Class 6 Homework

Morgan Black (PID A14904860)

```
#Original code supplied in the homework file, with typos/erros fixed

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

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

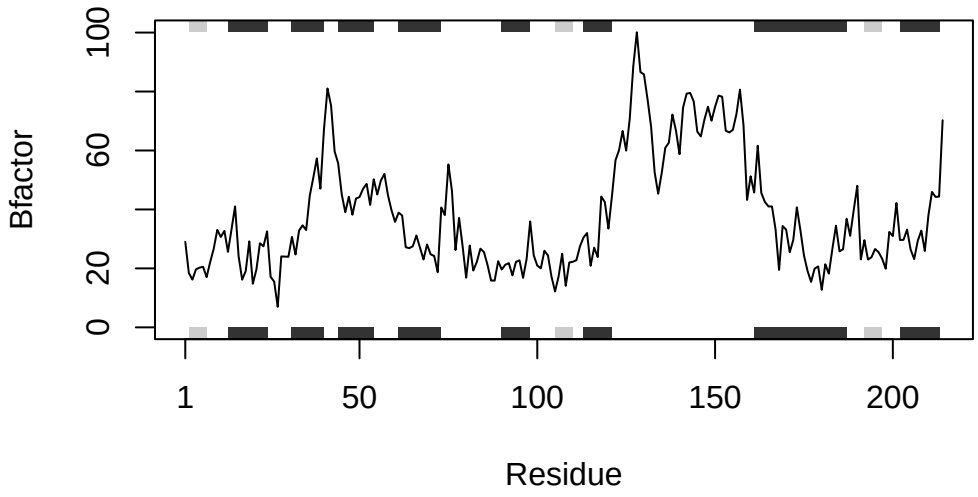
```
s2 <- read.pdb("1AKE") # kinase no drug
```

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

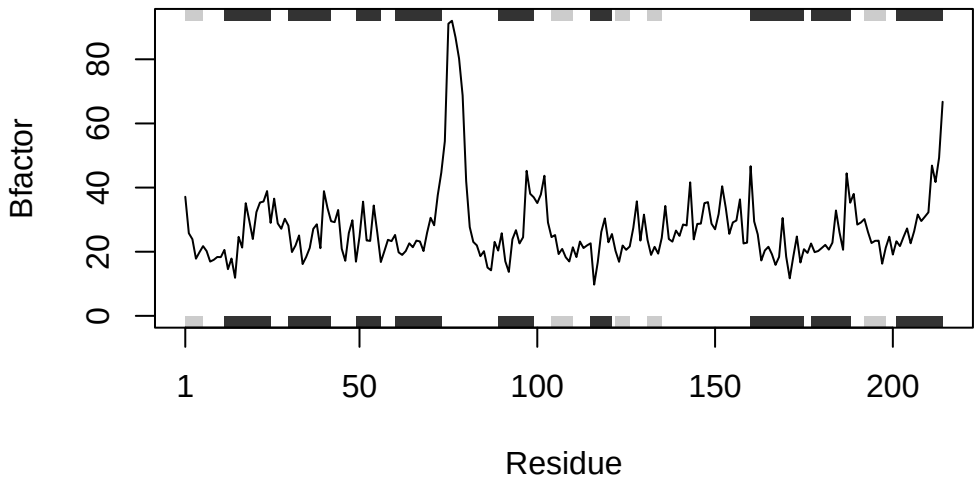
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

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

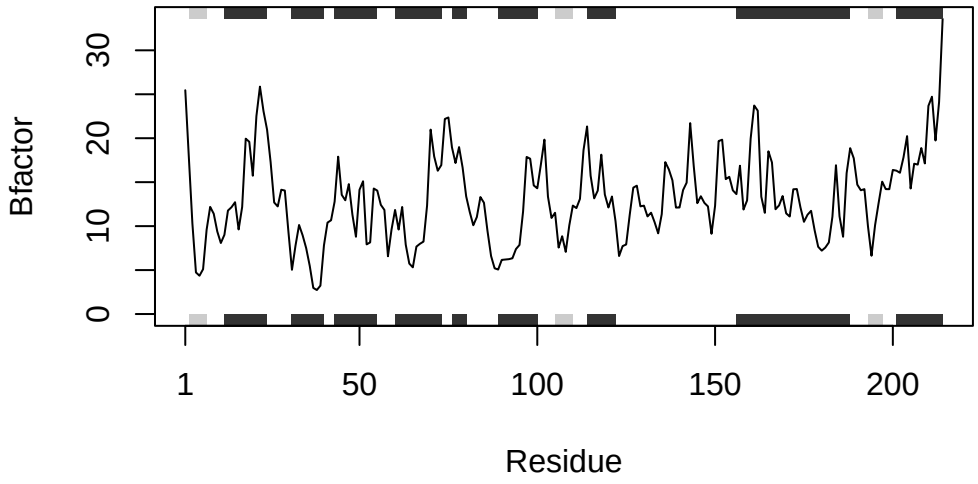
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```




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



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



##Write your own function starting from the code above that analyzes protein drug interactions by reading in any protein PDB data and outputs a plot for the specified protein.

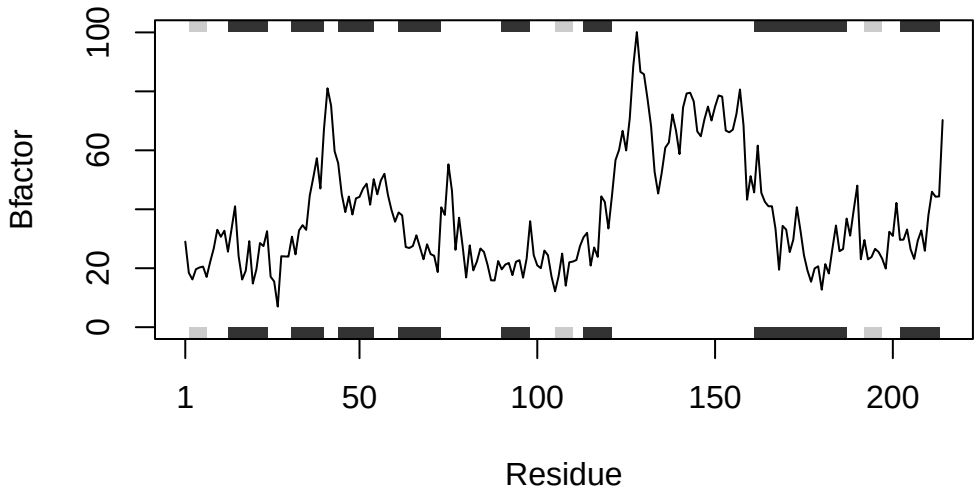
```
#Call the bio3d package to use in the function below
library(bio3d)

#Define the function name and input (protein identifier):
drug_interaction <- function(protein){
  #Read the structure of the input protein and assigns the data to "structure"
  structure <- read.pdb(protein)
  #Trim the protein data from the database to just look at the data in the
  #A chain of the protein and C-alpha atom type
  Achain <- trim.pdb(structure, chain="A", elety="CA")
  #Subset the Bfactor data from the Achain database above as a vector
  Bfactor <- Achain$atom$b
  #Plot the Bfactor response along the A chain amino acid sequence
  plotb3(Bfactor, sse=Achain, typ= "l", ylab="Bfactor")
}

drug_interaction("4AKE")
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/v3/7g0pvy6x6wsd_qvzzwc6snh80000gp/T//RtmpAa8kbp/4AKE.pdb exists.
Skipping download
```

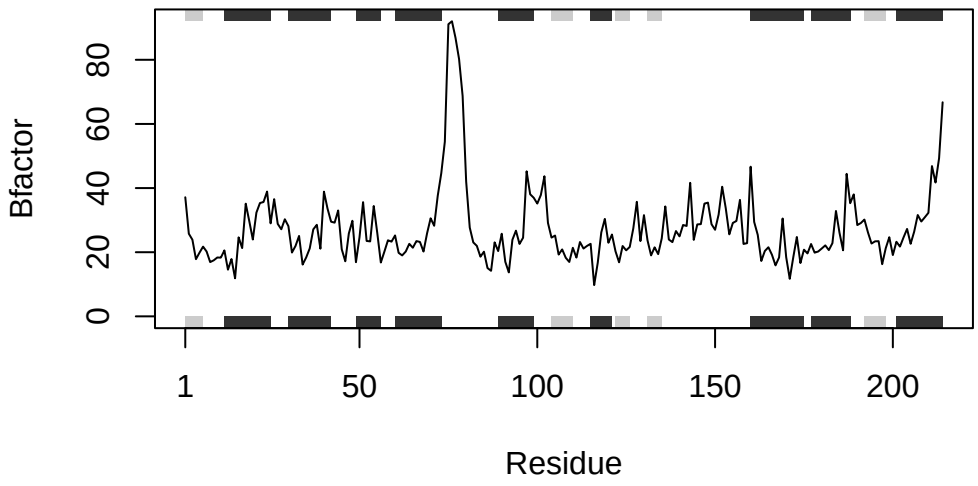



```
drug_interaction("1AKE")
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/v3/7g0pvy6x6wsd_qvzzwc6snh80000gp/T//RtmpAa8kbp/1AKE.pdb exists.
Skipping download
```

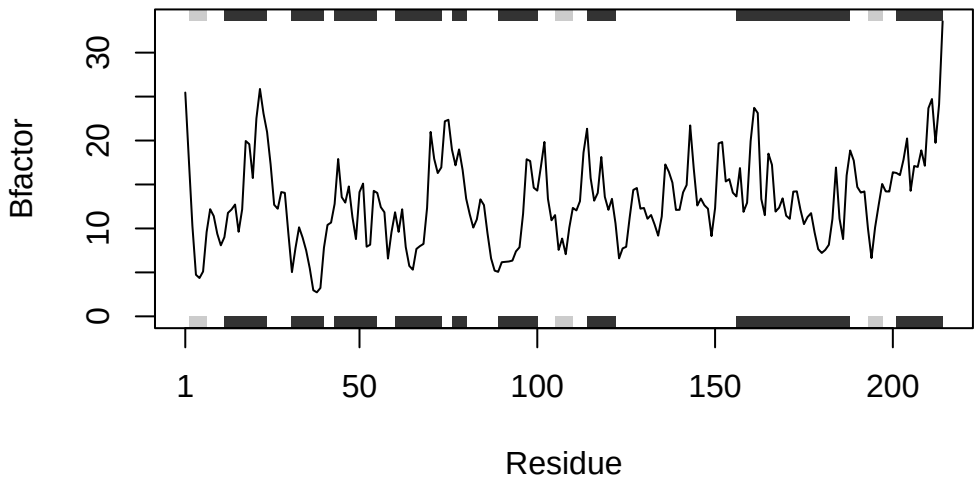
```
   PDB has ALT records, taking A only, rm.alt=TRUE
```




```
drug_interaction("1E4Y")
```

```
  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/v3/7g0pvy6x6wsd_qvzzwc6snh80000gp/T//RtmpAa8kbp/1E4Y.pdb exists.
Skipping download
```




```
#With this function, you can use any protein identifier name as the input.
#This function reads the input protein structure from a database, focuses
#in on just the A chain and B factor relevant portion of the protein, then
#plots the Bfactor response going along the length of the protein.

#The output of the function is a dot plot showing the Bfactor response
#at each amino acid position on the A chain of the protein sequence.
```