# Homework Class06

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## Question 6:

ORIGINAL CODE–

```
# 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")
str(s1)
```

```
List of 8
 $ atom  :'data.frame': 3459 obs. of  16 variables:
  ..$ type  : chr [1:3459] "ATOM" "ATOM" "ATOM" "ATOM" ...
  ..$ eleno : int [1:3459] 1 2 3 4 5 6 7 8 9 10 ...
  ..$ elety : chr [1:3459] "N" "CA" "C" "O" ...
  ..$ alt   : chr [1:3459] NA NA NA NA ...
  ..$ resid : chr [1:3459] "MET" "MET" "MET" "MET" ...
  ..$ chain : chr [1:3459] "A" "A" "A" "A" ...
  ..$ resno : int [1:3459] 1 1 1 1 1 1 1 2 2 ...
  ..$ insert: chr [1:3459] NA NA NA NA ...
  ..$ x     : num [1:3459] -10.93 -9.9 -9.17 -9.8 -10.59 ...
  ..$ y     : num [1:3459] -24.9 -24.4 -23.3 -22.3 -24 ...
  ..$ z     : num [1:3459] -9.52 -10.48 -9.81 -9.35 -11.77 ...
  ..$ o     : num [1:3459] 1 1 1 1 1 1 1 1 1 ...
  ..$ b     : num [1:3459] 41.5 29 27.9 26.4 34.2 ...
  ..$ segid : chr [1:3459] NA NA NA NA ...
  ..$ elesy : chr [1:3459] "N" "C" "C" "O" ...
  ..$ charge: chr [1:3459] NA NA NA NA ...
 $ xyz   : 'xyz' num [1, 1:10377] -10.93 -24.89 -9.52 -9.9 -24.42 ...
 $ seqres: Named chr [1:428] "MET" "ARG" "ILE" "ILE" ...
  ..- attr(*, "names")= chr [1:428] "A" "A" "A" "A" ...
 $ helix :List of 4
  ..$ start: Named num [1:19] 13 31 44 61 75 90 113 161 202 13 ...
  .. ..- attr(*, "names")= chr [1:19] "" "" "" "" ...
  ..$ end  : Named num [1:19] 24 40 54 73 77 98 121 187 213 24 ...
  .. ..- attr(*, "names")= chr [1:19] "" "" "" "" ...
  ..$ chain: chr [1:19] "A" "A" "A" "A" ...
  ..$ type : chr [1:19] "5" "1" "1" "1" ...
 $ sheet :List of 4
  ..$ start: Named num [1:14] 192 105 2 81 27 123 131 192 105 2 ...
  .. ..- attr(*, "names")= chr [1:14] "" "" "" "" ...
  ..$ end  : Named num [1:14] 197 110 7 84 29 126 134 197 110 7 ...
  .. ..- attr(*, "names")= chr [1:14] "" "" "" "" ...
  ..$ chain: chr [1:14] "A" "A" "A" "A" ...
  ..$ sense: chr [1:14] "0" "1" "1" "1" ...
 $ calpha: logi [1:3459] FALSE TRUE FALSE FALSE FALSE FALSE ...
 $ remark:List of 1
  ..$ biomat:List of 4
  .. ..$ num   : int 1
  .. ..$ chain :List of 1
  .. .. ..$ : chr [1:2] "A" "B"
  .. ..$ mat   :List of 1
  .. .. ..$ :List of 1
```

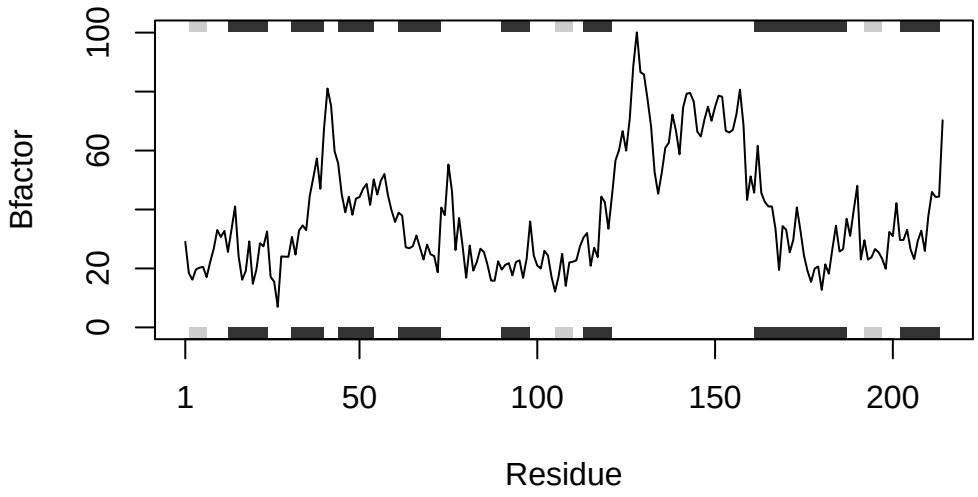
```
  .. .. .. ..$ A B: num [1:3, 1:4] 1 0 0 0 1 0 0 0 1 0 ...
  .. ..$ method: chr "AUTHOR"
 $ call  : language read.pdb(file = "4AKE")
 - attr(*, "class")= chr [1:2] "pdb" "sse"
```

```
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s3, chain="A", elety="CA") #changed s1 to s3!

s1.b <- s1.chainA$atom$b
str(s1)
```

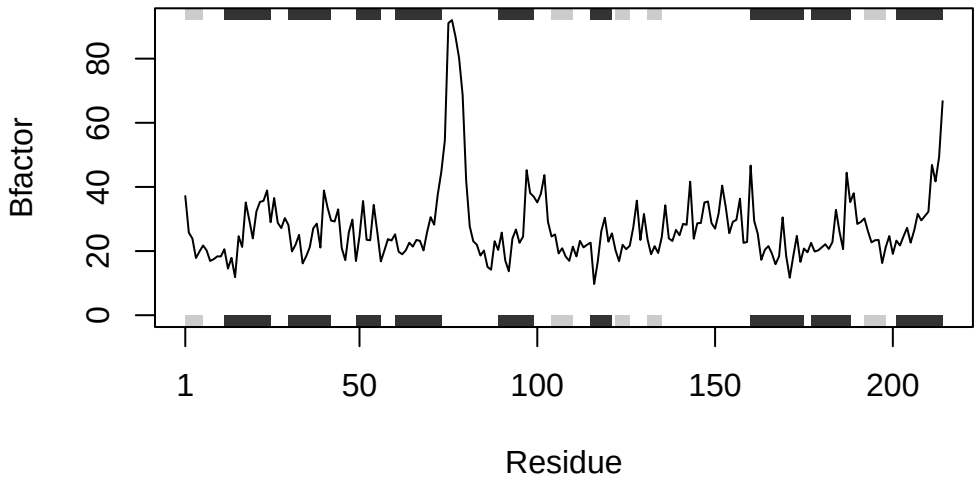
```
List of 8
 $ atom  :'data.frame': 3459 obs. of  16 variables:
  ..$ type  : chr [1:3459] "ATOM" "ATOM" "ATOM" "ATOM" ...
  ..$ eleno : int [1:3459] 1 2 3 4 5 6 7 8 9 10 ...
  ..$ elety : chr [1:3459] "N" "CA" "C" "O" ...
  ..$ alt   : chr [1:3459] NA NA NA NA ...
  ..$ resid : chr [1:3459] "MET" "MET" "MET" "MET" ...
  ..$ chain : chr [1:3459] "A" "A" "A" "A" ...
  ..$ resno : int [1:3459] 1 1 1 1 1 1 1 2 2 ...
  ..$ insert: chr [1:3459] NA NA NA NA ...
  ..$ x     : num [1:3459] -10.93 -9.9 -9.17 -9.8 -10.59 ...
  ..$ y     : num [1:3459] -24.9 -24.4 -23.3 -22.3 -24 ...
  ..$ z     : num [1:3459] -9.52 -10.48 -9.81 -9.35 -11.77 ...
  ..$ o     : num [1:3459] 1 1 1 1 1 1 1 1 1 ...
  ..$ b     : num [1:3459] 41.5 29 27.9 26.4 34.2 ...
  ..$ segid : chr [1:3459] NA NA NA NA ...
  ..$ elesy : chr [1:3459] "N" "C" "C" "O" ...
  ..$ charge: chr [1:3459] NA NA NA NA ...
 $ xyz   : 'xyz' num [1, 1:10377] -10.93 -24.89 -9.52 -9.9 -24.42 ...
 $ seqres: Named chr [1:428] "MET" "ARG" "ILE" "ILE" ...
  ..- attr(*, "names")= chr [1:428] "A" "A" "A" "A" ...
 $ helix :List of 4
  ..$ start: Named num [1:19] 13 31 44 61 75 90 113 161 202 13 ...
  .. ..- attr(*, "names")= chr [1:19] "" "" "" "" ...
  ..$ end  : Named num [1:19] 24 40 54 73 77 98 121 187 213 24 ...
  .. ..- attr(*, "names")= chr [1:19] "" "" "" "" ...
  ..$ chain: chr [1:19] "A" "A" "A" "A" ...
  ..$ type : chr [1:19] "5" "1" "1" "1" ...
 $ sheet :List of 4
  ..$ start: Named num [1:14] 192 105 2 81 27 123 131 192 105 2 ...
  .. ..- attr(*, "names")= chr [1:14] "" "" "" "" ...
```

```
  ..$ end  : Named num [1:14] 197 110 7 84 29 126 134 197 110 7 ...
  .. ..- attr(*, "names")= chr [1:14] "" "" "" "" ...
  ..$ chain: chr [1:14] "A" "A" "A" "A" ...
  ..$ sense: chr [1:14] "0" "1" "1" "1" ...
 $ calpha: logi [1:3459] FALSE TRUE FALSE FALSE FALSE FALSE ...
 $ remark:List of 1
  ..$ biomat:List of 4
  .. ..$ num   : int 1
  .. ..$ chain :List of 1
  .. .. ..$ : chr [1:2] "A" "B"
  .. ..$ mat   :List of 1
  .. .. ..$ :List of 1
  .. .. .. ..$ A B: num [1:3, 1:4] 1 0 0 0 1 0 0 0 1 0 ...
  .. ..$ method: chr "AUTHOR"
 $ call  : language read.pdb(file = "4AKE")
 - attr(*, "class")= chr [1:2] "pdb" "sse"
```

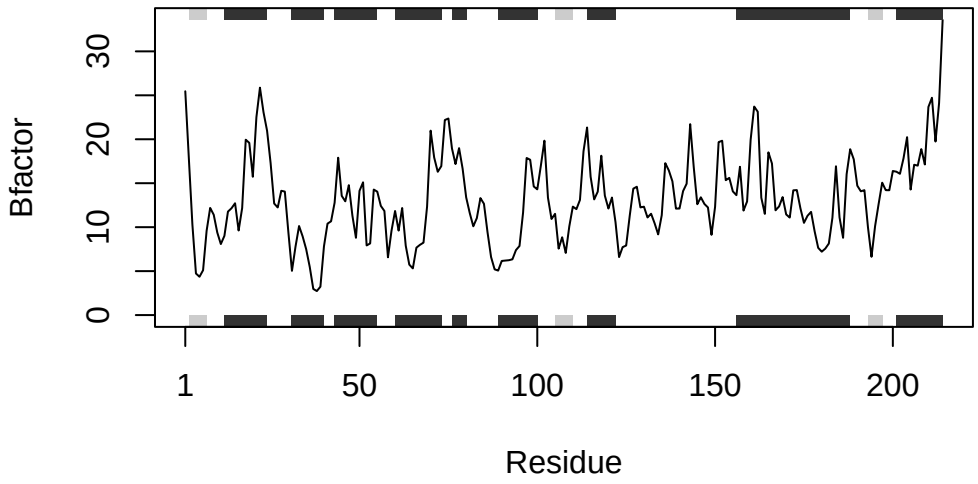
```
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b

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")
```

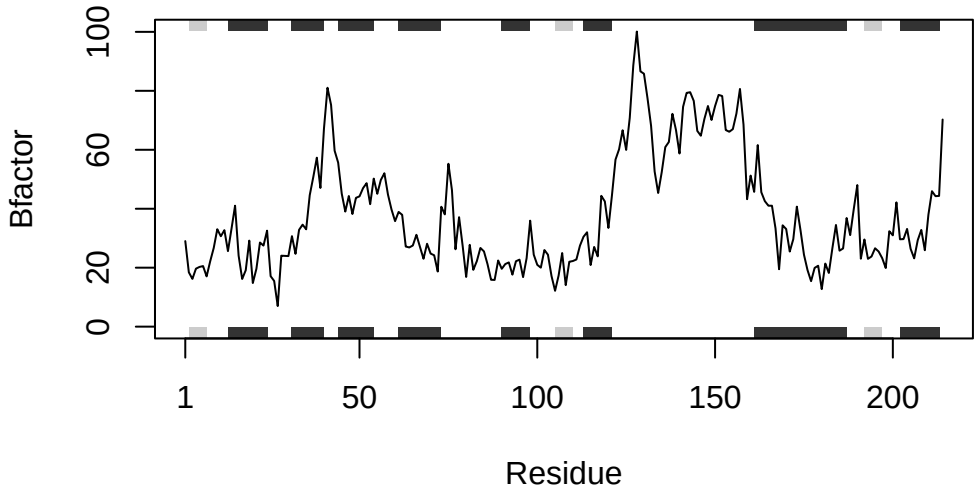


Q: How would you generalize the original code above to work with any set of input protein structures?

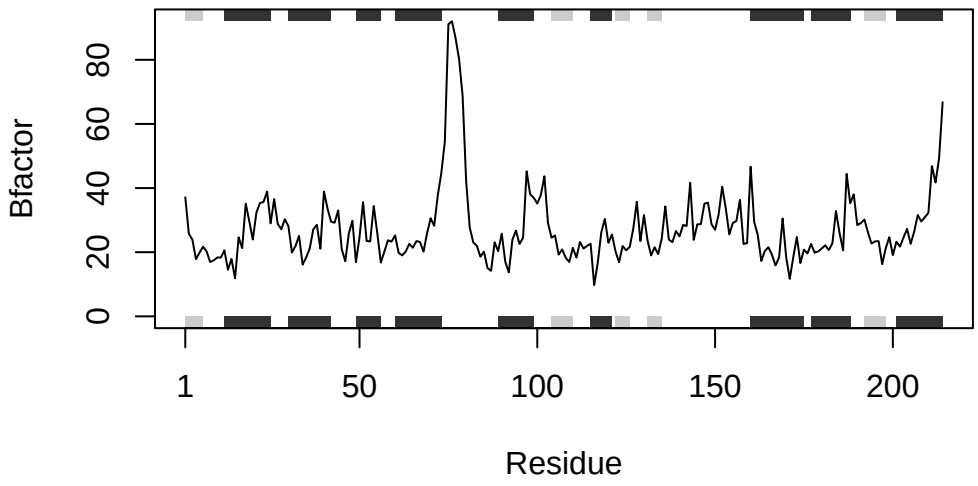
```
graph.cA.aB <- function(x) {
  x.chainA <- trim.pdb(x, chain="A", elety="CA")
  x.b <- x.chainA$atom$b
  plotb3(x.b, sse=x.chainA, typ="l", ylab="Bfactor")
}
```

I just made the s1, s2, s3 into one factor, x, that is variable according to what is inputted into the function.

```
graph.cA.aB(s1)
```




```
graph.cA.aB(s2)
```




```
graph.cA.aB(s3)
```