Class 11

```
data <- read.csv('Data Export Summary.csv', row.names = 1)
data
```

```
##                           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.

```
xray_percent <- 100 * sum(data$X.ray) / sum(data$Total)
xray_percent
```

```
## [1] 87.52836
```

```
em_perc <- 100 * sum(data$EM) / sum(data$Total)
em_perc
```

```
## [1] 4.94687
```

for every column

```
colSums(data) / sum(data$Total) * 100
```

```
##            X.ray              NMR               EM Multiple.methods
##      87.52836071       7.35991033       4.94686958       0.10555353
##          Neutron            Other            Total
##       0.03917451       0.02013134     100.00000000
```

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

```
prot_perc <- 100 * sum(data$Total[1]) / sum(data$Total)
prot_perc
```

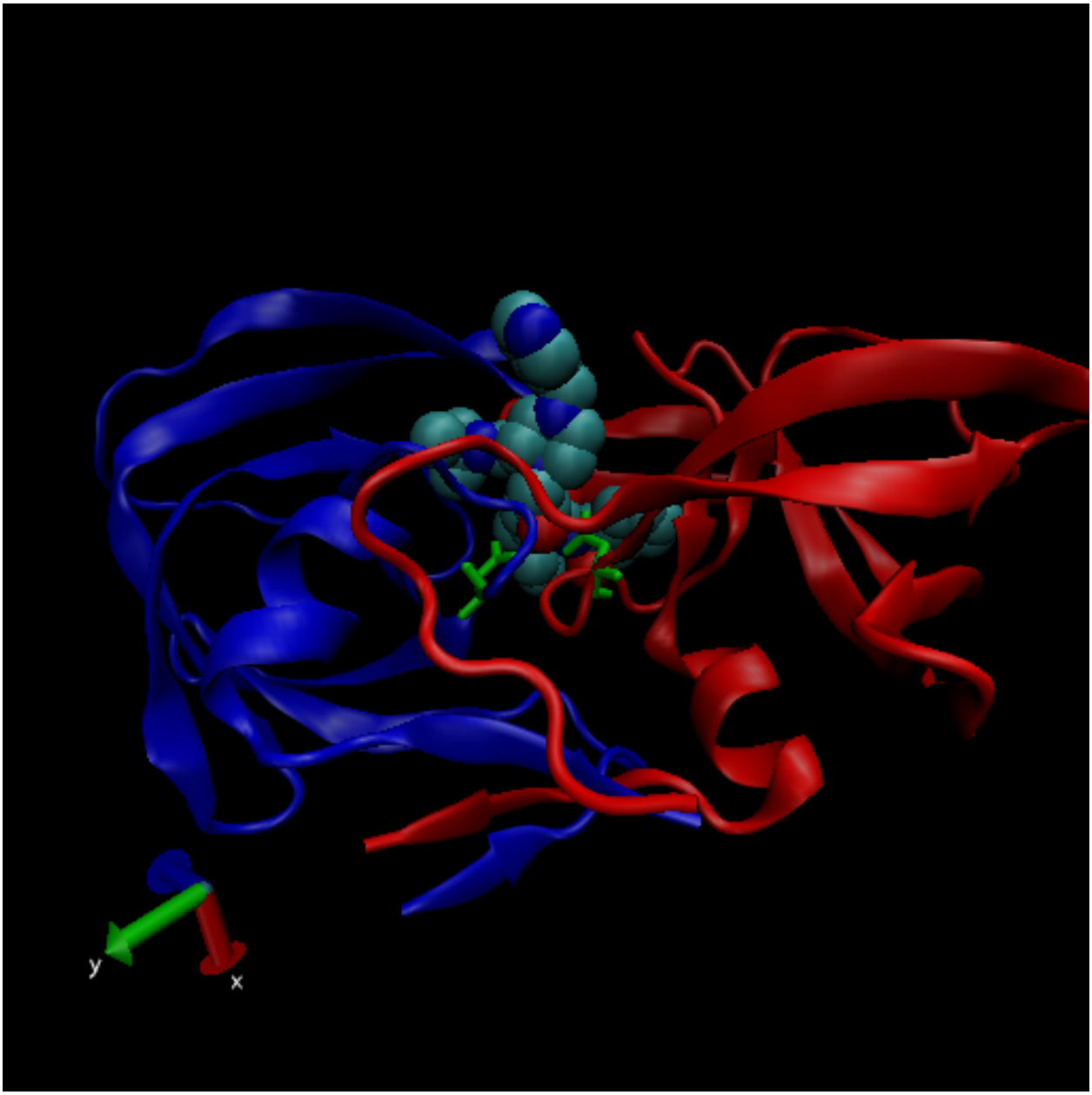
```
## [1] 87.3499
```

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?

23409

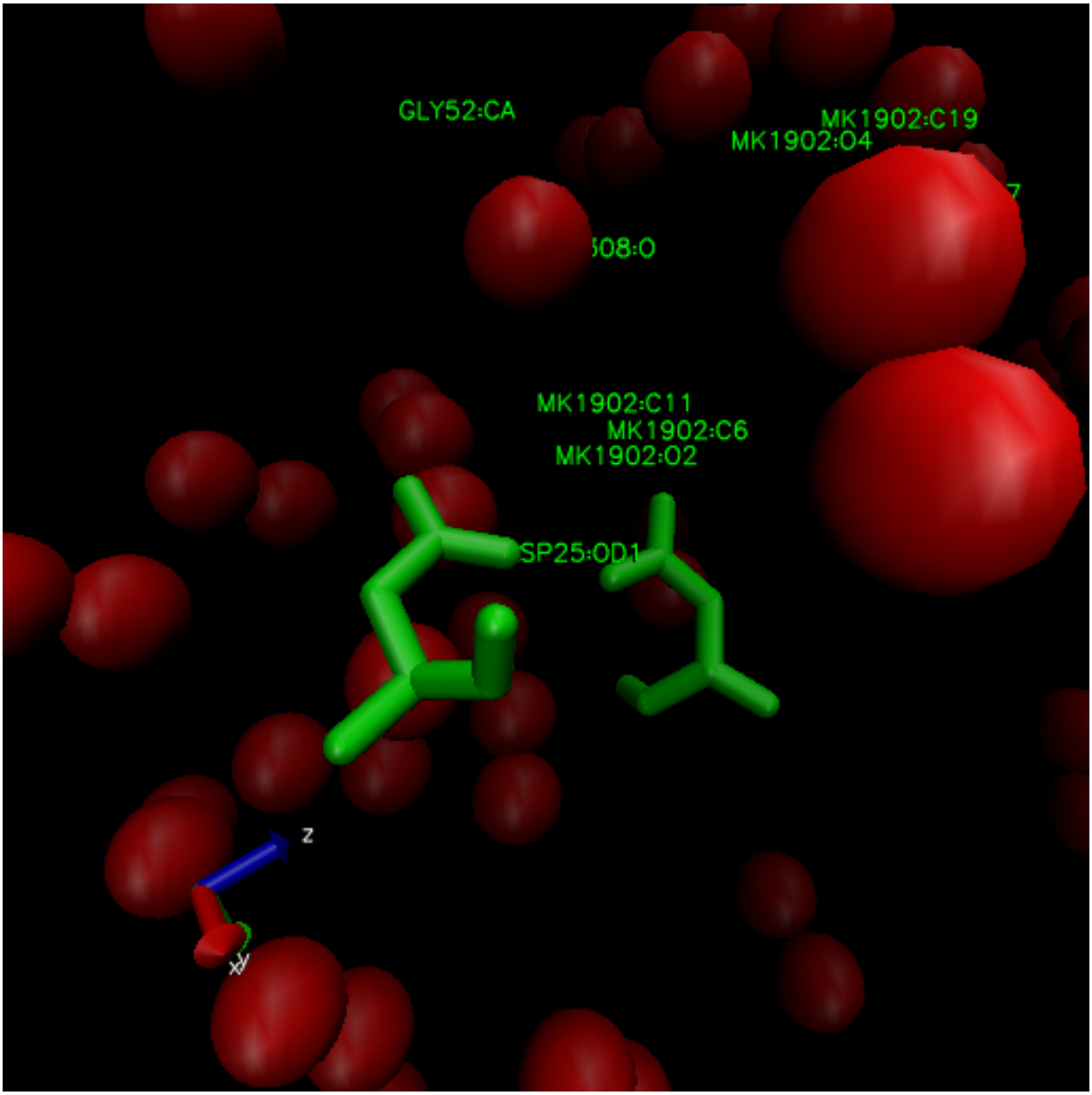
Q4: Water molecules normally have 3 atoms. Why do we see just one atom per water molecule in this structure?

The resolution is higher than the size of hydrogen



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)?

HOH 308




```
library(bio3d)
pdb <- read.pdb('1hel')
```

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

```
pdb
```

```
##
##  Call:  read.pdb(file = "1hel")
##
##    Total Models#: 1
##      Total Atoms#: 1186,  XYZs#: 3558  Chains#: 1  (values: A)
##
```

```
##      Protein Atoms#: 1001  (residues/Calpha atoms#: 129)
##      Nucleic acid Atoms#: 0  (residues/phosphate atoms#: 0)
##
##      Non-protein/nucleic Atoms#: 185  (residues: 185)
##      Non-protein/nucleic resid values: [ HOH (185) ]
##
##    Protein sequence:
##       KVFGRCELAAAMKRHGLDNYRGYSLGNWVCAAKFESNFNTQATNRNTDGSTDYGILQINS
##       RWWCNDGRTPGSRNLCNIPCSALLSSDITASVNCAKKIVSDGNGMNAWVAWRNRCKGTDV
##       QAWIRGCRL
##
## + attr: atom, xyz, seqres, helix, sheet,
##         calpha, remark, call
```

```
head(pdb$atom)
```

```
##   type eleno elety  alt resid chain resno insert      x      y      z o     b
## 1 ATOM     1     N <NA>   LYS     A     1   <NA>  3.294 10.164 10.266 1 11.18
## 2 ATOM     2    CA <NA>   LYS     A     1   <NA>  2.388 10.533  9.168 1  9.68
## 3 ATOM     3     C <NA>   LYS     A     1   <NA>  2.438 12.049  8.889 1 14.00
## 4 ATOM     4     O <NA>   LYS     A     1   <NA>  2.406 12.898  9.815 1 14.00
## 5 ATOM     5    CB <NA>   LYS     A     1   <NA>  0.949 10.101  9.559 1 13.29
## 6 ATOM     6    CG <NA>   LYS     A     1   <NA> -0.050 10.621  8.573 1 13.52
##   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>
```

Do a normal mode analysis (NMA), a prediction of the conformational variability and intrinsic dynamics of this protein

```
pdb <- read.pdb('1hel')
```

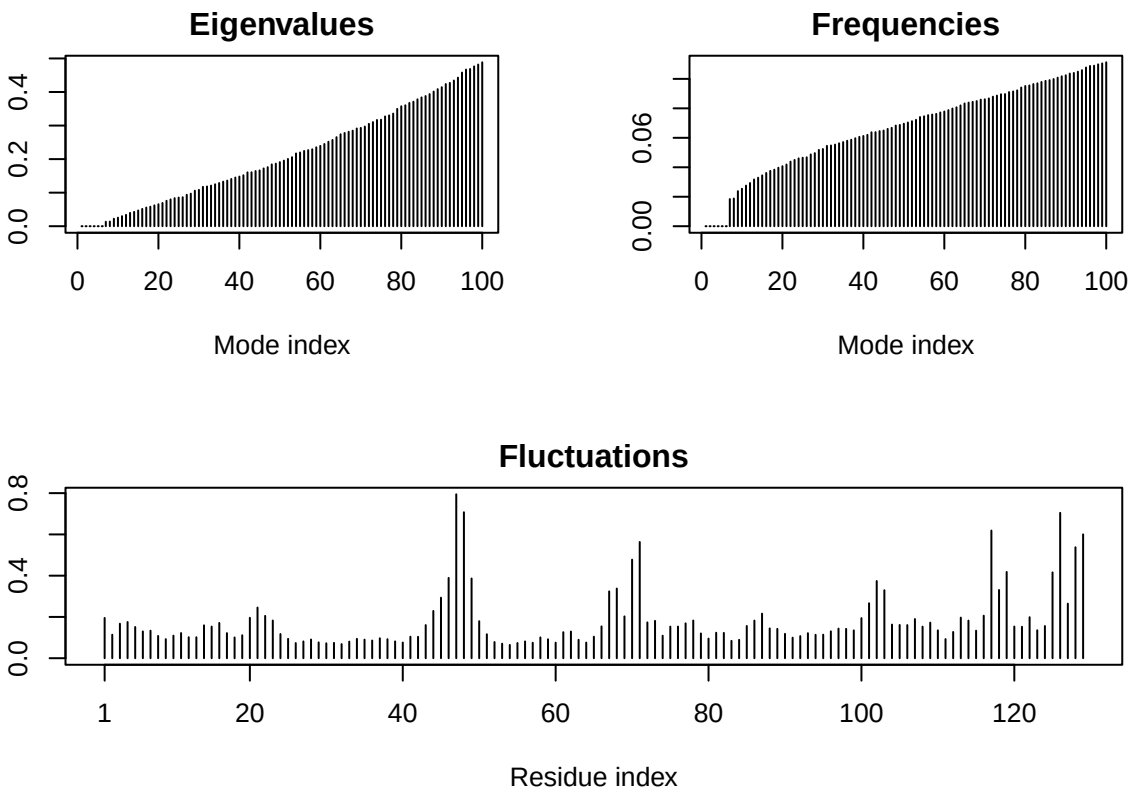
```
##   Note: Accessing on-line PDB file

## Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/5b/
## nx310gbn5pd_zqfnjpsgkt200000gn/T//Rtmpza3CdY/1hel.pdb exists. Skipping download
```

```
m <- nma(pdb)
```

```
##  Building Hessian...     Done in 0.049 seconds.
##  Diagonalizing Hessian...    Done in 0.151 seconds.
```

```
plot(m)
```



Make a little movie (trajectory) for viewing in VMD.

```
mktrj(m, file = 'nma.pdb')
```