.names=1)
head(pdbstats)
```

```
                         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.

My pdbstats data frame has numbers with commas in them. This may cause us problems. Let's see:

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

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

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

We found a function called `gsub()`. Now we can figure out how it works.

```
gsub(",", "", pdbstats$X.ray)
```

```
[1] "161663" "9348"   "8404"   "2758"   "164"    "11"
```

```
as.numeric(gsub(",", "", pdbstats$X.ray))
```

```
[1] 161663   9348   8404   2758    164     11
```

I can turn this snipet into a function that I can use for every column in the table.

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

commasum(pdbstats$X.ray)
```

```
[1] 182348
```

```
totals <- apply(pdbstats, 2, commasum)
totals
```

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

```
round(totals/totals["Total"]*100,2)
```

```
         X.ray             EM            NMR Multiple.methods
         84.54           8.72           6.57              0.11
      Neutron          Other          Total
          0.04           0.02         100.00
```

```
(commasum(pdbstats$X.ray) + commasum(pdbstats$EM)) / commasum(pdbstats$Total)*100
```

```
[1] 93.26839
```

93.27% of structures in PDB are solved by X-ray and electron microscopy. (84.54% was solved by X-ray and 8.72% was solved by EM).

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

```
prot <-commasum(pdbstats[1:3,7])

tot <- commasum(pdbstats$Total)

(prot/tot)*100
```

```
[1] 97.86447
```

97.86% 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?

26,204 structures in the current PDB are HIV-1 proteases.

2. Visualizing Protein Structure

We will learn the basics of Mol* (mol-star) homepage: https://molstar.org/viewer/

We will play with PDB code 1HSG.

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

- The hydrogen atoms are too small to visualize.

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

- Its residue number is 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.

Figure 1: HIV Pr

Back to R and working with PDB structures

Predict the dynamics (flexibility) of an important protein:

```
library(bio3d)
```

Figure 2: HIV Pr with the two critical ASP residues

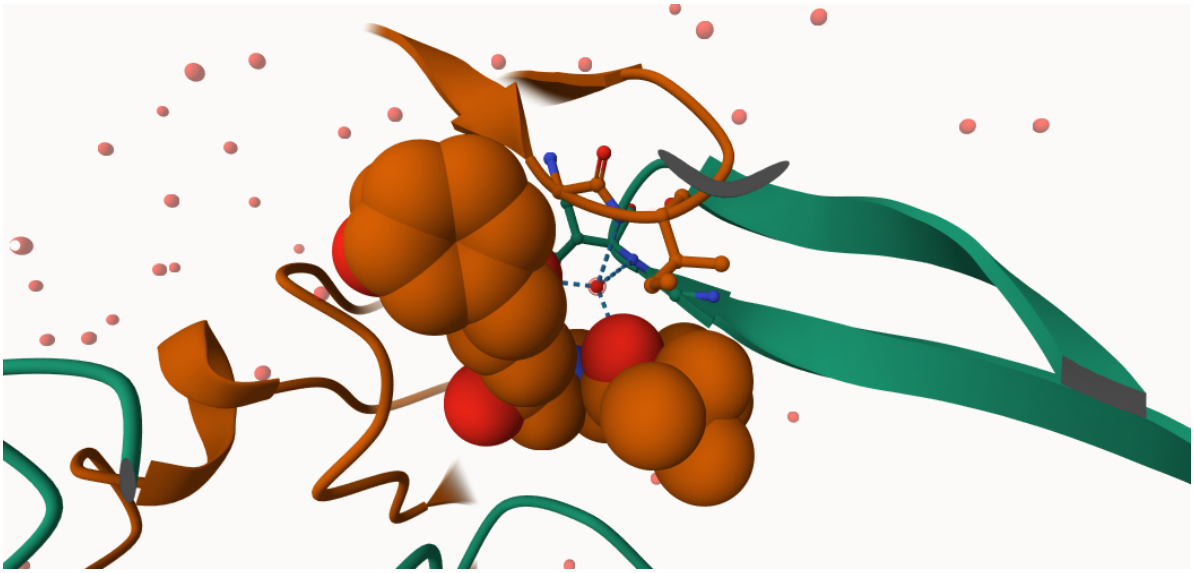


Figure 3: HIV Pr with the critical conserved water molecule

```
hiv <- read.pdb("1hsg")
```

```
  Note: Accessing on-line PDB file
```

```
hiv
```

```
 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(hiv$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(hiv)
```

```
  1   2   3   4   5   6   7   8   9  10  11  12  13  14  15  16  17  18  19  20
"P" "Q" "I" "T" "L" "W" "Q" "R" "P" "L" "V" "T" "I" "K" "I" "G" "G" "Q" "L" "K"
 21  22  23  24  25  26  27  28  29  30  31  32  33  34  35  36  37  38  39  40
"E" "A" "L" "L" "D" "T" "G" "A" "D" "D" "T" "V" "L" "E" "E" "M" "S" "L" "P" "G"
 41  42  43  44  45  46  47  48  49  50  51  52  53  54  55  56  57  58  59  60
"R" "W" "K" "P" "K" "M" "I" "G" "G" "I" "G" "G" "F" "I" "K" "V" "R" "Q" "Y" "D"
 61  62  63  64  65  66  67  68  69  70  71  72  73  74  75  76  77  78  79  80
"Q" "I" "L" "I" "E" "I" "C" "G" "H" "K" "A" "I" "G" "T" "V" "L" "V" "G" "P" "T"
 81  82  83  84  85  86  87  88  89  90  91  92  93  94  95  96  97  98  99   1
"P" "V" "N" "I" "I" "G" "R" "N" "L" "L" "T" "Q" "I" "G" "C" "T" "L" "N" "F" "P"
  2   3   4   5   6   7   8   9  10  11  12  13  14  15  16  17  18  19  20  21
"Q" "I" "T" "L" "W" "Q" "R" "P" "L" "V" "T" "I" "K" "I" "G" "G" "Q" "L" "K" "E"
 22  23  24  25  26  27  28  29  30  31  32  33  34  35  36  37  38  39  40  41
"A" "L" "L" "D" "T" "G" "A" "D" "D" "T" "V" "L" "E" "E" "M" "S" "L" "P" "G" "R"
 42  43  44  45  46  47  48  49  50  51  52  53  54  55  56  57  58  59  60  61
"W" "K" "P" "K" "M" "I" "G" "G" "I" "G" "G" "F" "I" "K" "V" "R" "Q" "Y" "D" "Q"
 62  63  64  65  66  67  68  69  70  71  72  73  74  75  76  77  78  79  80  81
"I" "L" "I" "E" "I" "C" "G" "H" "K" "A" "I" "G" "T" "V" "L" "V" "G" "P" "T" "P"
 82  83  84  85  86  87  88  89  90  91  92  93  94  95  96  97  98  99
"V" "N" "I" "I" "G" "R" "N" "L" "L" "T" "Q" "I" "G" "C" "T" "L" "N" "F"
```

Here we will do a Normal Mode Analysis (NMA) to predict functional motions of a kinase protein.

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

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

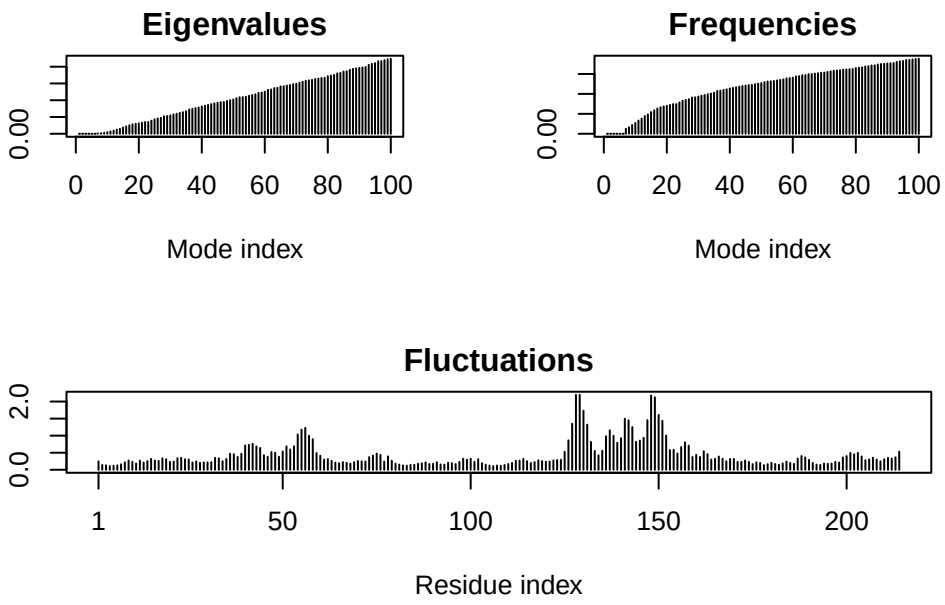
```
adk
```

```
 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
```

```
modes <- nma(adk)
```

```
 Building Hessian...        Done in 0.051 seconds.
 Diagonalizing Hessian...   Done in 0.395 seconds.
```

```
plot(modes)
```



Make a "movie" called a trajectory of the predicted motions:

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

Then I can open this file in Mol*…