

Homework Class 6 (R Functions)

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Section B: Improving analysis code of protein drug interactions

Function for plotting B-factor values given PDB data

Answer to Q6

Instructions: See Q6 of the hands-on lab supplement above. This entails turning a supplied code snippet into a more robust and re-usable function that will take any of the three listed input proteins and plot the effect of drug binding.

Input: `pdb_file` Output: Line Plot of Residue vs B factor `plot_b_factor()`

What this function do: This function read in the PDB file for the protein structure 4AKE, perform the analysis, and plot the Residual vs B factor line plot.

How we can use this function: This function can be used to analyze protein drug interaction from given PDB file and generate a line plot of residual vs b-factor for given proteins.

```
#start with install.packages("bio3d")

library(bio3d)

#' @param pdb_file PDB
#' @return Line Plot Residue with B factor
#' @export
#' @examples plot_b_factor("4AKE")

plot_b_factor <- function(pdb_file) {
  # Extract and read the PDB data

  p <- read.pdb(pdb_file)
```

```

# Trim the PDB file
p.chain <- trim.pdb(p, chain="A", eley="CA")

# Extract B factor values from PDB file
b_factors <- p.chain$atom$b

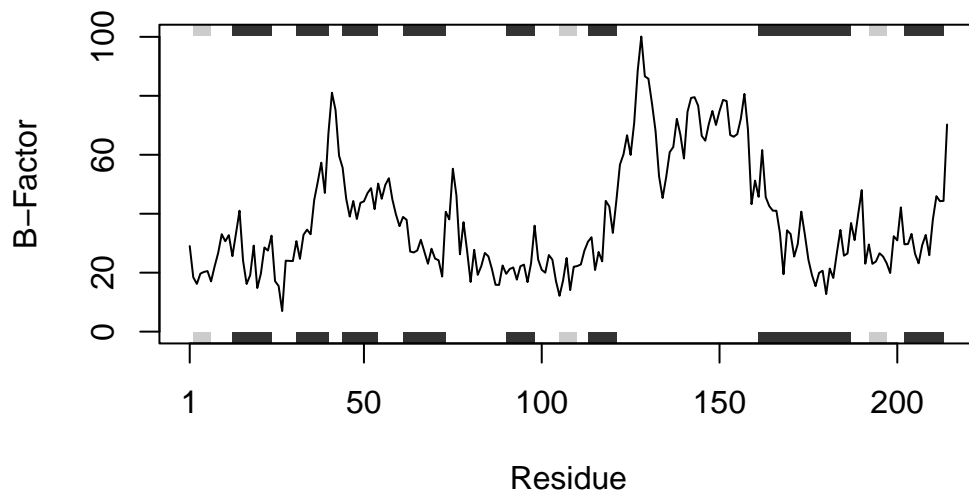
# Plot B factor values with line plot

plotb3(b_factors, sse=p.chain, typ="l", ylab="B-Factor")
}

plot_b_factor("4AKE")

```

Note: Accessing on-line PDB file



Overall, this function extract and read the PDB file, trims the PDB file, and extract the B factor values from the PDB file to generate a line plot of b factors for given residuals.