HW06

Danika

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

Note: Accessing on-line PDB file

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

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

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

Note: Accessing on-line PDB file

```r
# This is the input code
x <- "4AKE"
a <- read.pdb(x)
```

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose =
FALSE): /var/folders/x9/r3h9zcq9533g921wcjbjvh480000gn/T//RtmpAKXRT0/4AKE.pdb
exists. Skipping download

```
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")

a.chainA <- trim.pdb(a, chain="A", elety="CA")

s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b

a.b <- a.chainA$atom$b

plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```
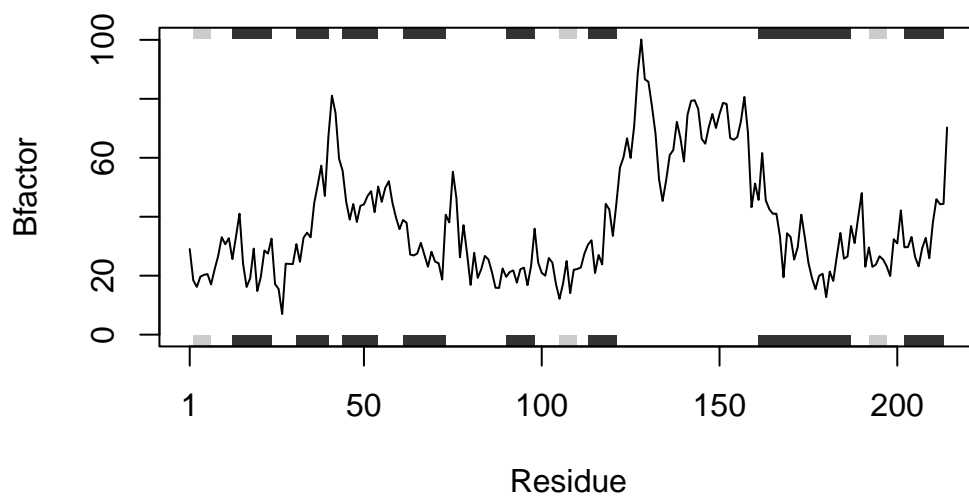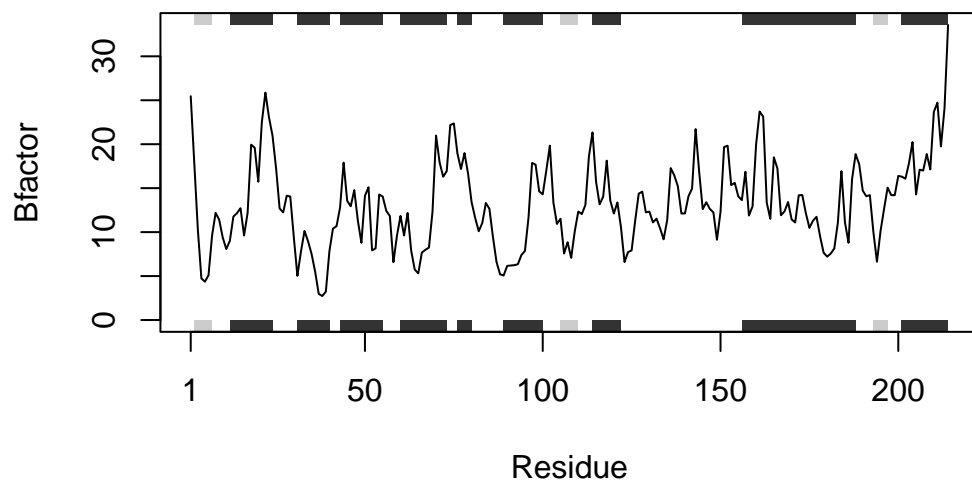


```
plotb3(s2.b, sse=s2.chainA, typ="l", ylab="Bfactor")
```
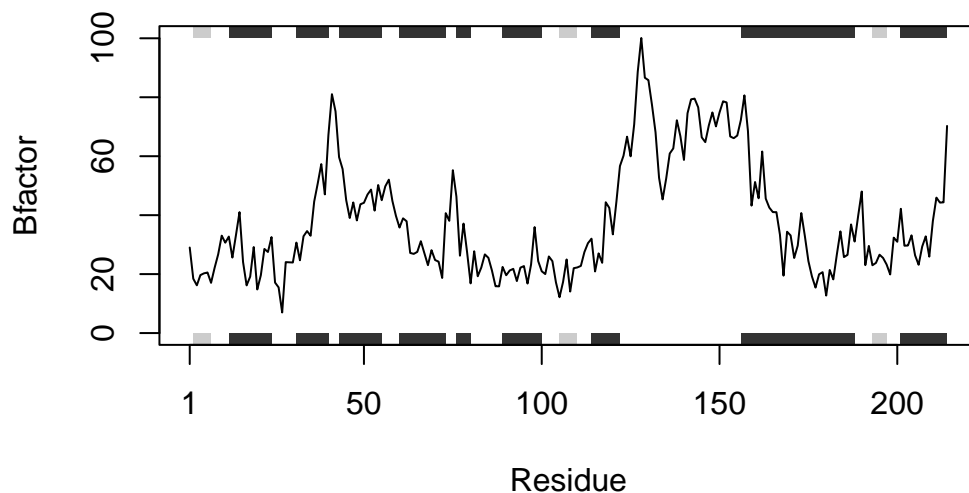
```
plotb3(s3.b, sse=s3.chainA, typ="l", ylab="Bfactor")
```

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


Should read any protein PDB data and outputs a plot
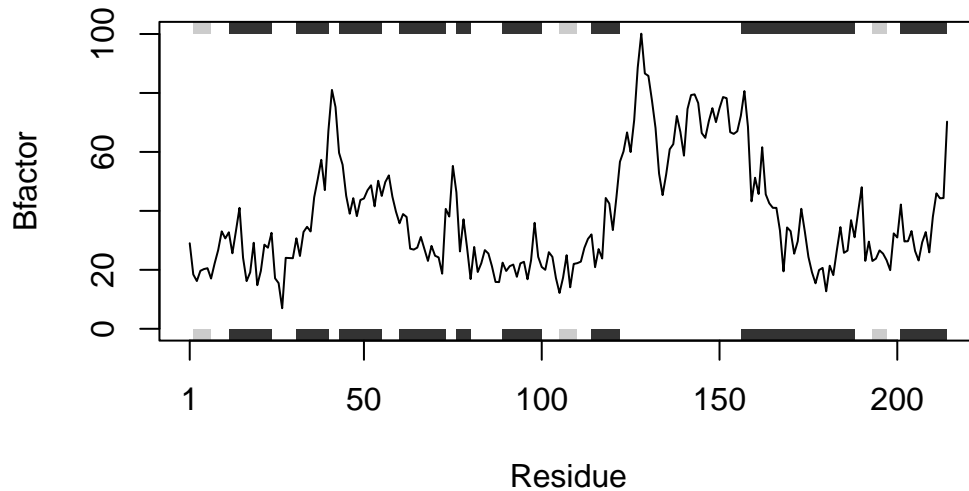
```
library(bio3d)
x <- "4AKE"

newfunction <- function(x){
  a <- read.pdb(x)
  a.chainA <- trim.pdb(a, chain="A", elety="CA")
  a.b <- a.chainA$atom$b
  plotb3(a.b, sse=s3.chainA, typ="l", ylab="Bfactor")
}

newfunction(x)
```

  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose =

4

FALSE): /var/folders/x9/r3h9zcq9533g921wcjbjvh480000gn/T//RtmpAKXRT0/4AKE.pdb
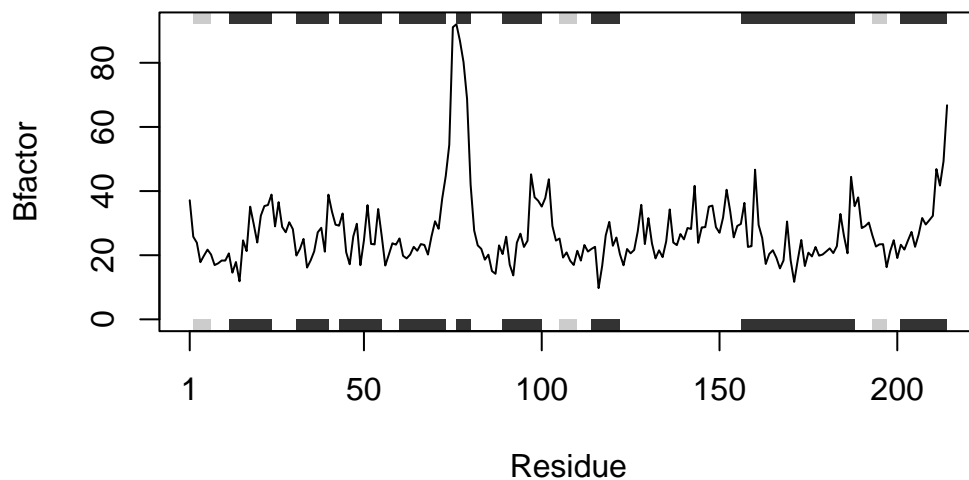exists. Skipping download


```
newfunction("1AKE")
```

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose =
FALSE): /var/folders/x9/r3h9zcq9533g921wcjbjvh480000gn/T//RtmpAKXRT0/1AKE.pdb
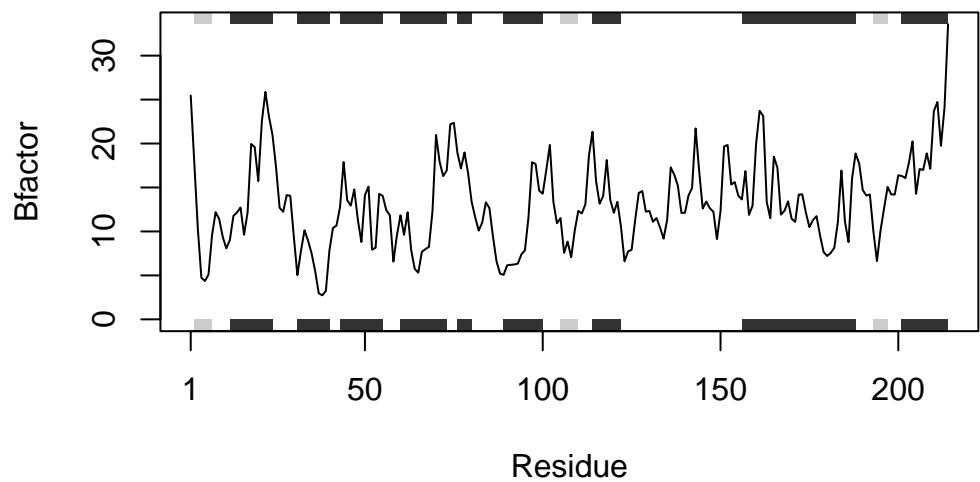exists. Skipping download

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

```
newfunction("1E4Y")
```

  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose =
FALSE): /var/folders/x9/r3h9zcq9533g921wcjbjvh480000gn/T//RtmpAKXRT0/1E4Y.pdb
exists. Skipping download

The graphs are the output