class11

A quick look at the 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.

```
methods.sums <- colSums(db)
round((methods.sums/methods.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
```

87.55% for X-Ray and **7.36%** for NMR

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

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

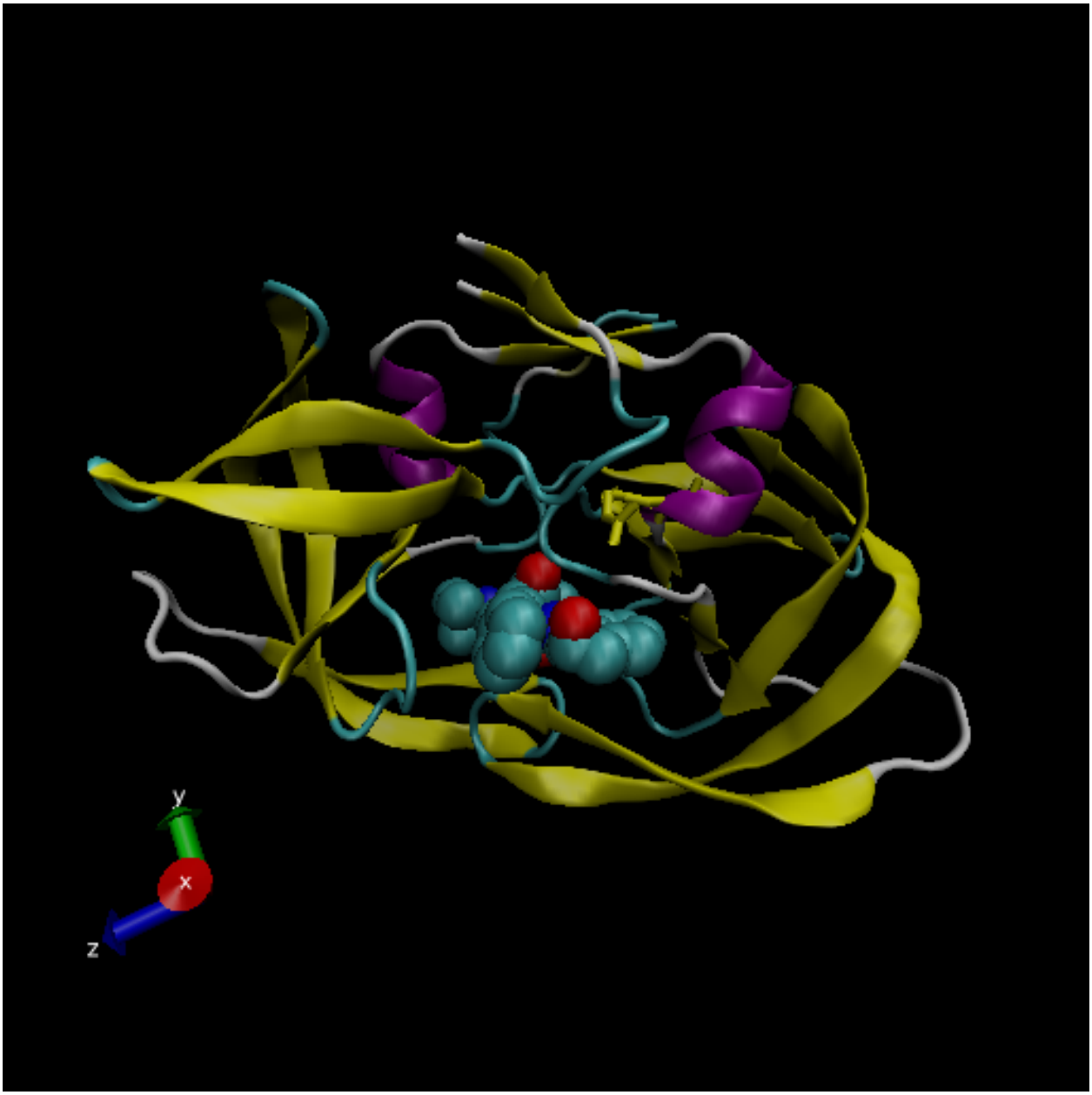
```
## [1] 87.36  5.14  5.31  2.08  0.10  0.01
```

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?

1828 HIV-1 protease structures

##VMD structure visualization image



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

The Hydrogen atom is too small to be seen through x-ray crystallography

> 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 MK1902:04

Using Bio3d

I need to load 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
```