class06_HW

Kalle Liimatta A59002114

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Q6.

Goal: Create a function that allows the user to input any protein PDB code and outputs a plot for the specified protein as done above.

We need to create functions that performs the code below.

- s1 <- read.pdb("4AKE") # kinase with drug
- s2 <- read.pdb("1AKE") # kinase no drug
- s3 <- read.pdb("1E4Y") # kinase with drug
- 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")

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

1) read_function: Input the protein PDB code into the read_function to download and access the PDB file of that protein

Turn the code below into a function:

- s1 <- read.pdb("4AKE") # kinase with drug
- s2 <- read.pdb("1AKE") # kinase no drug
- s3 <- read.pdb("1E4Y") # kinase with drug

```
#simplify to:  x <- read.pdb("x")

#input the protein PDB code where "x" is
read_function <- function(x) {
  sx <-read.pdb(x)
}
```

```
#test the read_function
s1 <- read_function("4AKE")
```

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

```
s1
```

```
Call:  read.pdb(file = x)

  Total Models#: 1
    Total Atoms#: 3459,  XYZs#: 10377  Chains#: 2  (values: A B)

    Protein Atoms#: 3312  (residues/Calpha atoms#: 428)
```

```
     Nucleic acid Atoms#: 0  (residues/phosphate atoms#: 0)

     Non-protein/nucleic Atoms#: 147  (residues: 147)
     Non-protein/nucleic resid values: [ HOH (147) ]

   Protein sequence:
      MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAAVKSGSELGKQAKDIMDAGKLVT
      DELVIALVKERIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVDRI
      VGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKDDQEETVRKRLVEYHQMTAPLIG
      YYSKEAEAGNTKYAKVDGTKPVAEVRADLEKILGMRIILLGAPGA...<cut>...KILG

+ attr: atom, xyz, seqres, helix, sheet,
        calpha, remark, call
```

```
#it works!
```

2) chain_function: add onto the read_function to build out the overall function

Turn the code below into a function:

- 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") #typo here, should be s3

```
#simplify to --> x.chainA <-trim.pdb(x, chain="A", elety="CA")
chain_function <- function(x) {
  x.chainA <-trim.pdb(read_function(x), chain="A", elety="CA")
}
```

```
#test the chain_function
s1.chainA <-chain_function("4AKE")
```

```
  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE): C:
\Users\kwlii\AppData\Local\Temp\RtmpI9YbrS/4AKE.pdb exists. Skipping download
```

```
s1.chainA
```

```
 Call:  trim.pdb(pdb = read_function(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
```

```
#it works!
```

3) atom_function: add onto the chain_function to build out the overall function

Turn the below code into a function:

- s1.b <- s1.chainA$atom$b
- s2.b <- s2.chainA$atom$b
- s3.b <- s3.chainA$atom$b

```
#simplify to --> x.b <- x.chainA$atom$b
atom_function <- function (x) {
  x.chainA <-chain_function(x)
  x.chainA$atom$b
}
```

```
#test the function
s1.b <- atom_function("4AKE")
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE): C:
\Users\kwlii\AppData\Local\Temp\RtmpI9YbrS/4AKE.pdb exists. Skipping download
```

```
  s1.b
```

```
  [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
```

```
  #it works!
```

4) plot_function: add onto the atom_function to make the overall function

Turn the below code into a function:

- 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")

```
#simplify to <-- plotb3(x.b, sse=x.chainA, typ="l", ylab="Bfactor")

plotb3_function <- function(x) {
           x.plotB3 <- plotb3(atom_function(x),
                     sse=chain_function(x),
                     typ="l",
                     ylab="Bfactor")}
```

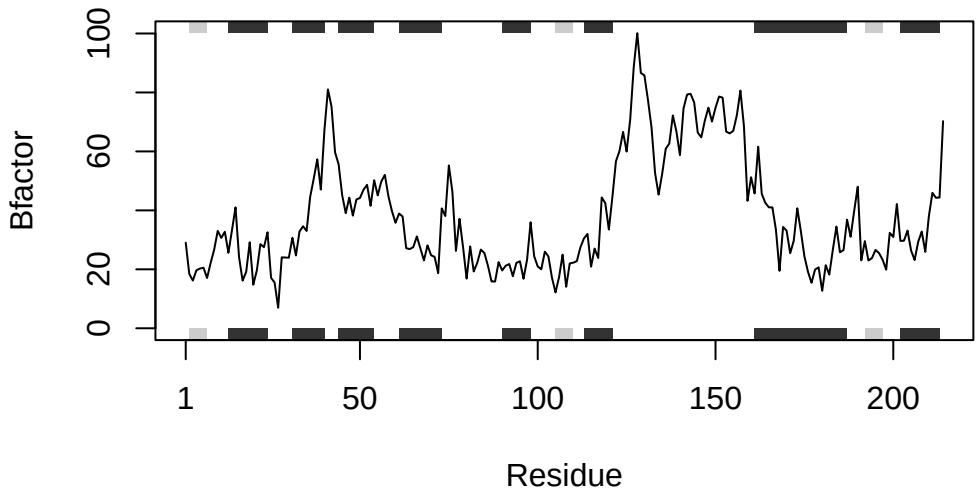
```
#test the function
plotb3_function("4AKE")
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE): C:
\Users\kwlii\AppData\Local\Temp\RtmpI9YbrS/4AKE.pdb exists. Skipping download
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE): C:
\Users\kwlii\AppData\Local\Temp\RtmpI9YbrS/4AKE.pdb exists. Skipping download
```



```
#it works!
```

5) Put all the functions together to create the final function

Final function:

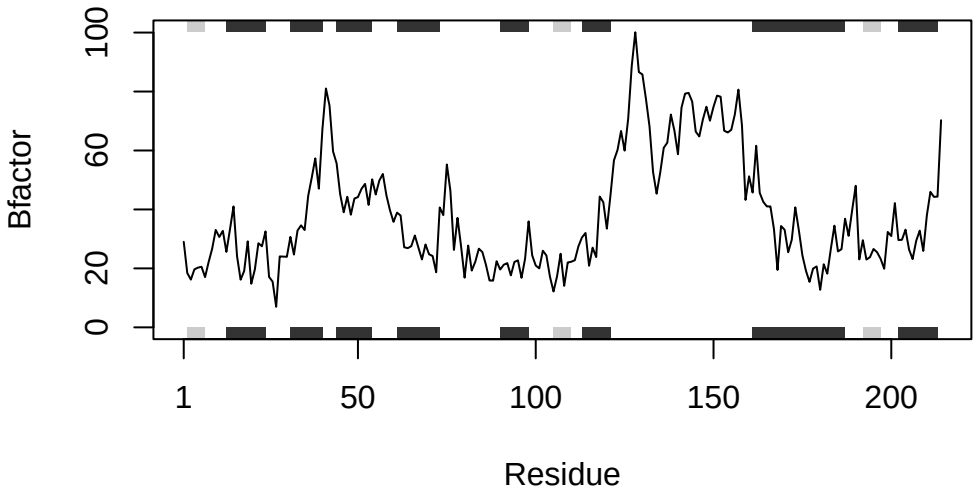
```
#input the protein PDB code where "x" is to get a plot for the specified protein

plotpdb <- function(x) {
    sx <-read.pdb(x)
    x.chainA <-trim.pdb(sx, chain="A", elety="CA")
    x.b <- x.chainA$atom$b
    x.plotB3 <- plotb3(x.b,
                       sse=x.chainA,
                       typ="l",
                       ylab="Bfactor")}
```

```
#Final test!
plotpdb("4AKE")
```

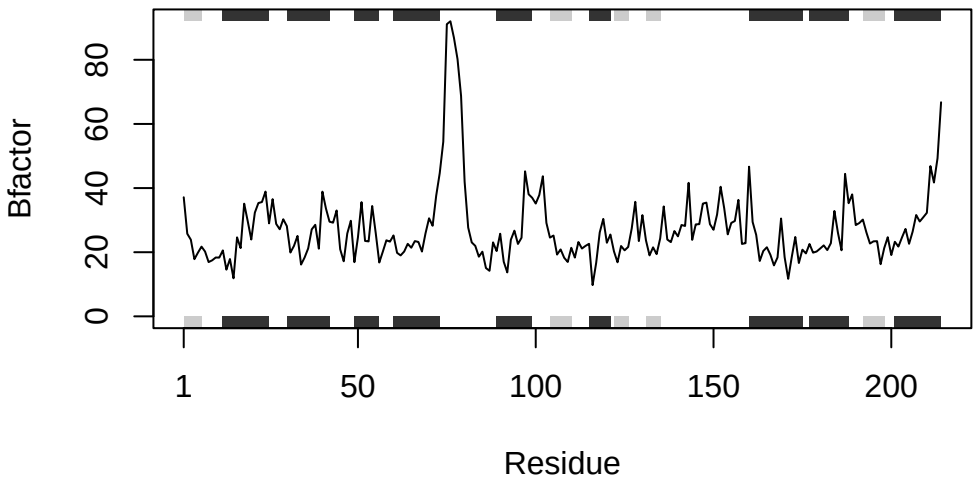
```
  Note: Accessing on-line PDB file
```

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE): C:
\Users\kwlii\AppData\Local\Temp\RtmpI9YbrS/4AKE.pdb exists. Skipping download
```



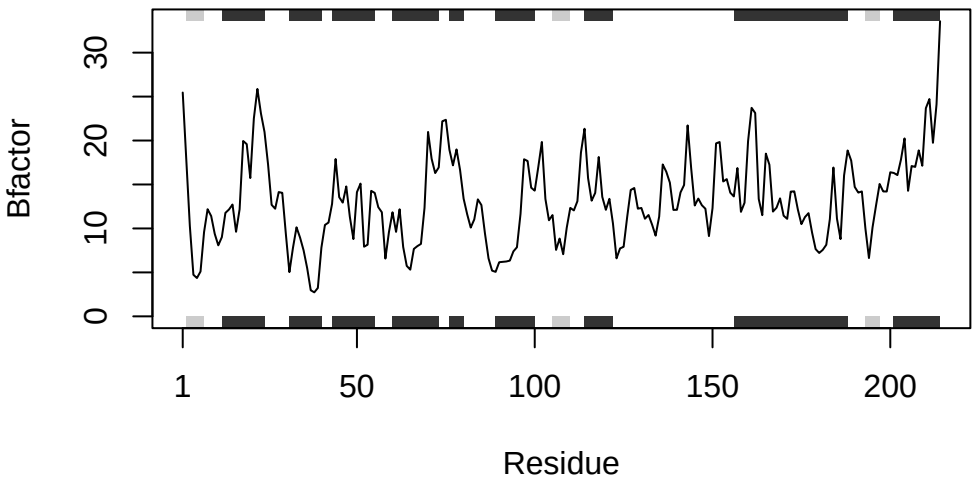

```
plotpdb("1AKE")
```

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




```
plotpdb("1E4Y")
```

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


Bfactor
0
10
20
30
1
50
100
150
200
Residue