

HW6

Youn Soo Na (PID:A17014731)

```
# 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

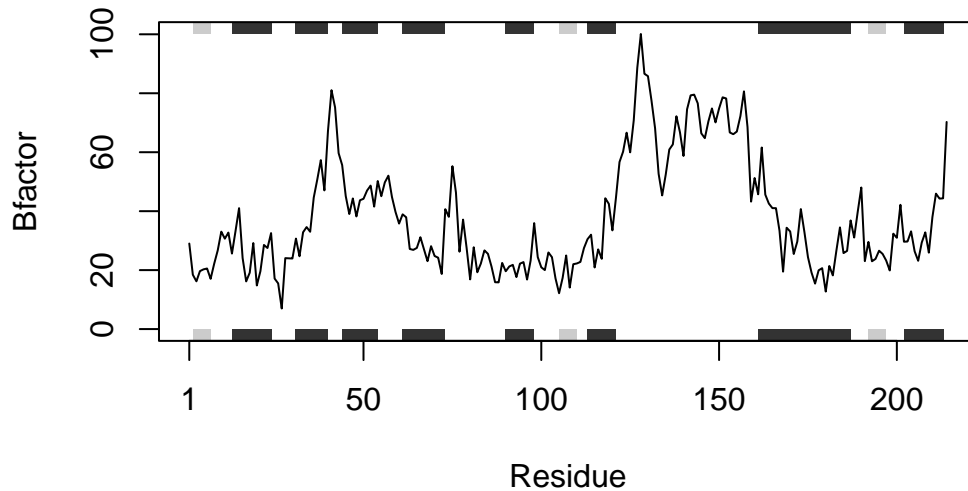
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")  
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")  
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")  
s1.b <- s1.chainA$atom$b  
s2.b <- s2.chainA$atom$b  
s3.b <- s3.chainA$atom$b  
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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



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



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

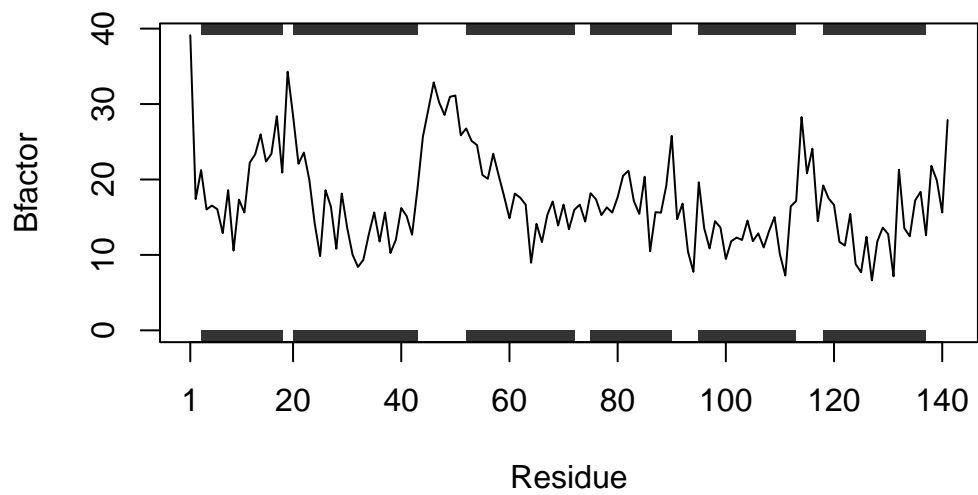
ANSWER

```
snippet <- function(x) {  
  y <- read.pdb(x)  
  y.chainA <- trim.pdb(y, chain="A", elety="CA")  
  y.b <- y.chainA$atom$b  
  plotb3(y.b, sse=y.chainA, typ="l", ylab="Bfactor")  
}
```

TESTING

```
snippet("1Y31")
```

Note: Accessing on-line PDB file



NOTE

Make this into a function

- 1st get a simple working snippet of code
- make it as simple as possible
- reduce code duplication
- then turn into a function
- test it then fix errors