

Class06 Homework

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Section 1: Improving analysis code by writing functions

Section B: Improve the below example code for the analysis of protein drug interactions by abstracting the main activities in your own new function.

Q6. How would you generalize the original code to work with any set of input protein structures?

We need to install the bio3d package using 'install.packages()'

- Had the code chunk with 'install.packages("bio3d")', but I had to remove it because it was causing problems when I tried to render

First run through the code to make sure it works:

```
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

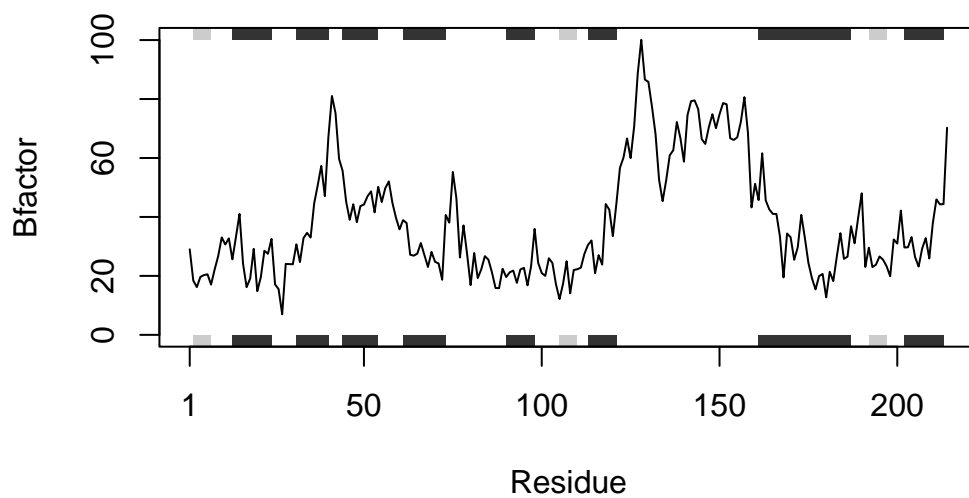
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

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")

```



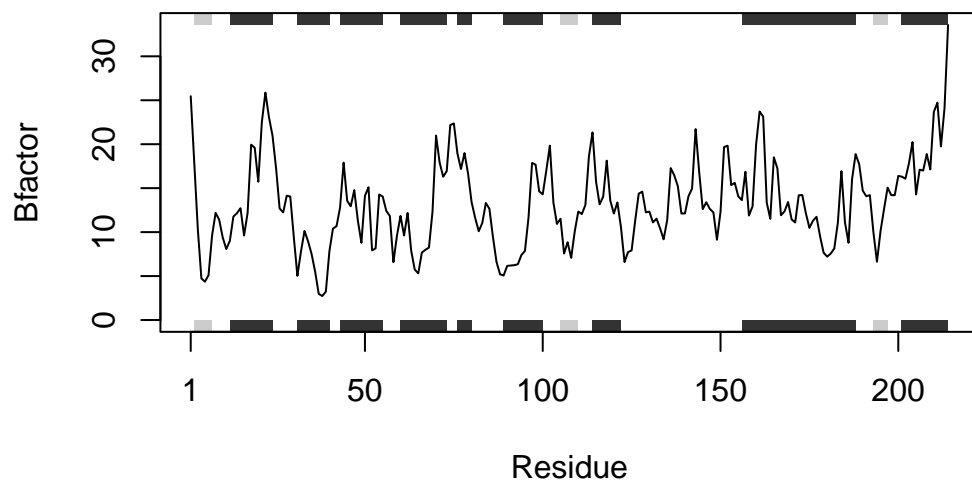
```

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

```



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



The first step to make an overall function is to combine ‘**read.pdb()**’ and ‘**trim.pdb()**’, into one function:

```
x <- "4AKE"
readntrim <- function(x) {
  trim.pdb(read.pdb(x), chain="A", elety="CA")
}

readntrim("4AKE")
```

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE): C:
\\Users\\ITSL0A~1\\AppData\\Local\\Temp\\RtmpaKqiSF\\4AKE.pdb exists. Skipping download

Call: trim.pdb(pdb = read.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:
MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMRLRAAVKSGSELGKQAKDIMDAGKLV
DELVIALVKERIAQEDCRNGFLDGFPR TIPQADAMKEAGINVDYVLEFDVPDELIVDRI
VGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKDDQEETVRKRLVEYHQMTAPLIG
YYSKEAEAGNTKYAKVDGTPVAEVRADLEKILG

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

- This function on its own gives information on the inputted protein.

Using ‘**plotb3()**’ and the original function, ‘**readntrim()**’, we can make another function for the final portion of the analysis:

```
x <- "4AKE"
final_function <- function(x) {
  plotb3(readntrim(x)$atom$b, sse=readntrim(x), typ="l", ylab="Bfactor")
}
```

Now we can easily input any protein and analyze their Bfactor trends using our 'final_function()'

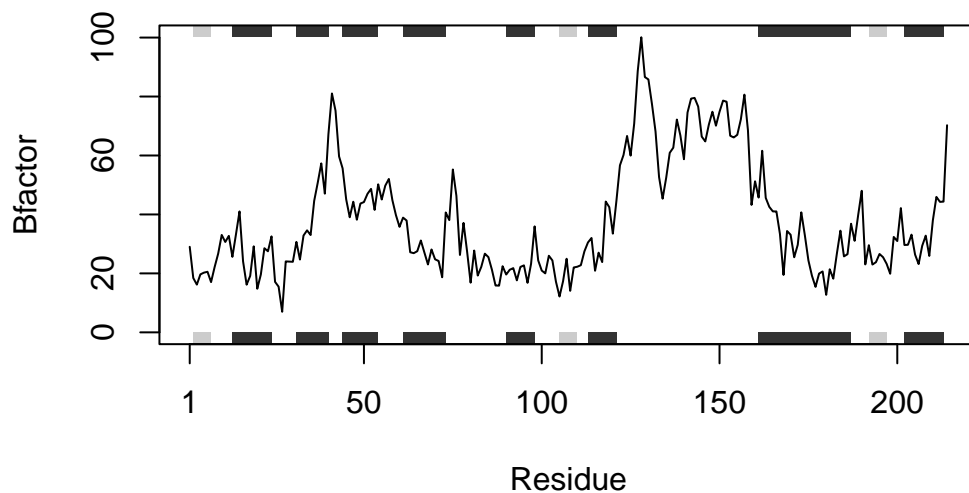
```
final_function("4AKE")
```

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE): C:
\Users\ITSL0A~1\AppData\Local\Temp\RtmpaKqiSF\4AKE.pdb exists. Skipping download

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE): C:
\Users\ITSL0A~1\AppData\Local\Temp\RtmpaKqiSF\4AKE.pdb exists. Skipping download



```
final_function("1AKE")
```

Note: Accessing on-line PDB file

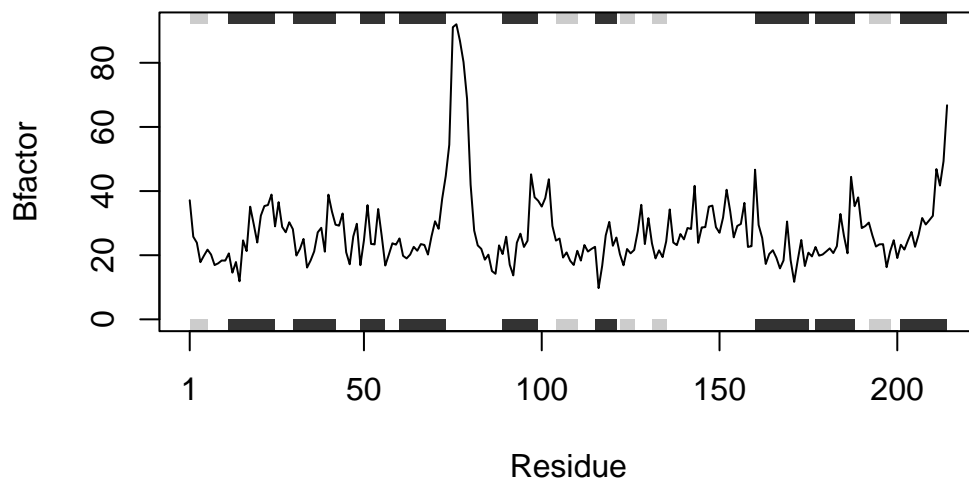
Warning in get.pdb(file, path = tempdir(), verbose = FALSE): C:\Users\ITSL0A~1\AppData\Local\Temp\RtmpaKqiSF\1AKE.pdb exists. Skipping download

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\ITSL0A~1\AppData\Local\Temp\RtmpaKqiSF\1AKE.pdb exists. Skipping download

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



```
final_function("1E4Y")
```

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE): C:\Users\ITSL0A~1\AppData\Local\Temp\RtmpaKqiSF\1E4Y.pdb exists. Skipping download

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE): C:\Users\ITSL0A~1\AppData\Local\Temp\RtmpaKqiSF\1E4Y.pdb exists. Skipping download

