class9

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```
db <- read.csv("Data Export Summary.csv")
knitr::kable(db)
```

Molecular.Type	X.ray	EM	NMR	Multiple.methods	Neutron	Other	Total
Protein (only)	154,766	10,155	12,187	191	72	32	177,403
Protein/Oligosaccharide	9,083	1,802	32	7	1	0	10,925
Protein/NA	8,110	3,176	283	6	0	0	11,575
Nucleic acid (only)	2,664	94	1,450	12	2	1	4,223
Other	163	9	32	0	0	0	204
Oligosaccharide (only)	11	0	6	1	0	4	22

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

```
gsub(",","", db$X.ray)
```

```
[1] "154766" "9083"   "8110"   "2664"   "163"    "11"
```

```
#globally substitutes comma with second argeument
xray.total <- sum(as.numeric(gsub(",","", db$X.ray)))
em.total <- sum(as.numeric(gsub(",","", db$EM)))

xray.total
```

```
[1] 174797
```

```
#turn into function
total <- function(col) {
  #substitute comma and conver to numeric
  sum(as.numeric(gsub(",","",col) ))
}

total(db$X.ray)
```

```
[1] 174797
```

```
#percentange of structures in PDB that are in X.ray and EM
paste("Percent X.ray:" , total(db$X.ray)/total(db$Total) * 100)
```

```
[1] "Percent X.ray: 85.5372103037895"
```

```
paste("Percent EM:" , total(db$EM)/total(db$Total) * 100)
```

```
[1] "Percent EM: 7.45576260569997"
```

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

```
#last column, first position
#convert to numeric using function
total(db$Total[1])
```

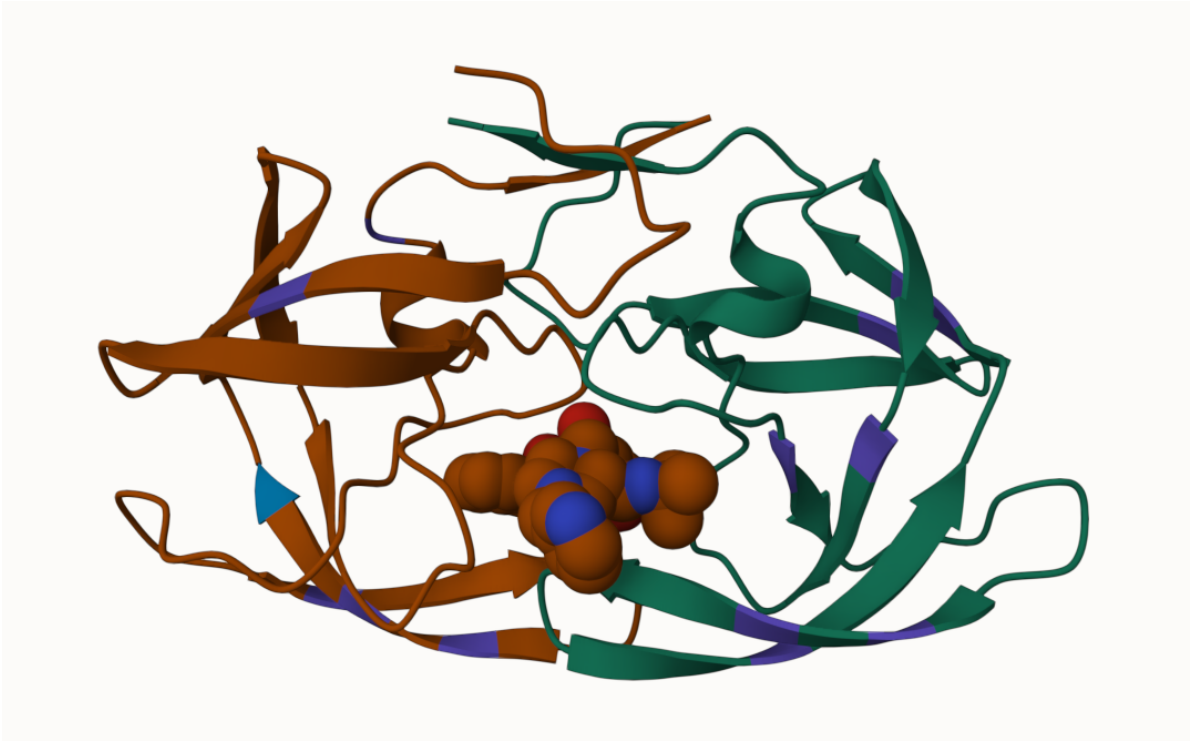
```
[1] 177403
```

```
#divide protein by total
round(total(db$Total[1])/ total(db$Total), 2)
```

```
[1] 0.87
```

> 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?

insert picture of protein instead



> **Q4: Water molecules normally have 3 atoms. Why do we see just one atom per water molecule?** The structure is too low a resolution to see H atoms. You need sub 1 Armstrong res to see H

> **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

Working with Structures in R

we can use `bio3d` package to read and perform bioinformatics calculations on PDB structures.

```
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
```

```
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
```

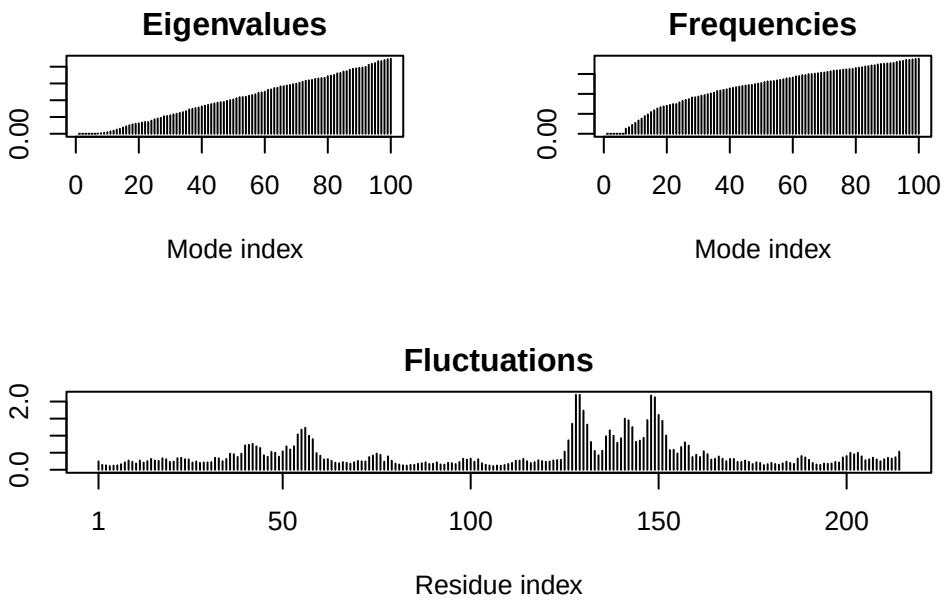
```
 Call:  read.pdb(file = "6s36")

   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
```

Perform a prediction of flexibility with a technique called NMA (normal mode analysis)

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

```
 Building Hessian...        Done in 0.013 seconds.
 Diagonalizing Hessian...   Done in 0.257 seconds.
```

```
plot(m)
```



Write out a "movie" (aka trajectory) of motion for veiwing MOLstar

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

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