

Class 6 Homework

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Original Code:

```
# 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

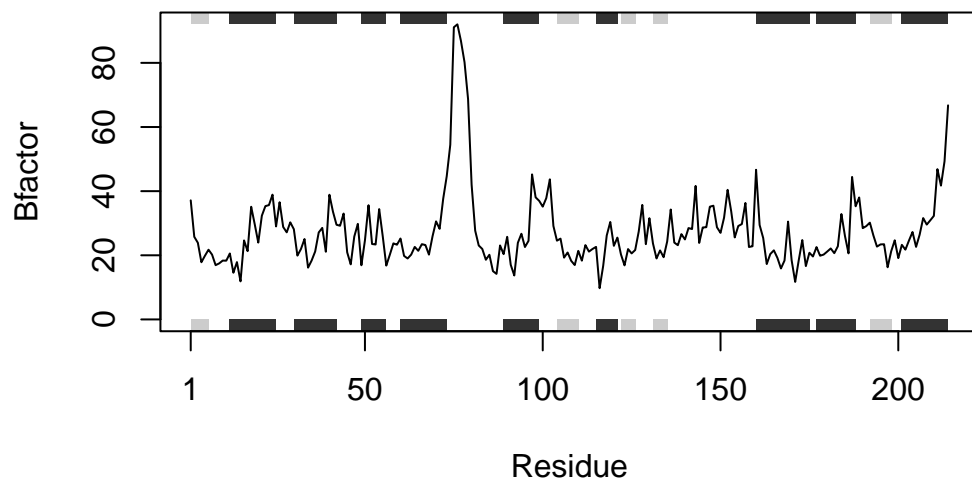
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

Note: Accessing on-line PDB file

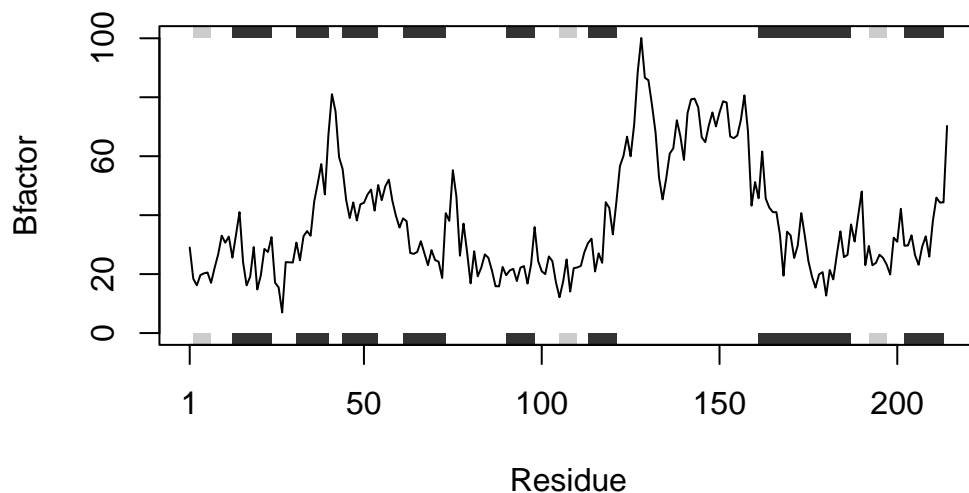
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")  
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")  
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")  
s1.b <- s1.chainA$atom$b  
s2.b <- s2.chainA$atom$b  
s3.b <- s3.chainA$atom$b  
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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



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



Writing the Function

```
library(bio3d) #loading bio3d package

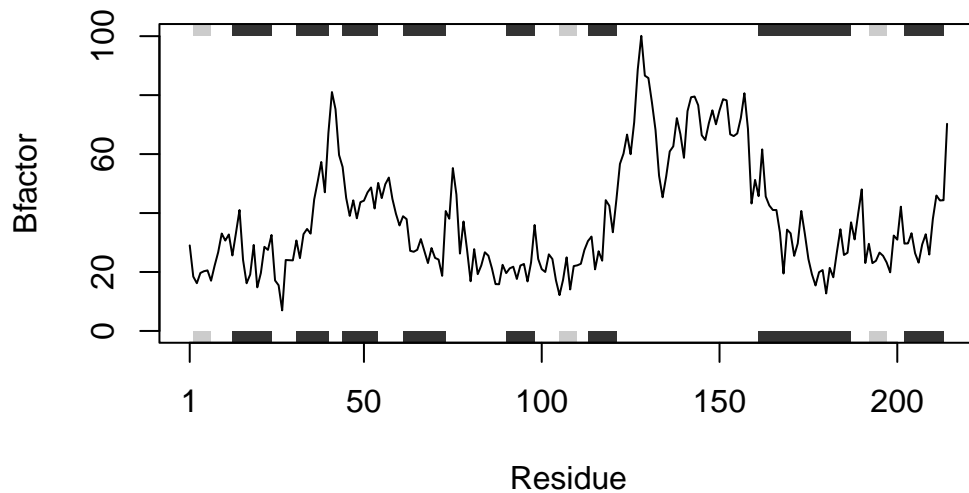
#Compressing the original code to a function called 'visualize()', which iterates
#pdb accession files through the functions defined below
visualize <- function(x) {
  pdb <- read.pdb(x) #reading pdb file
  trim <- trim.pdb(pdb, chain = "A", eley = "CA") #removing metadata
  atomb <- trim$atom$b #accessing atom level data
  plotb3(atomb, sse = trim, typ = "l", ylab = "Bfactor") #plotting bfactor
}
```

Testing, Testing, 1, 2, 3...

```
#Output of the function, inputting pdb accession codes into function  
visualize("4AKE")
```

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/wd/9lxssr4x6qj8knq0ng53tgqw0000gn/T//Rtmpx6Euod/4AKE.pdb exists.
Skipping download

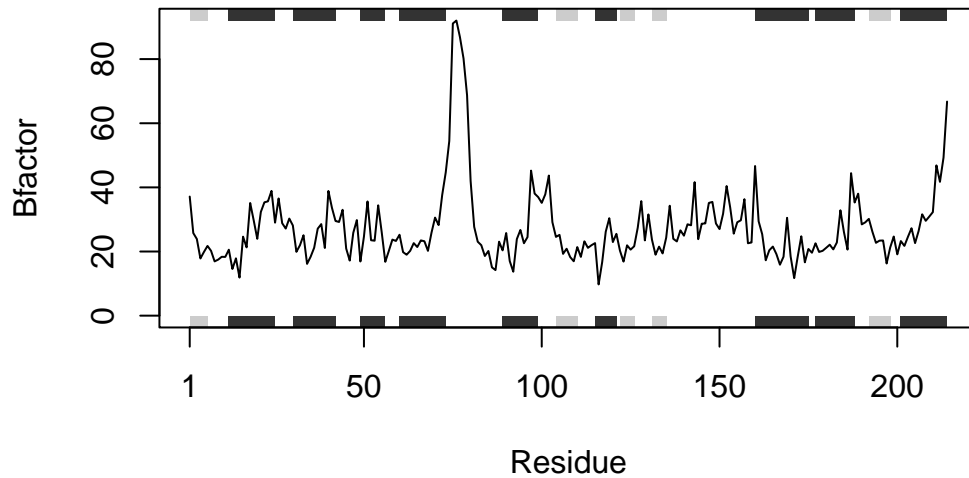


```
visualize("1AKE")
```

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/wd/9lxssr4x6qj8knq0ng53tgqw0000gn/T//Rtmpx6Euod/1AKE.pdb exists.
Skipping download

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



```
visualize("1E4Y")
```

Note: Accessing on-line PDB file

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):  
/var/folders/wd/9lxssr4x6qj8knq0ng53tgqw0000gn/T//Rtmpx6Euod/1E4Y.pdb exists.  
Skipping download
```

