

Class 6 Quesetion 6

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Q6. Write a function: See Q6 of the hands-on lab supplement above. This entails turning a supplied code snippet into a more robust and re-usable function that will take any of the three listed input proteins and plot the effect of drug binding. Note assessment rubric and submission instructions within document.

Can you improve this analysis 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

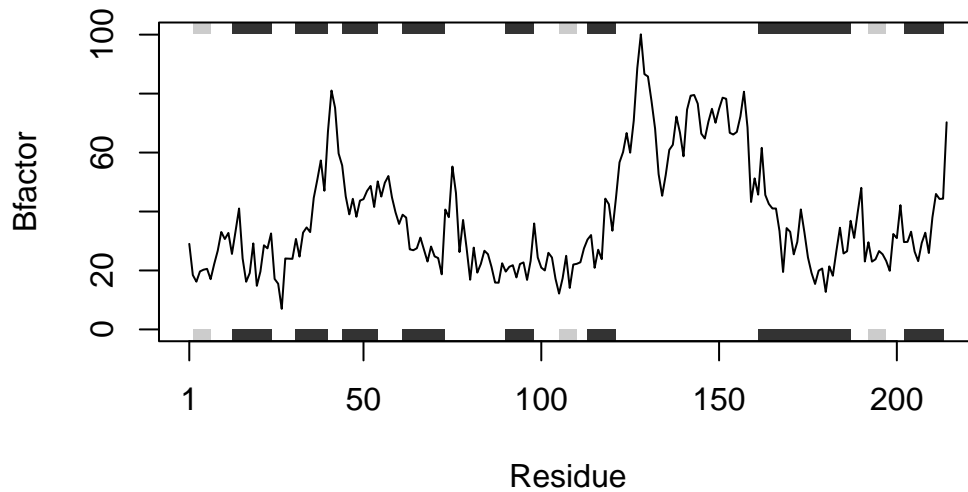
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

Note: Accessing on-line PDB file

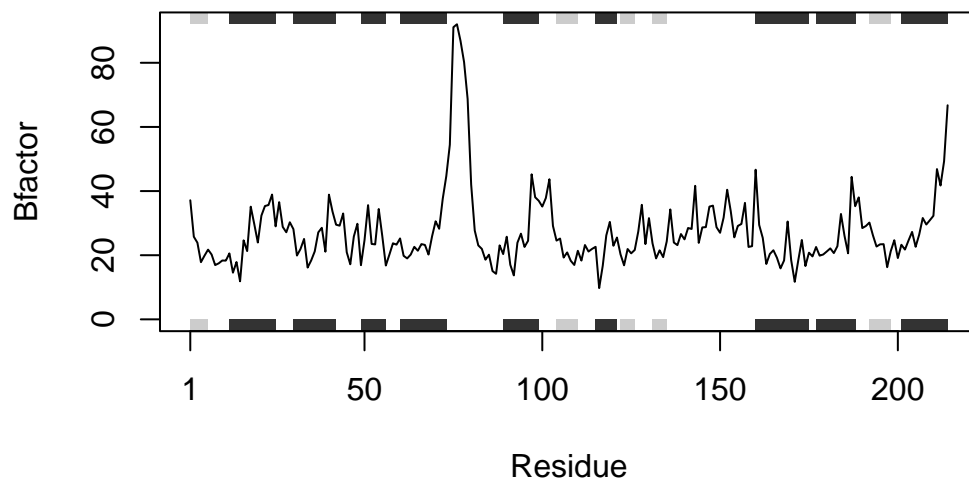
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")

s1.b <- s1.chainA$atom$b
```

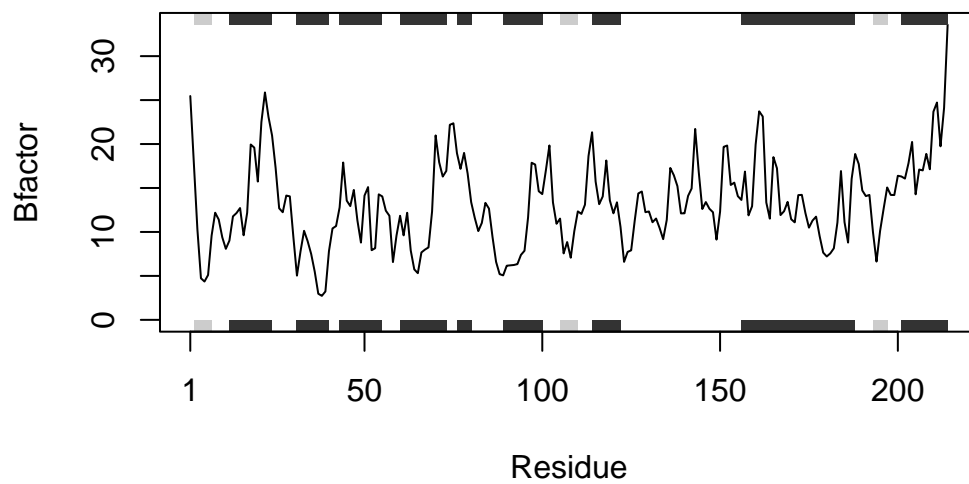
```
s2.b <- s2.chainA$atom$b  
s3.b <- s3.chainA$atom$b  
  
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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



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



There was a bug so I changed s1 to s3.

Shorted code:

```
library(bio3d)

functionQ6 <- function(protein) {

  ad <- read.pdb(protein) # this line reads the protein pdb file
  # ad stands for any database

  ad.chainA <- trim.pdb(ad, chain="A", elety="CA") # this line takes the chainA
  # from the database and trims it to a smaller subset of atoms

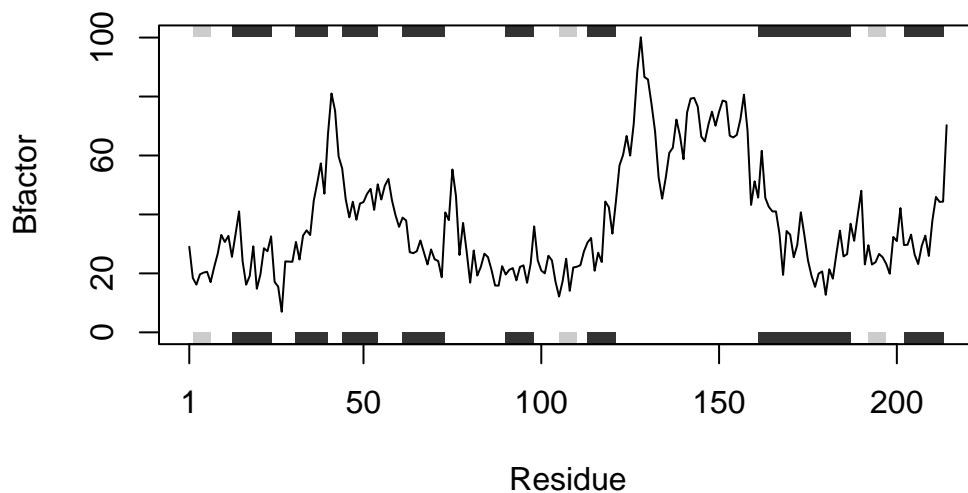
  ad.b <- ad.chainA$atom$b # this line assigns the ad.chainA from above
  # that have the b column to a new variable called ad.b

  plotb3(ad.b, sse=ad.chainA, typ="l", ylab="Bfactor") # this line plots the
  # numbers in the ad.b vector
}

# the input of the function is a pdb file of a specific protein
functionQ6("4AKE")
```

Note: Accessing on-line PDB file

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/0_/srr7hvg1jng7c1cd701sks00000gn/T//RtmpYDov8j/4AKE.pdb exists.
Skipping download
```

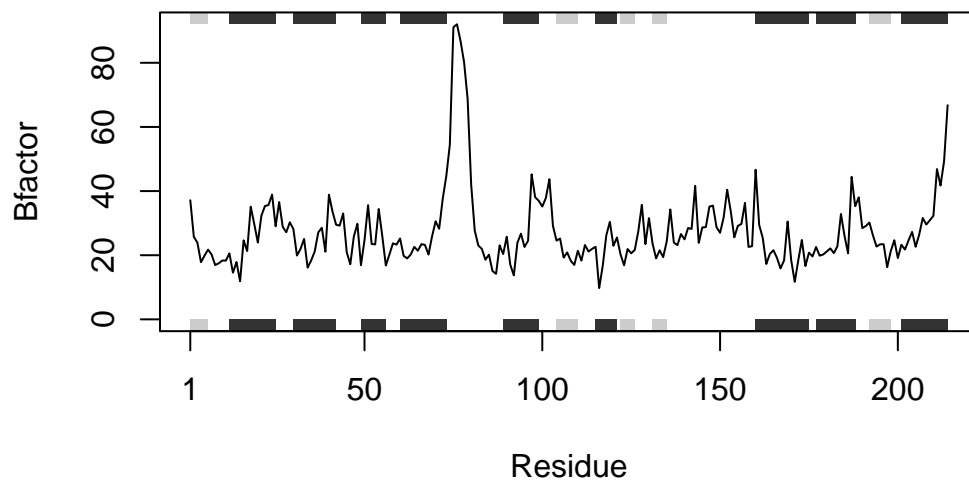


```
functionQ6("1AKE")
```

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/0_/srr7hvgn1jng7c1cd701sks00000gn/T/RtmpYDov8j/1AKE.pdb exists.
Skipping download

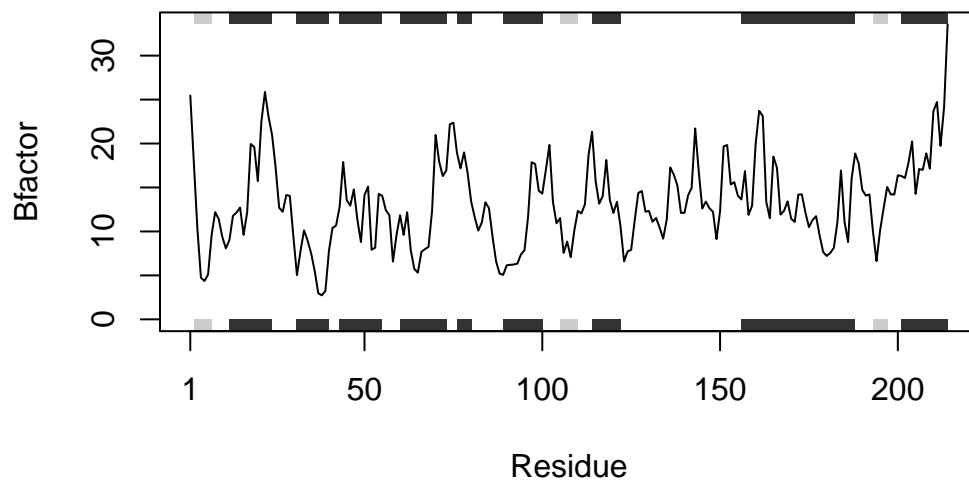
PDB has ALT records, taking A only, rm.alt=TRUE



```
functionQ6("1E4Y")
```

Note: Accessing on-line PDB file

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):  
/var/folders/0_/srr7hvgn1jng7c1cd701sks00000gn/T/RtmpYDov8j/1E4Y.pdb exists.  
Skipping download
```



```
# the output is a standard scatter plot with a line, of the chainA & b category
# of the protein with Beta factor on the y-axis and the residues of the protein
# on the x-axis.
```