class06_supplement

```
library(bio3d)
s1 <- read.pdb("4AKE") # kinase with drug
```

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

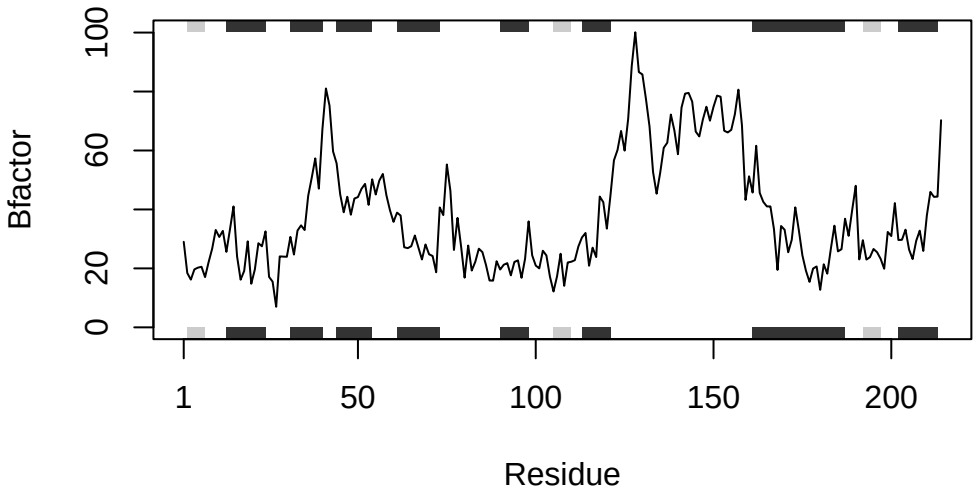
```
s2 <- read.pdb("1AKE") # kinase no drug
```

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

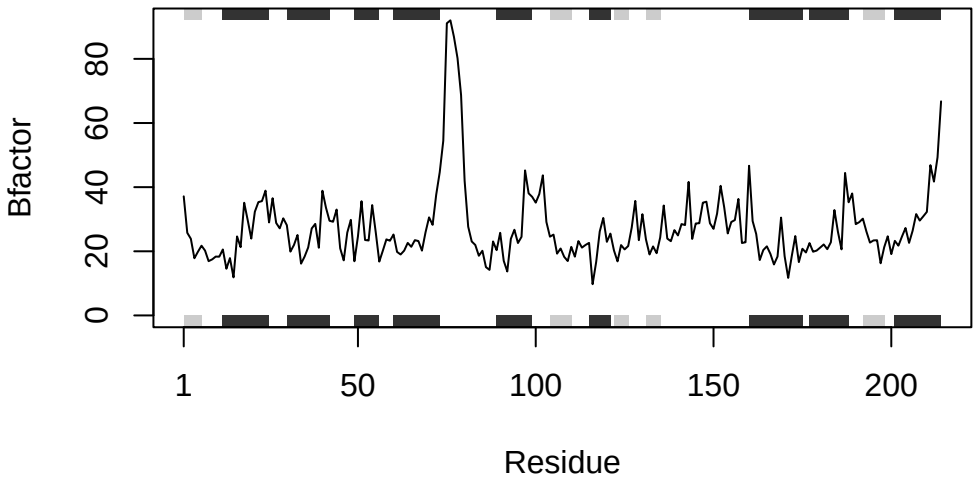
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

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

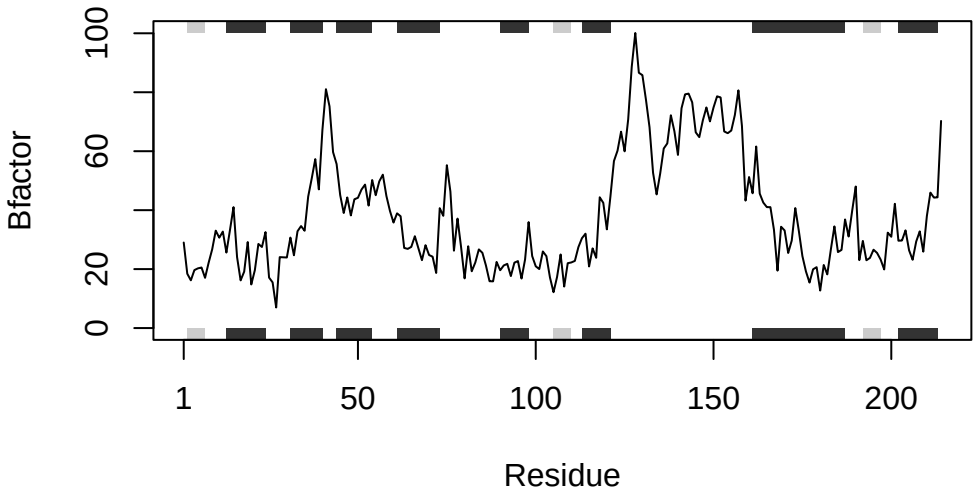
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```




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



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



The inputs are various accession values of proteins from PDB.

It appears that this function reads values from pdb, trims certain values from the dataset, compares two categories, and finally provides plots as the output.

The output are plots of bfactor of the given proteins with their residue number.

I will now attempt to rewrite this code, correcting for an error in one of the lines with a copy+paste error.

s1 <- read.pdb("4AKE") s1.chainA <- trim.pdb(s1, chain="A", elety="CA") s1.b <- s1.chainA*atom*b plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor") #input = "4AKE"

Simplified code:

pdbcode <- {("4AKE") pdb < - read.pdb (pdbcode) chain <- trim.pdb() s1.b <- s1.chainA*atom*b plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")} #input = "4AKE"