

Class06_homework

Fan Wu(PID:A15127541)

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

Note: Accessing on-line PDB file

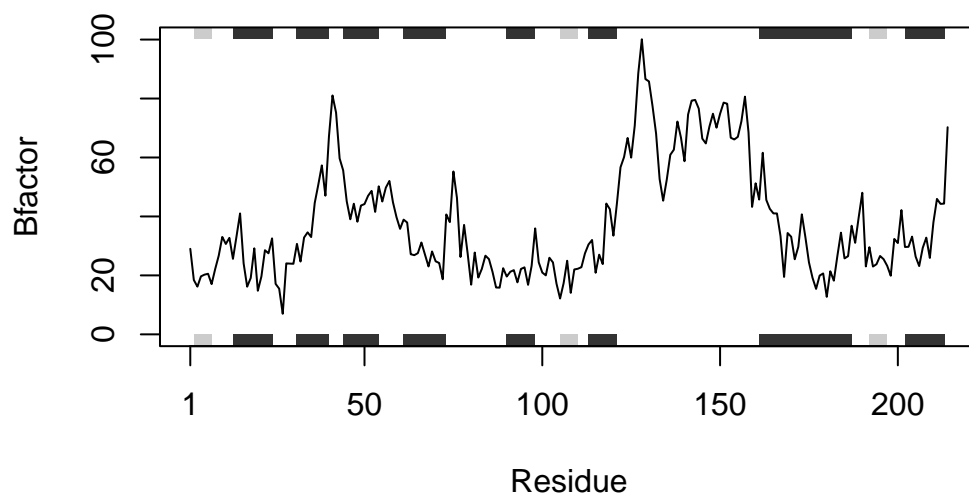
```
s2 <- read.pdb("1AKE") # kinase no drug
```

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

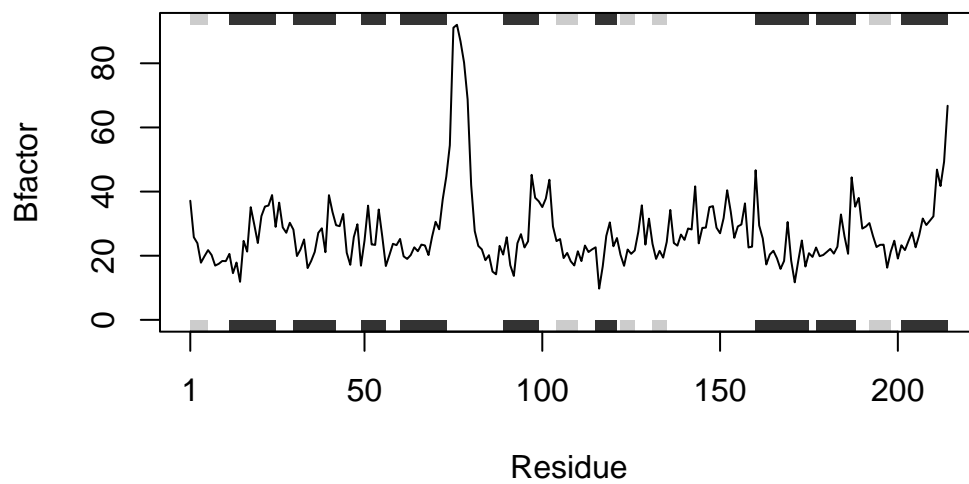
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

Note: Accessing on-line PDB file

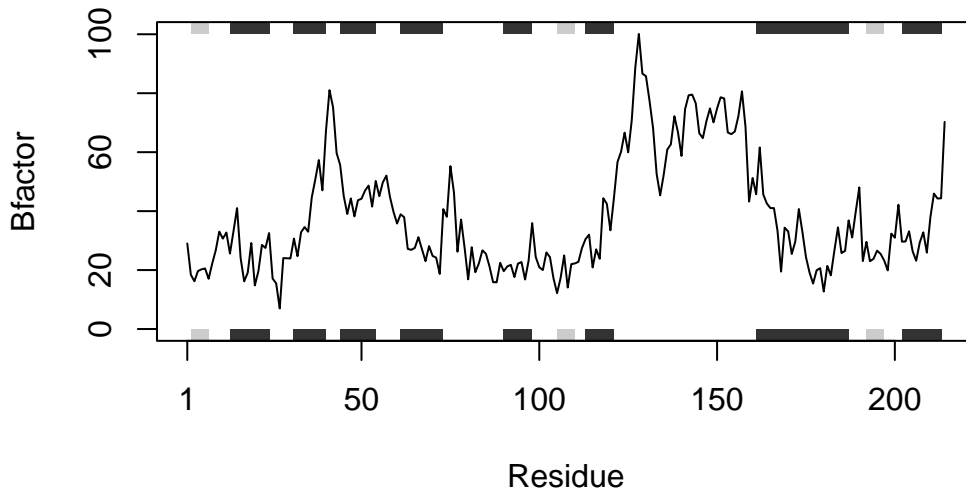
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")  
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")  
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")  
s1.b <- s1.chainA$atom$b  
s2.b <- s2.chainA$atom$b  
s3.b <- s3.chainA$atom$b  
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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



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



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

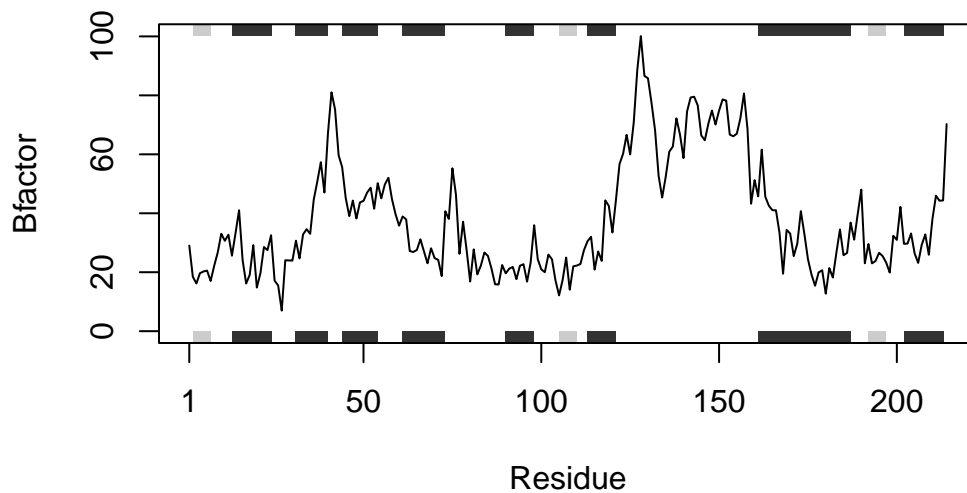
```
# input: in PDB format, any protein that contains a chain A and has alpha carbon atoms.
plot_chainA_Bfactor <- function(x){
  library(bio3d)
  protein_structure <- read.pdb(x)
  protein_structure.chainA <- trim.pdb(protein_structure,
                                     chain="A", eley="CA")
  protein_structure.b <- protein_structure.chainA$atom$b
  plotb3(protein_structure.b, sse=protein_structure.chainA,
         typ="l", ylab="Bfactor")
}
#output: a graph of the flexibility of chain A's backbone in the input protein structure
```

Outputs of the function `plot_chainA_Bfactor()` can be compared to that of original code

```
# demo1 of the function, can be compared to original code
plot_chainA_Bfactor ("4AKE")
```

Note: Accessing on-line PDB file

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):  
/var/folders/5z/1tx9n87953s0hzdmvns91c5w0000gn/T//RtmpCMfBG6/4AKE.pdb exists.  
Skipping download
```

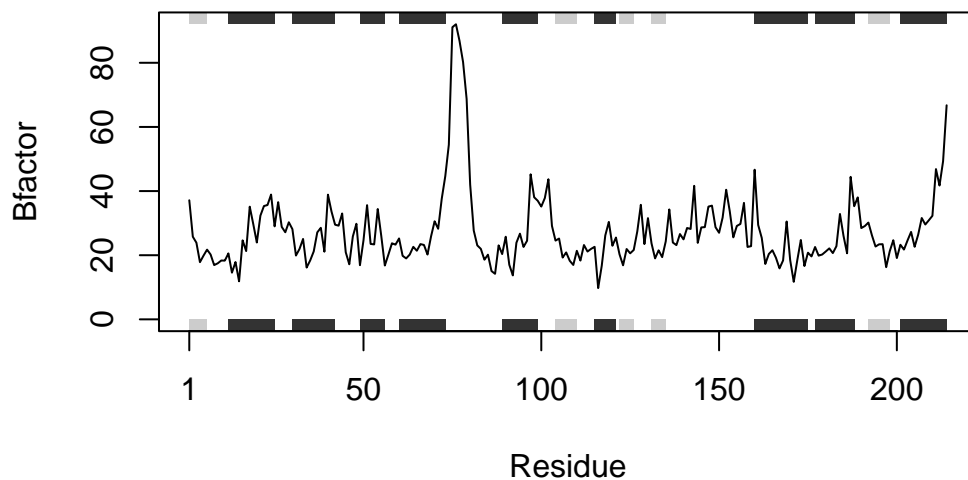


```
# demo2 of the function, can be compared to original code  
plot_chainA_Bfactor ("1AKE")
```

Note: Accessing on-line PDB file

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):  
/var/folders/5z/1tx9n87953s0hzdmvns91c5w0000gn/T//RtmpCMfBG6/1AKE.pdb exists.  
Skipping download
```

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



```
# demo3 of the function, can be compared to original code  
plot_chainA_Bfactor ("1E4Y")
```

Note: Accessing on-line PDB file

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):  
/var/folders/5z/1tx9n87953s0hzdmvns91c5w0000gn/T//RtmpCMfBG6/1E4Y.pdb exists.  
Skipping download
```

