Class10

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The main repository of structural data is the PDB. Let's examine what it contains.

I downloaded composition stats from < https://rcsb.org/stats/summary >

At the time of writing thjere are 183,201 protein structures. In UniProt there are 251600768 protein sequences.

```
round(183201/251600768*100, 2)
```

```
[1] 0.07
```

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

	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

Q. Write a function to fix this non numeric table.

We can use the `gsub()` function.

```
string <- c("10", "100", "1", "1000")
as.numeric(string) + 1
```

```
[1]   11  101    2 1001
```

```
x <- string
```

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

pdbstats <- apply(stats, 2, rm.comma)
```

Will add the rownames from the original wee table...

```
rownames(pdbstats) <- rownames(stats)
pdbstats
```

```
                         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.

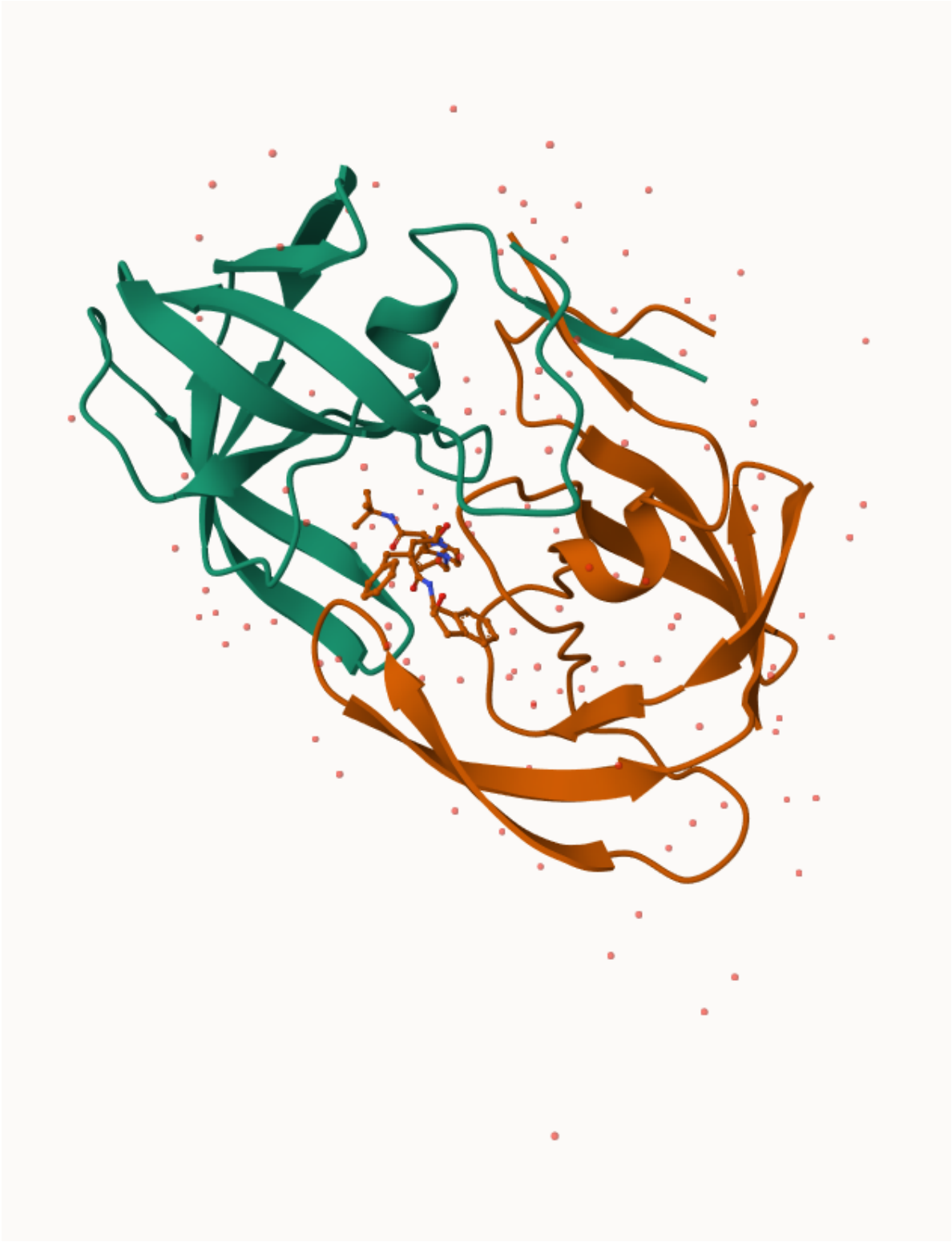
```
totals <- apply(pdbstats, 2, sum)
round(totals/totals["Total"] * 100, 2)
```

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

Q2-3 Let's skip these...

Using Mol* to examine HIV-Pr

Here is a rubish pic of HIV-Pr that is not very useful yet.



And a nicer pic colored by secondary structure with catalytic active site ASP 25 shown in each chain along with MK1 drug and all important water...

Using the bio3d package

```
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)
```

Figure 1: the prettiest image ever

```
$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"
```

Predicting funcitonal motions of a single structure

Run a Normal Mode Analysis (NMA) - a bioinformatics method to predict functional motions.

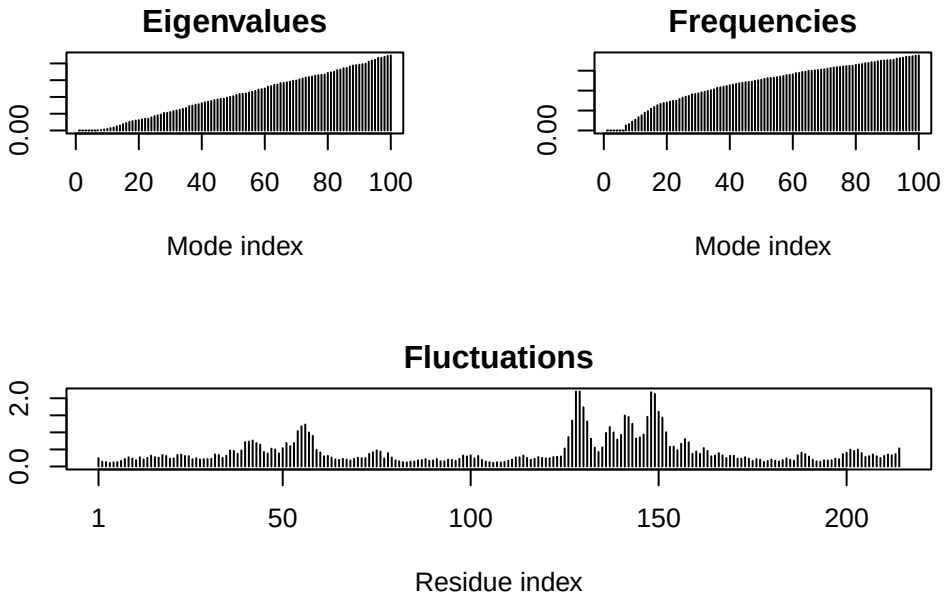
```
adk <- read.pdb("6s36")
```

```
 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 0.29 seconds.
```

```
plot(modes)
```




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