

Class 6 - Homework

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Instructions

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

```
library(bio3d)

s1 <- read.pdb("4AKE") # kinase with drug
s2 <- read.pdb("1AKE") # kinase no drug
s3 <- read.pdb("1E4Y") # kinase with drug

s1.chainA <- trim.pdb(s1, chain="A", eley="CA")
s2.chainA <- trim.pdb(s2, chain="A", eley="CA")
s3.chainA <- trim.pdb(s3, chain="A", eley="CA")

s1.b <- s1.chainA $\textit{atom}$ b
s2.b <- s2.chainA $\textit{atom}$ b
s3.b <- s3.chainA $\textit{atom}$ 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")
```

Function “protein”:

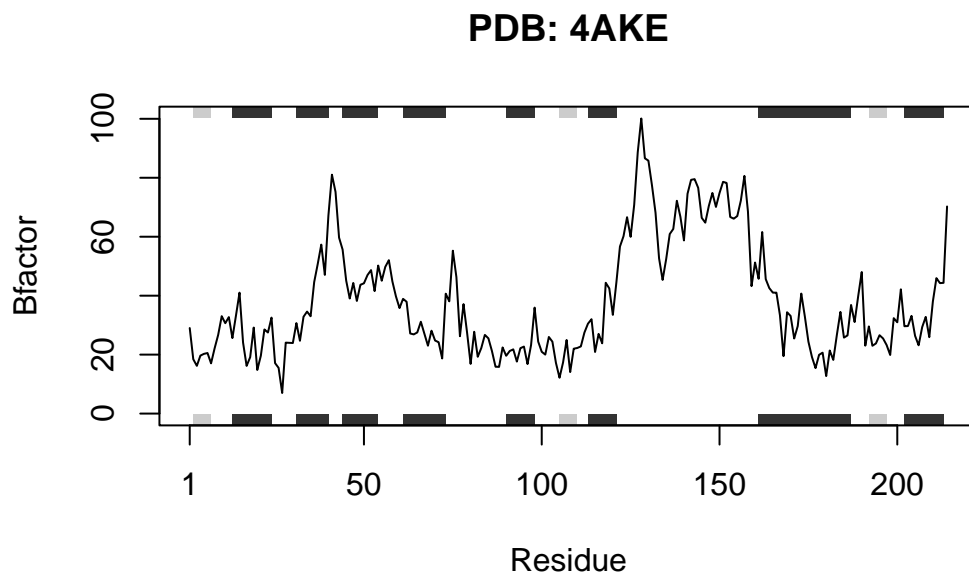
- “code” is the main argument of the function, requiring the PDB filename or the four letter PDB identifier.
- “chain”, “eley” and “typ” have defaults, but can be changed.

```
#install.packages('bio3d') # install package
library(bio3d) # load library

protein <- function(code, chain = "A", elety="CA", typ="l") {
  pdb <- read.pdb(code)
  # reads the pdb code for the desired protein
  chain <- trim.pdb(pdb, chain=chain, elety=elety)
  # loads the chain information
  plotb3(chain$atom$b, sse=chain, typ=typ, ylab="Bfactor", main = paste("PDB:", code))
  # returns the plot of B-factor values and PDB residue numbers.
  # the type of plot is changeable (e.g. line, points, etc.).
}

protein(code = "4AKE") # check if function is working for one code
```

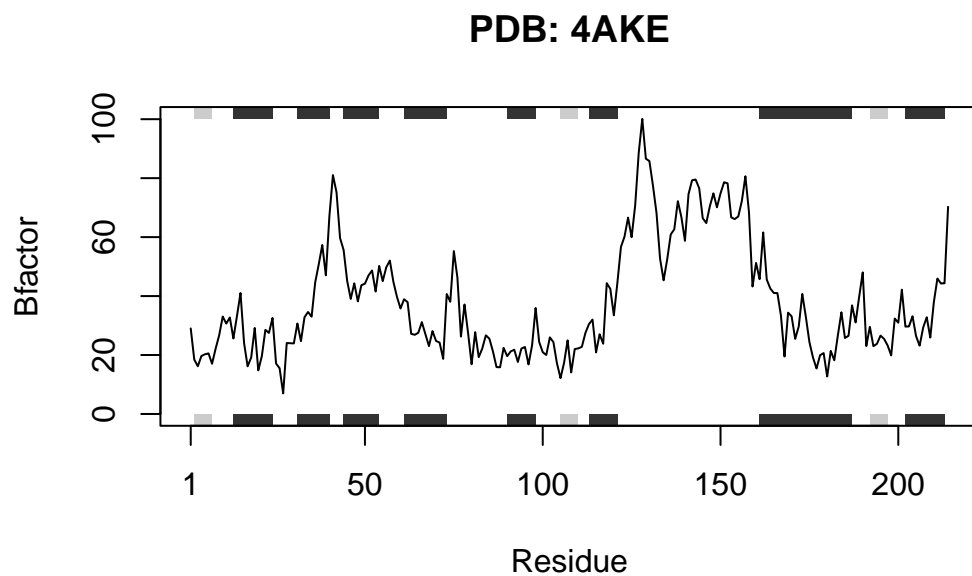
Note: Accessing on-line PDB file



Loading multiple proteins at the same time using the apply function.

```
files <- matrix(c("4AKE", "1AKE", "1E4Y"))  
apply((files), 1, protein)
```

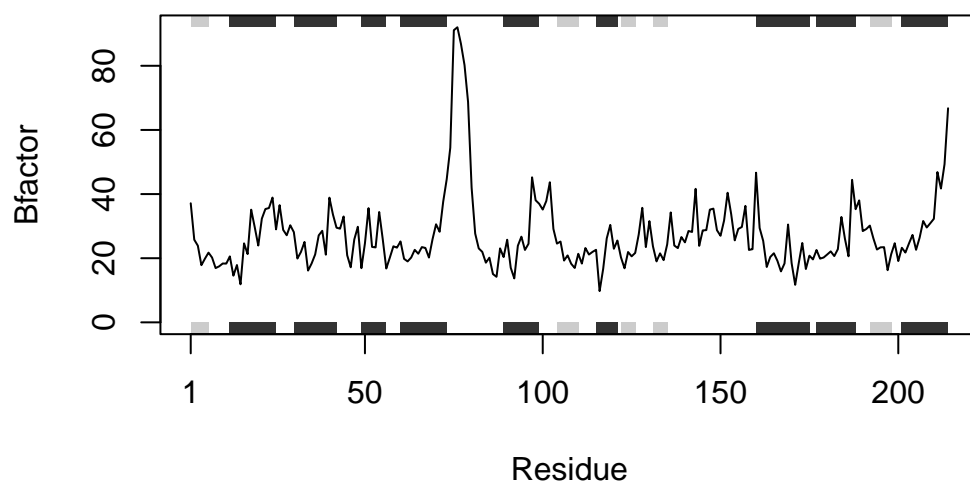
Note: Accessing on-line PDB file



Note: Accessing on-line PDB file

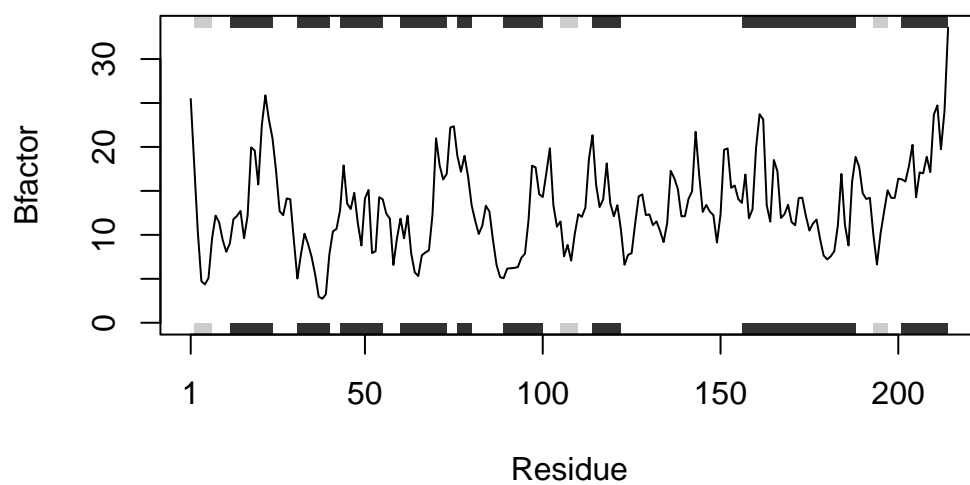
PDB has ALT records, taking A only, rm.alt=TRUE

PDB: 1AKE



Note: Accessing on-line PDB file

PDB: 1E4Y



NULL