Class 09: PDB

AUTHOR
Loreen A17059289

PDB Statistics:

The PDB is the main database for structural information on biomolecules.

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

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

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

```
xray.total <- sum(as.numeric(gsub(",", "", db$X.ray)))
em.total <- sum(as.numeric(gsub(",", "", db$EM)))
em.total
```

```
[1] 15236
```

```
xray.total
```

```
[1] 174797
```

Write a function to get rid of repetitive code:

```
# x is the input.
sum_comma <- function(x) {
  # Substitute the comma and covert to numeric.
  sum(as.numeric(gsub(",", "", x)))
}

sum_comma(db$X.ray)
```

```
[1] 174797
```

```
sum_comma(db$EM)
```

```
[1] 15236
```

```
sum_comma(db$Total)
```

```
[1] 204352
```

For Xray:

```
sum_comma(db$X.ray) / sum_comma(db$Total)
```

```
[1] 0.8553721
```

For EM:

```
sum_comma(db$EM) / sum_comma(db$Total)
```

```
[1] 0.07455763
```

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

```
round(sum_comma(db$Total[1]) / sum_comma(db$Total), 2)
```

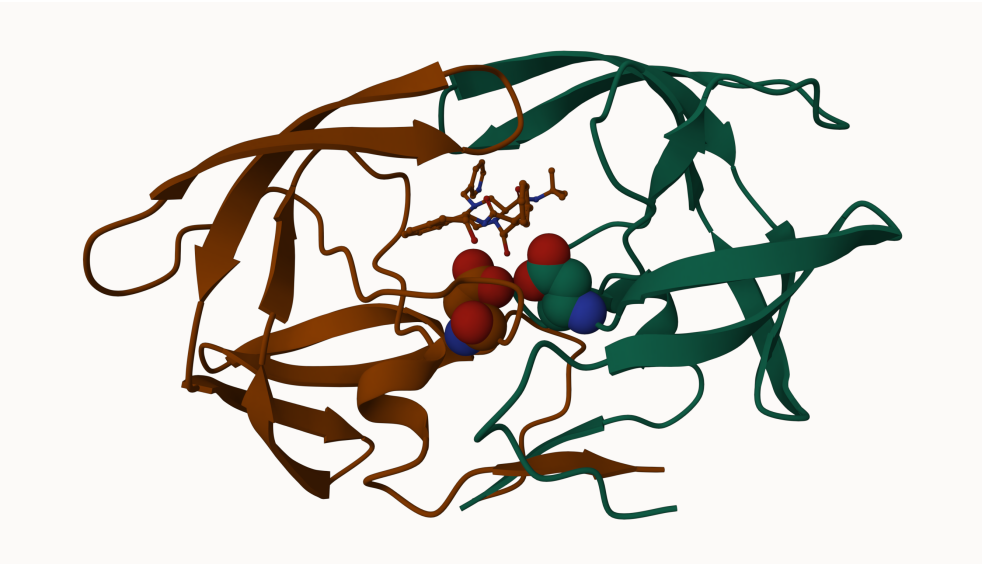
```
[1] 0.87
```

> 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?

skip

Visualizing the HIV-1 protease structure:

> Q6.



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

This structure is too low a resolution to see H atoms. You need a sub Angstrom resolution to see Hydrogen.

> 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?

HOH308

Working with Structures in R

We can use the `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
```

```
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>
```

Read an ADK structure:

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

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

```
adk
```

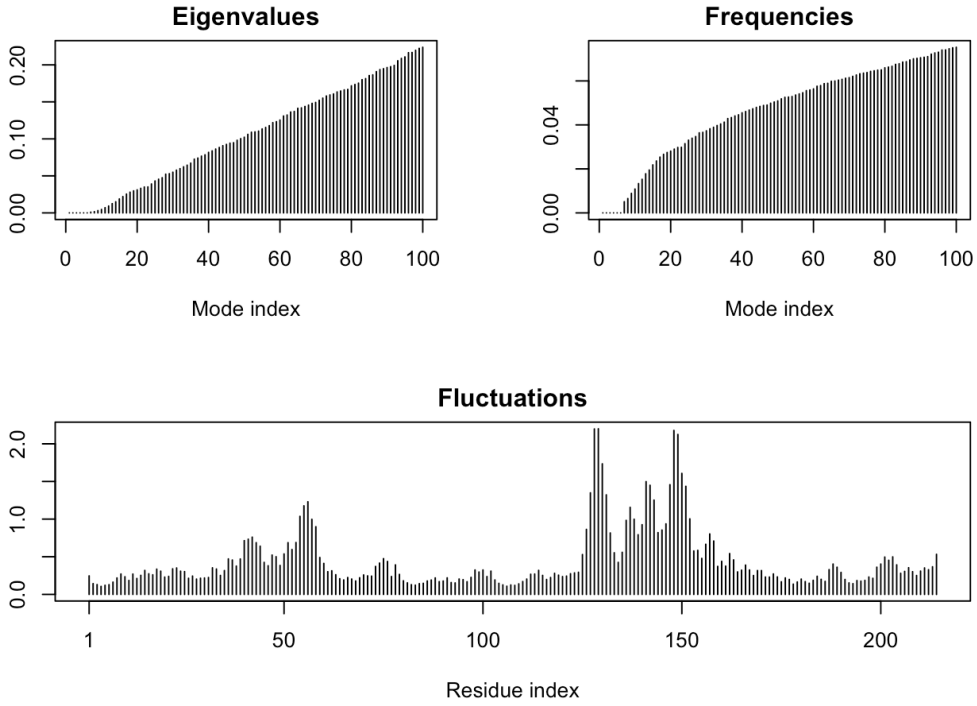
```
 Call:  read.pdb(file = "6s36")

   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 code analysis):

```
# Perform flexibility prediction
m <- nma(adk)
```

```
 Building Hessian...        Done in 0.047 seconds.
 Diagonalizing Hessian...   Done in 0.499 seconds.
```

```
plot(m)
```



Write out. "movie" (a.k.a trajectory) of the motion for viewing in M0lstar:

```
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

> Q9: How many protein chains are in this structure?

2