

Class 6 Function Homework

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Q Write a function of the supplied code.

Supplied code :

```
library(bio3d)
s1 <- read.pdb("4AKE") # kinase with drug
```

Note: Accessing on-line PDB file

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

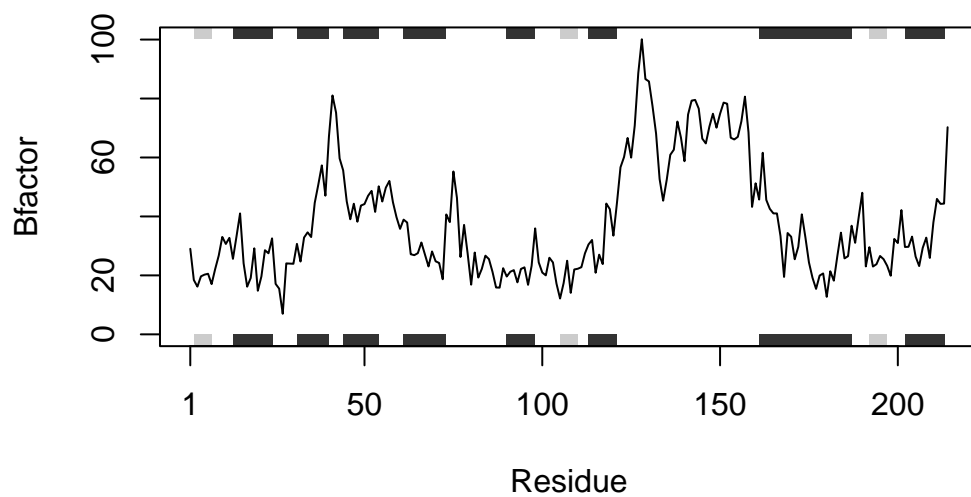
Note: Accessing on-line PDB file

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

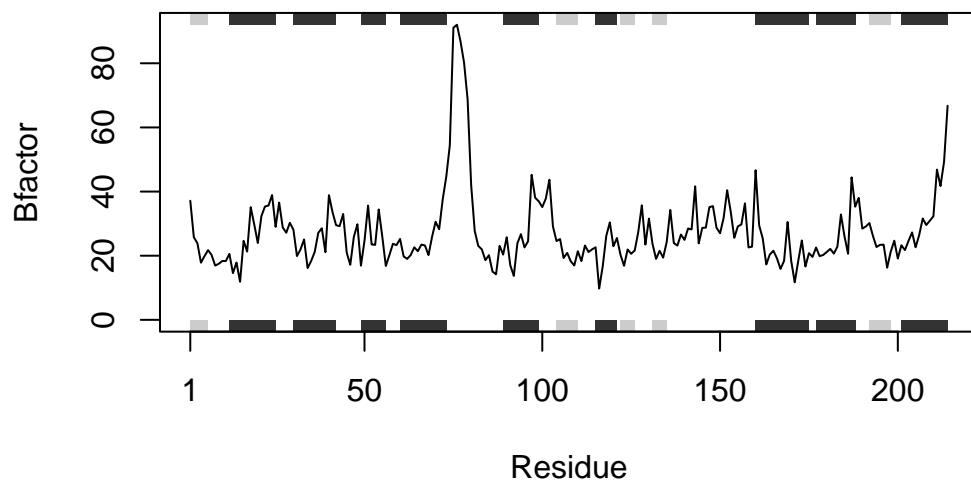
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

Note: Accessing on-line PDB file

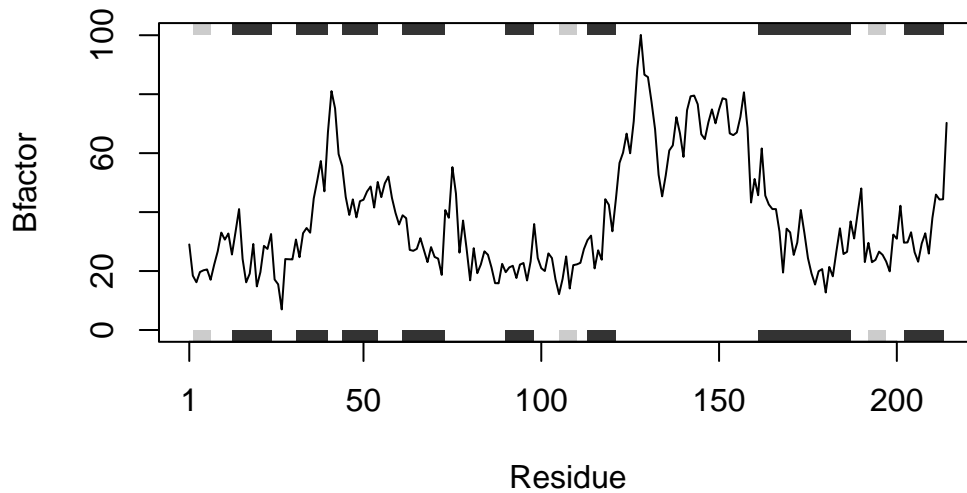
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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



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



Can you improve this analysis code?

Assignment :

```
Plot_Bfactor <- function(pdb) {  
  
  #the input to this function is pdb, the 4 Character pdb ID (e.g. "4AKE")  
  
  ans <- read.pdb(pdb)  
  ans <- trim.pdb(ans, chain = "A", elety = "CA")  
  
  # repeated parts of code taken and applied to ans  
  
  # 1) Function now reads input pdbfile  
  # 2) trims to chain A and alpha carbon atoms  
  # 3) applies both to ans
```

```

b <- ans$atom$b

# B factors are extracted out of our trimmed pdb file , set to b

plotb3(b, sse = ans, type="l", ylab = "Bfactor")

# produces plot using :
# B factors (b)
# our trimmed, input pdb file (ans)
# same parameters as original code
}

#Function output :
# Plot of B-factors vs residues
# Set to our input pdbfile

Plot_Bfactor("4AKE")

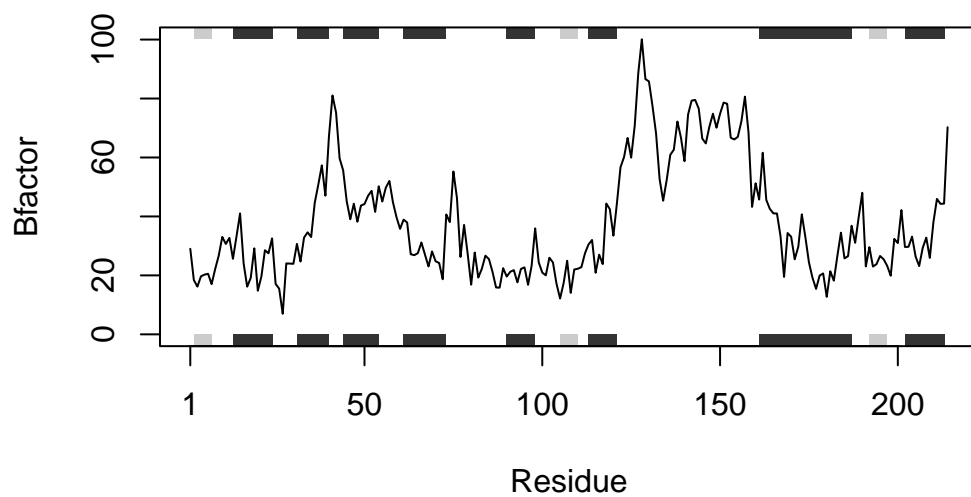
```

Note: Accessing on-line PDB file

```

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/gp/8szl16kd5bq7qnbbt4s9l44m0000gn/T//RtmpJ9gcQn/4AKE.pdb exists.
Skipping download

```



```
#This is an example of the function reading in the "4AKE" pdb file  
# Returns a B-factor plot for the protein.
```