Class11: Structural Bioinformatics

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```
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
```

```
method.sums<- colSums(db)
method.sums
```

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

#Q1.87.55% by X-ray and 4.92% by EM

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

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

```
type.sums <- rowSums(db)
round((type.sums/method.sums["Total"])*100,2)
```

```
##         Protein (only) Protein/Oligosaccharide              Protein/NA
##                 174.73                   10.27                   10.63
##    Nucleic acid (only)                   Other  Oligosaccharide (only)
##                   4.15                    0.20                    0.02
```
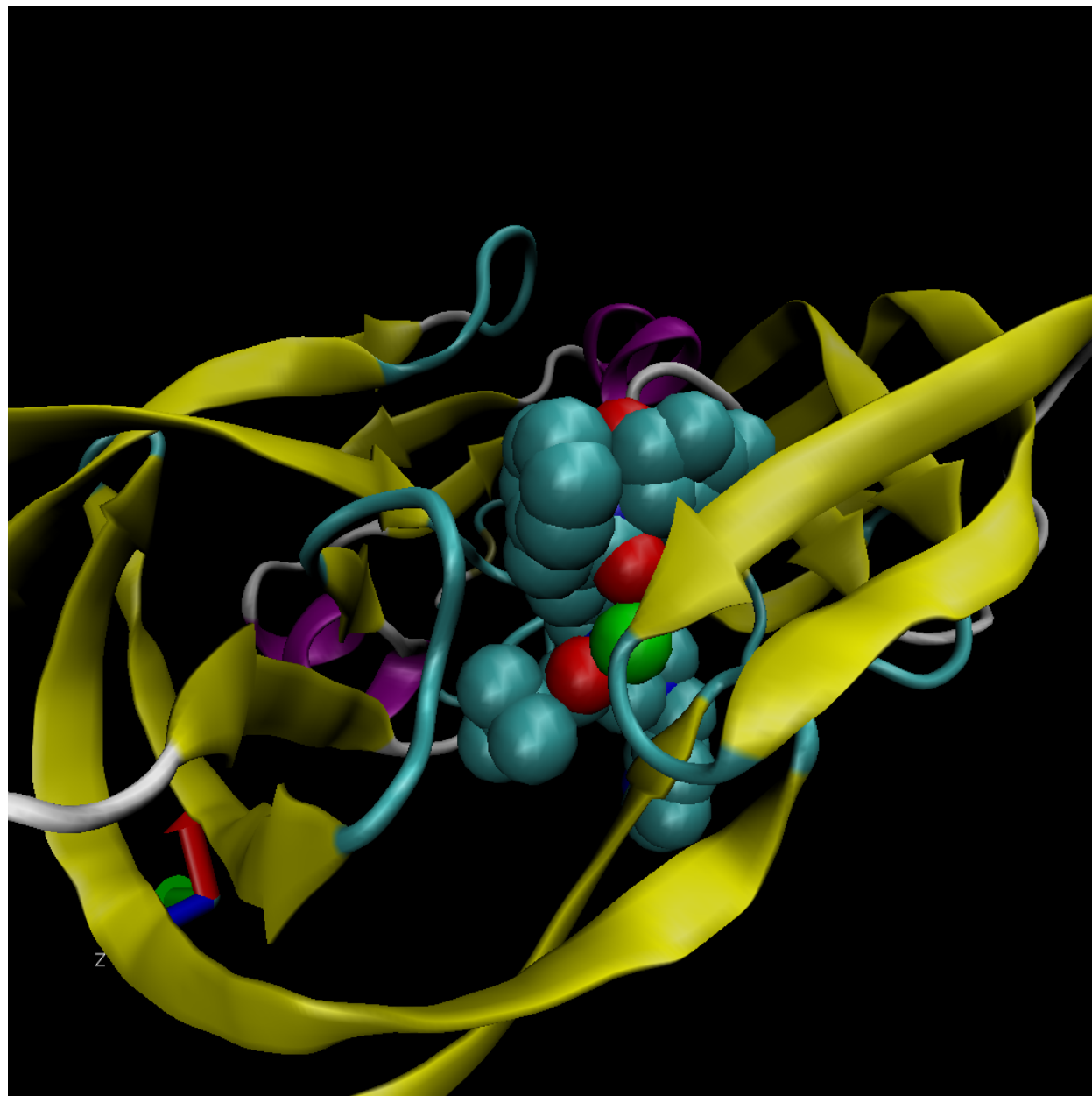
```
round((db$Total/method.sums["Total"])*100,2)
```

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

```
87.36+5.14+5.31
```

```
## [1] 97.81
```

#Q2: 87.36% of structures are protein only, 97.81% of structures contain proteins.

#Q3:1828 structures

#Q4: the hydrogen atoms are very small, and since no hydrogen atoms are shown, each water molecule will only show 1 atom which is the oxygen.

#Q5:the water molecule in MK1 ligand binding site is HOH308:0

#Q6: it is the alpha helix with loops on both of its ends