Supplement

Laura Sun (PID: A17923552)

Q1: Input of the function?

The inputs of the function are the names of protein structure. User can input the ones they are looking for.

Q2: what the function does and how to use it?

This function reads the user input proteins from protein data base. It then get the alpha carbon, get B-factor value, and make a plot. User can call protein() and input the protein names with " " into the bracket to use it.

Q3: - what is the output of the function.

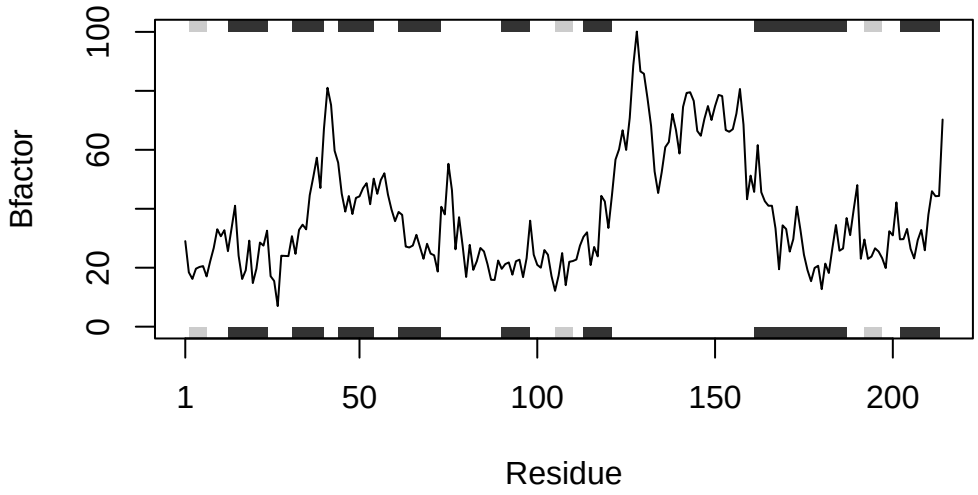
The output of the function is a plot of residue vs. Bfactor. It shows the effect of drug binding.

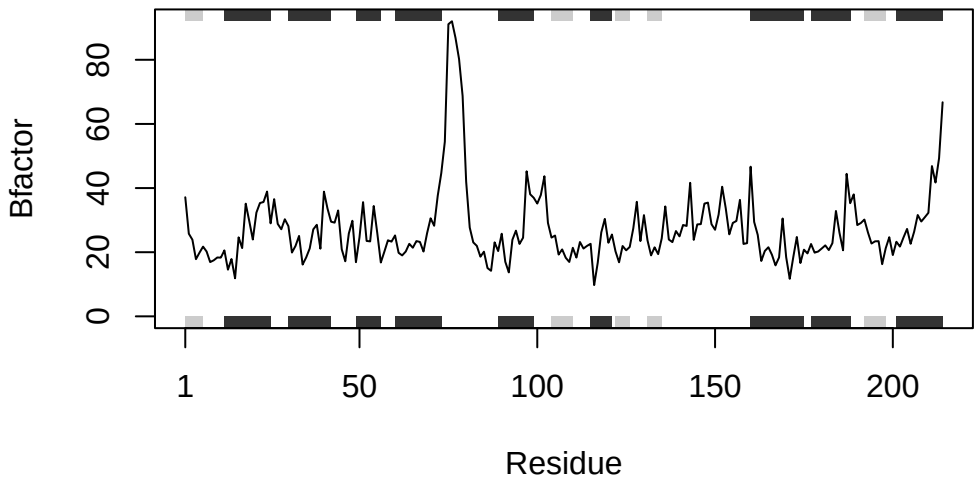
```
library(bio3d)

protein <- function(drug1, drug2, drug3){ #input protein names
  s1 <- read.pdb(drug1)
  s2 <- read.pdb(drug2)
  s3 <- read.pdb(drug3)
  s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
  s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
  s3.chainA <- trim.pdb(s3, chain="A", elety="CA")
  s1.b <- s1.chainA$atom$b
  s2.b <- s2.chainA$atom$b
  s3.b <- s3.chainA$atom$b
  plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
  plotb3(s2.b, sse=s2.chainA, typ="l", ylab="Bfactor")
  plotb3(s3.b, sse=s3.chainA, typ="l", ylab="Bfactor")
}
```

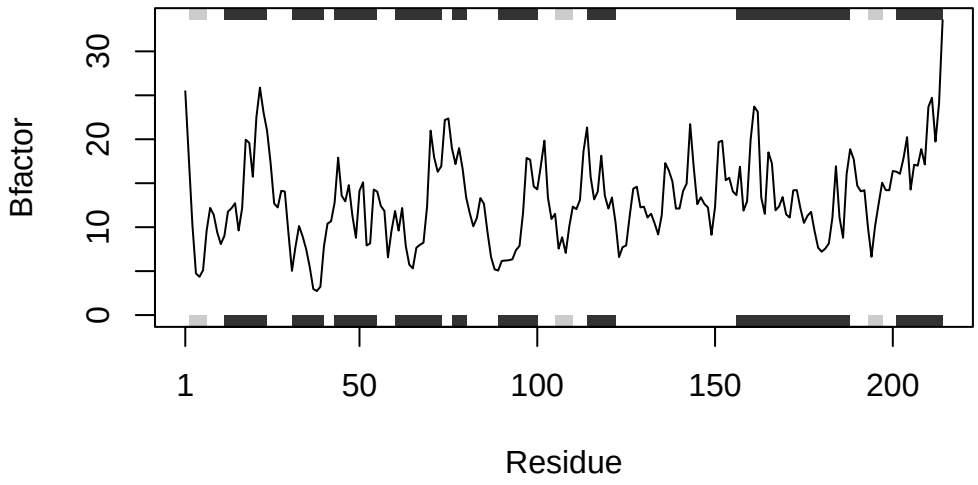
Test to check:

```
# Input protein names
protein("4AKE", "1AKE", "1E4Y")
```

```
  Note: Accessing on-line PDB file
  Note: Accessing on-line PDB file
   PDB has ALT records, taking A only, rm.alt=TRUE
  Note: Accessing on-line PDB file
```




Bfactor
0
20
40
60
80
1
50
100
150
200
Residue


Bfactor
0
10
20
30
1
50
100
150
200
Residue