HW Class 6

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##Original code:

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

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

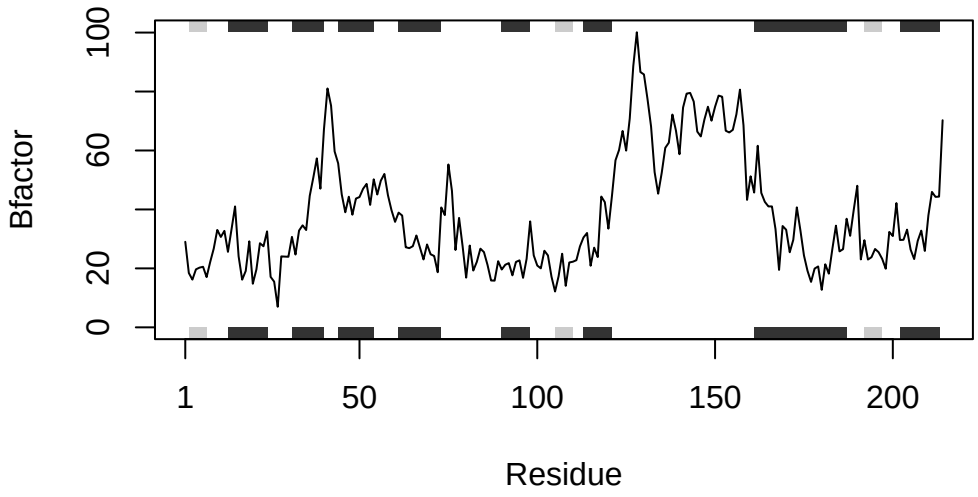
```
s2 <- read.pdb("1AKE")  # kinase no drug
```

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

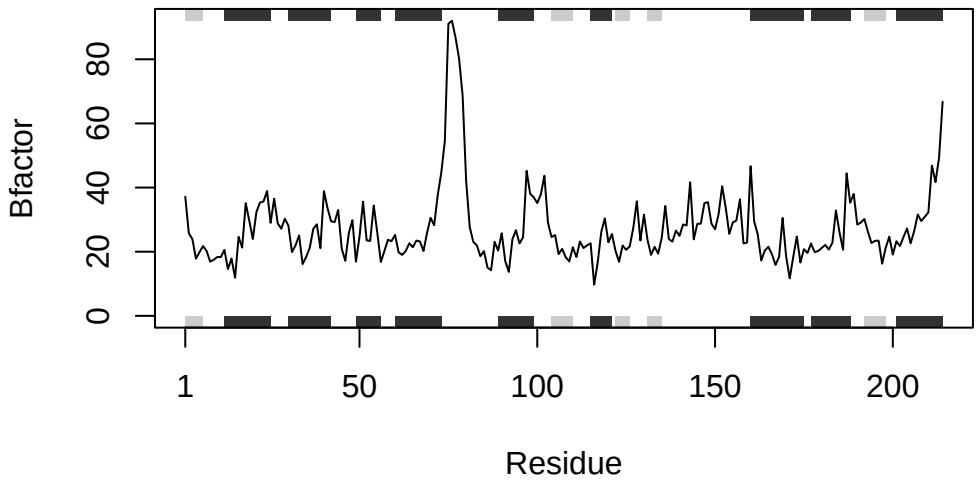
```
s3 <- read.pdb("1E4Y")  # kinase with drug
```

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

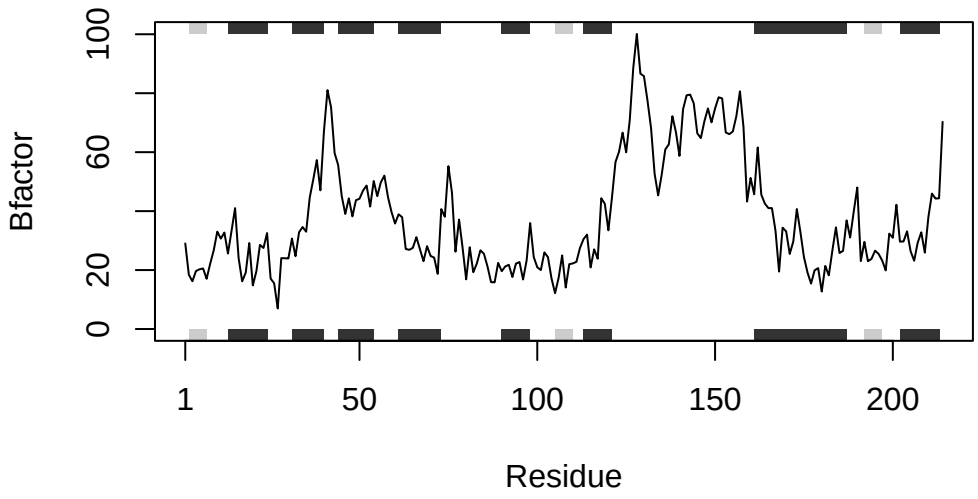
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```




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



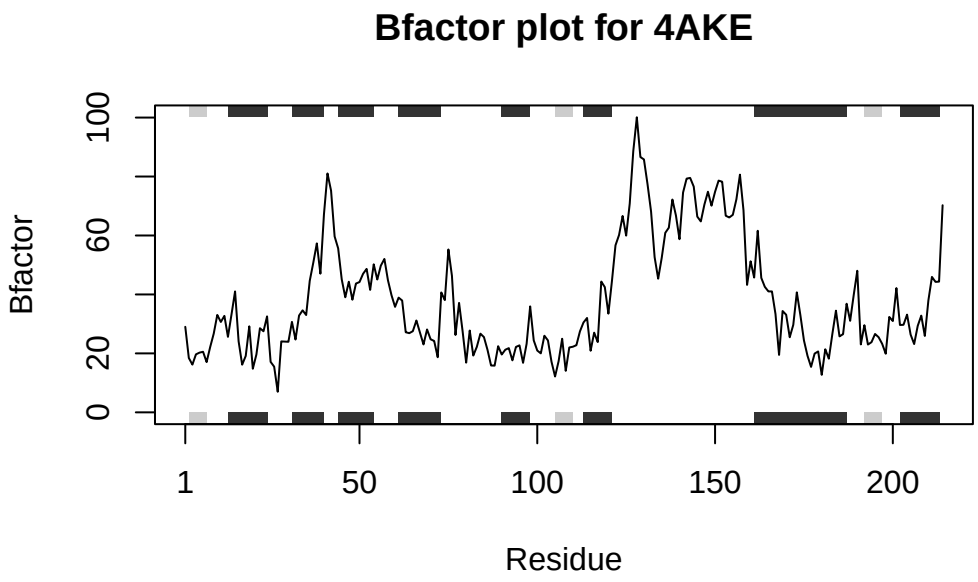
```
plotb3(s3.b, sse=s3.chainA, typ="l", ylab="Bfactor")
```



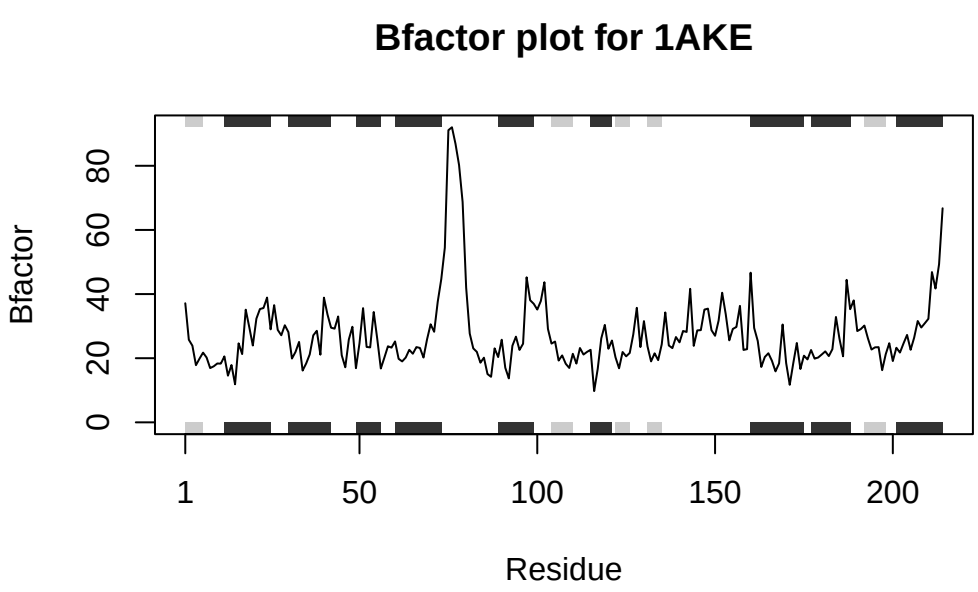
##Improved code:

```
library(bio3d)
plotb3factor <- function(protein_id){
  for (id in protein_id){
    protein <- read.pdb(id)
    chainA <- trim.pdb(protein, chain="A", elety="CA")
    bfactor <- chainA$atom$b
    plotb3(bfactor,sse=chainA,typ="l", ylab="Bfactor", main=paste("Bfactor plot for", id))
  }
}
#Test
plotb3factor(c("4AKE", "1AKE", "1E4Y"))
```

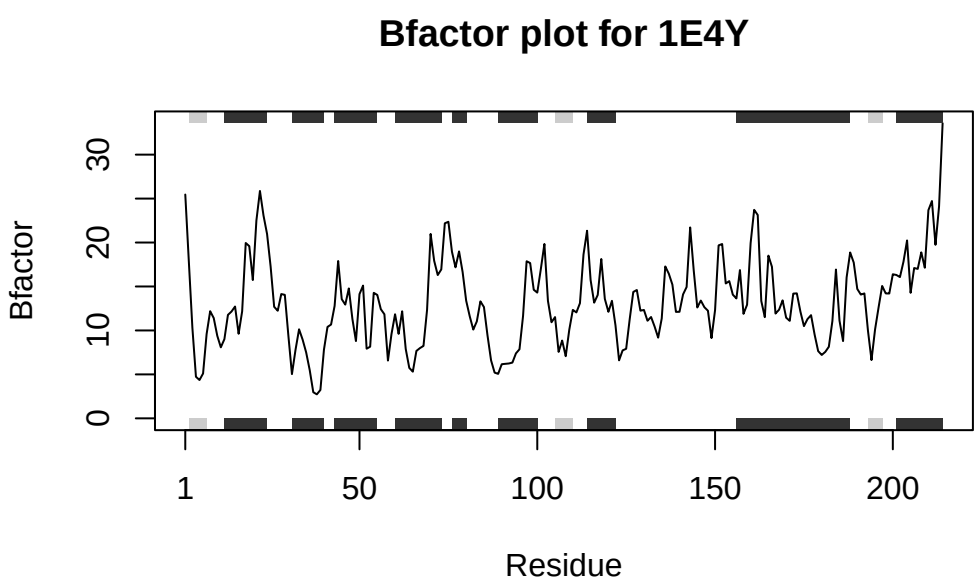
```
  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/hf/y1pqvvwd0v11pdxh10fw5hy80000gn/T//RtmpsUflj4/4AKE.pdb exists.
Skipping download
```




```
  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/hf/y1pqvvwd0v11pdxh10fw5hy80000gn/T//RtmpsUflj4/1AKE.pdb exists.
Skipping download

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




```
  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/hf/y1pqvvwd0v11pdxh10fw5hy80000gn/T//RtmpsUflj4/1E4Y.pdb exists.
Skipping download
```



##Documentation question The inputs are protein information obtained from PDB. The function takes in the protein and trim it to leave only chain A. The element type is set to the alpha carbon atom. Then, the function extracts column B information from chain A atoms, and names as bfactor. The function next uses chain A as the secondary structure element to construct a line plot. The label on the y axis is set to Bfactor and on the top the function prints Bfactor plot for a given PDB id. The output is a line graph entailing the Bfactor information of each residue of chain A of a given PDB id.