HW Class 6: R Functions

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#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.

```
#install.packages("bio3d")
#library("bio3d")
```

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

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

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

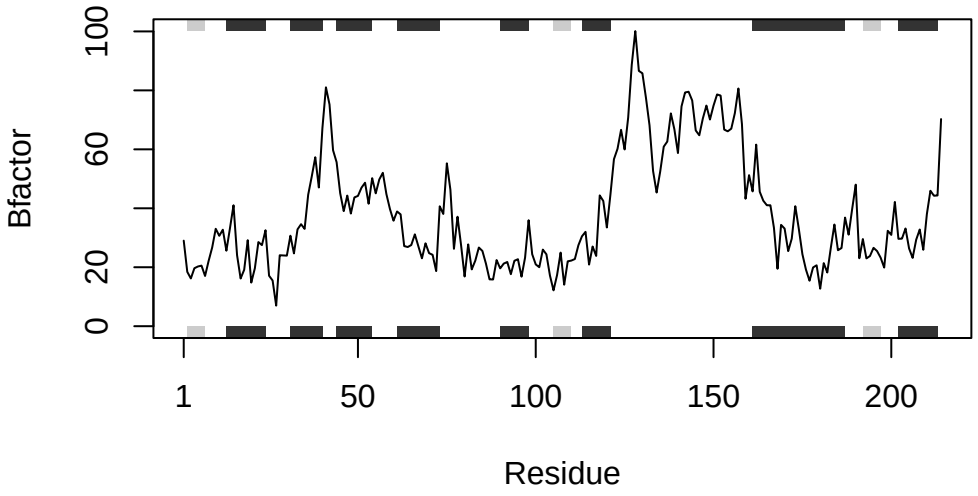
```
Note: Accessing on-line PDB file
 PDB has ALT records, taking A only, rm.alt=TRUE
```

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

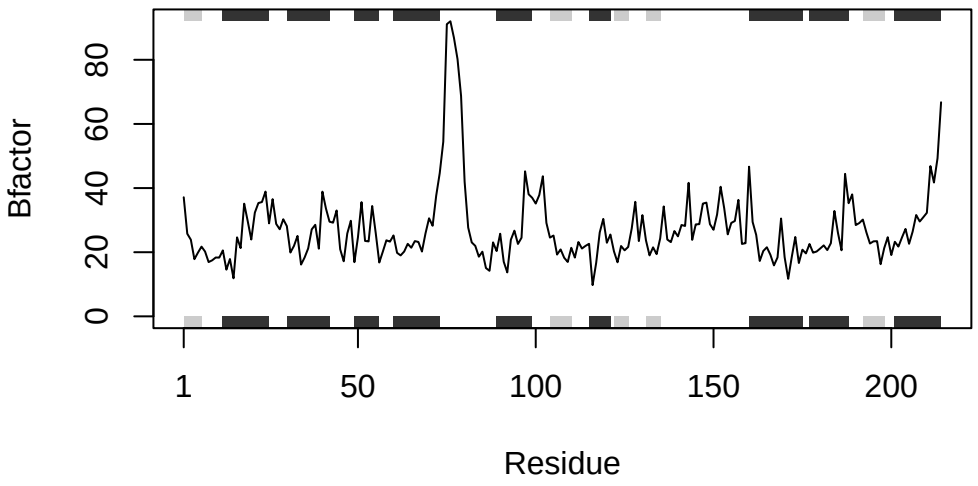
```
Note: Accessing on-line PDB file
```

```
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
```

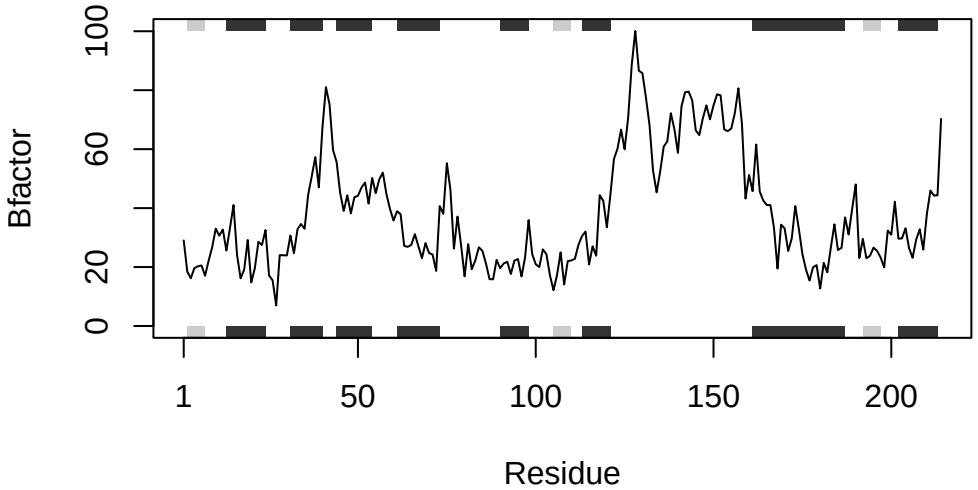
```
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```




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




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

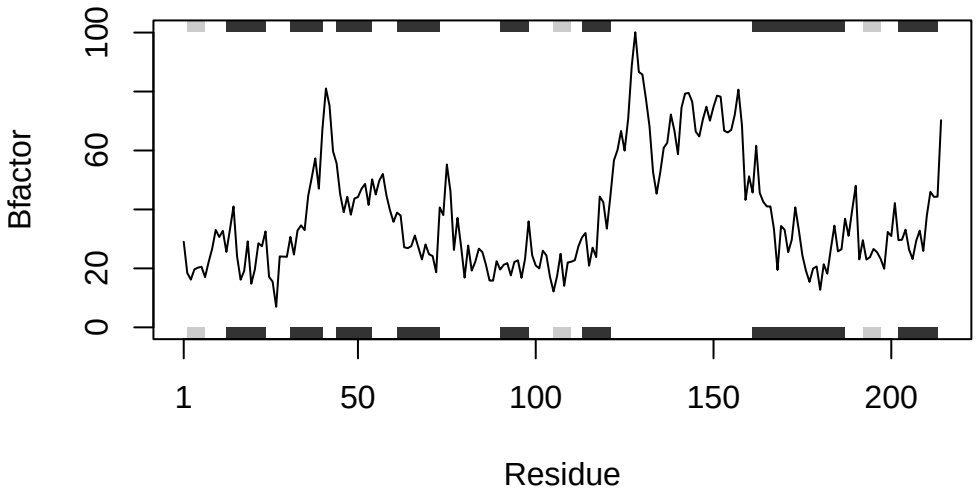


Q6. How would you generalize the original code above to work with any set of input protein structures?

```
library(bio3d)

generate_Bfactor_plot <- function(protein_pdb) {
  # Load the PDB file
  read_pdb <- read.pdb(protein_pdb)

  # Trim the PDB, keeping the structure of chain A and alpha carbons (CA)
  chain <- trim.pdb(read_pdb, chain = "A", elety = "CA")

  # Extract the "B-factor" from the chain
  read_pdb.b <- chain$atom$b

  # Create a B-factor plot as a line plot with annotations of secondary structure elements
  plotb3(read_pdb.b, sse = chain, typ = "l", ylab = "Bfactor")
}

# Example usage:
generate_Bfactor_plot("4AKE")  # Replace with the PDB file name of your choice
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/7h/wt3v3bgj3bq8wxjl8gcbt0fw0000gn/T//RtmpvilnTP/4AKE.pdb exists.
Skipping download
```



Documentation: This function reads a PDB file and creates a B-factor plot for the protein structure using the bio3D library.

An identifer, representing a protein, in the PDB database is inputted into the function. You can call the function by typing `generate_Bfactor_plot(___)` with the underlines replaced with the desired input (i.e. "1AKE"). The output should be a b-factor plot with Bfactor graphed on the y-axis and residue graphed on the x-axis.