Class 11: Structural Bioinformatics

Angelita Rivera (PID A15522236)

11/2/2021

A quick look into PDB

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

##		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)</pre>
```

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

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

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

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

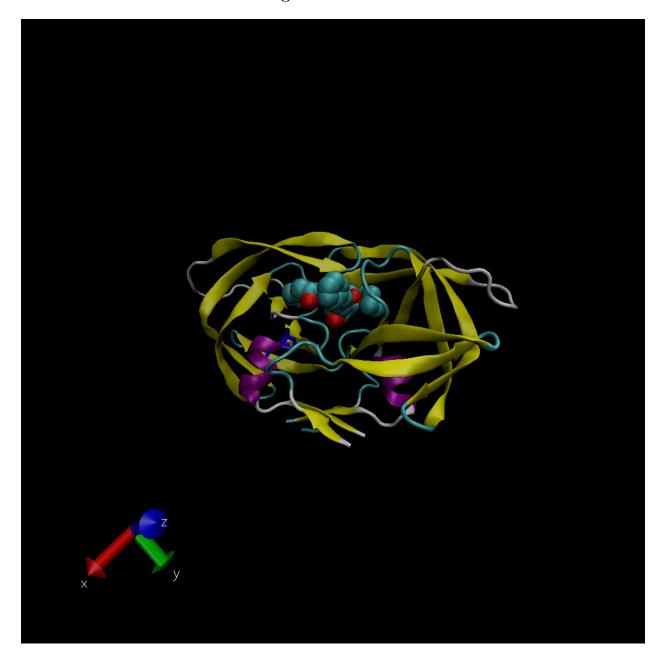
```
## [1] 87.36 5.14 5.31 2.08 0.10 0.01
```

87.36% are protein.

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.

VMD structure visualization image



 $\mathbf{Q4}$: Water molecules normally have 3 atoms. Why do we see just one atom per water molecule in this structure?

Hydrogen atoms are too small to see compared to oxygen, since it is the smallest atom.

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)?

MK1902.

Using Bio3D

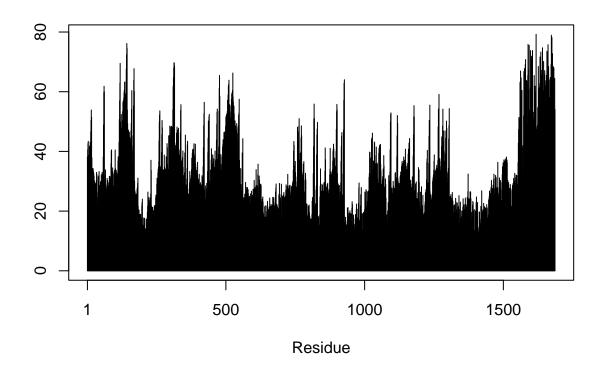
I need to load the library.

```
library(bio3d)
pdb <- read.pdb("1hsg")</pre>
     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
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" "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" "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.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
                                                            х
                                                                    У
                                                                          z o
## 1 ATOM
              1
                     N <NA>
                              PRO
                                       Α
                                             1
                                                  <NA> 29.361 39.686 5.862 1 38.10
## 2 ATOM
              2
                    CA <NA>
                              PRO
                                       Α
                                                  <NA> 30.307 38.663 5.319 1 40.62
                                             1
                                                  <NA> 29.760 38.071 4.022 1 42.64
## 3 ATOM
              3
                     C <NA>
                              PRO
                                       Α
                                             1
## 4 ATOM
              4
                     O <NA>
                              PRO
                                       Α
                                                  <NA> 28.600 38.302 3.676 1 43.40
                                             1
## 5 ATOM
                                                  <NA> 30.508 37.541 6.342 1 37.87
              5
                    CB <NA>
                              PRO
                                       Α
                                             1
## 6 ATOM
              6
                    CG <NA>
                              PRO
                                             1
                                                  <NA> 29.296 37.591 7.162 1 38.40
##
     segid elesy charge
## 1
      <NA>
               N
                    <NA>
## 2
               С
                    <NA>
      <NA>
## 3
      <NA>
               С
                    <NA>
                    <NA>
## 4
      <NA>
               0
## 5
      <NA>
               C
                    <NA>
## 6
      <NA>
               С
                    <NA>
```