HW6

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Original code:

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

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

```
s2 <- read.pdb("1AKE") # kinase no drug
```
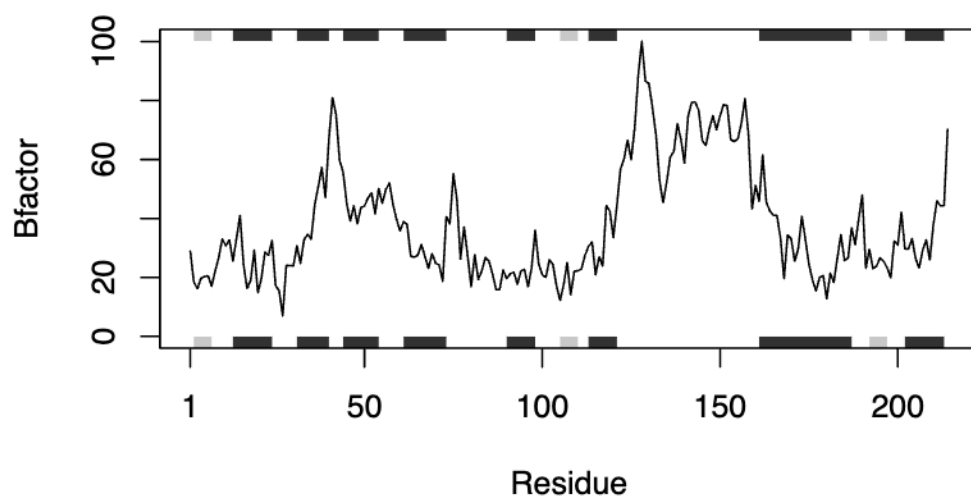
```
  Note: Accessing on-line PDB file
   PDB has ALT records, taking A only, rm.alt=TRUE
```
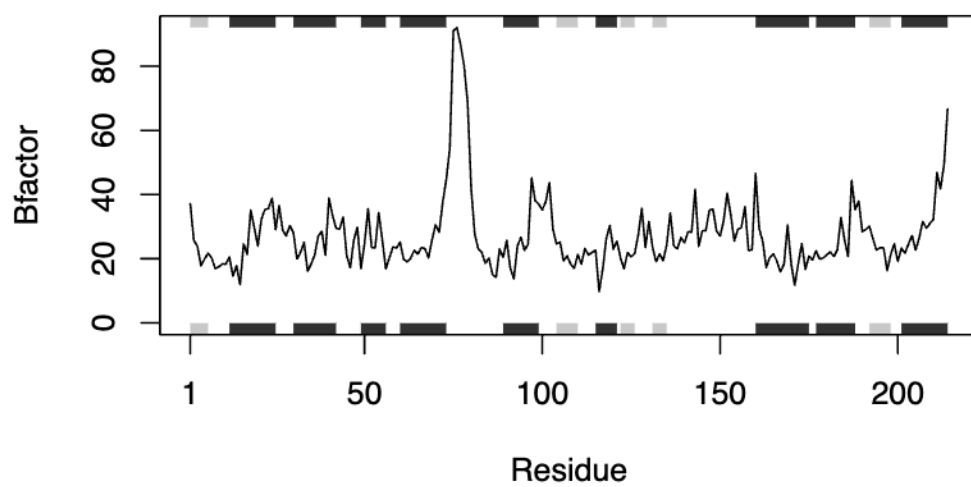
```
s3 <- read.pdb("1E4Y") # kinase with drug
```
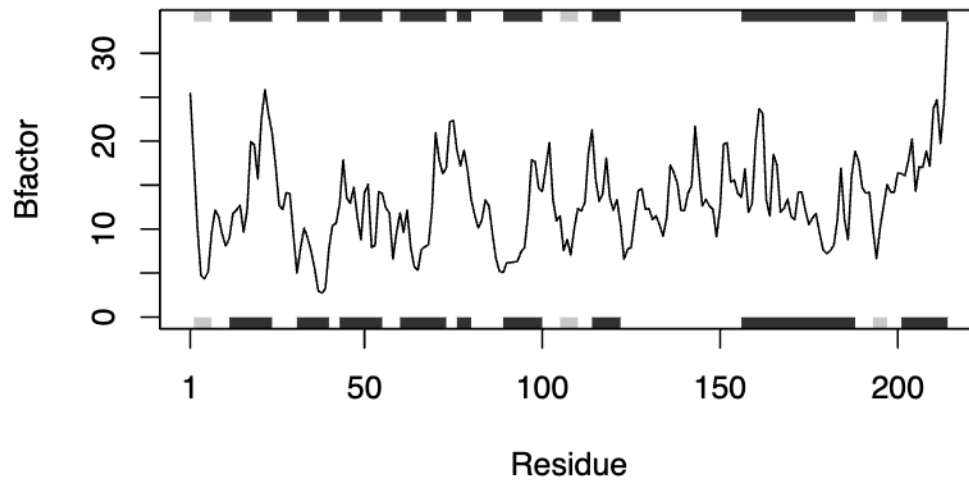
```
  Note: Accessing on-line PDB file
```

```
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)
```

Cluster Dendrogram

dist(rbind(s1.b, s2.b, s3.b))
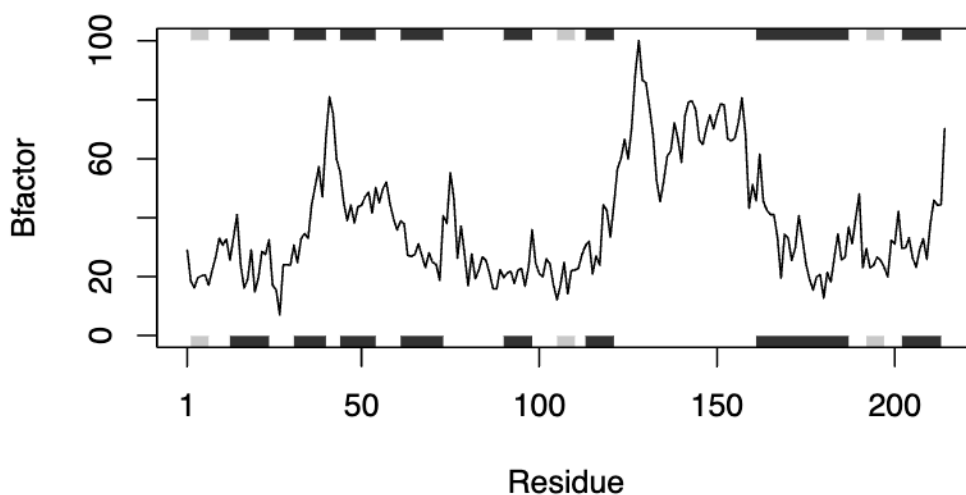hclust (*, "complete")

My code:

```r
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
```