

Class 6 function homework

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Write a function from the supplied code

```
# Can you improve this analysis code?  
  
library(bio3d)  
s1 <- read.pdb("4AKE") # kinase with drug
```

Note: Accessing on-line PDB file

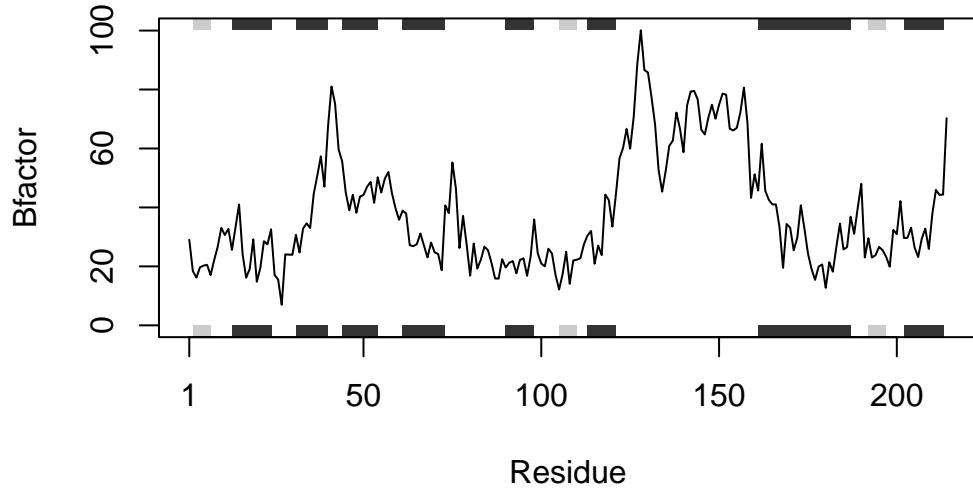
```
s2 <- read.pdb("1AKE") # kinase no drug
```

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

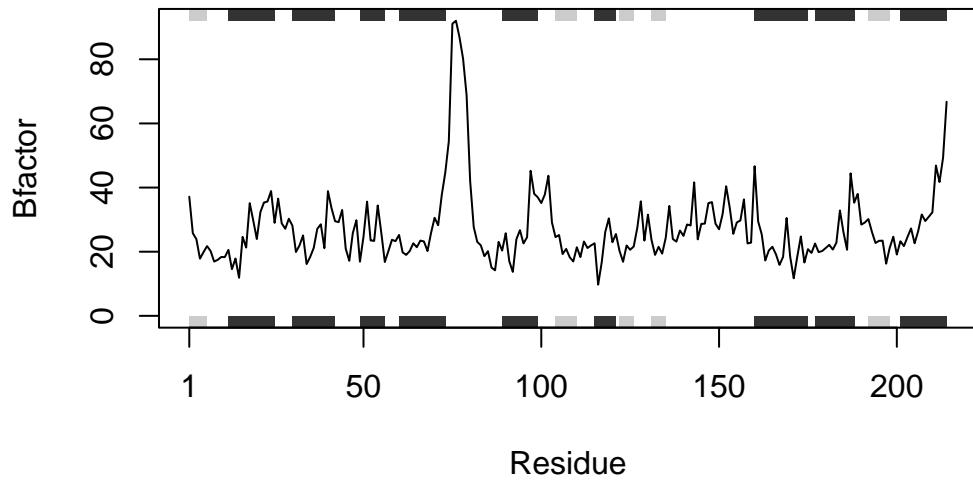
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

Note: Accessing on-line PDB file

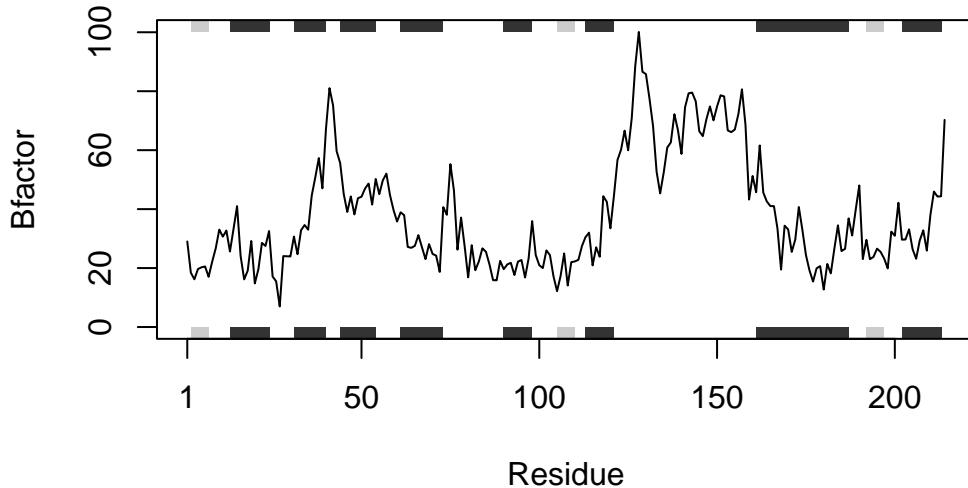
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")  
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")  
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")  
s1.b <- s1.chainA$atom$b  
s2.b <- s2.chainA$atom$b  
s3.b <- s3.chainA$atom$b  
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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



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



First I need to install it and then load it up... `install.packages("bio3d")` and then `library(bio3d)`

```
library(bio3d)
```

All functions in R have at least 3 things:

- A **name** that we use to call the function
- One or more input **arguments**
- The **body** the lines of R code that do the work

An improved line of code to produce a more proper function may look like this

The original codes shows operations (reading a PDB file, trimming, extracting and plotting B factors) that are repeating three times.

This can be improved by putting these sequence of events or pipeline into a `function()`.

The Function `lapply()` is used to apply the function to each element of a list or a vector and return a list of the same length into a vector.

```
library(bio3d)

protein_interactions <- function(pdb_IDs,elety = "CA", chain = "A", length=3, plot=TRUE)
{
  pdb <- lapply(pdb_IDs, read.pdb)
  trimmed <- lapply(pdb, trim.pdb, elety = elety, chain = chain)
  Bfactors <- lapply(trimmed, function(protein) protein$atom$b)

  if (plot) {
    for (i in seq_along(Bfactors)) {
      plotb3(
        Bfactors[[i]],
        sse = trimmed[[i]],
        typ = "l",
        ylab = "B-factor",
        main = pdb_IDs[i]
      )
    }
  }
}
```