Class 6: Homework Function

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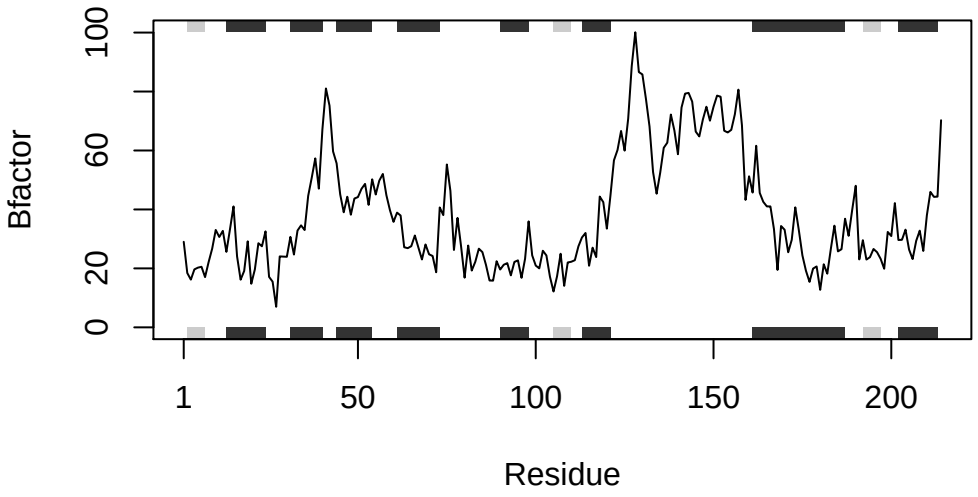
The provided code that we want to improve and adapt to be more general for any protein-drug combination. Install package bio3D with install.packages() before running code.

```
library(bio3d)

id <- "4AKE"
pdb <- read.pdb(id)
```

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

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

plotb3(pdb.chainA$atom$b, sse=pdb.chainA, typ="l", ylab="Bfactor")
```

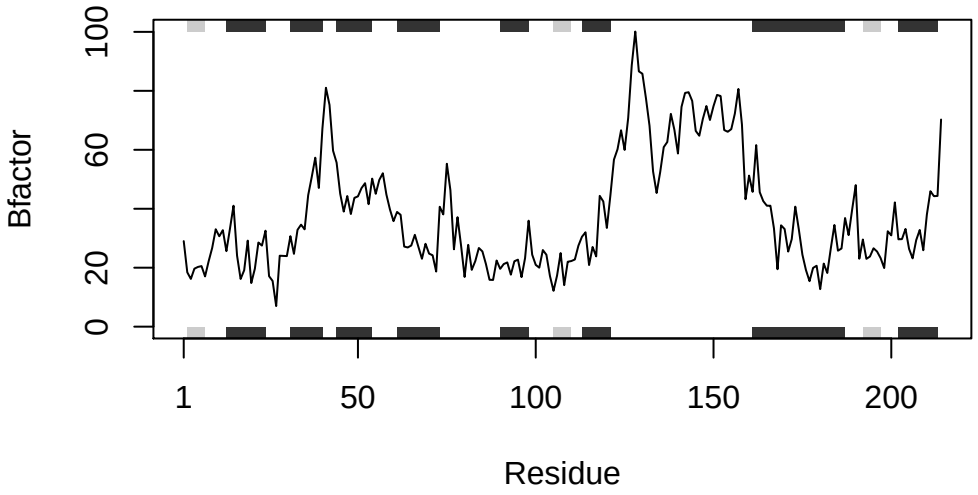



```
#' Produce a B-factor plot of a PDB file
#'
#'@param id The pdb code of your input structure.
#'
#'@return a plot of B-factor favlues
#'
#'@examples
#'  pdbplot("4AKE")

plotpdb <- function(id) {
  # Read the input PDB file
  pdb <- read.pdb(id)
  # Extract a subset of chain A
  pdb.chain <- trim.pdb(pdb, chain="A", elety="CA")
  plotb3(pdb.chain$atom$b, sse=pdb.chain, typ="l", ylab="Bfactor")
}
```

```
plotpdb('4AKE')
```

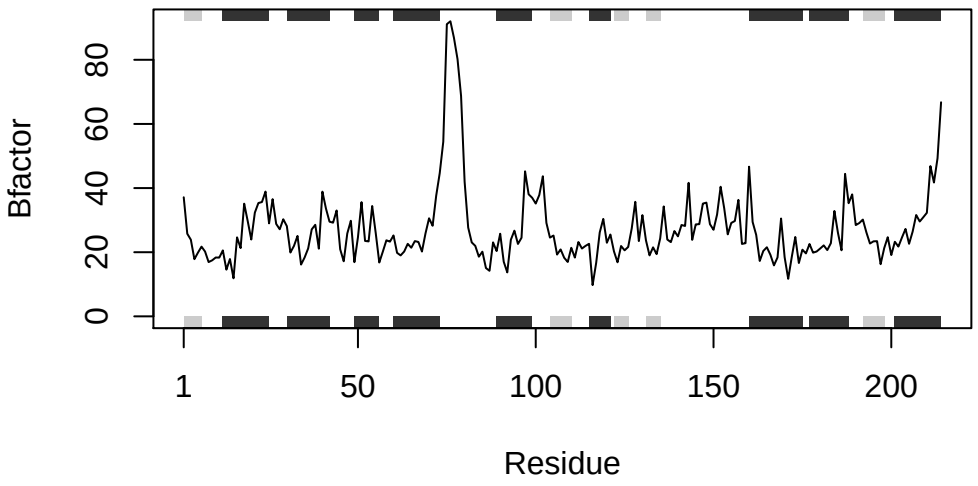
```
  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/rr/
```

```
3rx969893_df30kbjzv323480000gn/T//Rtmpbd1dH8/4AKE.pdb exists. Skipping download
```



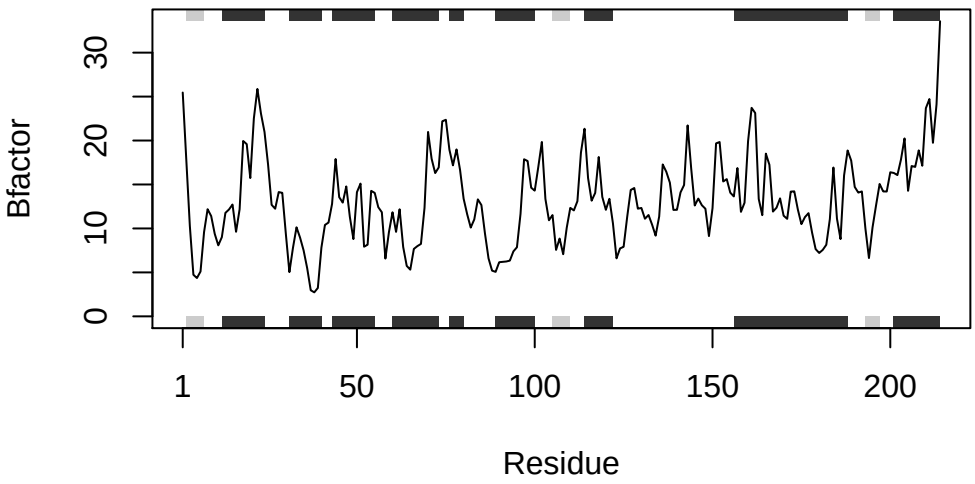

```
plotpdb('1AKE')
```

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




```
plotpdb('1E4Y')
```

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


Bfactor
0
10
20
30
1
50
100
150
200
Residue