Week 5 R functions Q6

Qiyu Chen

11/8/2020

Example codes to improve upon

```r
library(bio3d)
s1 <- read.pdb("4AKE") # kinase with drug
```

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

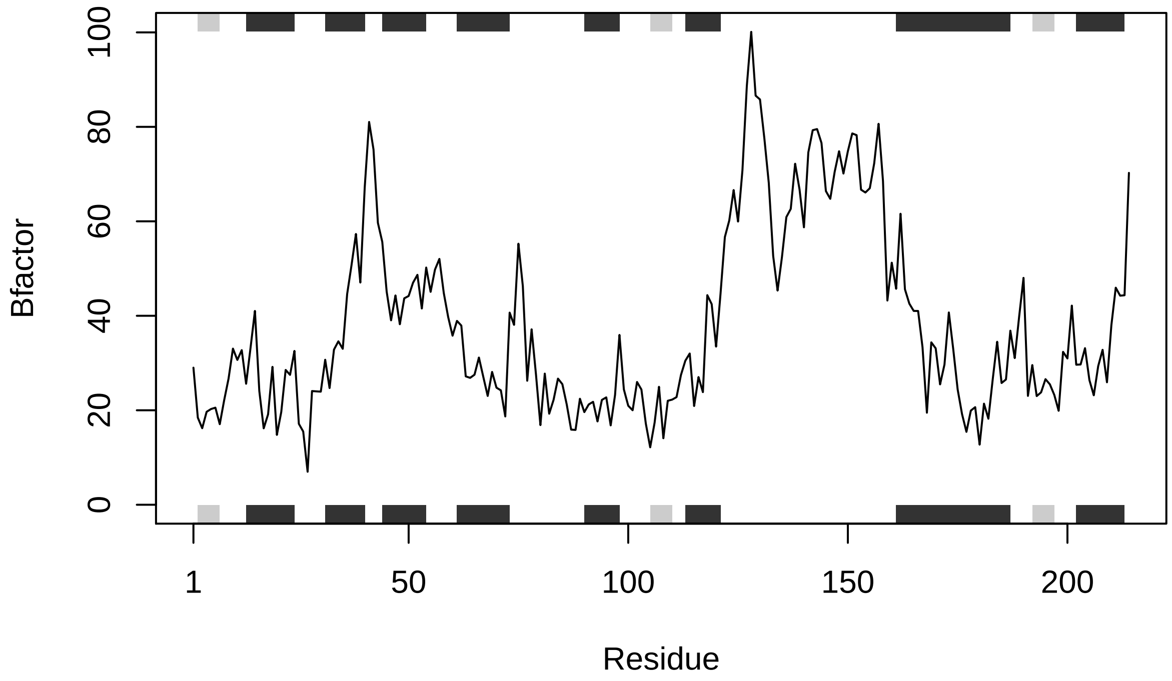
```r
s2 <- read.pdb("1AKE") # kinase no drug
```

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

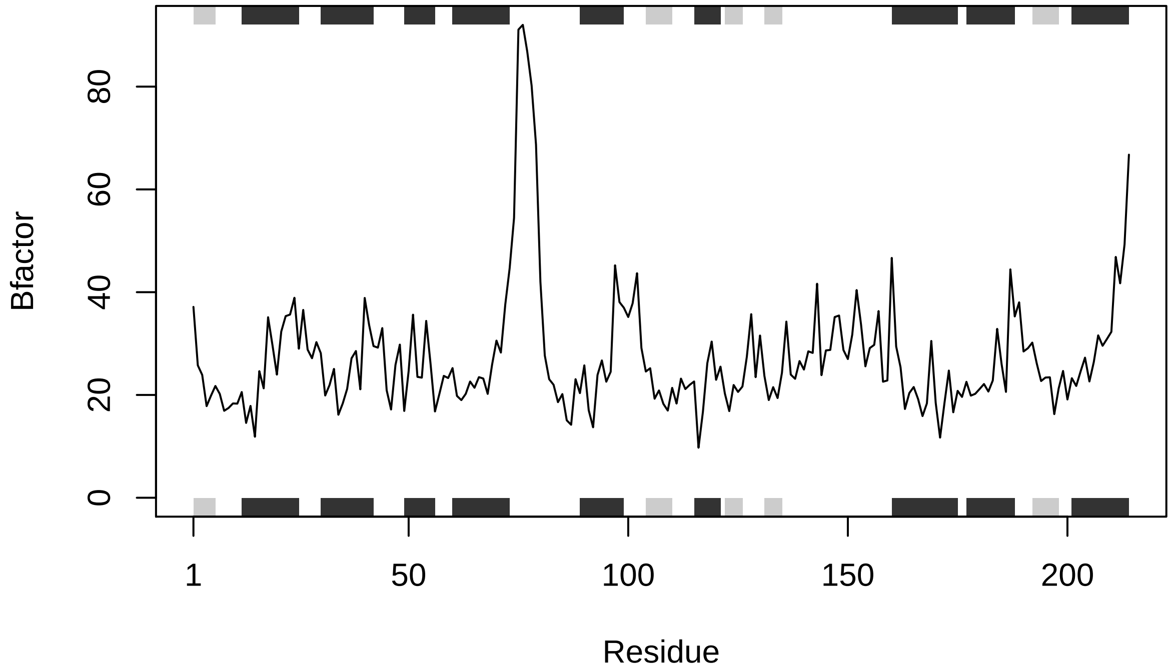
```r
s3 <- read.pdb("1E4Y") # kinase with drug
```

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

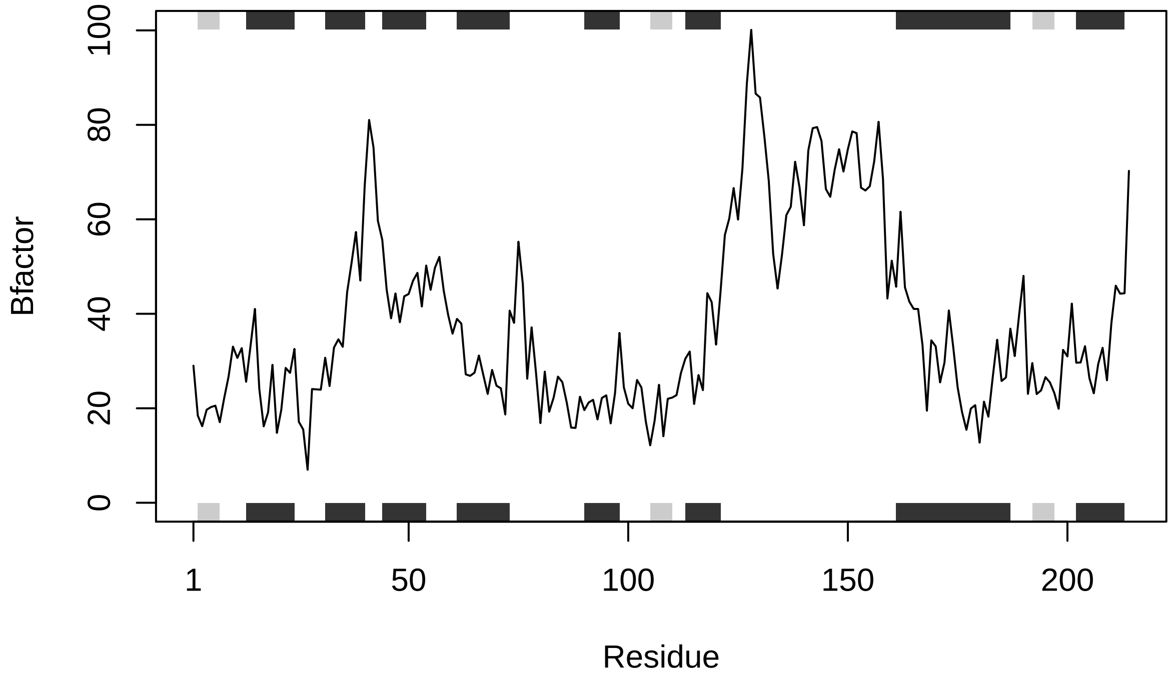
```r
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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



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



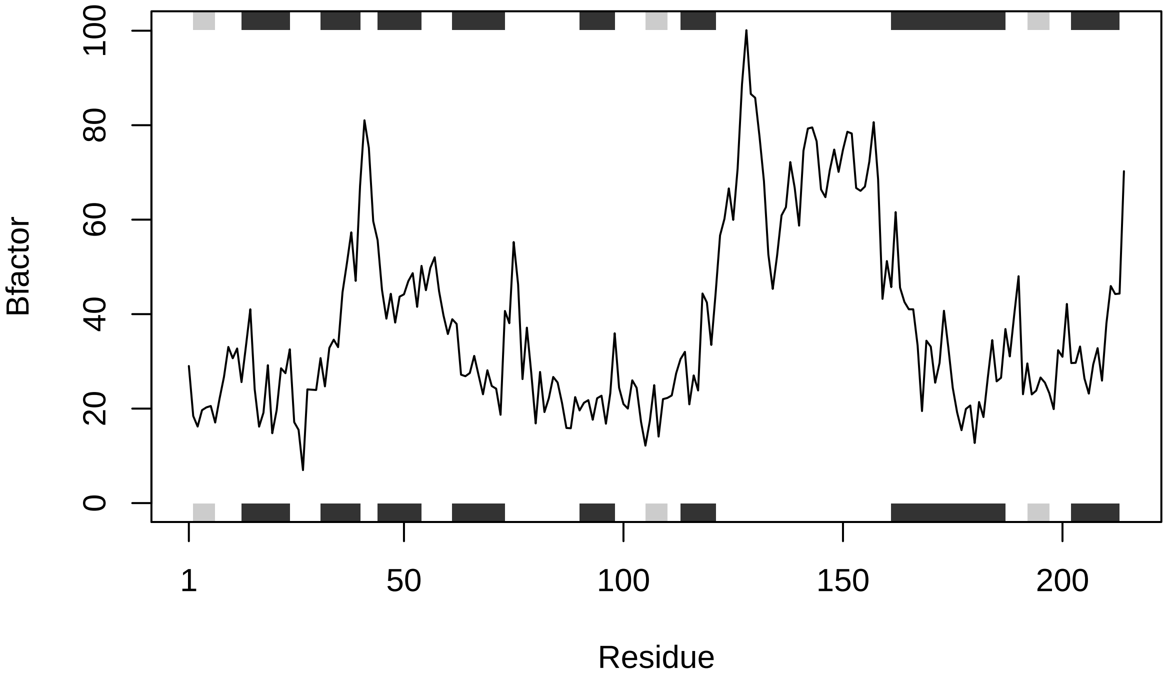
Q6. How would you generalize the original code above to work with any set of input protein structures?

```
# generate the plots of the B-factor trends of specific proteins from PDB files

#' plot_Bfactor
#'
#' @param x a character vector of the name of PDB file
#'
#' @return a plot of the B-factor trend
#' @export
#'
#' @examples
#'  pdb_file <- "4AKE"
#'  plot_Bfactor(pdb_file) or
#'  plot_Bfactor("4AKE")

plot_Bfactor <- function(x){
  # read a Protein Data Bank file
  s <- read.pdb(x)
  # trim PDB object
  s.chainA <- trim.pdb(s, chain="A", elety="CA")
  # obtain b-factor values
  s.b <- s.chainA$atom$b
  # plot the trend of B-factor
  plotb3(s.b, sse=s.chainA, typ="l", ylab="Bfactor")
}
```

```r
# use plot_Bfactor function on 4AKE as an example
plot_Bfactor("4AKE")
```

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

```
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/54/
## wtm5nzr57lg3k_qg656222w00000gn/T//Rtmpw9q3Je/4AKE.pdb exists. Skipping download
```


Bfactor
Residue