

# Lab 6 Homework: R Functions

Clarissa Savko (PID:A69028482)

```
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

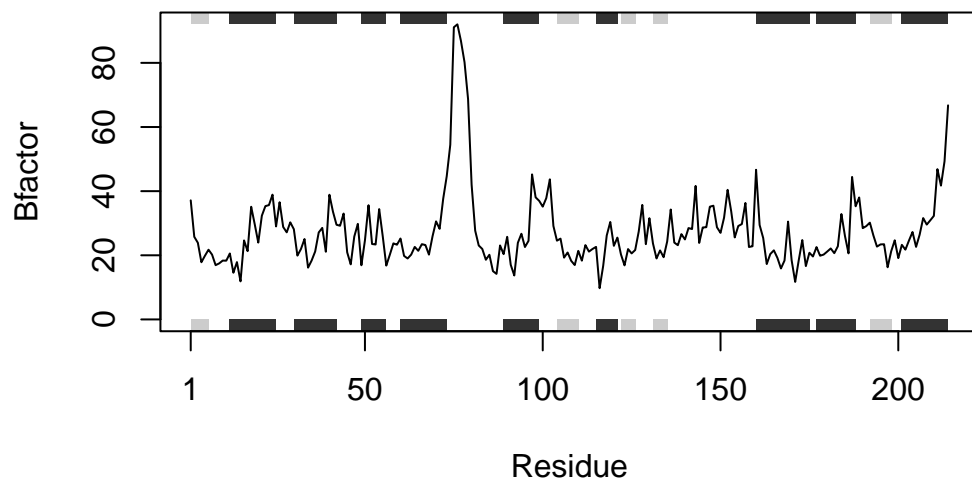
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

Note: Accessing on-line PDB file

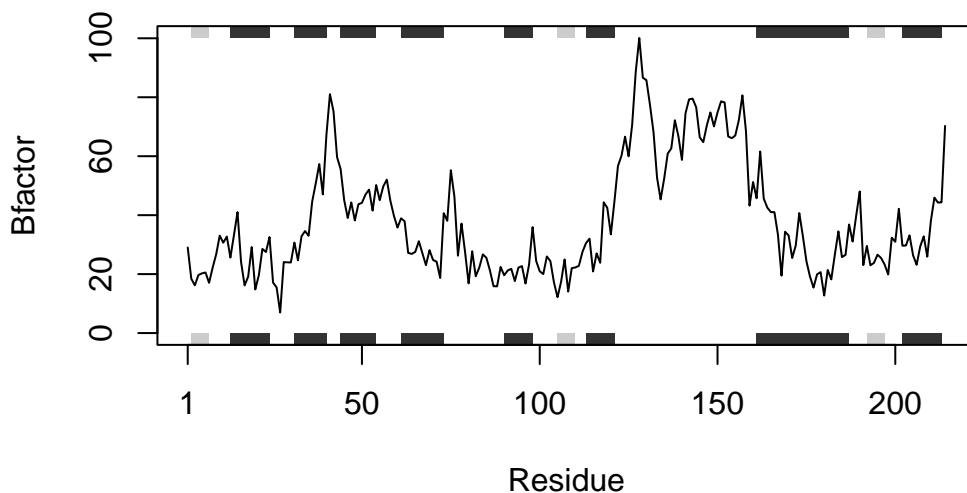
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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



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



`read.pdb()` returns a list. `trim.pdb()` subsets a desired portion of the PDB object `top=FALSE` and `bot=false` would remove the marginal rectangles at the top and bottom of the plot. They represent the secondary structure elements of alpha helices and beta strands. Points rather than lines would make a better plot so you can see the individual data points.

```
library(bio3d)
s1 <- read.pdb("4AKE") # kinase with drug
```

Note: Accessing on-line PDB file

Warning in `get.pdb(file, path = tempdir(), verbose = FALSE)`:  
C:\Users\clari\AppData\Local\Temp\RtmpSEP8m8\4AKE.pdb exists. Skipping download

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

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):  
C:\Users\clari\AppData\Local\Temp\RtmpSEP8m8\1AKE.pdb exists. Skipping download

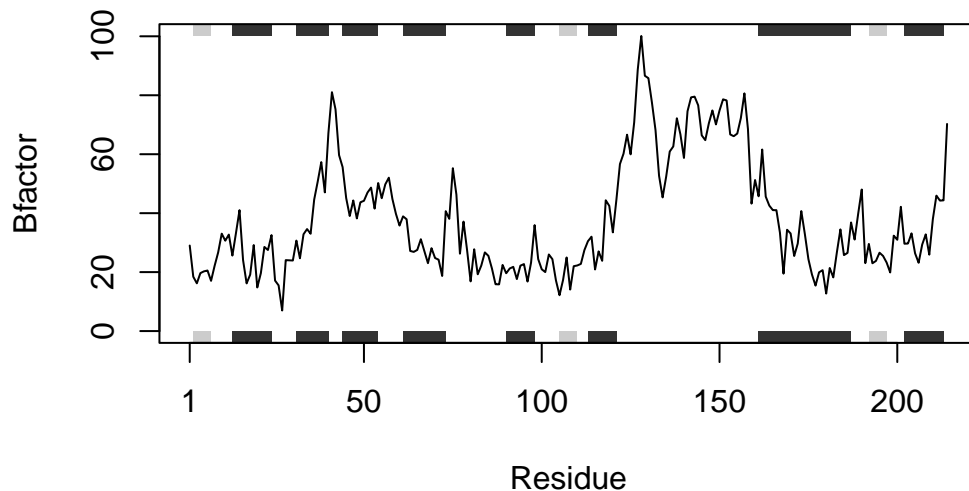
PDB has ALT records, taking A only, rm.alt=TRUE

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

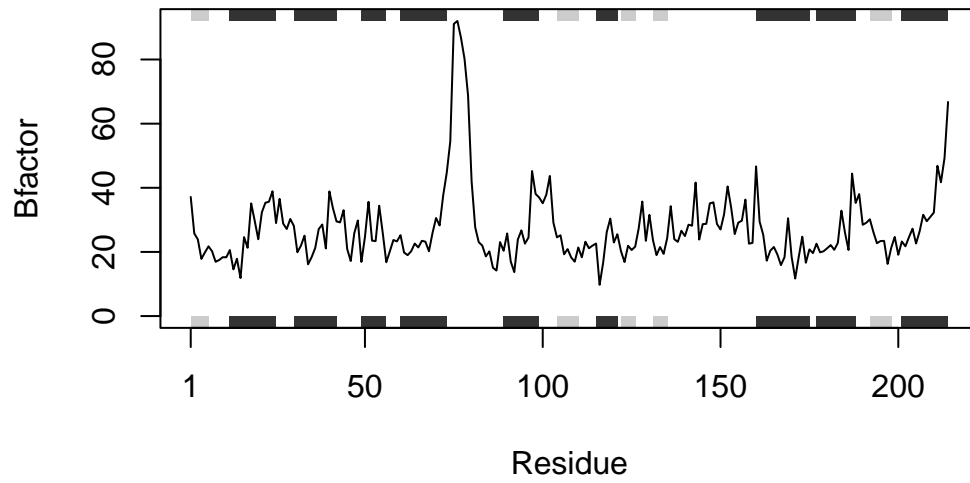
Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):  
C:\Users\clari\AppData\Local\Temp\RtmpSEP8m8\1E4Y.pdb exists. Skipping download

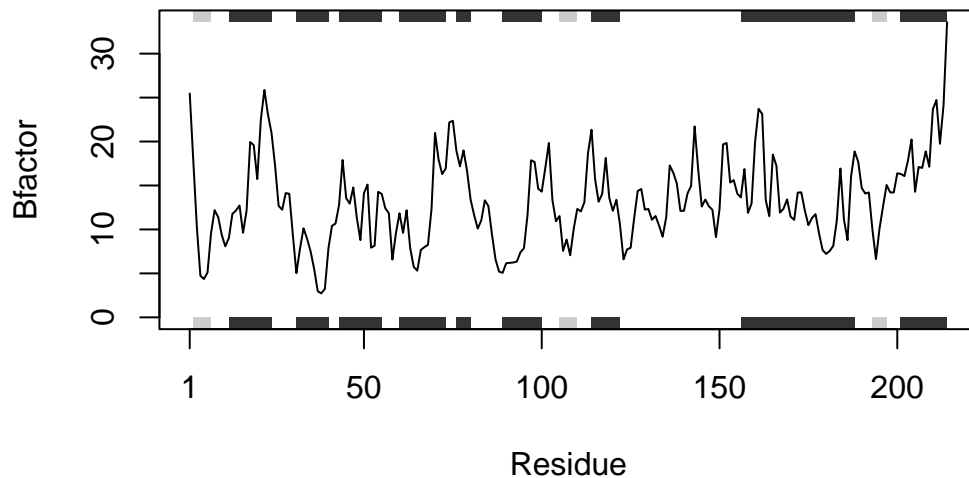
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")  
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")  
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")  
s1.b <- s1.chainA$atom$b  
s2.b <- s2.chainA$atom$b  
s3.b <- s3.chainA$atom$b  
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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



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



```
library(bio3d)
s1 <- read.pdb("4AKE") # kinase with drug
```

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):  
C:\Users\clari\AppData\Local\Temp\RtmpSEP8m8\4AKE.pdb exists. Skipping download

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

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):  
C:\Users\clari\AppData\Local\Temp\RtmpSEP8m8\1AKE.pdb exists. Skipping download

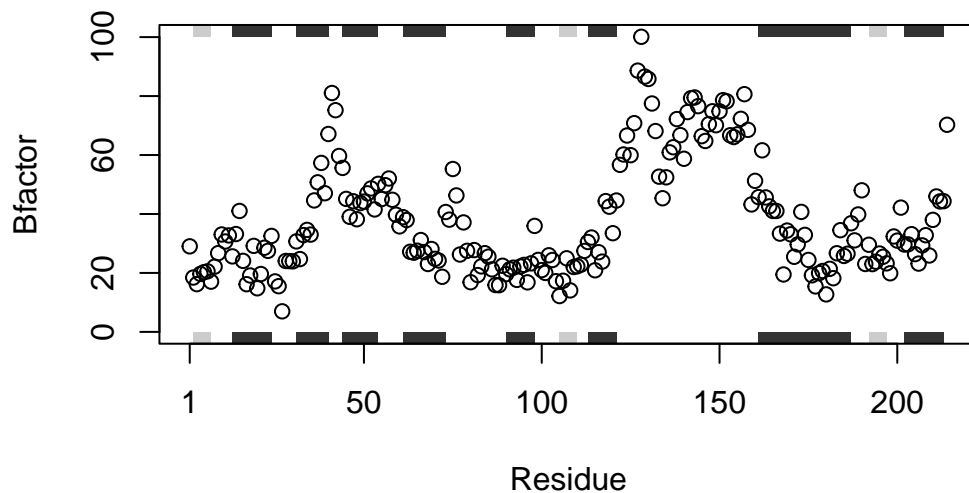
PDB has ALT records, taking A only, rm.alt=TRUE

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

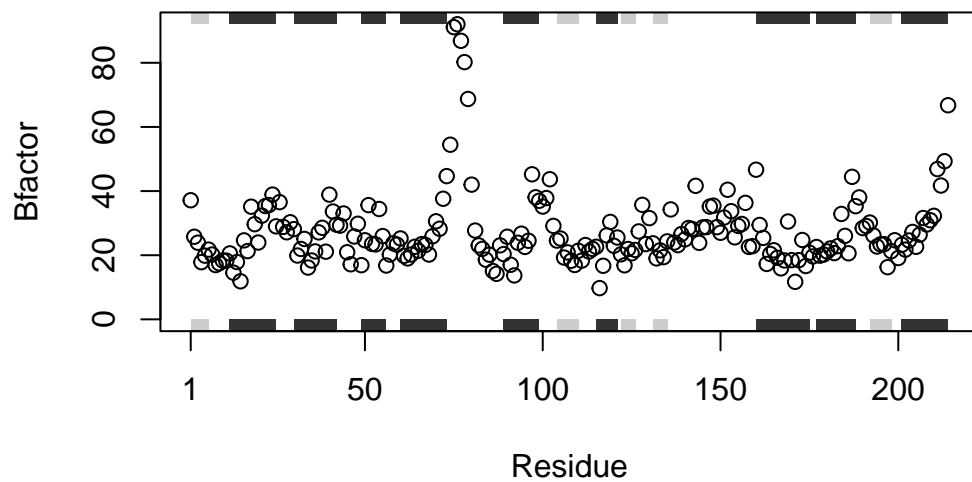
Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):  
C:\Users\clari\AppData\Local\Temp\RtmpSEP8m8\1E4Y.pdb exists. Skipping download

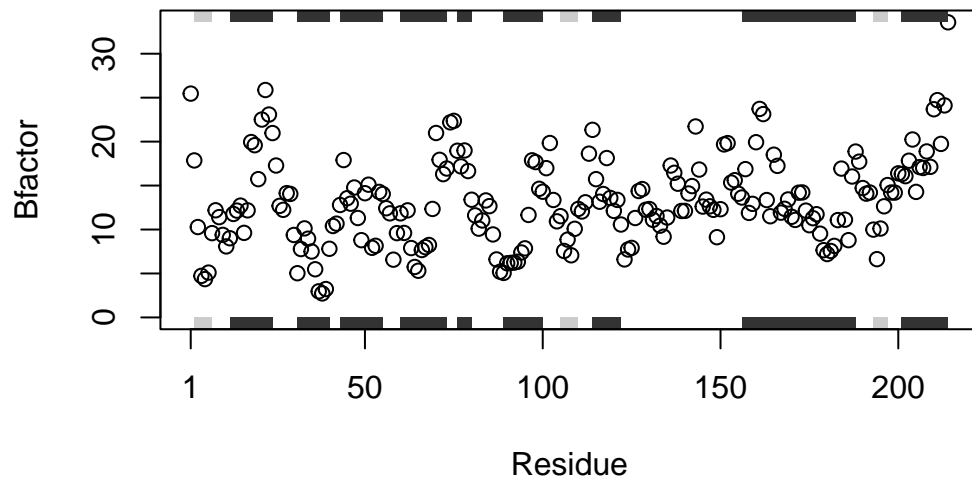
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")  
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")  
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")  
s1.b <- s1.chainA$atom$b  
s2.b <- s2.chainA$atom$b  
s3.b <- s3.chainA$atom$b  
plotb3(s1.b, sse=s1.chainA, typ="p", ylab="Bfactor")
```



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

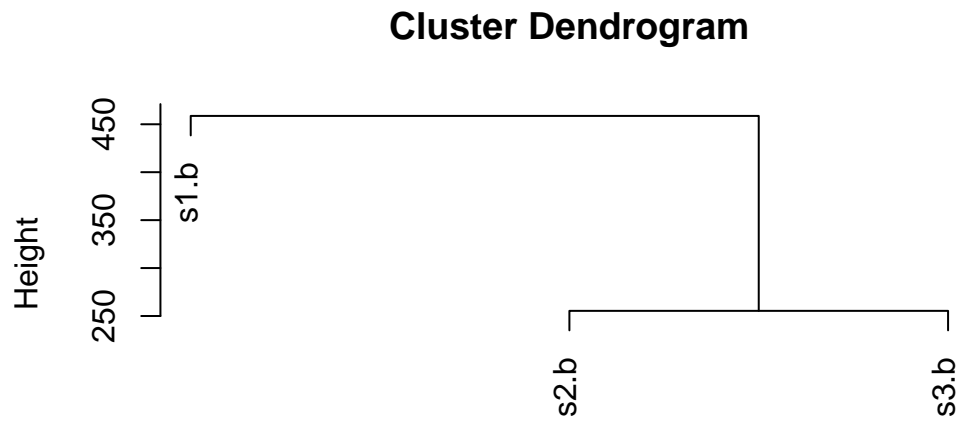


```
plotb3(s3.b, sse=s3.chainA, typ="p", ylab="Bfactor")
```





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



```
dist(rbind(s1.b, s2.b, s3.b))  
hclust (*, "complete")
```