homework6

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R Markdown

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

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
```

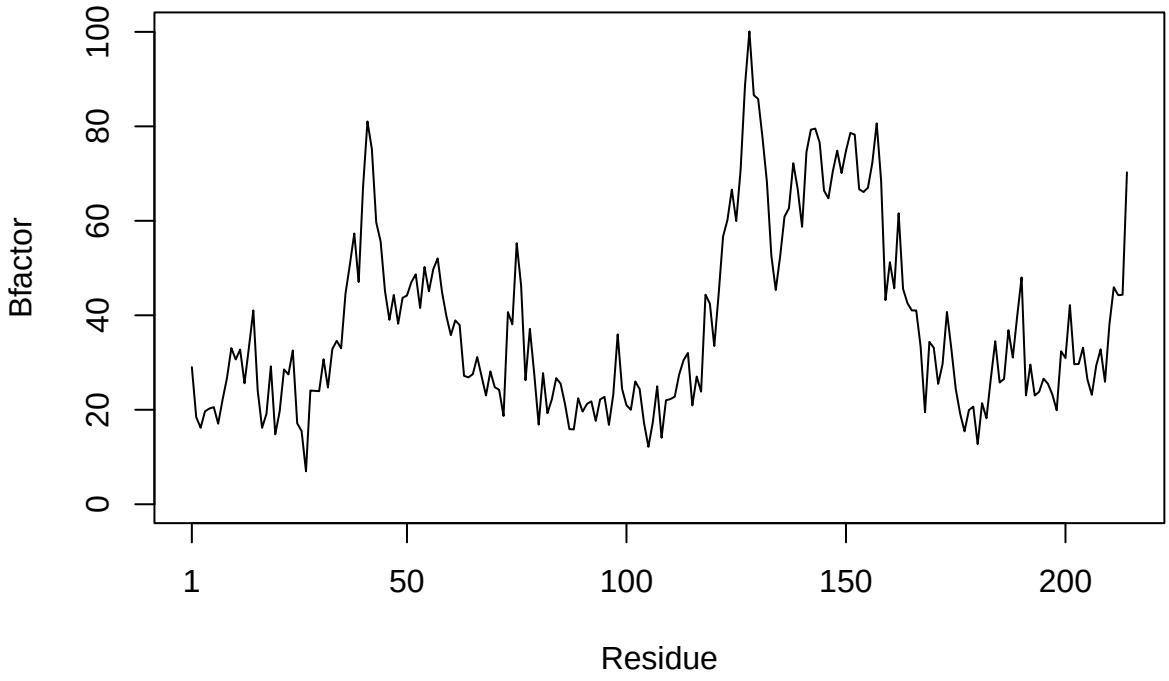
```
##   Note: Accessing on-line PDB file
```

```
typeof(s1)
```

```
## [1] "list"
```

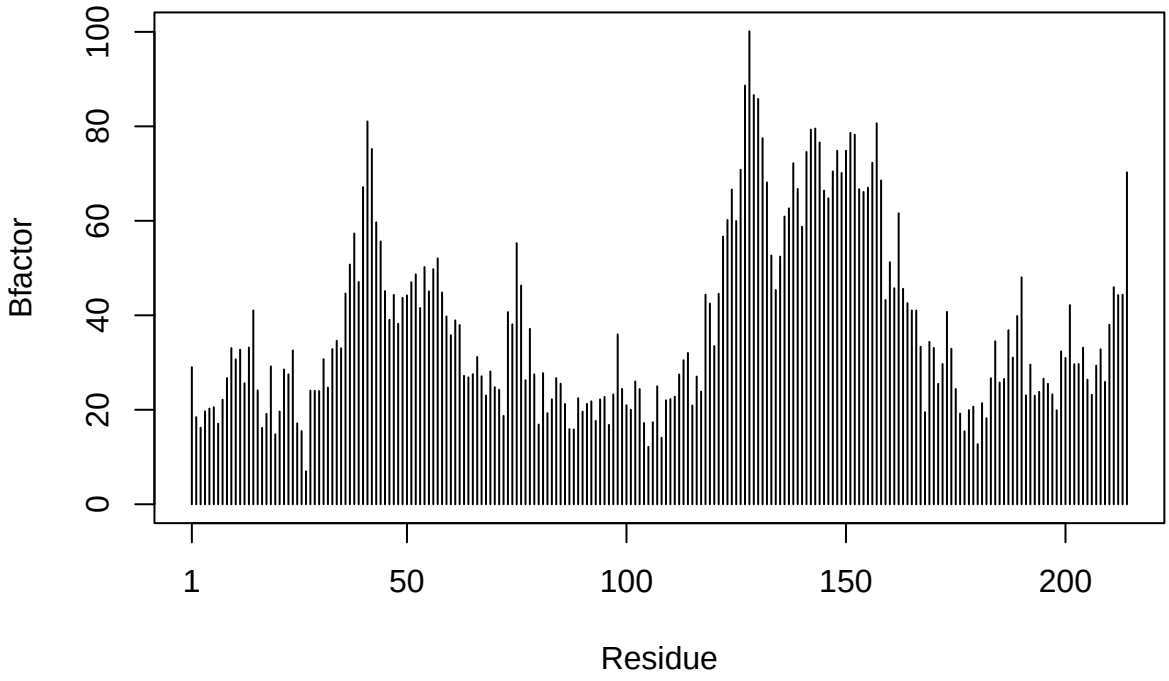
```
# Q2. What does the trim.pdb() function do?
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")
# It searches through the list and keeps the parts of the list in which the chain = "A" and elety = "CA
```

```
# Q3. What input parameter would turn off the marginal black and grey rectangles in the plots and what
s1.b <- s1.chainA$atom$b

s2.b <- s2.chainA$atom$b

s3.b <- s3.chainA$atom$b

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



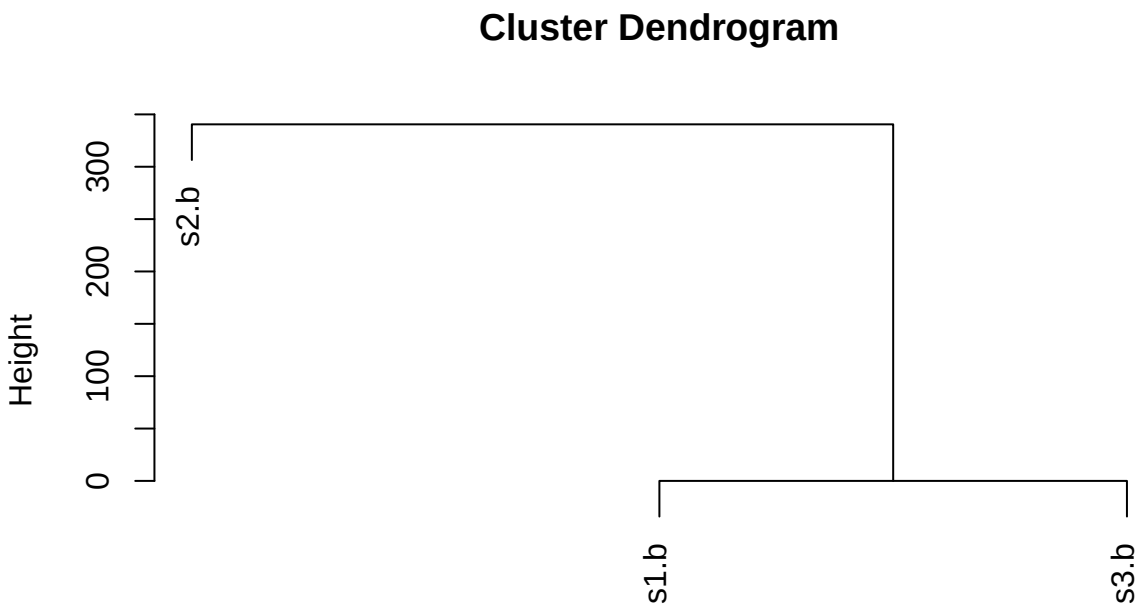

```
# Removing the sse=s1.chainA parameter turns off the marginal black and grey rectangles. They represent
```

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

plotb3(s1.b, typ="h", ylab="Bfactor")
```




```
# A histogram would be a better plot to compare across the different proteins
```

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

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

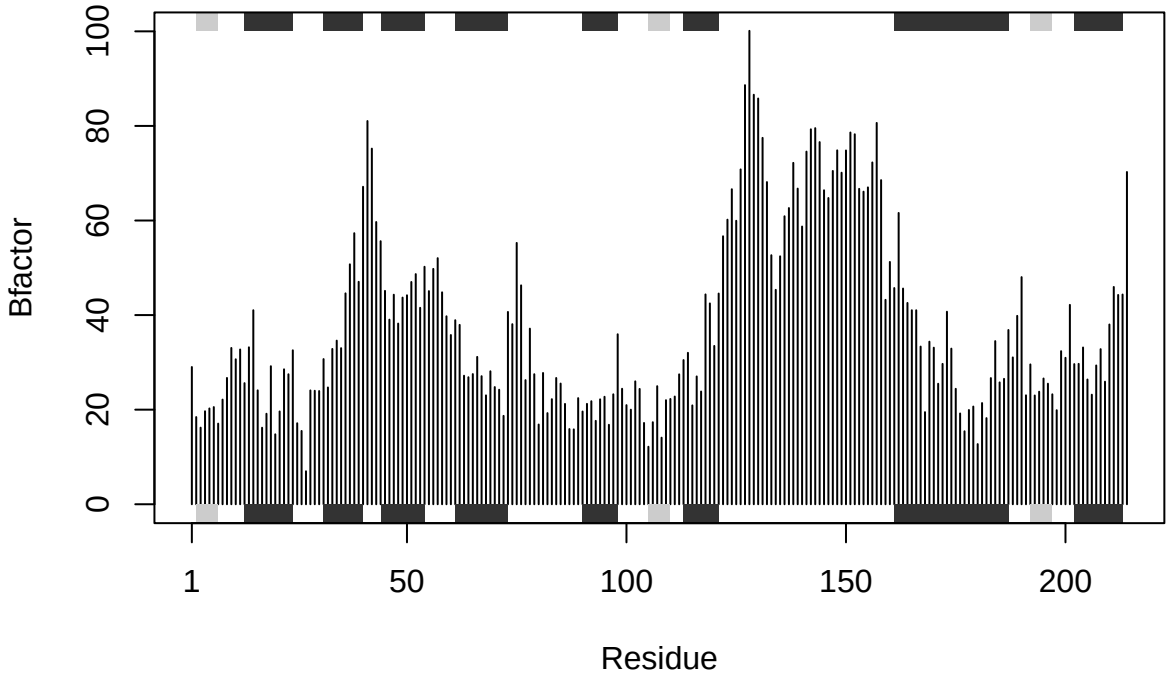



```
# The "4AKE" and "1E4Y" proteins are more similar to each other in their B-factor trends. They both hav
```

```
# Name of the function is analyzeProtein
# The arguments are the name of the protein = x, the chain = y, the elety = z, and the atom = a.

analyzeProtein <- function(x, y, z, a) {
  # Access the protein database for protein x
  s <- read.pdb(x)
  # Access the parts of protein x with the chain y and elety z
  s.chain <- trim.pdb(s, chain = y, elety = z)
  # Access the atom a from the protein x with the chain y and elety z
  s.atom <- s.chain$atom[,a];
  # Plot the histogram of the Bfactor of the atom a from protein x with chain y and elety z
  plotb3(s.atom, sse=s.chain, typ="h", ylab="Bfactor", ylim = c(0, 100))
}
# Example of the function being used
analyzeProtein("4AKE", "A", "CA", "b")
```

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

```
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
## C:\Users\jorda\AppData\Local\Temp\Rtmp4AGDAT/4AKE.pdb exists. Skipping download
```


Bfactor
0
20
40
60
80
100
1
50
100
150
200
Residue