Class09

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

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

```
for (i in as.vector(colnames(PDB_Data))){
  PDB_Data[,i] <- as.numeric(gsub(",","",PDB_Data[,i]))
}

sum(PDB_Data$X.ray)/sum(PDB_Data$Total)
```

```
[1] 0.8483231
```

```
sum(PDB_Data$EM)/sum(PDB_Data$Total)
```

```
[1] 0.08327301
```

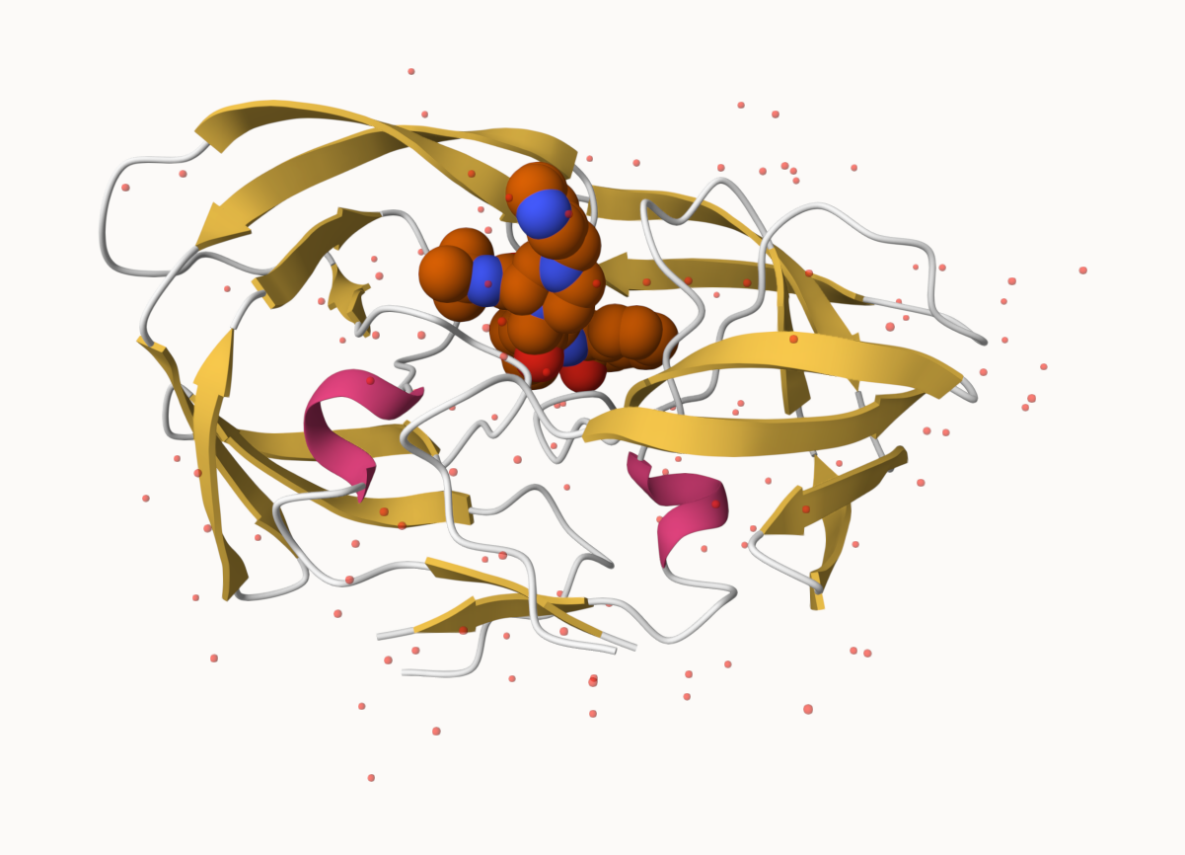
Q2: What proportion of structures in the PDB are protein?

```
PDB_Data["Protein (only)", "Total"]/sum(PDB_Data$Total)
```

```
[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?

211,377 (PDB search for “HIV-1 protease”)



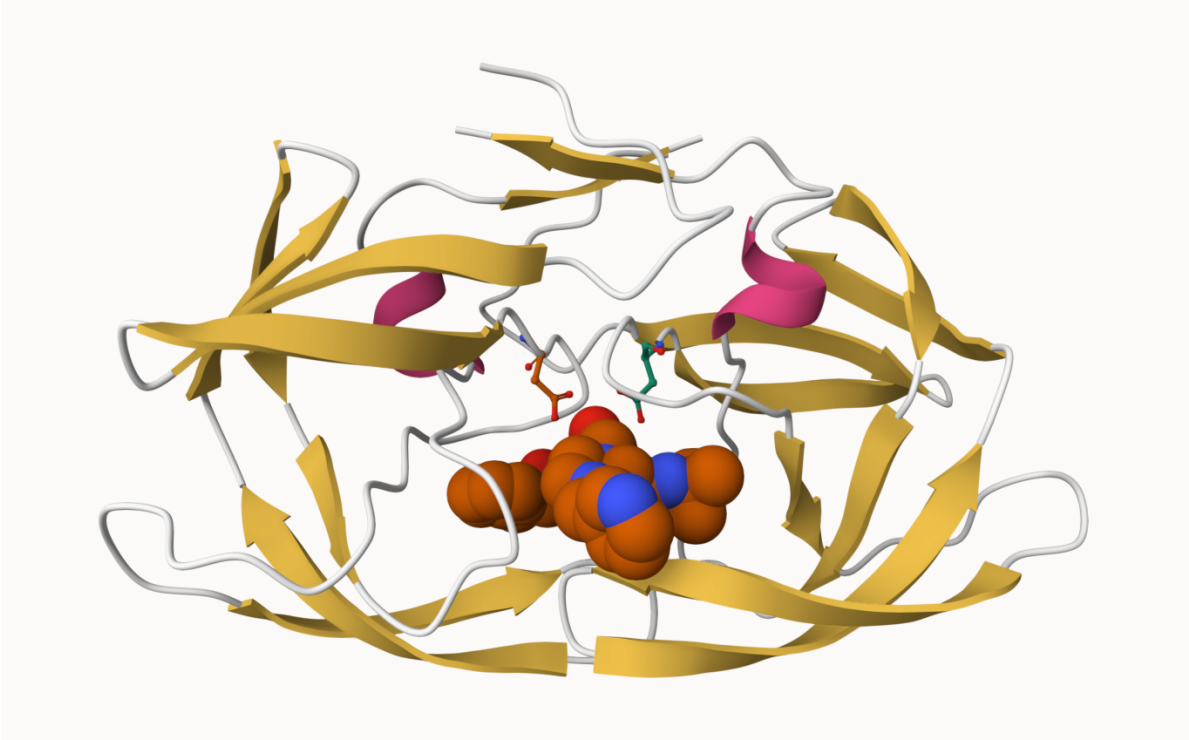
Q4: Water molecules normally have 3 atoms. Why do we see just one atom per water molecule in this structure?

Hydrogen atoms are not usually displayed in the default setting, because their size are smaller than the resolution of the data.

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

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?

Q7: [Optional] As you have hopefully observed HIV protease is a homodimer (i.e. it is composed of two identical chains). With the aid of the graphic display can you identify secondary structure elements that are likely to only form in the dimer rather than the monomer?

```
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?

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