Structural Bioinformatics

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#1. Introduction to RCSB Protein Data Bank (PDB)

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

```
                           X.ray     EM    NMR Multiple.methods Neutron Other
Protein (only)           158,844 11,759 12,296              197      73    32
Protein/Oligosaccharide    9,260  2,054     34                8       1     0
Protein/NA                 8,307  3,667    284                7       0     0
Nucleic acid (only)        2,730    113  1,467               13       3     1
Other                        164      9     32                0       0     0
Oligosaccharide (only)        11      0      6                1       0     4
                           Total
Protein (only)           183,201
Protein/Oligosaccharide   11,357
Protein/NA                12,265
Nucleic acid (only)        4,327
Other                        205
Oligosaccharide (only)        22
```

At the time of writing, there are 183,201 protein structures. In Uniport, there are 251600,768 protein sequences.

```
round(183201/251600768*100,2)
```

```
[1] 0.07
```

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

```
total <- data["Protein (only)", "Total"]
total <- as.numeric(gsub(",", "", total))

total_xray_em <- as.numeric(gsub(",","",data["Protein (only)", "X.ray"])) +
                      as.numeric(gsub(",","",data["Protein (only)", "EM"]))

perc <- round(total_xray_em/total*100,2)
perc
```

```
[1] 93.12
```

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

```
all_structures <- as.numeric(gsub(",","",data[,"Total"]))
all_structures
```

```
[1] 183201  11357  12265   4327    205     22
```

```
prop_proteins <- round(all_structures[1]/sum(all_structures)*100,2)
prop_proteins
```

```
[1] 86.67
```

Making a function to remove commas

```
rm.comma <- function(x){
  as.numeric(gsub(",","",x))
}

pdbstats <- apply(data, 2, rm.comma)
```

Will add the rownames from the origianl table.

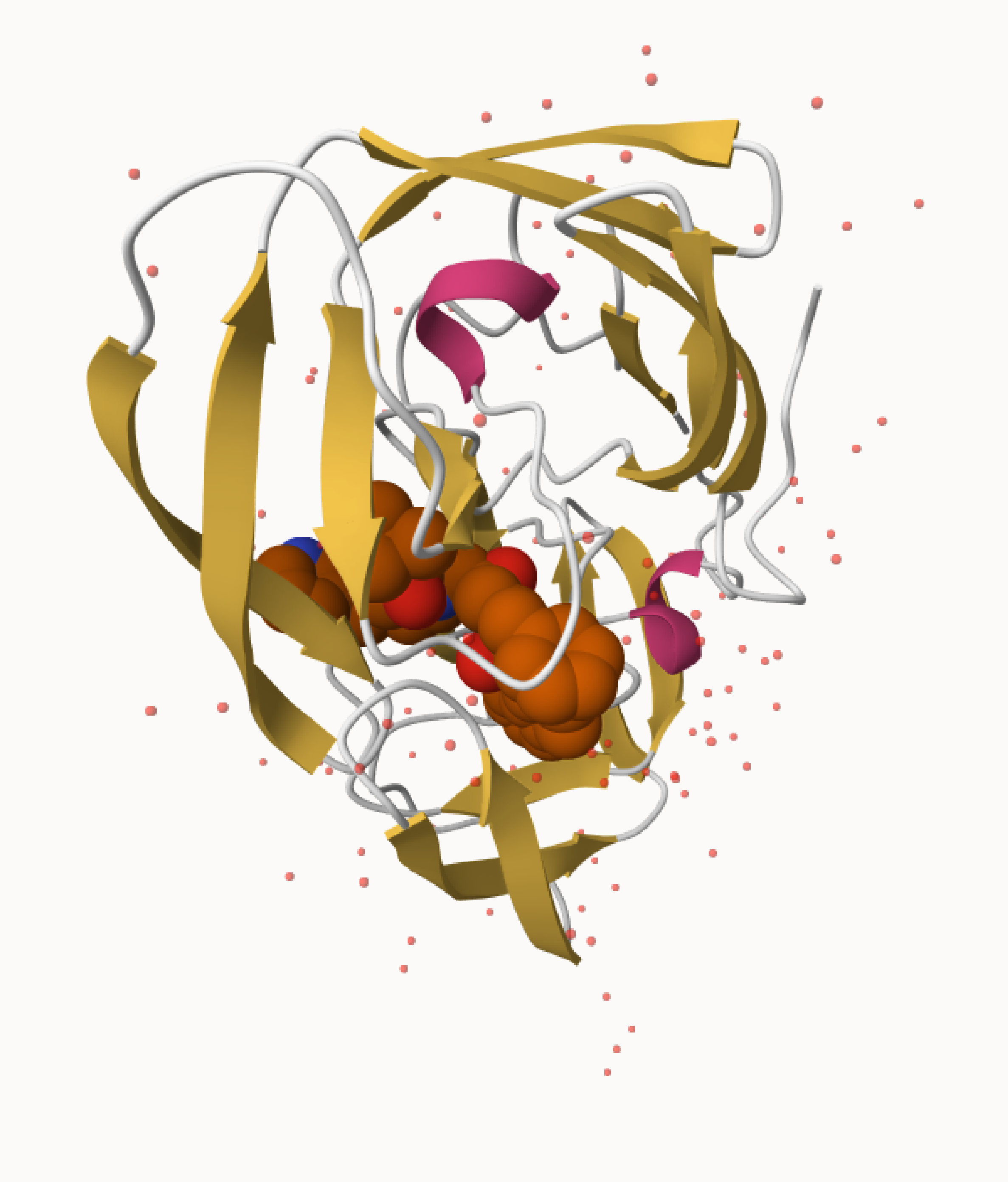
```
rownames(pdbstats) <- rownames(data)
pdbstats
```

```
                         X.ray    EM   NMR Multiple.methods Neutron Other
Protein (only)          158844 11759 12296              197      73    32
Protein/Oligosaccharide   9260  2054    34                8       1     0
Protein/NA                8307  3667   284                7       0     0
Nucleic acid (only)       2730   113  1467               13       3     1
Other                      164     9    32                0       0     0
Oligosaccharide (only)      11     0     6                1       0     4
                         Total
Protein (only)          183201
Protein/Oligosaccharide  11357
Protein/NA               12265
Nucleic acid (only)       4327
Other                      205
Oligosaccharide (only)      22
```

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?

There are 200 HIV-1 protease structures.

Here is a pic of HIV-Pr.



And a nicer pic is:

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

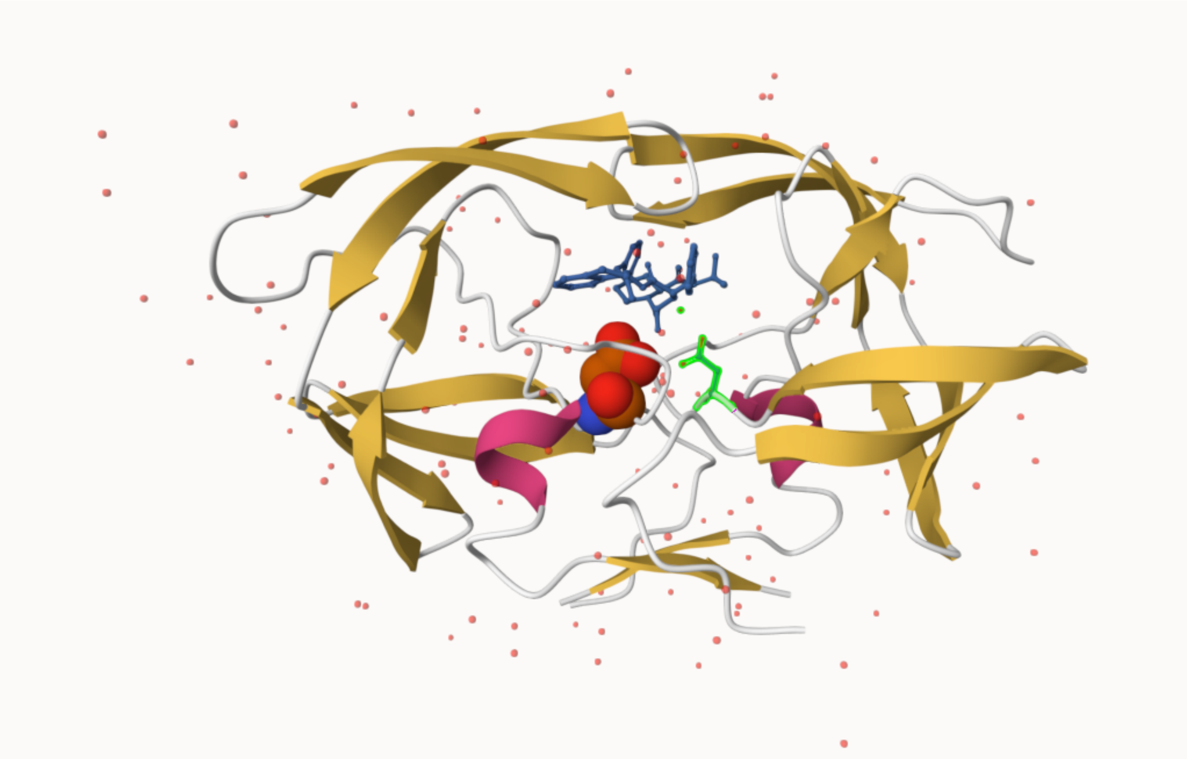


Figure 1: A lovely Image

The resolution at which the structure of 1HSG was resolved is 2A but hydrgen atoms are of the size 0.5A. Hence, water molecules appear as just 1 atom.

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

HOH 308

#3. Introduction to Bio3D

```
library(bio3d)
```

Reading PDB data file into R:

```
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, MK1

Q9: How many protein chains are in this structure? 2

Observing the attributes:

```
attributes(pdb)
```

```
$names
[1] "atom"   "xyz"    "seqres" "helix"  "sheet"  "calpha" "remark" "call"  

$class
[1] "pdb" "sse"
```

```
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>
```

```
head(pdb$atom$resid)
```

```
[1] "PRO" "PRO" "PRO" "PRO" "PRO" "PRO"
```

```
aa321(pdb$atom$resid[pdb$calpha])
```

```
  [1] "P" "Q" "I" "T" "L" "W" "Q" "R" "P" "L" "V" "T" "I" "K" "I" "G" "G" "Q"
 [19] "L" "K" "E" "A" "L" "L" "D" "T" "G" "A" "D" "D" "T" "V" "L" "E" "E" "M"
 [37] "S" "L" "P" "G" "R" "W" "K" "P" "K" "M" "I" "G" "G" "I" "G" "G" "F" "I"
 [55] "K" "V" "R" "Q" "Y" "D" "Q" "I" "L" "I" "E" "I" "C" "G" "H" "K" "A" "I"
 [73] "G" "T" "V" "L" "V" "G" "P" "T" "P" "V" "N" "I" "I" "G" "R" "N" "L" "L"
 [91] "T" "Q" "I" "G" "C" "T" "L" "N" "F" "P" "Q" "I" "T" "L" "W" "Q" "R" "P"
[109] "L" "V" "T" "I" "K" "I" "G" "G" "Q" "L" "K" "E" "A" "L" "L" "D" "T" "G"
[127] "A" "D" "D" "T" "V" "L" "E" "E" "M" "S" "L" "P" "G" "R" "W" "K" "P" "K"
[145] "M" "I" "G" "G" "I" "G" "G" "F" "I" "K" "V" "R" "Q" "Y" "D" "Q" "I" "L"
[163] "I" "E" "I" "C" "G" "H" "K" "A" "I" "G" "T" "V" "L" "V" "G" "P" "T" "P"
[181] "V" "N" "I" "I" "G" "R" "N" "L" "L" "T" "Q" "I" "G" "C" "T" "L" "N" "F"
```

Predicting functional motions of a single structure:

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

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

```
adk
```

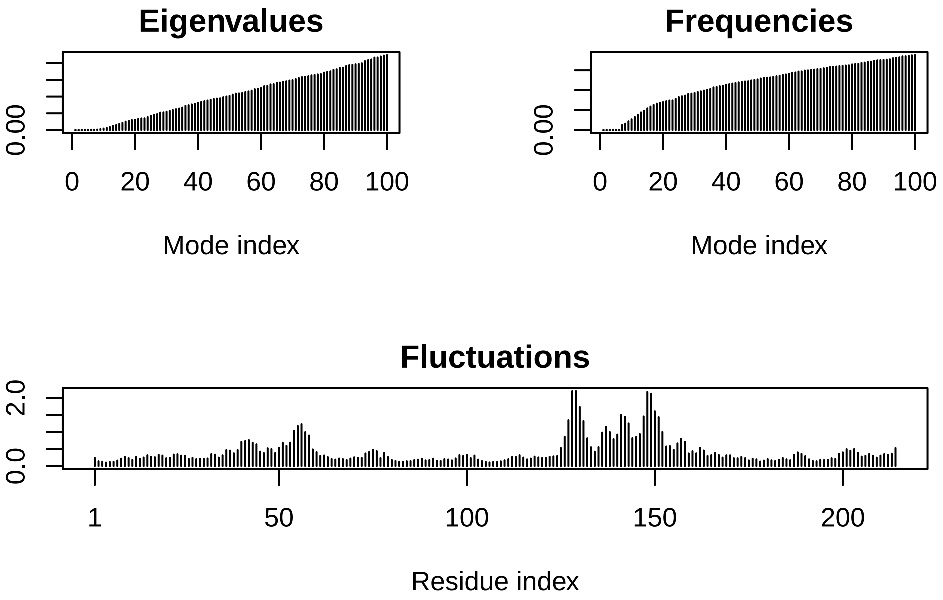
```


 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
```

Normal Mode Analysis:

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

```
 Building Hessian...        Done in 0.03 seconds.
 Diagonalizing Hessian...   Done in 0.33 seconds.
```

```
plot(m)
```



View the movie:

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