Class 6 Homework

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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
```

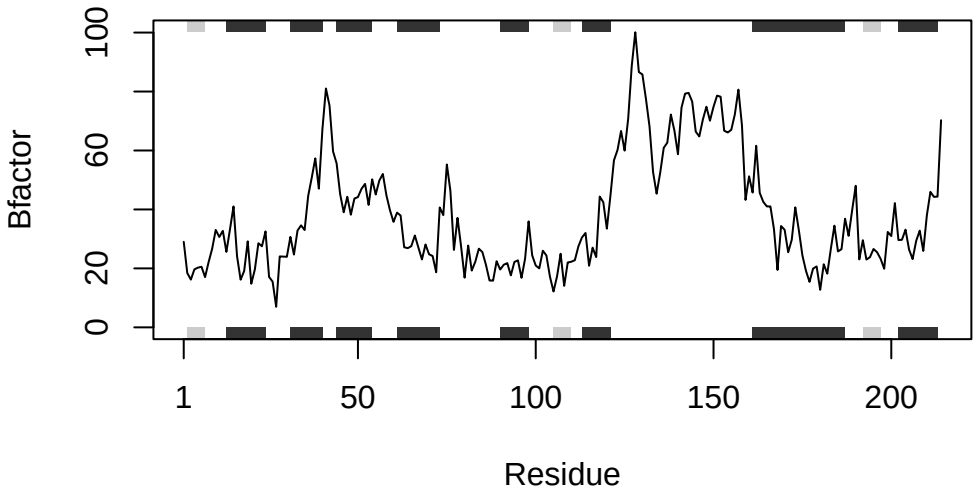
```
s2 <- read.pdb("1AKE")  # kinase no drug
```

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

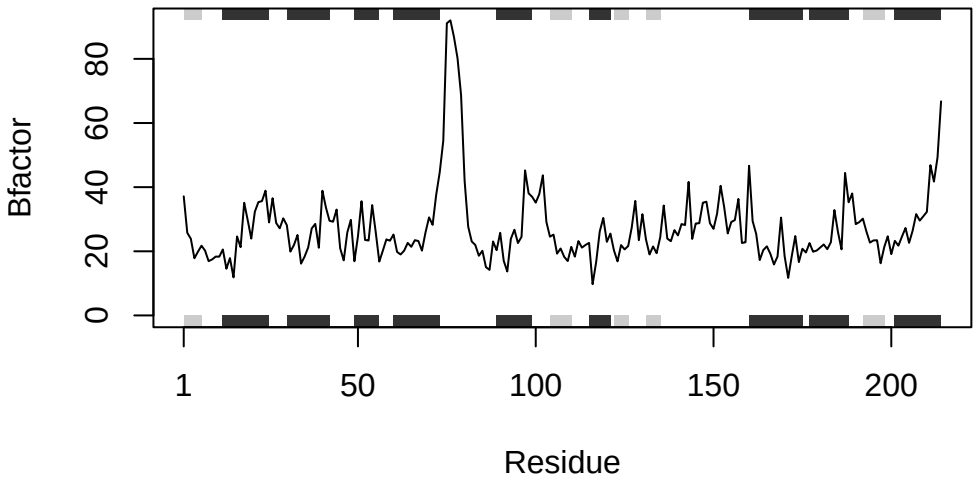
```
s3 <- read.pdb("1E4Y")  # kinase with drug
```

```
Note: Accessing on-line PDB file
```

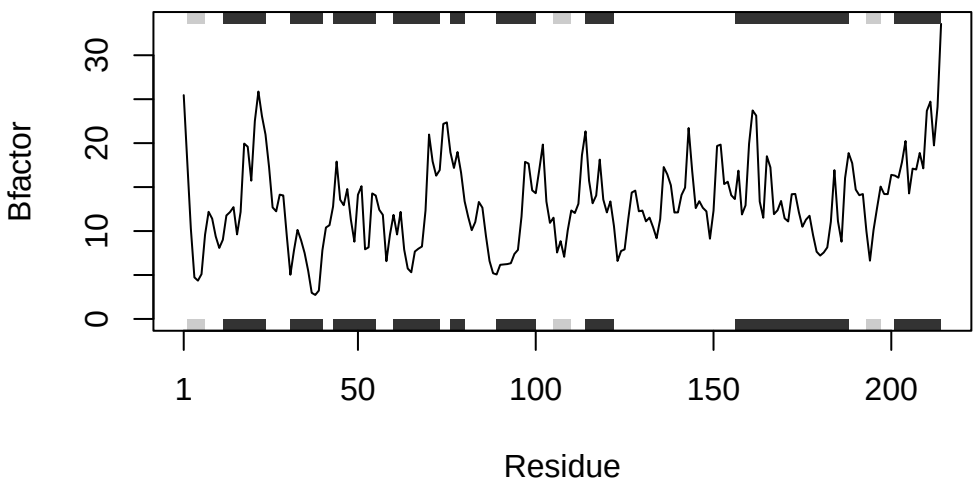
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```




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



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



We will start by using `read.pdb` to read the protein.

```
protein_x <- read.pdb("1E4Y")
```

```
  Note: Accessing on-line PDB file
```

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/g7/6kj1lwl51s7_mw596z6h96y40000gn/T//RtmpcIe2ll/1E4Y.pdb exists.
Skipping download
```

We will then use `trim.pdb` with chain ("A") and elety ("CA").

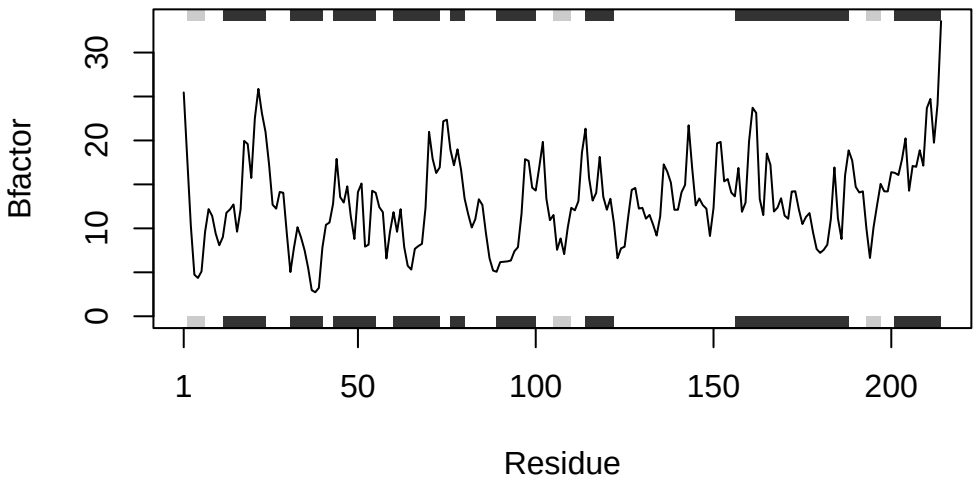
```
protein_x.chainA <- trim.pdb(protein_x, chain="A", elety="CA")
```

In order to for chain A to be specific to an atom, we must call this function.

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

Finally, we will plot a line graph (typ="l")

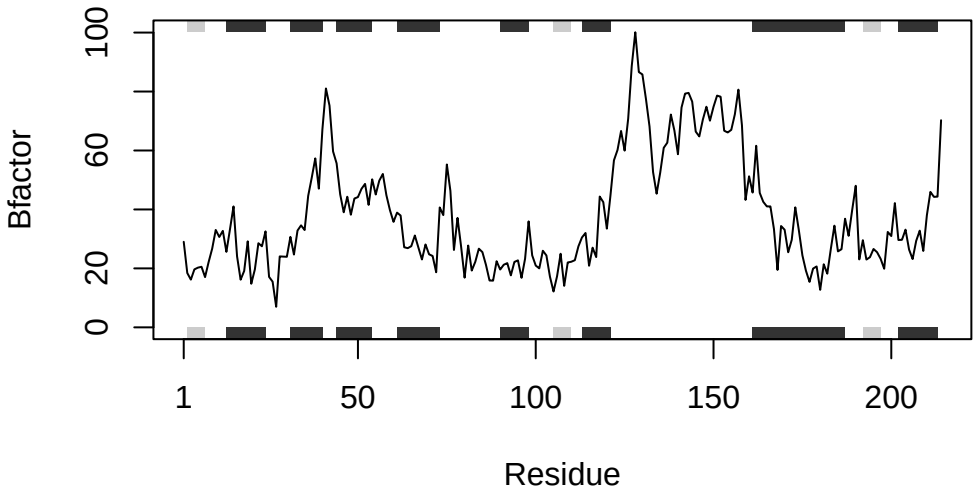
```
plotb3(protein_x.b, sse=protein_x.chainA, typ="l", ylab="Bfactor")
```




```
# we are turning this into a function
plot_protein_x <- function(x){
  protein_x <- read.pdb(x)
  protein_x.chainA <- trim.pdb(protein_x, chain="A", elety="CA")
  protein_x.b <- protein_x.chainA$atom$b
  plotb3(protein_x.b, sse=protein_x.chainA, typ="l", ylab="Bfactor")


}
```

```
# test to see if the functoin can be generalized to work with any set of input protein str

plot_protein_x("4AKE")
```

```
  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/g7/6kj1lwl51s7_mw596z6h96y40000gn/T//RtmpcIe2ll/4AKE.pdb exists.
Skipping download
```

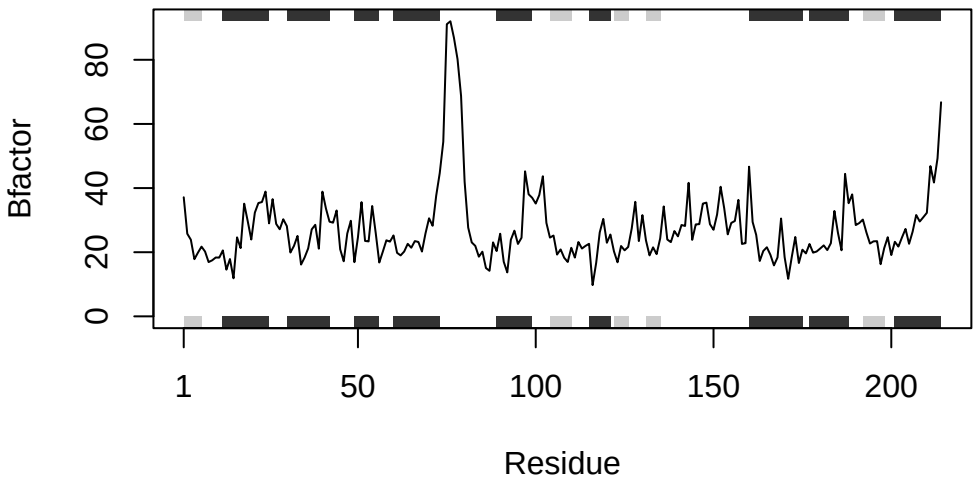



```
plot_protein_x("1AKE")
```

```
  Note: Accessing on-line PDB file
```

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/g7/6kj1lwl51s7_mw596z6h96y40000gn/T//RtmpcIe2ll/1AKE.pdb exists.
Skipping download
```

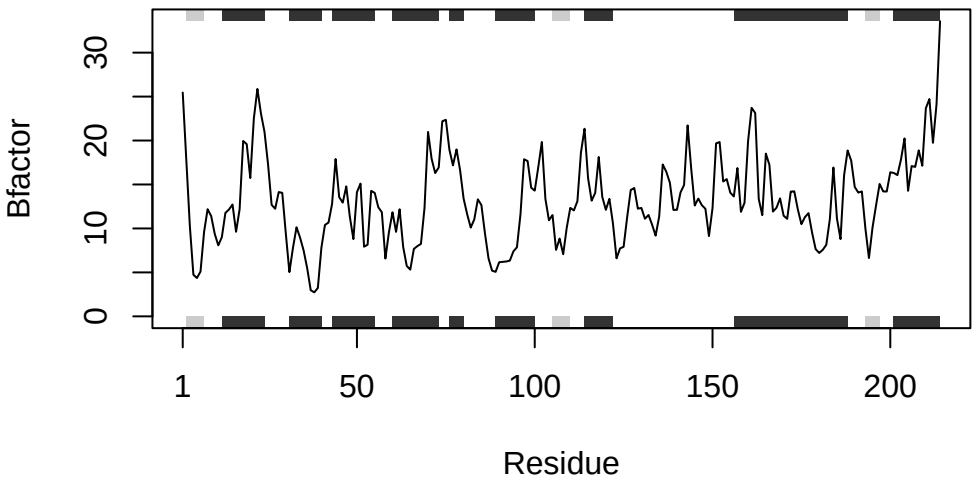
```
   PDB has ALT records, taking A only, rm.alt=TRUE
```




```
plot_protein_x("1E4Y")
```

```
  Note: Accessing on-line PDB file
```

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/g7/6kj1lwl51s7_mw596z6h96y40000gn/T//RtmpcIe2ll/1E4Y.pdb exists.
Skipping download
```


Bfactor
0
10
20
30
1
50
100
150
200
Residue