Bio3D Tutorial

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Bio3D

This is an R package to analyse protein structure, sequence and trajectory. For more details on using Bio3D please see http://thegrantlab.org/bio3d/index.php.

Load bio3d library

```
library("bio3d")
```

Read a pdb file.

```
pdb<-read.pdb("Files/1MNZ_refmac1_highR.pdb")
```

```
##   HEADER    ISOMERASE                               06-SEP-02   1MNZ
```

```
## Warning in read.table(text = sapply(raw.atom, split.fields),
## stringsAsFactors = FALSE, : not all columns named in 'colClasses' exist
```

```
##    PDB has ALT records, taking A only, rm.alt=TRUE
```

Use the function 'atom.select' to select the C-aplha of your chain.

```
calpha<-atom.select(pdb,"calpha")
```

Before to write your new pdb in a new file, use the function trim.pdb(), which will create a new pdb object based on the C-alpha.

```
calpha_pdb<-trim.pdb(pdb,calpha)
```

Now output your new pdb object to a file using the function write.pdb()

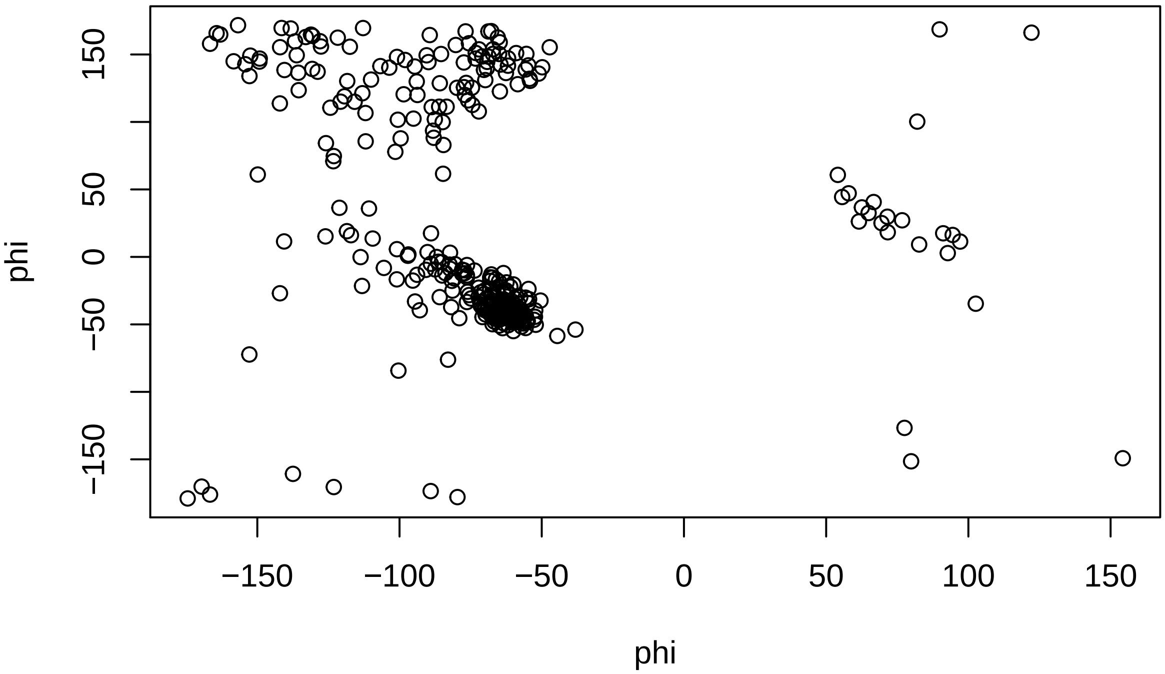
```
write.pdb(calpha_pdb, file="Files/calpha_1MNZ.pdb")
```

Calculate the torsion angle

```
tor<-torsion.pdb(pdb)
```

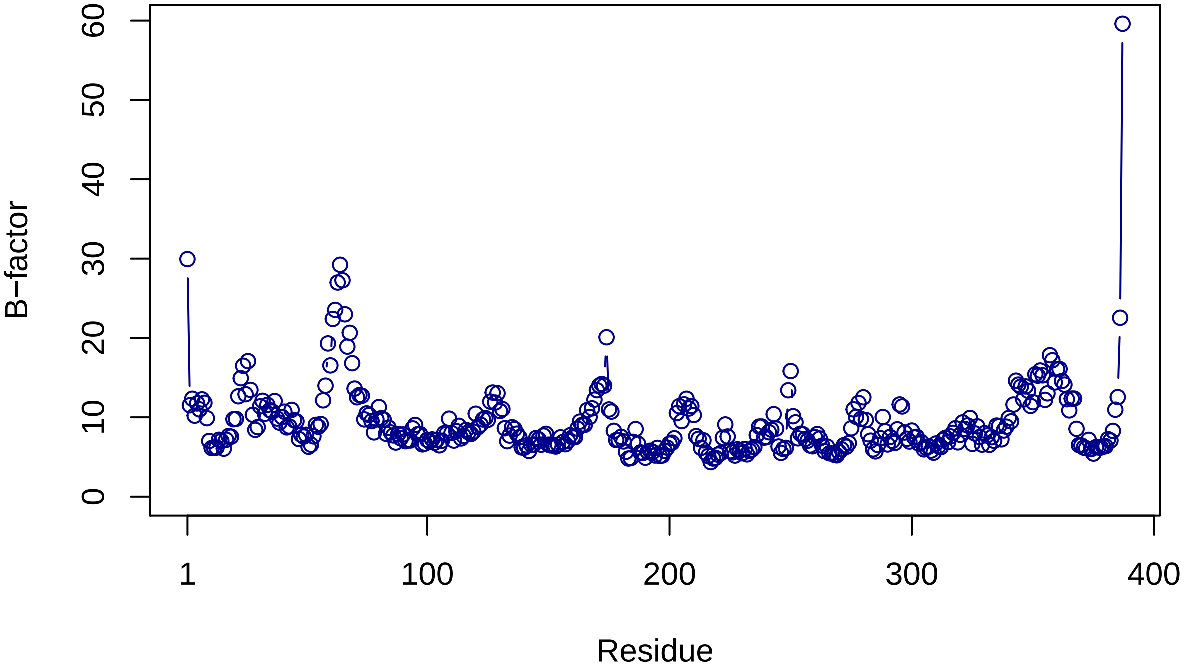
Plot the Ramachandran plot

```
plot(tor$phi,tor$psi, xlab="phi",ylab="phi")
```



Plot of B-factor values for C-alpha atoms

```
plot.bio3d(pdb$atom[pdb$calpha, "b"], ylab="B-factor", type="b", col="darkblue")
```



Read protein sequence. NOTE: Before use the function read.fasta rename your file as “sequence_name.fa”

```
seq <-read.fasta("Files/1MNZ_A.fa")
```

Or you can read the protein sequence directly from the pdb using the function pdbseq()

```
seq_pdb <- pdbseq(pdb)
```