

# HW6

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## N.B. Homework with scoring rubric.

**Q6. How would you generalize the original code above to work with any set of input protein structures?**

```
library(bio3d)
#must load `bio3d` otherwise you cannot access the data on an empty Rstudio tab
```

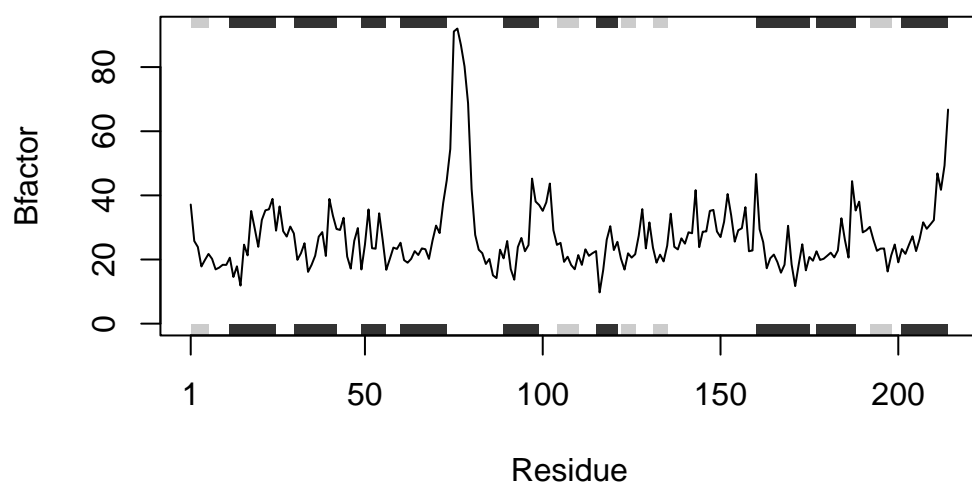
## Original Code to use for analysis

```
protein.and.drug.analysis <- function(protein.list) {
  for (x in protein.list) {
    #read the pdb and shortcut it
    pdb <- read.pdb(x)
    # search for the specifications
    s1.chainA <- trim.pdb(pdb, chain = "A", elety = "CA")
    s1.b <- s1.chainA$atom$b
    #plot
    plotb3(s1.b, sse = s1.chainA, type = "l", ylab = "Bfactor")
  }
}
#need to set x for the sources
x <- c("4AKE", "1AKE", "1E4Y")
#display the function
protein.and.drug.analysis(x)
```

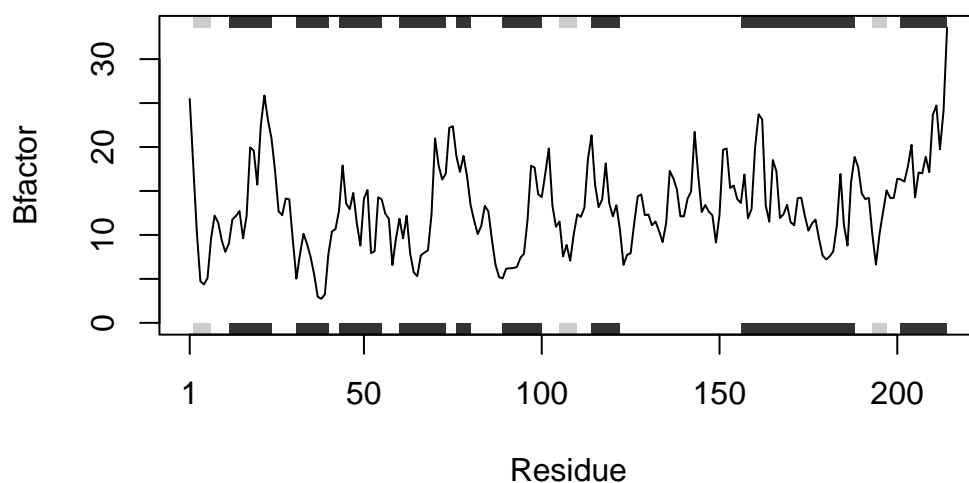
Note: Accessing on-line PDB file



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



Note: Accessing on-line PDB file



## Comments on what are the inputs to the function.

The input of this function are protein data bank (pdb) structures of a protein either with or without a drug.

## What the function does and how to use it.

The function reads through a list of protein codes, pulling their pdb files and stores them in the new variable “pdb”. We trim the data for the data we want to analyze using the `trim.pdb()` function to pull data for an Alpha Chain of a protein and store in “s1.chainA”. We filter for B factors in the atom column of the data. The plot is generated for B-Factor (atomic mobility) vs the residues of a protein structure with/without a drug.

## What is the output of the function.

The output of the function is a plot of B-factor vs protein alpha chain residues of all the proteins in the list of proteins that matches the specifications we called for.