question06

Kyle Alvarez

Example Code To Be Reduced

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

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

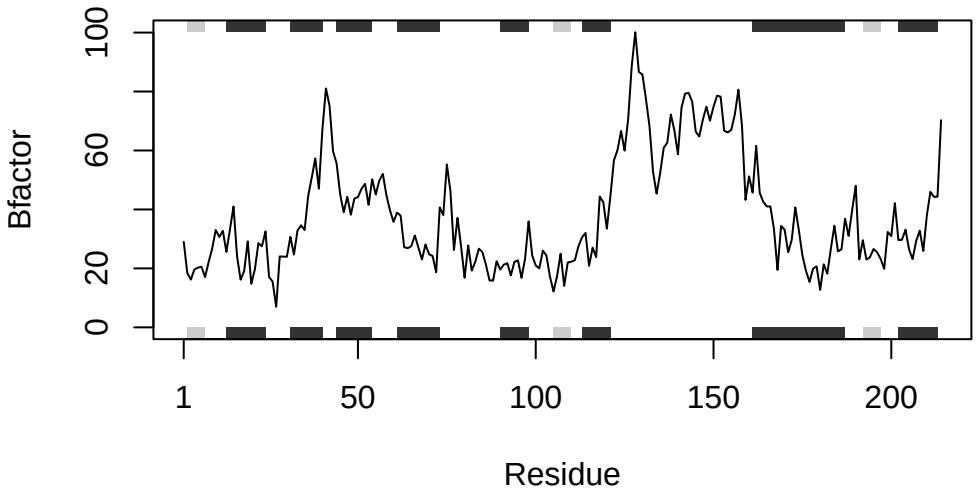
```
s2 <- read.pdb("1AKE") # kinase no drug
```

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

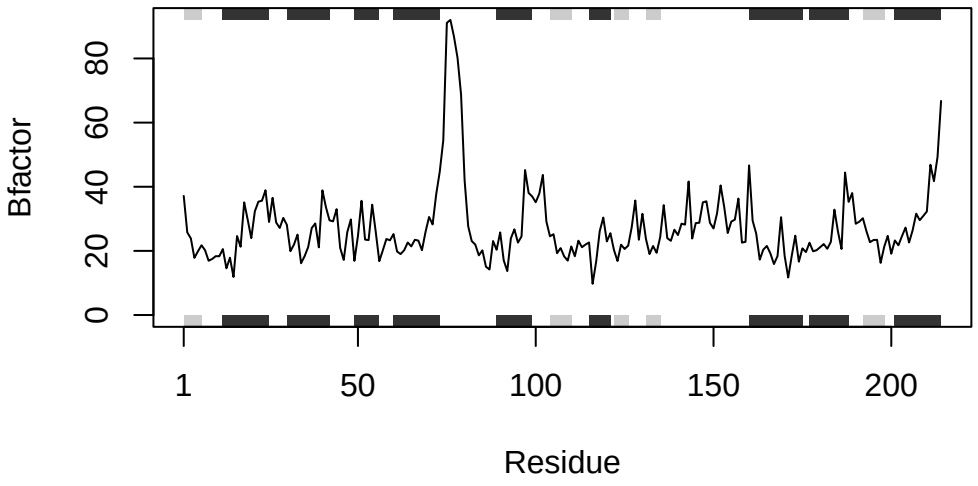
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

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

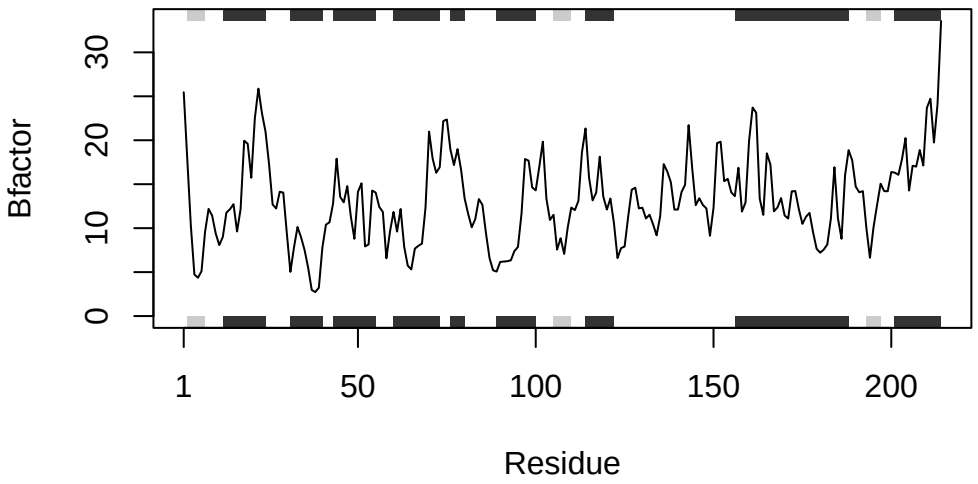
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```




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



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



Example Code Reduced to a Function

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

```
analyzePDI <- function(kinase){ # Takes a kinase as its argument
  structure <- read.pdb(kinase) # Reads the protein data bank of the kinase and stores it
  structure.chainA <- trim.pdb(structure, chain="A", elety="CA") # Trims the PDB object of
  structure.b <-  structure.chainA$atom$b # Assigns the specific atom from the proteins's
  plotb3(structure.b, sse=structure.chainA, type="l", ylab="Bfactor") # Plots the data of
}
```

In order to use this function all you have to do is type `analyzePDI()` and insert the kinase/protein that you want to be analyzed in quotations within the parentheses of the argument.

The output of the function is a line graph that plots the residue against the Bfactor of a kinase/protein.

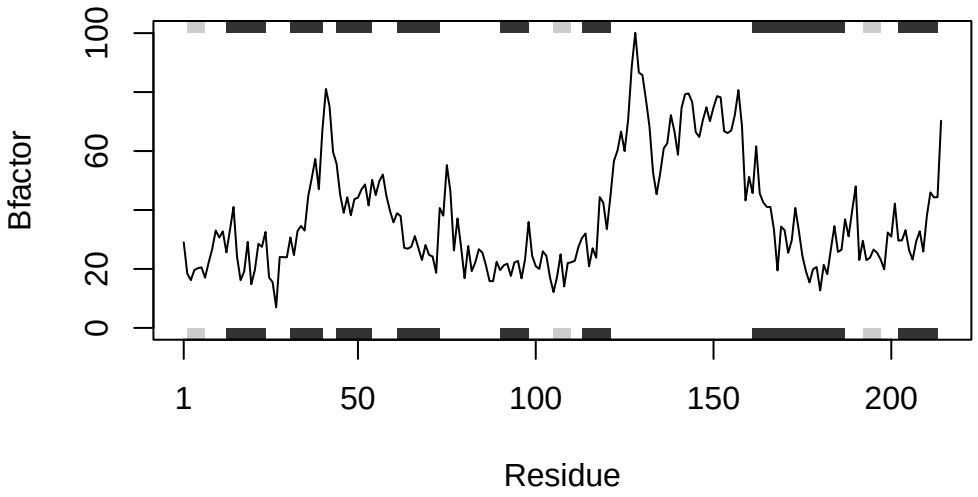
Using the simplified function for the example kinases

Tests the function against the example kinases to see if the graphs are the same, in this case it is. Hence we have a simplified function in which we can use to plot different kinases instead of having to manually type out every step subsequently.

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

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/3v/
_2psgc5x25jbg4hscbfbqz_00000gn/T//Rtmp2XNadz/4AKE.pdb exists. Skipping download
```

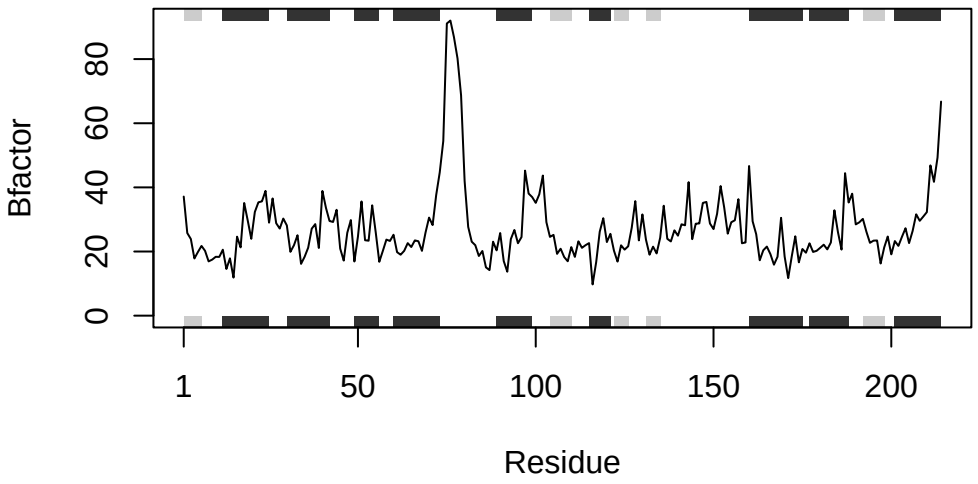



```
analyzePDI("1AKE")
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/3v/
_2psgc5x25jbg4hscbfbqz_00000gn/T//Rtmp2XNadz/1AKE.pdb exists. Skipping download
```

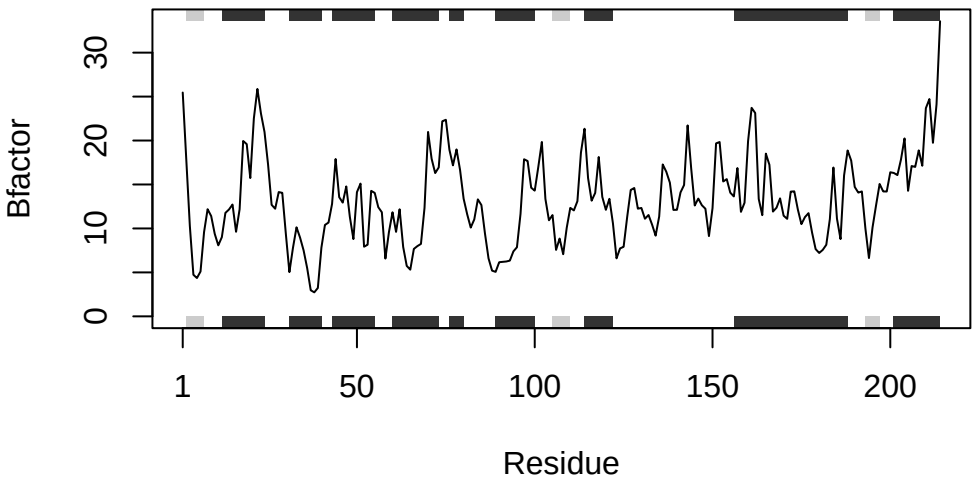
```
PDB has ALT records, taking A only, rm.alt=TRUE
```




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

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/3v/
_2psgc5x25jbg4hscbfbqz_00000gn/T//Rtmp2XNadz/1E4Y.pdb exists. Skipping download
```


Bfactor
0
10
20
30
1
50
100
150
200
Residue