inclass09

Quarto

Quarto enables you to weave together content and executable code into a finished document. To learn more about Quarto see https://quarto.org.

Running Code

When you click the **Render** button a document will be generated that includes both content and the output of embedded code. You can embed code like this:

```
1 + 1
```

```
[1] 2
```

You can add options to executable code like this

```
[1] 4
```

The `echo: false` option disables the printing of code (only output is displayed).

```
db<- read.csv("Data Export Summary.csv")
db
```

```
           Molecular.Type   X.ray     EM    NMR Multiple.methods Neutron Other
1          Protein (only) 154,766 10,155 12,187              191      72    32
2 Protein/Oligosaccharide   9,083  1,802     32                7       1     0
3              Protein/NA   8,110  3,176    283                6       0     0
4     Nucleic acid (only)   2,664     94  1,450               12       2     1
5                   Other     163      9     32                0       0     0
```

```
6  Oligosaccharide (only)      11       0      6                1       0     4
    Total
1 177,403
2  10,925
3  11,575
4   4,223
5     204
6      22
```

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

```
sum_xray <- sum(as.numeric( gsub(",","", db$X.ray) ))
sum_em <- sum(as.numeric( gsub(",","", db$EM) ))
```

How can we make this into a fucntion?

```
#x is a column from a matrix that is specified, in the format : matrix$columntitle
#function substitues comma for an empty string, makes it into a number, and sums the value
sum_comma<- function(x) {
  return(sum(as.numeric( gsub(",","", x) )))
}
```

Now we can answer Q1

```
#for xray
sum_comma(db$X.ray)/sum_comma(db$Total)
```

```
[1] 0.8553721
```

```
#for EM
round(sum_comma(db$EM)/sum_comma(db$Total),2 )
```

```
[1] 0.07
```

> 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? Q6. Generate and save a figure clearly showing the two distinct chains of HIV-protease along with the ligand. You might also consider showing the catalytic residues ASP 25 in each chain and the critical water (we recommend "Ball & Stick" for these side-chains). Add this figure to your Quarto document.

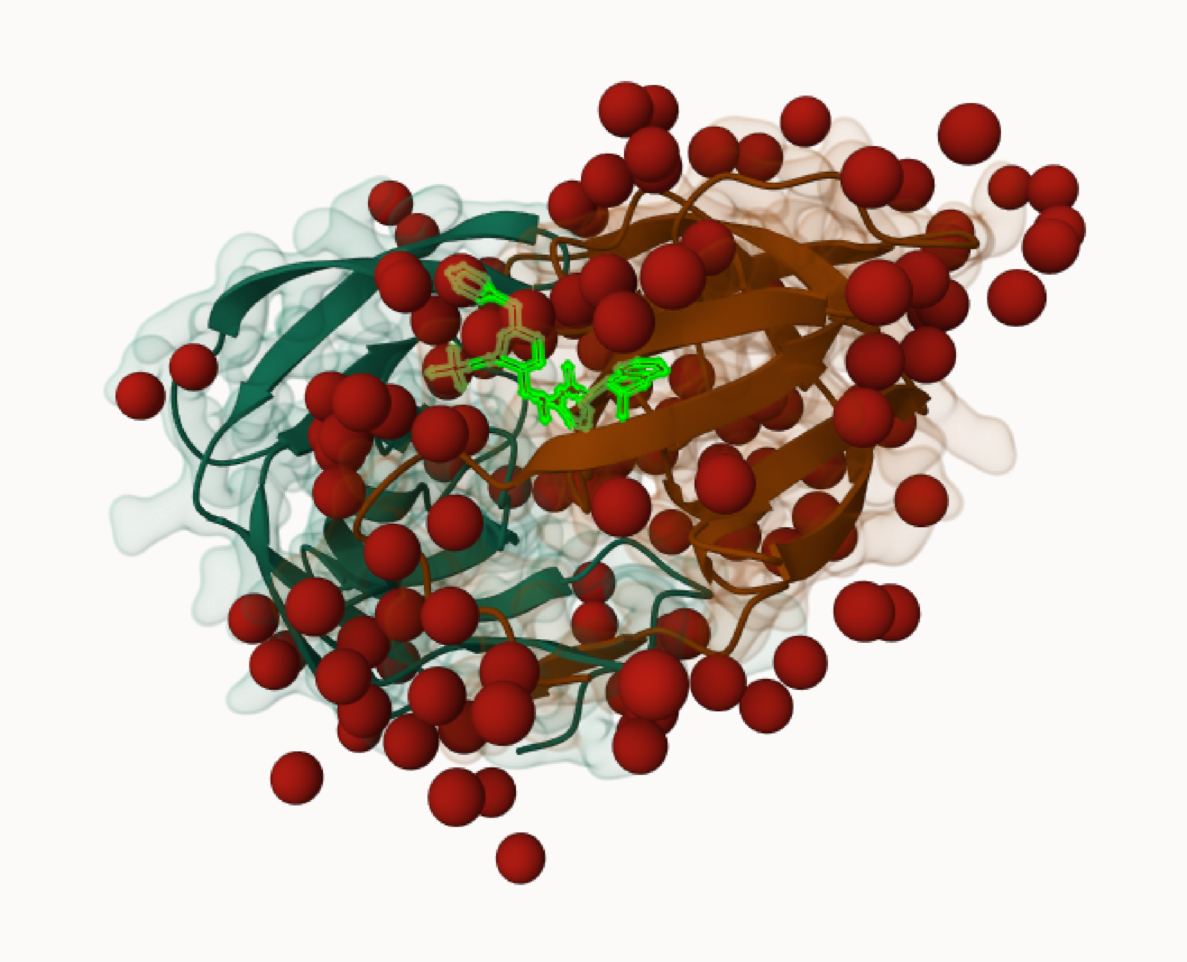


Figure 1: HIV-PR structure rom MERK with a bound drug

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

Because the resolution is too low to see all three atoms. You need a sub 1 Angstrom resolution to see them.

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

#Section 3: Workigm with structures in R

We can use the `bio3d` package to read and perfrom bioinformatics calculations on PDG structures

```r
library(bio3d)

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

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

```r
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
```

```r
attributes(pdb)
```

```
$names
[1] "atom"   "xyz"    "seqres" "helix"  "sheet"  "calpha" "remark" "call"  

$class
[1] "pdb" "sse"
```

```r
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

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

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

```r
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
```

> Q7: How many amino acid residues are there in this pdb object? 198

> Q8: Name one of the two non-protein residues? HOH, MK1

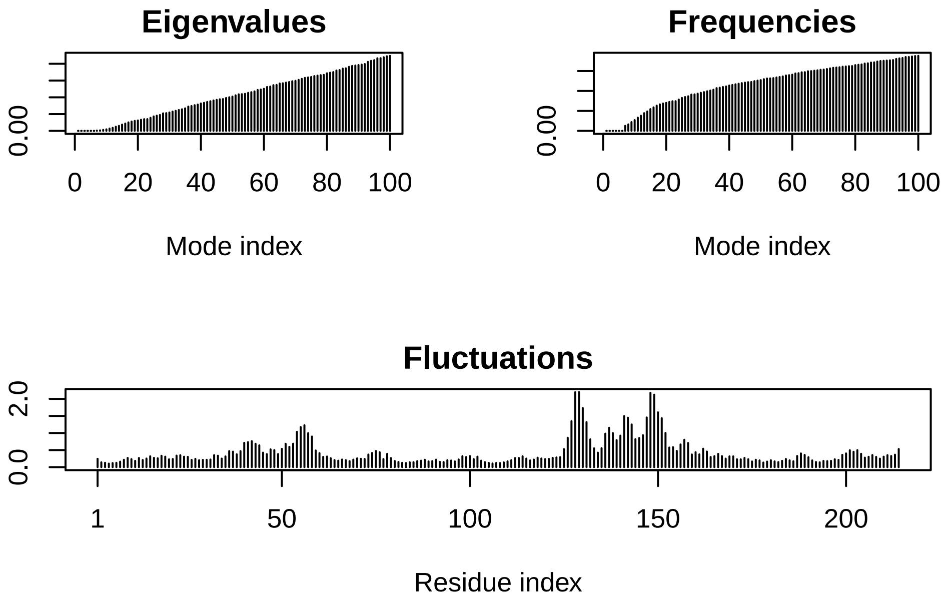
> Q9: How many protein chains are in this structure? 2

Perfrom a predcition of felxibility with a technique called NMA (normal mode analysis)

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

```
 Building Hessian...        Done in 0.064 seconds.
 Diagonalizing Hessian...   Done in 0.633 seconds.
```

```r
plot(m)
```



Write out a “movie” (aka trajectory) if tge motion forr viewing in MOL star

```
mktrj(m, file="adk_m7.pdb")
```