class 09

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##Download a CSV file from the PDB site (accessible from "Analyze" > "PDB Statistics" > "by Experimental Method and Molecular Type". Move this CSV file into your RStudio project and use it to answer the following questions:

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

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

a function to drop the comma :(

```
rm.comma<-function(x){
  as.numeric(gsub(",","",x))
}
PDB_summary1<-apply(PDB_summary, 2, rm.comma)
rownames(PDB_summary1)<-rownames(PDB_summary)
PDB_summary1
```

```
                        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
```

```
PDB_summary1_total <-apply(PDB_summary1, 2, sum)
round(PDB_summary1_total/PDB_summary1_total["Total"]*100, 2)
```

```
        X.ray            EM           NMR Multiple.methods
        84.83          8.33          6.68             0.11
      Neutron         Other         Total
         0.04          0.02        100.00
```

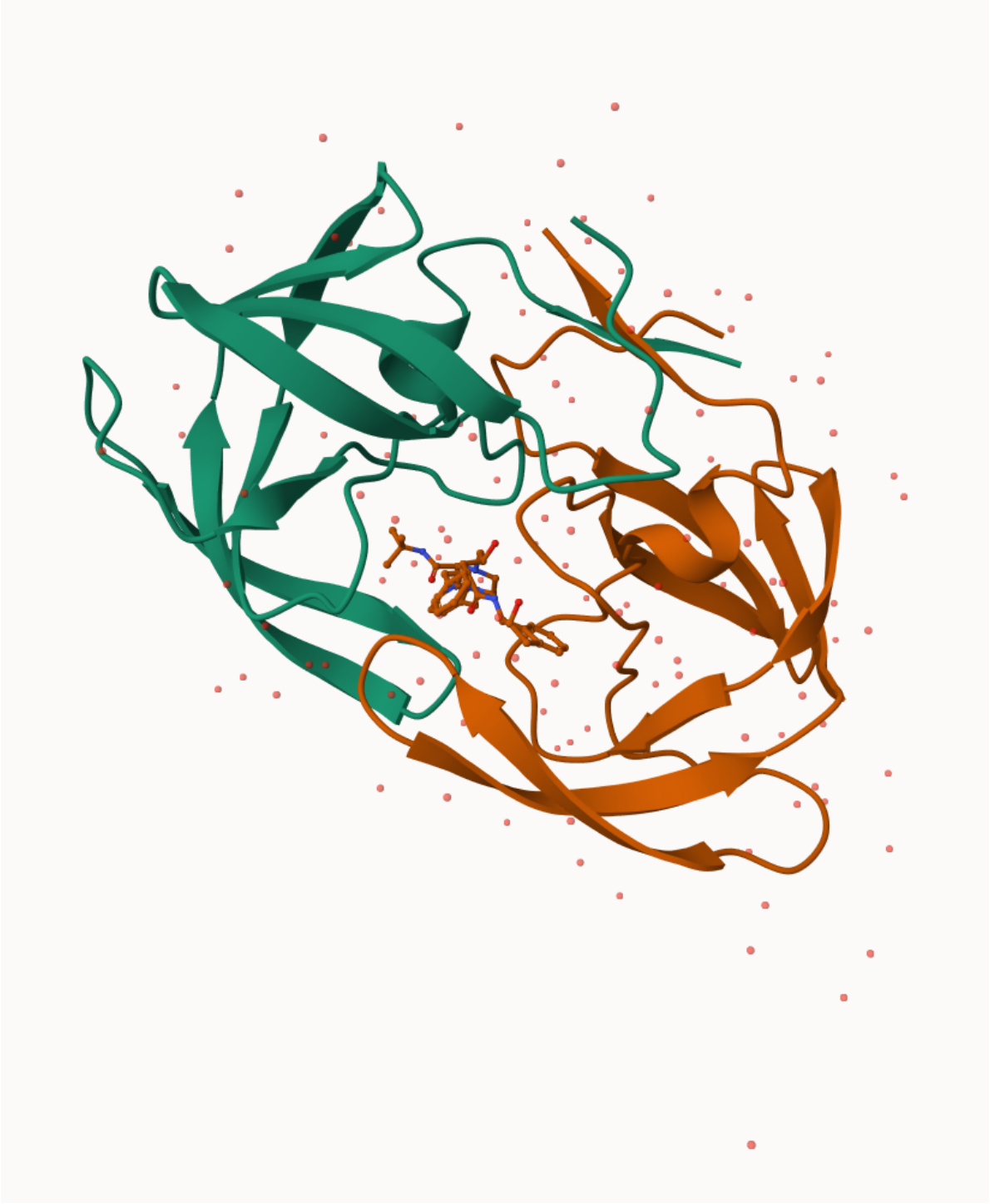
Q2: What proportion of structures in the PDB are protein?

Skipped

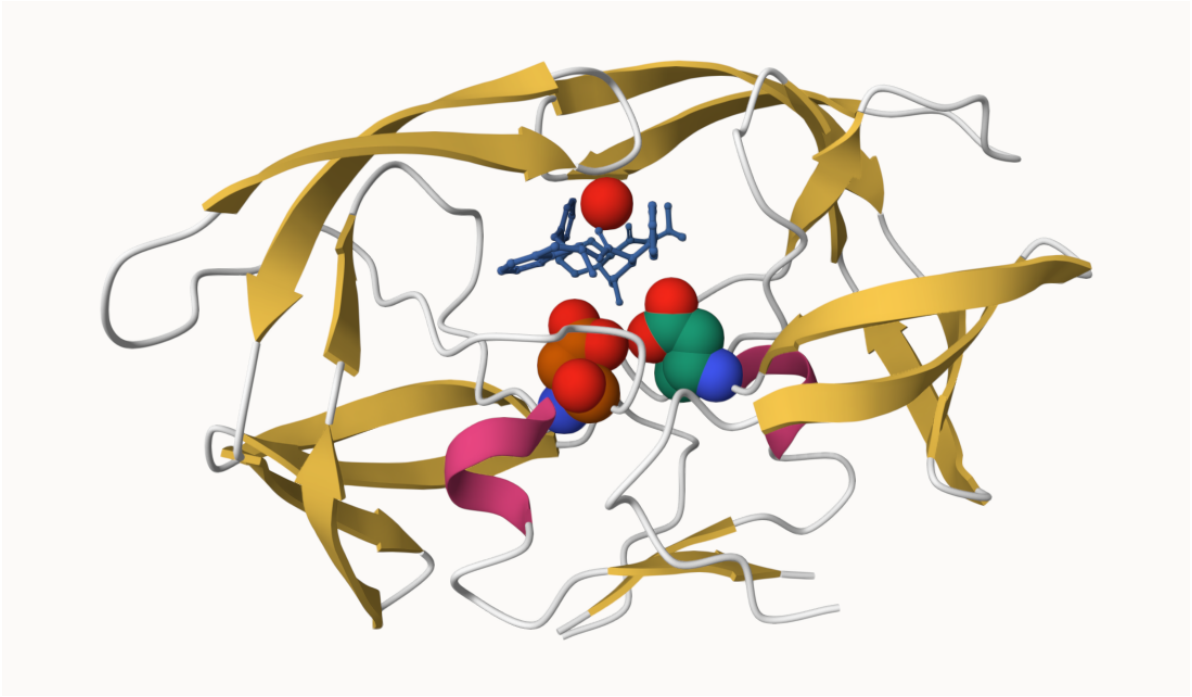
Q3: Type HIV in the PDB website search box on the home page and determine how many HIV-1 protease structures are in the current PDB?

Skipped

#Using Mol to examine HIV-Pr



HIV-PR Picture
#Prettier image with the water and 2 sidechains



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

Because the cystrallography only have resolution of 2A, which is bigger than the H atom so therefore H is not showing in here.

> 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

See above images, Water 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.

See above images.

##BIO3D!!!!!

```
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
```

```
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"
```

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

```
[1] 198
```

#Run a normal mode analysis(NMA)- a bioinfomatic prediction

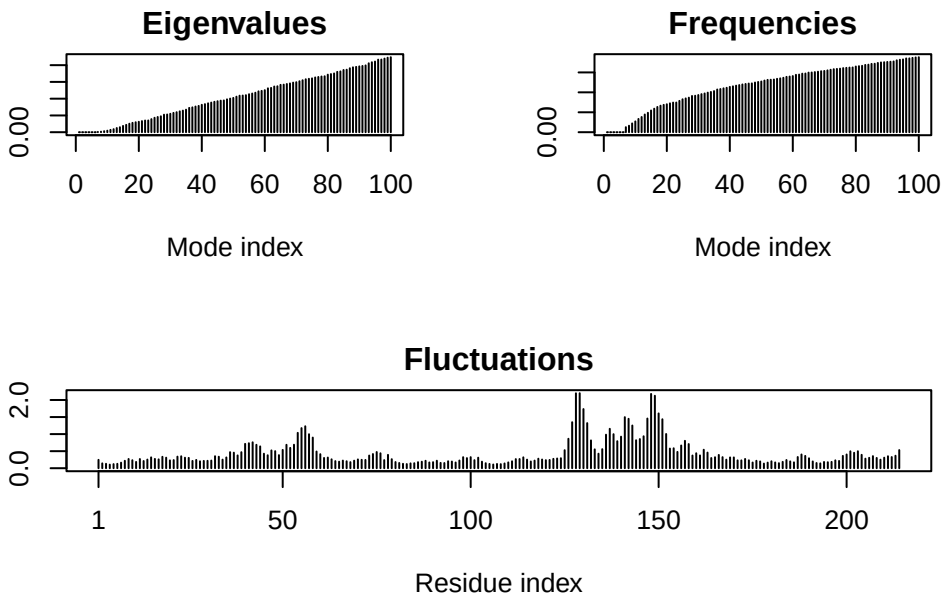
```
adk<-read.pdb("6s36")
```

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

```
modes<-nma(adk)
```

```
 Building Hessian...        Done in 0.031 seconds.
 Diagonalizing Hessian...   Done in 0.469 seconds.
```

```
plot(modes)
```




```
mktrj(modes, file="modes.pdb")
```

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?

2