Class 10

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Reading CSV File

```
#Loading in data
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
```

```
#Removing commas and changing character vectors into numeric vectors
rm.com <- function(x) {
  as.numeric(gsub(",","", x))
}

pdbstats <- apply(stats, 2, rm.com)
pdbstats #there's no row names!
```

```
      X.ray    EM   NMR Multiple.methods Neutron Other  Total
[1,] 158844 11759 12296              197      73    32 183201
[2,]   9260  2054    34                8       1     0  11357
[3,]   8307  3667   284                7       0     0  12265
[4,]   2730   113  1467               13       3     1   4327
[5,]    164     9    32                0       0     0    205
[6,]     11     0     6                1       0     4     22
```

```
#adding row names back in
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)
rounded <- round(totals/totals["Total"] * 100, 2)

rounded["X.ray"] + rounded["EM"]
```

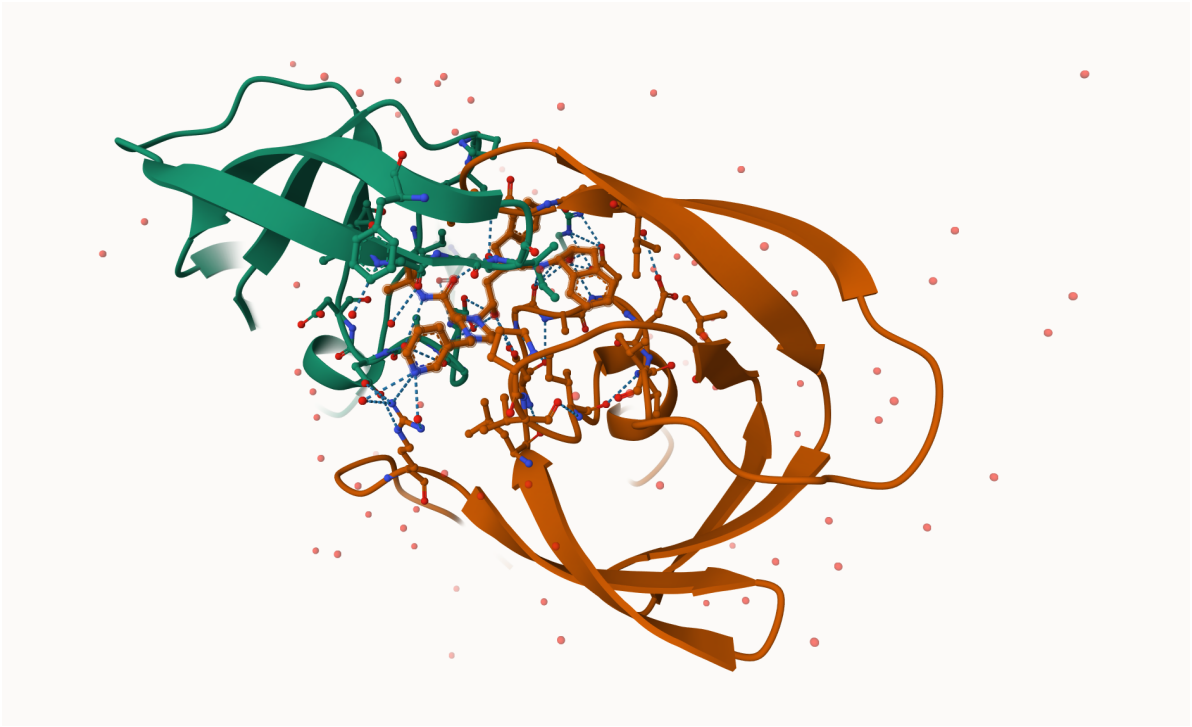
```
X.ray
93.16
```

93.16%

Q2-Q3: Skipping...

Using Mol* to examine HIV-Pr

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



Refined...

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

Because the resolution of the structure is larger than the size of hydrogen atoms.

> 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

408

> Q6: Below...

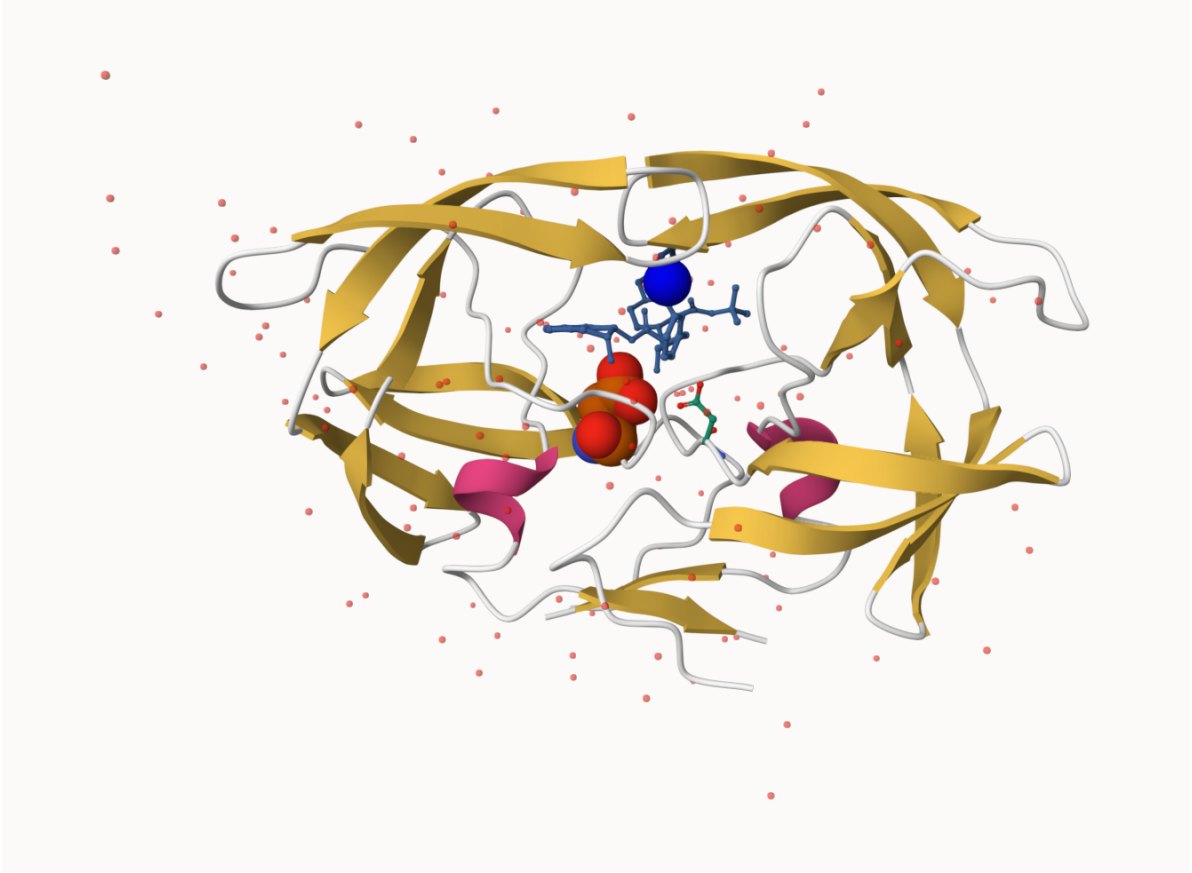


Figure 1: I want to be a structural bioinformatician :)

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
```

```
head(pdb$atom) #full atom list
```

```
  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) #residue names (not all are amino acids)
```

```
[1] "PRO" "PRO" "PRO" "PRO" "PRO" "PRO"
```

```
pdb$calpha #which atoms in the file are residues?
```

```
  [1] FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE
 [13] FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE
 [25] FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE
 [37] FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
 [49] FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE
 [61] FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
 [73] FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE
 [85] FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE
 [97]  TRUE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE
[109] FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
[121]  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE
[133]  TRUE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
[145] FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE
[157] FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE
[169] FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE
[181] FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
[193]  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE
[205] FALSE FALSE FALSE  TRUE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE
[217]  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE
[229] FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE
[241] FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE
[253] FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE
[265] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE
[277] FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE
```

```
[289] FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE
[301] FALSE  TRUE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE
[313] FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
[325] FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE
[337] FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE
[349] FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE
[361] FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE
[373] FALSE FALSE FALSE  TRUE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE
[385] FALSE FALSE FALSE  TRUE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE  TRUE
[397] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE
[409] FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE
[421] FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE
[433] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE
[445] FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE
[457] FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE
[469] FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE
[481] FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE
[493] FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE
[505] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE
[517] FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE
[529] FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
[541]  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE
[553] FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE
[565] FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE
[577] FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
[589]  TRUE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE  TRUE
[601] FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE
[613] FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE
[625] FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE
[637] FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE
[649] FALSE FALSE FALSE  TRUE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE
[661] FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE
[673] FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE
[685] FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE
[697] FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE
[709] FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE  TRUE FALSE
[721] FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE
[733] FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE
[745] FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
[757] FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE
[769] FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE
[781] FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE
[793] FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE
```

```
 [805] FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE
 [817] FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
 [829] FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE
 [841] FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE
 [853] FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE
 [865] FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
 [877] FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE
 [889] FALSE  TRUE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE
 [901] FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE
 [913] FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE
 [925] FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE
 [937] FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE
 [949] FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE
 [961] FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE
 [973] FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE
 [985] FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE
 [997]  TRUE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE
[1009] FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
[1021]  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE
[1033] FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE  TRUE
[1045] FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE
[1057] FALSE FALSE  TRUE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE
[1069] FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE
[1081] FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE
[1093] FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE
[1105] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE
[1117] FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
[1129]  TRUE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE
[1141] FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE
[1153]  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE
[1165] FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE
[1177] FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE
[1189] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE
[1201] FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE
[1213] FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE
[1225] FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
[1237]  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE
[1249] FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
[1261]  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE
[1273] FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE  TRUE
[1285] FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
[1297] FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE
[1309] FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE
```

```
[1321] FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE
[1333] FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE
[1345] FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE
[1357]  TRUE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE
[1369] FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE
[1381] FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
[1393]  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE
[1405] FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE
[1417] FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE
[1429] FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE
[1441] FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE
[1453] FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE
[1465] FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE  TRUE
[1477] FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE
[1489]  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE
[1501] FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
[1513] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
[1525] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
[1537] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
[1549] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
[1561] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
[1573] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
[1585] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
[1597] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
[1609] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
[1621] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
[1633] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
[1645] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
[1657] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
[1669] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
[1681] FALSE FALSE FALSE FALSE FALSE FALSE
```

```
aa321( pdb$atom$resid[ pdb$calpha ] ) #using aa321() to get 1 letter AA code of amino acid
```

```
  [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 functional motions of a single strucutre

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

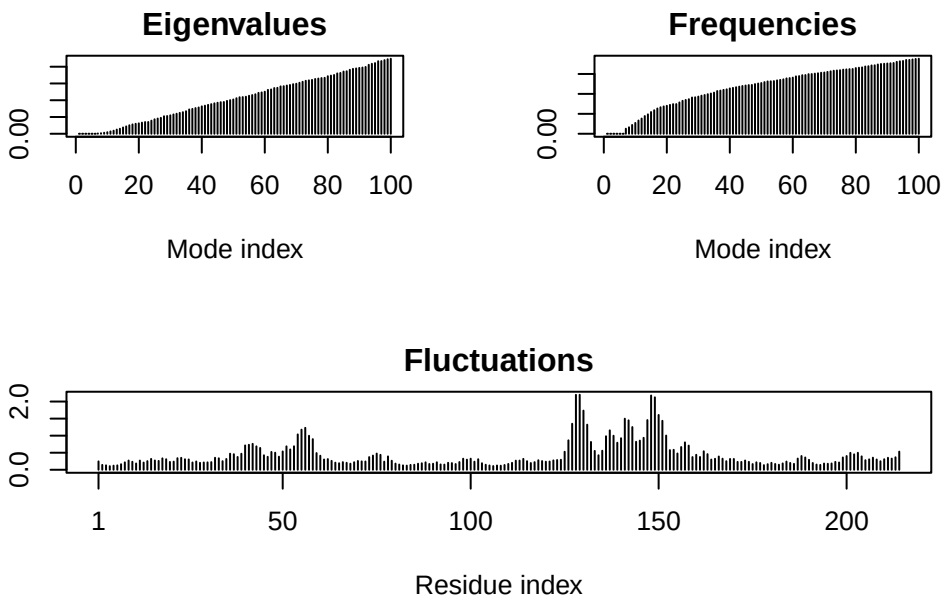
```
adk <- read.pdb("6s36")
```

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

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

```
Building Hessian...        Done in 0.014 seconds.
Diagonalizing Hessian...   Done in 0.255 seconds.
```

```
plot(modes)
```



Make a trajectory in time to visualize…

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