

# class06Hmwk

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Original

```
# Can you improve this analysis code?  
library(bio3d)  
s1 <- read.pdb("4AKE") # kinase with drug
```

Note: Accessing on-line PDB file

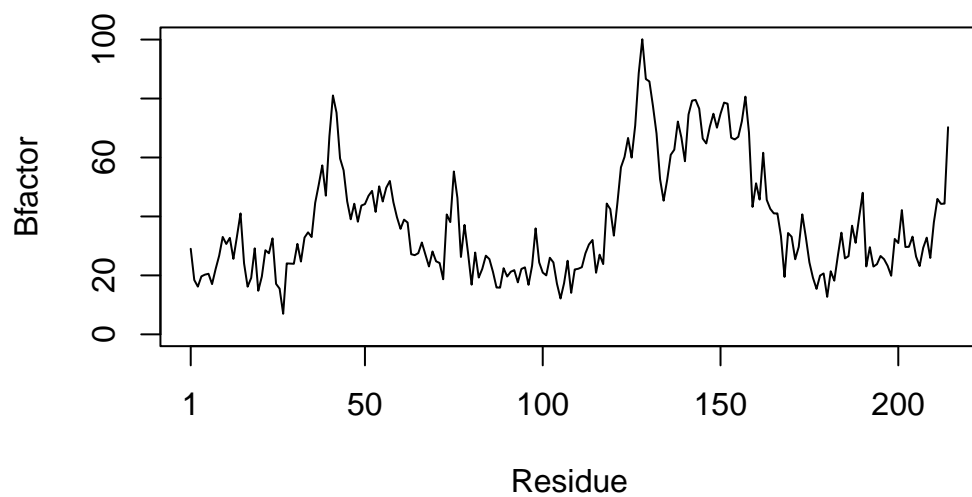
```
s2 <- read.pdb("1AKE") # kinase no drug
```

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

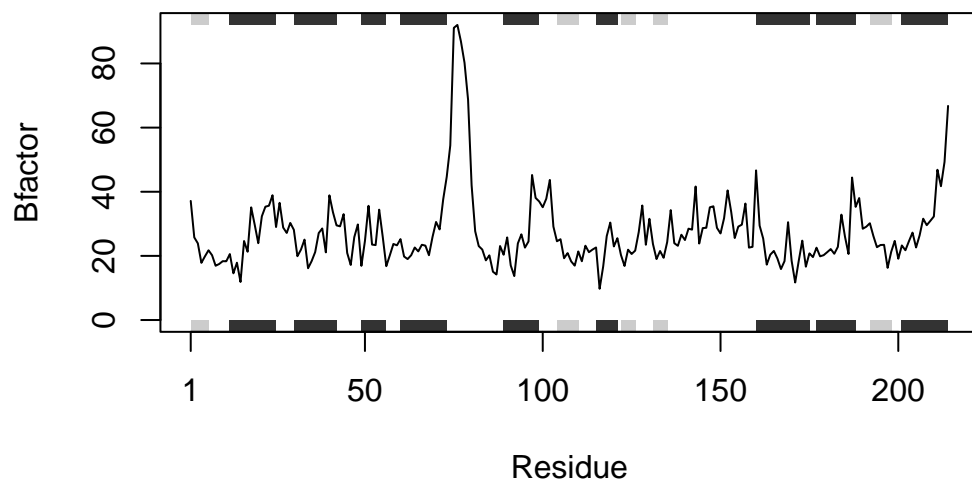
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

Note: Accessing on-line PDB file

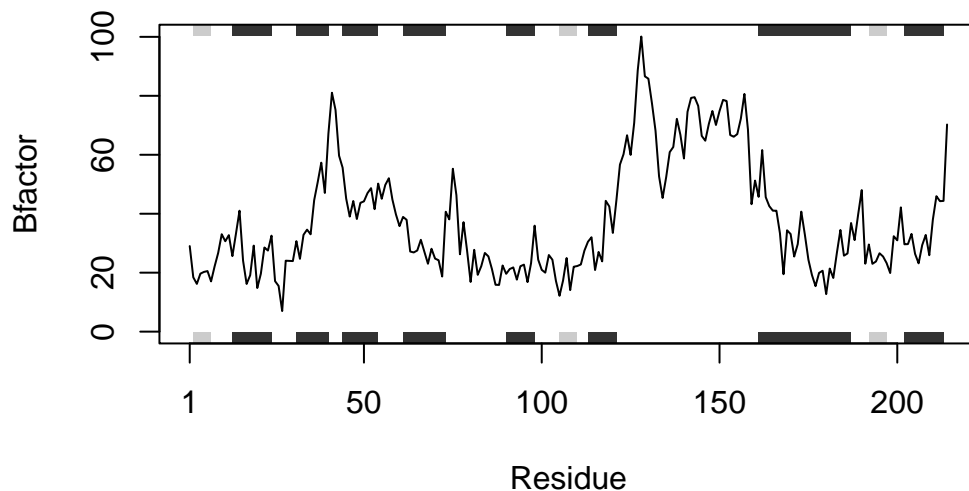
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")  
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")  
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")  
s1.b <- s1.chainA$atom$b  
s2.b <- s2.chainA$atom$b  
s3.b <- s3.chainA$atom$b  
plotb3(s1.b, typ="l", ylab="Bfactor")
```



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



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



changed function

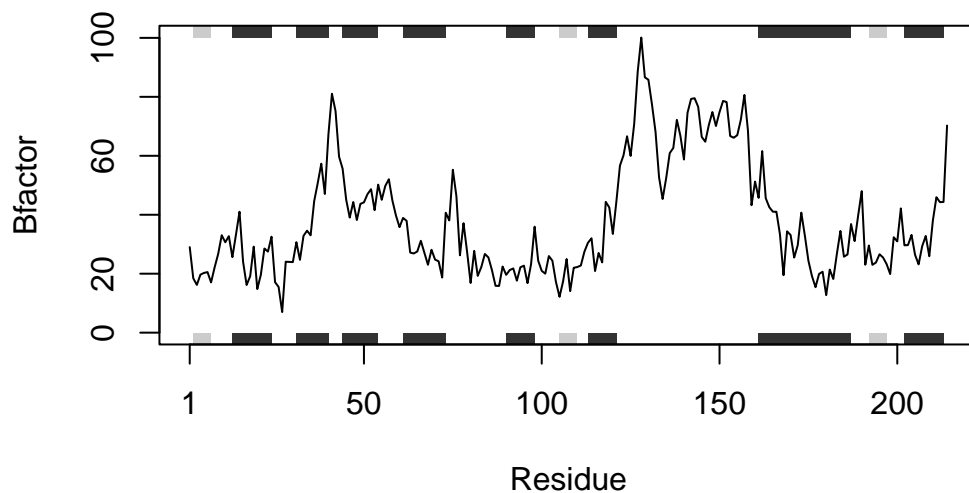
```
#takes in the string pdb code
#it will output a pdb object corresponding to that string,
#the trimmed A chain of that object, and the atom b values of that chain.
# it will then print a lineplot of b atom values

pdbPlot<-function(string){
  protein<-read.pdb(string)
  protein.chainA<- trim.pdb(protein, chain="A", elety="CA")
  protein.b <- protein.chainA$atom$b
  plotb3(protein.b, sse=protein.chainA, typ="l", ylab="Bfactor")
}
#test to see if it produces same output
pdbPlot("4AKE")
```

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE): C:

\\Users\\danie\\AppData\\Local\\Temp\\Rtmpe2sXR8\\4AKE.pdb exists. Skipping download

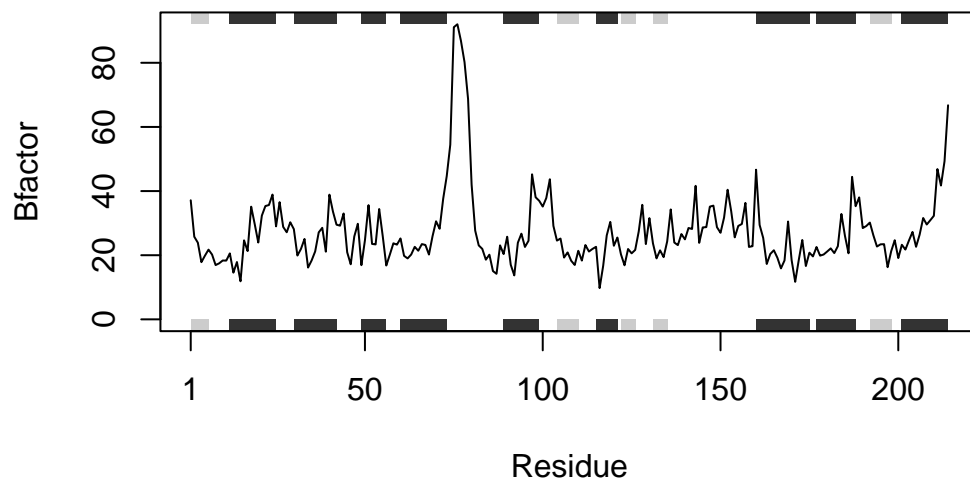


```
pdbPlot("1AKE")
```

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE): C:  
\\Users\\danie\\AppData\\Local\\Temp\\Rtmpe2sXR8\\1AKE.pdb exists. Skipping download

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



```
pdbPlot("1E4Y")
```

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE): C:\Users\danie\AppData\Local\Temp\Rtmpe2sXR8\1E4Y.pdb exists. Skipping download

