Untitled

The PDB database

```
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.

```
(sum(db$X.ray)/ sum(db$Total)) *100
```

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

How about doing this over every method? (i.e. column in the little table)

```
(colSums(db) / sum(db$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?

```
(db$Total[1] / sum(db$Total)) *100
```

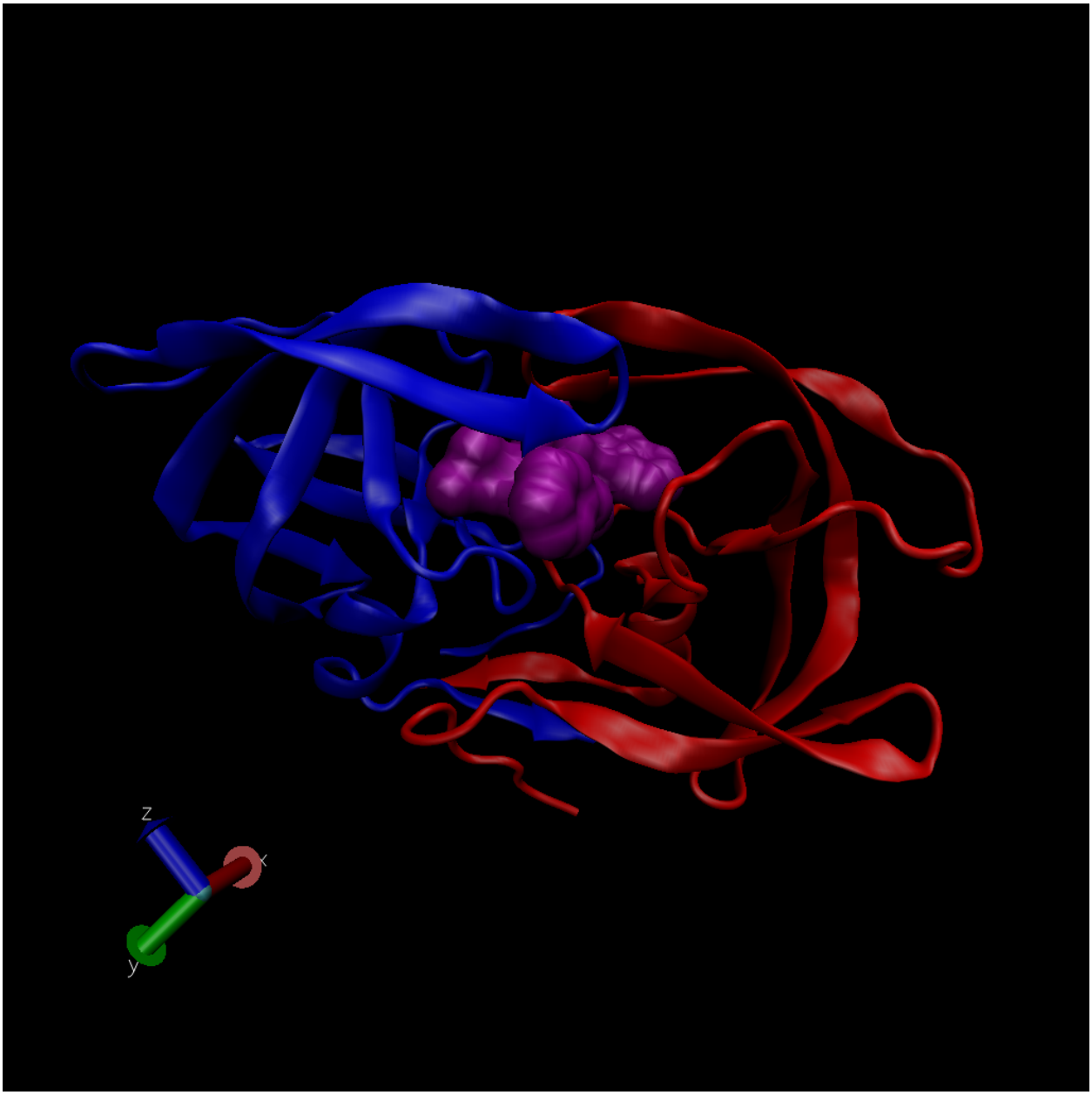
```
## [1] 87.3499
```

```
(db[1,ncol(db)] / sum(db$Total)) *100
```

```
## [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?

23,409 structures



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

Otherwise they would be so small and hard to visualize so it simplifies it some.

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)?

Within the conserved Aspertate. . . ?

Using Bio3D in R for structural bioinformatics

Do a Normal Mode Analysis (NMA) a prediction of the conformational variability and intrinsic dynamics of this protein.

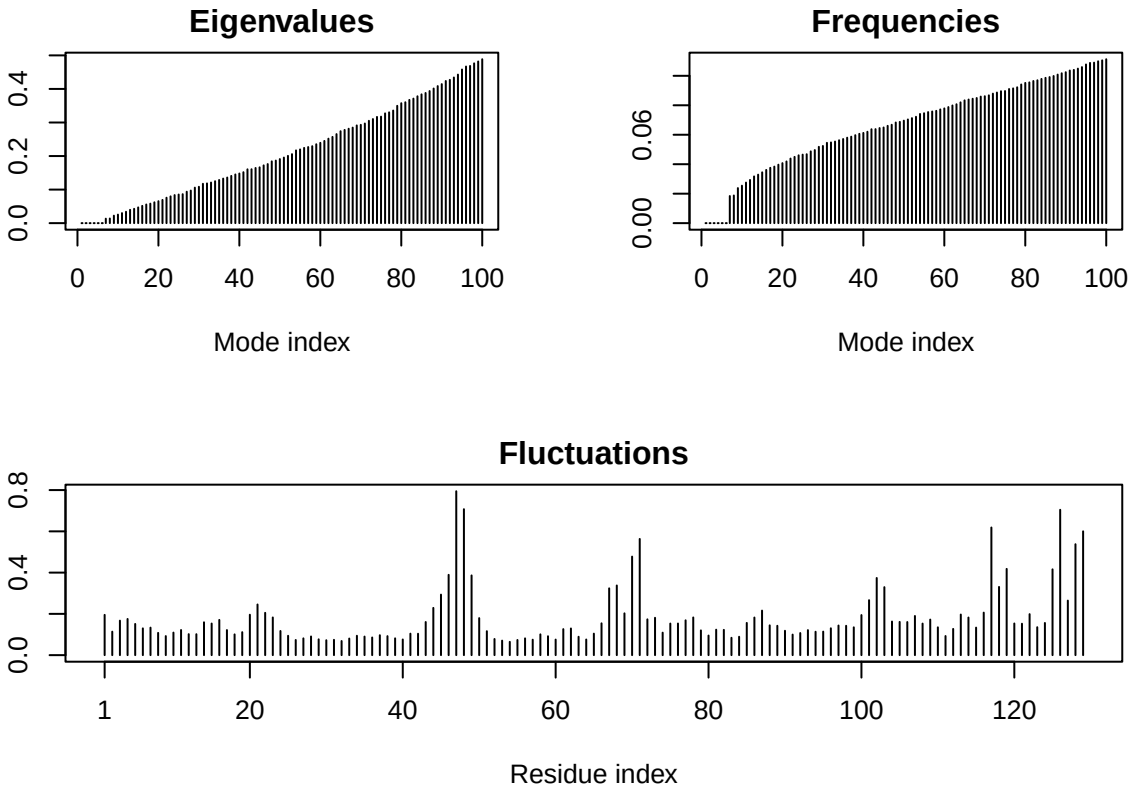
```
library(bio3d)

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

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

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

```
##  Building Hessian...     Done in 0.034 seconds.
##  Diagonalizing Hessian...    Done in 0.077 seconds.
```

```
plot(m)
```



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

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