HW Assignment Class 6

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> Q6. How would you generalize the original code above to work with any set of input protein structures?

The following function generalizes the code provided in HW6 such that it can be called with any specified PDB file as a parameter as long as it is entered in the form of a String.

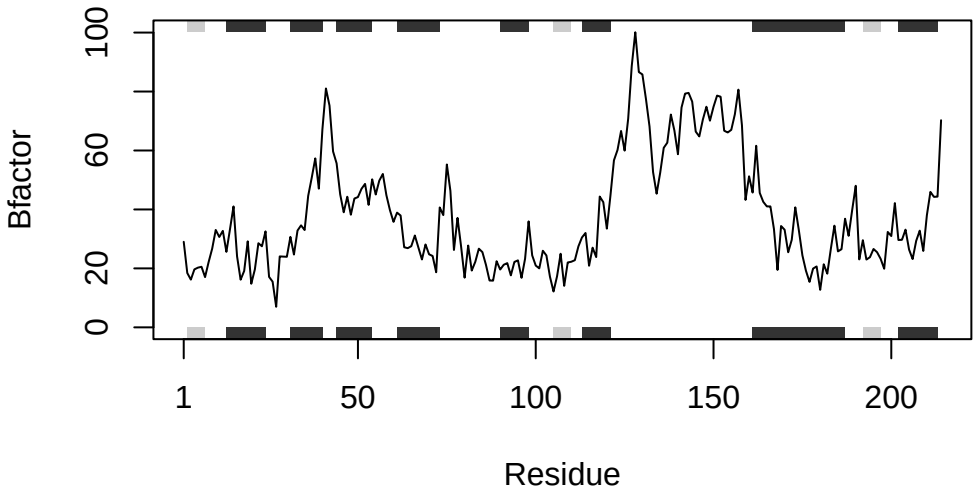
The function first reads the PDB file, and then generates a graph based on the parameters defined by the variables created in the function.

```
library(bio3d)
analyzePDI <- function(fileToCall) {
  s1 <- read.pdb(fileToCall) #Reads PDB file
  s1.chainA <- trim.pdb(s1, chain = "A", elety = "CA") #Trims data
  s1.b <- s1.chainA$atom$b #Assigns our required X-axis to a variable
  plotb3(s1.b, sse=s1.chainA, type = "l", ylab="Bfactor") #Plots line graph
}
```

The code block below calls the function for the PDB file of the kinase with drug "4AKE". The graph is generated by our function.

```
analyzePDI("4AKE")
```

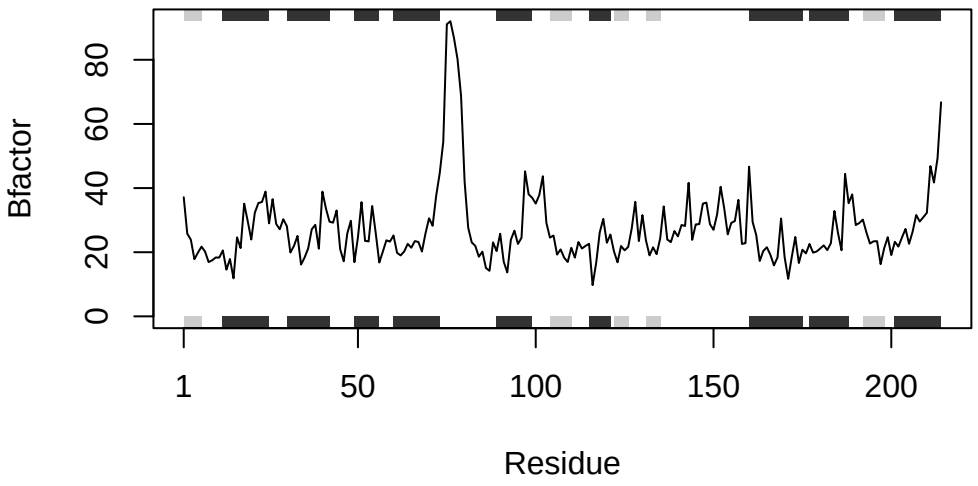
```
Note: Accessing on-line PDB file
```



The following code block calls the function for two other PDB files.

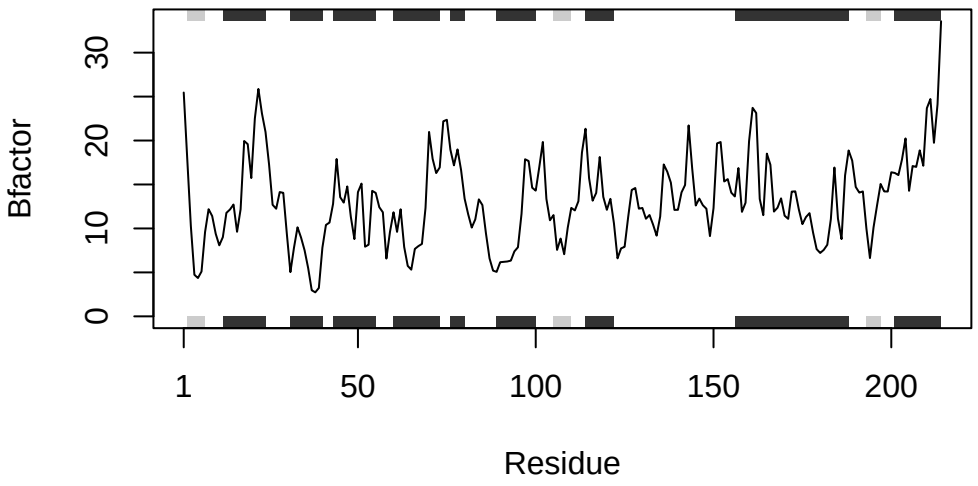
```
analyzePDI("1AKE")
```

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




```
analyzePDI("1E4Y")
```

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


Bfactor
0
10
20
30
1
50
100
150
200
Residue