lab6HW

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Library Installation

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

Orignal 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
```

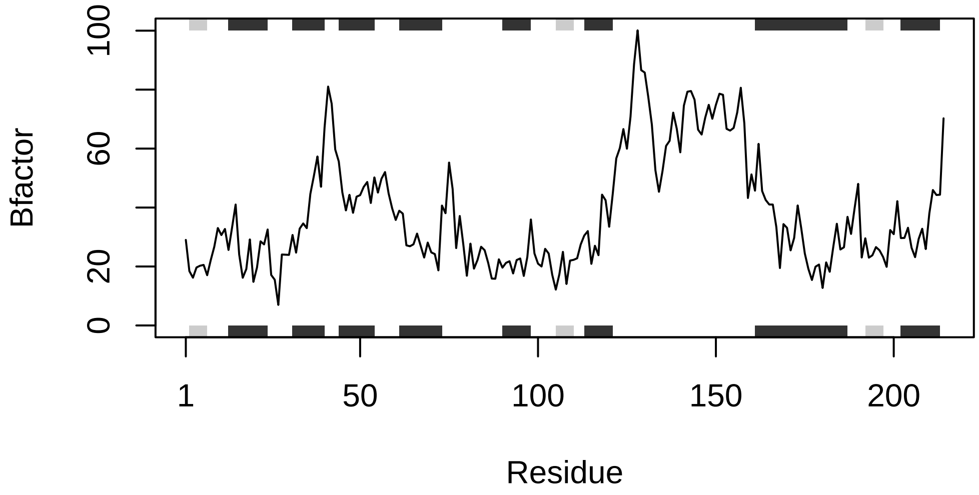
```
Note: Accessing on-line PDB file
 PDB has ALT records, taking A only, rm.alt=TRUE
```

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

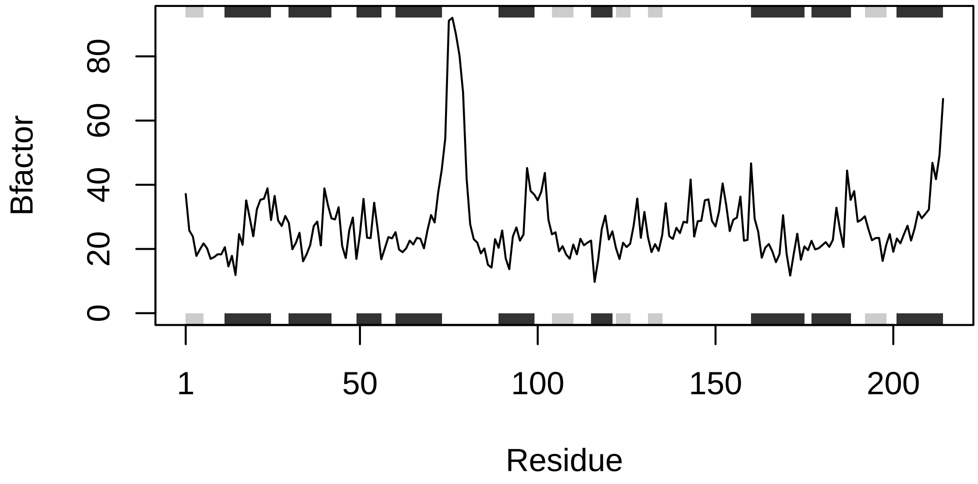
```
Note: Accessing on-line PDB file
```

```
#s1
#s2
#s3
```

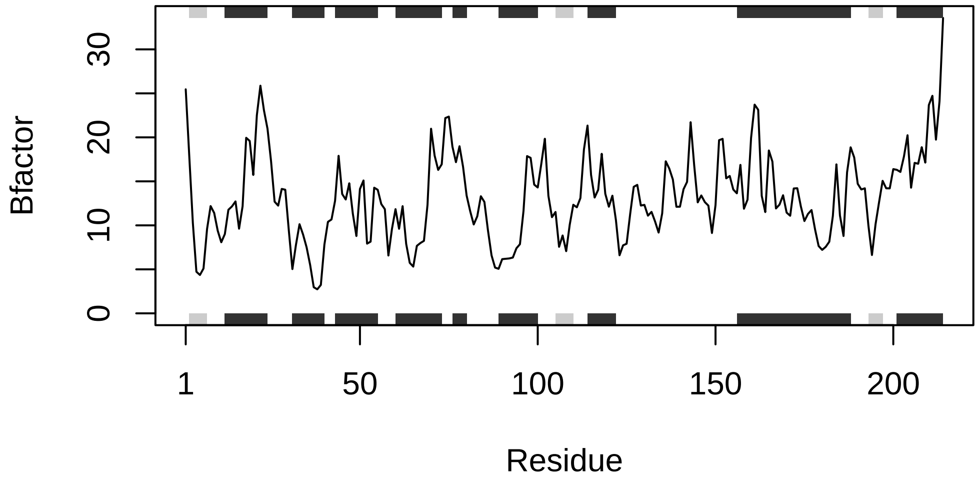
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")

#s1
#s1.chainA

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")
```



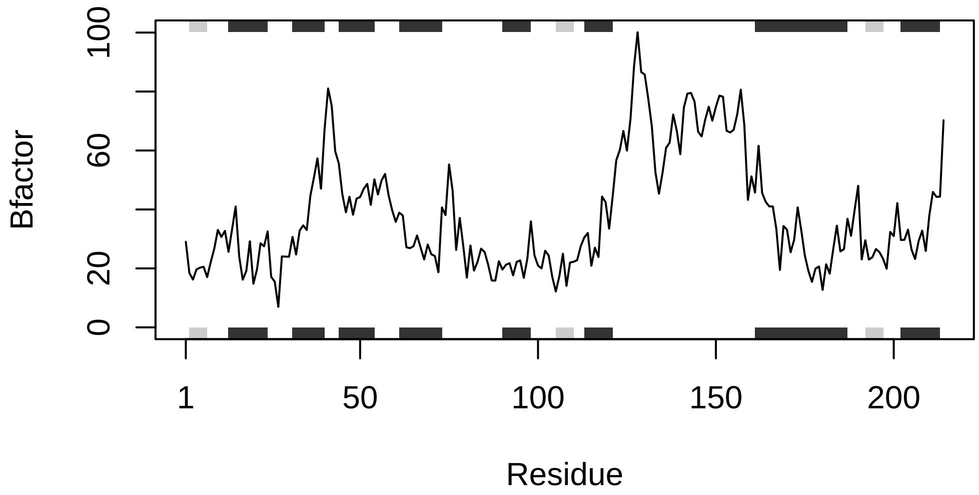
Question 6: Generalized Function

```
# The plotBFactor function takes an input of protein structures as a
# vector of strings, trims the protein sequence based on desired parameters.
# It then plots B Factor (y) to Residue (x).
#
# parameter input: a string vector of protein structures
# return: plot(s) of protein B Factor vs. Residue
plotBFactor <- function(input) {

  vecLength <- length(input)

  # Iterate over input vector to plot each protein structure given
  for (x in 1:vecLength) {

    # If input is not a character vector, break the loop (invalid input)
    if (is.character(input[x]) != T) {
      break
    }

    # read protein structure at index x
    curr <- read.pdb(input[x])

    # trim the chain
    curr.chainA <- trim.pdb(curr, chain="A", elety="CA")
    curr.b <- curr.chainA$atom$b

    # plot b factor against residue
    plotb3(curr.b, sse=curr.chainA, typ="l", ylab="Bfactor")
  }

}
```

Run function with original inputs

```
plotBFactor("4AKE")
```

```
  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\iWumb\AppData\Local\Temp\Rtmp0ehKnH/4AKE.pdb exists. Skipping download
```

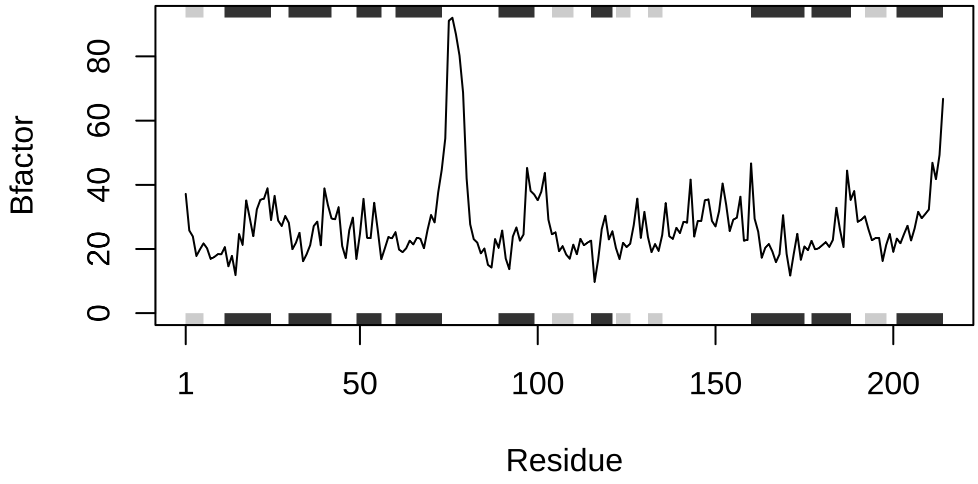


```
plotBFactor("1AKE")
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\iWumb\AppData\Local\Temp\Rtmp0ehKnH/1AKE.pdb exists. Skipping download
```

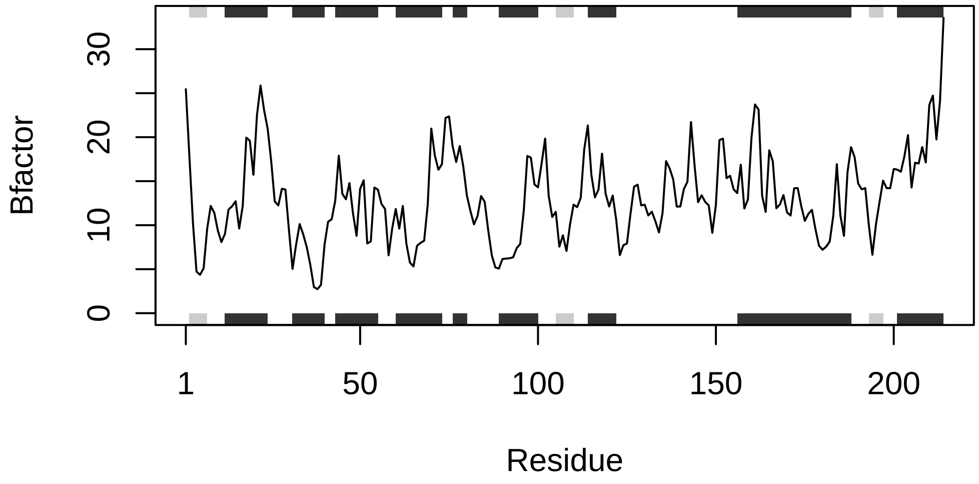
```
   PDB has ALT records, taking A only, rm.alt=TRUE
```



```
plotBFactor("1E4Y")
```

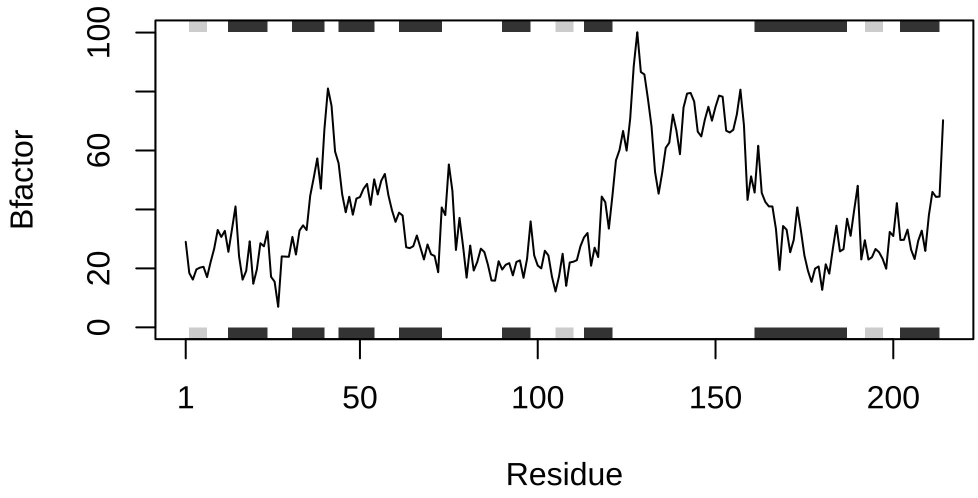
```
  Note: Accessing on-line PDB file
```

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\iWumb\AppData\Local\Temp\Rtmp0ehKnH/1E4Y.pdb exists. Skipping download
```



```r
vec <- c("4AKE", "1AKE", "1E4Y")
plotBFactor(vec)
```

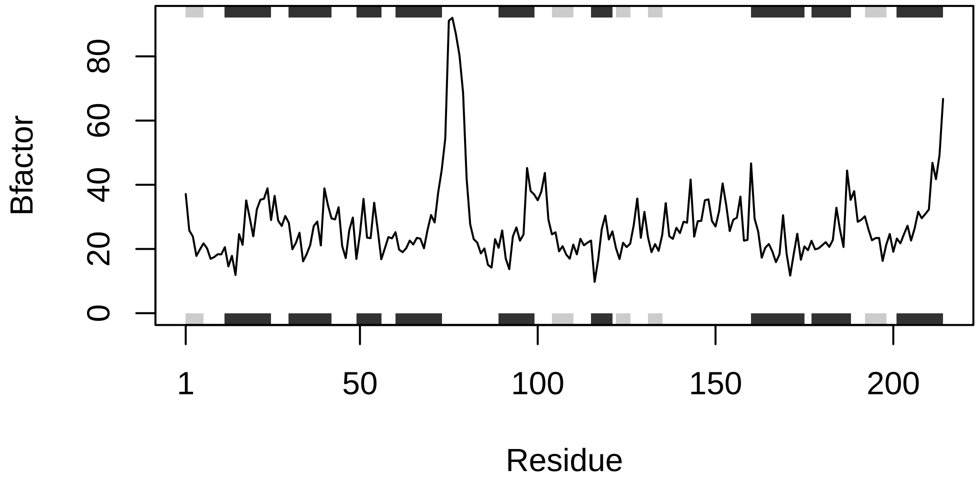
```
  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\iWumb\AppData\Local\Temp\Rtmp0ehKnH/4AKE.pdb exists. Skipping download

  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\iWumb\AppData\Local\Temp\Rtmp0ehKnH/1AKE.pdb exists. Skipping download
```

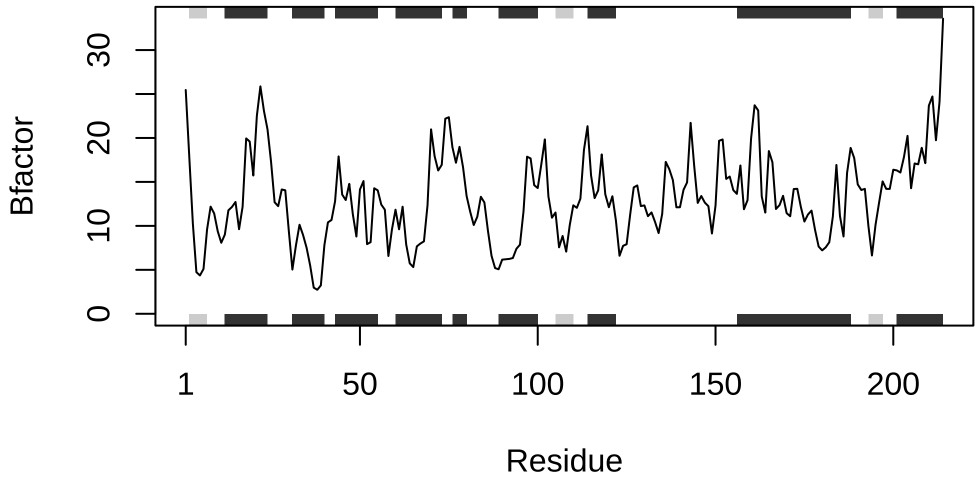


```
   PDB has ALT records, taking A only, rm.alt=TRUE
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\iWumb\AppData\Local\Temp\Rtmp0ehKnH/1E4Y.pdb exists. Skipping download
```


Bfactor
0
20
40
60
80
1
50
100
150
200
Residue


Bfactor
0
10
20
30
1
50
100
150
200
Residue