HW Class6 (Write a function)

L.Cruz PID: A59006931

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```
# install.packages("bio3d")
```

```
# Can you improve this analysis code?
library(bio3d)
s1 <- read.pdb("4AKE")  # kinase with drug
```

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

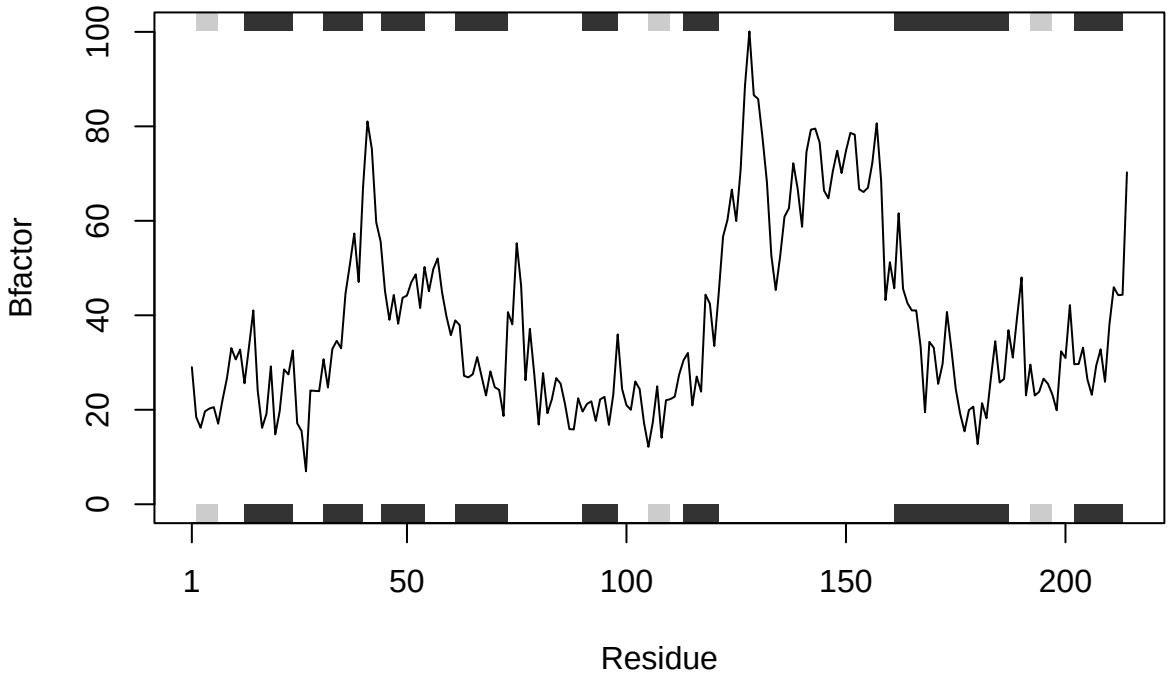
```
s2 <- read.pdb("1AKE")  # kinase no drug
```

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

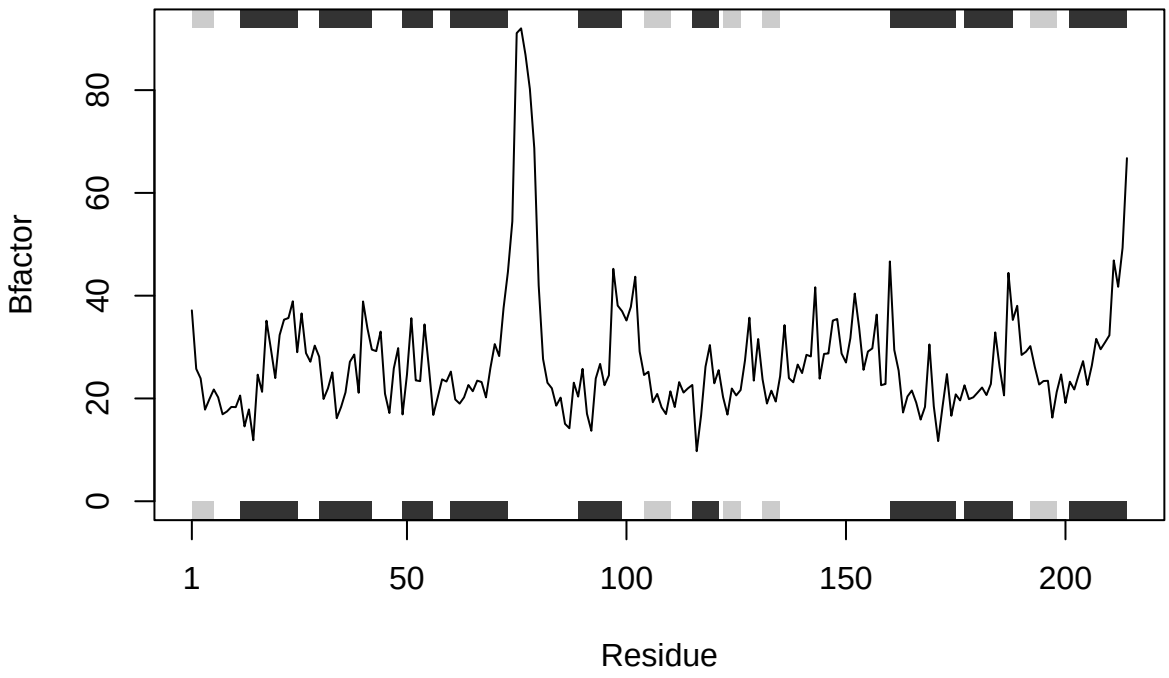
```
s3 <- read.pdb("1E4Y")  # kinase with drug
```

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

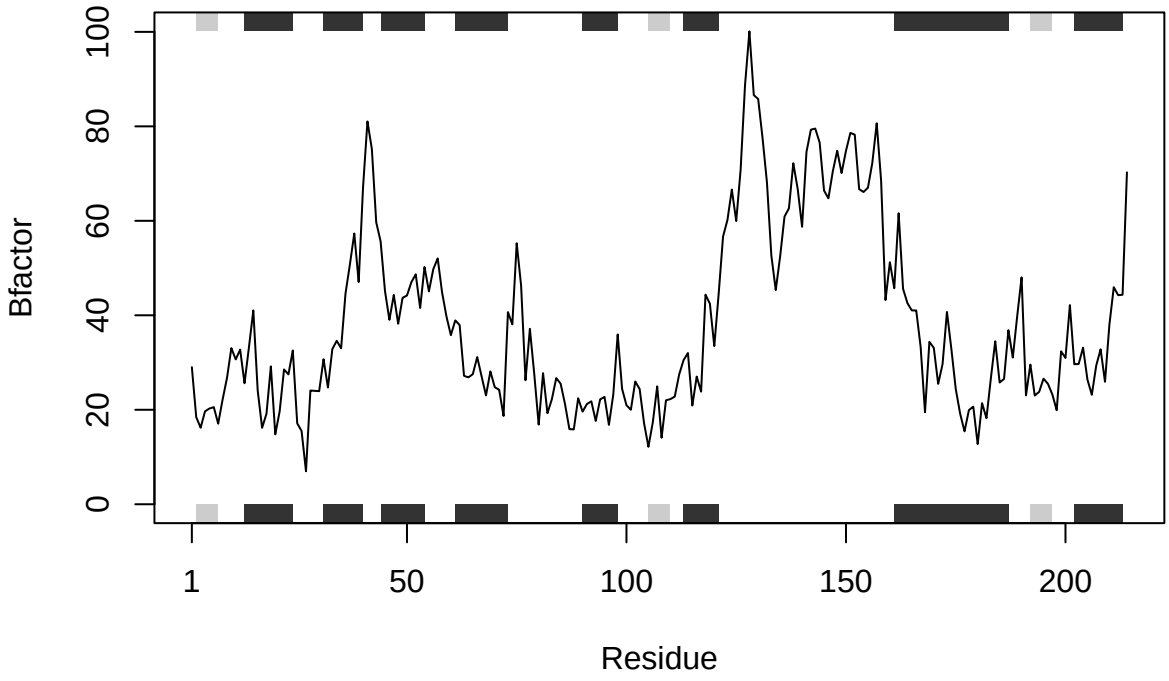
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```




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




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




```
##Make a Function to visualize the data better:
all.drug.plot <- function(file, chain, elmnt, fctr){
##Give data different colors to better vizualize:
  plot_colors <- c("NAVY", "DARK RED", "DARK GREEN")
## This will help  to repeat through every value of the "file" vector
  for (i in 1:length(file)) {
  s1 <- read.pdb(file[i])
  s1.chain <- trim.pdb(s1, chain = chain, elety = elmnt)
  atom_df <- s1.chain$atom
##Made a variable so "s1.fctr" takes in all the element information
##This will also select the entire columns, respectively, based on the factor input
  s1.fctr <- atom_df[, fctr]
##First plot
  if (i == 1) {
    plotb3(s1.fctr, sse = s1.chain, typ = "l", ylab = paste(toupper(fctr), "factor", sep = ""), col = pl
##Other plots are then added to the first plot
  } else {lines(s1.fctr, col = plot_colors[i])}}
##Add legends for the graph and other aesthetics
  legend("topright", title = "PDB File Name", file, fill = plot_colors, horiz=TRUE, cex = 0.5, inset = c
}
```

```
##This will test the new function and see if we can identify the protein drug iterations
files <- c("4AKE", "1AKE", "1E4Y")
chains <- "A"
elements <- "CA"
factors <- "b"
```

```
all.drug.plot(files, chains, elements, factors)
```

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

## Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/ly/
## 21877hyn0q72js2x6r9k91w40000gn/T//Rtmpf46KDw/4AKE.pdb exists. Skipping download

##   Note: Accessing on-line PDB file

## Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/ly/
## 21877hyn0q72js2x6r9k91w40000gn/T//Rtmpf46KDw/1AKE.pdb exists. Skipping download

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

## Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/ly/
## 21877hyn0q72js2x6r9k91w40000gn/T//Rtmpf46KDw/1E4Y.pdb exists. Skipping download
```