Class 6 Homework: Writing a Function

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Create a function to improve this code.

```
#original code
library(bio3d)

s1 <- read.pdb("4AKE") # kinase with drug
```

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

```
s2 <- read.pdb("1AKE") # kinase no drug
```

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

```
s3 <- read.pdb("1E4Y") # kinase with drug
```

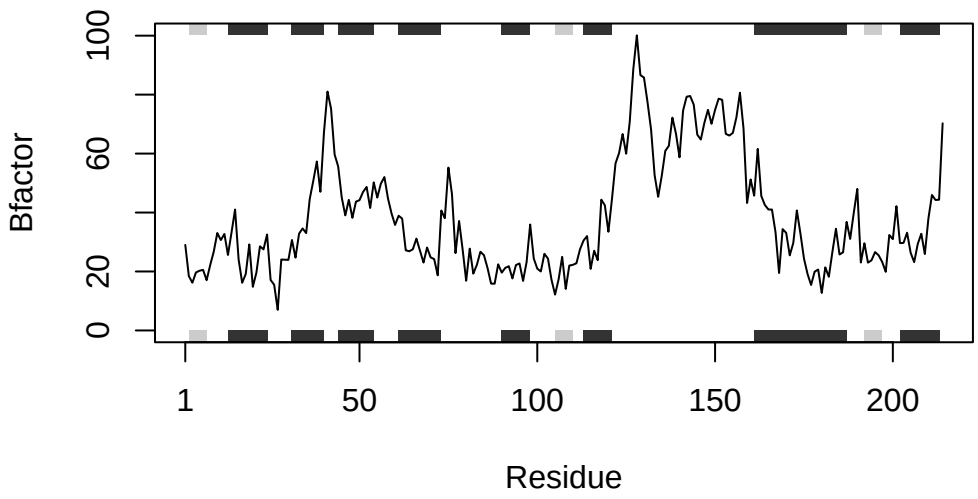
```
  Note: Accessing on-line PDB file
```

```
#this reads the pdb files
```

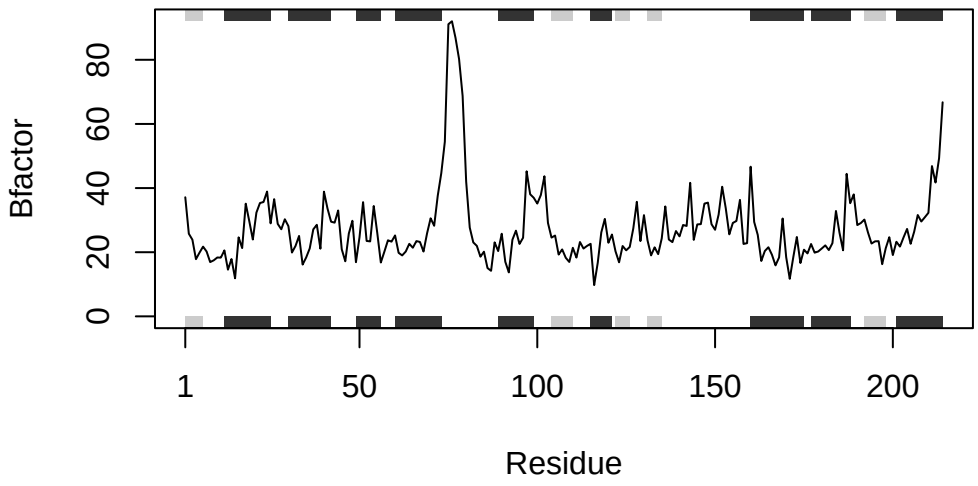
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")

#this one creates a data frame that trims does the file to just chain A and elety "CA" for ea
```

```
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b

#this one parses out just the "b" column from the data frame and assigns it to a list
```

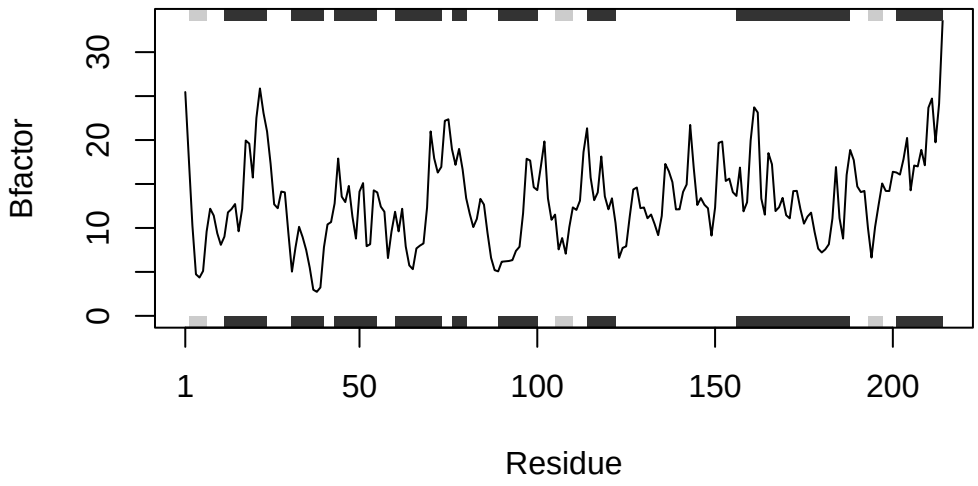
```
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```




```
plotb3(s2.b, sse=s2.chainA, typ="l", ylab="Bfactor")
```




```
plotb3(s3.b, sse=s3.chainA, typ="l", ylab="Bfactor")
```



```
#this creates a line graph of the "b" column against "sse=__.chainA" and labels the y axis
```

Lets combine these into a single function.

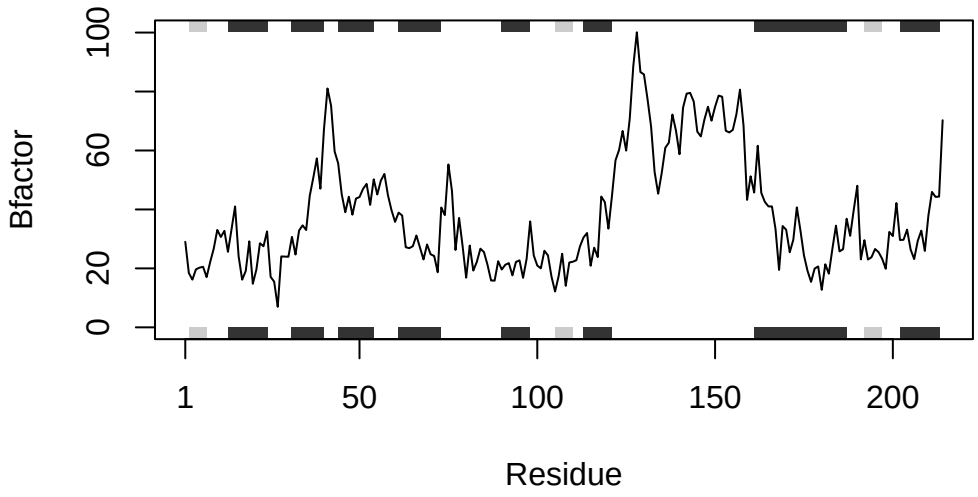
inputs and **explanation of code**

```
plot_b_atoms <- function(name){

  library(bio3d)
  s <- read.pdb(name)
  #reads the file based on the protein id

  s.chainA <- trim.pdb(s, chain="A", elety="CA")
  #trims the data frame to just include the A chain data with elety of "CA"

  s.b <- s.chainA$atom$b
  #this sections out just the "b" column of the new data frame

  final_plot <- plotb3(s.b, sse=s.chainA, typ="l", ylab="Bfactor")
  #this plots a line graph of the b column data

  return(final_plot)
  # this returns the final plot as the output of the function

}

#the input "name" refers to the 4 letter protein id from the bio3d database

#each line in the function performs the same thing as each "chunk" in the original code, now
```

outputs and **how to use the function**

```
plot_b_atoms("4AKE")
```

```
  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\obald\AppData\Local\Temp\Rtmp2HaYZh/4AKE.pdb exists. Skipping download
```



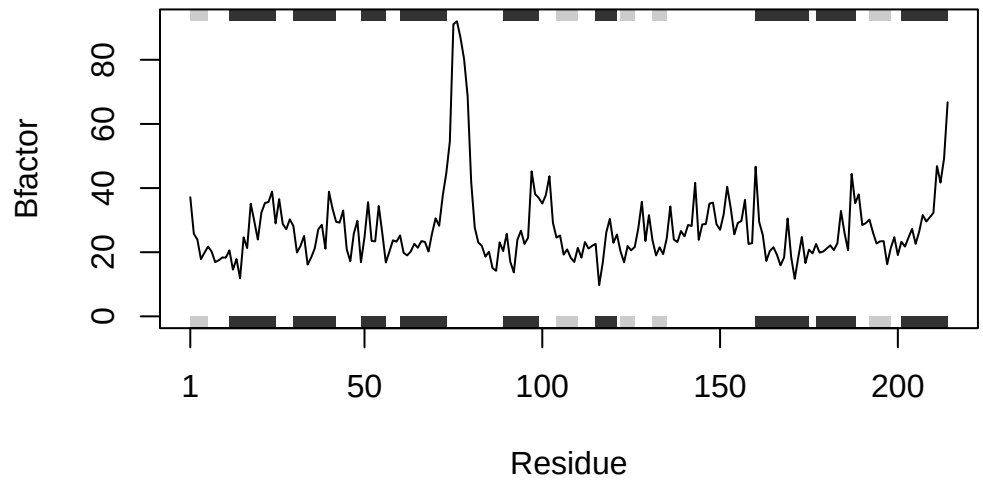

```
NULL
```

```
plot_b_atoms("1AKE")
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\obald\AppData\Local\Temp\Rtmp2HaYZh/1AKE.pdb exists. Skipping download
```

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

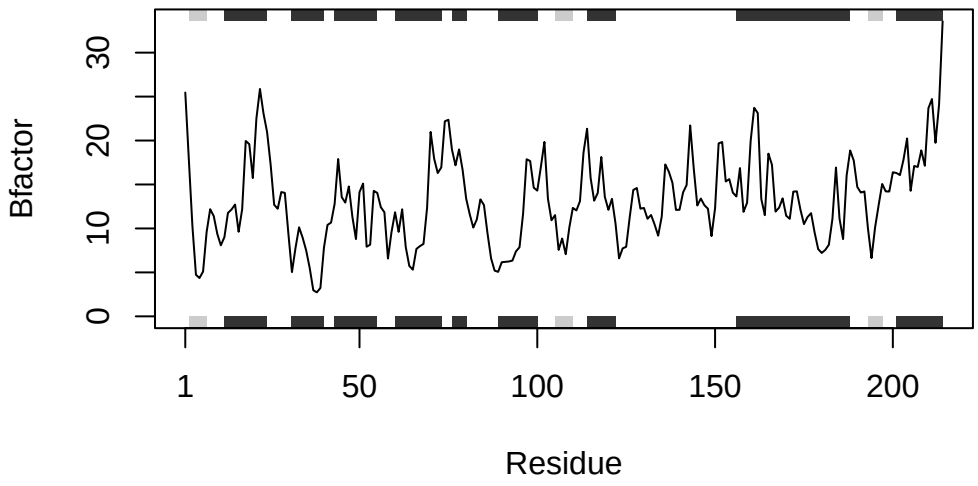



```
NULL
```

```
plot_b_atoms("1E4Y")
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\obald\AppData\Local\Temp\Rtmp2HaYZh/1E4Y.pdb exists. Skipping download
```




```
NULL
```

```
#to use this function, just input the 4 letter id from the bio3d data base

#this will output a plot of the "b" atoms from the A chain of the protein input
```