Class 10: Structural Bioinformatics (Pt. 1)

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The PDB database

The Protein Data Bank (PDB)

```
stats <- read.csv("PDB Stats Structural Bioinformatics.csv", row.names=1)
stats
```

```
                        X.ray    EM   NMR Integrative Multiple.methods Neutron
Protein (only)         178795 21825 12773         343               226      84
Protein/Oligosaccharide  10363  3564    34           8                11       1
Protein/NA                9106  6335   287          24                 7       0
Nucleic acid (only)       3132   221  1566           3                15       3
Other                      175    25    33           4                 0       0
Oligosaccharide (only)      11     0     6           0                 1       0
                        Other  Total
Protein (only)             32 214078
Protein/Oligosaccharide     0  13981
Protein/NA                  0  15759
Nucleic acid (only)         1   4941
Other                       0    237
Oligosaccharide (only)      4     22
```

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

```
n.sums <- colSums(stats)
n.sums/n.sums["Total"]
```

```
          X.ray              EM             NMR      Integrative
    0.8095077464     0.1283842935     0.0590278614     0.0015340257
Multiple.methods         Neutron           Other            Total
    0.0010441012     0.0003533881     0.0001485836     1.0000000000
```

```
round(n.sums, digits=2)
```

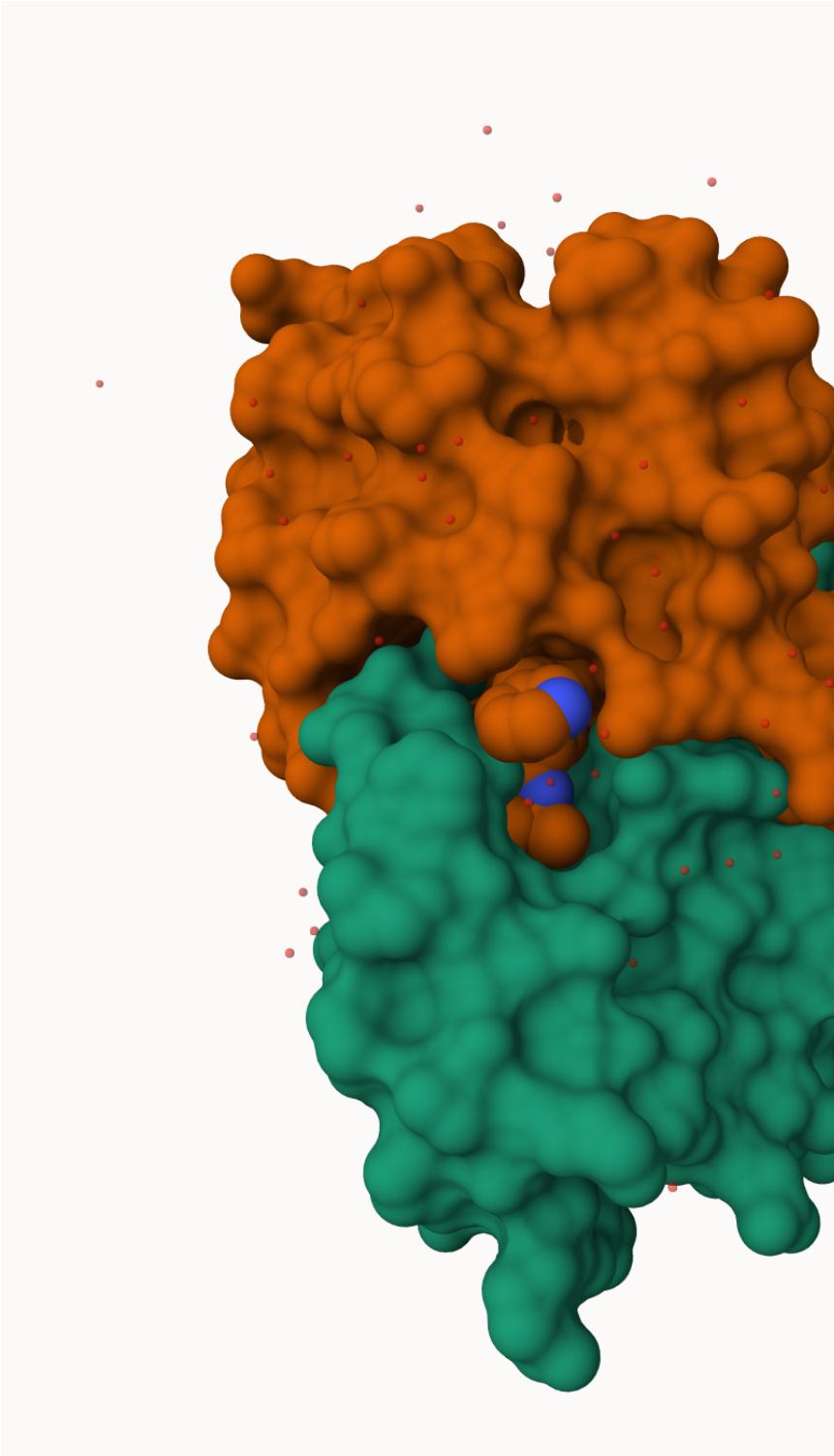
```
          X.ray              EM             NMR      Integrative
         201582           31970           14699             382
Multiple.methods         Neutron           Other           Total
            260              88              37          249018
```

X-Ray: 80.9% EM: 12.8%

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

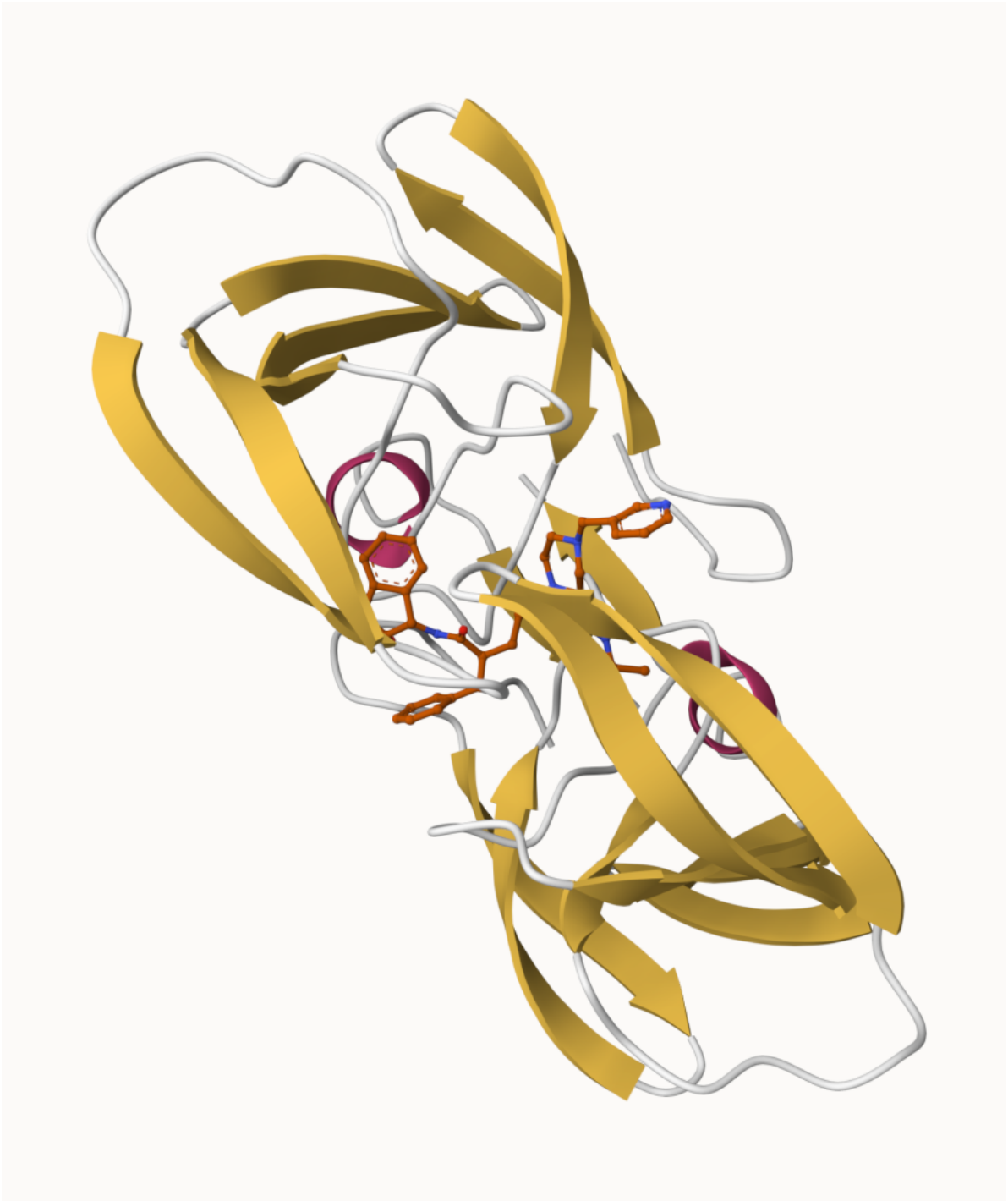
85.9%

Using Molstar

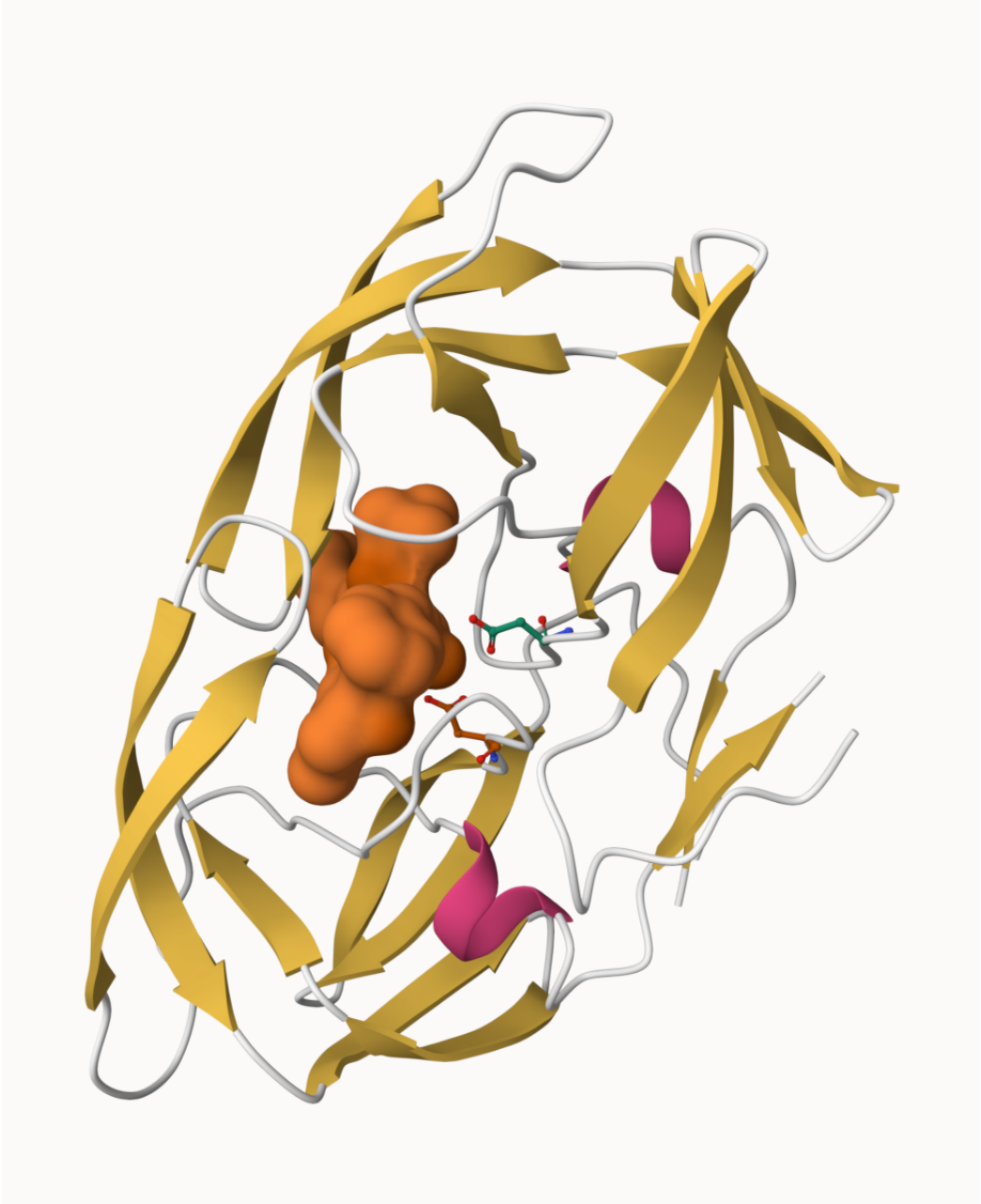


We can use the main Molstar Viewer Online:

Q. Generate and insert an image of teh HIV-pr cartoon colored by secondary structure, showing the inhibitor (ligand) in ball and stick.



Q. One final image showing catalytic APS 25 as ball and stick and the all-important



```
library(bio3d)
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"
```

Let's try out the new **bio3dview** package that is not yet on CRAN. We can use the **remotes** package to install any R package from GitHub.

Quick viewing of PDBs

```
library(bio3dview)
sele <- atom.select(hiv, resno=25)
#view.pdb(hiv, backgroundColor = "lightpink", highlight = sele, highlight.style = "spacefill"
```

Prediction of Protein Flexibility

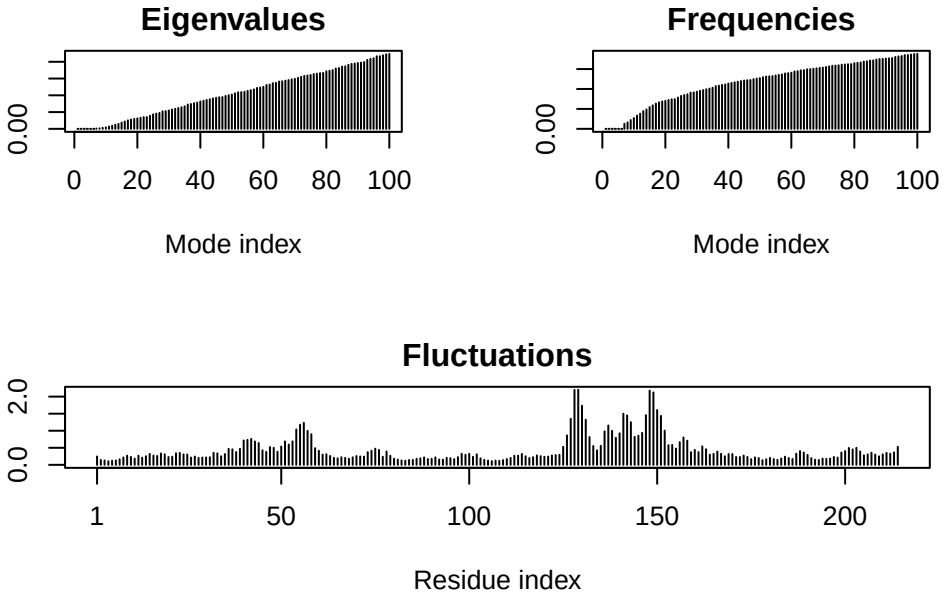
```
adk <- read.pdb("6s36")
```

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

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

```
 Building Hessian...     Done in 0.021 seconds.
 Diagonalizing Hessian...   Done in 0.09 seconds.
```

```
plot(m)
```



Lets write out our results as a trajectory movie:

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

```
#view.nma(m)
```