BGGN213: Lab 6 Supplement

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This is the supplement to Lab 6: R Functions

Section 1: Improving analysis code by writing functions

A. Improve this regular R code by abstracting the main activities in your own new function. (Note: we will go through this example together in the formal lecture.)

The main steps should entail running through the code to see if it works,...

```
# I had to make some edits in the code to get it to work correctly (i.e. store the 5 appropriate data a

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$b - min(df$b)) / (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$d) - min(df$d))
df$a
```

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

A. (continued) ... simplifying to a core working code snippet,

```
x <- df$a
x2 <- (x - min(x)) / (max(x) - min(x))
x2
```

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

A. (continued) ... reducing any calculation duplication,

```
# Setting 'min(x)' and 'max(x)' as "range" functions will reduce calculation duplication
x <- df$a
rng <- range(x)
# where the function ends up looking like this...
x2 <- (x - rng[1]) / (rng[2] - rng[1])
x2
```

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

A. (continued) ... and finally transferring your new streamlined code into a more useful function.

```
# This code streamlined the previous code into a more useful function that accounts for 'NA' values.
rescale <- function(x) {
  rng <- range(x, na.rm=TRUE)
  (x - rng[1]) / (rng[2] - rng[1])
}
# Example showing function is functional
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
```

```
# Now that we know this function works we can save the function either as an R file and source it each
```

B. Next improve the below example code for the analysis of protein drug interactions by abstracting the main activities in your own new function. Then answer questions 1 to 6 below. It is recommended that you start a new Project in RStudio in a new directory and then install the bio3d package noted in the R code below (N.B. you can use the command 'install.packages("bio3d")' or the RStudio interface to do this).

Installing the bio3d package (Note: This code is not within a "code chunk" to avoid installing packages multiple times) 'install.packages("bio3d")'

B. (continued) ... Then run through the code to see if it works, fix any copy/paste errors before simplifying to a core working code snippet...

```
library(bio3d)
# Overall Goal: Can you improve this analysis code?
# First corrected any copy/paste errors
s1 <- read.pdb("4AKE") # kinase with drug
```

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

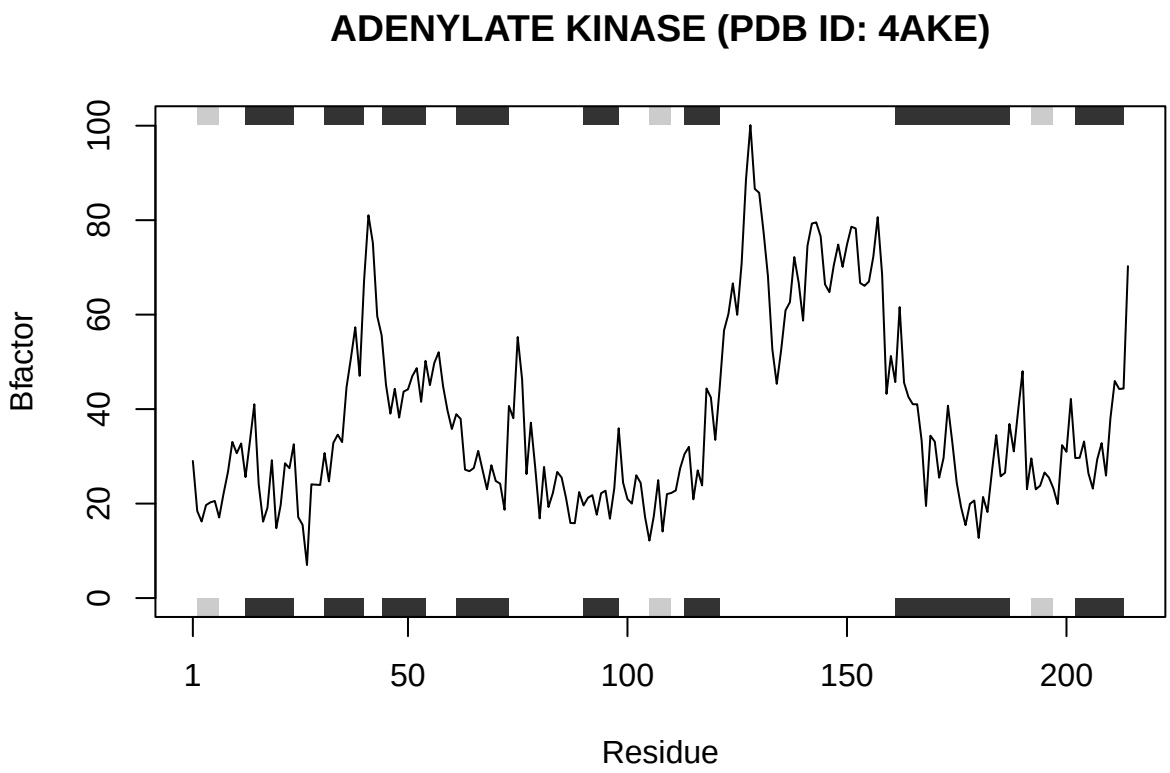
```
s2 <- read.pdb("1AKE") # kinase no drug
```

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

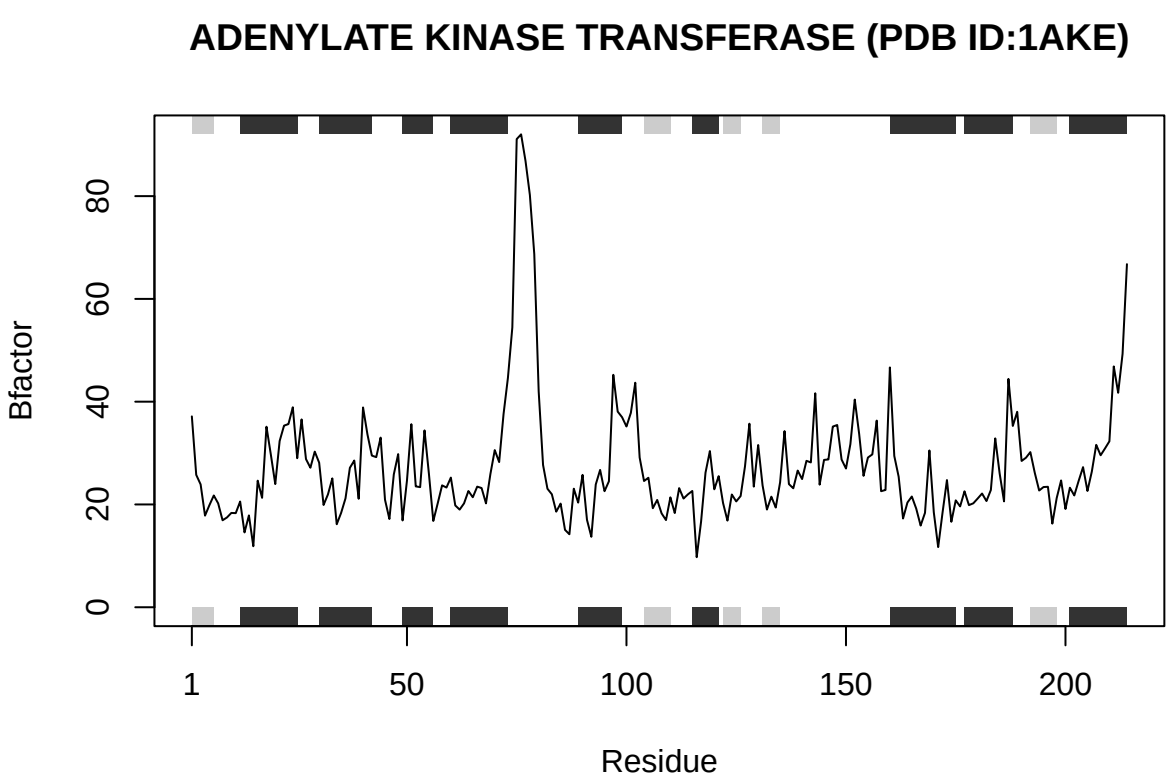
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

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

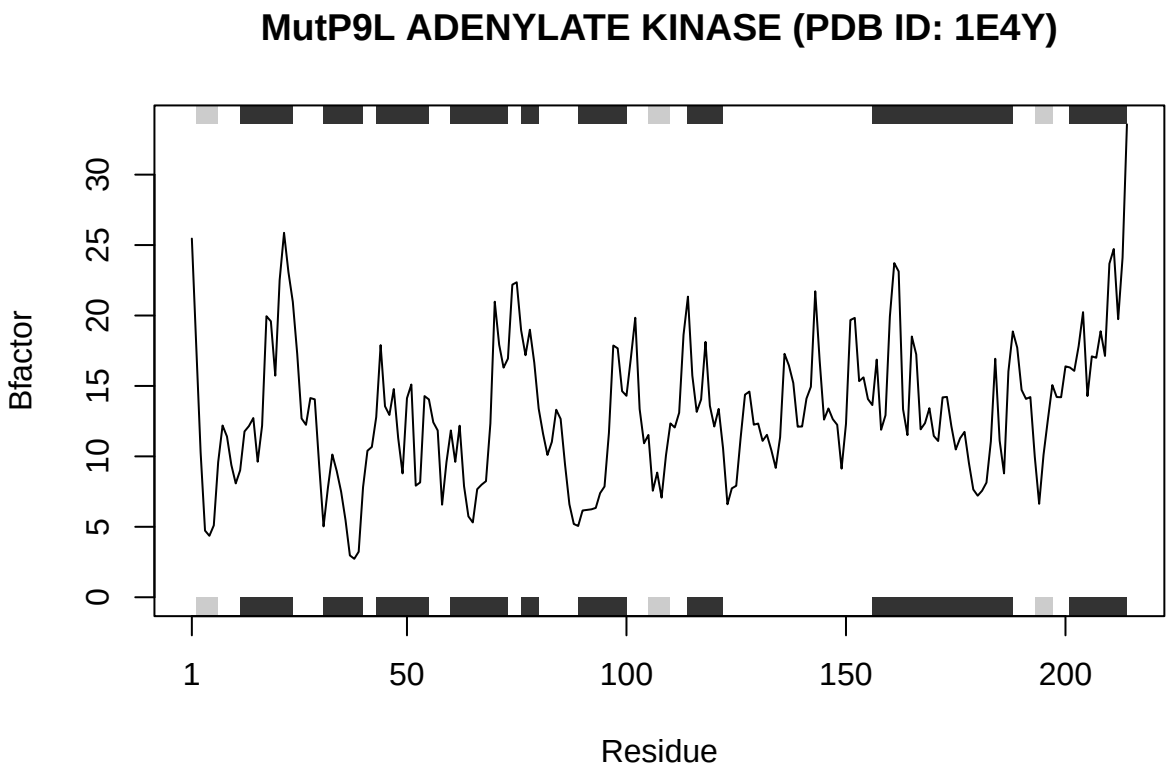
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b

# Then plotted each dataset individually and added titles
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor", main = "ADENYLATE KINASE (PDB ID: 4AKE)")
```




```
plotb3(s2.b, sse=s2.chainA, typ="l", ylab="Bfactor", main = "ADENYLATE KINASE TRANSFERASE (PDB ID:1AKE)
```




```
plotb3(s3.b, sse=s3.chainA, typ="l", ylab="Bfactor", main = "MutP9L ADENYLATE KINASE (PDB ID: 1E4Y)")
```



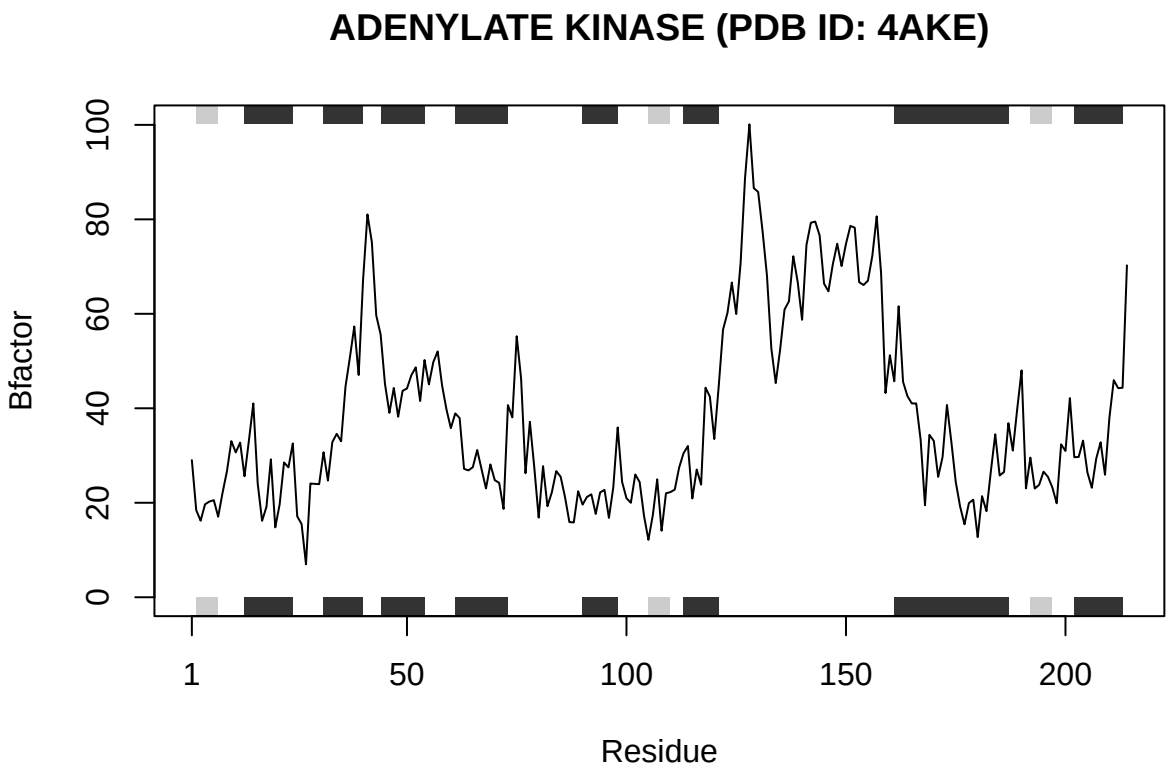
B. (continued) . . . simplifying to a core working code snippet, reducing any calculation duplication, . . .

```
# First, I reduced the amount of calculations by inserting 'read.pdb()' directly into the 'trim.pdb()'
s1.chainA <- trim.pdb((read.pdb("4AKE")), chain="A", elety="CA")
```

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

```
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE): C:
## \Users\colta\AppData\Local\Temp\RtmpEx8Lmx/4AKE.pdb exists. Skipping download
```

```
s1.b <- s1.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor", main = "ADENYLATE KINASE (PDB ID: 4AKE)")
```



B. (continued) ... and finally transferring it into a more useful function for you.

```
# I transferred the main part of the function (didn't include plotting) into a more useful function nam
lab6 <- function(x) {
  chainA <- trim.pdb((read.pdb(x)), chain="A", elety="CA")
  chainA$atom$b
}
```

```
# Then I plotted each PDB ID onto one plot
plotb3(lab6("4AKE"), typ="l", ylab="Bfactor", main = "ADENYLATE KINASES")
```

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

## Warning in get.pdb(file, path = tempdir(), verbose = FALSE): C:
## \Users\colta\AppData\Local\Temp\RtmpEx8Lmx/4AKE.pdb exists. Skipping download
```

```
lines(lab6("1AKE"), col="red")
```

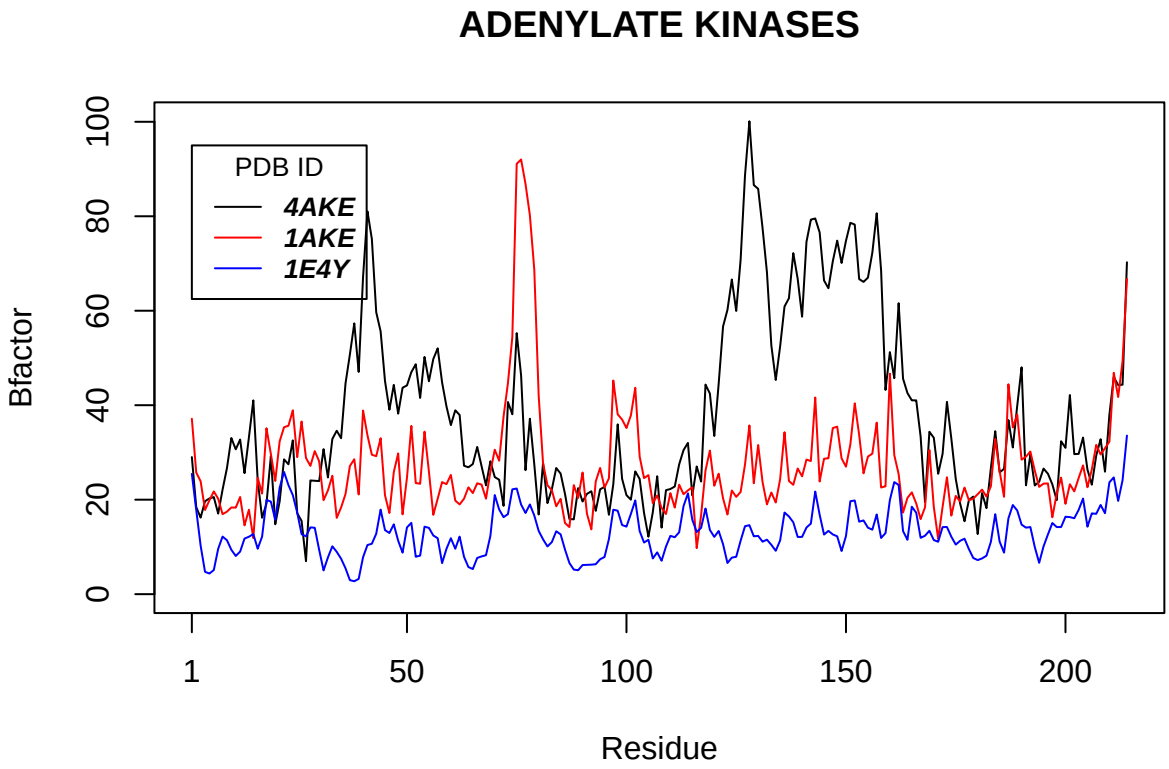
```
##   Note: Accessing on-line PDB file

## Warning in get.pdb(file, path = tempdir(), verbose = FALSE): C:
## \Users\colta\AppData\Local\Temp\RtmpEx8Lmx/1AKE.pdb exists. Skipping download

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

```
lines(lab6("1E4Y"), col="blue")
```

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

```
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE): C:
## \Users\colta\AppData\Local\Temp\RtmpEx8Lmx/1E4Y.pdb exists. Skipping download
```

```
# Then added a legend
legend(1, 95, legend=c("4AKE", "1AKE", "1E4Y"),
       col=c("black", "red", "blue"), lty = 1, cex=0.8,
       title="PDB ID", text.font=4)
```



Q1. What type of object is returned from the read.pdb() function?

'read.pdb()' retrieves data from the specified PDB format file from Protein Data Bank

Q2. What does the trim.pdb() function do?

'trim.pdb()' retrieves a specified subset of atoms from the original Protein Data Bank file

Q3. What input parameter would turn off the marginal black and grey rectangles in the plots and what do they represent in this case?

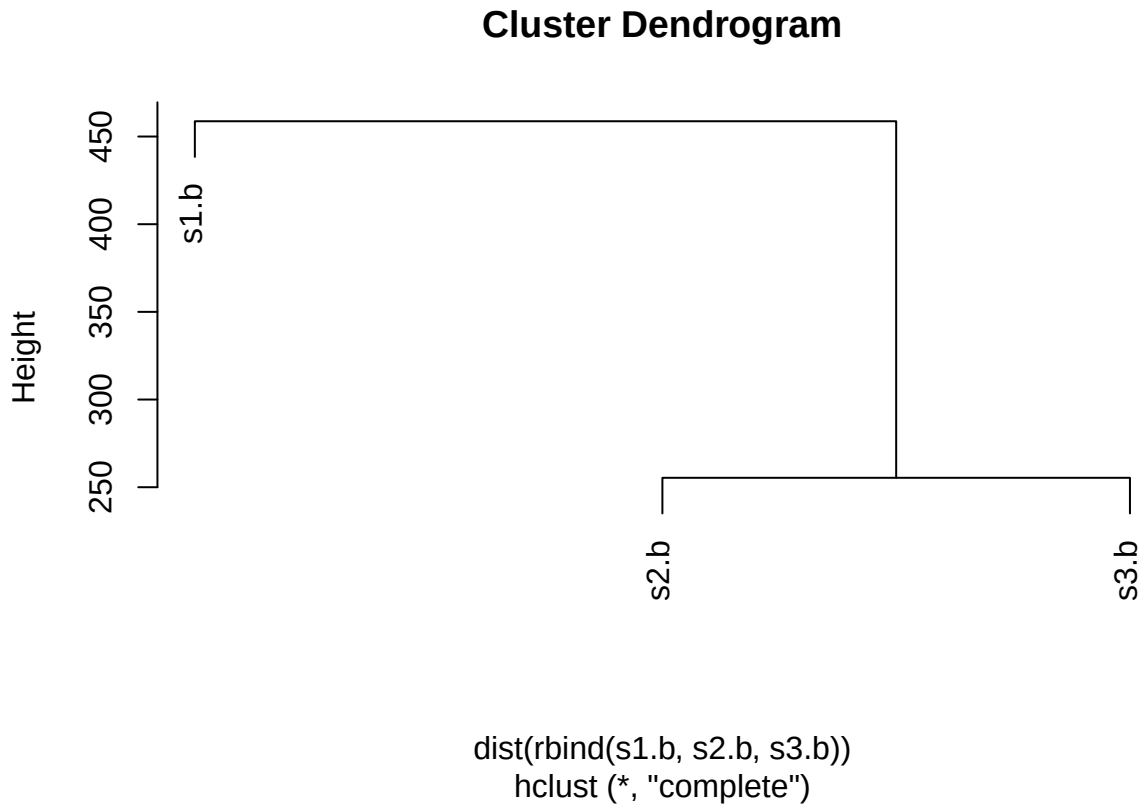
Taking out 'sse=' turns off the marginal black and grey rectangles. These rectangles represent secondary structures.

Q4. What would be a better plot to compare across the different proteins?

PCA with a cluster diagram would probably be the best because you could easily visualize and quantify relationships between multiple parameters.

Q5. Which proteins are more similar to each other in their B-factor trends. How could you quantify this?

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



Answer: "1AKE" (i.e. "s2.b", and red) and "1E4Y" (i.e. "s3.b", and blue) are more similar to each other in their B-factor trends. You can quantify this by the height of each branch.

Q6. How would you generalize the original code above to work with any set of input protein structures?

I already did. Using my function 'lab6()' you just put the PDB ID into the parenthesis within quotes.