HW_6

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Generalizing R code using a function

The original code looks like this:

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

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

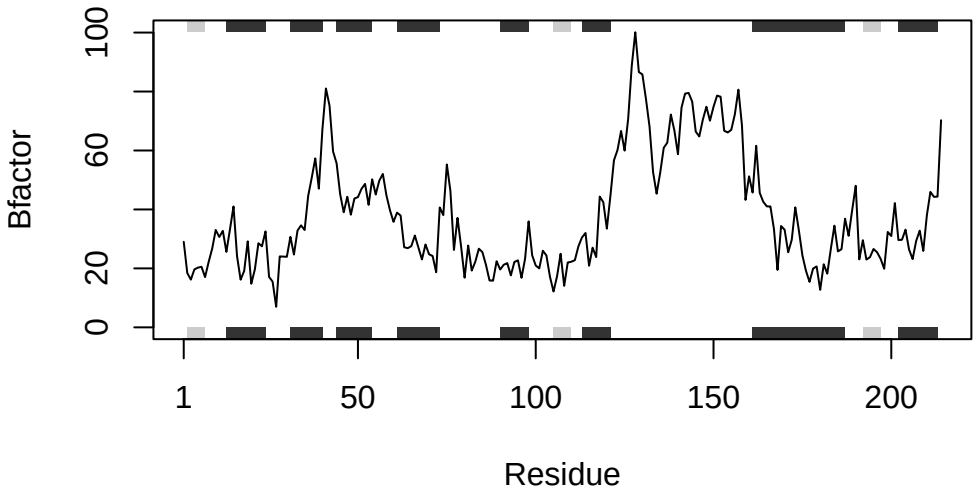
```
s2 <- read.pdb("1AKE") # kinase no drug
```

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

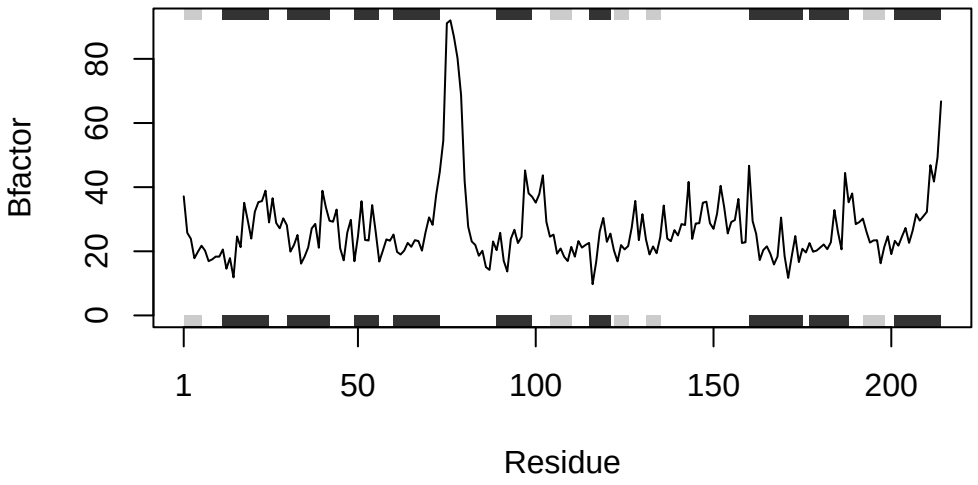
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

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

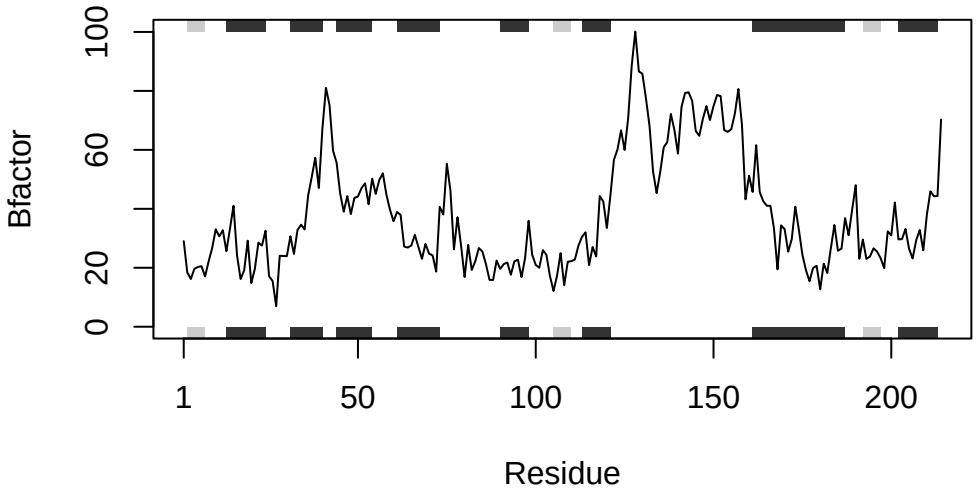
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```




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



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



We can generalize this code so that we don't have to copy and paste the previous code every time we want to analyze a protein.

Here is the function to do that:

```
analyze_protein_drug_interaction <- function(protein) {
  # this function takes in the protein name as input

  # read in the PDB object for the input protein
  s <- read.pdb(protein)

  # trim the PDB object to contain a subset
  s.chainA <- trim.pdb(s, chain="A", elety="CA")

  # select desired B-factor data series
  s.b <- s.chainA$atom$b

  # lineplot with standard error and y labeled
  plotb3(s.b, sse=s.chainA, typ="l", ylab="Bfactor")
```

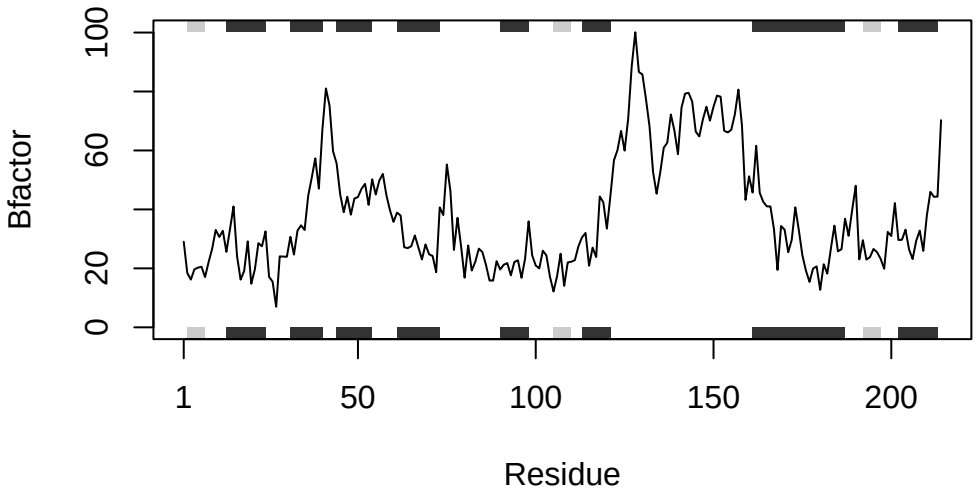
```
  # this plot serves as the sole output of the function
}
```

Let's test the function on the previous inputs.

```
# we can use the function by typing the function name and providing the protein name (text
analyze_protein_drug_interaction("4AKE")
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\soysa\AppData\Local\Temp\RtmpqcmoaY/4AKE.pdb exists. Skipping download
```

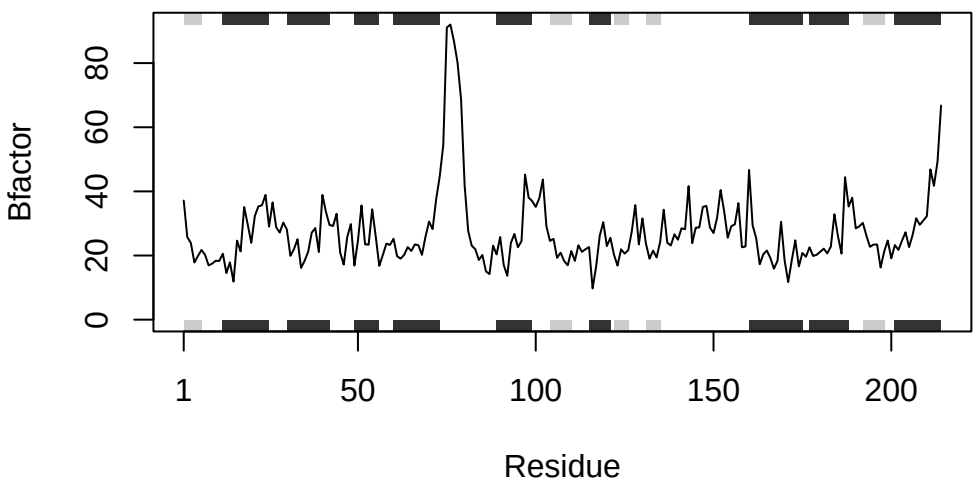



```
analyze_protein_drug_interaction("1AKE")
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\soysa\AppData\Local\Temp\RtmpqcmoaY/1AKE.pdb exists. Skipping download
```

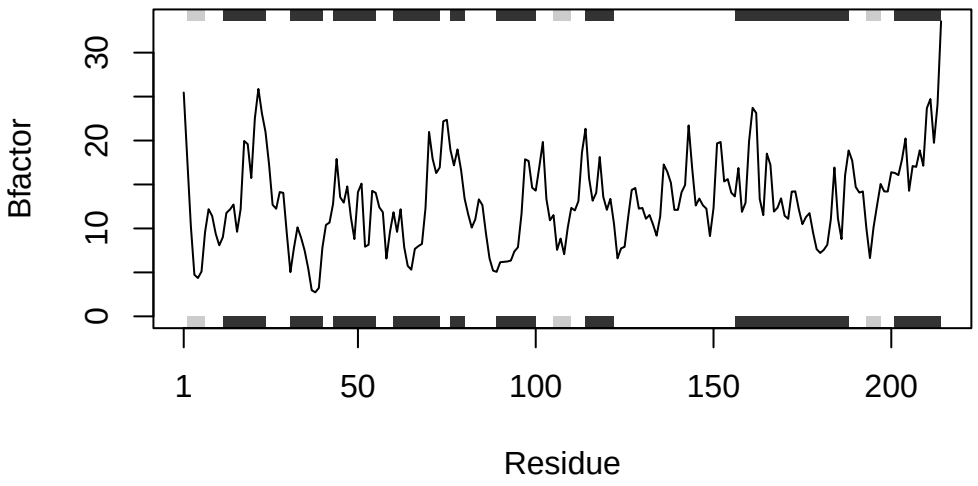
```
PDB has ALT records, taking A only, rm.alt=TRUE
```




```
analyze_protein_drug_interaction("1E4Y")
```

```
  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\soysa\AppData\Local\Temp\RtmpqcmoaY/1E4Y.pdb exists. Skipping download
```



Looks like it works!