Hw06

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Q6: Optimization

Here we will make a more robust version of the following code which analyzes a given protein's drug interactions and plots it...

```
# install.packages("bio3d")
# 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
```

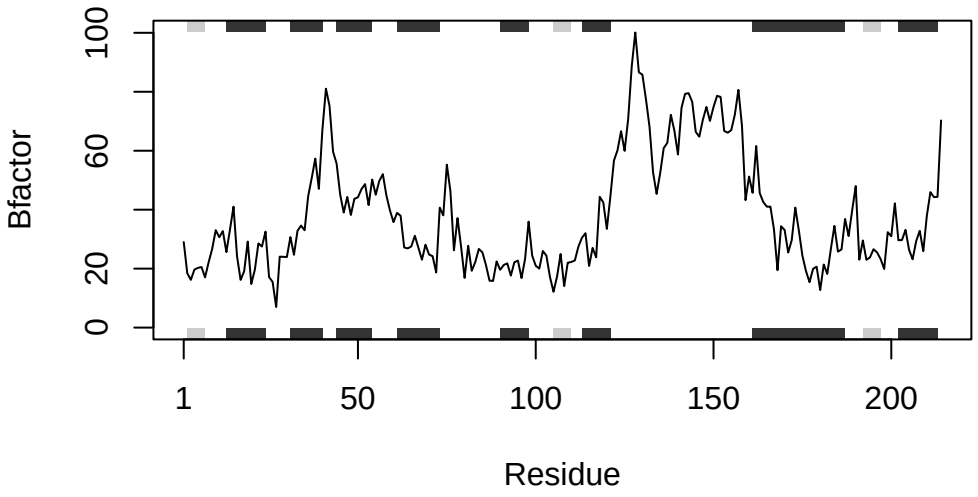
```
Note: Accessing on-line PDB file
 PDB has ALT records, taking A only, rm.alt=TRUE
```

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

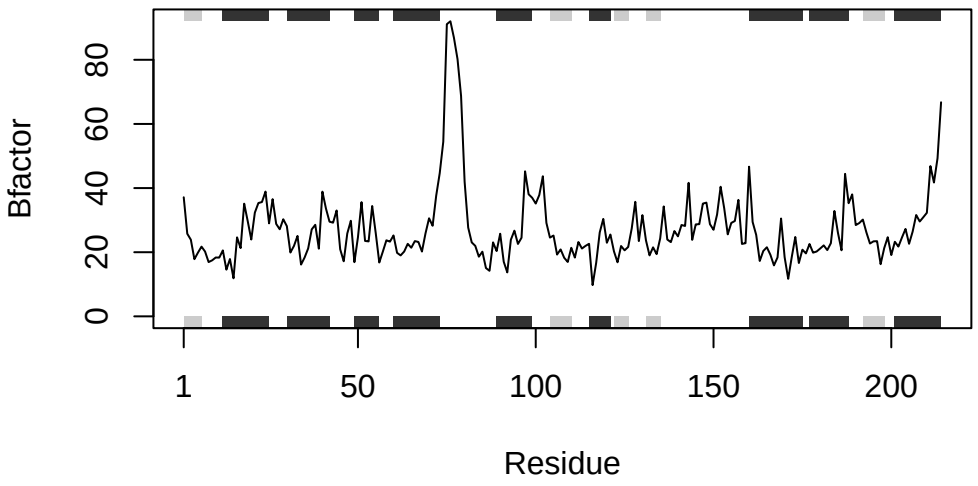
```
Note: Accessing on-line PDB file
```

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

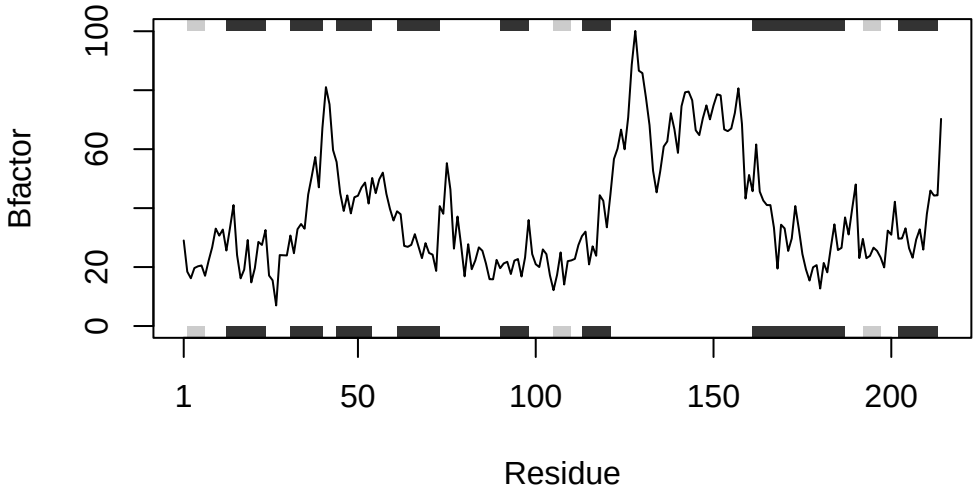
```
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b

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")
```



I will write a function that serves the same purpose as the above code and also is more concise and reusable. The function will take an input of any given protein's 4 digit PDB code and outputs a plot outlining the drug B factor interactions plotted against specific residues of the protein.

Shortened code

`plotBfactor()`

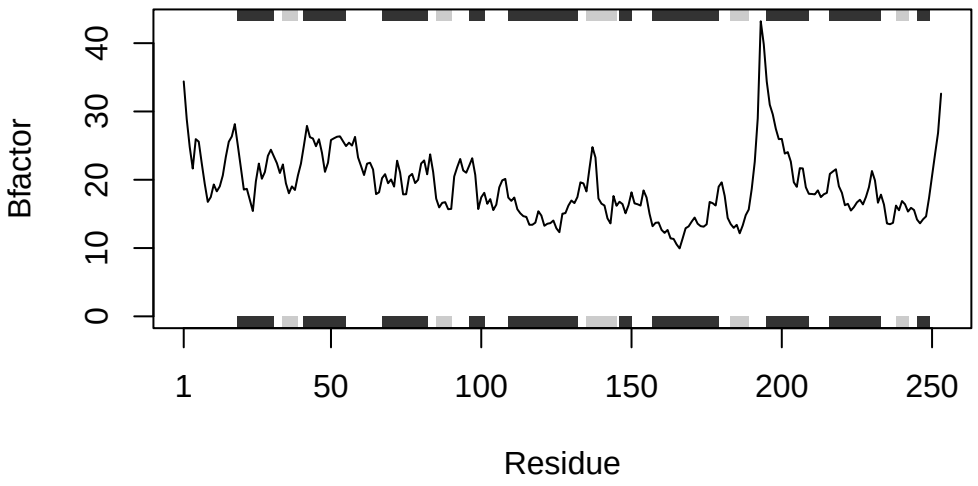
```
#This function takes input prot which is the 4 letter PDB code
#It will output a plot of Bfactor interactions vs amino acid residue position of prot

plotBfactor <- function(prot) {
  #input: prot = "____" PDB code

  s <- read.pdb(prot) #reads the argument PDB code
  s.chainA <- trim.pdb(s, chain="A", elety="CA")
  s.b <- s.chainA$atom$b

  #creates plot of Bfactor vs amino acid position of prot
  plotb3(s.b, sse=s.chainA, typ="l", ylab="Bfactor")
}
```

Now let's test our `plotBfactor()` function.

To use it, you just have to pass an existing 4 letter PDB code as a string argument to the function. The output will be a Bfactor vs Amino Acid Residue plot showing the relative mobility or rigidity of a protein.

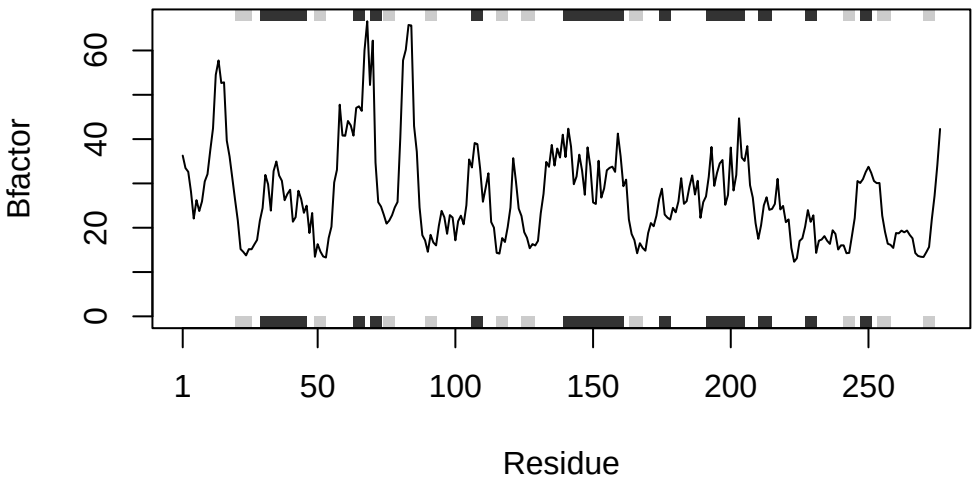
```
#Example: To generate plot for PDB code 3EK2
plotBfactor("3EK2")
```

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




```
#Example: To generate plot for PDB code 7TR7
plotBfactor("7TR7")
```

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


Bfactor
0
20
40
60
1
50
100
150
200
250
Residue