

# HW Class 06

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##B # Can you improve this analysis code? Q6.

```
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

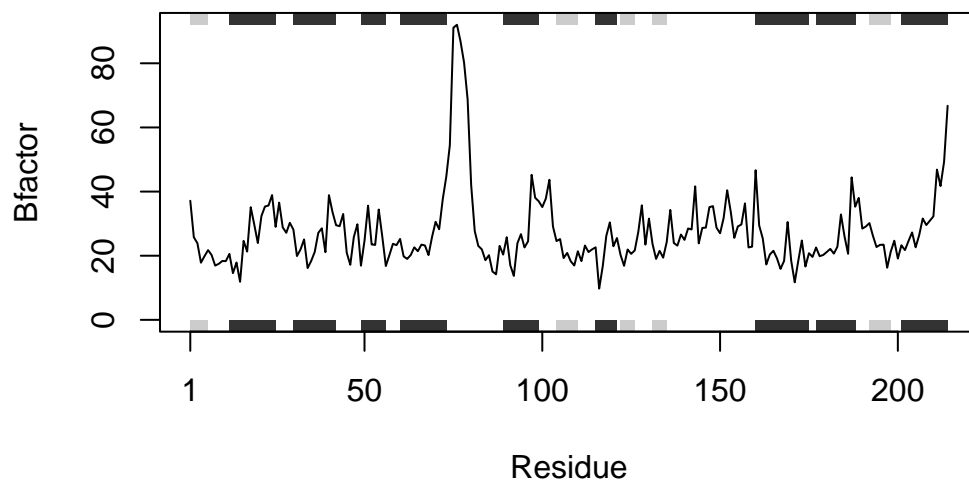
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

Note: Accessing on-line PDB file

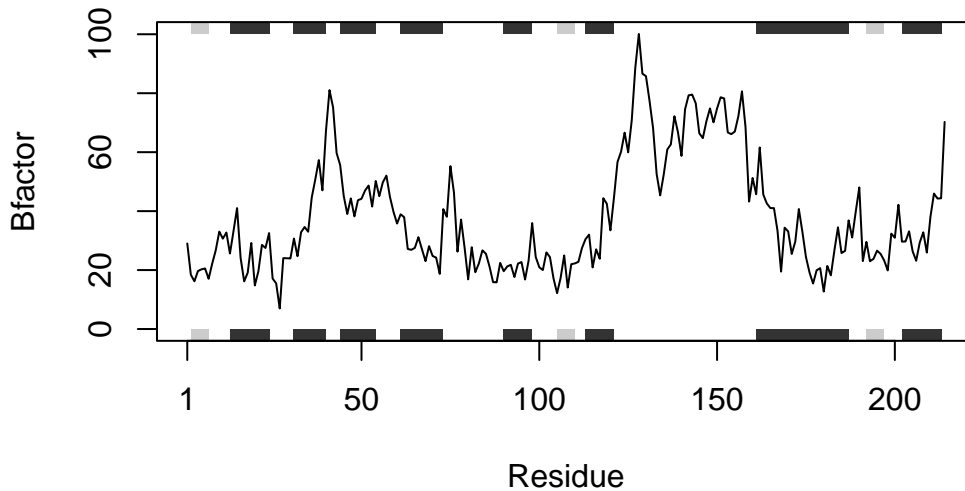
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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



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



##Solving process:

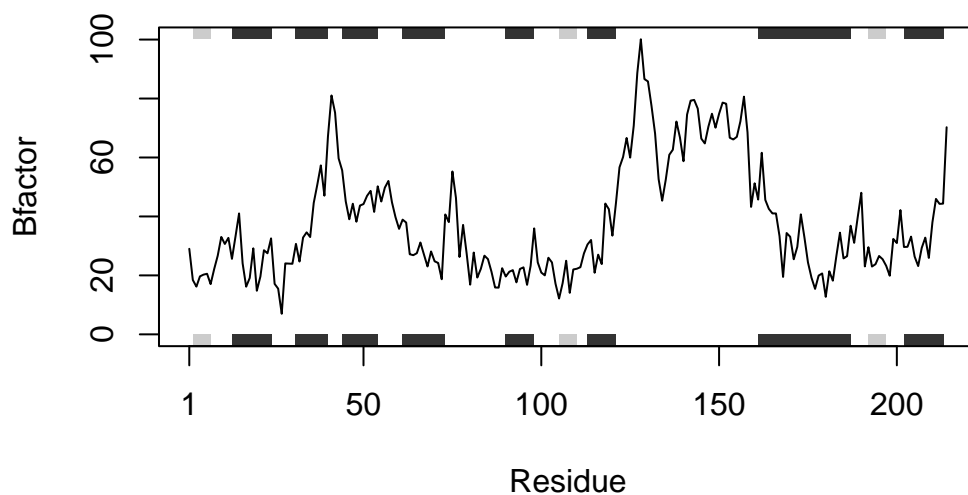
```
#First make a vector list of pdb to be processed and plotted
pdb_id <- c("4AKE", "1AKE", "1E4Y")
```

```
plotfunc <- function(pdb_id){ #name the function and use the function on pdb_id
  step1 <- read.pdb(pdb_id) #Step 1 read each pdb_id
  step2 <- trim.pdb(step1, chain="A", elety="CA") #Step 2 trim the read pdb in step 1
  step3 <- step2$atom$b #Step 3 select the data to be plotted
  plotb3(step3, sse=step2, typ="l", ylab="Bfactor") #Plot
}
```

```
lapply(pdb_id, plotfunc) #apply the defined function "plotfunc" onto the vector list of pdb_id
```

Note: Accessing on-line PDB file

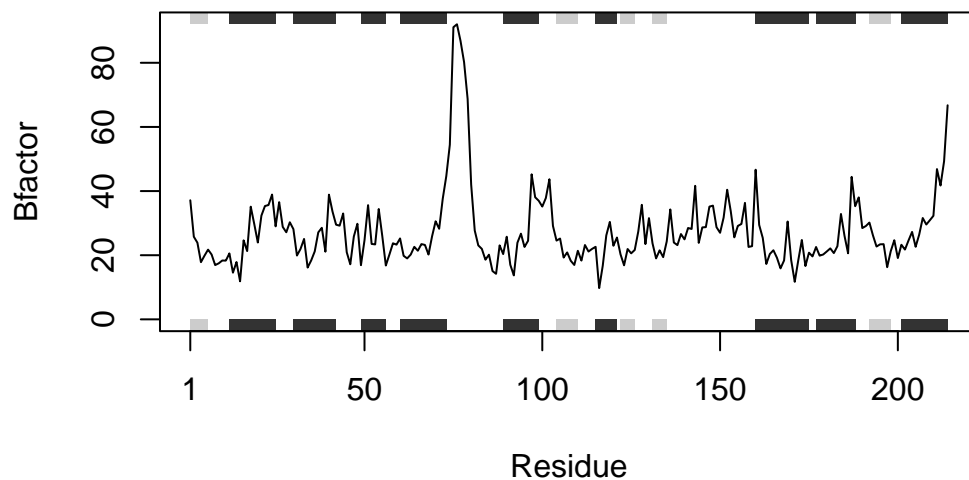
```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/5j/c5tk4s8x0h55tjhjchdchws40000gn/T//RtmpHe9KmM/4AKE.pdb exists.
Skipping download
```



Note: Accessing on-line PDB file

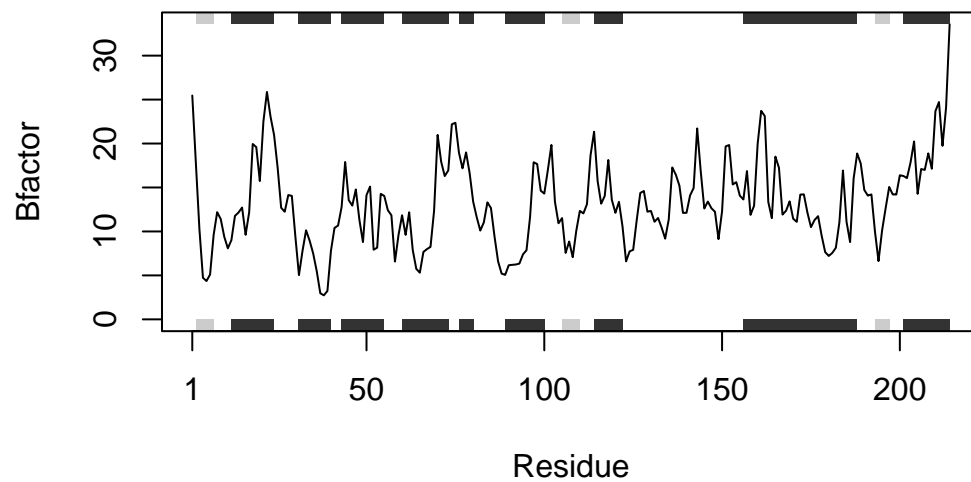
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):  
/var/folders/5j/c5tk4s8x0h55tjhjchdchws40000gn/T//RtmpHe9KmM/1AKE.pdb exists.  
Skipping download

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):  
/var/folders/5j/c5tk4s8x0h55tjhjchdchws40000gn/T//RtmpHe9KmM/1E4Y.pdb exists.  
Skipping download



[[1]]  
NULL

[[2]]  
NULL

[[3]]  
NULL