HW 06

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Can you improve this analysis code?

Previous Code

```
library(bio3d)

s1 <- read.pdb("4AKE") # kinase with drug
```

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

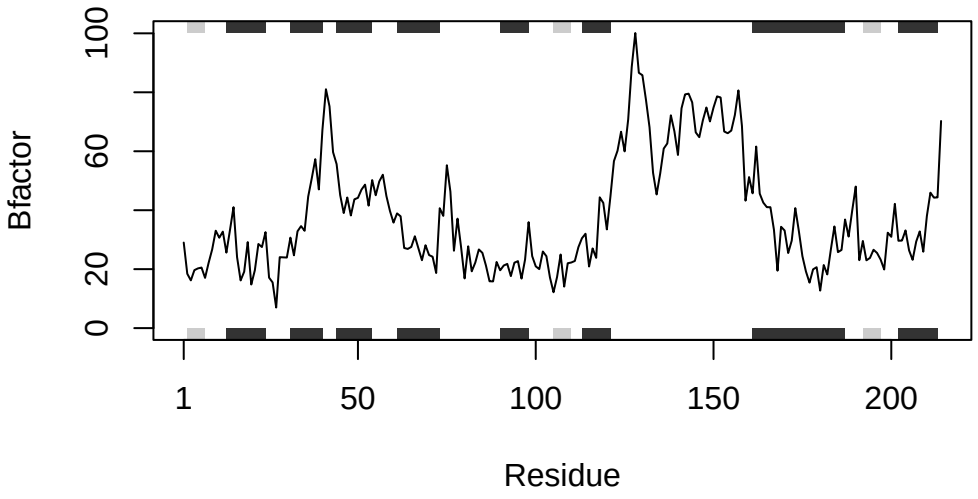
```
s2 <- read.pdb("1AKE") # kinase no drug
```

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

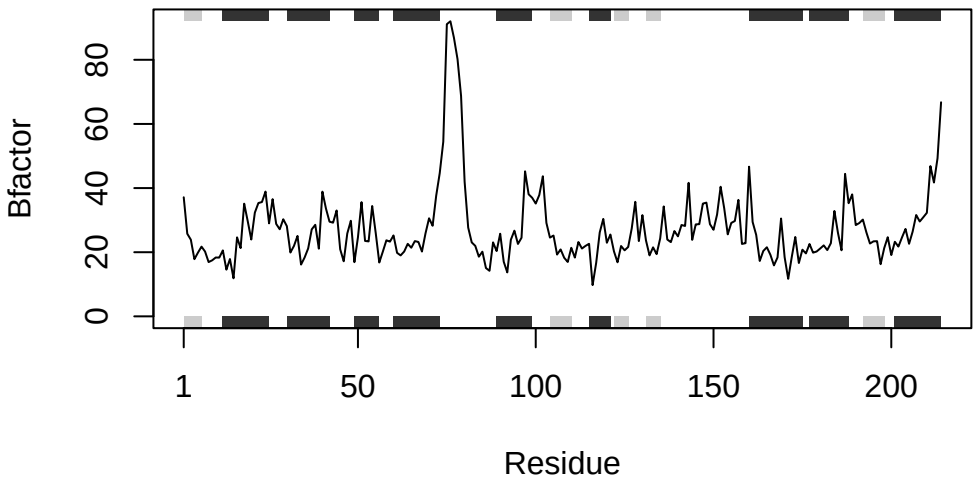
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

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

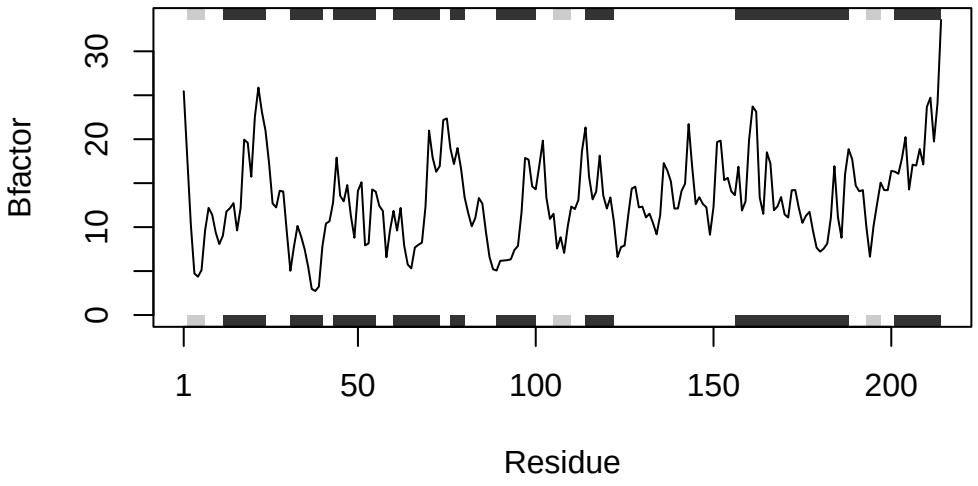
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")

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")
```



New Function

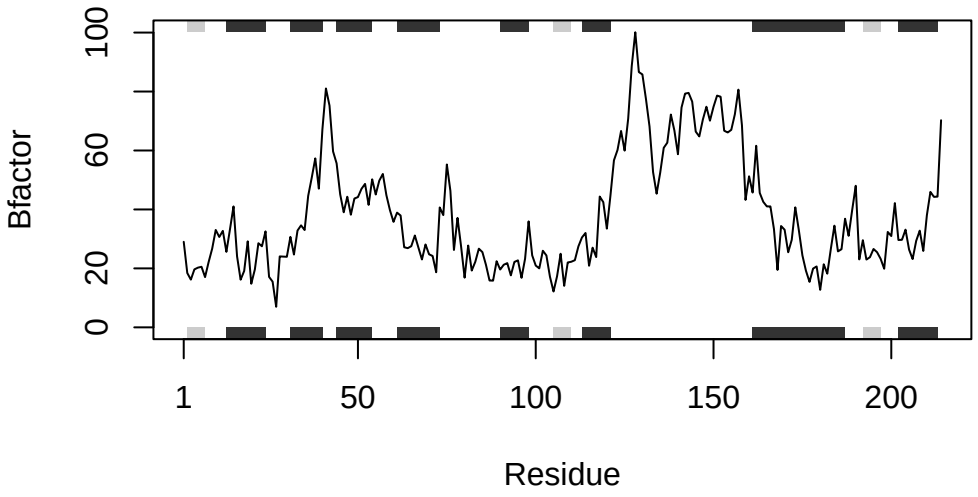
```
library(bio3d)

plot_pdb_id <- function(pdb_id) {
  #Reading pdb file
  pdb_id <- read.pdb(pdb_id)
  #Extracting the A chain
  s.chainA <- trim.pdb(pdb_id, chain="A",elety="CA")
  #Extracting the atom (Bfactor)
  s.b <- s.chainA$atom$b
  #Plot Bfactor vs. Residue
  plotb3(s.b, sse =s.chainA, typ="l", ylab="Bfactor")}
```

Now a user can use the "plot_pbd_id" function to plot any 4 character pdb identifier to get a plot of the Bfactor to the residue of the chain. (Ex. "4AKE" is shown below)

```
plot_pdb_id("4AKE")
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/3_/
4g_tn94d3jd95tzqfht5kqjh0000gn/T//Rtmpqipqnq/4AKE.pdb exists. Skipping download
```

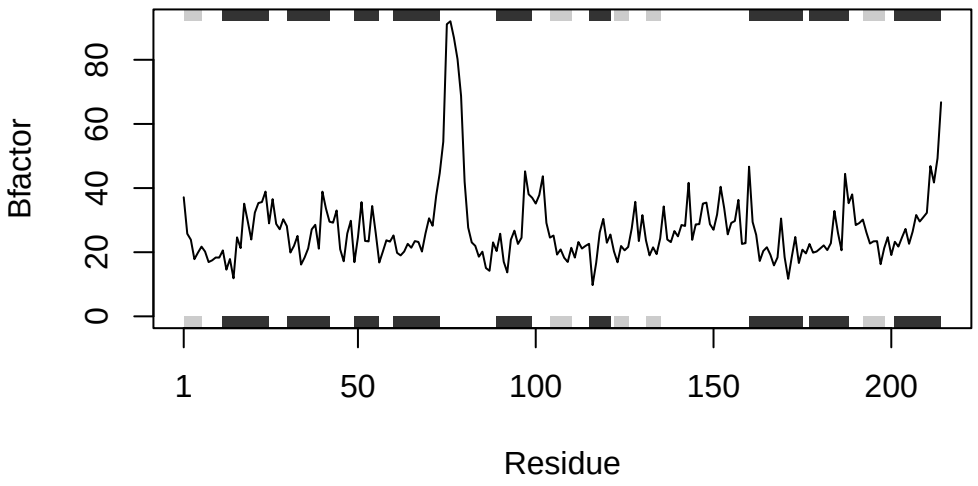



```
plot_pdb_id("1AKE")
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/3_/
4g_tn94d3jd95tzqfht5kqjh0000gn/T//Rtmpqipqnq/1AKE.pdb exists. Skipping download
```

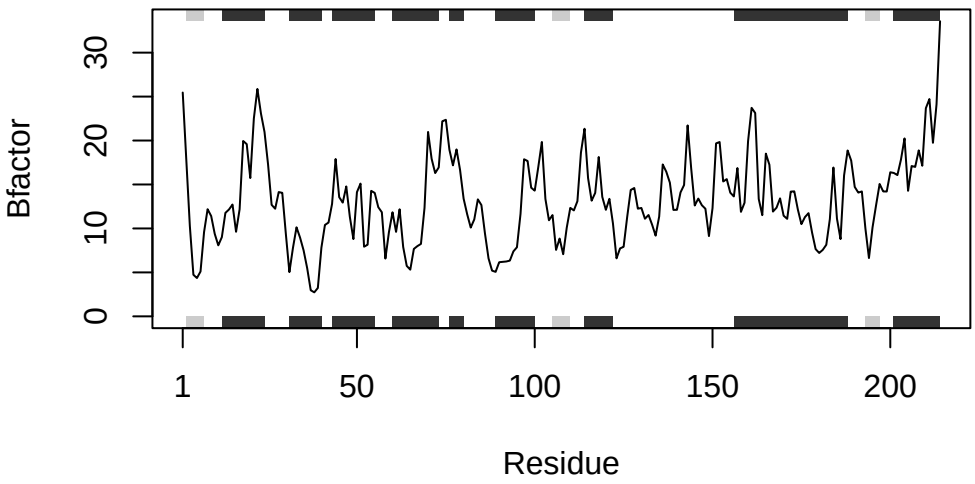
```
   PDB has ALT records, taking A only, rm.alt=TRUE
```




```
plot_pdb_id("1E4Y")
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/3_/
4g_tn94d3jd95tzqfht5kqjh0000gn/T//Rtmpqipqnq/1E4Y.pdb exists. Skipping download
```


Bfactor
0
10
20
30
1
50
100
150
200
Residue