HW06

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Question: 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
```
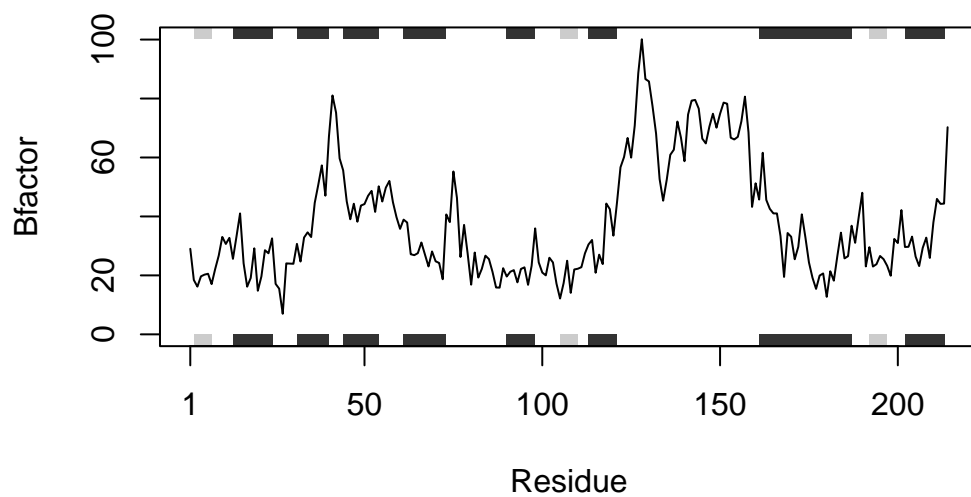
```
s3 <- read.pdb("1E4Y") # kinase with drug
```
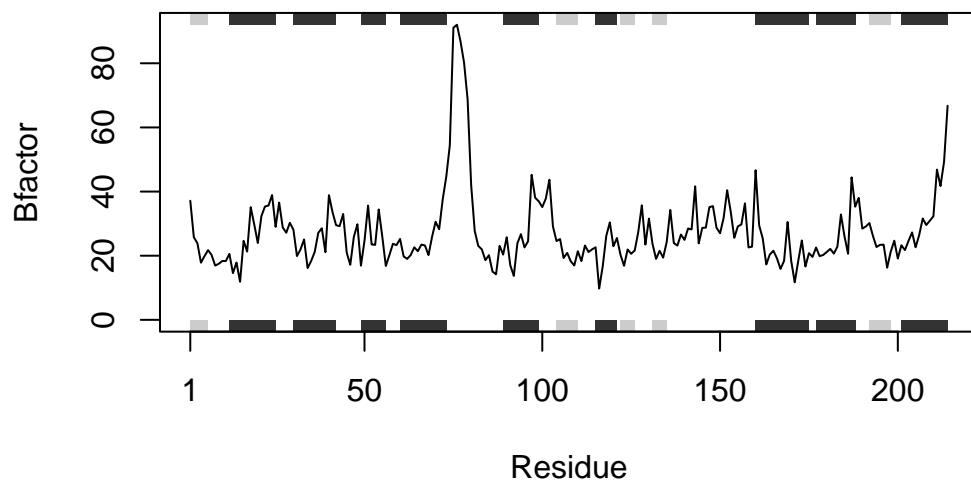
```
  Note: Accessing on-line PDB file
```

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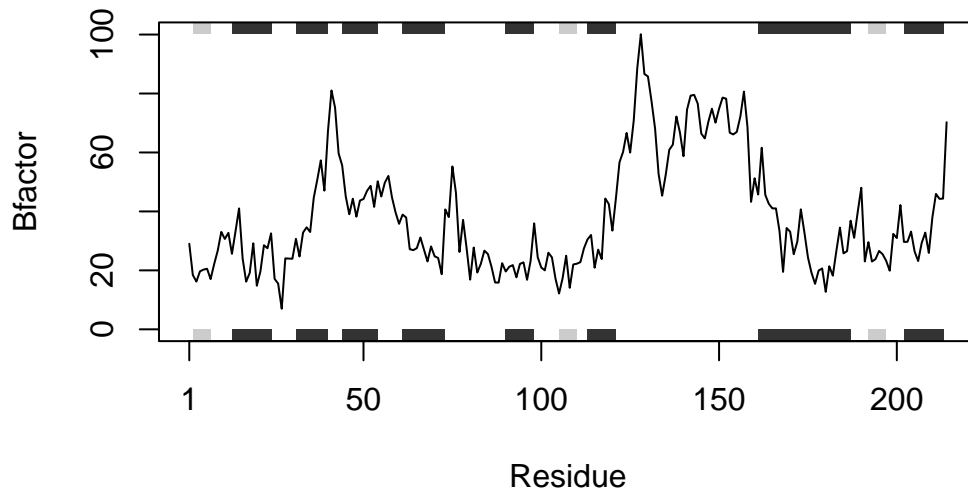
```
plotb3(s2.b, sse=s2.chainA, typ="l", ylab="Bfactor")
```


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


ANSWER:

```
# goal of function: read each .pdb file, then trim the .pdb file to pick out rows where chai

#input: name of pdb file
func <- function(x="4AKE") {
  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, type ="l", ylab="Bfactor")
}
```

Test:

```
#to use function, put in name of the pdb file; output should be the corresponding plot
func("1E4Y")
```

  Note: Accessing on-line PDB file