

Class06.HW

Sharlene Yang

Class 06 HW

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

```
# Can you improve this analysis code?  
library(bio3d)  
s1 <- read.pdb("4AKE") # kinase with drug
```

Note: Accessing on-line PDB file

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

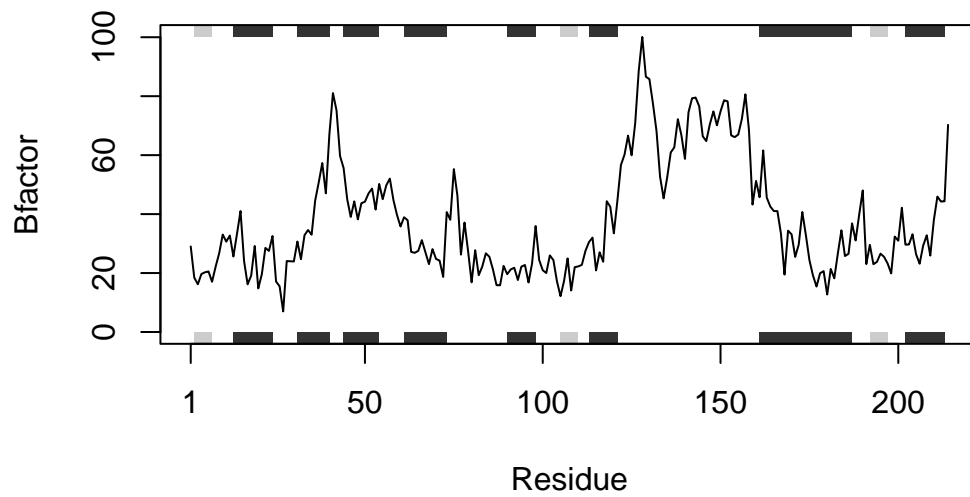
Note: Accessing on-line PDB file
PDB has ALT records, taking A only, rm.alt=TRUE

```
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
```

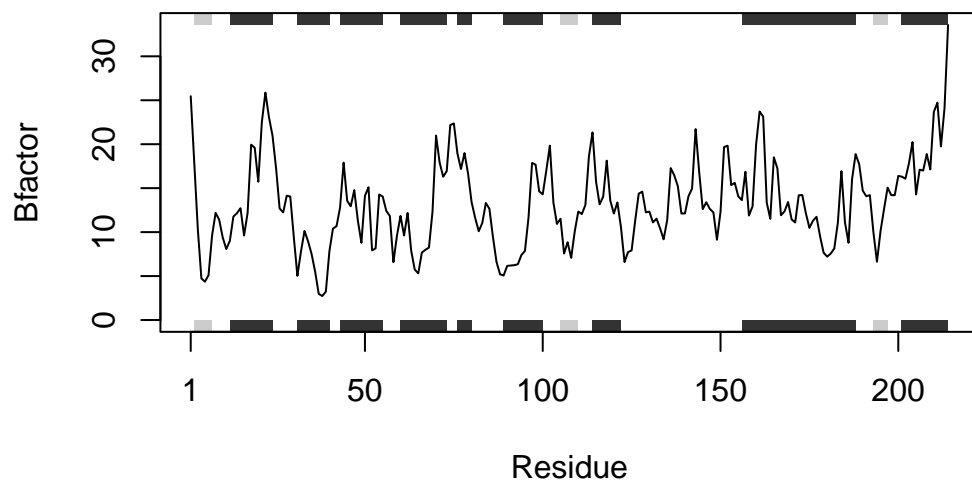
```
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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



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



The generalized function:

```
library(bio3d)

plotkinase <- function(x) {
  #This function takes x, where x is the accession number
  #This function reads the accession number into the database
  #The output is s which reads the file for the inserted accession number
  s <- read.pdb(x)

  #This function takes the s variable as the input
  #This function produces a smaller PDB object, containing a subset of atoms as its output
  #The output is chainA which is the shorter PDB of the accession number
  chainA <- trim.pdb(s, chain="A", elty = "CA")

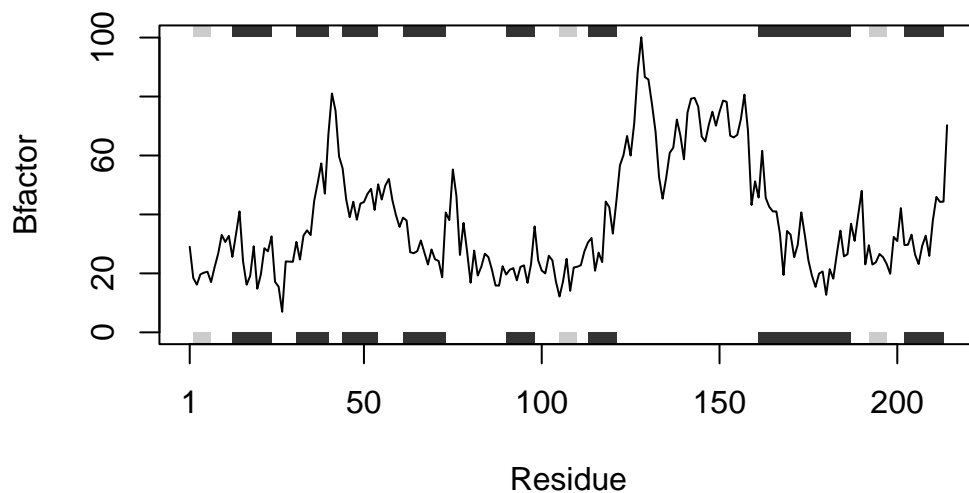
  #The input of this function will be chainA
  #The function is used to access the variable "b" in the list of "atoms" in chainA
  #The output is s.b
  s.b <- chainA$atom$b

  #The inputs for this function are s.b and chainA
  #This function plots the data onto a graph
  #The output will be the graph
  plotb3(s.b, sse= chainA, typ="l", ylab="Bfactor")
}

library(bio3d)
plotkinase("4AKE")
```

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\sharl\AppData\Local\Temp\Rtmp8gkwSY\4AKE.pdb exists. Skipping download

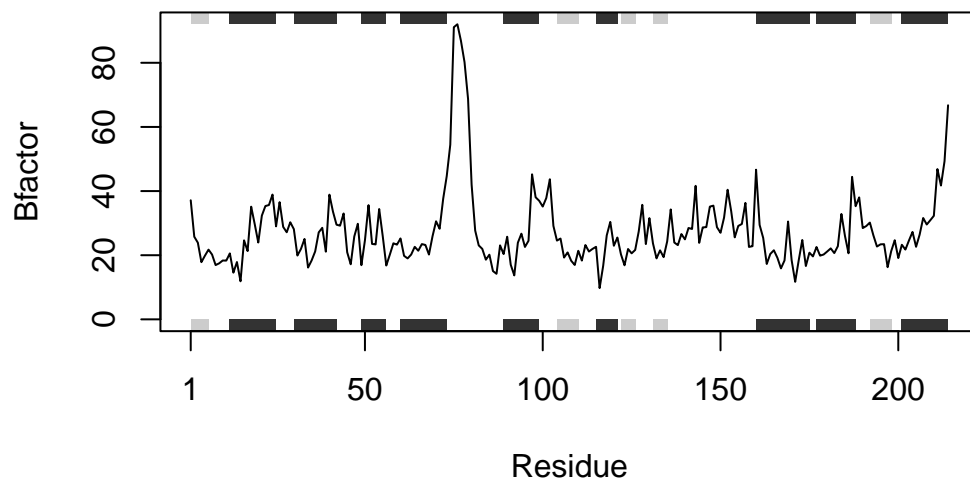


```
plotkinase("1AKE")
```

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\sharl\AppData\Local\Temp\Rtmp8gkwSY\1AKE.pdb exists. Skipping download

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



```
plotkinase("1E4Y")
```

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\sharl\AppData\Local\Temp\Rtmp8gkwSY\1E4Y.pdb exists. Skipping download

