HW6

Elsa Quillin (PID: A69043008)

Original code:

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

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

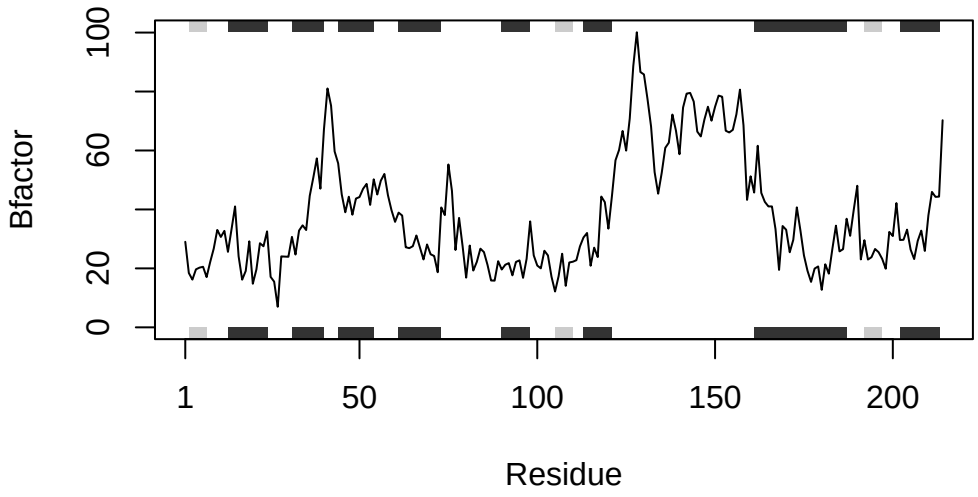
```
s2 <- read.pdb("1AKE") # kinase no drug
```

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

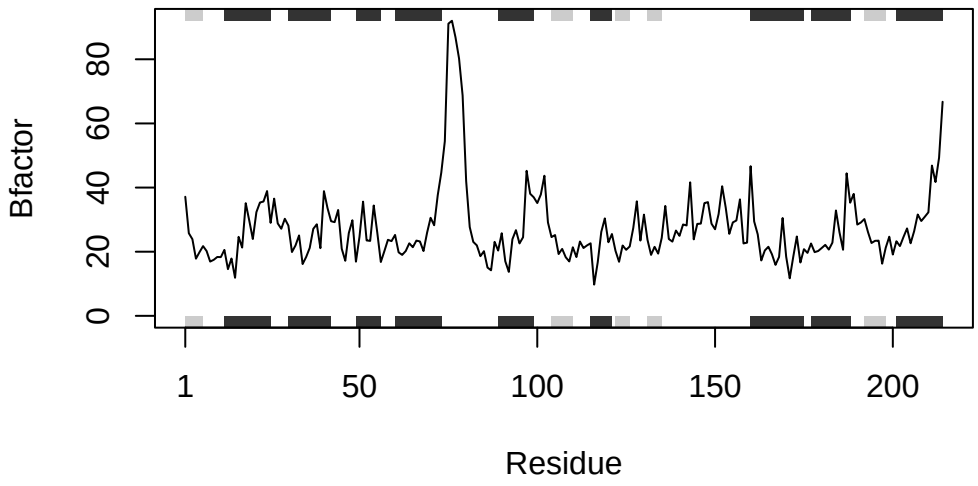
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

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

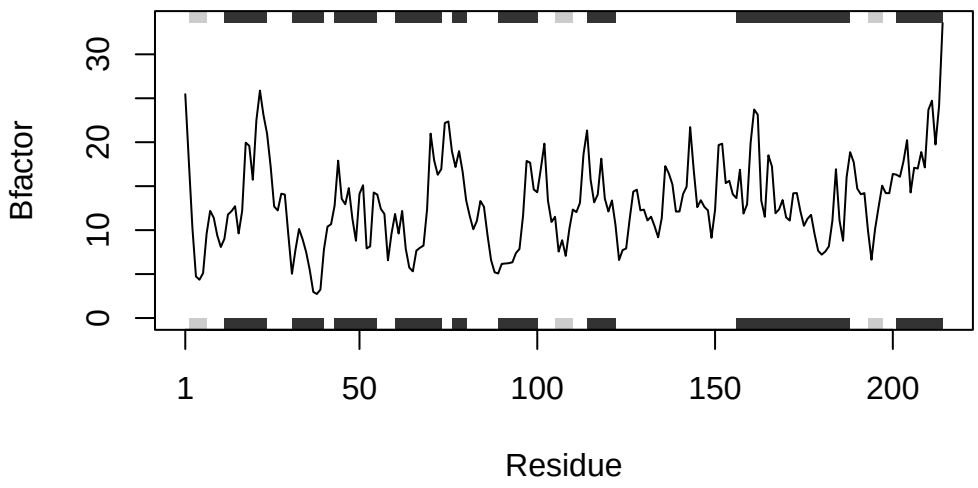
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



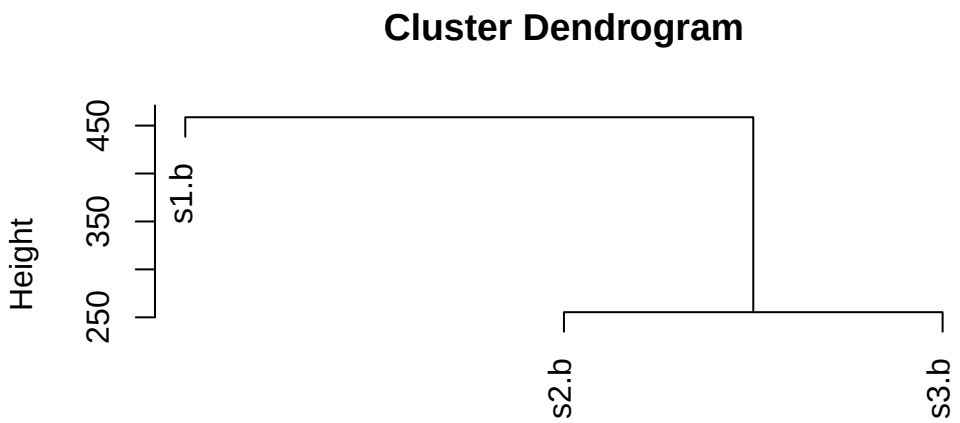

```
plotb3(s2.b, sse=s2.chainA, typ="l", ylab="Bfactor")
```



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




```
hc <- hclust( dist( rbind(s1.b, s2.b, s3.b) ) )
plot(hc)
```



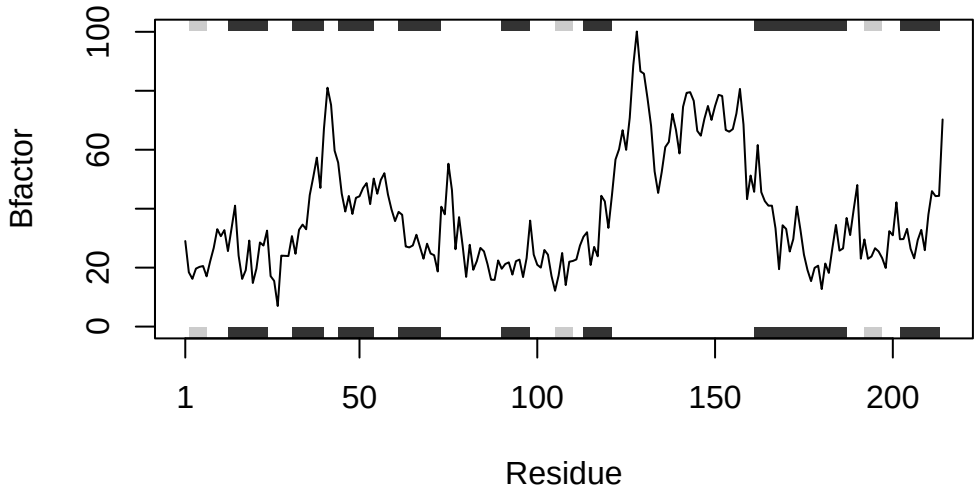
My code:

```
library(bio3d)

#input for pdb_code is the 4 digit protein specific code
#This is a function that will read pdb for the protein you enter
analysis <- function(pdb_code){
  pdb <- read.pdb(pdb_code)
#here the code will trim the output from pdb for chain A and the alpha carbon element
chainA <- trim.pdb(pdb, chain="A", elety="CA")
#here it will create a new definition "b" which is only the Bfactor
b <- chainA$atom$b
#this code is creating a plot of the residues against the B factor
plotb3(b, sse=chainA, typ="l", ylab="Bfactor")
#the return is showing the data
return(b)
}
```

Test:

```
analysis("4AKE")
```

```
  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/c9/jwxkdfxj1g16bppyf8tl9yfh0000gn/T//RtmpwstC46/4AKE.pdb exists.
Skipping download
```




```
  [1]  29.02  18.44  16.20  19.67  20.26  20.55  17.05  22.13  26.71  33.05
 [11]  30.66  32.73  25.61  33.19  41.03  24.09  16.18  19.14  29.19  14.79
 [21]  19.63  28.54  27.49  32.56  17.13  15.50   6.98  24.07  24.00  23.94
 [31]  30.70  24.70  32.84  34.60  33.01  44.60  50.74  57.32  47.04  67.13
 [41]  81.04  75.20  59.68  55.63  45.12  39.04  44.31  38.21  43.70  44.19
 [51]  47.00  48.67  41.54  50.22  45.07  49.77  52.04  44.82  39.75  35.79
 [61]  38.92  37.93  27.18  26.86  27.53  31.16  27.08  23.03  28.12  24.78
 [71]  24.22  18.69  40.67  38.08  55.26  46.29  26.25  37.14  27.50  16.86
 [81]  27.76  19.27  22.22  26.70  25.52  21.22  15.90  15.84  22.44  19.61
 [91]  21.23  21.79  17.64  22.19  22.73  16.80  23.25  35.95  24.42  20.96
[101]  20.00  25.99  24.39  17.19  12.16  17.35  24.97  14.08  22.01  22.26
[111]  22.78  27.47  30.49  32.02  20.90  27.03  23.84  44.37  42.47  33.48
[121]  44.56  56.67  60.18  66.62  59.95  70.81  88.63 100.11  86.60  85.80
```

```
[131]  77.48  68.13  52.66  45.34  52.43  60.90  62.64  72.19  66.75  58.73
[141]  74.57  79.29  79.53  76.58  66.40  64.76  70.48  74.84  70.11  74.82
[151]  78.61  78.24  66.70  66.10  67.01  72.28  80.64  68.54  43.23  51.24
[161]  45.72  61.60  45.61  42.57  41.03  41.02  33.34  19.48  34.38  33.11
[171]  25.48  29.68  40.71  32.91  24.41  19.20  15.43  19.93  20.66  12.72
[181]  21.40  18.21  26.68  34.50  25.77  26.52  36.85  31.05  39.84  48.03
[191]  23.04  29.57  23.00  23.80  26.59  25.49  23.25  19.89  32.37  30.97
[201]  42.16  29.64  29.69  33.15  26.38  23.17  29.35  32.80  25.92  38.01
[211]  45.95  44.26  44.35  70.26
```