Class10: Structural Bioinformatics

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

```
                         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
```

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

Write a function to fix this non-numeric table.

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

PDB.df <- apply(PDB, 2, rm.comma)
PDB.df
```

```
      X.ray    EM   NMR Multiple.methods Neutron Other  Total
[1,] 158844 11759 12296              197      73    32 183201
[2,]   9260  2054    34                8       1     0  11357
[3,]   8307  3667   284                7       0     0  12265
[4,]   2730   113  1467               13       3     1   4327
[5,]    164     9    32                0       0     0    205
[6,]     11     0     6                1       0     4     22
```

Add original row names

```
rownames(PDB.df) <- rownames(PDB)
PDB.df
```

```
                         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
```

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

93%

```
x <- sum(PDB.df[,1:2])
y <- sum(PDB.df[,1:6])
(x/y)*100
```

```
[1] 93.15962
```

```
totals <- apply(PDB.df, 2, sum)
totals/totals["Total"]*100
```

```
          X.ray              EM             NMR Multiple.methods
   84.83231383      8.32730146      6.67953467      0.10691797
        Neutron           Other           Total
    0.03642780      0.01750427    100.00000000
```

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

86%

```
x <- sum(PDB.df[1,])
y <- sum(PDB.df[1:6,])
(x/y)*100
```

```
[1] 86.67026
```

```
totals <- apply(PDB.df, 1, sum)
sum(PDB.df[1,])
```

```
[1] 366402
```

```
sum(PDB.df[1:6,])
```

```
[1] 422754
```

```
x/y
```

```
[1] 0.8667026
```

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?

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

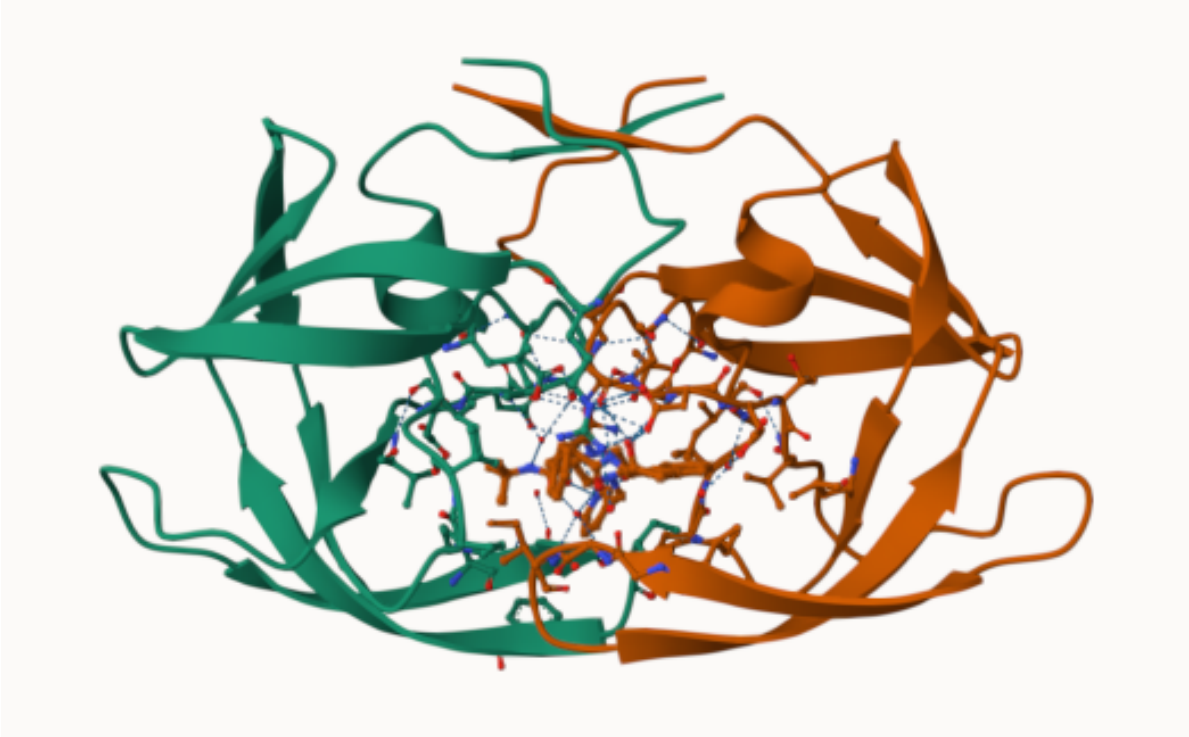
Hydrogen is only one 1A and the resolution for this is 2A.

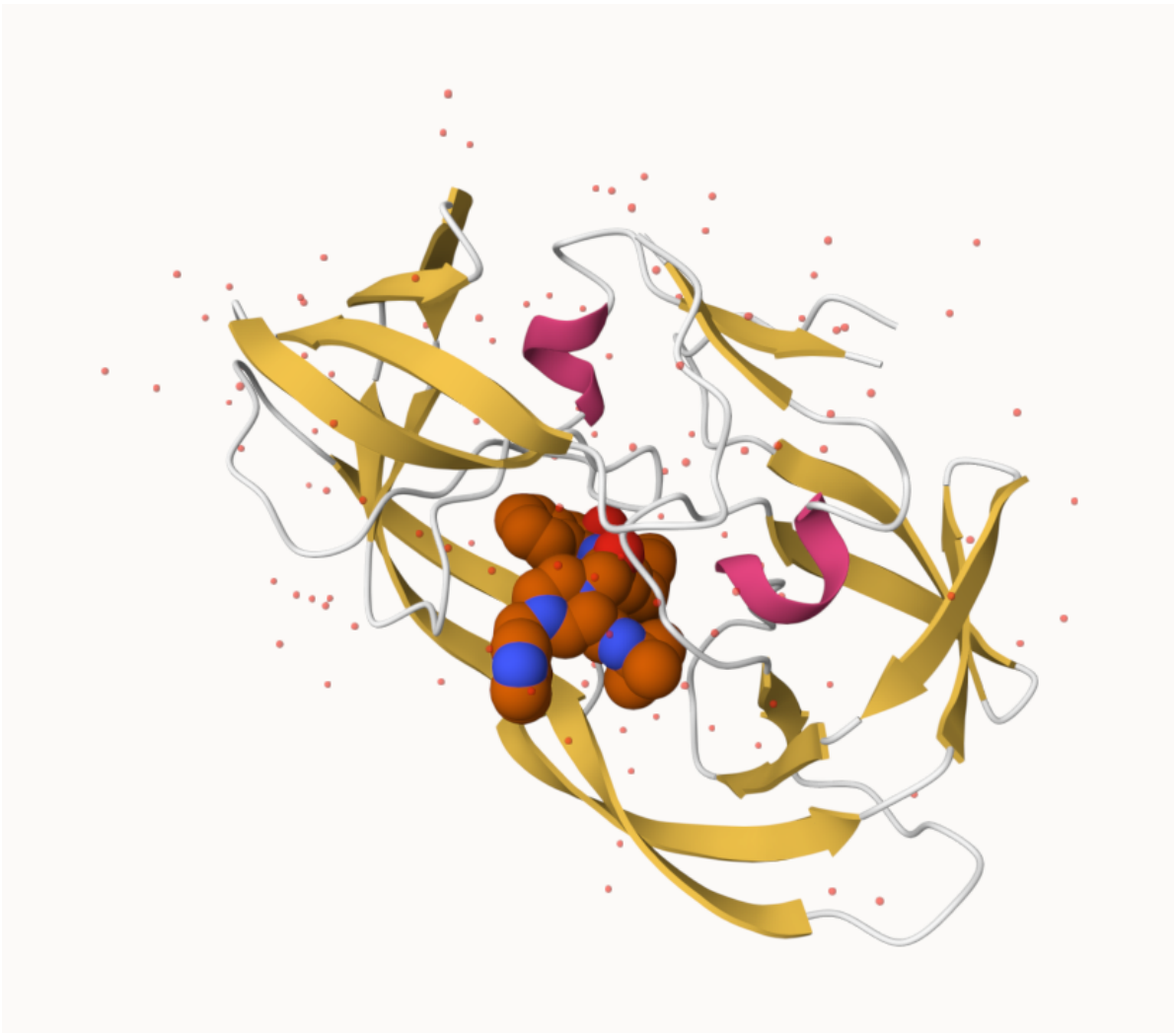
Q5: There is a critical "conserved" water molecule in the binding site. Can you identify this water molecule? What residue number does this water molecule have

H0H - 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.

Discussion Topic: Can you think of a way in which indinavir, or even larger ligands and substrates, could enter the binding site?





```
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

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

```
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>
```

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

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

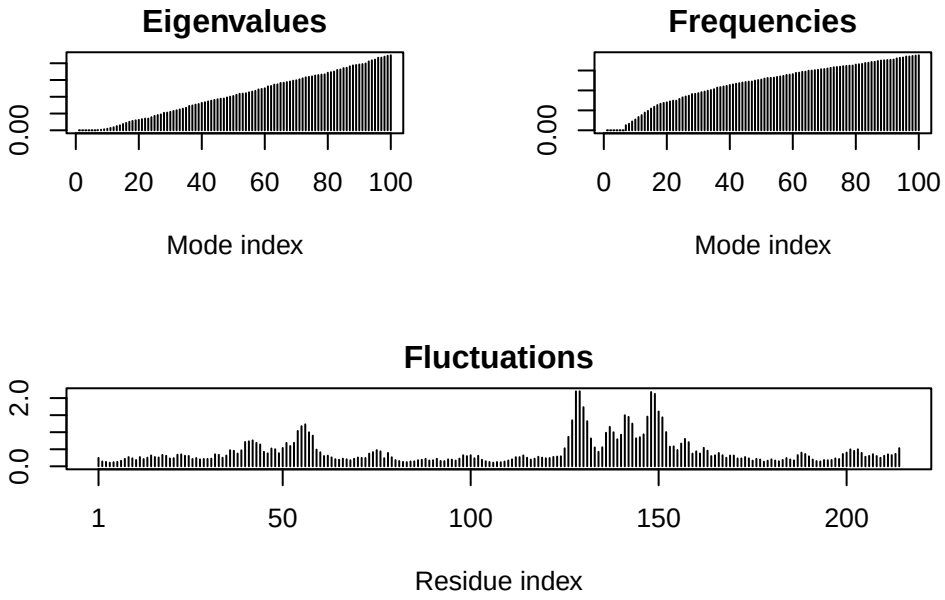
```
adk
```

```
 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 0.013 seconds.
 Diagonalizing Hessian...   Done in 0.254 seconds.
```

```
plot(m)
```




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

Q10. Which of the packages above is found only on BioConductor and not CRAN? msa.

Q11. Which of the above packages is not found on BioConductor or CRAN?: bio3D-view.

Q12. True or False? Functions from the devtools package can be used to install packages from GitHub and BitBucket? TRUE.

```
#library(bio3d)
#aa <- get.seq("1ake_A")
```

```
#install.packages("bio3d")
#install.packages("devtools")
#install.packages("BiocManager")

#BiocManager::install("msa")
#devtools::install_bitbucket("Grantlab/bio3d-view")
```

```
#library(bio3d)

#aa <- get.seq("1ake_A")
#aa
```

Q13. How many amino acids are in this sequence, i.e. how long is this sequence? 214.