Lab 11: Structural Bioinformatics II

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1.1 Obtaining and inspecting our input structure

```
library(bio3d)
```

```
file.name <- get.pdb("1hsg")
```

```
## Warning in get.pdb("1hsg"): ./1hsg.pdb exists. Skipping download
```

```
hiv <- read.pdb(file.name)
```

```
hiv
```

```
##
##  Call:  read.pdb(file = file.name)
##
##    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
```

Q1: What is the name of the two non protein resid values in this structure? What does resid correspond to and how would you get a listing of all reside values in this structure?

The two non protein resid values are HOH and MK1. Resid corresponds to the residues within the structure. To get a list of all residue values in the structure look at the variable through: hiv*atom*resid

```
head(hiv$atom$resid, n = 20)
```

```
##  [1] "PRO" "PRO" "PRO" "PRO" "PRO" "PRO" "PRO" "GLN" "GLN" "GLN" "GLN" "GLN"
## [13] "GLN" "GLN" "GLN" "GLN" "ILE" "ILE" "ILE" "ILE"
```

1.2 Prepare initial protein and ligand input files

```
prot <- trim.pdb(hiv, "protein")
lig <- trim.pdb(hiv, "ligand")

write.pdb(prot, file="1hsg_protein.pdb")
write.pdb(lig, file="1hsg_ligand.pdb")
```

1.3 Using AutoDockTools to setup protein docking input

Q2: Can you locate the binding site visually? Note that crystal structures normally lack hydrogen atoms, why?

Yes, you can locate the binding site visually. The hydrogen atoms are not generally required to represent the structure, and normally crystal structures lack hydrogen atoms.

Q3: Look at the charges. Does it make sense (e.g. based on your knowledge of the physiochemical properties of amino acids)?

Yes,the charges make sense