class11_bimm143

Hope (PID: A15652616)

11/3/2021

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

```
##                           X.ray   NMR   EM Multiple.methods Neutron Other  Total
## Protein (only)           142419 11807 6038              177      70    32 160543
## Protein/Oligosaccharide    8426    31  991                5       0     0   9453
## Protein/NA                 7498   274 2000                3       0     0   9775
## Nucleic acid (only)        2368  1378   60                8       2     1   3817
## 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
##            87.53             7.36             4.95             0.11
##          Neutron            Other            Total
##             0.04             0.02           100.00
```

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

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

```
## [1] 87.35  5.14  5.32  2.08  0.10  0.01
```

The proportion is 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 protease structures

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

The red spheres are being shown as the 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)?

Residue number is 135

```
library(bio3d)
```

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

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

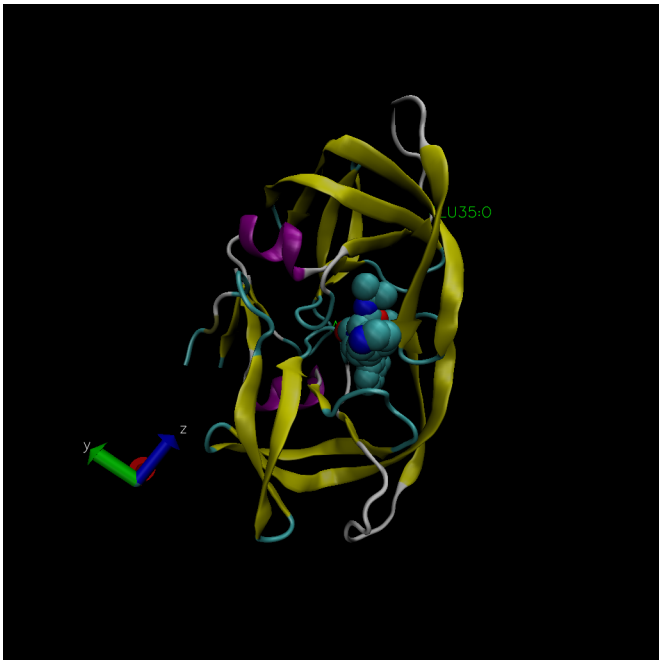
```
read.pdb(file = "1hsg")
```

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

## Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/
## _5/3_f7ytg129xbjldn046wvxkw0000gn/T//RtmpYckWpV/1hsg.pdb exists. Skipping
## download

##
##  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
```

```
print(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?

HOH

Q9: How many protein chains are in this structure?

2

```
attributes(pdb)
```

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