Bimm 143 Class 11

Anika Bhattacharjya (A15459876)

Introduction to the RCSB Protein Data Bank (PDB)

```
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)
method.sums
```

```
##            X.ray              NMR               EM Multiple.methods
##           160736            13518             9027              194
##          Neutron            Other            Total
##               72               37           183584
```

```
method.sums/method.sums["Total"]
```

```
##            X.ray              NMR               EM Multiple.methods
##     0.8755447098     0.0736338679     0.0491709517     0.0010567370
##          Neutron            Other            Total
##     0.0003921910     0.0002015426     1.0000000000
```

X-Ray = 87.6%, EM = 4.92%

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

```
column.sums <- rowSums(db[ ,c(1:5)])
column.sums
```

```
##          Protein (only) Protein/Oligosaccharide              Protein/NA
##                  160353                    9429                    9754
##     Nucleic acid (only)                   Other  Oligosaccharide (only)
##                    3810                     183                      18
```

```
column.sums/method.sums["Total"]*100
```

```
##          Protein (only) Protein/Oligosaccharide              Protein/NA
##            87.345847133             5.136068503             5.313099181
##     Nucleic acid (only)                   Other  Oligosaccharide (only)
##             2.075344257             0.099681889             0.009804776
```

87% of PDB structures are protein only, 97% of the structures contain some 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 83790 structures that result when I search for HIV-1 protease structures.

Visualizing the HIV-1 protease structure

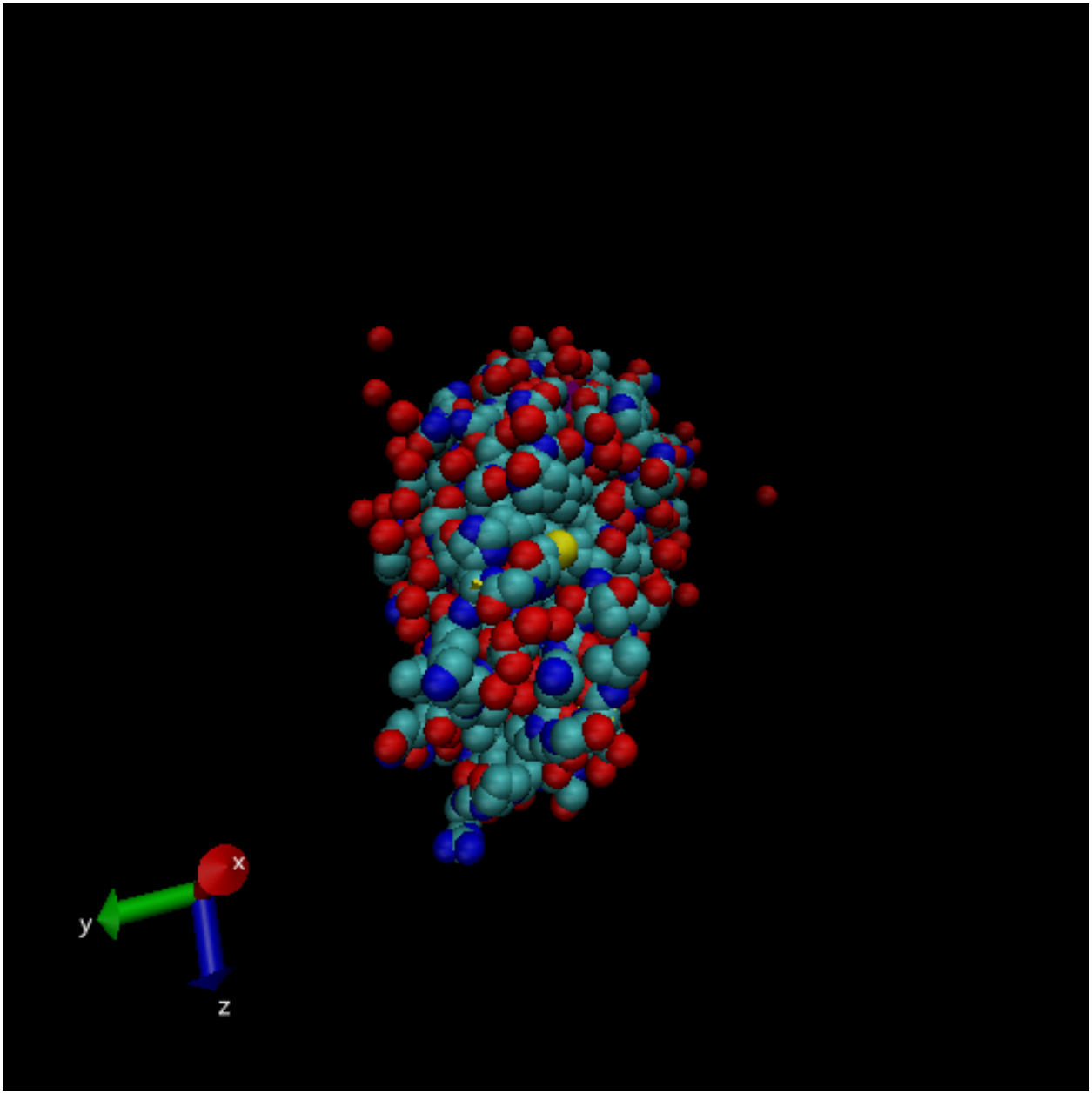
> Q4: Water molecules normally have 3 atoms. Why do we see just one atom per water molecule in this structure?

We just see the oxygen atom in the water molecule because the size of a hydrogen atom is smaller than the smallest representation VMD can provide.

> 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)?

The water molecule is on residue 308.

VMD structure visualization image



Introduction to Bio3D in R

```
# load the library
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
```

```
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"
```

```
# 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>
```

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

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

HOH

Q9: How many protein chains are in this structure?

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