

class06_hw

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```
# 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

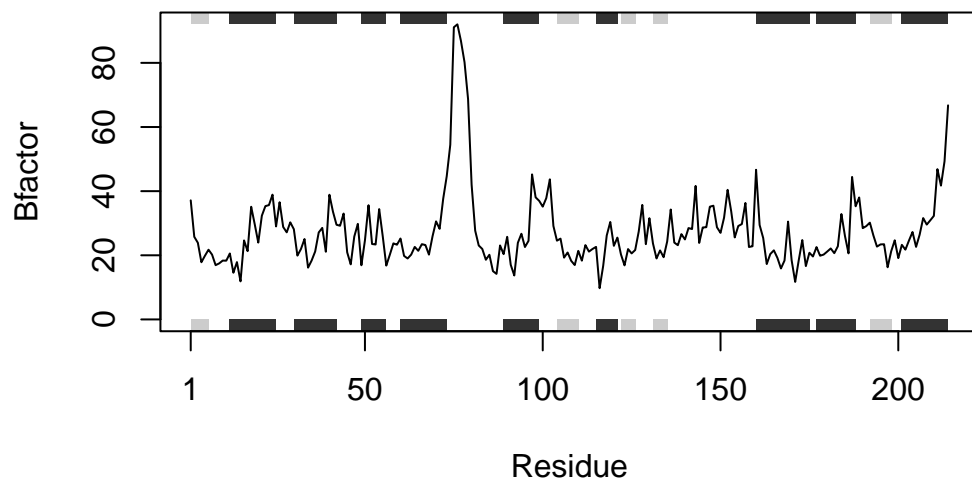
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

Note: Accessing on-line PDB file

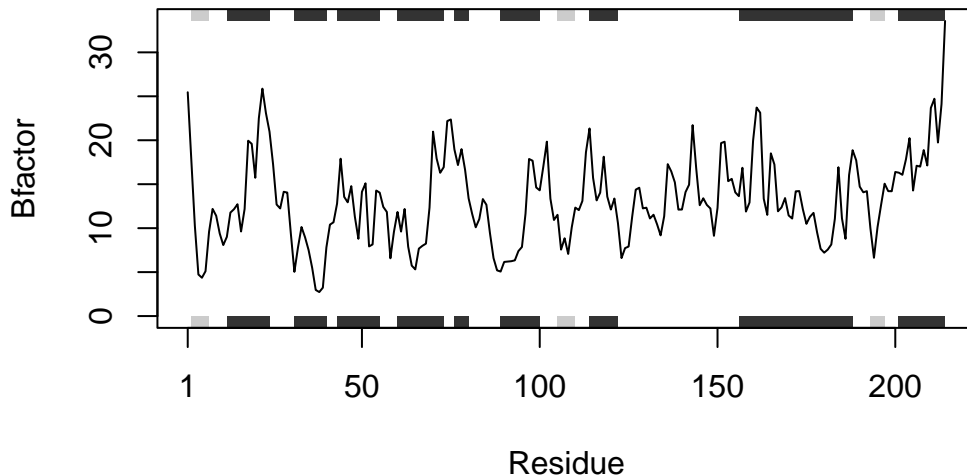
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")  
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")  
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")  
  
s1.b <- s1.chainA$atom$b  
s2.b <- s2.chainA$atom$b  
s3.b <- s3.chainA$atom$b  
  
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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



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



the first step is to use `read.pdb` to read the protein.

```
protein <- read.pdb("4AKE")
```

Note: Accessing on-line PDB file

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/6b/30swmpb11hj19z5zb0w2bt80000gn/T/RtmpkFI30y/4AKE.pdb exists.
Skipping download
```

Next step is using `trim.pdb` and using `chain` and `elety`, specifically for chain A and elety CA

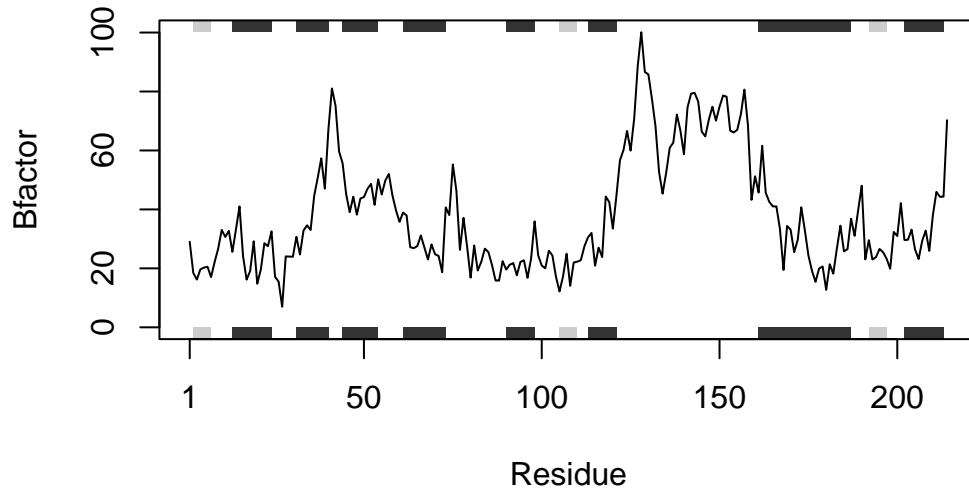
```
protein.chainA <- trim.pdb(protein, chain="A", elety="CA")
```

The next step is calling a specific atom from chainA

```
protein.b <- protein.chainA$atom$b
```

The final step is to plot with optional secondary structures in the marginal regions. we will be plotting a line graph (typ="l")

```
plotb3(protein.b, sse=protein.chainA, type="l",ylab="Bfactor")
```



Now we will input all of this information in the format of a function.

```
#what the function does and how to use it AND what is the output of the function

##this function reads proteins from a database and then plots the output as the Bfactor us

plot_protein <- function(x) {
  #use read.pdb to read the protein
  protein <- read.pdb(x)

  #using trim.pdb and using chain and elety, specifically for chain A and elety CA
  protein.chainA <- trim.pdb(protein, chain="A", elety="CA")

  #calling a specific atom from chainA
  protein.b <- protein.chainA$atom$b
```

```

#plot with optional secondary structures in the marginal regions, using a line graph
plotb3(protein.b, sse=protein.chainA, type="l",ylab="Bfactor")
}

```

In the function, we wrote all the necessary statements required to generalize the function for any protein. now we will plot the protein using the function above

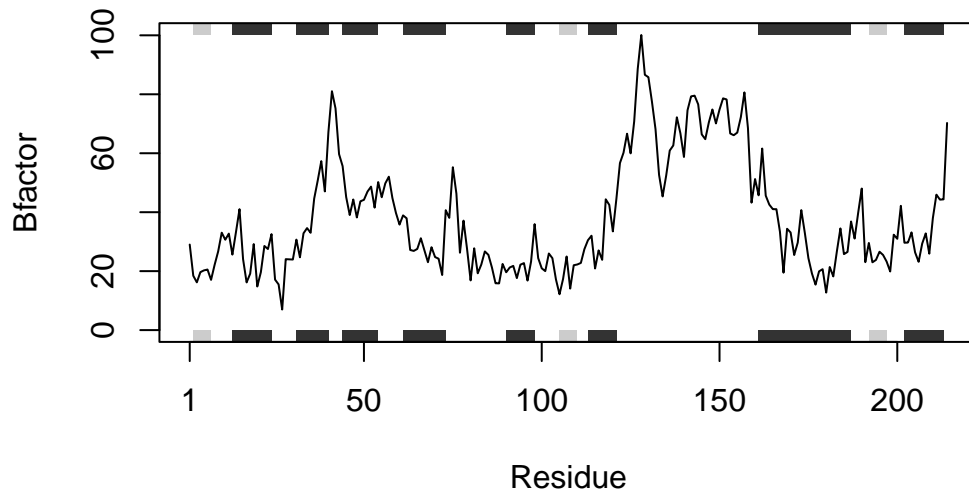
```

# functions match and desired outputs are produced
plot_protein("4AKE")

```

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/6b/30swmpb11hj19z5zb0w2btx80000gn/T//RtmpkFI30y/4AKE.pdb exists.
Skipping download



```

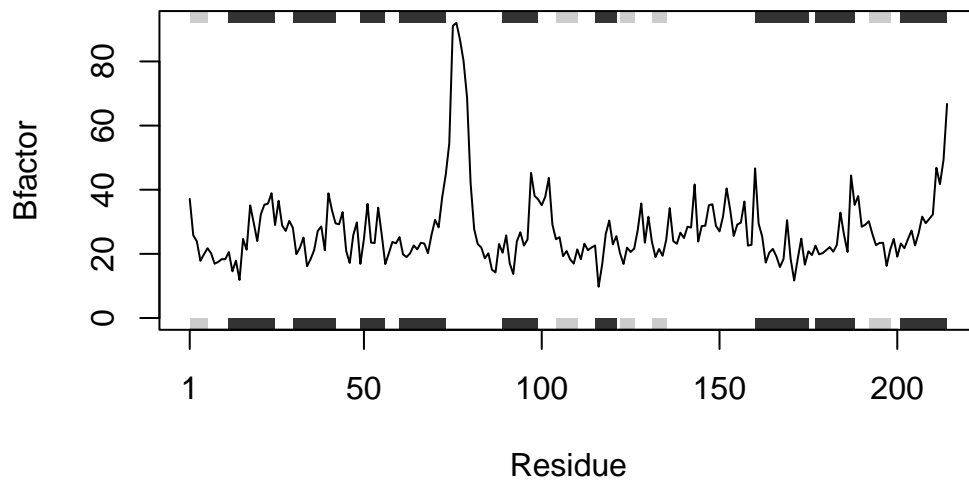
plot_protein("1AKE")

```

Note: Accessing on-line PDB file

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):  
/var/folders/6b/30swmpb11hj19z5zb0w2btx80000gn/T//RtmpkFI30y/1AKE.pdb exists.  
Skipping download
```

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



```
plot_protein("1E4Y")
```

Note: Accessing on-line PDB file

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):  
/var/folders/6b/30swmpb11hj19z5zb0w2btx80000gn/T//RtmpkFI30y/1E4Y.pdb exists.  
Skipping download
```

