Class 6 Homework

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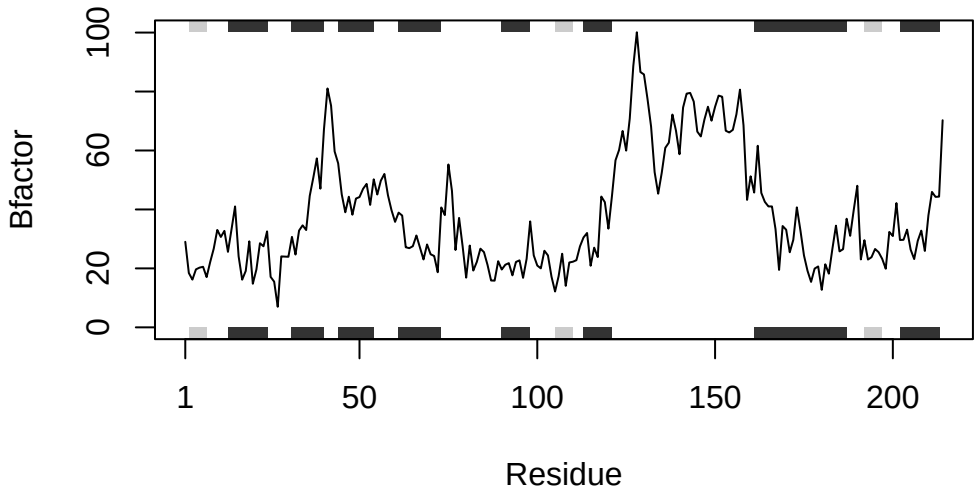
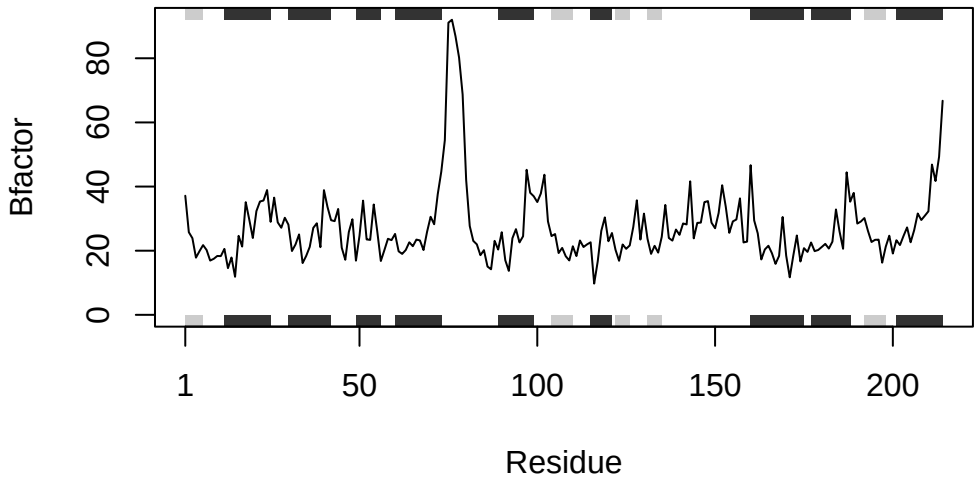
```
#The new function (for processing and plotting B-factor vs residue)

library(bio3d)
graph_pdb <- function (pdb){
  pbd_file <- read.pdb(pdb)
  trimmed_file.chainA <- trim.pdb(pbd_file, chain="A", elety="CA")
  pdb_b <- trimmed_file.chainA$atom$b
  plotb3(pdb_b, sse= trimmed_file.chainA, typ="l", ylab="Bfactor")
}

# The function graph_pdb takes PDB ID of a protein-drug interaction as input.

# The new function graph_pdb() graphs the B-factor in a protein vs residue.

#In the function, read.pdb is used to read a protein data bank file (PDB) with a given PDB
#Trim.pdb is used to keep only the atoms in chain A and the carbon alpha atoms
#$atom$b extracts the B-factors
#Plotb3() is used to plot the B-factors in a line plot.

# The output is the graph of the B-factor vs residue graph of each PDB ID.
```

```
#For plotting the B-factor vs residue for any set of IDs:
#we can use sapply() to create the graphs for multiple IDs at once.

pdb_ids <- c("4AKE", "1AKE", "1E4Y")
graphs <- sapply(pdb_ids, graph_pdb)
```

```
  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
```