Homework Q6

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The below code chunk contains a function that analyzes protein drug interactions by reading in any protein PDB data and outputting a plot of the B-factor trend for the specified protein. Simply input the PDB identifier of the protein to obtain this plot.

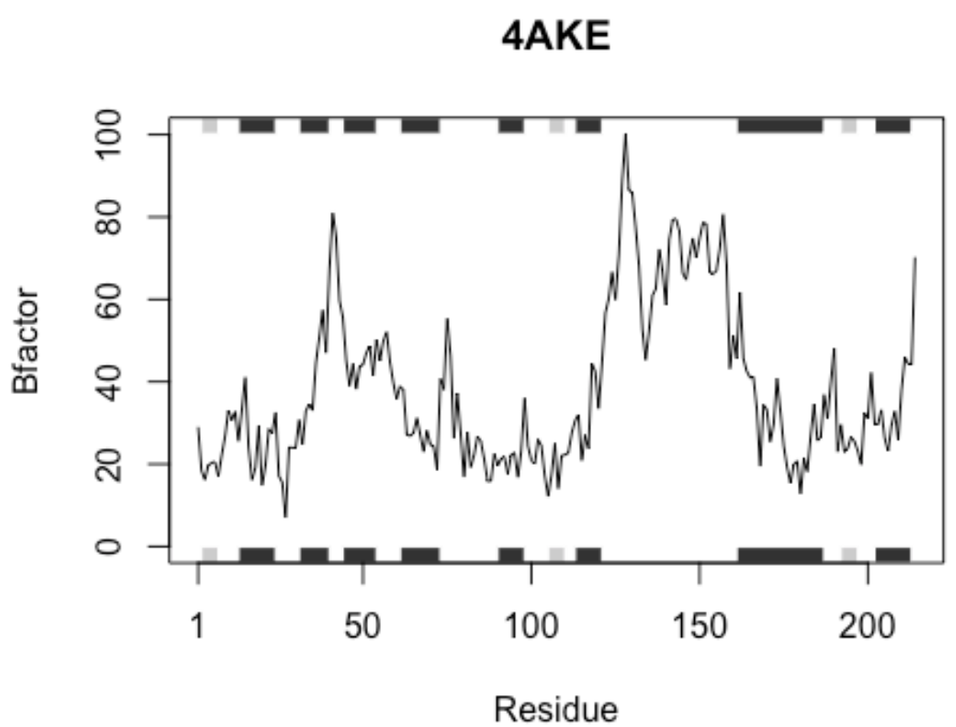
Input: a single element character vector containing the four letter PDB identifier for online file access.

Output: Plot with the B-factor trend of the protein.

```
btrend <- function(x){

 library("bio3d") #loads bio3d package
 s <- read.pdb(x) #reads in specified protein

 s.chainA <- trim.pdb(s, chain="A", elety="CA") #trims protein to subset of its atoms in chain A of type "CA"

 s.b <- s.chainA$atom$b #assigns vector of b-factors of each atom to variable

 plotb3(s.b, sse=s.chainA, typ="l", ylab="Bfactor", main = x) #plots the trend of the b-factor
}
```

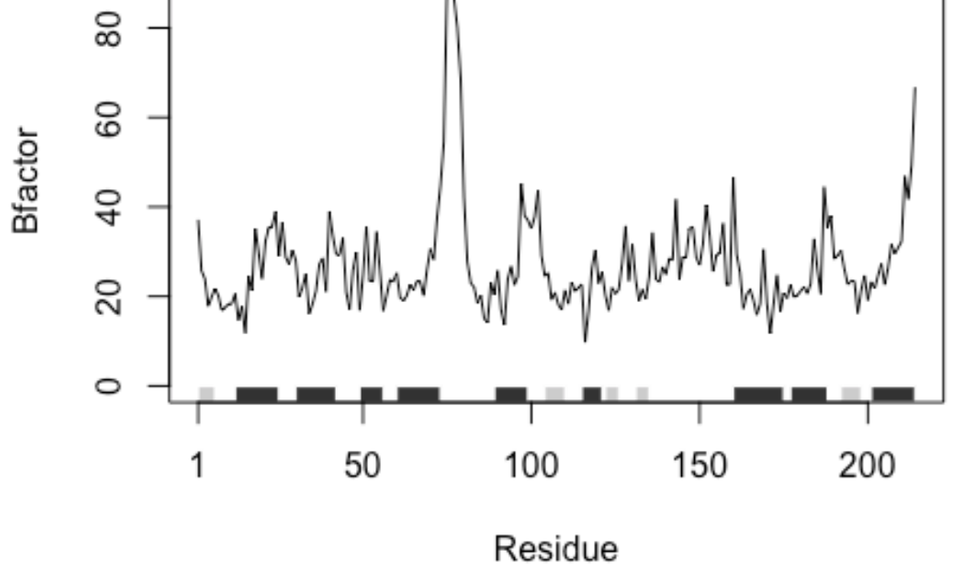
Test Case #1

```
btrend("4AKE")
##   Note: Accessing on-line PDB file
```



Test Case #2

```
btrend("1AKE")
##   Note: Accessing on-line PDB file
##    PDB has ALT records, taking A only, rm.alt=TRUE
```



Test Case #3

```
btrend("1E4Y")
##   Note: Accessing on-line PDB file
```