HW06

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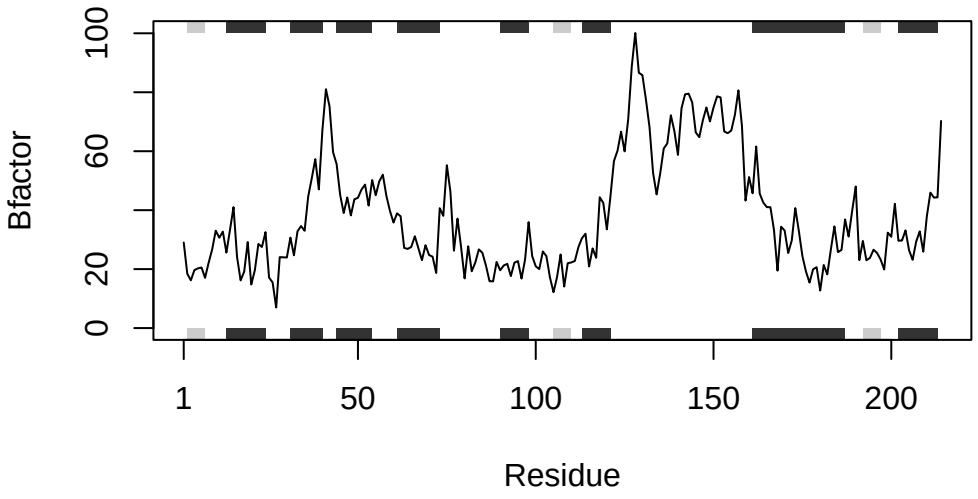
```
# install.packages("bio3d") in console first, then library
library(bio3d)

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

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

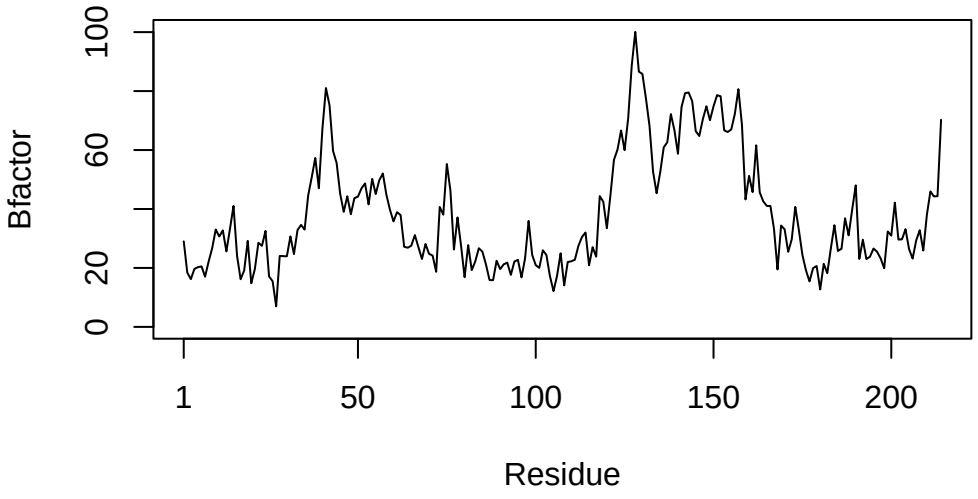
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



```
#Q1. What type of object is returned from the read.pdb() function?
# it returns a pdb file, which is a list containing 8 elements.

# Q2. What does the trim.pdb() function do?
# the function produces a new smaller PDB object, containing a subset of atoms, from a giv
```

```
#Q3. What input parameter would turn off the marginal black and grey rectangles in the plo
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor", top = FALSE, bot = FALSE)
```



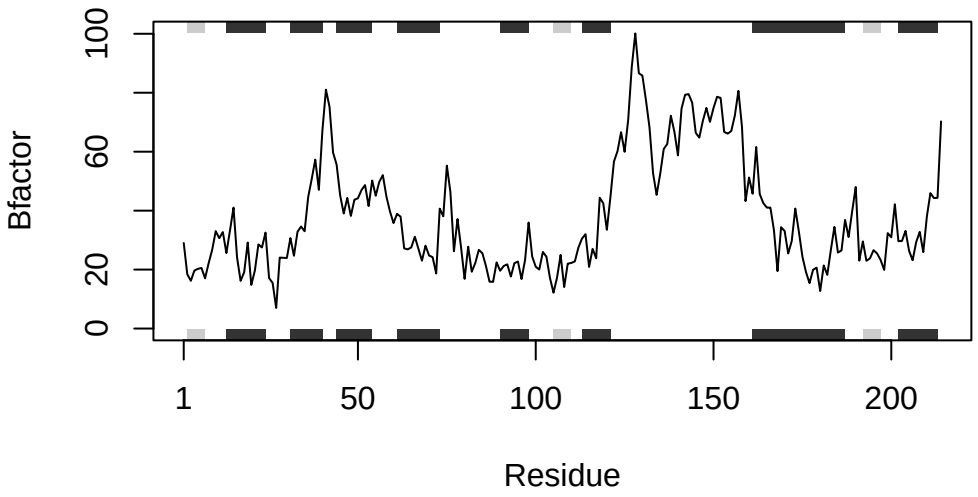

```
# top and bot. set both argument to FALSE to turn off the marginal black and grey rectangl
```

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

```
  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose =
FALSE): /var/folders/_2/rqml3ksd3l999_13212061zc0000gn/T//RtmpfVaTSc/4AKE.pdb
exists. Skipping download
```

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




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

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

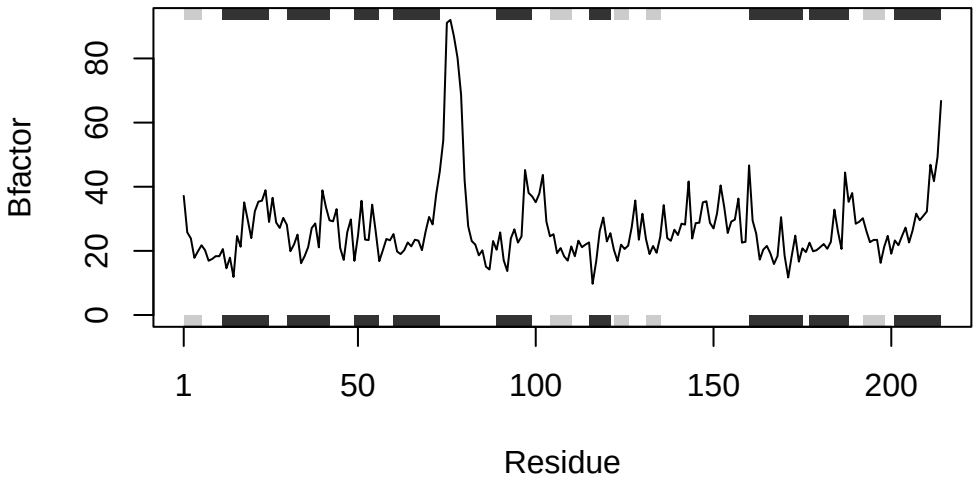
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

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

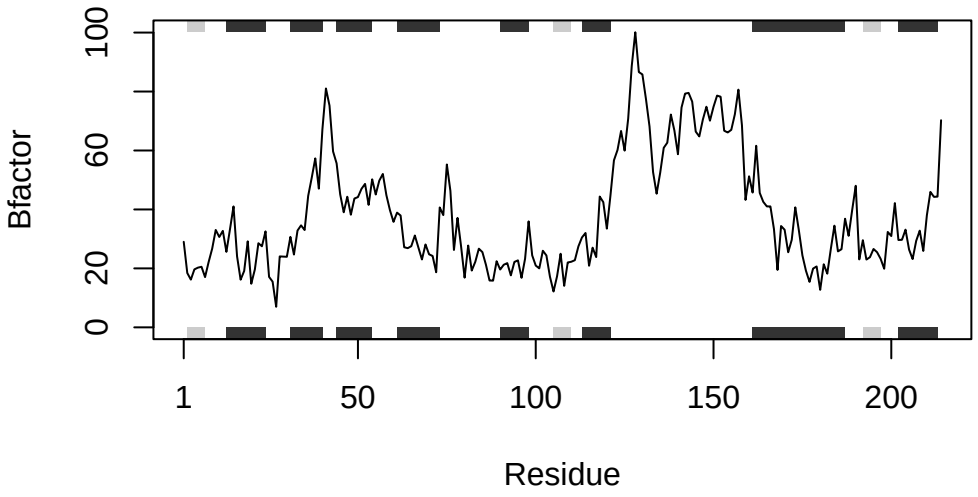
```
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")

s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
```

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

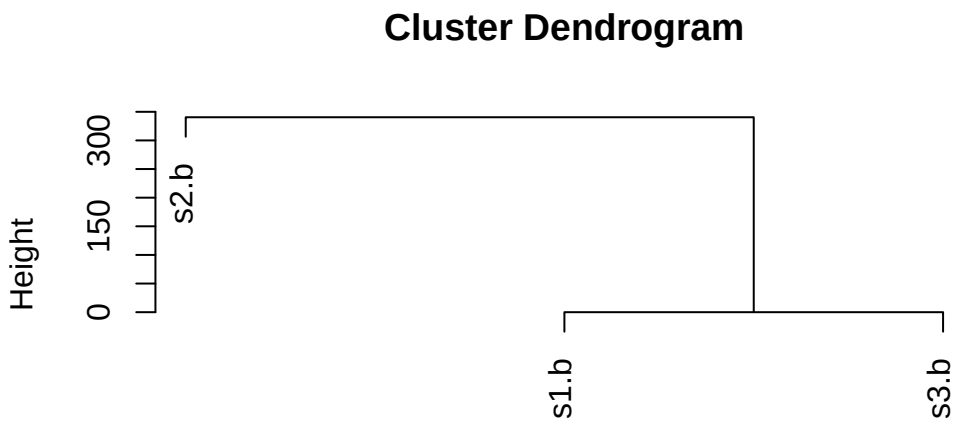



```
plotb3(s3.b, sse=s3.chainA, typ="l", ylab="Bfactor")
```




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

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



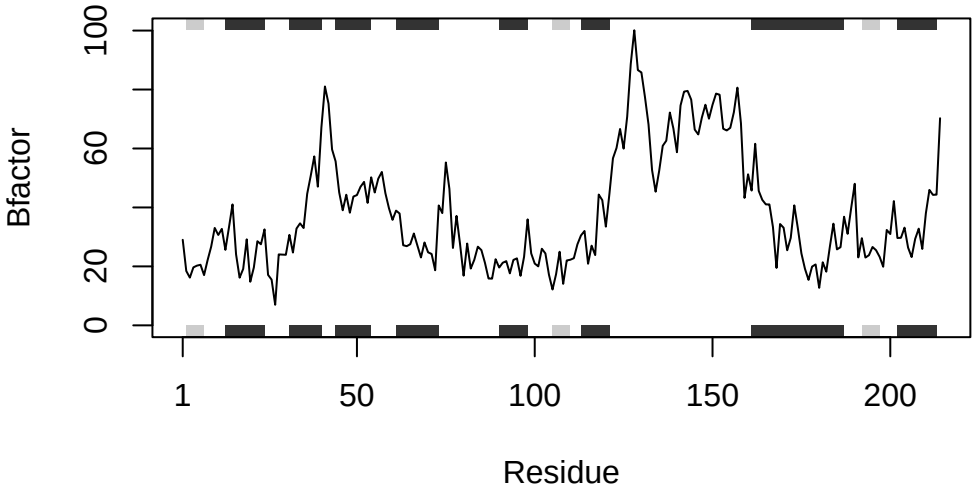

```
#Q5. Which proteins are more similar to each other in their B-factor trends. How could you
# protein 1 and protein 3 (4AKE and 1E4Y)
```

```
#Generalize the code (write a funcrion)
plot_pdb <- function(x){
  s <- read.pdb(x)
  s.chainA <- trim.pdb(s, chain="A", elety="CA")
  s.b <- s.chainA$atom$b
  plotb3(s.b, sse=s.chainA, typ="l", ylab="Bfactor")
}

plot_pdb("4AKE")
```

```
  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose =
FALSE): /var/folders/_2/rqml3ksd3l999_132l2061zc0000gn/T//RtmpfVaTSc/4AKE.pdb
exists. Skipping download
```


Bfactor
0
20
60
100
1
50
100
150
200
Residue