Class 11 - Structural Bioinformatics (Pt. 1)

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1: Introduction to the RCSB Protein Data Bank (PDB)

- PDB statistics
- 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:

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

```
##                          X.ray   NMR   EM Multiple.methods Neutron Other  Total
## Protein (only)          142303 11804 5999              177      70    32 160385
## Protein/Oligosaccharide   8414    31  979                5       0     0   9429
## Protein/NA                7491   274 1986                3       0     0   9754
## Nucleic acid (only)       2368  1372   60                8       2     1   3811
## Other                      149    31    3                0       0     0    183
## Oligosaccharide (only)      11     6    0                1       0     4     22
```

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

```
method.sums <- colSums(db)
round((method.sums/method.sums["Total"]) * 100, 2)
```

```
##            X.ray              NMR               EM Multiple.methods
##            87.55             7.36             4.92             0.11
##          Neutron            Other            Total
##             0.04             0.02           100.00
```

- 87.55% by X-ray and 4.92% by EM.

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

```
round((db$Total/method.sums["Total"]) * 100, 2)
```

```
## [1] 87.36  5.14  5.31  2.08  0.10  0.01
```

- 87.36%

> 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?

- There are 1828 HIV-1 protease structures in the current PDB
- *The PDB format*

  2. Visualizing the HIV-1 protease structure

- Using Atom Selections

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

- We only see just one atom per water molecule because the VMD application/viewer only displays the oxygen atom of each water molecule.

> Q5: There is a conserved water molecule in the binding site. Can you identify this water molecule? What residue number does this water molecule have (see note below)?

- This water molecule binds at the MK1 binding site and has residue number HOH308:O.

VMD Structure visualization image

```
#![](vmdscene.png)
```

Rmd will not knit with the insertion of this picture as a png file so I inserted it as a code chunk. . . .

> Q6: As you have hopefully observed HIV protease is a homodimer (i.e. it is composed of two identical chains). With the aid of the graphic display and the sequence viewer extension can you identify secondary structure elements that are likely to only form in the dimer rather than the monomer?

- Isolated bridges are likely to only form in the dimer rather than the monomer.

  3. Introduction to Bio3D in R

```
library(bio3d)
```

- Reading PDB file data into R

```
pdb <- read.pdb("1hsg")
```

```
##   Note: Accessing on-line PDB file
```

- To get a quick summary of the contents of the pdb object you just created you can issue the command print(pdb) or simply type pdb (which is equivalent in this case):

```
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
```

Q7: How many amino acid residues are there in this pdb object?

- 198

Q8: Name one of the two non-protein residues?

- MK1

Q9: How many protein chains are in this structure?

- 2

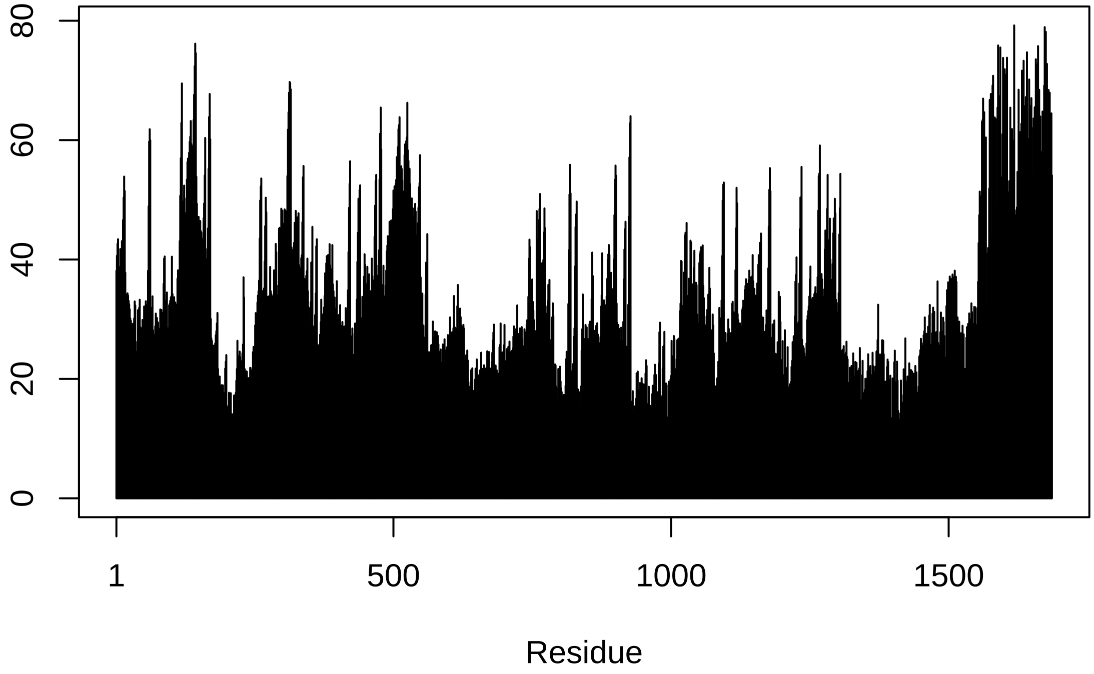
```
aa123(pdbseq(pdb))
```

```
##   [1] "PRO" "GLN" "ILE" "THR" "LEU" "TRP" "GLN" "ARG" "PRO" "LEU" "VAL" "THR"
##  [13] "ILE" "LYS" "ILE" "GLY" "GLY" "GLN" "LEU" "LYS" "GLU" "ALA" "LEU" "LEU"
##  [25] "ASP" "THR" "GLY" "ALA" "ASP" "ASP" "THR" "VAL" "LEU" "GLU" "GLU" "MET"
##  [37] "SER" "LEU" "PRO" "GLY" "ARG" "TRP" "LYS" "PRO" "LYS" "MET" "ILE" "GLY"
##  [49] "GLY" "ILE" "GLY" "GLY" "PHE" "ILE" "LYS" "VAL" "ARG" "GLN" "TYR" "ASP"
##  [61] "GLN" "ILE" "LEU" "ILE" "GLU" "ILE" "CYS" "GLY" "HIS" "LYS" "ALA" "ILE"
##  [73] "GLY" "THR" "VAL" "LEU" "VAL" "GLY" "PRO" "THR" "PRO" "VAL" "ASN" "ILE"
##  [85] "ILE" "GLY" "ARG" "ASN" "LEU" "LEU" "THR" "GLN" "ILE" "GLY" "CYS" "THR"
##  [97] "LEU" "ASN" "PHE" "PRO" "GLN" "ILE" "THR" "LEU" "TRP" "GLN" "ARG" "PRO"
## [109] "LEU" "VAL" "THR" "ILE" "LYS" "ILE" "GLY" "GLY" "GLN" "LEU" "LYS" "GLU"
## [121] "ALA" "LEU" "LEU" "ASP" "THR" "GLY" "ALA" "ASP" "ASP" "THR" "VAL" "LEU"
## [133] "GLU" "GLU" "MET" "SER" "LEU" "PRO" "GLY" "ARG" "TRP" "LYS" "PRO" "LYS"
## [145] "MET" "ILE" "GLY" "GLY" "ILE" "GLY" "GLY" "PHE" "ILE" "LYS" "VAL" "ARG"
## [157] "GLN" "TYR" "ASP" "GLN" "ILE" "LEU" "ILE" "GLU" "ILE" "CYS" "GLY" "HIS"
## [169] "LYS" "ALA" "ILE" "GLY" "THR" "VAL" "LEU" "VAL" "GLY" "PRO" "THR" "PRO"
## [181] "VAL" "ASN" "ILE" "ILE" "GLY" "ARG" "ASN" "LEU" "LEU" "THR" "GLN" "ILE"
## [193] "GLY" "CYS" "THR" "LEU" "ASN" "PHE"
```

Plot of B-factor

```
plot.bio3d(pdb$atom$b, sse=pdb)
```

```
## Warning in plotb3(...): Length of input 'sse' does not equal the length of input
## 'x'; Ignoring 'sse'
```



The ATOM records

```
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>
```

Note that the attributes (+ attr:) of this object are listed on the last couple of lines. To find the attributes of any such object you can use:

```
attributes(pdb)
```

```
## $names
## [1] "atom"   "xyz"    "seqres" "helix"  "sheet"  "calpha" "remark" "call"
##
## $class
## [1] "pdb" "sse"
```

To access these individual attributes we use the dollar-attribute name convention that is common with R list objects. For example, to access the atom attribute or component use pdb$atom:

```
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>
```