lab09

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Contents

Introduction to PDB

Importing the PDB statistics data file.

```
#Installing the 'READR' Package
library(readr)
```

```
#import data and convert into integer format for numeric operations
PDB_stats <- read_csv("Data Export Summary.csv")
```

```
## Rows: 6 Columns: 9
## -- Column specification --------------------------------------------------------
## Delimiter: ","
## chr (1): Molecular Type
## dbl (4): Integrative, Multiple methods, Neutron, Other
## num (4): X-ray, EM, NMR, Total
##
## i Use `spec()` to retrieve the full column specification for this data.
## i Specify the column types or set `show_col_types = FALSE` to quiet this message.
```

```
#PDB_stats <- read.csv("Data Export Summary.csv", row.names = 1)
#PDB_stats <- lapply(PDB_stats, gsub, pattern = ',', replacement = '')
#PDB_stats <- lapply(PDB_stats, as.integer)
```

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

81.4% of the structures in the PDB are solved by X-ray 12.3% of the strucutres in the PDB are solved by electron microscopy.

```
total_xray <- sum(PDB_stats$`X-ray`)
total_EM <- sum(PDB_stats$EM)
total_entries <- sum(PDB_stats$Total)

total_xray/total_entries
```

```
## [1] 0.8143231
```

```
total_EM/total_entries
```

```
## [1] 0.1227148
```

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

86.0% of the structures in the PDB are protein.

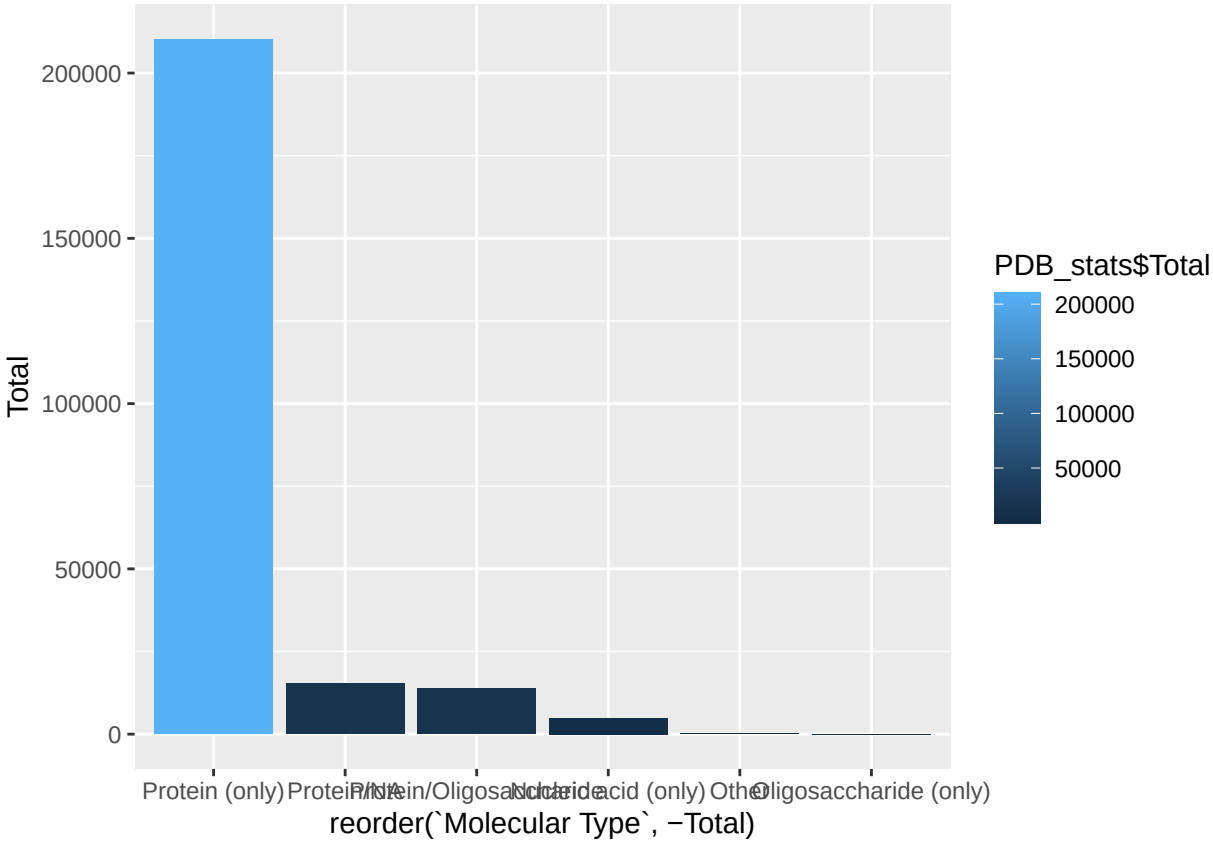
```
PDB_stats$Total[1]/sum(PDB_stats$Total)
```

```
## [1] 0.860465
```

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?

Q3: Make a bar plot overview of Molecular type

```
library(ggplot2)

ggplot(PDB_stats) + aes(reorder(`Molecular Type`, -Total), Total, fill=PDB_stats$Total) + geom_col()
```




```
#ggplot(PDB_stats) + aes(reorder(`Molecular Type`, -Total), Total) + geom_bar(stat = "identity", positi
```

Visualizing structure data with the Mol* viewer

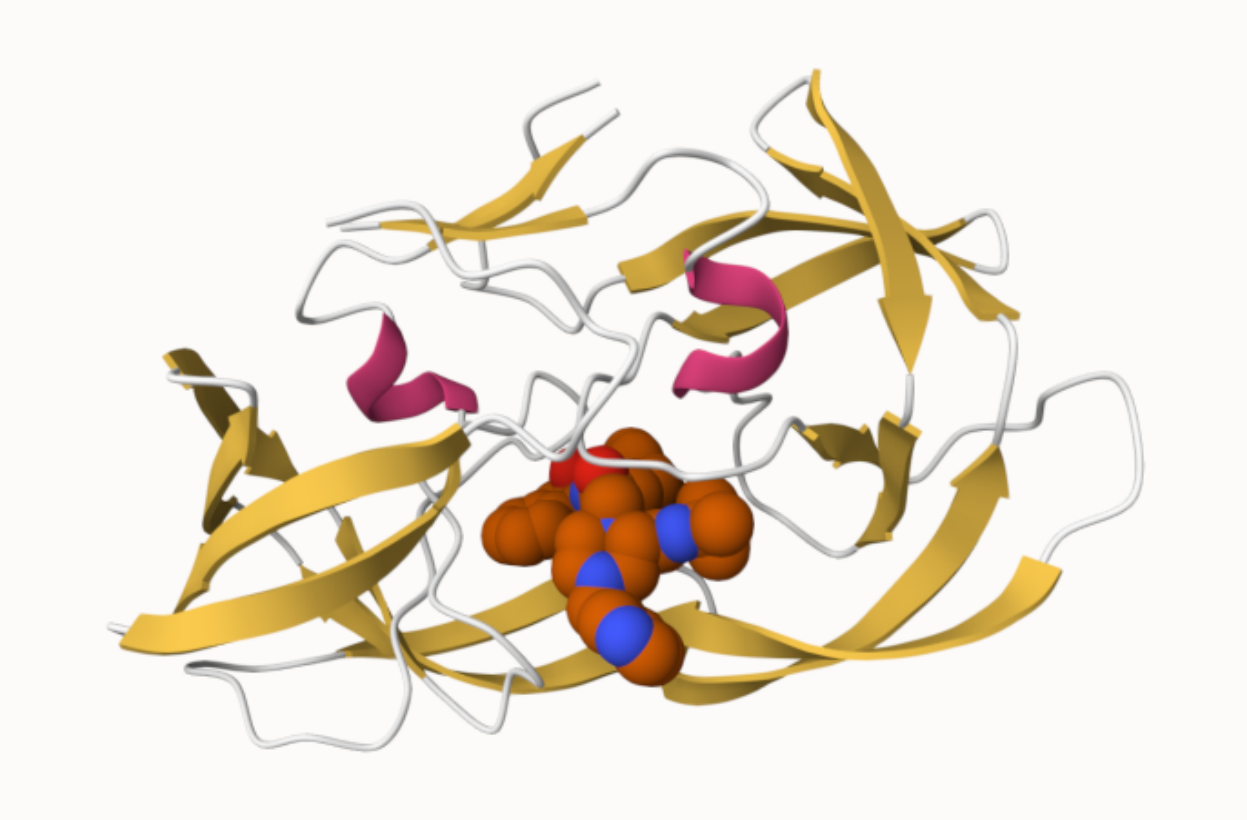
The Mol* viewer is embeded in the website of many bioinformatics websites, like PDB

We will use it on the https://molstar.org/ website

Let's look at the x-ray crystal structure of the HIV-1 protease bound with the drug indinavir (PDB ID: 1HSG)

Figures or images can be inserted using markdown format.

Updated image of the protease with the spacefill model representation of the drug



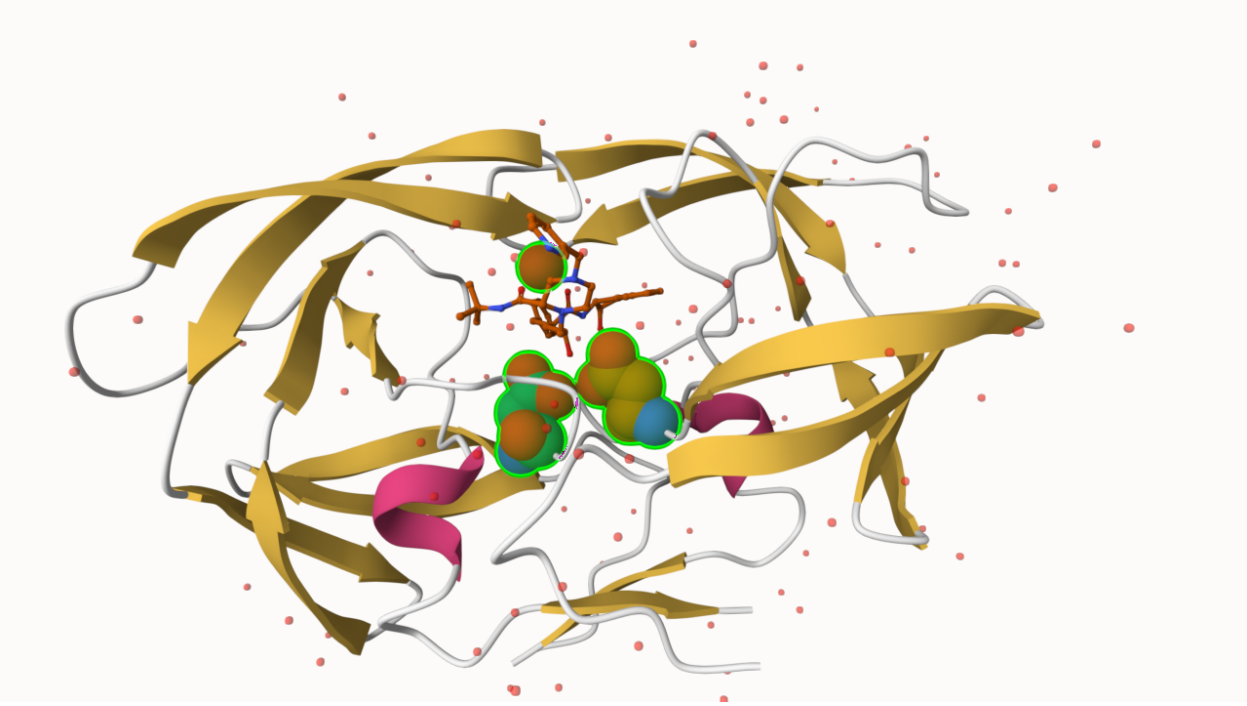
Q4: Water molecules normally have 3 atoms. Why do we see just one atom per water molecule in this structure?

We chose to display the water molecules in a way that is less obtrusive when observing the rest of the structure.

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

This water molecule has residue number 308.

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.



Bio3D package for structural bioinformatics

We can use the bio3d package to read and analyze biomolecular data in R.

```
library(bio3d)

hiv <- read.pdb("1HSG")
```

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

```
hiv
```

```
##
##  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?

There are 128 residues in this pdb object

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

HOH

Q9: How many protein chains are in this structure?

2, chains A and B.

Let's get the sequence

```
pdbseq(hiv)
```

```
##   1   2   3   4   5   6   7   8   9  10  11  12  13  14  15  16  17  18  19  20
## "P" "Q" "I" "T" "L" "W" "Q" "R" "P" "L" "V" "T" "I" "K" "I" "G" "G" "Q" "L" "K"
##  21  22  23  24  25  26  27  28  29  30  31  32  33  34  35  36  37  38  39  40
## "E" "A" "L" "L" "D" "T" "G" "A" "D" "D" "T" "V" "L" "E" "E" "M" "S" "L" "P" "G"
##  41  42  43  44  45  46  47  48  49  50  51  52  53  54  55  56  57  58  59  60
## "R" "W" "K" "P" "K" "M" "I" "G" "G" "I" "G" "G" "F" "I" "K" "V" "R" "Q" "Y" "D"
##  61  62  63  64  65  66  67  68  69  70  71  72  73  74  75  76  77  78  79  80
## "Q" "I" "L" "I" "E" "I" "C" "G" "H" "K" "A" "I" "G" "T" "V" "L" "V" "G" "P" "T"
##  81  82  83  84  85  86  87  88  89  90  91  92  93  94  95  96  97  98  99   1
## "P" "V" "N" "I" "I" "G" "R" "N" "L" "L" "T" "Q" "I" "G" "C" "T" "L" "N" "F" "P"
##   2   3   4   5   6   7   8   9  10  11  12  13  14  15  16  17  18  19  20  21
## "Q" "I" "T" "L" "W" "Q" "R" "P" "L" "V" "T" "I" "K" "I" "G" "G" "Q" "L" "K" "E"
##  22  23  24  25  26  27  28  29  30  31  32  33  34  35  36  37  38  39  40  41
## "A" "L" "L" "D" "T" "G" "A" "D" "D" "T" "V" "L" "E" "E" "M" "S" "L" "P" "G" "R"
##  42  43  44  45  46  47  48  49  50  51  52  53  54  55  56  57  58  59  60  61
## "W" "K" "P" "K" "M" "I" "G" "G" "I" "G" "G" "F" "I" "K" "V" "R" "Q" "Y" "D" "Q"
##  62  63  64  65  66  67  68  69  70  71  72  73  74  75  76  77  78  79  80  81
## "I" "L" "I" "E" "I" "C" "G" "H" "K" "A" "I" "G" "T" "V" "L" "V" "G" "P" "T" "P"
##  82  83  84  85  86  87  88  89  90  91  92  93  94  95  96  97  98  99
## "V" "N" "I" "I" "G" "R" "N" "L" "L" "T" "Q" "I" "G" "C" "T" "L" "N" "F"
```

Let's trim to chain A and get just it's sequence:

```
chainA <- trim.pdb(hiv, chain = "A")
chainA.seq <- pdbseq(chainA)
```

Let's blast

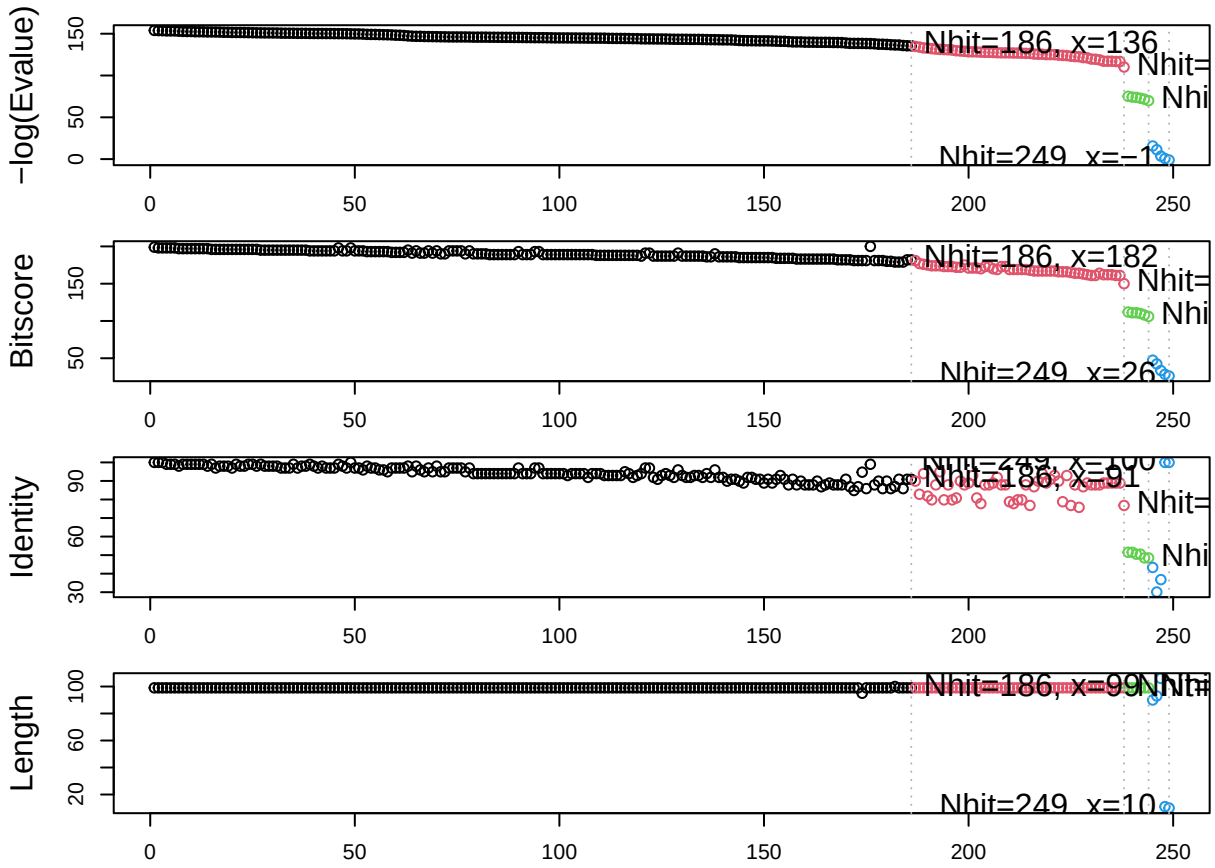
```
#These results will be cached so that it does not re-do the blast search every time

blast <- blast.pdb(chainA.seq)
```

```
##  Searching ... please wait (updates every 5 seconds) RID = G54Y91G4016
##  ..............................
##  Reporting 249 hits
```

Plot a quick overview of blast results

```
hits <- plot(blast)
```

```
##   * Possible cutoff values:    135 110 69 -2
##              Yielding Nhits:    186 238 244 249
##
##   * Chosen cutoff value of:    69
##              Yielding Nhits:    244
```



Prediciton of functional motions

We can run a normal mode analysis (NMA) to predict large scale motions/flexibility/dynamics of any biomolecule that we can read into R.

Let's look at ADK chain A

```
adk <- read.pdb("1ake")
```

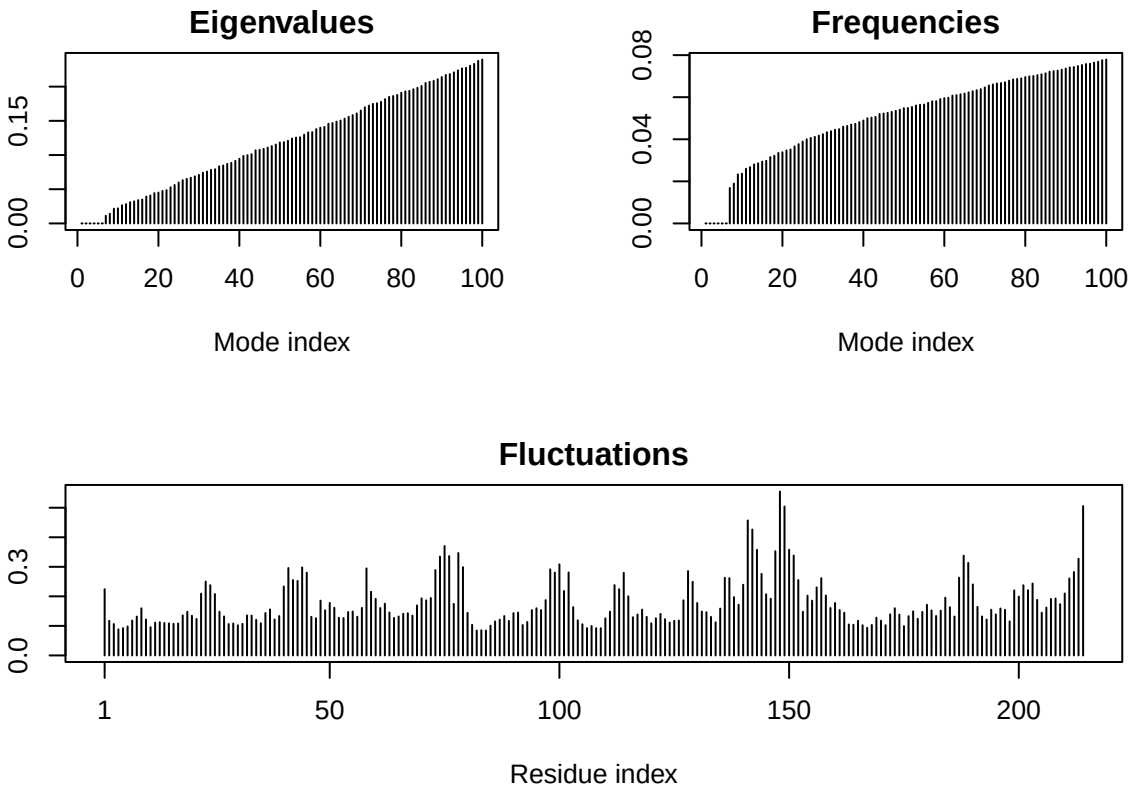
```
##   Note: Accessing on-line PDB file
##    PDB has ALT records, taking A only, rm.alt=TRUE
```

```
adk_A <- trim.pdb(adk, chain="A")
```

```
m <- nma(adk_A)
```

```
##  Building Hessian...     Done in 0.05 seconds.
##  Diagonalizing Hessian...    Done in 0.49 seconds.
```

```
plot(m)
```



Let's write out a "trajectory" of predicted motion that we can open in Mol*

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

Play with 3D viewing in R

We can use the new **bio3dview** package, which is not yet on CRAN, to render interactive 3D views in R and HTML output reports.

To install from GitHub we can use the **pak* package

```
#pak::pak("bioboot/bio3dview")
```