HW6

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A. Can you improve this analysis code?

```
df <- data.frame(a=1:10, b=seq(200,400,length=10),c=11:20,d=NA)
df$a <- (df$a - min(df$a)) / (max(df$a) - min(df$a))
df$b <- (df$b - min(df$a)) / (max(df$b) - min(df$b))
df$c <- (df$c - min(df$c)) / (max(df$c) - min(df$c))
df$d <- (df$d - min(df$d)) / (max(df$a) - min(df$d))
```

Firstly, we see that there is an error in the line with df$d as an a has not been changed into a d. Thus is important to generalize this process into a function to reduce errors arising from copy and paste. We first simply to work with a generic vector x.

```
x <- 1:5
x <- (x - min(x)) / (max(x) - min(x))

#since min(x) is repeated, we can simplify by saving it into a variable

xmin <- min(x)
x <- (x - xmin) / (max(x) - xmin)

#since function range() also outputs the minimum and maximum, we can further simplify:

rng = range(x)
x <- (x-rng[1]) / (rng[2] - rng[1])
```

Writing a function to emulate the repeated process

```
rescale <- function(x){
  rng = range(x)
  (x-rng[1]) / (rng[2] - rng[1])
}
```

Let's test on a small example where we know the answer

```
rescale(1:10)
```

```
 [1] 0.0000000 0.1111111 0.2222222 0.3333333 0.4444444 0.5555556 0.6666667
 [8] 0.7777778 0.8888889 1.0000000
```

It seems that the rescale function works on our small test. How about when the example has NAs?

```
rescale(c(1,2,3, NA, 10))
```

```
[1] NA NA NA NA NA
```

Why? Let's see how `range()` deals with NA

```
range(c(1,2,3,NA,10))
```

```
[1] NA NA
```

Turns out `range()` has an argument na.rm which will be useful

```
range(c(1,2,3,NA,10), na.rm = T)
```

```
[1]  1 10
```

Let's rewrite the rescale function

```
rescale <- function(x){
  rng = range(x, na.rm = T)
  (x-rng[1]) / (rng[2] - rng[1])
}
```

and retry on our example with an NA

```
rescale(c(1,2,3, NA, 10))
```

```
[1] 0.0000000 0.1111111 0.2222222        NA 1.0000000
```

Great! Note that some potential problems with this code though are that if there are strings in the vector the function won't know how to deal with those

```
#rescale(c(1,2,3, "cat"))
#returns "Error in x - rng[1] : non-numeric argument to binary operator"
```

B. Can you improve this analysis code?

First fix the error in s3.chainA

```
library(bio3d)
```

```
Warning: package 'bio3d' was built under R version 4.0.5
```

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

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

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

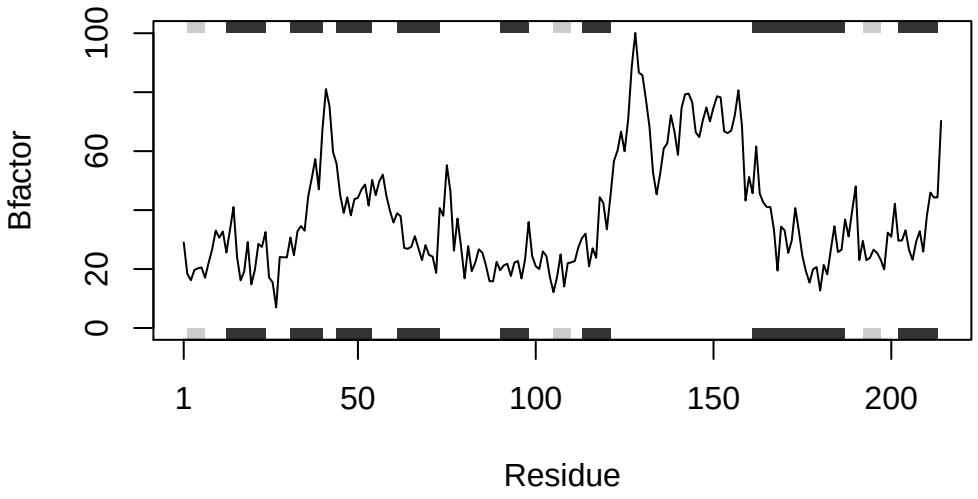
```
  Note: Accessing on-line PDB file
   PDB has ALT records, taking A only, rm.alt=TRUE
```

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

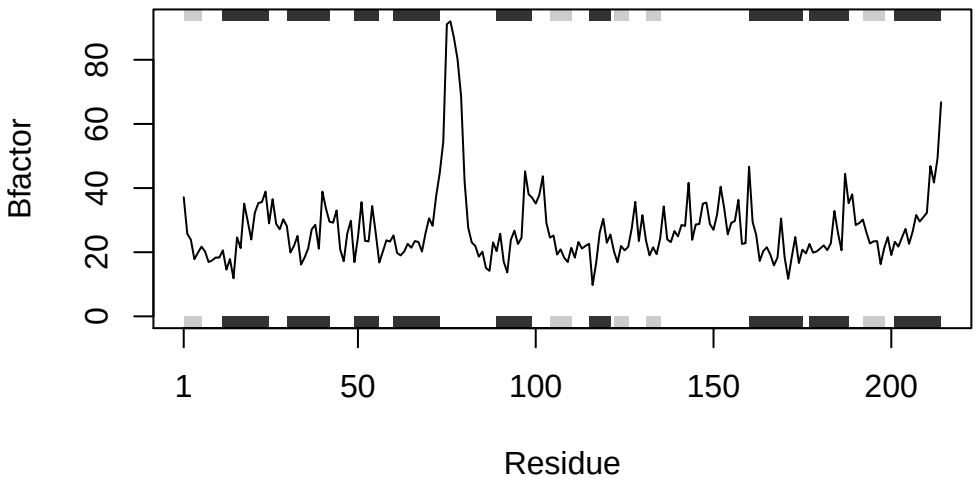
```
  Note: Accessing on-line PDB file
```

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

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

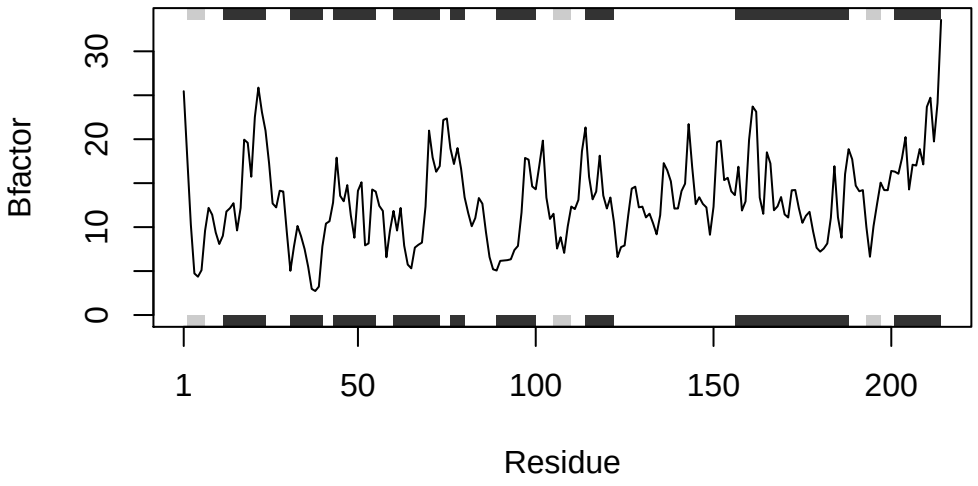
```
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```




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




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



SHORT QUESTIONS

Q1 The object returned from the `read.pdb()` function is a Protein Data Bank (PDB) coordinate file.

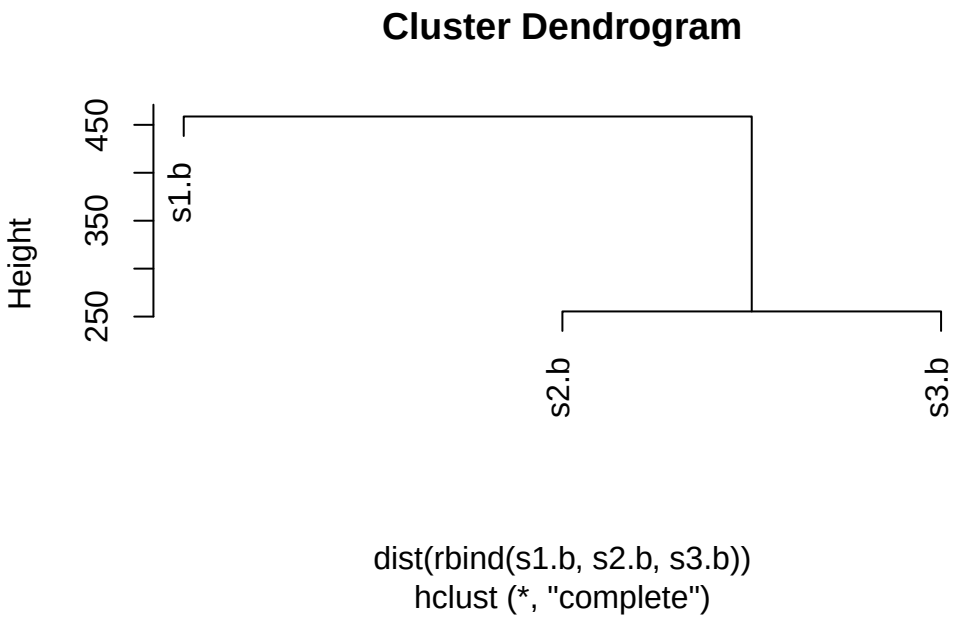
Q2 The function `trim.pdb()` produces a smaller PDB object by subsetting certain atoms from a larger PDB object, for example by specifying a chain of a protein

Q3 Setting the input parameter "sse" to NULL would remove the black and grey rectangles in the plots. These rectangles represent the secondary structure of the protein

Q4 A better plot to compare across the different proteins might be to overlay these scatter plots over one another

Q5

```
hc <- hclust( dist( rbind(s1.b, s2.b, s3.b) ) )

plot(hc)
```



One might compare/quantify the similarity of the proteins based on heirarchal clustering. With some metric of distance, the b-factor at each position/residue on the protein is compared, where proteins more similar will score lower distance scores, and vice versa. Hierarchal clustering will group similar proteins (based on distance) together and form a sort of tree showing the

comparative distances between such proteins. Based on the hierarchal clustering of the b-factor trends of the three proteins, we see that s2.b and s3.b are the most structurally similar.

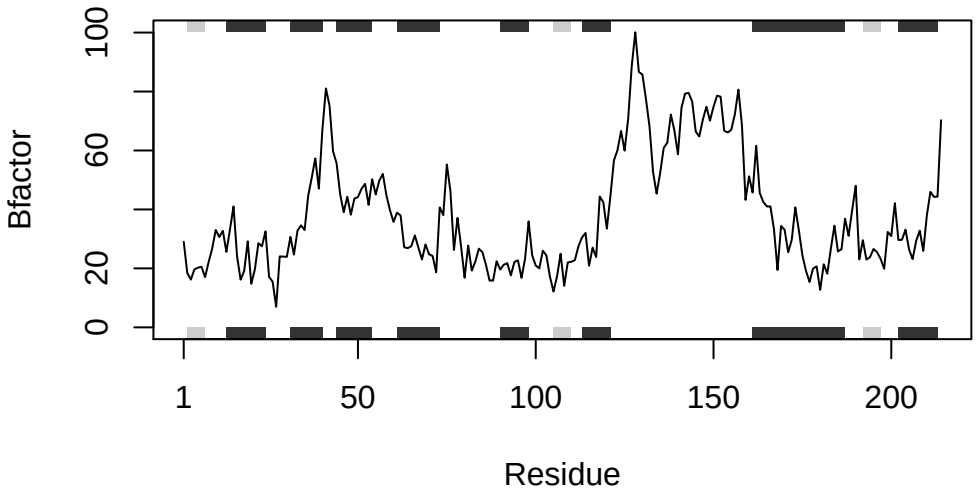
Q6

```
#It seems that the purpose of this code/analysis chunk isto plot
#the b-factor scores of a protein along with annotations of the secondary structure

#This function will take in a protein with identifier PID.
#It will first access the PDB file of this protein using the read.pdb() function
#then it will then trim it using trim.pdb in accordance with the specifications of the
#protein chain and the atom type.
#Lastly it will plot, using plotb3, a scatterplot of the b-score along the protein chain
#with annotations of the secondary structure specified by the trimmed object.
#The output of this function is this plot.

#The input of the function are the unique identifier of the protein, PID
#the chain specified,which by default is set to "A",
#and the atom name "elety" which by default is set to "CA"

plotb3_new <- function(PID, chain = "A", elety = "CA"){
  #this loads the PDB coordinate file of the protein specified by PID into protein
  protein <- read.pdb(PID)
  #variable protein trimmed by chain and atom type, by default "A" and "CA"
  protein.chain <- trim.pdb(protein, chain = chain, elety = elety)
  #the b-factor score of the protein chain is plotted alongside the sse protein.chain
  plotb3(protein.chain$atom$b, sse = protein.chain, typ = "l", ylab = "Bfactor")
}
```

Let's try with our known protein samples to compare our results

```
plotb3_new("4AKE")  # kinase with drug
```

```
  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE): C:
\Users\Joshua\AppData\Local\Temp\RtmpO46oeN/4AKE.pdb exists. Skipping download
```

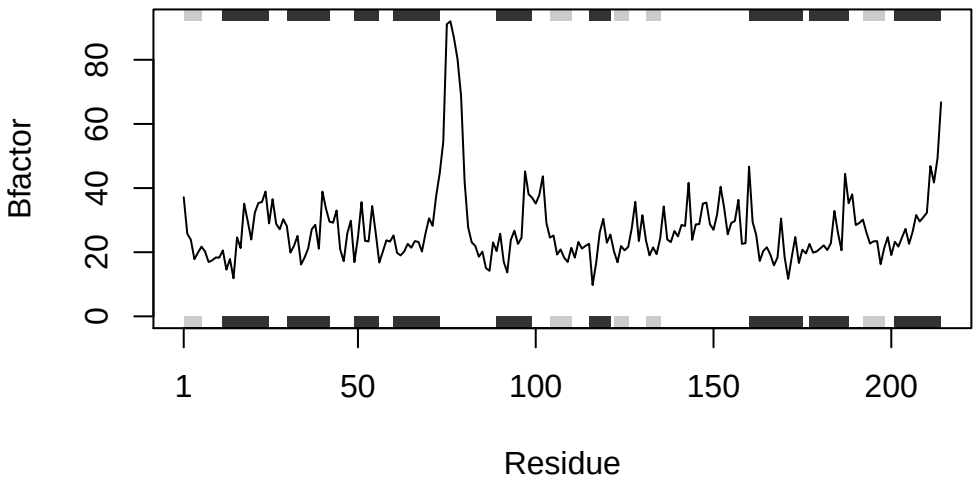



```
plotb3_new("1AKE")  # kinase no drug
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE): C:
\Users\Joshua\AppData\Local\Temp\RtmpO46oeN/1AKE.pdb exists. Skipping download
```

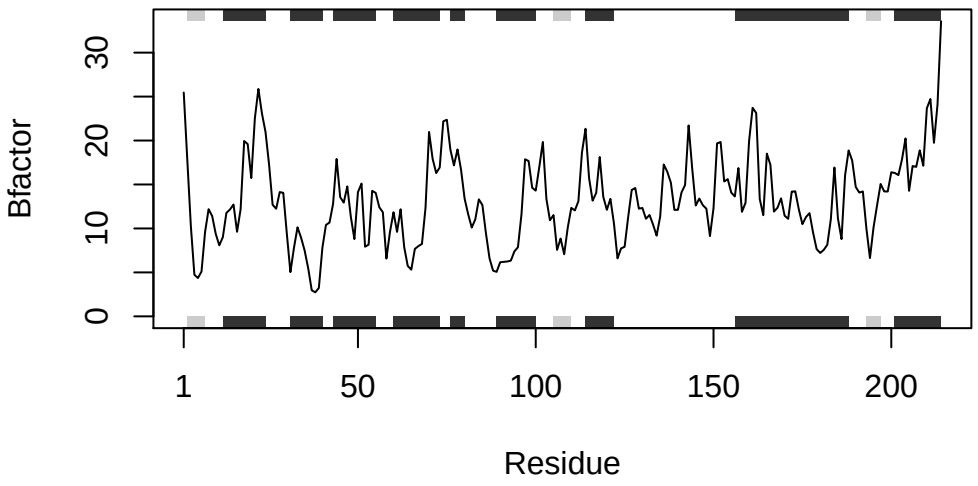
```
   PDB has ALT records, taking A only, rm.alt=TRUE
```




```
plotb3_new("1E4Y")  # kinase with drug
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE): C:
\Users\Joshua\AppData\Local\Temp\RtmpO46oeN/1E4Y.pdb exists. Skipping download
```



Looks like everything matches up with the results of the original analysis!