HW06

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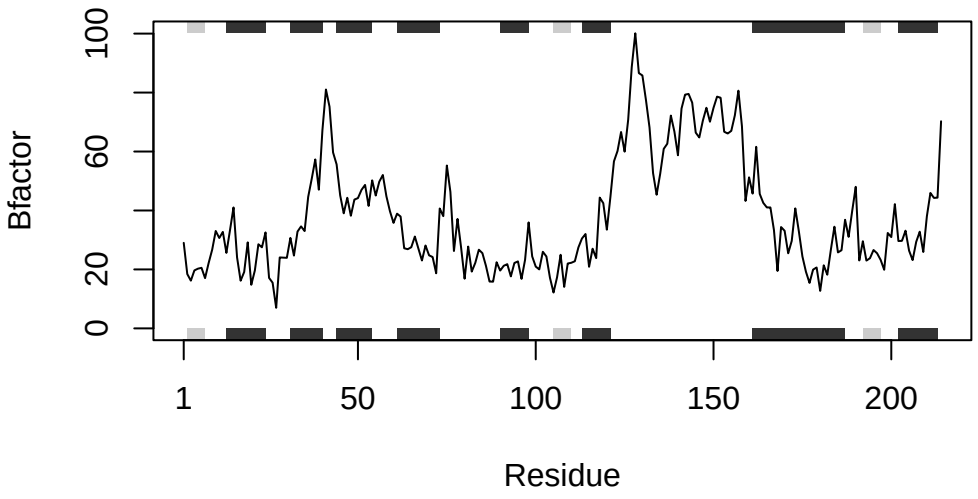
Q6. How would you generalize the original code above to work with any set of input protein structures?

To generalize the original code to work with any protein structures as input, I wrote a function that takes a list of pdb file names as input. It then read in each pbd file, trims it to chain A, and then plots it.

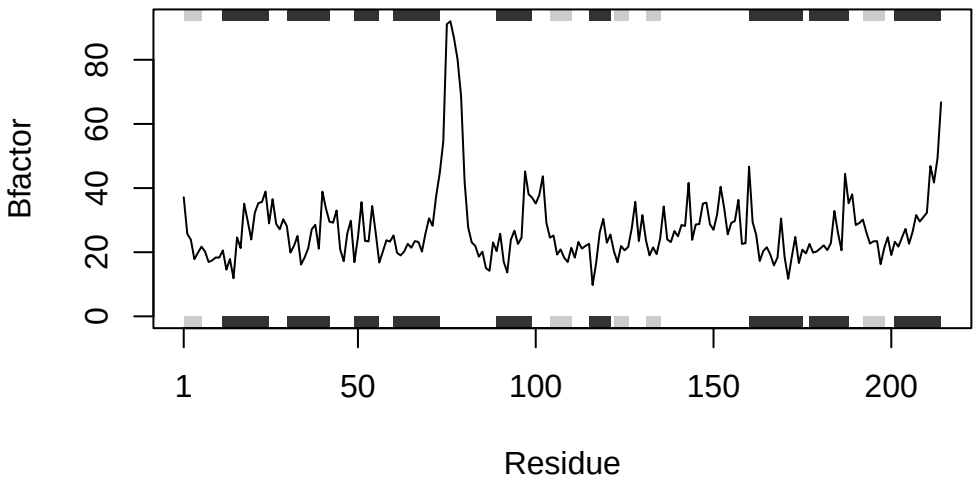
```
#install.packages("bio3d")
library(bio3d)

# The input is a list of pdb file names. The function plot_B_factors then reads in each
#file, trims it to chain A and then plots the B factors using 'plotB3' function.
plot_B_factors <- function(file_list) {
  for (file in file_list) {
    # read in pdb file and trim to chain A
    s <- read.pdb(file)
    s.chainA <- trim.pdb(s, chain="A", elety="CA")

    # plot B-factors
    s.b <- s.chainA$atom$b
    plotb3(s.b, sse=s.chainA, typ="l", ylab="Bfactor")
  }
}

#A list for the provided file names.
file_list <- c("4AKE", "1AKE", "1E4Y")

# Applied the plot_b_factors function. By providing the list of files names rather
#than single files, the function can be applied to any protein structures without
```

```
#editing the code each time.
plot_B_factors(file_list)
```

```
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
```