Class06: Function Homework

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My Own Function to Analyze Protein-Drug Interactions

Write a function from the supplied code:

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

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

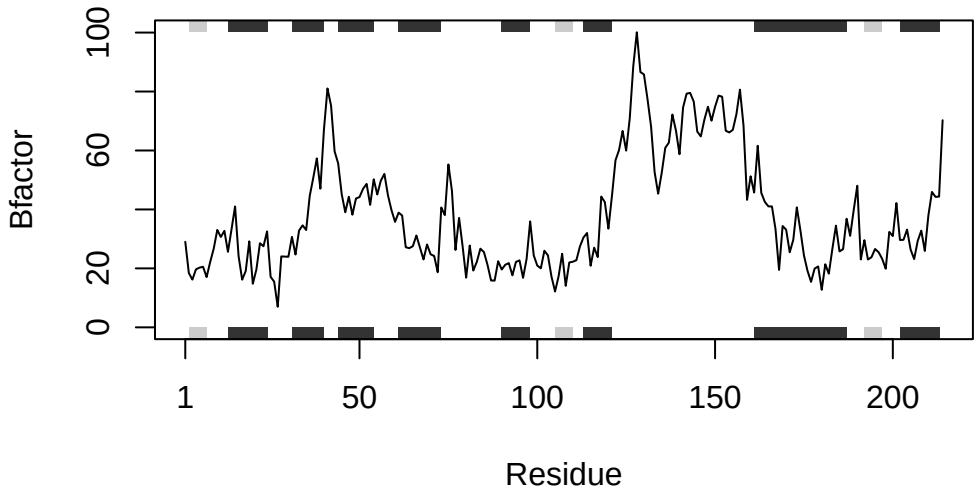
```
s2 <- read.pdb("1AKE") # kinase no drug
```

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

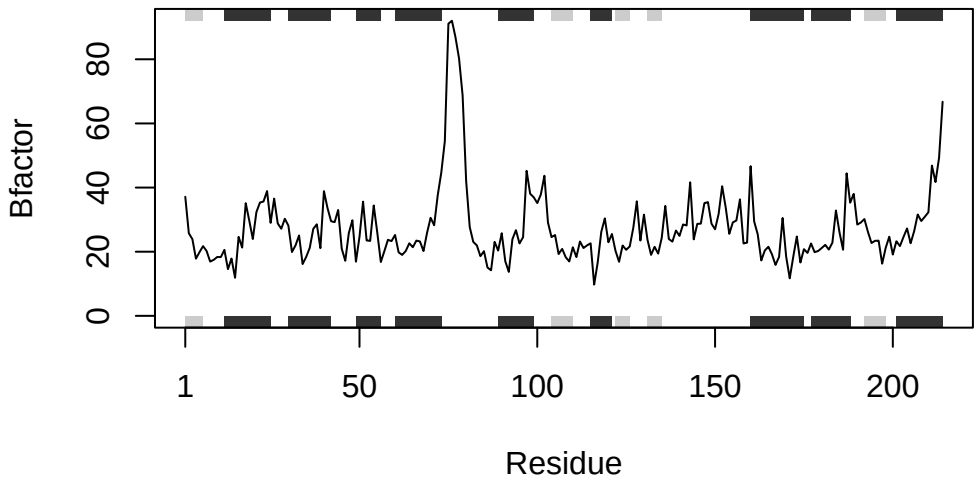
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

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

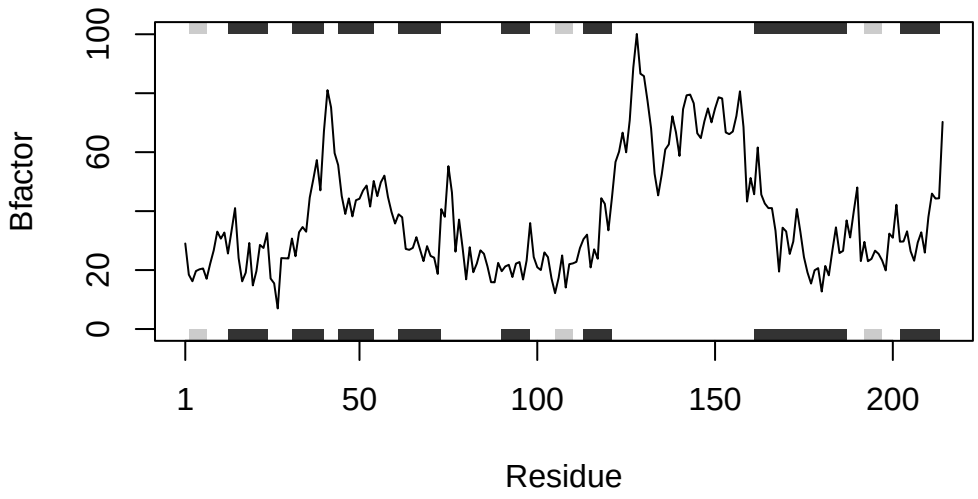
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")

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")
```



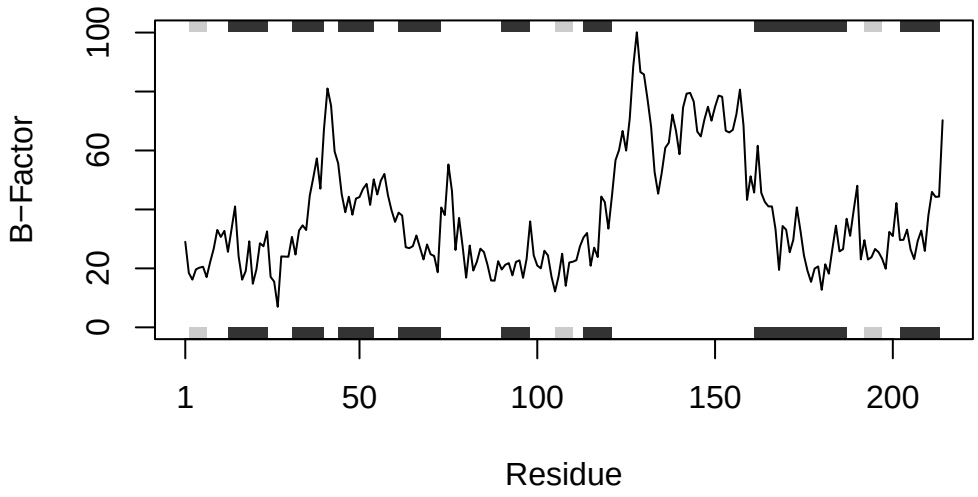
```
plotb3(s3.b, sse=s3.chainA, typ="l", ylab="Bfactor")
```



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

Q6. I began by inputing the "s1" or "4AKE" kinase with the drug into my function. I compared the new resulting plot to the original plot and obtained the same visual.

```
protein_plot <- function(x, y, title="Protein Drug Interaction") {
  s1 <- read.pdb("4AKE")
  s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
  s1.b <- s1.chainA$atom$b
  x=s1.b
  y=s1.chainA
}
plot.bio3d(s1.b, sse=s1.chainA, xlab="Residue", ylab="B-Factor", typ="l")
```



I decided to try this function out with a different PDB code "6TPK" and referred to this PDB code as "s4"

> I first needed to define "s4", "s4.chainA", and "s4.b" to store this data in the R "Environment"

```
s4 <- read.pdb("6TPK")
```

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

```
s4.chainA <- trim.pdb(s4, chain="A", elety="CA")
```

```
s4.b <- s4.chainA$atom$b
```

I obtained a graph of the protein "6TPK" to be able to analyze protein-drug interaction.

> Note: I removed the "sse=s4.chainA" information from the "plot.bio3d()" because it did not align properly with the other plot properties.

```
protein_plot <- function(x, y, title="Protein Drug Interaction") {
  s4 <- read.pdb("6TPK")
  s4.chainA <- trim.pdb(s4, chain="A", elety="CA")
  s4.b <- s4.chainA$atom$b
  x=s4.b
  y=s4.chainA
}
plot.bio3d(s4.b, xlab="Residue", ylab="B-Factor", typ="l")
```