HW 06

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

First to load the bio3d package using ***`library()`****.*

```
library(bio3d)
```

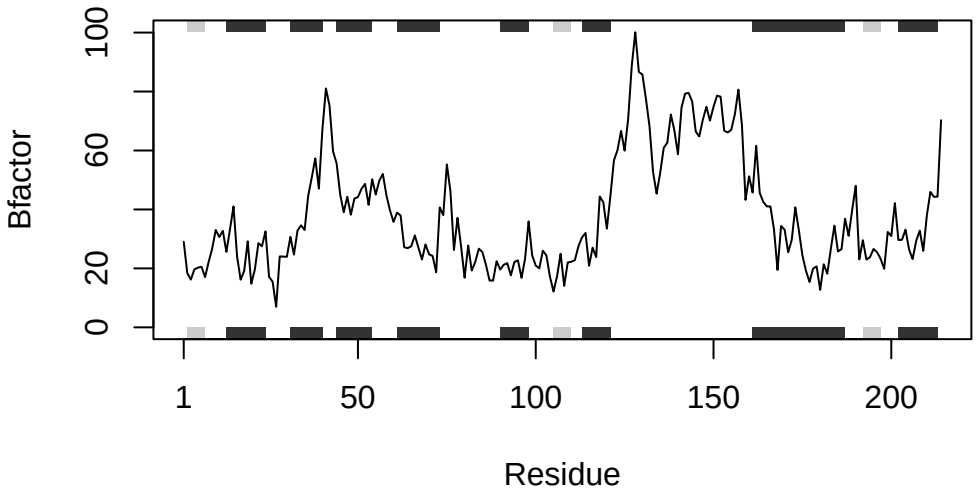
Below is the code for creating the new function to plot Bfactor for a PDB structure.

```
#Enter the name of the protein (PDB ID) in x
Bfar.plot <- function(x) {
  #Read in PDB file
  s1 <- read.pdb(x)
  #Extract CA atoms from chain A
  s1.chainA <- trim.pdb(s1, chain = "A", elety = "CA")
  #Get Bfactor data for each chain
  s1.b <- s1.chainA$atom$b
  #Plot Bfactor profile
  plotb3(s1.b, sse = s1.chainA, typ = "l", ylab = "Bfactor")
}
```

Now we can plot each Bfactor for PDB structure using ***`Bfar.plot`*** *function.*

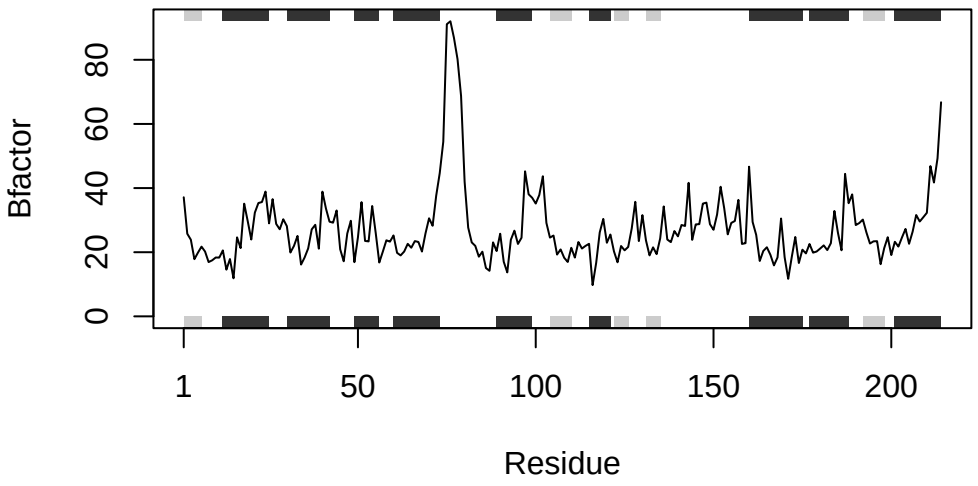
```
Bfar.plot("4AKE")
```

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



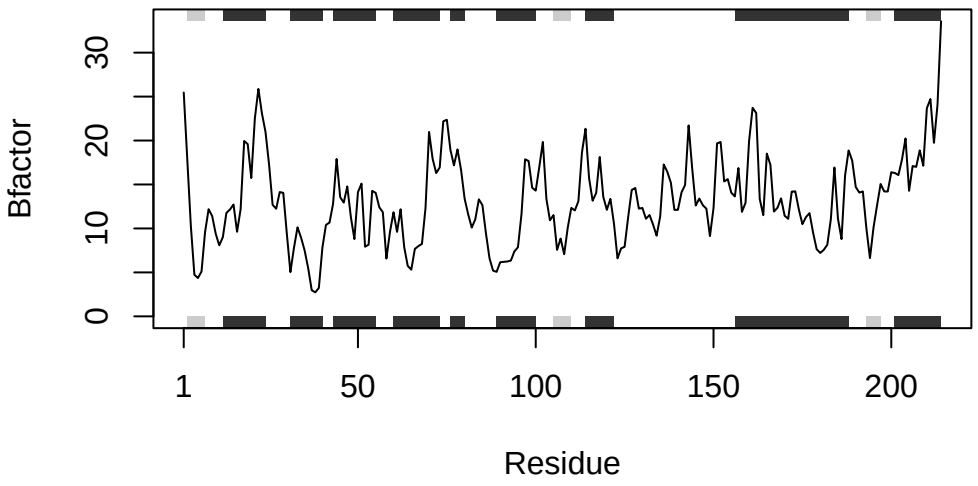

```
Bfar.plot("1AKE")
```

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




```
Bfar.plot("1E4Y")
```

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


Bfactor
0
10
20
30
1
50
100
150
200
Residue