Class06_Homework

Gregory Jordan

PDB Kinase Analyzer Function Homework 06

Prompt:

Can you improve this analysis code? library(bio3d) 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")

Problem to address:

The previous code requires you to repeat it for every pdb object, as we see below. We want to make a function that you can simply call with your PDB object 4 letter name so no coding is involved :)

4 functions to create:

1. read in the PDB file
2. get the chain A from the pdb object
3. get the atom and b columns from chain A
4. plot the chainA/atom and b columns

Solution:

First step is to load in the bio3d library

```
#install.packages(bio3d) if not already installed
library(bio3d)
```

Next make a function to read in any pdb file by only having to input the 4 letter PDB code

```
#input is PDB 4 letter code
kinase <- function(x){
  read.pdb(x)
}
```

Now make a function to trim the pdb file and get chain A

```
#input is PDB 4 letter code
trimmed_kinase <- function(x){
  trim.pdb(kinase(x), chain="A",elety="CA")
}
```

Now make a function to get the b column from atom column from chain A

```
#input is PDB 4 letter code
atom_b <- function(x){
  a<-trimmed_kinase(x)
  a$atom$b
}
```

Finally, make a function to plot the atom_b and trimmed_kinase as done in the examples

```
#input is PDB 4 letter code
plot_kinase <- function(x){
  plotb3(atom_b(x), sse=trimmed_kinase(x),typ="l",ylab="Bfactor")
}
```

Note: I made the input for each of these functions the 4 letter PDB code to make it easier on the user so they only need to know the PDB code.

Testing the code:

1.Read File

```
#using 4AKE PDB code
#kinase("4AKE")
```

2.Trimmed_kinase

```
#trimmed_kinase("4AKE")
```

3.Atom_b

```
#atom_b("4AKE")
```

I am only going to display the plot_kinase result as a test because it involves the other functions working and displaying the other functions returns way too much output to keep the final pdf to submit clean looking.

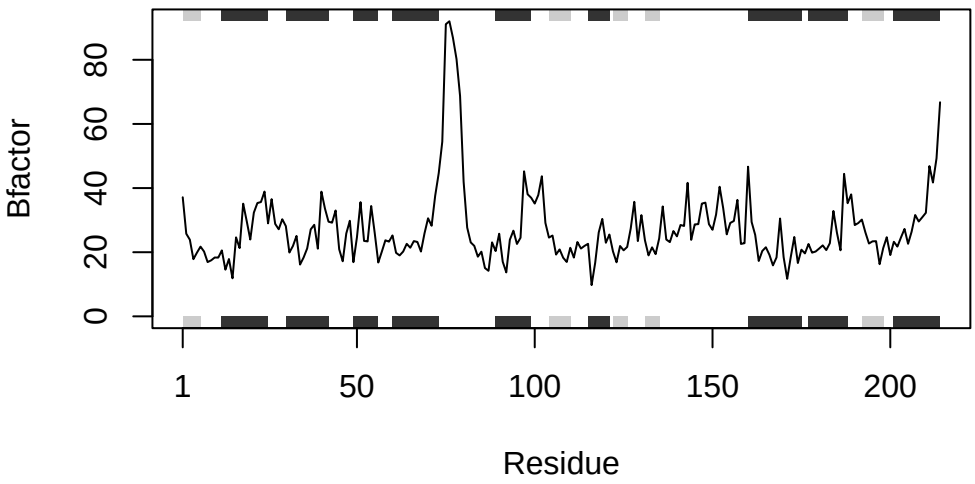
4.Plot

```
plot_kinase("1AKE")
```

```
  Note: Accessing on-line PDB file
   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): /var/folders/
x7/31_d9zdx01j16mvpmr7t07lh0000gn/T//RtmpBRUqvv/1AKE.pdb exists. Skipping
download

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


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