class6_HW

2025-01-27

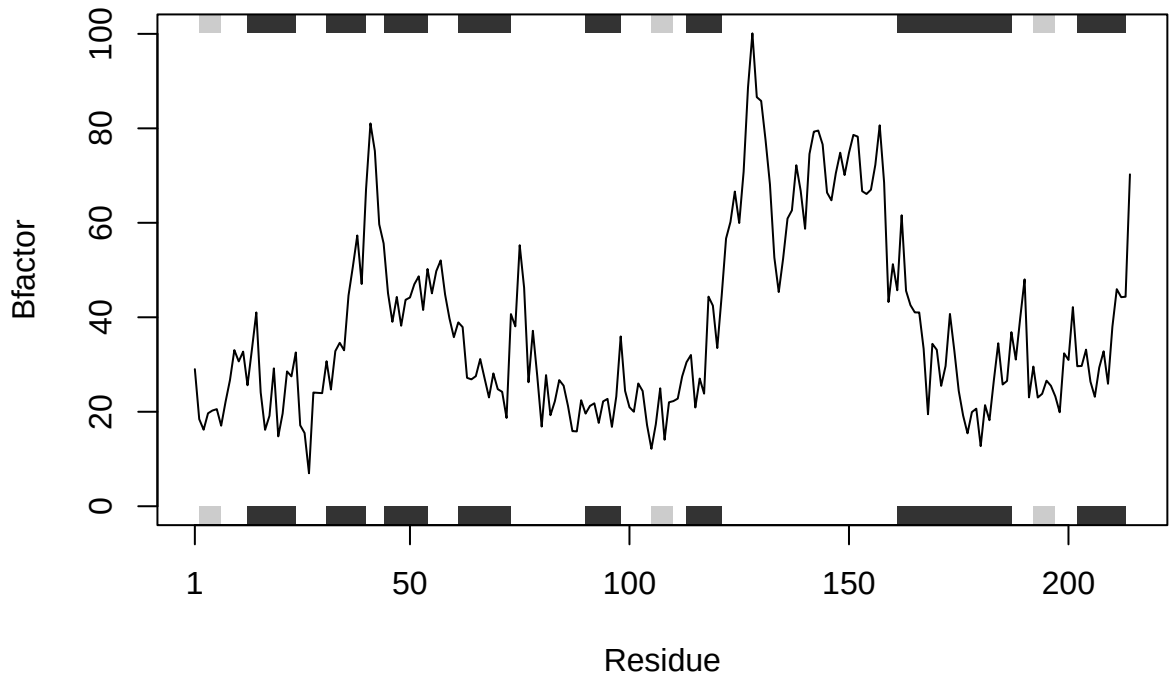
Using the provided code, I will make a function that can read in any protein PDB data and output a plot for the specified drug interactions.

This is what the provided code does, not as a function.

```
library(bio3d)

#reads in the pdb and stores it in a variable
s1 <- read.pdb("4AKE")
```

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

```
  s1.chainA <- trim.pdb(s1, chain="A", elety="CA") #extracts a specific part of the structure
  s1.b <- s1.chainA$atom$b
  plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor") #plots the interactions in a line chart
```

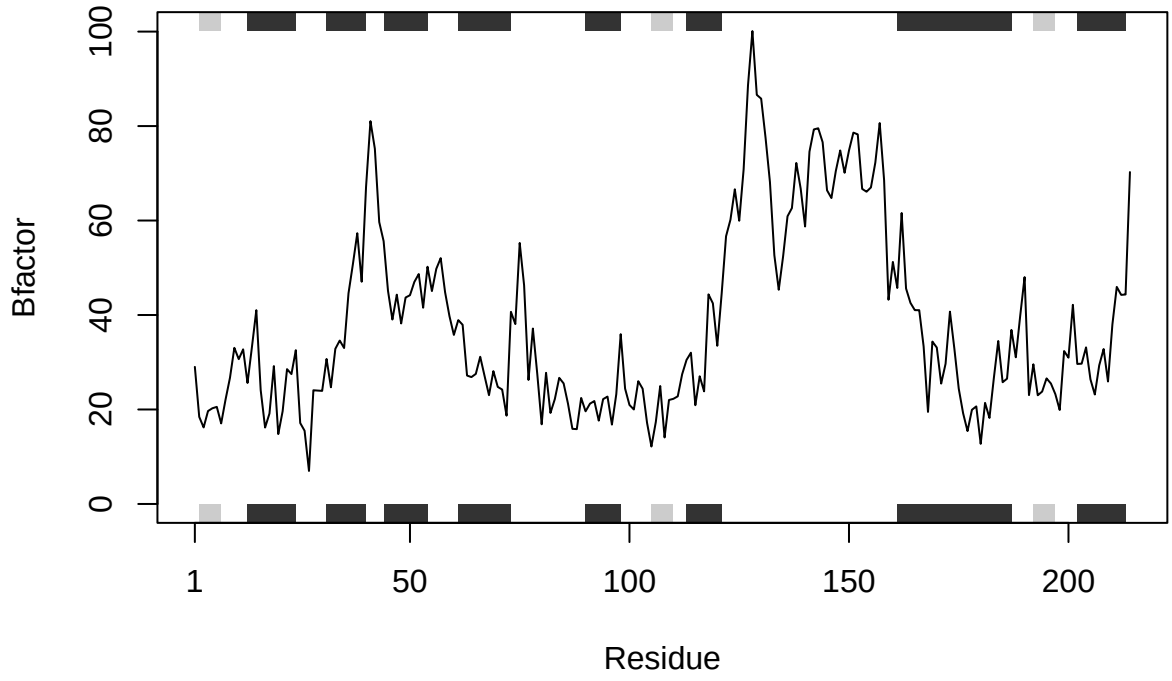



```
library(bio3d)

#a function to plot protein drug interactions, input can be any protein pdb data as a string value, suc
```

```
drug_analysis <- function(x) {
  s1 <- read.pdb(x)
  s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
  s1.b <- s1.chainA$atom$b
  plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
}

#function works for the following calls
drug_analysis("4AKE")
```

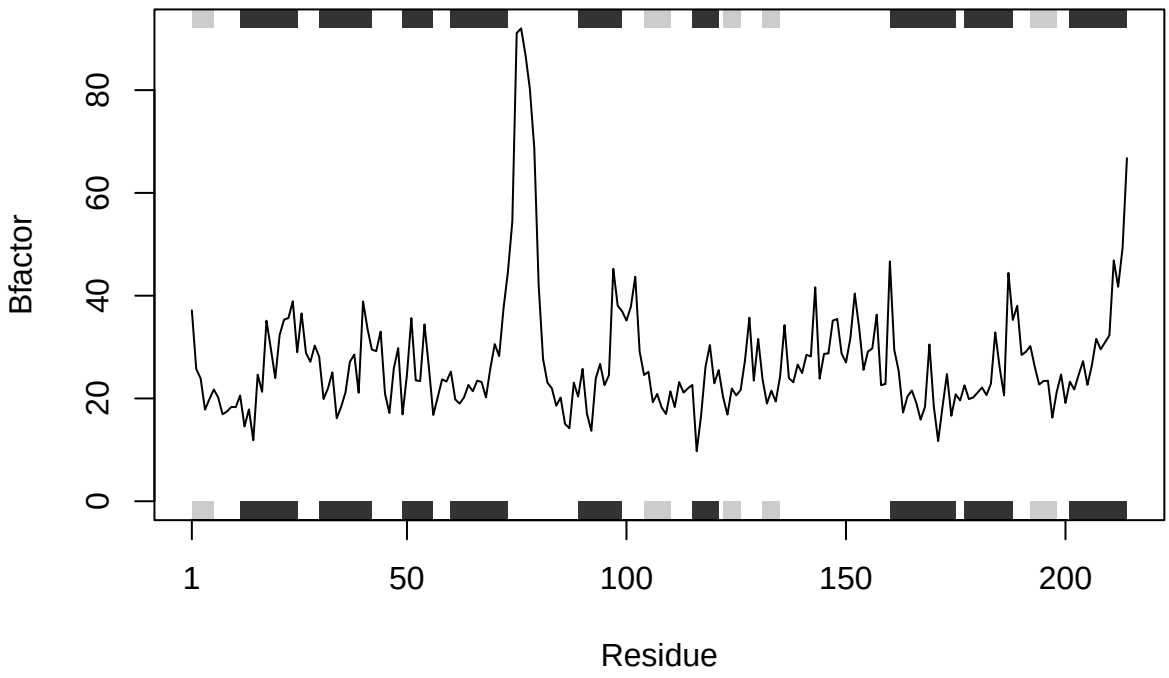
```
##   Note: Accessing on-line PDB file
```

```
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
## /var/folders/_d/vvmf9_l90rd4kq5m6g3dy9s00000gn/T//Rtmp44fn2u/4AKE.pdb exists.
## Skipping download
```



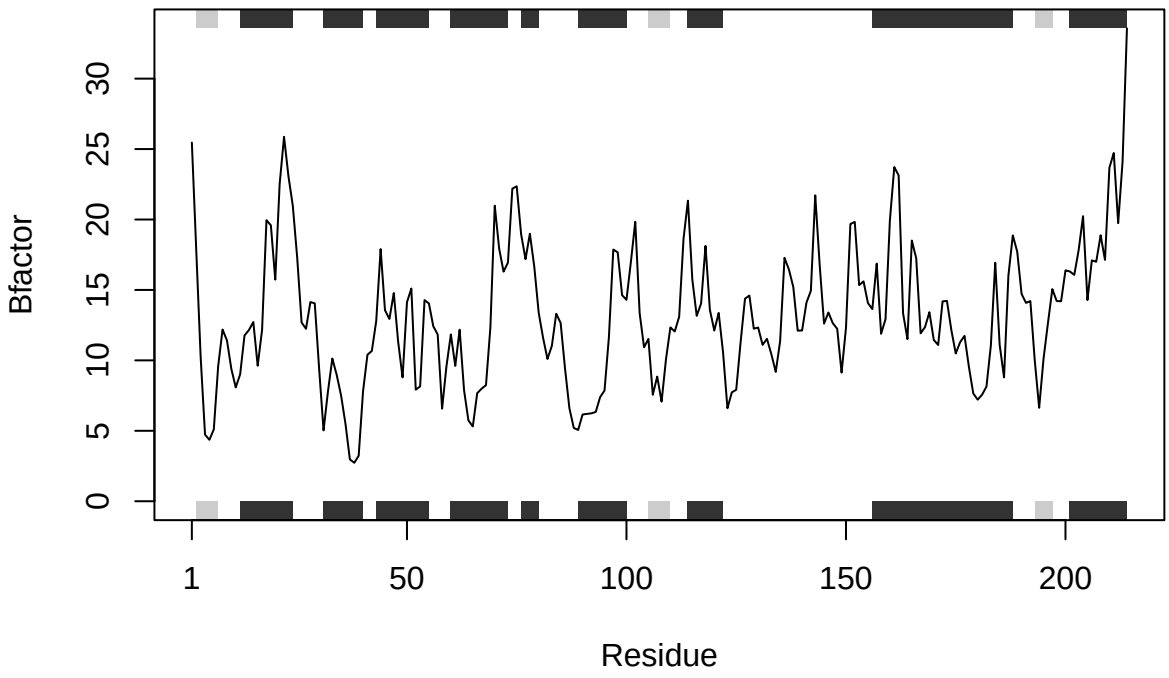

```
drug_analysis("1AKE")
```

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




```
drug_analysis("1E4Y")
```

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


Bfactor
0
5
10
15
20
25
30
1
50
100
150
200
Residue