

Homework 6

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The following code declares the library packages that are needed to be used. Installation of the package was conducted through `install.packages("bio3d")`.

```
library(bio3d)
```

The following code gives a breakdown of the proposed function.

The function is aimed to take a specified protein of interest and generate a plot based on the protein structure of chain A and the targeted column of focus.

```
#the input of the function is the specified protein of interest
newfun <- function(input) {

  #reads the input protein and assigns it to variable s
  s <- read.pdb(input)

  #isolates the protein structure to the targeted chain
  s.chainA <- trim.pdb(s, chain="A", eley="CA")

  #assigns a variable to the targeted column of focus
  s.b <- s.chainA$atom$b

  #plots the vector, adding the secondary structure,
  #assigning the type of plot and the title of the y-axis
  plotb3(s.b, sse=s.chainA, typ="l", ylab="Bfactor")
}
```

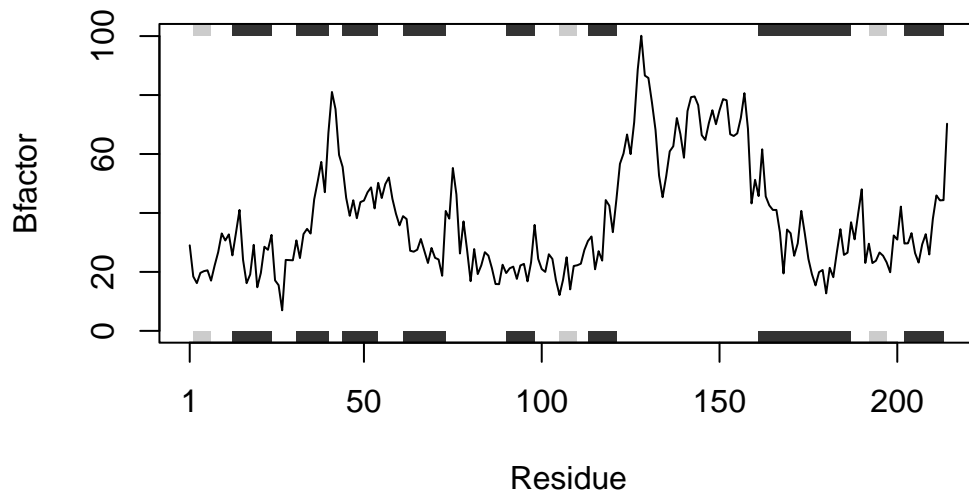
The following code runs the function to make sure it is successful.

```
#the sample list of variables to be inputted
protein_list <- c("4AKE", "1AKE", "1E4Y")
```

```
#run
for (i in protein_list) {
  print(i)
  newfun(i)
}
```

[1] "4AKE"

Note: Accessing on-line PDB file



[1] "1AKE"

Note: Accessing on-line PDB file

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



[1] "1E4Y"

Note: Accessing on-line PDB file

