Homework6

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The original code

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

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

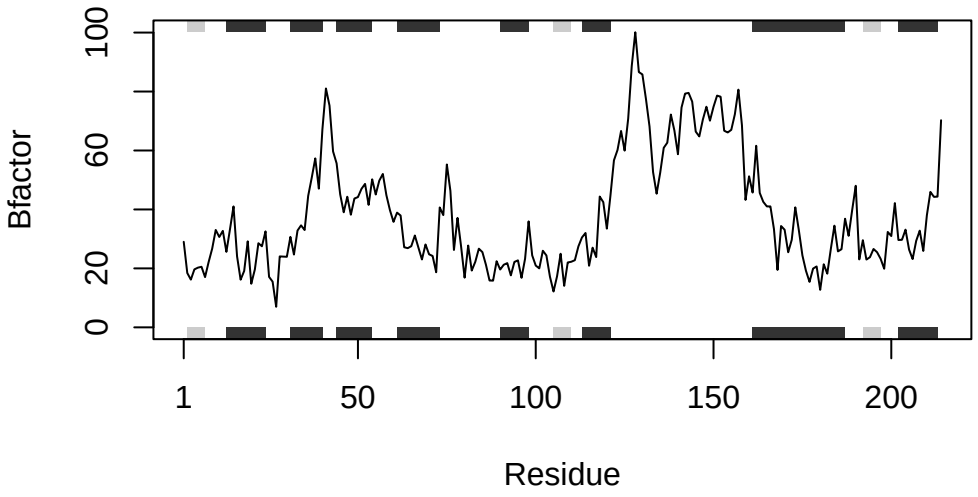
```
s2 <- read.pdb("1AKE")  # kinase no drug
```

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

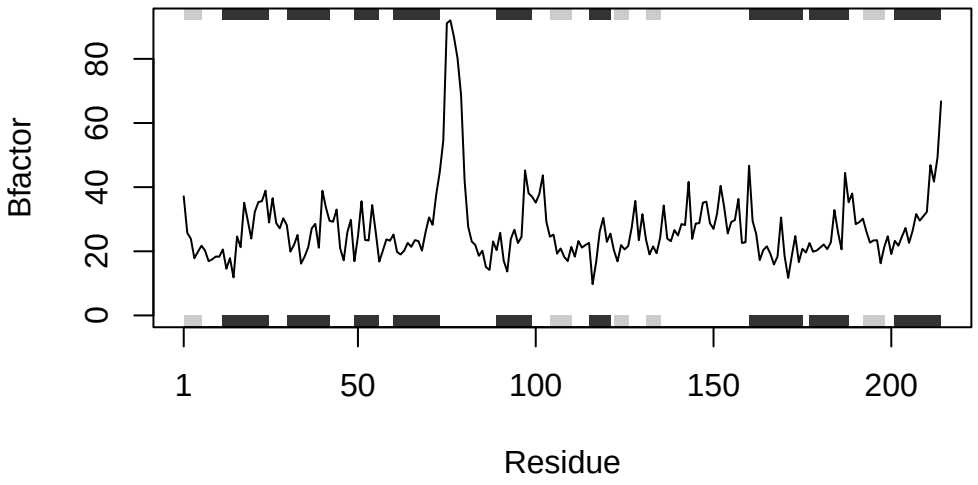
```
s3 <- read.pdb("1E4Y")  # kinase with drug
```

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

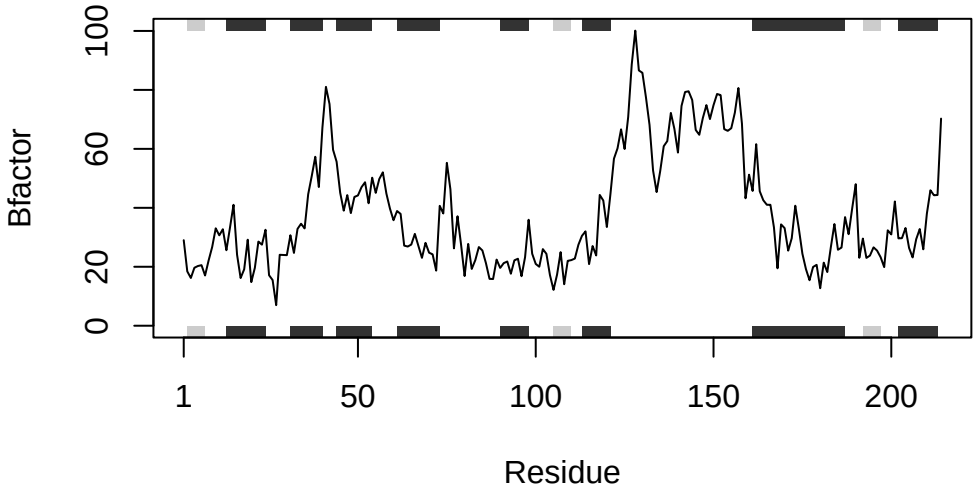
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```




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



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



Q6. How would you generalize the original code above to work with any set of input protein structures?

My generalized version

The following function takes a PDB coordinate as the argument and analyzes protein drug interactions and outputs a plot for the specified protein.

```
# 'input' is the PDB coordinate
plot <- function(input) {
  # reads the PDB coordinate file and stores it in the 'protein' object
  protein <- read.pdb(input)

  # trims the original protein into a smaller subset that only contains
  # chain A of the protein
  chainA <- trim.pdb(protein, chain="A", elety="CA")

  # extracts the B factor information from chain A
```

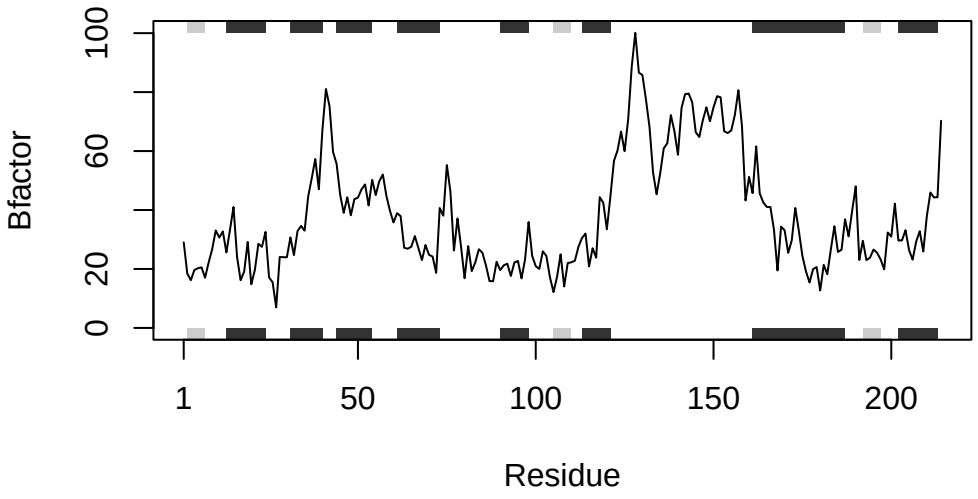
```
  Bfactor <- chainA$atom$b

  # plots the B-factor value against the residue positions
  # The type of plot is set to a line plot
  plotb3(Bfactor, sse=chainA, typ="l", ylab="Bfactor")
}

plot("4AKE")
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/t8/g2cm39vx0blc9lrx93xwqy5m0000gn/T//RtmpqWuXku/4AKE.pdb exists.
Skipping download
```

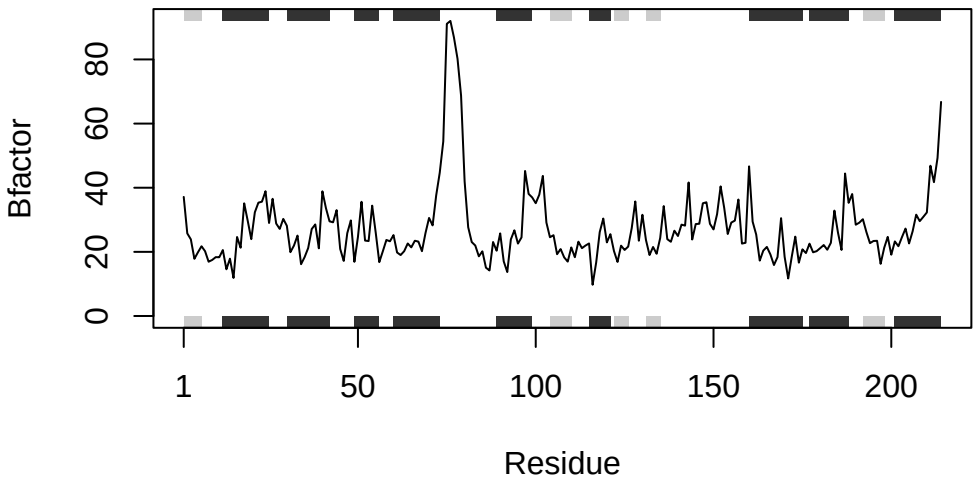



```
plot("1AKE")
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/t8/g2cm39vx0blc9lrx93xwqy5m0000gn/T//RtmpqWuXku/1AKE.pdb exists.
Skipping download
```

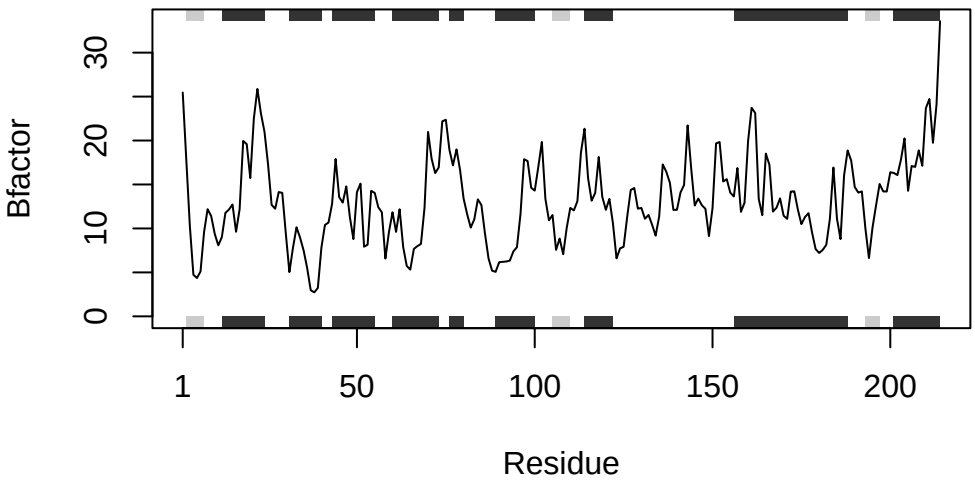
```
   PDB has ALT records, taking A only, rm.alt=TRUE
```




```
plot("1E4Y")
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/t8/g2cm39vx0blc9lrx93xwqy5m0000gn/T//RtmpqWuXku/1E4Y.pdb exists.
Skipping download
```


Bfactor
0
10
20
30
1
50
100
150
200
Residue