Lab 6 homework

Jazz Zhang (A16149005)

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

```
Warning: package 'bio3d' was built under R version 4.3.1
```

```
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
```

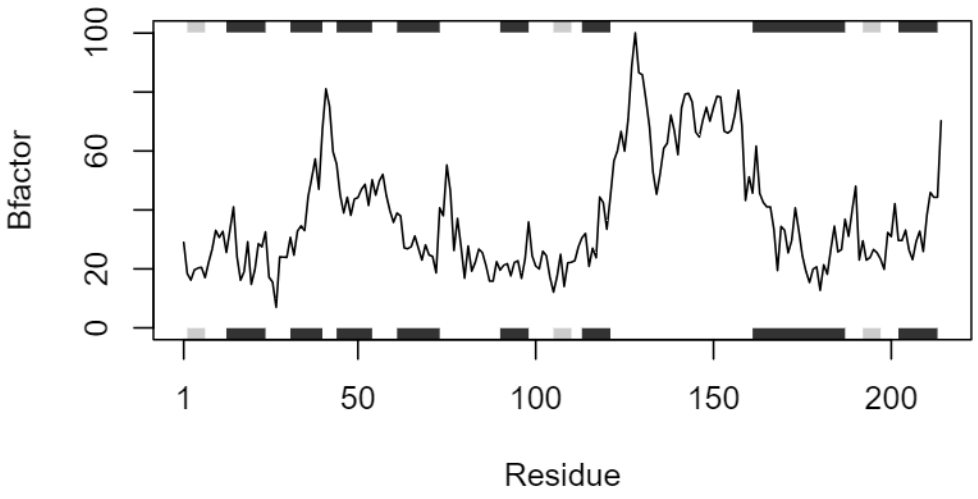
```
class(s1)
```

```
[1] "pdb" "sse"
```

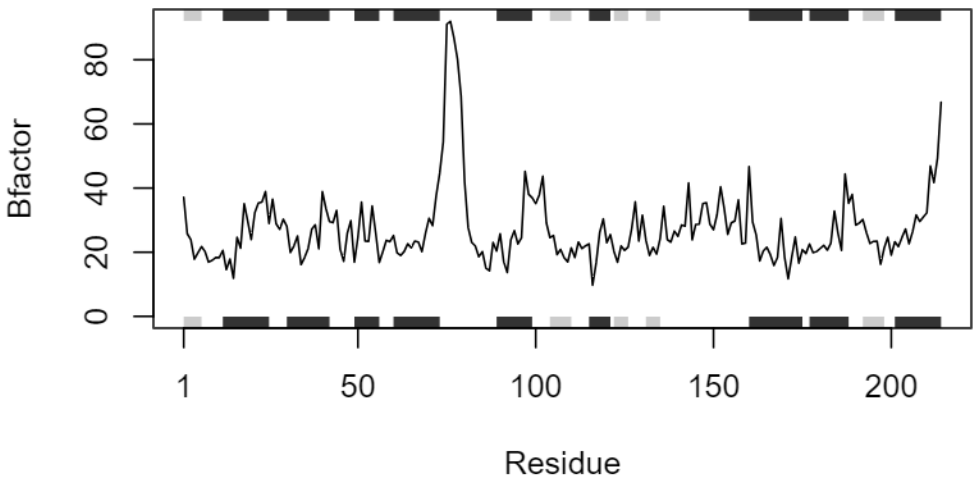
```
?trim.pdb()
```

```
starting httpd help server ... done
```

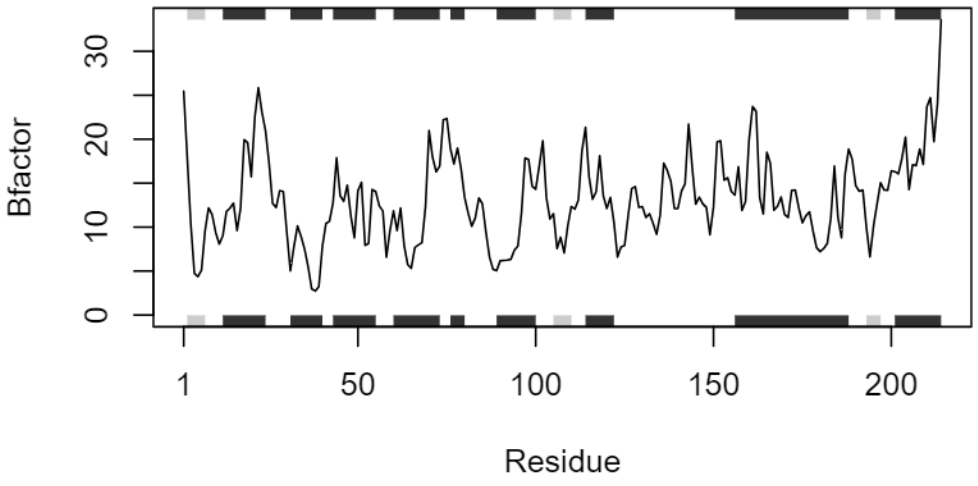
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
s1.plot <- plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```




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




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

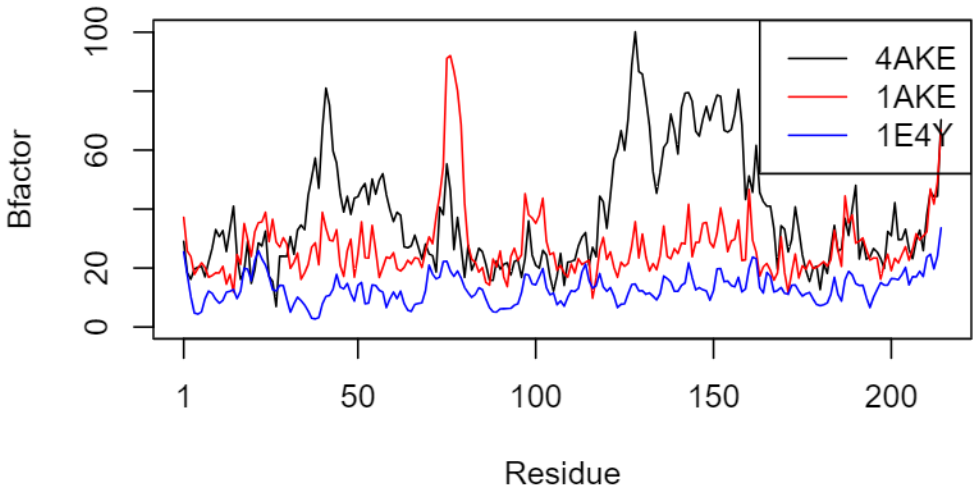


Q1: pdb and sse

Q2: it produce a new smaller PDB object, containing a subset of atoms, from a given larger PDB object, according to input selection (in this case: chain A)

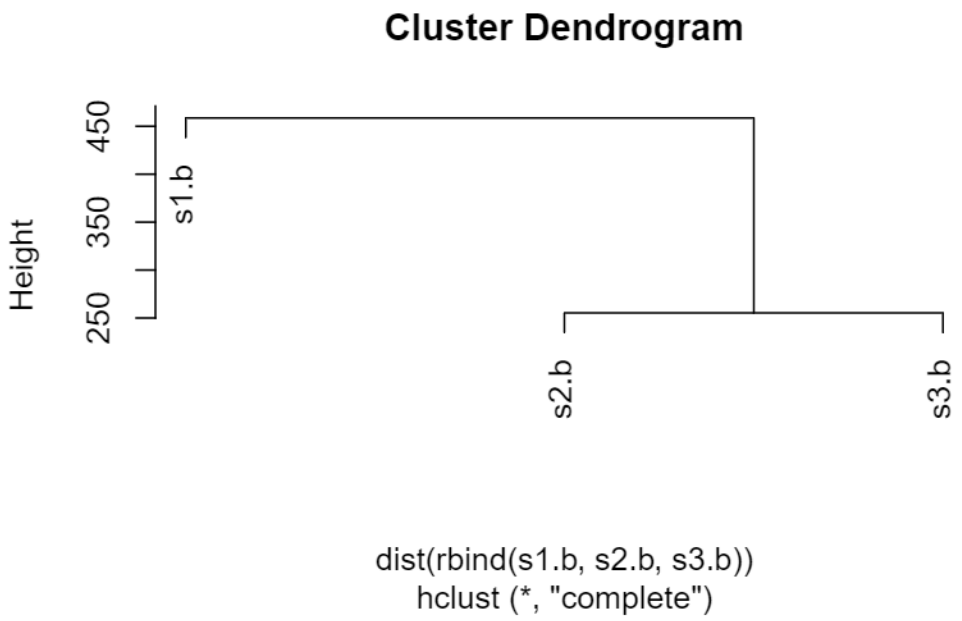
Q3: top and bot (to turn off, both arguments should be set to "FALSE"), they represent secondary structures (alpha helices and beta sheets)

```
# code chunk completed with help from Alex Liu
# Plot the s1 protein
plotb3(s1.b, sse = s1.chainA, typ = "l", ylab = "Bfactor", top=FALSE, bot=FALSE)

# stack s2 and s3 to the plot
lines(s2.b, col = "red")
lines(s3.b, col = "blue")

# add legend
legend("topright", legend = c("4AKE", "1AKE", "1E4Y"), col = c("black", "red", "blue"), lt
```



Q4: Instead of creating 3 separated plots, we can stack the lines representing B-factor in the same plot so it's easier to compare. Also a dendrogram plot could be made to compare similarity between each protein.

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

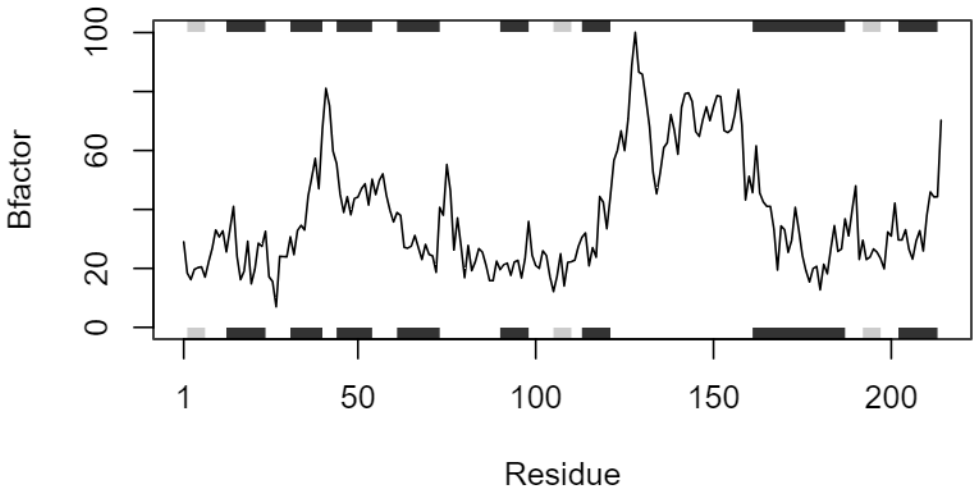


Q5: protein s2 and s3 are similar to each other

```
# function protein() for plotting B-factor of chain A from a give PDB file
protein <- function(PDB){
  s <- read.pdb(PDB) #read pdb files of protein of interest
  s.chainA <- trim.pdb(s, chain="A", elety="CA") # extract chain A from protein
  s.b <- s.chainA$atom$b # extract B-factor of chain A of protein
  plotb3(s.b, sse=s.chainA, typ="l", ylab="Bfactor") # plot B-factor
}

protein("4AKE")
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\jz644\AppData\Local\Temp\Rtmp6ZdToA/4AKE.pdb exists. Skipping download
```

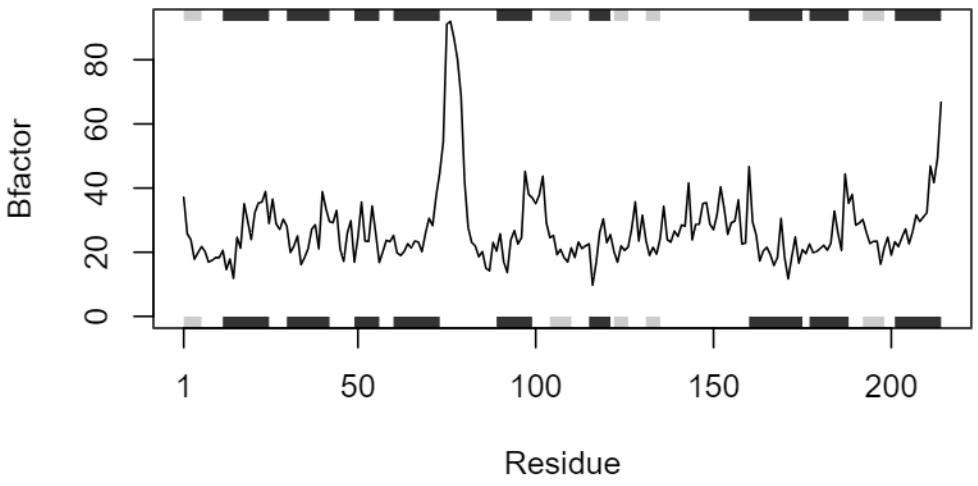



```
protein("1AKE")
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\jz644\AppData\Local\Temp\Rtmp6ZdToA/1AKE.pdb exists. Skipping download
```

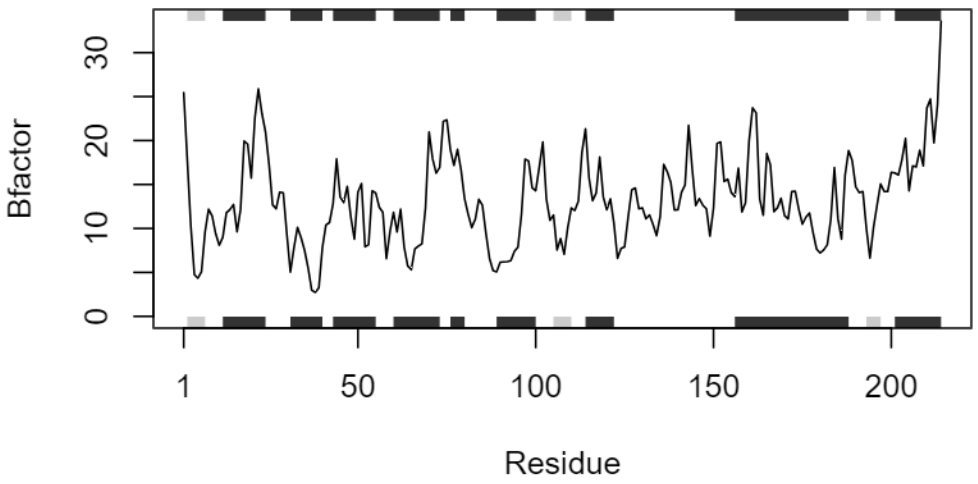
```
   PDB has ALT records, taking A only, rm.alt=TRUE
```




```
protein("1E4Y")
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\jz644\AppData\Local\Temp\Rtmp6ZdToA/1E4Y.pdb exists. Skipping download
```


Bfactor
0
10
20
30
1
50
100
150
200
Residue