Class 6 Homework

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Original code

```
library(bio3d)
```

```
Warning: package 'bio3d' was built under R version 4.4.3
```

```
s1 <- read.pdb("4AKE") # kinase with drug
```

```
  Note: Accessing on-line PDB file
```

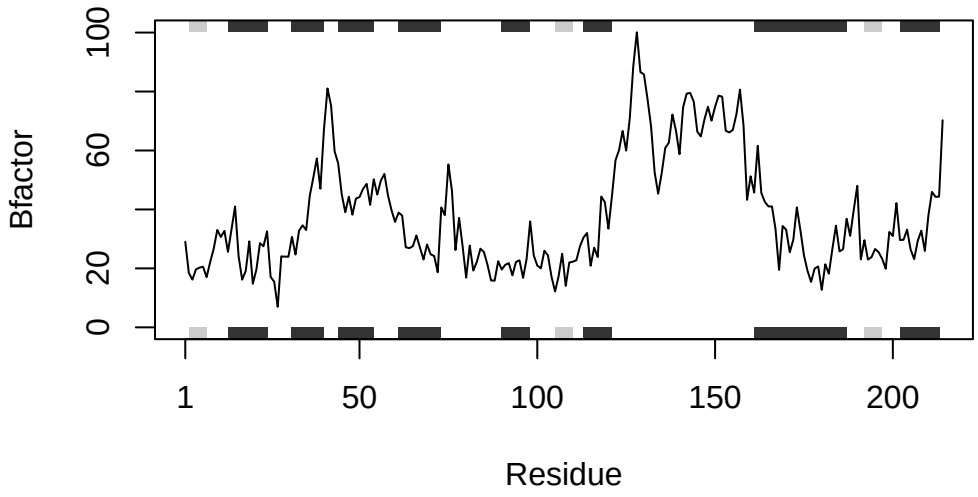
```
s2 <- read.pdb("1AKE") # kinase no drug
```

```
  Note: Accessing on-line PDB file
   PDB has ALT records, taking A only, rm.alt=TRUE
```

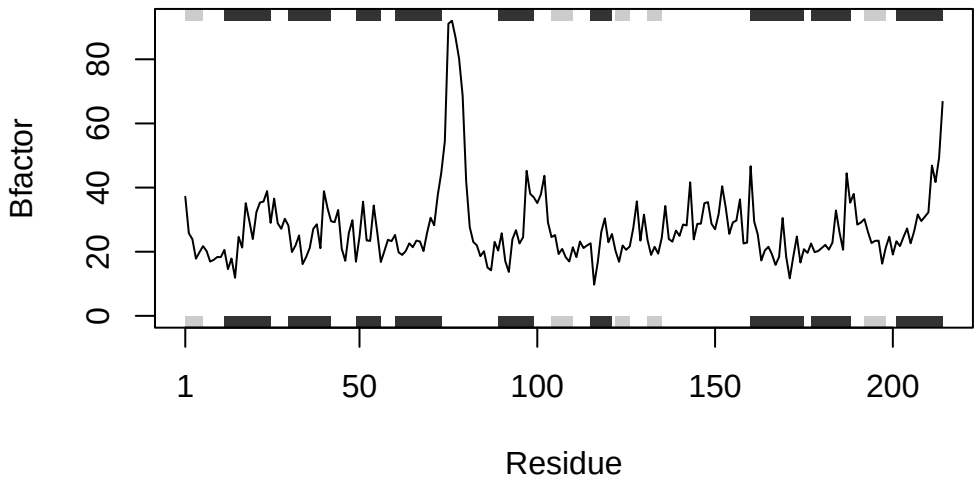
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

```
  Note: Accessing on-line PDB file
```

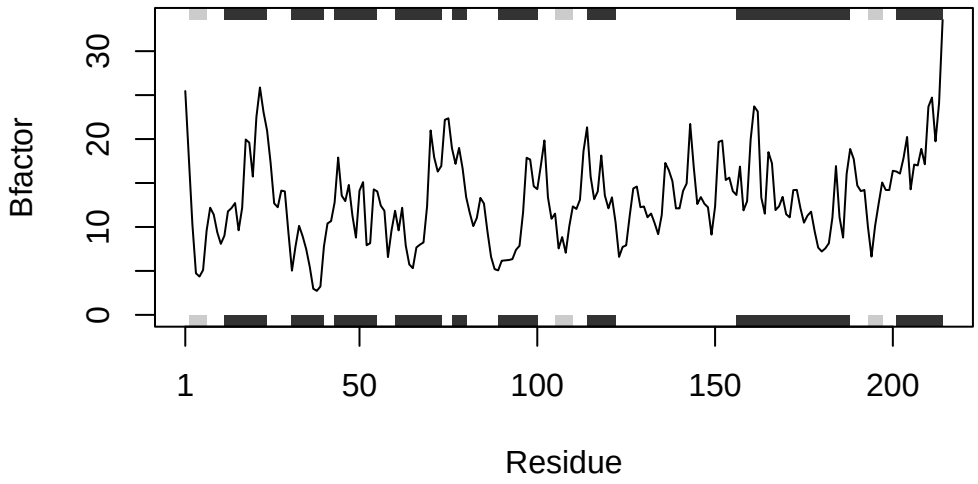
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```




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



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



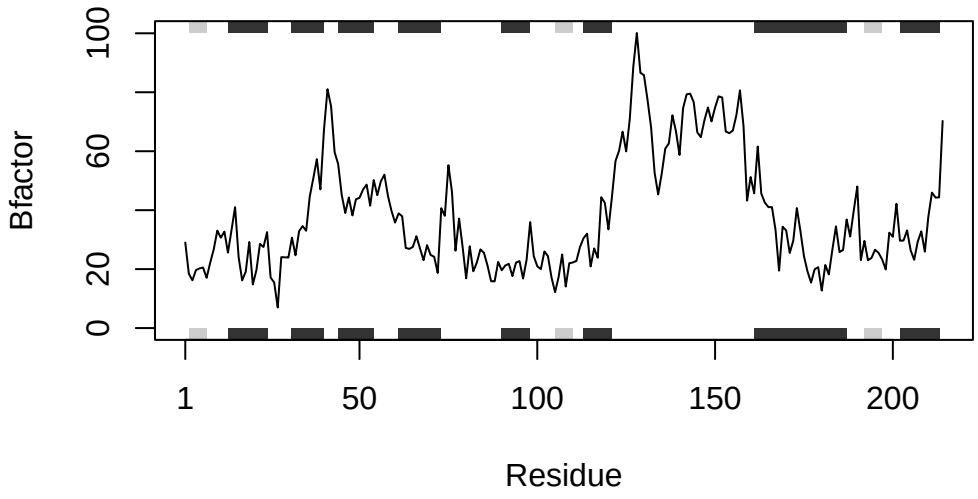
New function

```
rm(list=ls())

#Function to plot B-factor of a protein chain

  #Inputs:
    #input - PDB code as string
    #chain - which chain from PDB to use, default A
    #sse - whether to display secondary structures on plot, default T
    #typ - plot type, taken from bio3d plotb3, default l (lines)

  #Output: plot of B-factor for each residue in a protein chain

bfactorplot <- function(input, chain = "A", sse = T, typ = "l"){

  #Read in PDB file
  prot <- read.pdb(input)
```

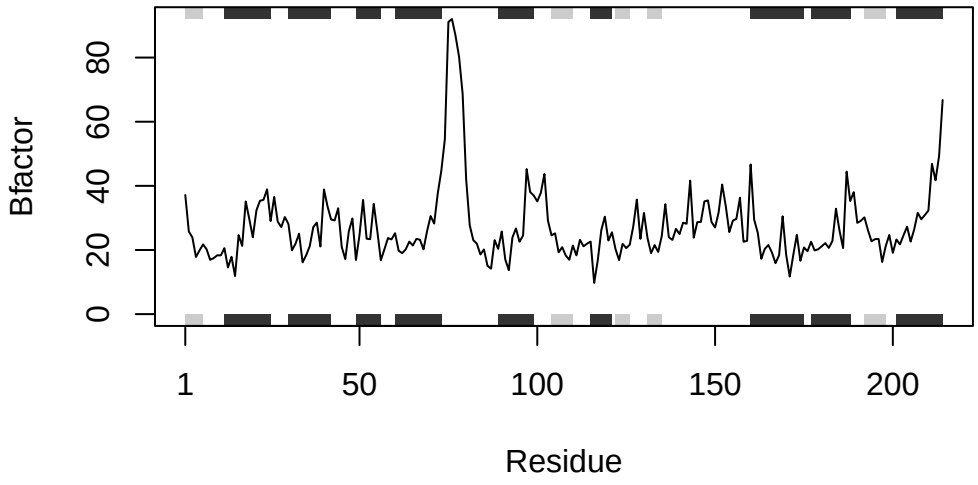
```
  #Identify alpha carbons in designated chain
  prot.chain <- trim.pdb(prot, chain = chain,  elety = "CA")

  #Make vector of B-factors
  prot.b <- prot.chain$atom$b

  #If sse == F, remove secondary structure annotation
  if(sse == F){
    prot.chain <- NULL
  }

  #Plot B-factors
  plotb3(prot.b, sse = prot.chain, typ = typ, ylab = "Bfactor")
}
```

```
#test function
sapply(c("4AKE", "1AKE", "1E4Y"), bfactorplot)
```

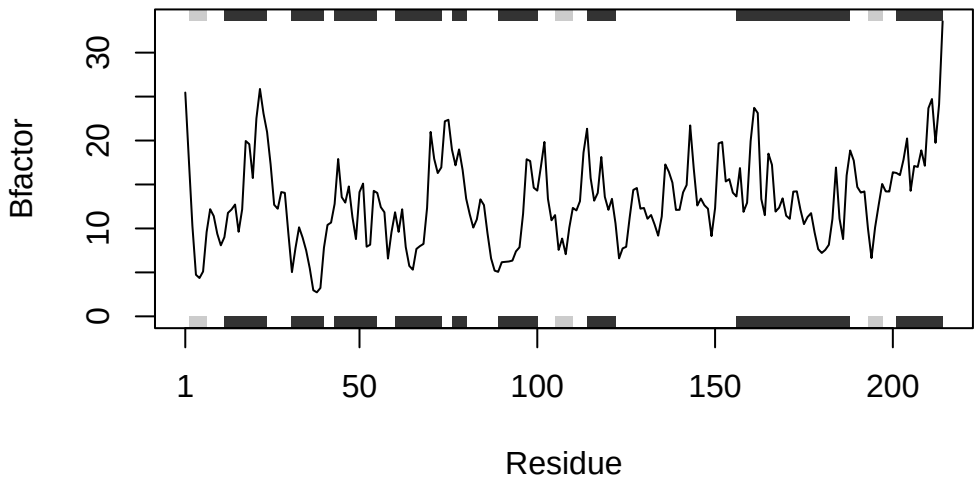
```
  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\grace\AppData\Local\Temp\RtmpmYKqwN/4AKE.pdb exists. Skipping download
```



```
  Note: Accessing on-line PDB file

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

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



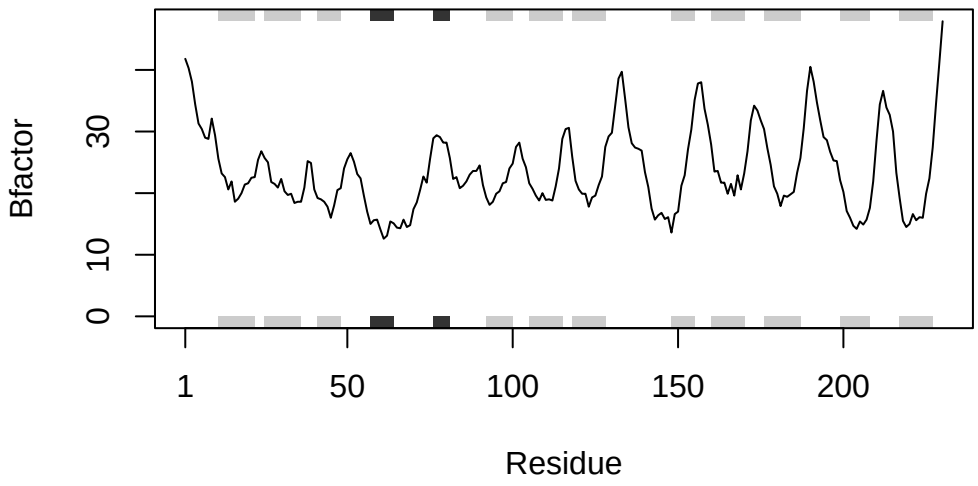

```
  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\grace\AppData\Local\Temp\RtmpmYKqwN/1E4Y.pdb exists. Skipping download
```




```
$`4AKE`
NULL

$`1AKE`
NULL

$`1E4Y`
NULL
```

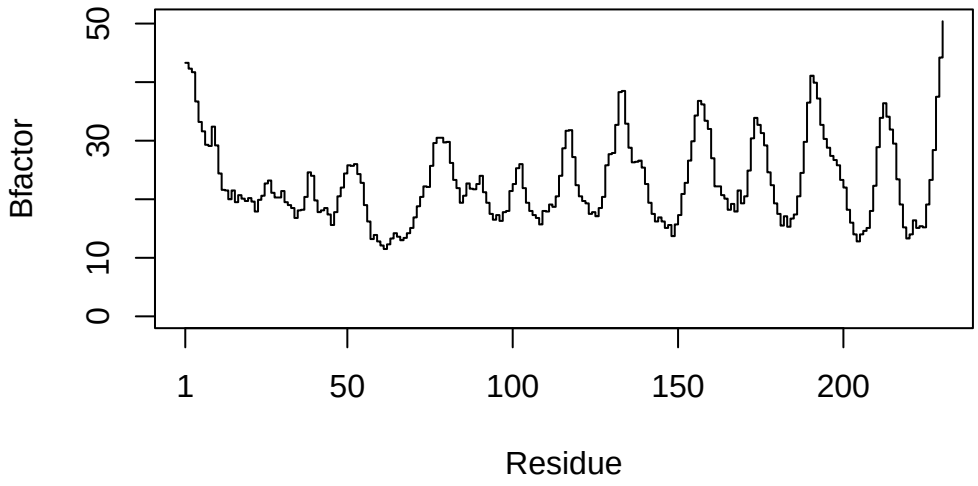
```
#test with different protein
bfactorplot("1GFL")
```

```
  Note: Accessing on-line PDB file
```




```
#test non-default inputs
bfactorplot("1GFL", chain = "B", sse = F, typ = "s")
```

```
  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\grace\AppData\Local\Temp\RtmpmYKqwN/1GFL.pdb exists. Skipping download
```


Bfactor
0
10
30
50
1
50
100
150
200
Residue