HW Class 6: Write a Function

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```
library(bio3d)
```

Section 1: Improving analysis code by writing functions

A

Improve the below 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$b)) / (max(df$b) - min(df$b))

df$a <- (df$c - min(df$c)) / (max(df$c) - min(df$c))

df$a <- (df$d - min(df$d)) / (max(df$d) - min(df$d))
```

Analysis code to improve

```
s1 <- read.pdb("4AKE") # kinase with drug
s2 <- read.pdb("1AKE") # kinase no drug
s3 <- read.pdb("1E4Y") # kinase with drug
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")
```

Question 1:

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

```
s1 <- read.pdb("4AKE")
```

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

```
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /tmp/RtmpD2QBEI/
## 4AKE.pdb exists. Skipping download
```

```
str(s1)
```

```
## List of 8
##  $ atom  :'data.frame':  3459 obs. of  16 variables:
##   ..$ type  : chr [1:3459] "ATOM" "ATOM" "ATOM" "ATOM" ...
##   ..$ eleno : int [1:3459] 1 2 3 4 5 6 7 8 9 10 ...
##   ..$ elety : chr [1:3459] "N" "CA" "C" "O" ...
##   ..$ alt   : chr [1:3459] NA NA NA NA ...
##   ..$ resid : chr [1:3459] "MET" "MET" "MET" "MET" ...
##   ..$ chain : chr [1:3459] "A" "A" "A" "A" ...
##   ..$ resno : int [1:3459] 1 1 1 1 1 1 1 2 2 ...
##   ..$ insert: chr [1:3459] NA NA NA NA ...
##   ..$ x     : num [1:3459] -10.93 -9.9 -9.17 -9.8 -10.59 ...
##   ..$ y     : num [1:3459] -24.9 -24.4 -23.3 -22.3 -24 ...
##   ..$ z     : num [1:3459] -9.52 -10.48 -9.81 -9.35 -11.77 ...
##   ..$ o     : num [1:3459] 1 1 1 1 1 1 1 1 1 1 ...
##   ..$ b     : num [1:3459] 41.5 29 27.9 26.4 34.2 ...
##   ..$ segid : chr [1:3459] NA NA NA NA ...
##   ..$ elesy : chr [1:3459] "N" "C" "C" "O" ...
##   ..$ charge: chr [1:3459] NA NA NA NA ...
##  $ xyz   : 'xyz' num [1, 1:10377] -10.93 -24.89 -9.52 -9.9 -24.42 ...
##  $ seqres: Named chr [1:428] "MET" "ARG" "ILE" "ILE" ...
##   ..- attr(*, "names")= chr [1:428] "A" "A" "A" "A" ...
##  $ helix :List of 4
##   ..$ start: Named num [1:19] 13 31 44 61 75 90 113 161 202 13 ...
##   .. ..- attr(*, "names")= chr [1:19] "" "" "" "" ...
##   ..$ end  : Named num [1:19] 24 40 54 73 77 98 121 187 213 24 ...
##   .. ..- attr(*, "names")= chr [1:19] "" "" "" "" ...
##   ..$ chain: chr [1:19] "A" "A" "A" "A" ...
##   ..$ type : chr [1:19] "5" "1" "1" "1" ...
##  $ sheet :List of 4
##   ..$ start: Named num [1:14] 192 105 2 81 27 123 131 192 105 2 ...
##   .. ..- attr(*, "names")= chr [1:14] "" "" "" "" ...
##   ..$ end  : Named num [1:14] 197 110 7 84 29 126 134 197 110 7 ...
##   .. ..- attr(*, "names")= chr [1:14] "" "" "" "" ...
##   ..$ chain: chr [1:14] "A" "A" "A" "A" ...
##   ..$ sense: chr [1:14] "0" "1" "1" "1" ...
##  $ calpha: logi [1:3459] FALSE TRUE FALSE FALSE FALSE FALSE ...
##  $ remark:List of 1
##   ..$ biomat:List of 4
##   .. ..$ num   : int 1
##   .. ..$ chain :List of 1
##   .. .. ..$ : chr [1:2] "A" "B"
##   .. ..$ mat   :List of 1
##   .. .. ..$ :List of 1
##   .. .. .. ..$ A B: num [1:3, 1:4] 1 0 0 0 1 0 0 0 1 0 ...
##   .. ..$ method: chr "AUTHOR"
##  $ call  : language read.pdb(file = "4AKE")
##  - attr(*, "class")= chr [1:2] "pdb" "sse"
```

Returns a list.

Question 2:

What does the trim.pdb() function do?

```
help("trim.pdb")
```

It trims the original PDB object to contain a subset of the original atoms.

Question 3:

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

```
help("plotb3")
```

The *sse* parameter is what sets the marginal grey and black rectangles, which represents the major secondary structure elements (SSEs) of the protein.

Question 4:

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

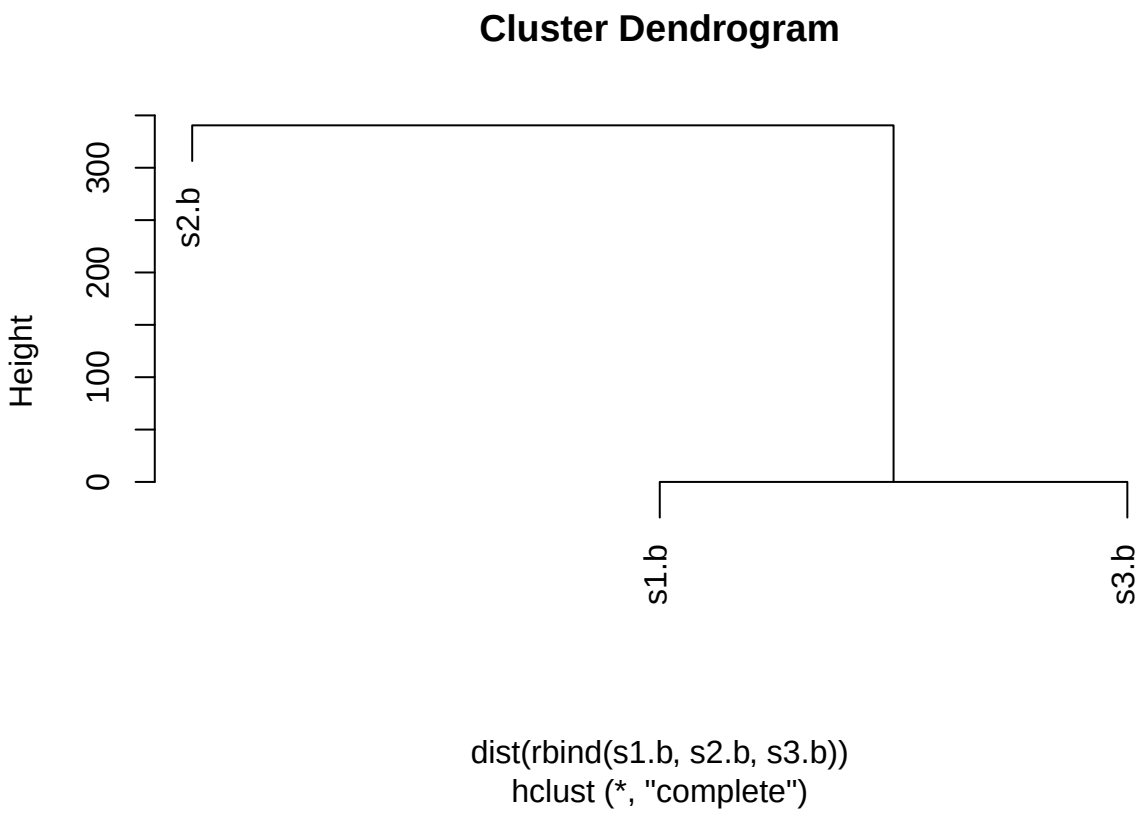
A scatterplot of RMSD data from aligned protein sequences. Alignment would allow for significant residue-residue comparisons.

Question 5:

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

Use hierarchical clustering with the calculated distances between protein structures to identify which are more similar.

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



The kinases with drugs (4AKE and 1E4Y) are more similar to each other than to the kinase without drugs (1AKE).

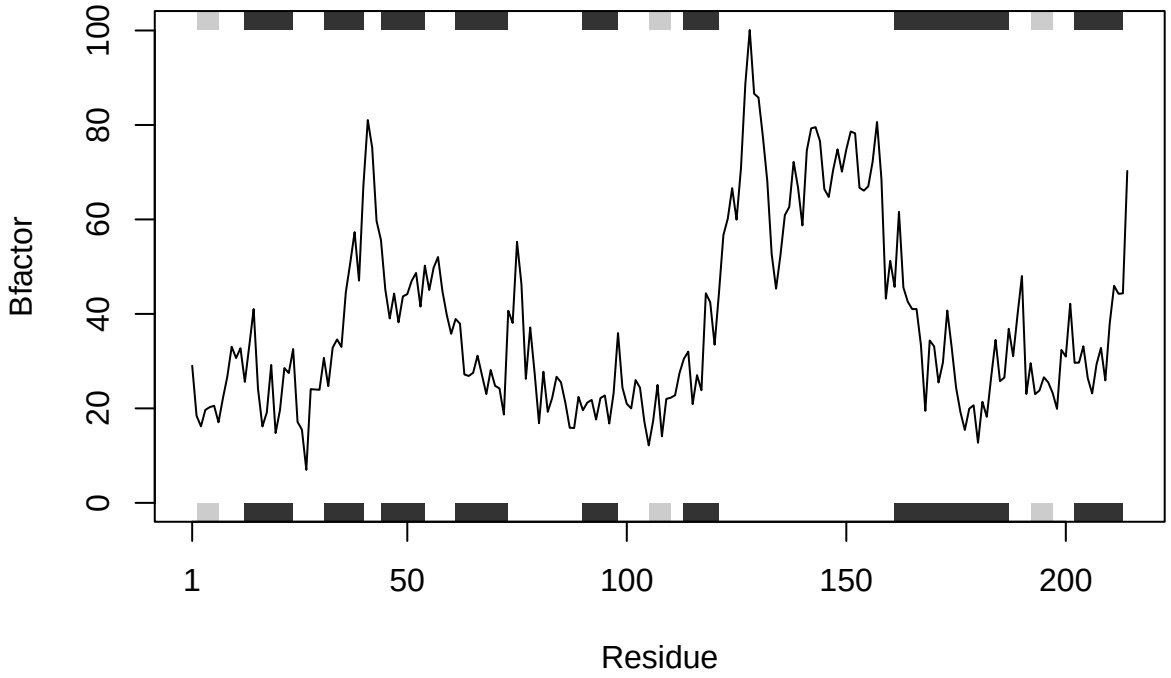
Question 6:

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

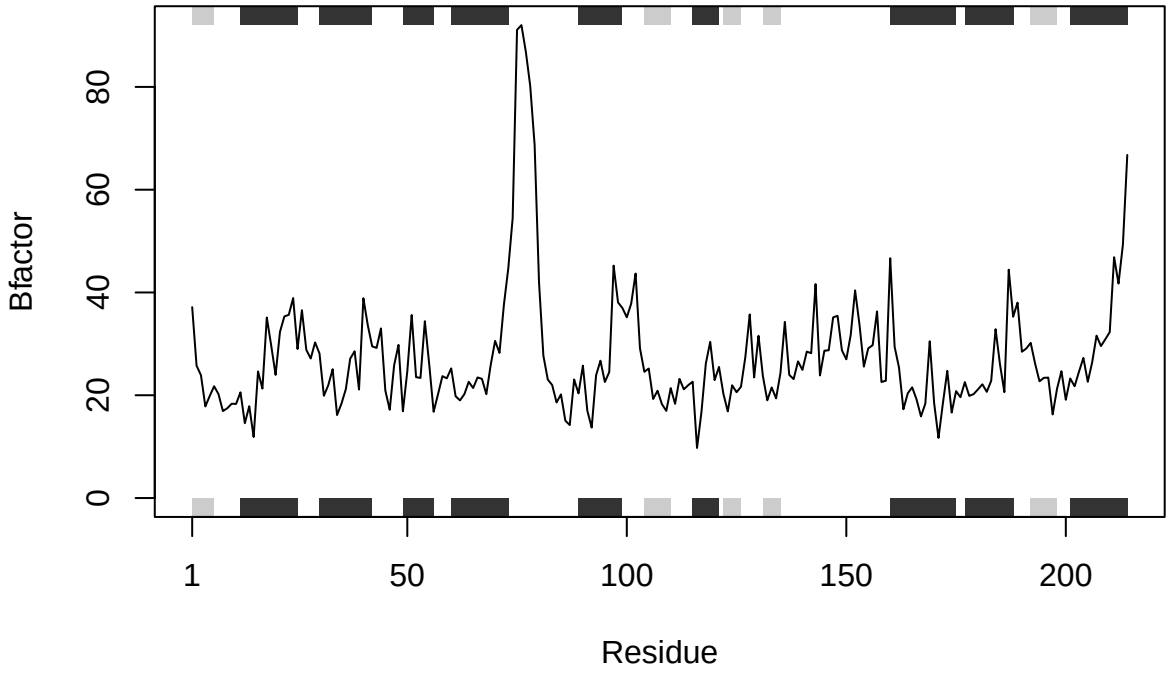
```
structure_analysis <- function(protein_vector,
                               trim_chain = "A", trim_elety = "CA",
                               plotb3_typ = "l", plotb3_ylab = "Bfactor") {
  for(protein in protein_vector) {
    structure <- read.pdb(protein)
    structure.chainA <- trim.pdb(structure, chain=trim_chain, elety=trim_elety)
    structure.b <- structure.chainA$atom$b
    plotb3(structure.b, sse=structure.chainA, typ=plotb3_typ, ylab=plotb3_ylab)

  }
}

structure_analysis(c("4AKE", "1AKE", "1E4Y"))
```

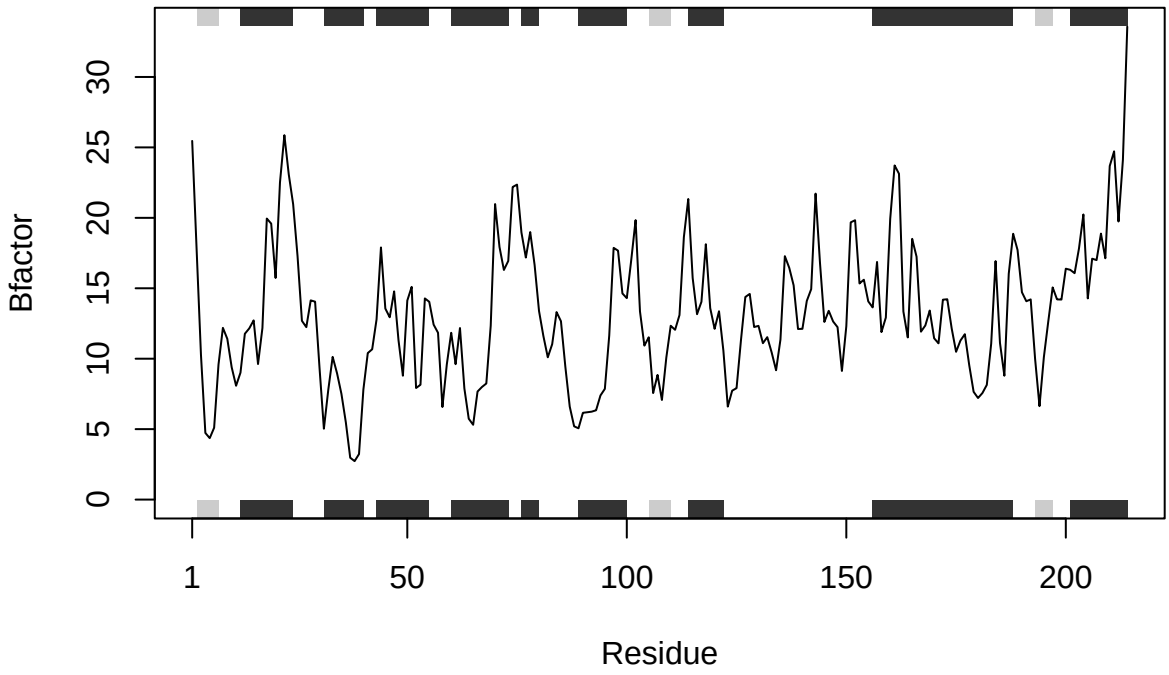
```
##   Note: Accessing on-line PDB file
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /tmp/RtmpD2QBEI/
## 4AKE.pdb exists. Skipping download
##   Note: Accessing on-line PDB file
```

```
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /tmp/RtmpD2QBEI/
## 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): /tmp/RtmpD2QBEI/
## 1E4Y.pdb exists. Skipping download
```




Bfactor
0
5
10
15
20
25
30
1
50
100
150
200
Residue