Class 10

Yanlin

Q1: What percentage of structures in the PDB are solved by X-Ray and Electron Microscopy. –83.255 and 10.234 respectively.

Q2: What proportion of structures in the PDB are protein? –protein only is 86.4%

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? –4,563

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

	X.ray	EM	NMR	Multiple.methods	Neutron	Other
Protein (only)	167,317	15,698	12,534	208	77	32
Protein/Oligosaccharide	9,645	2,639	34	8	2	0
Protein/NA	8,735	4,718	286	7	0	0
Nucleic acid (only)	2,869	138	1,507	14	3	1
Other	170	10	33	0	0	0
Oligosaccharide (only)	11	0	6	1	0	4

	Total
Protein (only)	195,866
Protein/Oligosaccharide	12,328
Protein/NA	13,746
Nucleic acid (only)	4,532
Other	213
Oligosaccharide (only)	22

```
x <- pdbsum$Total
x
```

```
[1] "195,866" "12,328"  "13,746"  "4,532"   "213"     "22"
```

```r
convert_comma_number <- function(x) {
  x <- gsub(',','', x)
  x <- as.numeric(x)
  return(x)
}

n.tot <- sum(convert_comma_number(x))
```

The `apply()` function takes any function and "apply" it over either the ROWs or COLs of a data.frame

```r
n.pdbsum <- apply(pdbsum, 2, convert_comma_number)
colSums(apply(pdbsum, 2, convert_comma_number)) / n.tot
```

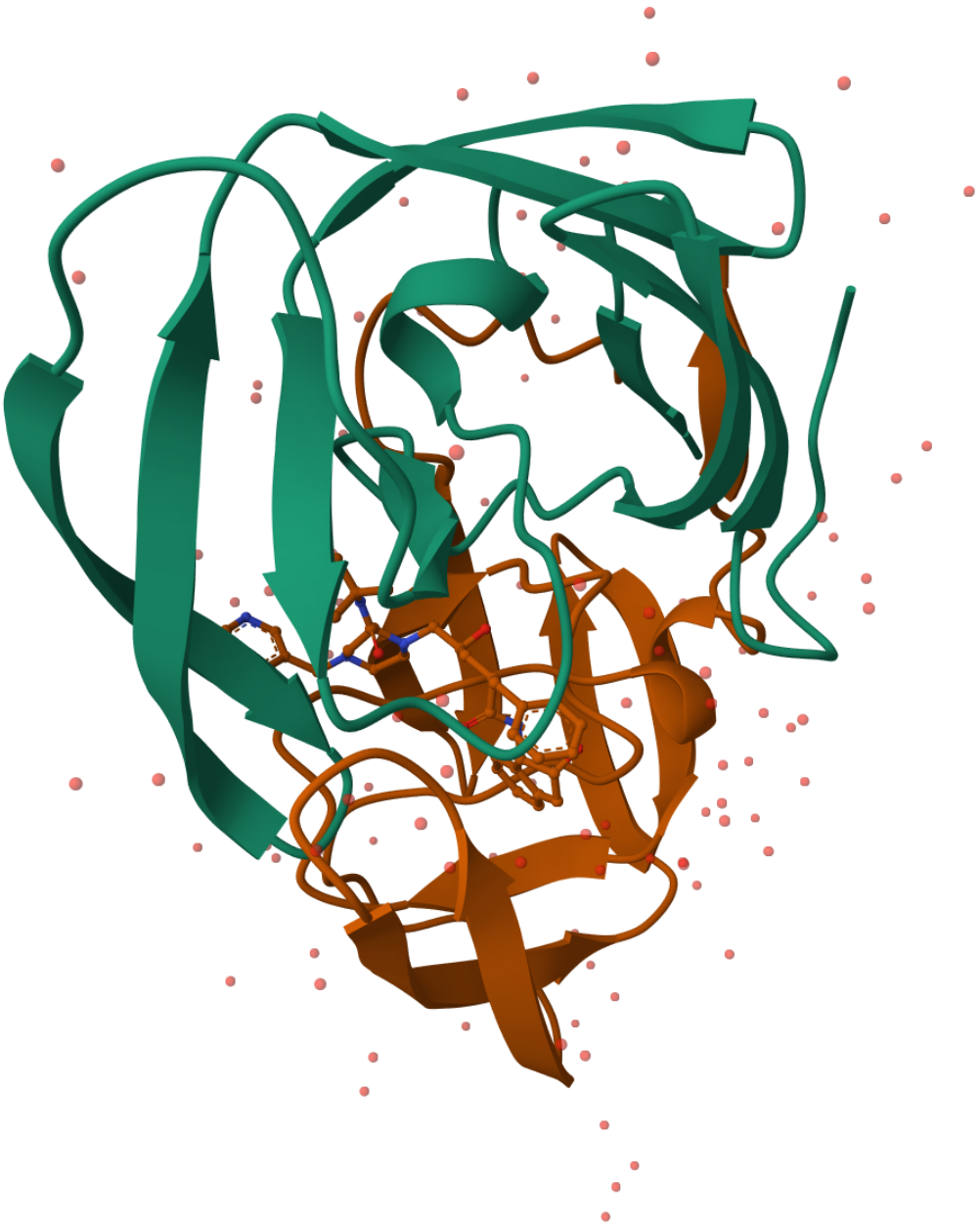
```
          X.ray              EM             NMR Multiple.methods
    0.8325592064    0.1023479646    0.0635181093    0.0010498132
        Neutron           Other           Total
    0.0003617003    0.0001632063    1.0000000000
```

```r
n.pdbsum[1, "Total"]/n.tot
```

```
   Total
0.863961
```

`read_csv()` from library `readr` can remove `,` in the numeric data automatically

Using Mol*



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

in this structure? – H is too small

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 –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)

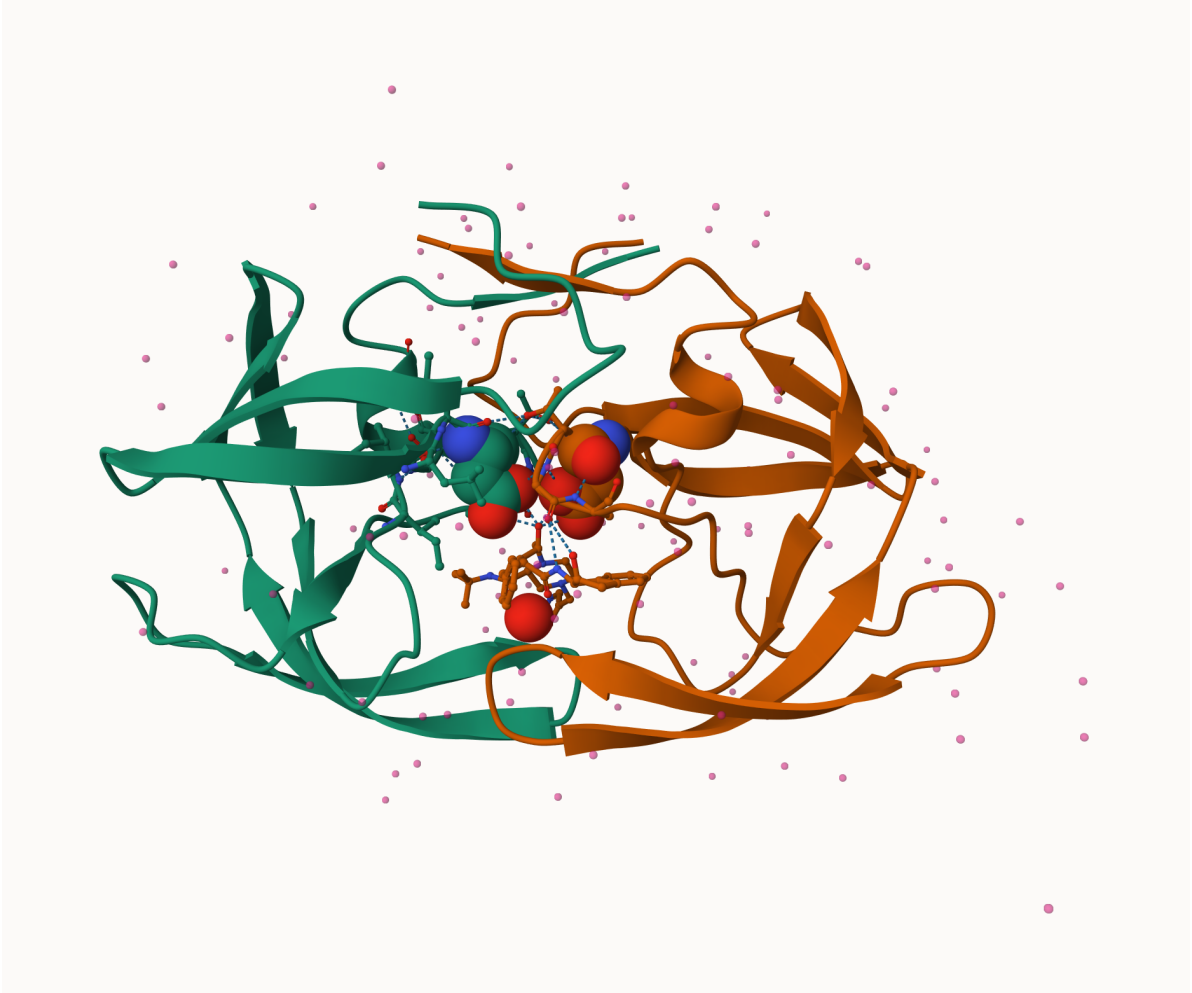


Figure 1: The all important ASP25 amino acids and HOH 308

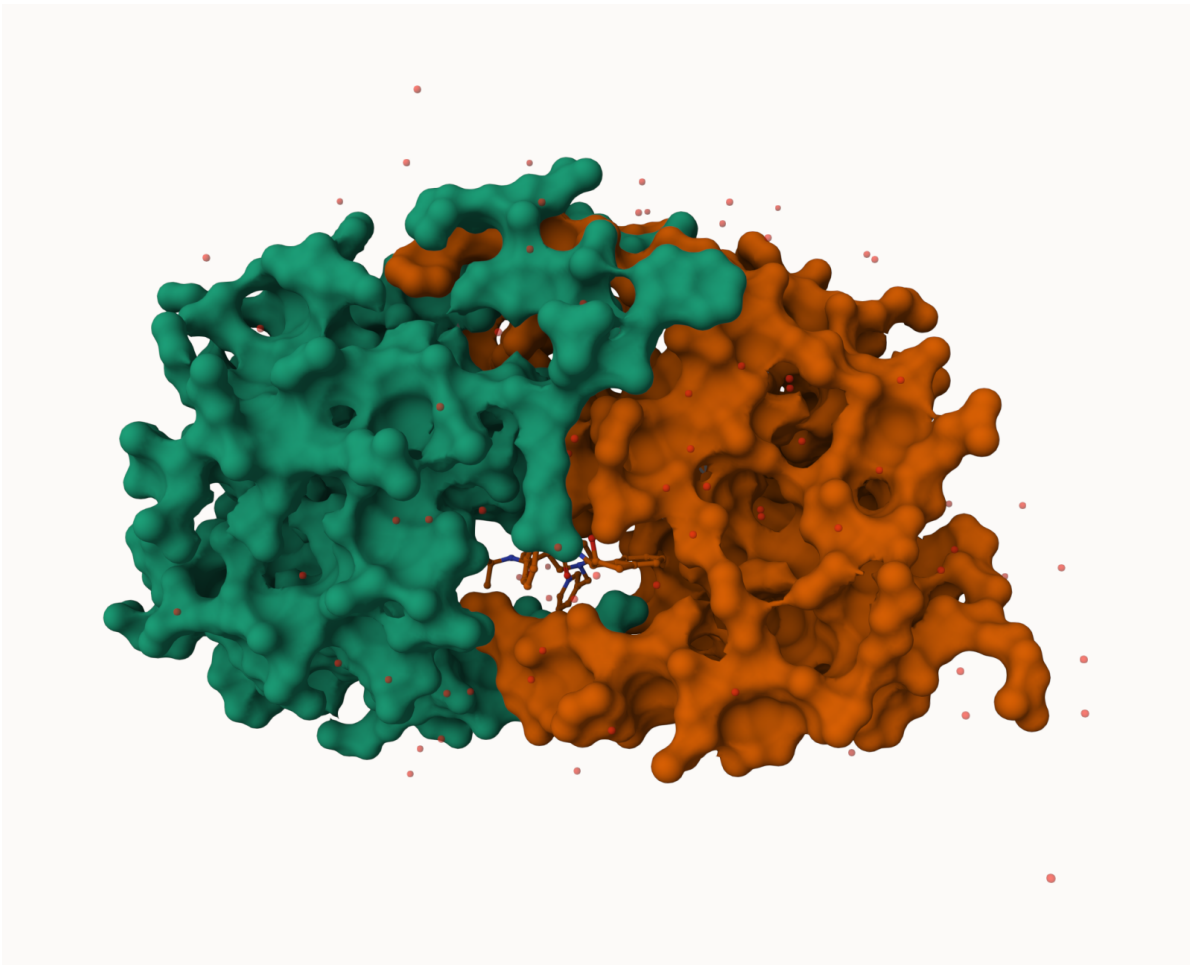


Figure 2: Surface representation showing the binding cleft

Q7: How many amino acid residues are there in this pdb object? –198

Q8: Name one of the two non-protein residues? –HOH (127), MK1 (1)

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

```
library(bio3d)
library(shiny)
library(r3dmol)
```

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

```
 Call:  read.pdb(file = "1hsg.pdb")

   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
```

```
attributes(pdb)
```

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

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

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

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

```
adk
```

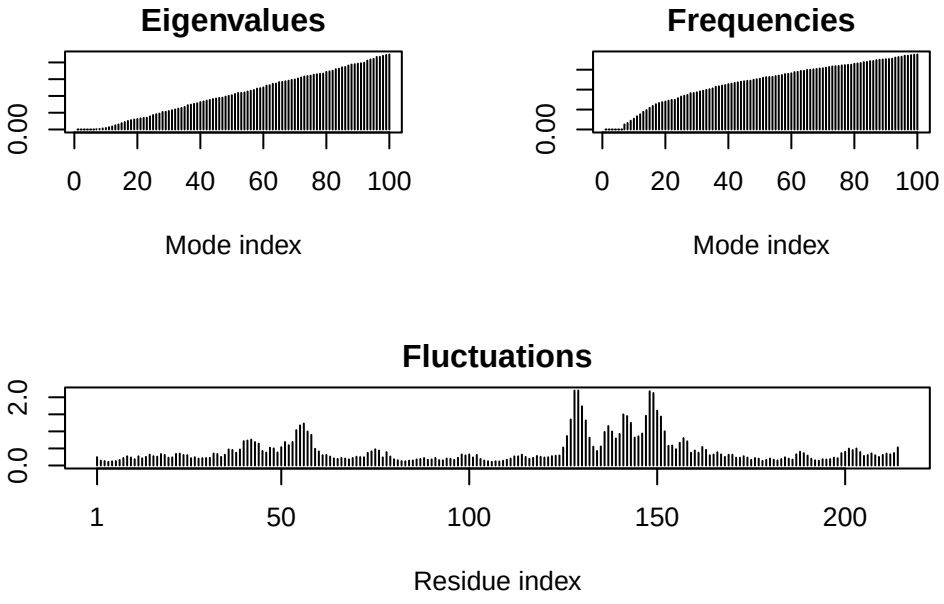
```
 Call:  read.pdb(file = "6s36")

   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 0.033 seconds.
 Diagonalizing Hessian...   Done in 0.306 seconds.
```

```
plot(m)
```



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