

# Lab Supplement

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Original code to make function from:

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

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

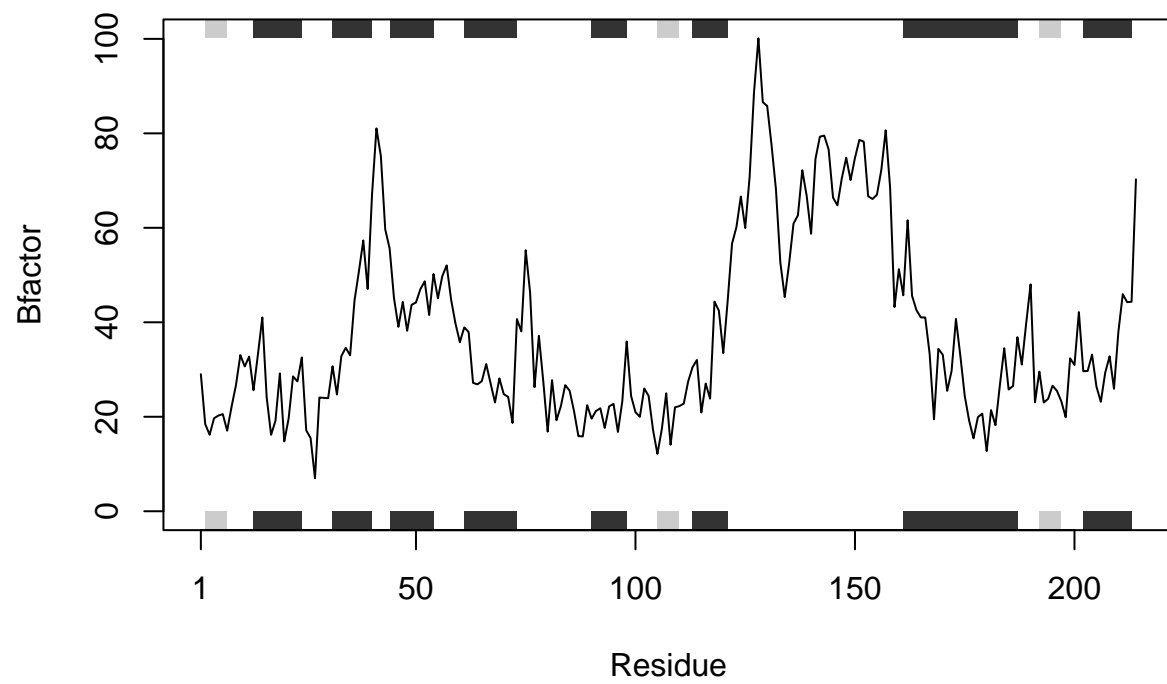
```
s2 <- read.pdb("1AKE") # kinase no drug
```

```
## 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
```

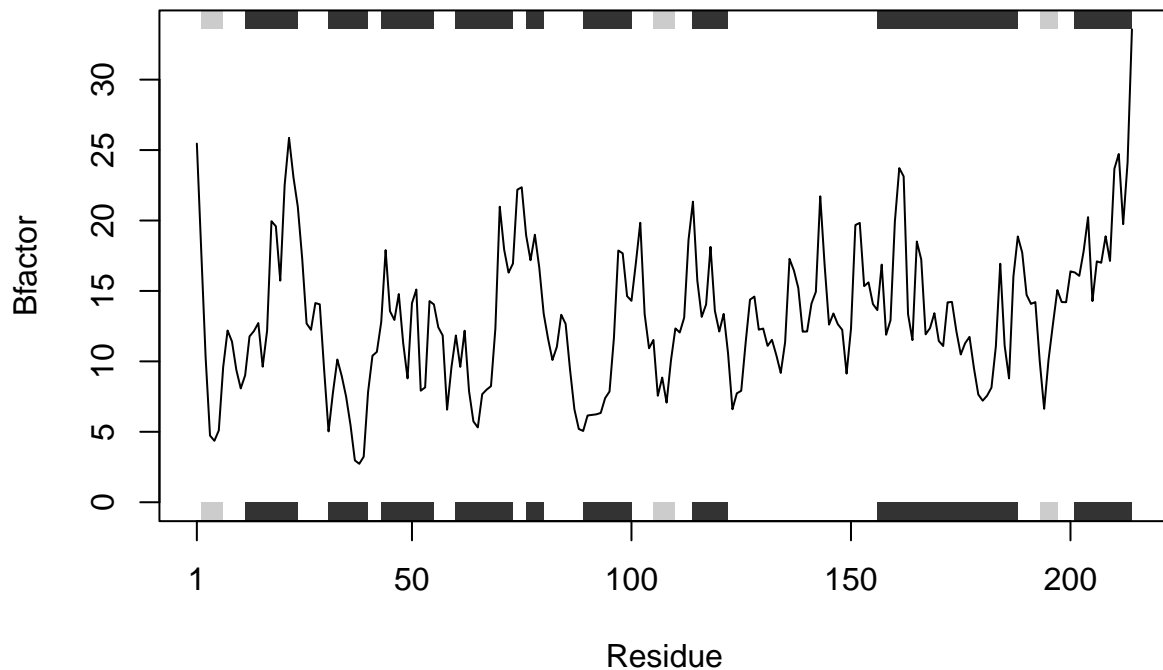
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")  
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")  
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")  
  
s1.b <- s1.chainA$atom$b  
s2.b <- s2.chainA$atom$b  
s3.b <- s3.chainA$atom$b  
  
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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



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



To make function, let's make a PDB code the argument/input (pdbCode) for the function.

This function will output the Bfactor by residue line plot for the particular protein PDB code entered. Specifically, this is done by first excluding all but the 'A' chain of the protein.

Since in the example, each 'block' of the function is written three times for three different PDB codes, I just took one of each and generalized these lines to 's' rather than 's1', 's2', or 's3'. This is because the new function only takes in one PDB code.

To call the function, just write improvedPDBFunc() and write the desired PDB code in quotes inside the parenthesis.

```
improvedPDBFunc <- function(pdbCode) {
  s <- read.pdb(pdbCode)
  s.chainA <- trim.pdb(s, chain="A", elety="CA")
  s.b <- s.chainA$atom$b
  plotb3(s.b, sse=s.chainA, typ="l", ylab="Bfactor")
}
```

Example function run:

```
improvedPDBFunc('4AKE')
```

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

```
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/5b/
## nx310gbn5pd_zqfnjpsgkt200000gn/T//Rtmp9jZ5jI/4AKE.pdb exists. Skipping download
```

