hw_week3

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Homework: Simplifying the given chunk of code

First, install the pdb package

```
#install.packages("bio3d")
```

Given code:

The code that needs to be simplified:

```
library(bio3d)

#including protein names
s1 <- read.pdb("4AKE") # kinase with drug
```

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

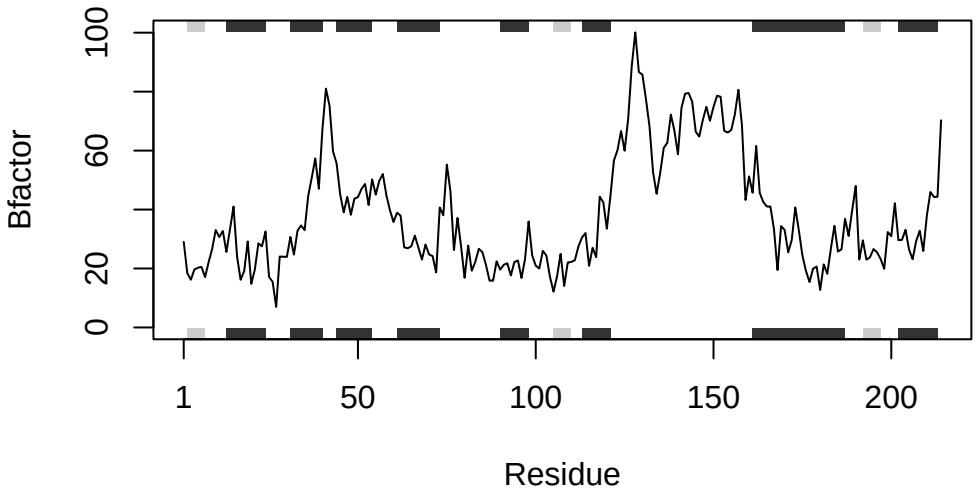
```
s2 <- read.pdb("1AKE") # kinase no drug
```

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

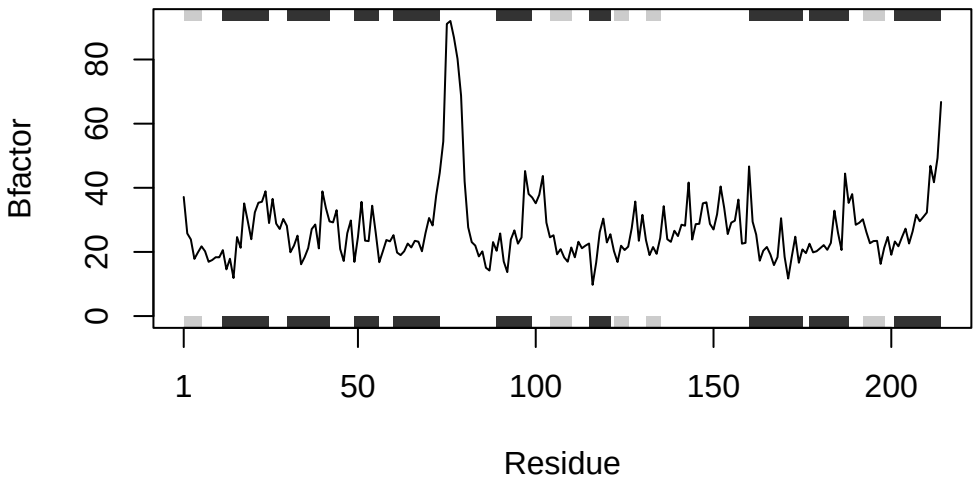
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

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

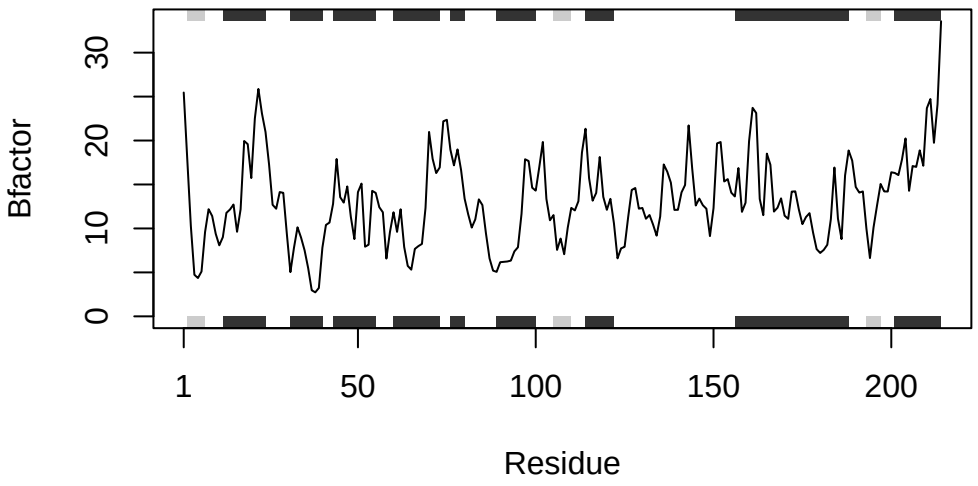
```
#extracting the A chain from each protein
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")

#extracting atom b from the A chain
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b

#plotting 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")
```



Simplified code

Simplifying the above function by condensing three lines of code into a singular function.

```
library(bio3d)

pdb_plot <-function(x) {
  #reading the pdb file to store it in x
  x <- read.pdb(x)
  #extracting chain A
  x.chainA <- trim.pdb(x, chain="A", elety="CA")
  #extracting atom b (Bfactor) from chain A
  x.b <- x.chainA$atom$b
  #plotting the B atom factors against the chain residues as a line graph
  plotb3(x.b, sse=x.chainA, typ="l", ylab="Bfactor")
}
```

Now, a user can input the 4 digit PDB code within the function ***'pdb_plot()'*** to get a plot of the B factor vs Residue on the A chain. e.g.

```
pdb_plot("1AKE")
```

```
  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/wk/
g99jn15131xdpvglxz6x448c0000gn/T//RtmpPrDctq/1AKE.pdb exists. Skipping download

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