

# Lec6HW\_Phoebe\_He

Phoebe He

1/25/2019

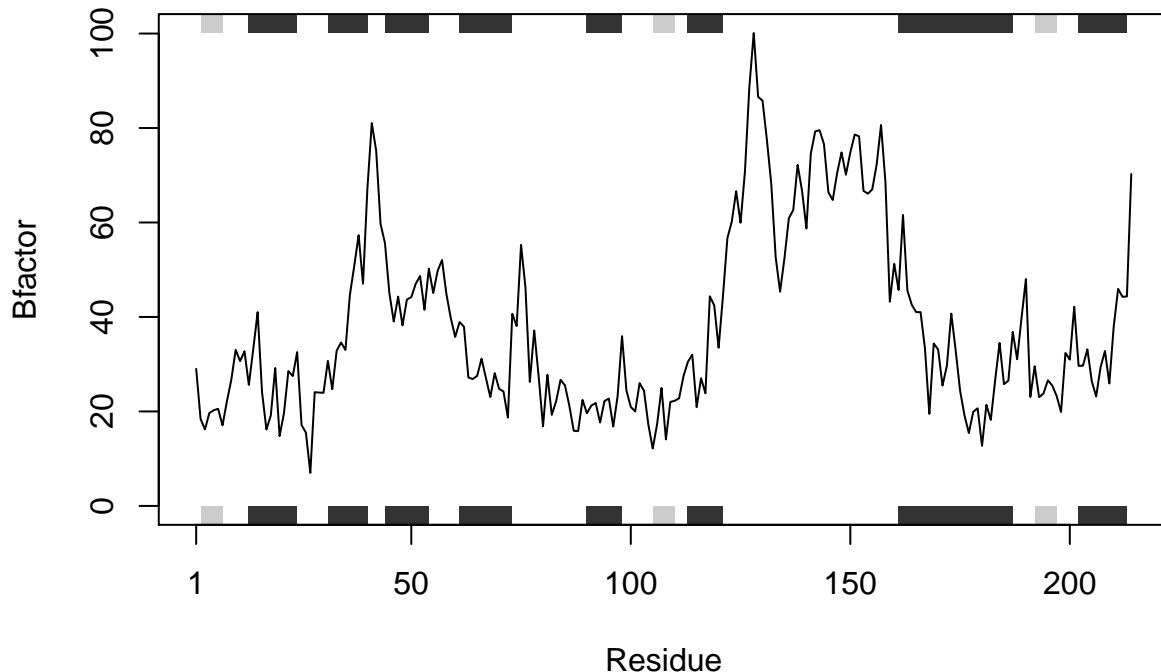
## Define function

The function below is able to take in an ID from PDB and plot out the corresponding protein's chain A's alpha carbon's Bfactor level. The inputs are the PDB ID of the desired protein, in string. To use the function, simply put in the PDB ID of your desired protein and run `plot_pdb(your_input_PDB_ID)`. The output is a plot showing the Bfactor trend levels of the alpha carbons on chain A of the input protein. The plot also marks the regions for alpha helices and beta sheets.

```
# Below defines function plot_pdb
library(bio3d)
plot_pdb <- function(x) {# The inputs are the PDB ID of the protein
  s1.chainA <- trim.pdb(read.pdb(x), chain="A", eley="CA")
  s1.b <- s1.chainA$atom$b
  plotb3(s1.b,
    sse=s1.chainA, # This line of code makes the grey/black boxes on the top and bottom of the ch
    typ="l",
    ylab="Bfactor")
}

# Test the function with three different inputs
plot_pdb("4AKE")
```

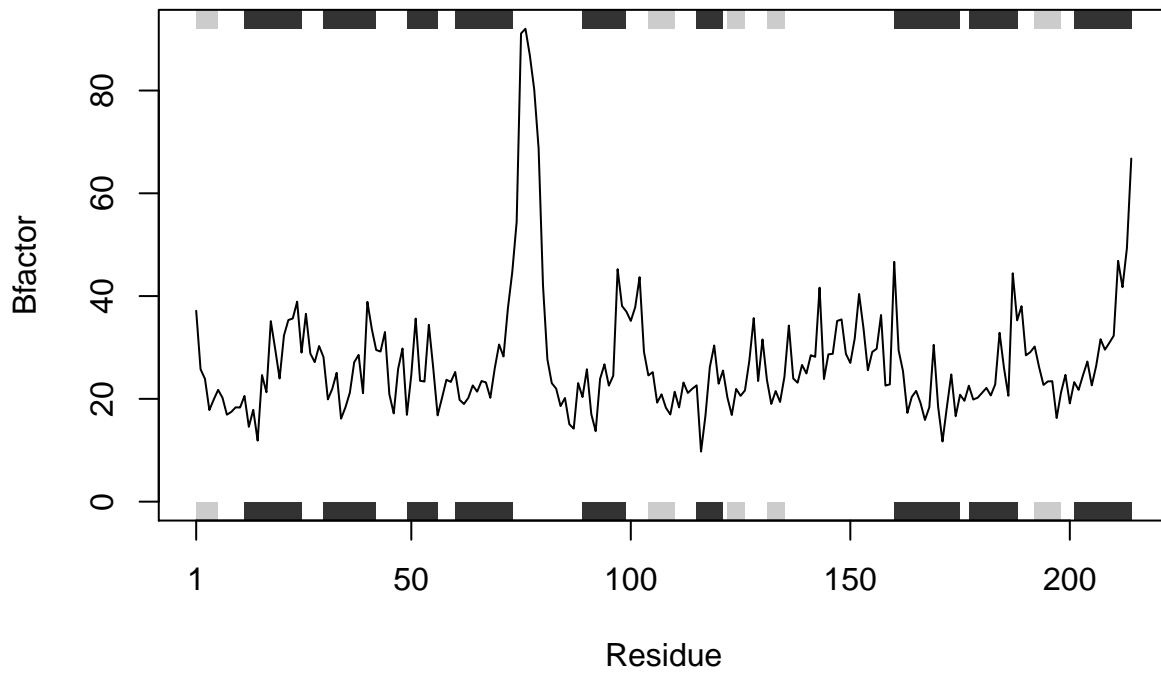
## Note: Accessing on-line PDB file



```
plot_pdb("1AKE")
```

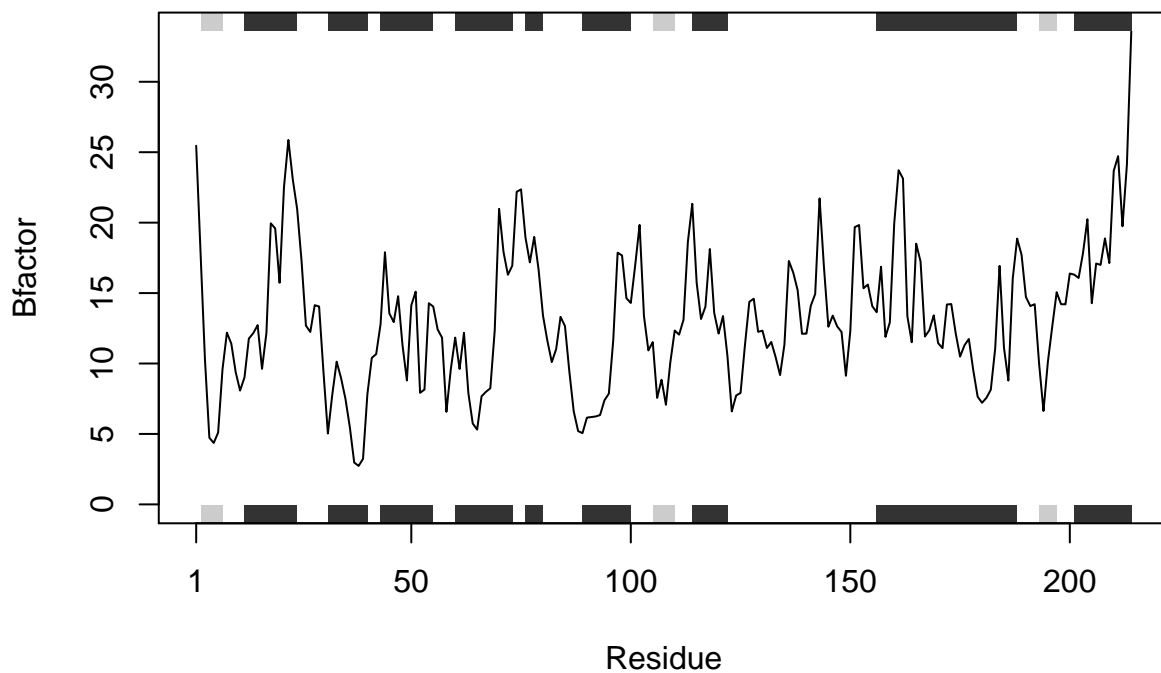
## Note: Accessing on-line PDB file

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



```
plot_pdb("1E4Y")
```

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



### Mock Bonus: plot overlays

This mock bonus uses points to overlay the Bfactor plots of chain A carbon items of protien B(red) on top of same plot of protein A(black). However, only protein A's alpha helices and beta sheets are labeled in the graph.

```
s3 <- read.pdb("1E4Y") # this is protein B
```

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

```
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/  
## tx/55gs511d5ls6vjxcgp47h5sc0000gp/T/Rtmpg0GMli/1E4Y.pdb exists. Skipping  
## download
```

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

```
s3.b <- s3.chainA$atom$b
```

```
plot_pdb("1AKE") # this is protein A
```

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

```
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/  
## tx/55gs511d5ls6vjxcgp47h5sc0000gp/T/Rtmpg0GMli/1AKE.pdb exists. Skipping  
## download
```

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

```
points(s3.b, typ='l', col="red")
```

