Hands-on Lab Supplement Q6

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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
```

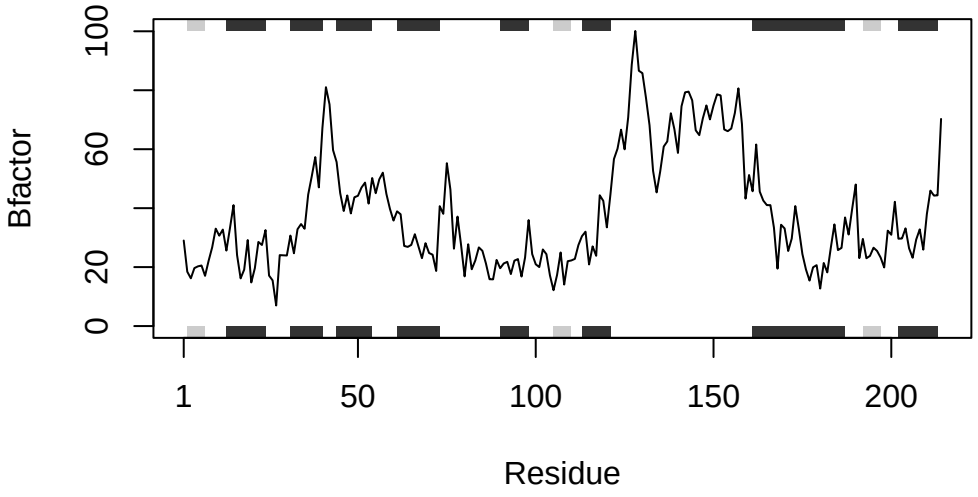
```
Note: Accessing on-line PDB file
 PDB has ALT records, taking A only, rm.alt=TRUE
```

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

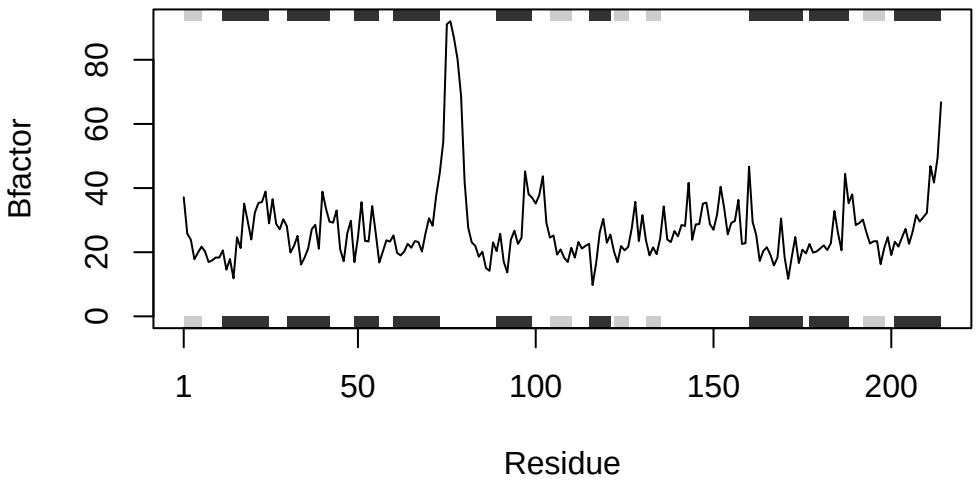
```
Note: Accessing on-line PDB file
```

```
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
```

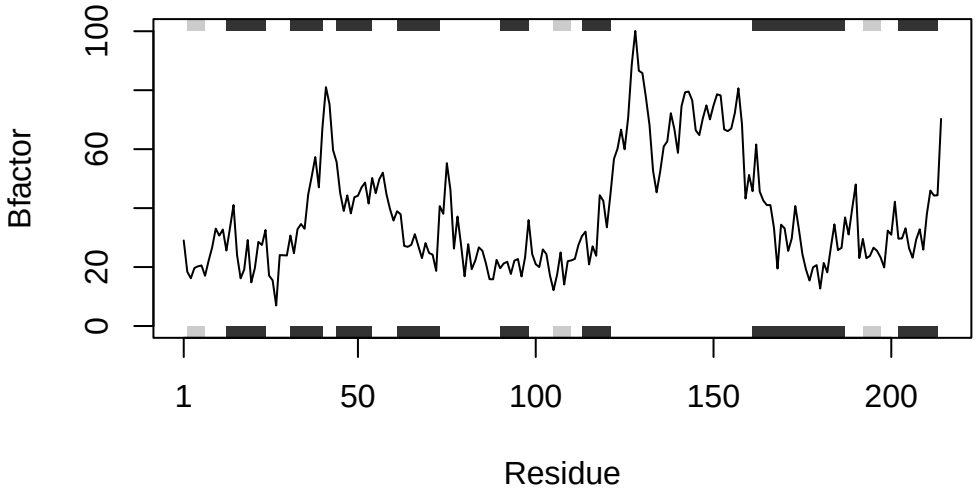
```
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```




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




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



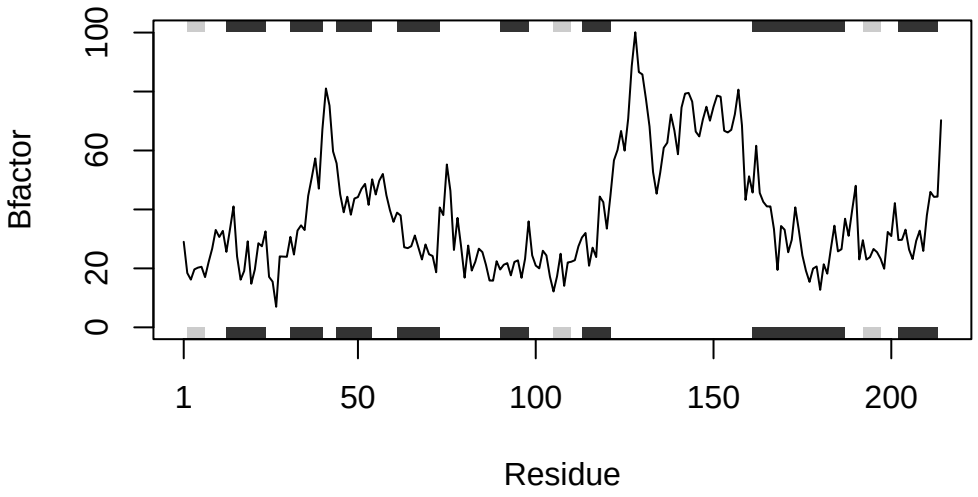
Generalized Code for any Protein Input:

```
# install bio3d package; once in script or more preferably, in the R Console
## install.packages("bio.3d)
library(bio3d)

# create the function for the  pdb analysis with the pdb file name, x, as the input
gen.pdb.analysis <- function(x) {
  # assign a vector that will read the pdb file being inputted
  pdb <- read.pdb(x)

  # trim the pdb object by its chain type (chain="A") & its atom type (elety="CA")
  chainA <- trim.pdb(pdb, chain="A", elety="CA")

  #extract the b-factors from the trimmed pdb vector
  b.factor <- chainA$atom$b

  # create a plot using these extracted b-factors, setting the secondary structure object
    # (sse) as chain, typ="l" for a line plot, & setting the y-label as "Bfactor"
  plotb3(b.factor, sse=chainA, typ="l", ylab="Bfactor")
}
```

Example of function use:

```
# Input desired pdb file into function
gen.pdb.analysis("4AKE")
```

```
  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\helxn\AppData\Local\Temp\RtmpGurzAF/4AKE.pdb exists. Skipping download
```


Bfactor
0
20
60
100
1
50
100
150
200
Residue