Class10

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Introduction to the RCSB Protein Data Bank (PDB)

The Protein Data Bank(PDB) is the main repository of biomolecular structure. ### PDB statistics

```
PDB.data <- read.csv('Data Export Summary.csv',row.names = 1)
PDB <- data.frame(PDB.data)
PDB
```

```
                         X.ray     EM    NMR Integrative Multiple.methods
Protein (only)         178,795 21,825 12,773         343              226
Protein/Oligosaccharide 10,363  3,564     34           8               11
Protein/NA               9,106  6,335    287          24                7
Nucleic acid (only)      3,132    221  1,566           3               15
Other                      175     25     33           4                0
Oligosaccharide (only)      11      0      6           0                1
                        Neutron Other   Total
Protein (only)               84    32 214,078
Protein/Oligosaccharide       1     0  13,981
Protein/NA                    0     0  15,759
Nucleic acid (only)           3     1   4,941
Other                         0     0     237
Oligosaccharide (only)        0     4      22
```

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

The comma in these numbers leads to the numbers here being read as character.

```
library(readr)
stats <- read_csv('Data Export Summary.csv')
stats
```

```
# A tibble: 6 x 9
  `Molecular Type`    `X-ray`    EM   NMR Integrative `Multiple methods` Neutron
  <chr>                 <dbl> <dbl> <dbl>       <dbl>               <dbl>   <dbl>
1 Protein (only)       178795 21825 12773         343                 226      84
2 Protein/Oligosacch~   10363  3564    34           8                  11       1
3 Protein/NA             9106  6335   287          24                   7       0
4 Nucleic acid (only)    3132   221  1566           3                  15       3
5 Other                   175    25    33           4                   0       0
6 Oligosaccharide (o~      11     0     6           0                   1       0
# i 2 more variables: Other <dbl>, Total <dbl>
```

```
n.Xray <- sum(stats$`X-ray`)
n.Total <- sum(stats$`Total`)
per.Xray <- n.Xray/n.Total
per.Xray
```

```
[1] 0.8095077
```

80.95% of structures in the PDB are solved by X-Ray and Electron Microscopy.

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

```
per.protein <- stats[1,'Total']/n.Total
per.protein
```

```
      Total
1 0.8596889
```

85.97% of structures in the PDB are protein (only).

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?

644 HIV-1 protease structures are in the current PDB.

Visualizing the HIV-1 protease structure

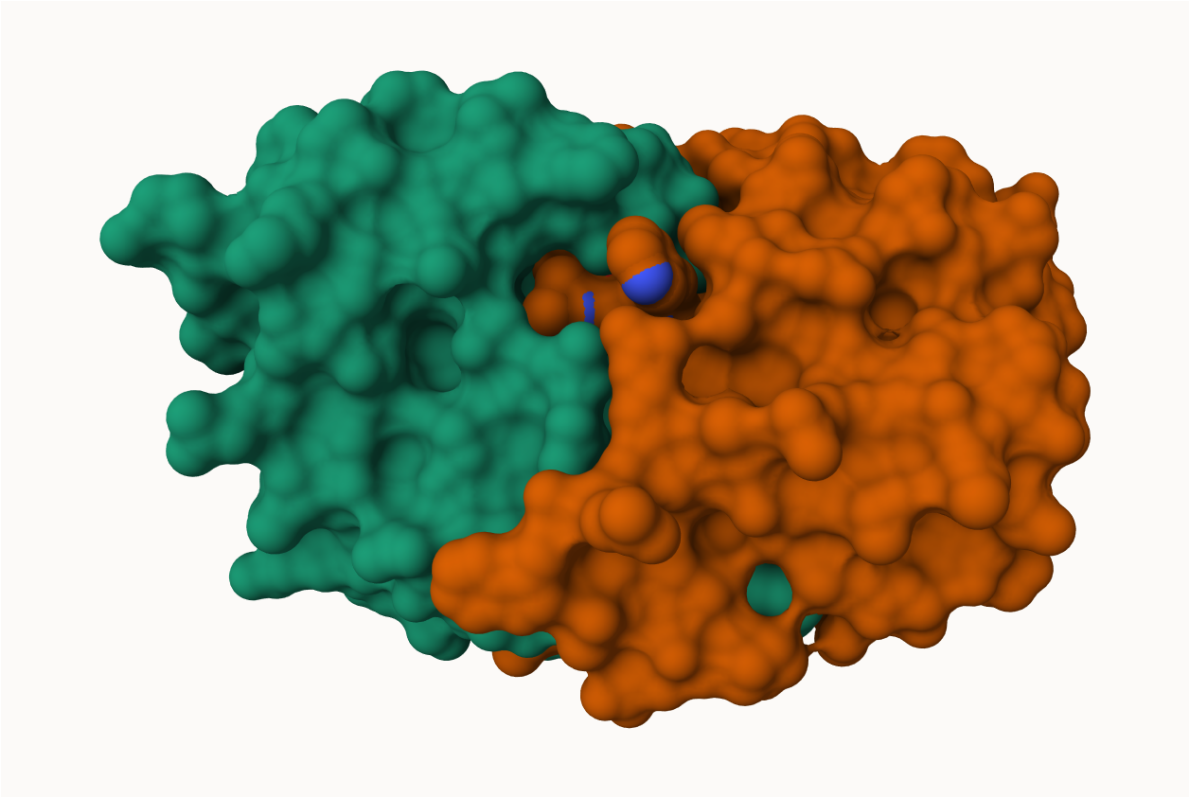


Figure 1: HIV-pr 1HSG with surface display showing ligand binding

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

The structure was constructed using X-RAY DIFFRACTION according to the PDB website. As the electron density of hydrogen atoms was too weak to be detected, the X-RAY DIFFRACTION only showed the oxygen atoms as the have a much stronger electron density.

> 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

HOH308

> 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.

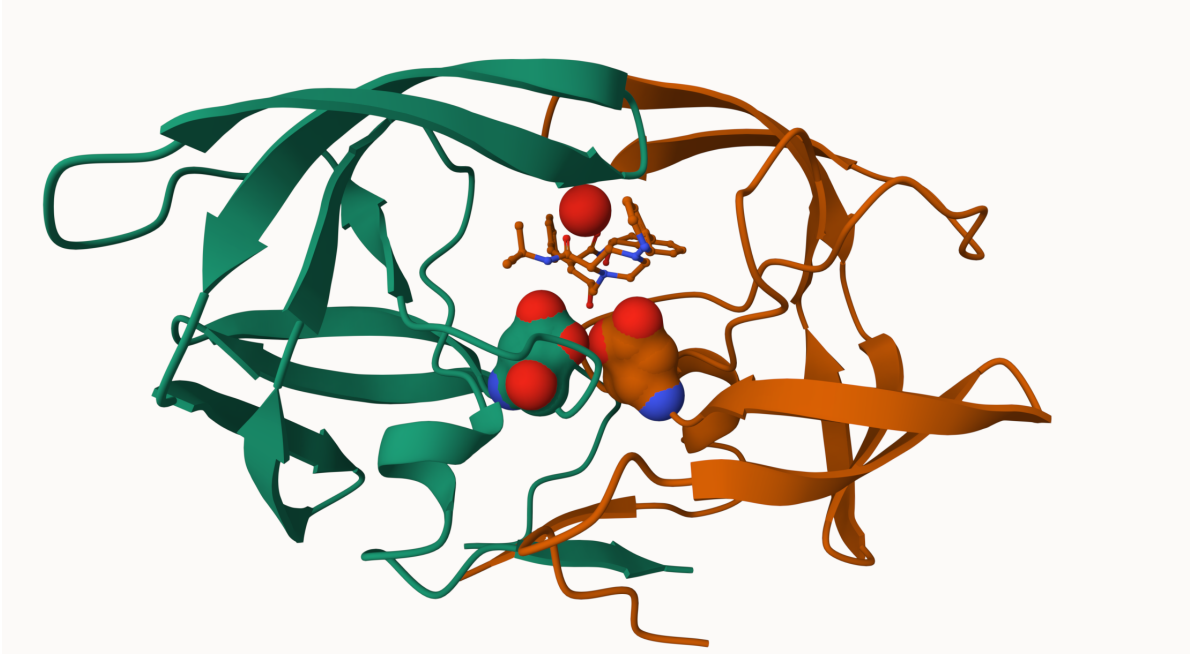


Figure 2: HIV-pr 1HSG highlighting ASP25 amino acids in both chains of the HIV-PR dimer along with the inhibitor and the all important active site water

Bio3D package for structural bioinformatics

```
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
```

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

198

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

HOH (127)

Q9: How many protein chains are in this structure?

2 (chain A &B)

```
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>
```

```
#library(bio3dview)
#library(NGLVieweR)
#view.pdb(pdb) |>
#  setSpin()
```

```
# Select the important ASP 25 residue
#sele <- atom.select(pdb, resno=25)

# and highlight them in spacefill representation
#view.pdb(pdb, cols=c("navy","teal"),
#         highlight = sele,
#         highlight.style = "spacefill") |>
#  setRock()
```

Predicting functional motions of a single structure

Read an ADK structure from the PDB database:

```
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
```

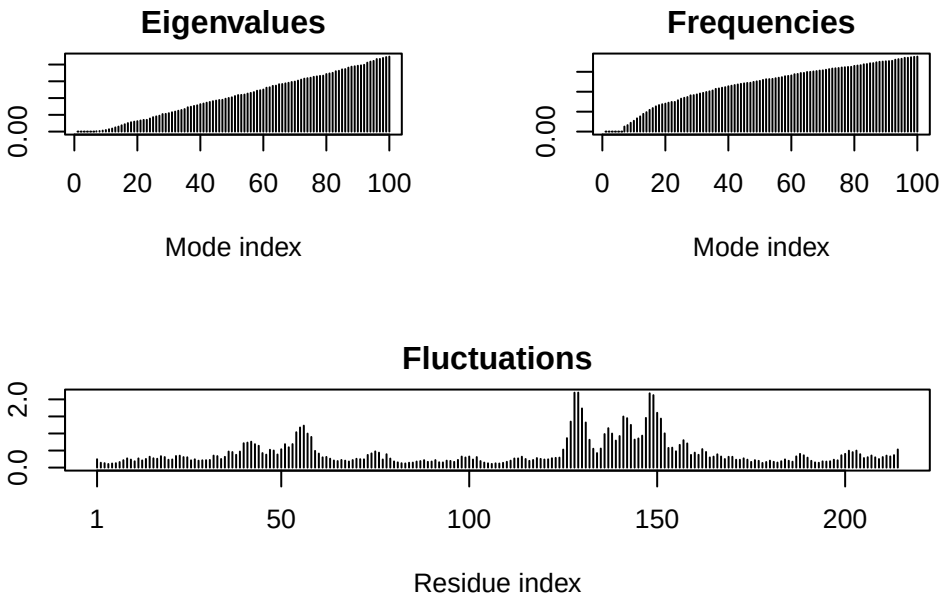
```
      VGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKDDQEETVRKRLVEYHQMTAPLIG
      YYSKEAEAGNTKYAKVDGTKPVAEVRADLEKILG

+ attr: atom, xyz, seqres, helix, sheet,
        calpha, remark, call
```

```
m <- nma(adk)
```

```
 Building Hessian...        Done in 0.012 seconds.
 Diagonalizing Hessian...   Done in 0.052 seconds.
```

```
plot(m)
```



Write out our results as we trajectory/movie of predicted motions:

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