

Lab06 part II

WBray

```
# 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

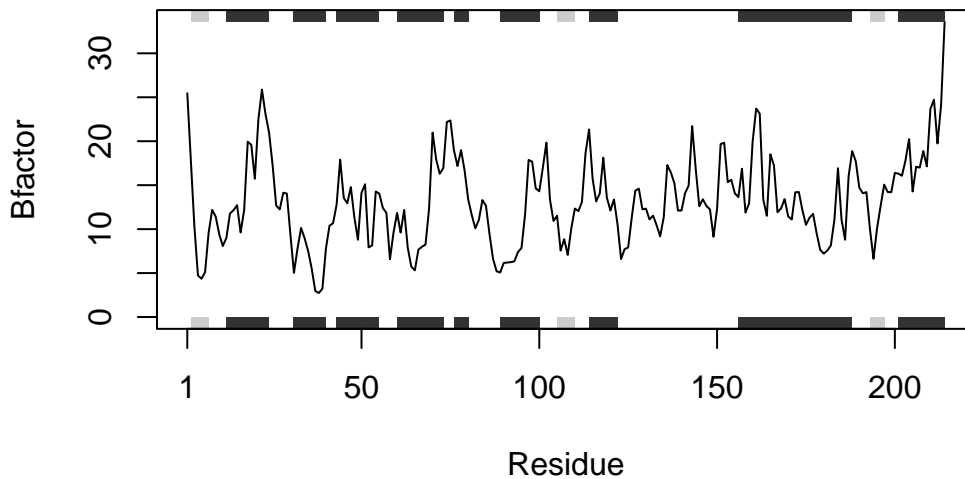
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")  
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")  
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")  
s1.b <- s1.chainA$atom$b  
s2.b <- s2.chainA$atom$b  
s3.b <- s3.chainA$atom$b  
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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



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

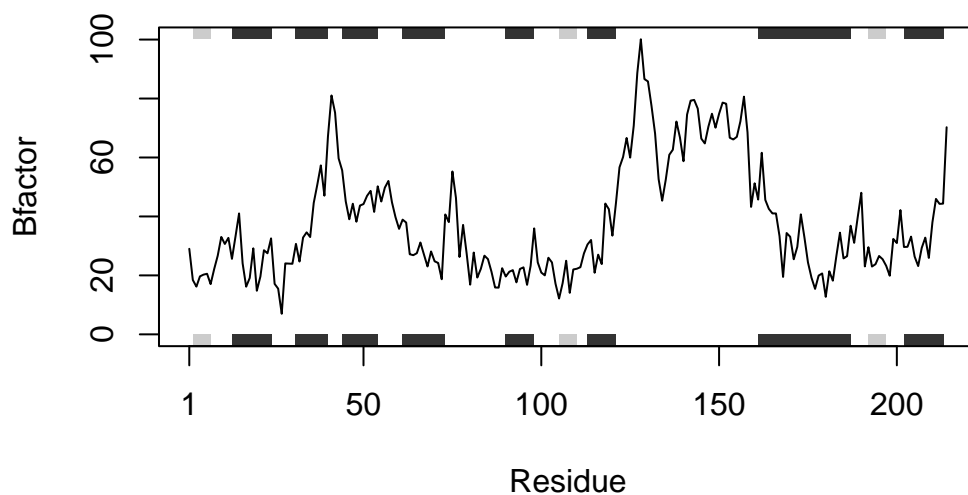


```
#generating a function to collapse above example; calling bio3d library, using the .pdb read
funcy <- function(pID){
  library(bio3d)
  s <- read.pdb(pID)
  s.ChainA <- trim.pdb(s, chain = "A", elety = "CA")
  s.b <- s.ChainA$atom$b
  plotb3(s.b, sse=s.ChainA, typ="l", ylab="Bfactor")
}
```

```
#concatinating a vector of the protein input, running "funcy" function above on input sequen
#\ warning: false
seq_vec <- c("4AKE", "1AKE", "1E4Y")
sapply(seq_vec, funcy)
```

Note: Accessing on-line PDB file

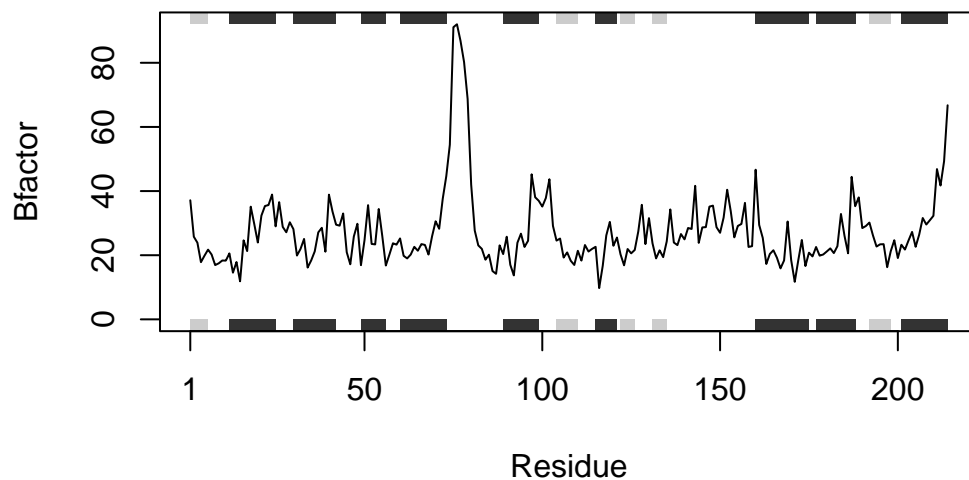
```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\MOTZU~1\AppData\Local\Temp\Rtmp0Q7Lbm\4AKE.pdb exists. Skipping
download
```



Note: Accessing on-line PDB file

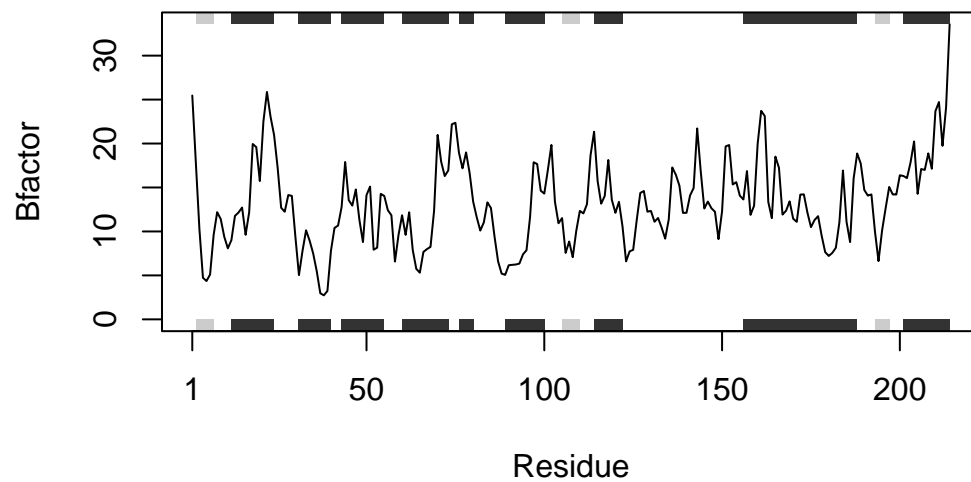
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\MOTZU~1\AppData\Local\Temp\Rtmp0Q7Lbm\1AKE.pdb exists. Skipping
download

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



Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\MOTZU~1\AppData\Local\Temp\Rtmp0Q7Lbm\1E4Y.pdb exists. Skipping
download



\$`4AKE`
NULL

\$`1AKE`
NULL

\$`1E4Y`
NULL