HW 06

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Protein Code

First install and load the bio3d package

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

I will begin by running the code provided

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

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

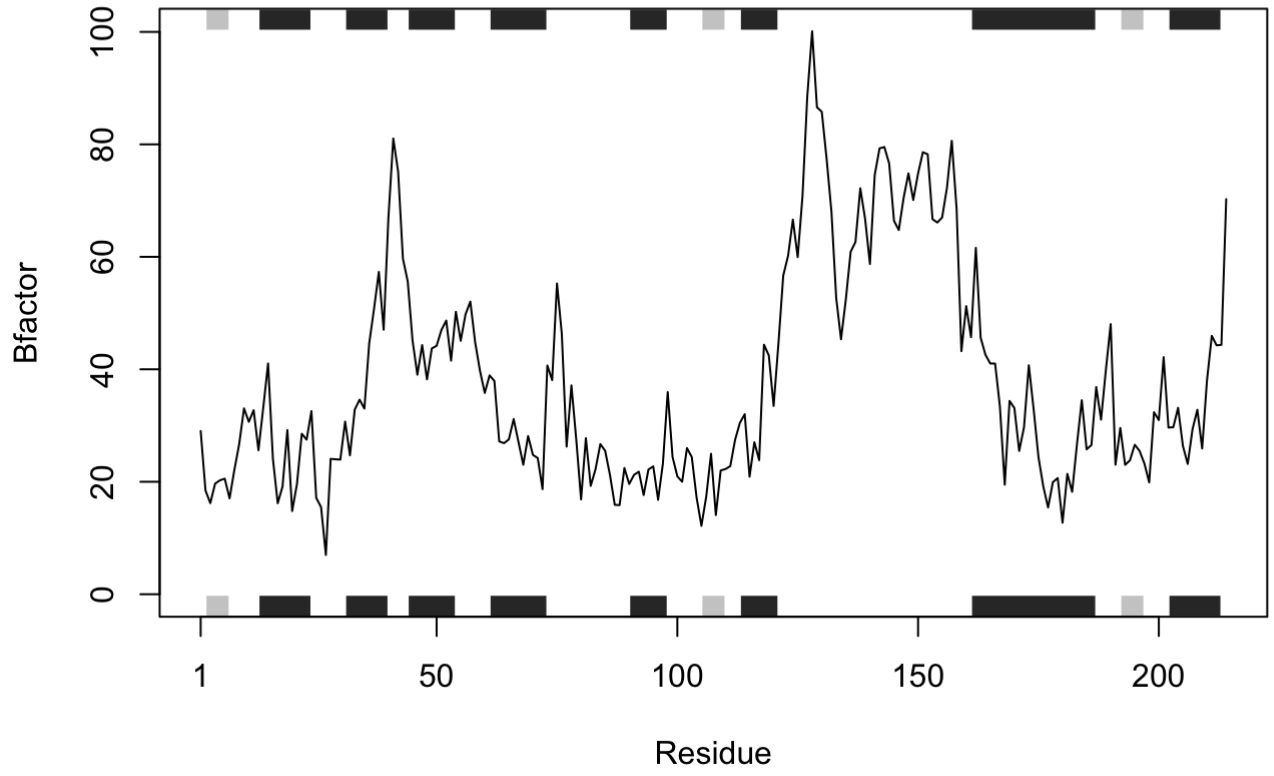
```
s2 <- read.pdb("1AKE") # kinase no drug
```

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

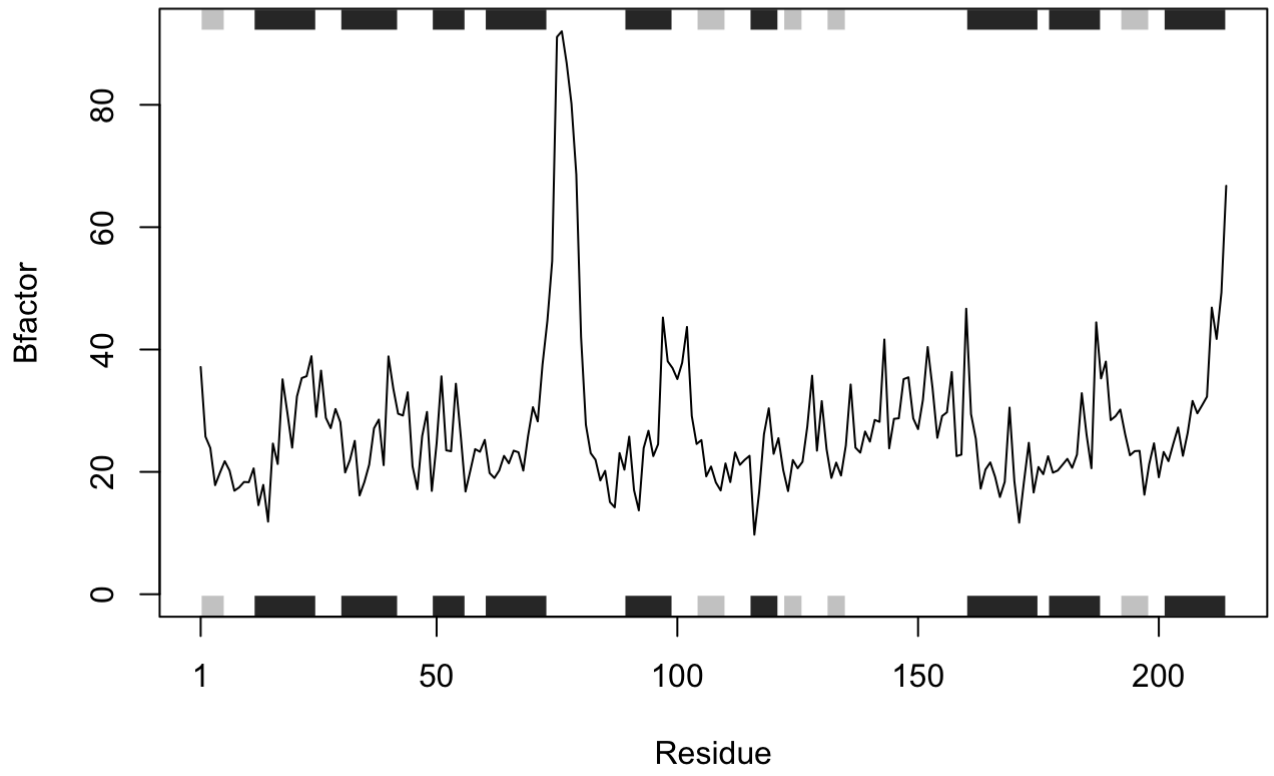
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

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

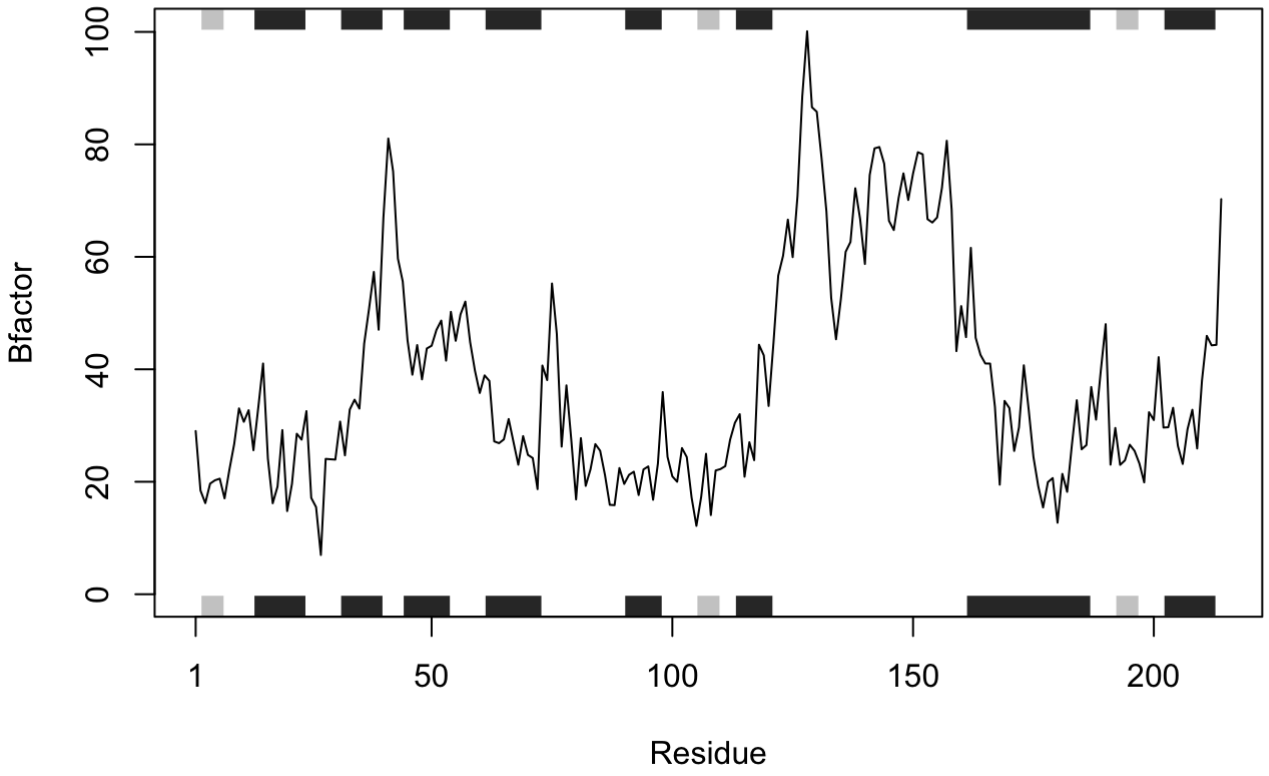
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")

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")
```



I will start by trying to apply all portions to “4AKE” or “s1”

Firstly starting with trim in the function

```
trimpro = function(x){ #naming the function for trimming protein
  trim.pdb(x, chain="A", elety="CA") #using trim function on pdb input
}
trimpro(s1)
```

```
##
##  Call:  trim.pdb(pdb = x, chain = "A", elety = "CA")
##
##    Total Models#: 1
##      Total Atoms#: 214,  XYZs#: 642  Chains#: 1  (values: A)
##
##      Protein Atoms#: 214  (residues/Calpha atoms#: 214)
##      Nucleic acid Atoms#: 0  (residues/phosphate atoms#: 0)
##
##      Non-protein/nucleic Atoms#: 0  (residues: 0)
##      Non-protein/nucleic resid values: [ none ]
##
##    Protein sequence:
##       MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAAVKSGSELGKQAKDIMDAGKLVT
##       DELVIALVKERIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVDRI
##       VGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKDDQEETVRKRLVEYHQMTAPLIG
##       YYSKEAEAGNTKYAKVDGTKPVAEVRADLEKILG
##
## + attr: atom, helix, sheet, seqres, xyz,
##         calpha, call
```

The function is providing a trim of each pdb file.

```
trimpro(s2)
```

```
##
##  Call:  trim.pdb(pdb = x, chain = "A", elety = "CA")
##
##    Total Models#: 1
##      Total Atoms#: 214,  XYZs#: 642  Chains#: 1  (values: A)
##
##      Protein Atoms#: 214  (residues/Calpha atoms#: 214)
##      Nucleic acid Atoms#: 0  (residues/phosphate atoms#: 0)
##
##      Non-protein/nucleic Atoms#: 0  (residues: 0)
##      Non-protein/nucleic resid values: [ none ]
##
##    Protein sequence:
##       MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAAVKSGSELGKQAKDIMDAGKLVT
##       DELVIALVKERIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVDRI
##       VGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKDDQEETVRKRLVEYHQMTAPLIG
##       YYSKEAEAGNTKYAKVDGTKPVAEVRADLEKILG
##
## + attr: atom, helix, sheet, seqres, xyz,
##         calpha, call
```

Now we will try to implement the “$atom$b” into the function

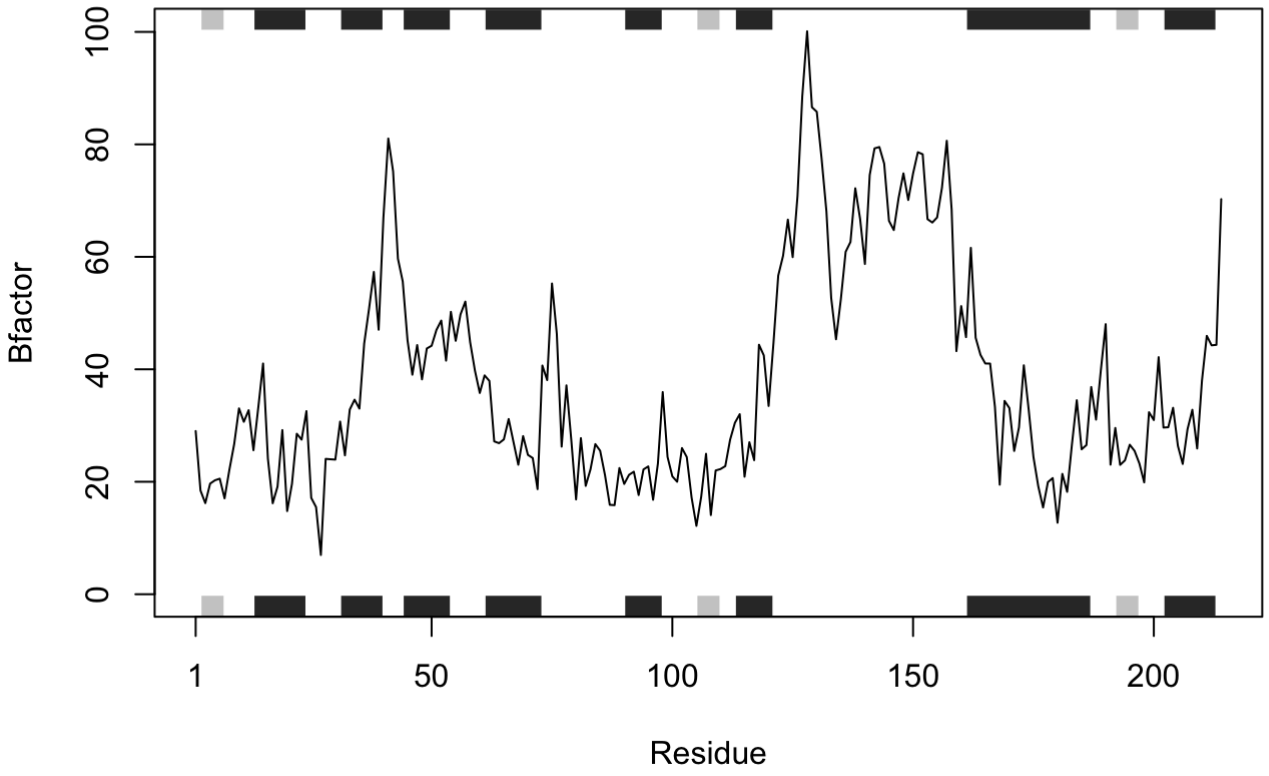
```
atom = function(x){ #naming the function protein
  trimpro(x)$atom$b #adding the atom portion
}
atom(s1)
```

```
##   [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
```

The function provides the atom numbers.

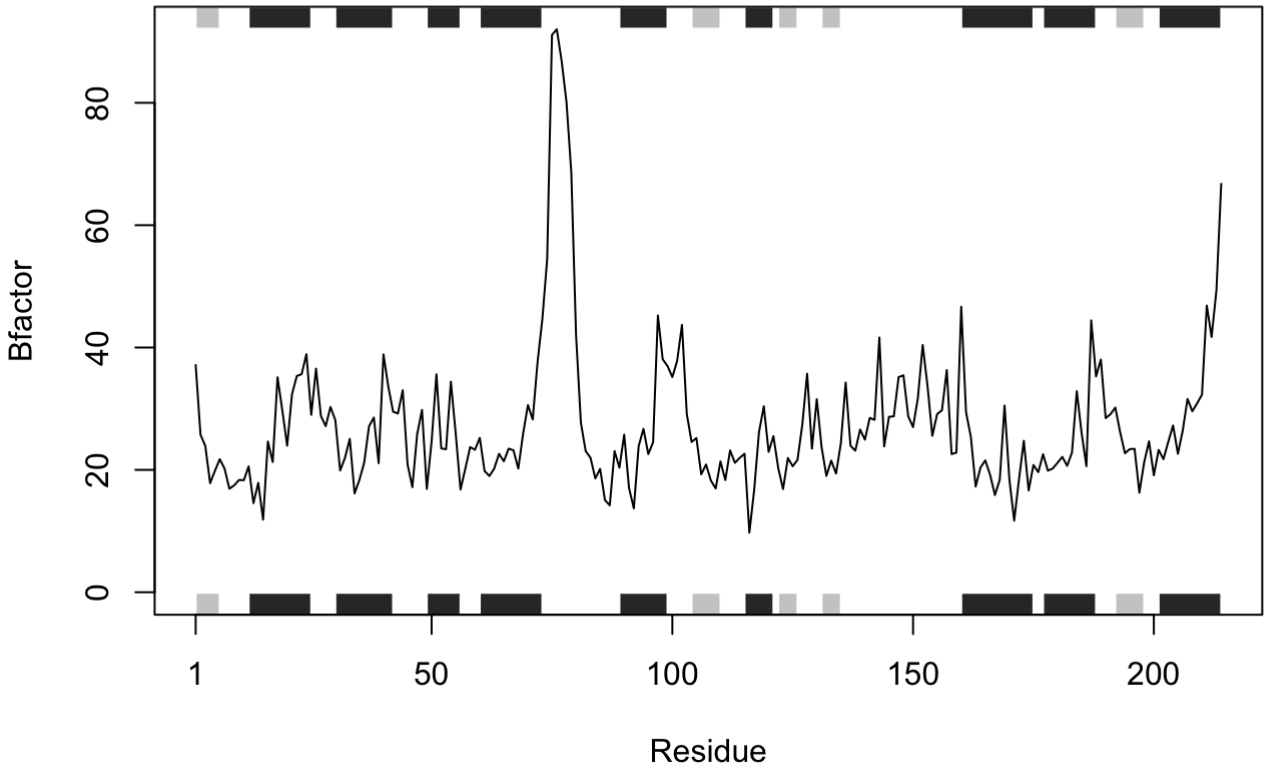
Now we will try to add the plot portion to the function

```
#' Protein function to provide a plot
#'
#' @param x, or input is a loaded pdb file. For Example: s1 is a loaded file from bio3d
using function read.pdb()
#'
#' @return returns a plot for specified protein
#'
#'
#' @examples
protein = function(x){ #naming the function protein
  plotb3(atom(x), sse = trimpro(x), typ="l", ylab="Bfactor") #implementing both function
s I had previously written in order to make a plot
}
protein(s1)
```



Now it will test on the rest of the proteins

```
protein(s2)
```


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