Class 6 Homework Function

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The provided code that we want to improve and adopt to be more general for any protein-drug combination.

```
library(bio3d)
s1 <- read.pdb("4AKE") # kinase with drug
```

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

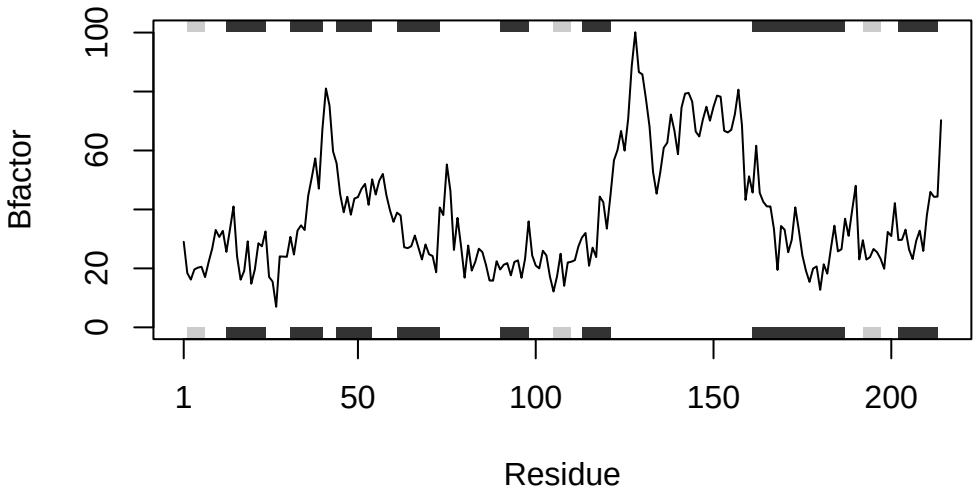
```
s2 <- read.pdb("1AKE") # kinase no drug
```

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

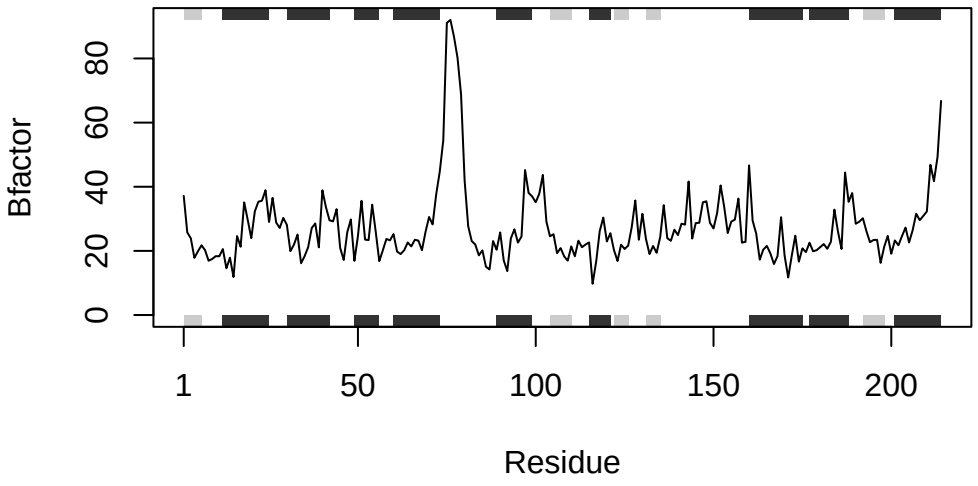
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

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

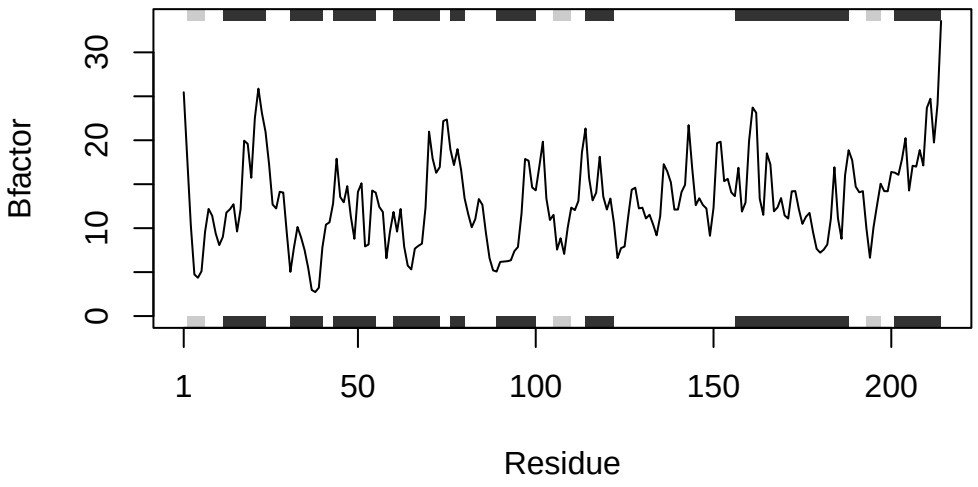
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")

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")
```

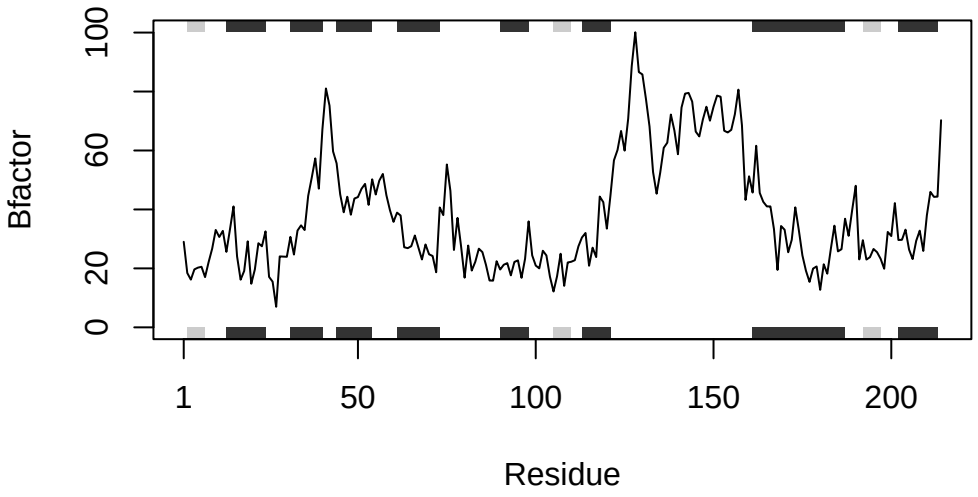



```
#test run for just one protein
id <- "4AKE"
pdb <- read.pdb(id) # kinase with drug
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose =
FALSE): /var/folders/5w/y1lm5qmx3r5fqyf39_mvjhvm0000gn/T//Rtmpn4JNMw/4AKE.pdb
exists. Skipping download
```

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

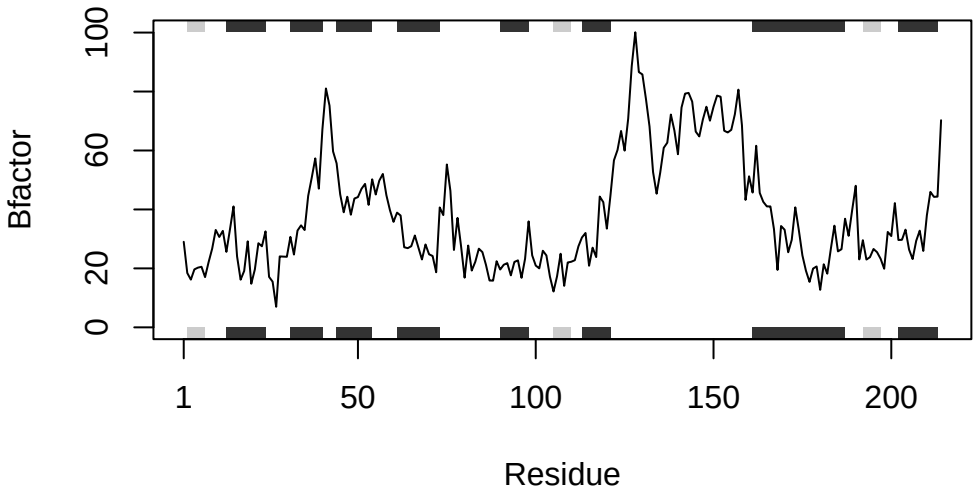



```
#function to make a plot when you input a PDB code as 'x'
plotpdb <- function(x){
  # read the input PDB file
  pdb <- read.pdb(x)
  #trim down the protein to only chain A
  chainA <- trim.pdb(pdb, chain="A", elety="CA")
  #retrieve b-factor values under atom in the chain A and make the b-factor plot
  plotb3(chainA$atom$b, sse=chainA, typ="l", ylab="Bfactor")
}
```

```
#execute the function `plotpdb` using input of PDB codes, and it will output the b-factor
plotpdb("4AKE")
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose =
FALSE): /var/folders/5w/y1lm5qmx3r5fqyf39_mvjhvm0000gn/T//Rtmpn4JNMw/4AKE.pdb
exists. Skipping download
```

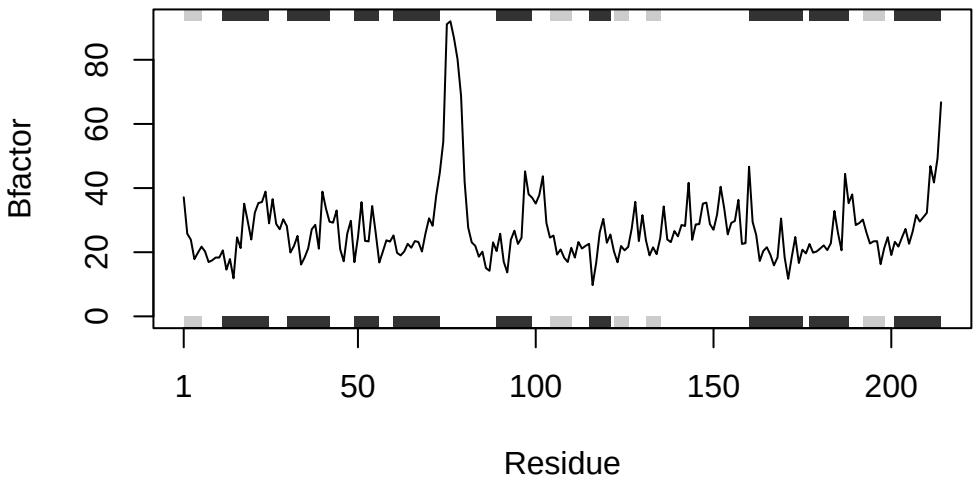



```
plotpdb("1AKE")
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose =
FALSE): /var/folders/5w/y1lm5qmx3r5fqyf39_mvjhvm0000gn/T//Rtmpn4JNMw/1AKE.pdb
exists. Skipping download
```

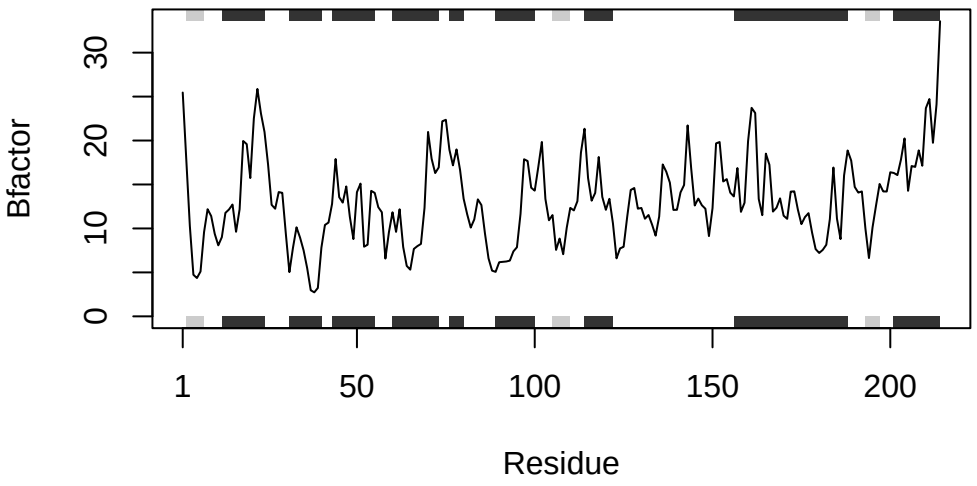
```
   PDB has ALT records, taking A only, rm.alt=TRUE
```




```
plotpdb("1E4Y")
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose =
FALSE): /var/folders/5w/y1lm5qmx3r5fqyf39_mvjhvm0000gn/T//Rtmpn4JNMw/1E4Y.pdb
exists. Skipping download
```


Bfactor
0
10
20
30
1
50
100
150
200
Residue