Lab6_supplementHW

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2023-05-01

```
# Can you improve this analysis code?
library(bio3d)
s1 <- read.pdb("4AKE")  # kinase with drug
```

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

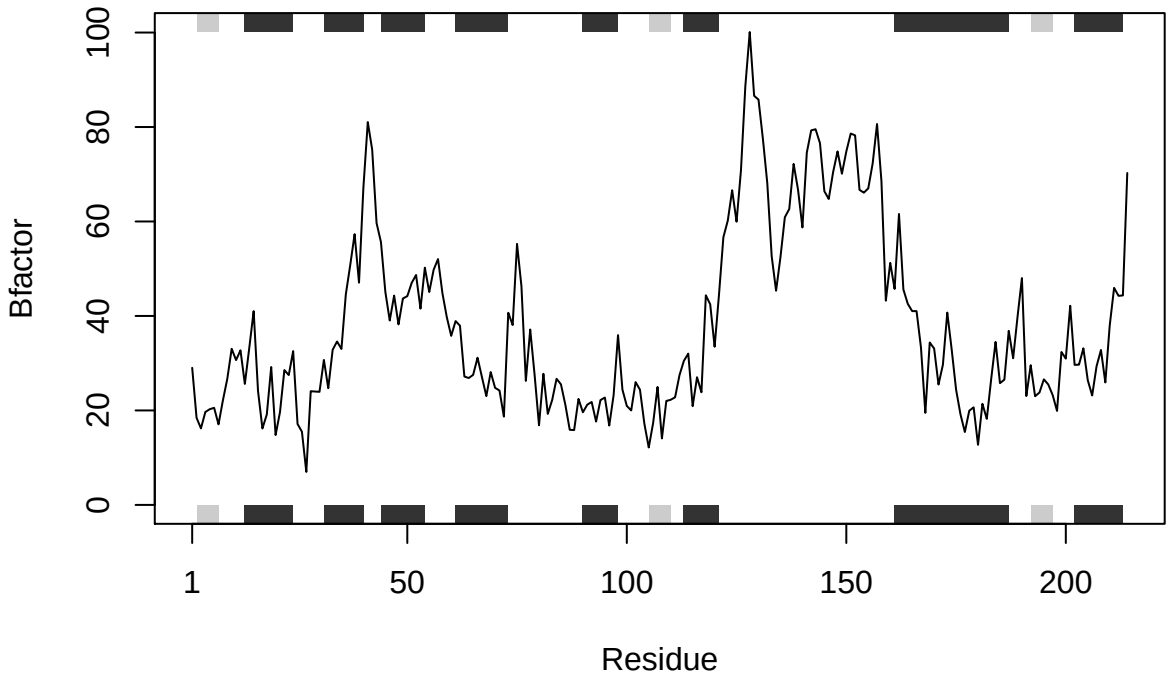
```
s2 <- read.pdb("1AKE")  # kinase no drug
```

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

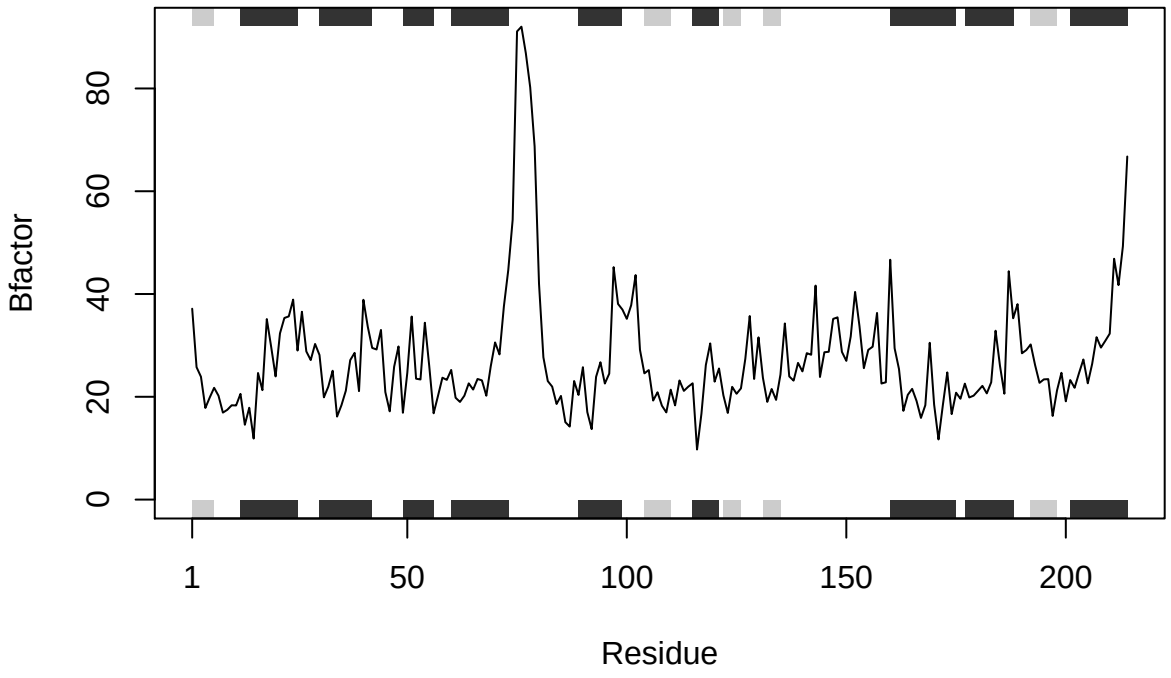
```
s3 <- read.pdb("1E4Y")  # kinase with drug
```

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

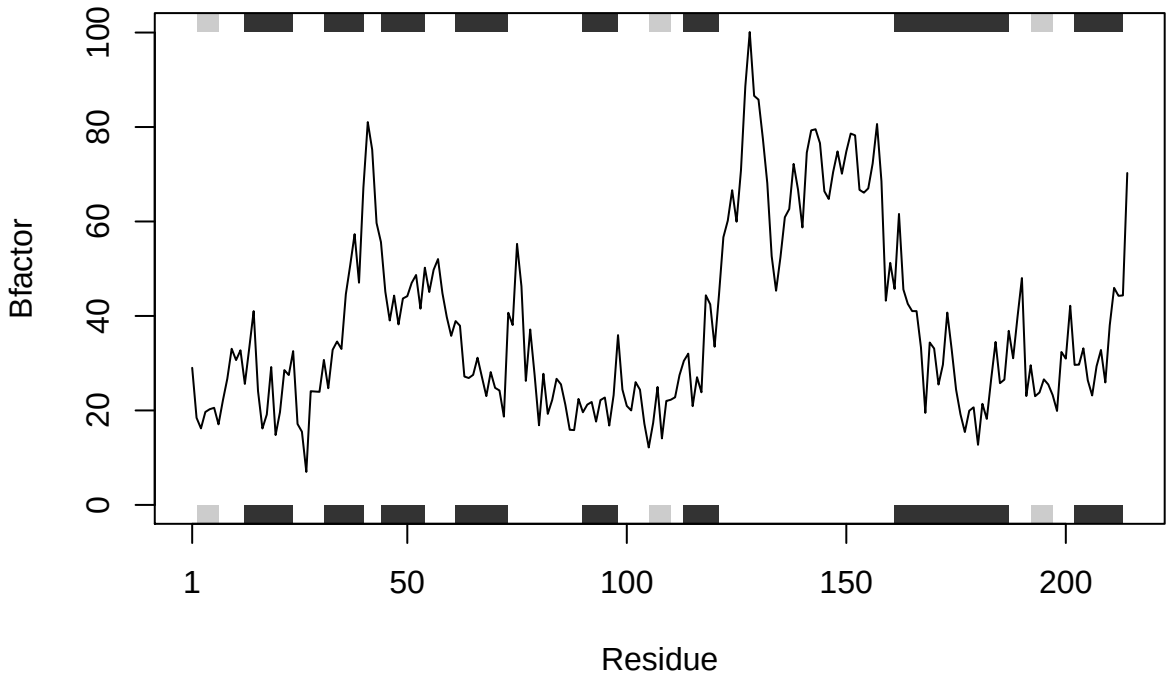
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```




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




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



Q1.

read.pdb() reads a Protein Data Bank (PDB) coordinate file and returns a list of class "pdb" with 8 components.

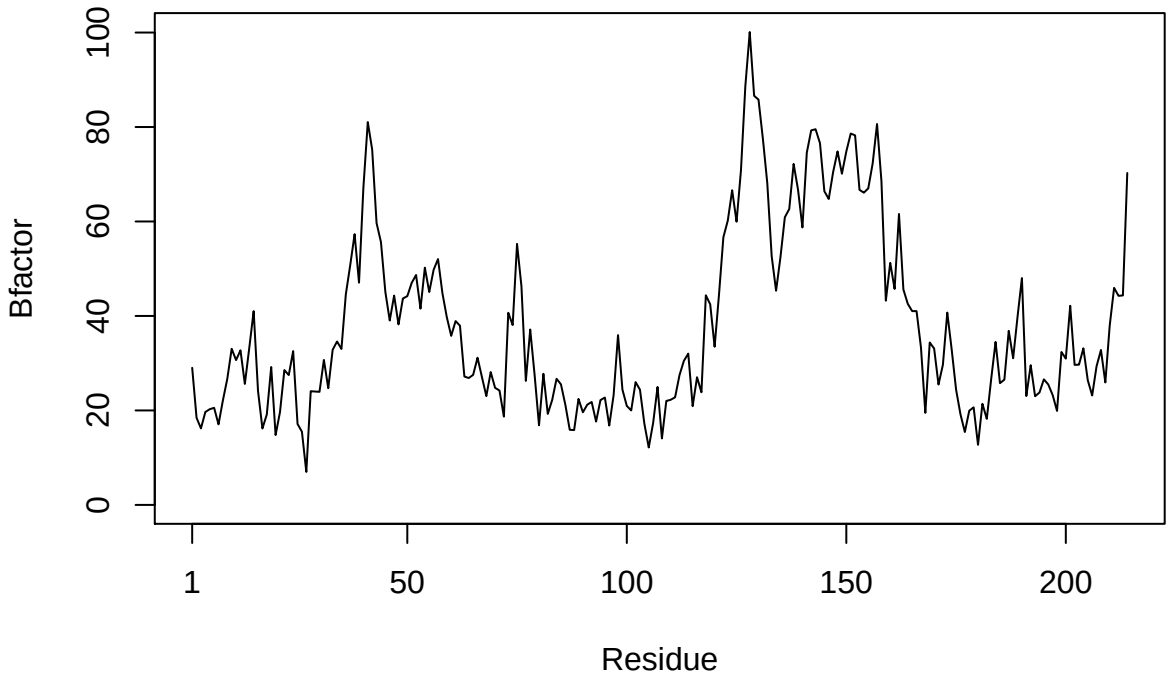
Q2.

trim.pdb() trims a pdb object to a subset of atoms.

Q3.

Deleting "sse=s1.chainA" would turn off the marginal black and grey rectangles. "sse" represents secondary structure object as returned from read.pdb.

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



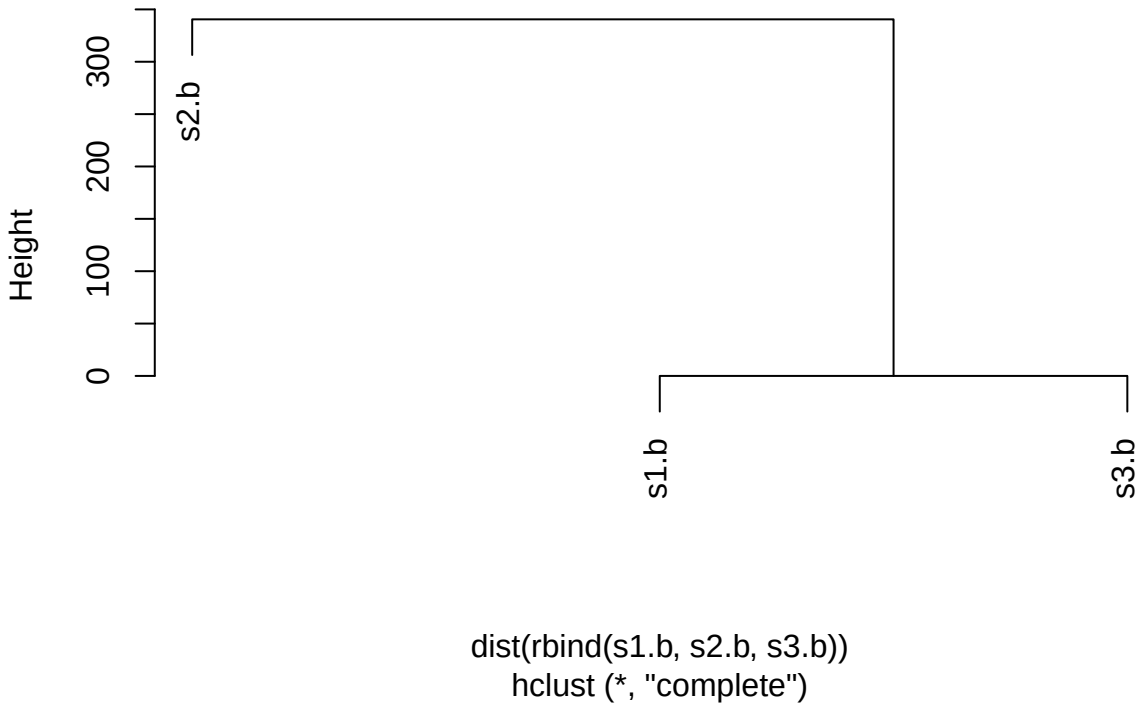
> Q4.

A plot that combines the above plots together but shows them in different colors.

Q5.

Protein 1 and protein 3 are more similar to each other.

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



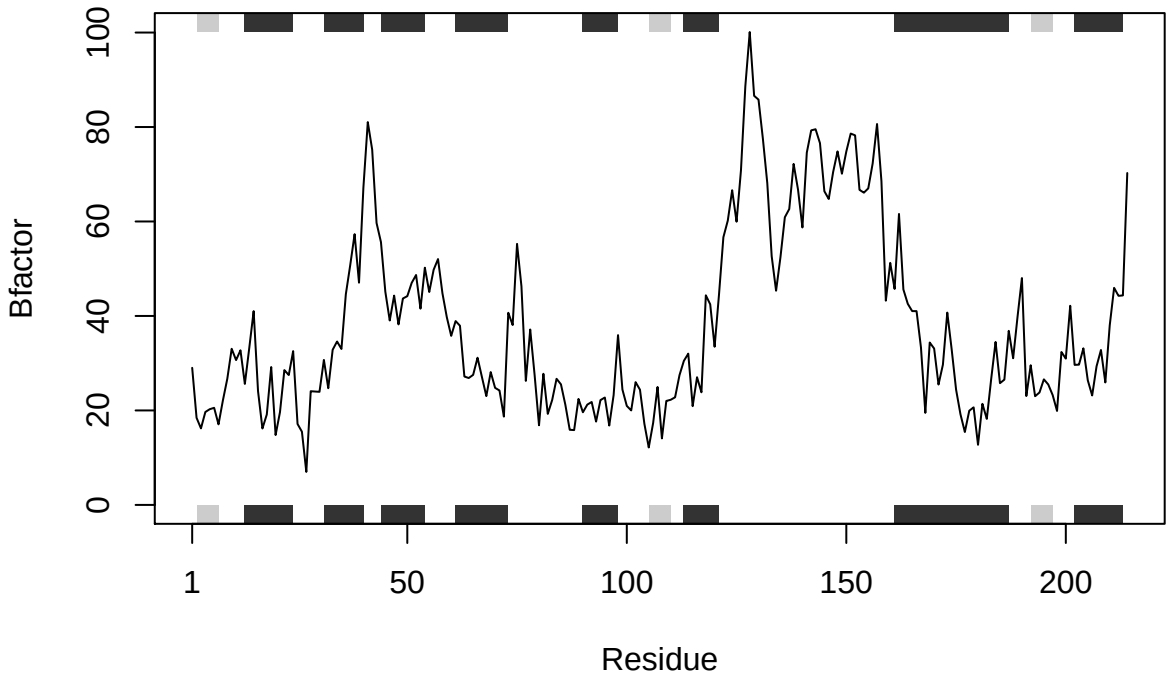
Q6.

```
#This is a function that takes a pdb file name as input and generate a plot as the output.
analysis_code <- function(pdb){
  #Input a pdb file name with quotation marks, e.g. pdb <- "4AKE"
  protein <- read.pdb(pdb)
  protein.chainA <- trim.pdb(protein, chain="A", elety="CA")
  protein.b <- protein.chainA$atom$b
  #Generate a plot as the output
  plotb3(protein.b, sse=protein.chainA, typ="l", ylab="Bfactor")
}

analysis_code("4AKE")
```

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

## Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/3v/
## bfp1dcl15f146gpllv3mfl300000gn/T//RtmpVxwfV0/4AKE.pdb exists. Skipping download
```

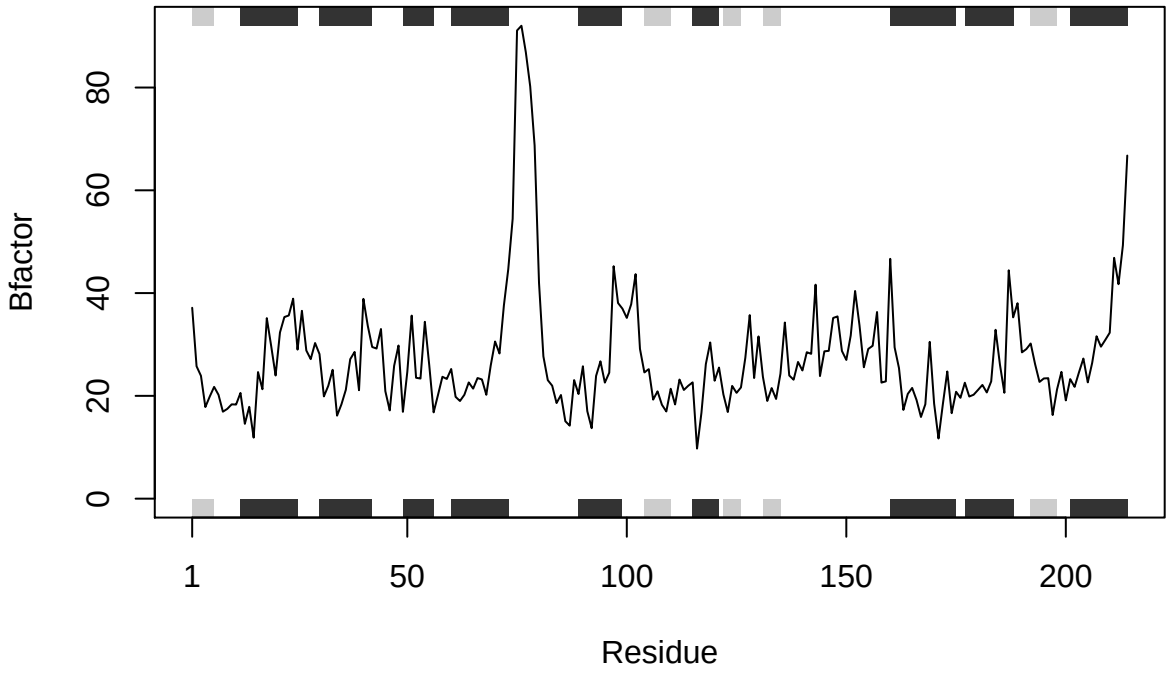



```
analysis_code("1AKE")
```

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

```
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/3v/
## bfp1dcl15f146gpllv3mfl300000gn/T//RtmpVxwfV0/1AKE.pdb exists. Skipping download
```

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



```
analysis_code("1E4Y")
```

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

```
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/3v/
## bfp1dcl15f146gpllv3mfl300000gn/T//RtmpVxwfV0/1E4Y.pdb exists. Skipping download
```