

HW6

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#Q6

Original 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

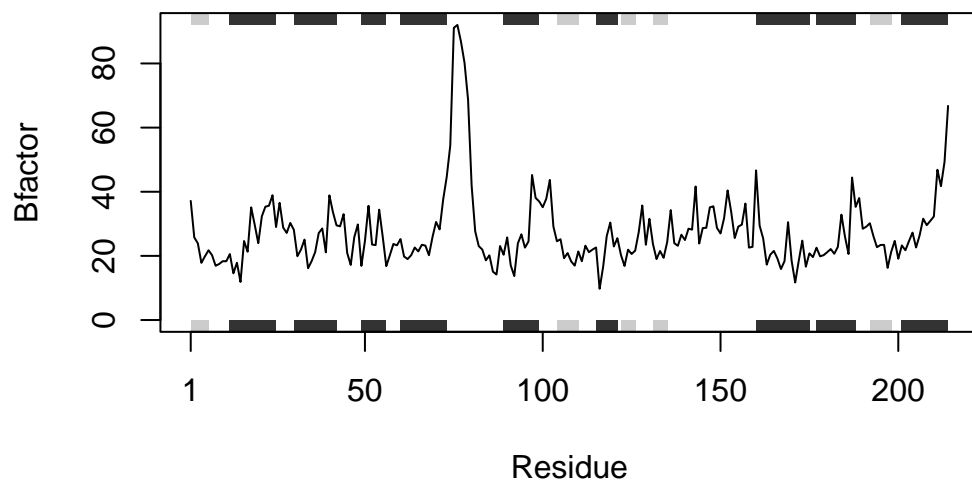
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

Note: Accessing on-line PDB file

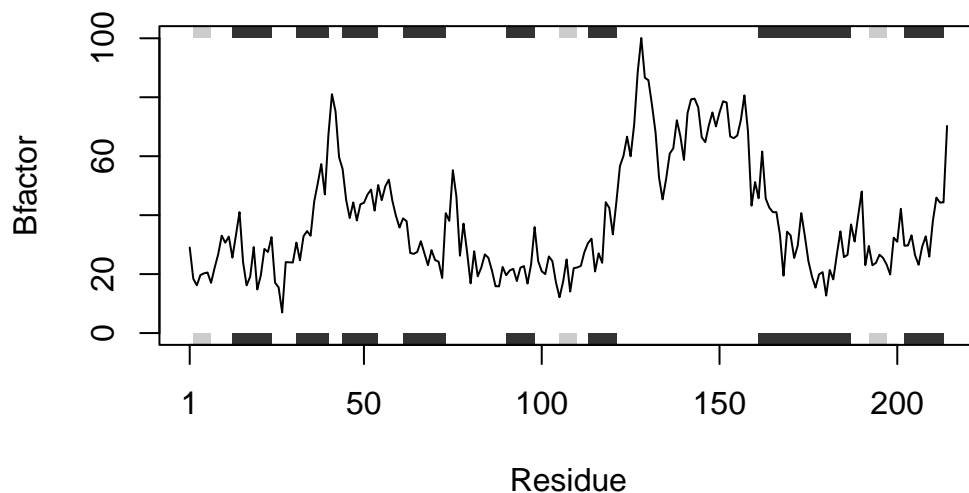
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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



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



Input: PDB accession code WITH “ ” Output: plot of residue position v. Bfactor Method:

1. Read PDB file into variable
2. Trim PDB file of all atoms except for alpha carbons in chain A (CA)
3. Store Bfactor as variable
4. Plot residue position v. stored Bfactor

Improved code:

```
#load bio3d package into environment
library(bio3d)

#create function to automate PDB analysis
plot_Bfactor <- function(x){
  #read and store PDB file from PDB accession code
  pdb <- read.pdb(x)

  #trim stored pdb file for alpha carbons in chain A
```

```

pdb_chainA <- trim.pdb(pdb, chain="A", eley="CA")

#store Bfactors so they can be easily passed to function for creation of plot
pdb_Bfactor <- pdb_chainA$atom$b

#plot residue position v. Bfactor for input PDB
plotb3(pdb_Bfactor, sse=pdb_chainA, typ="l", ylab="Bfactor")
}

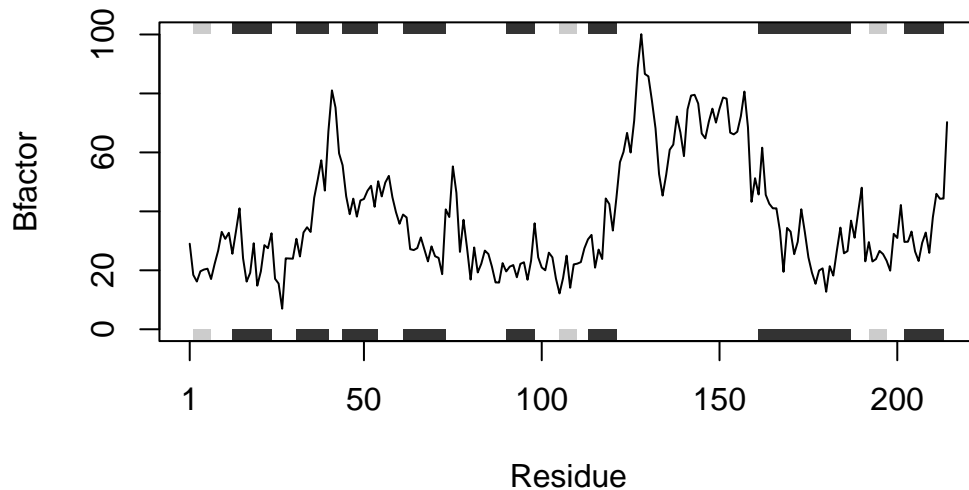
```

Testing code:

```
plot_Bfactor("4AKE")
```

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\NATETR~1\AppData\Local\Temp\RtmpILvqzF\4AKE.pdb exists. Skipping
download

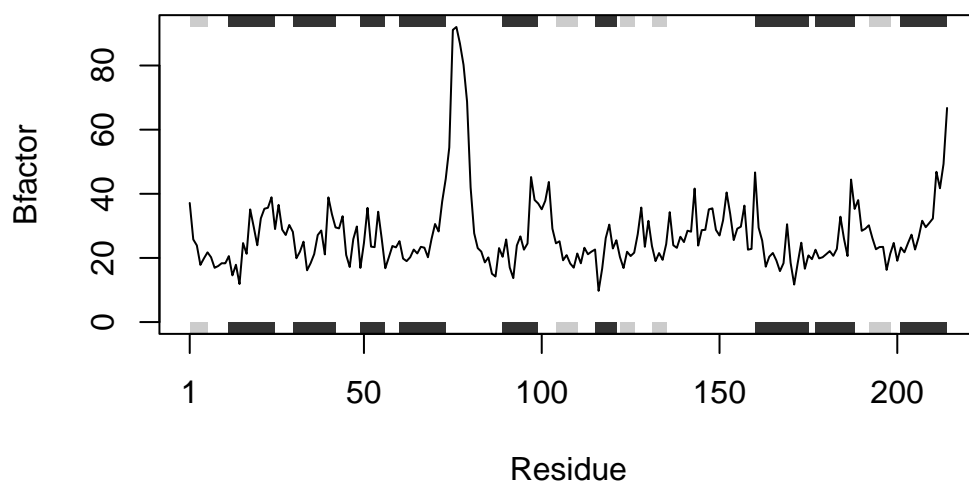


```
plot_Bfactor("1AKE")
```

Note: Accessing on-line PDB file

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

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



```
plot_Bfactor("1E4Y")
```

Note: Accessing on-line PDB file

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

