

HW 6 Class Functions

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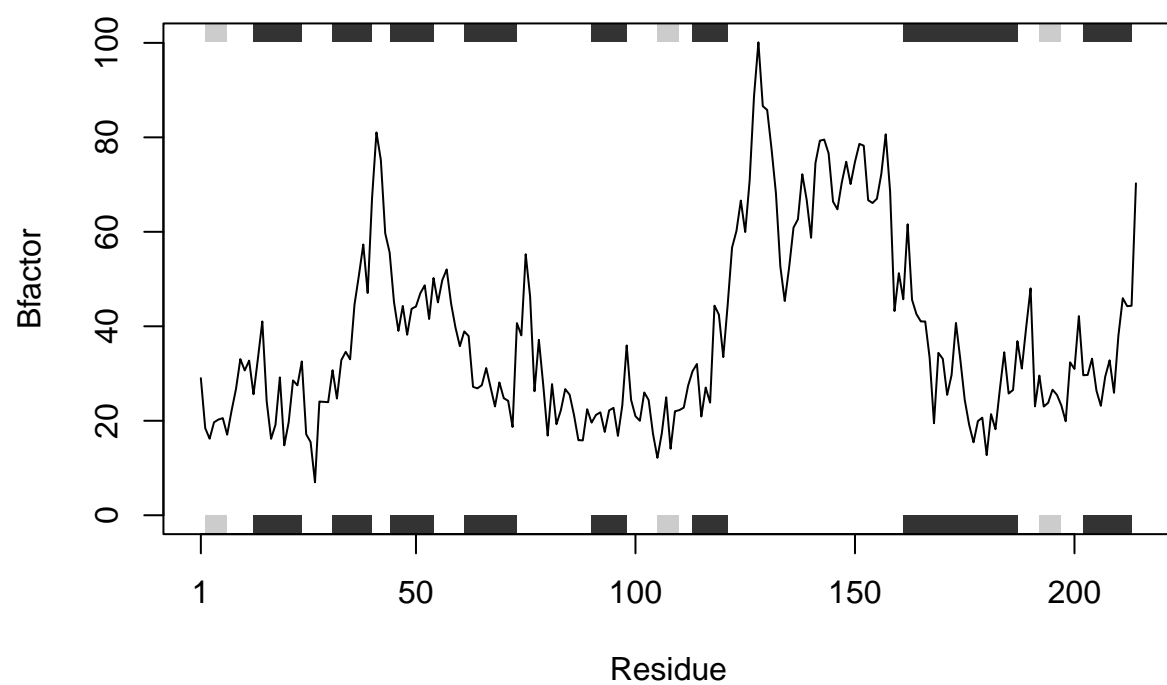
```
# (A. Can you improve this analysis code?)
library(bio3d)
s1 <- read.pdb("4AKE") # kinase with drug

## Note: Accessing on-line PDB file

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

## Note: Accessing on-line PDB file
## PDB has ALT records, taking A only, rm.alt=TRUE
s3 <- read.pdb("1E4Y") # kinase with drug

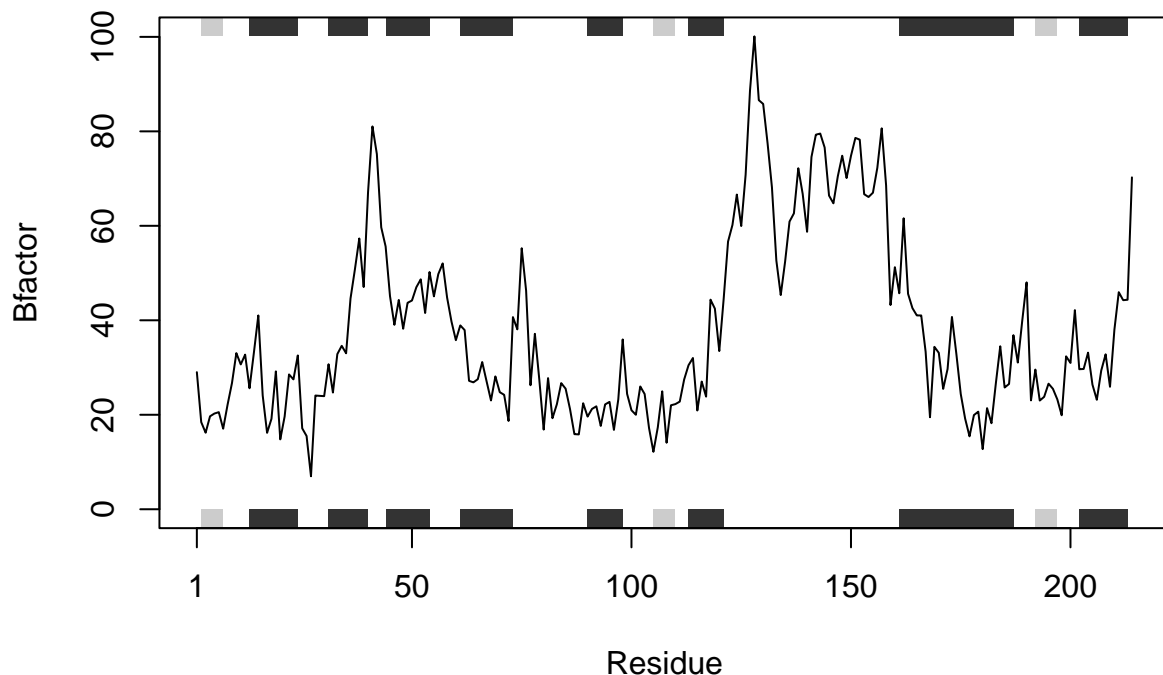
## Note: Accessing on-line PDB file
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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



```
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?

```
# Define a function to analyze protein-drug interactions and plot B-factors
# Input: pdb_id - the PDB ID of the protein (e.g., "4AKE")
#         chain - the protein chain we want to analyze (i.e. "A" in this example)
#         plot_type - the type of plot (i.e. "l" in this example)
plot_bfactor_interaction <- function(pdb_id, chain = "A", plot_type = "l") {

  # Read the PDB file into R using the PDB ID
  # This step loads the protein structure into R
  pdb <- read.pdb(pdb_id)

  # Trim the PDB data to focus on only C-alpha atoms from the specified chain
  # Trimming helps reduce the amount of data, focusing on specific parts of the protein
  chain_data <- trim.pdb(pdb, chain = chain, elty = "CA")

  # Extract the B-factors (which indicate the flexibility of each atom)
  # B-factors show how much atoms move.
  b_factors <- chain_data$atom$b

  # Plot the B-factors to visualize which parts of the protein are flexible/rigid
  # The plot shows flexibility in the protein structure. B-factors are directly correlated
  # with more flexibility.
  plotb3(b_factors, sse = chain_data, typ = plot_type, ylab = "B-factor",
         main = paste("B-factor Plot for", pdb_id))
}
```

```

# Return the B-factors so they can be used later
return(b_factors)
}

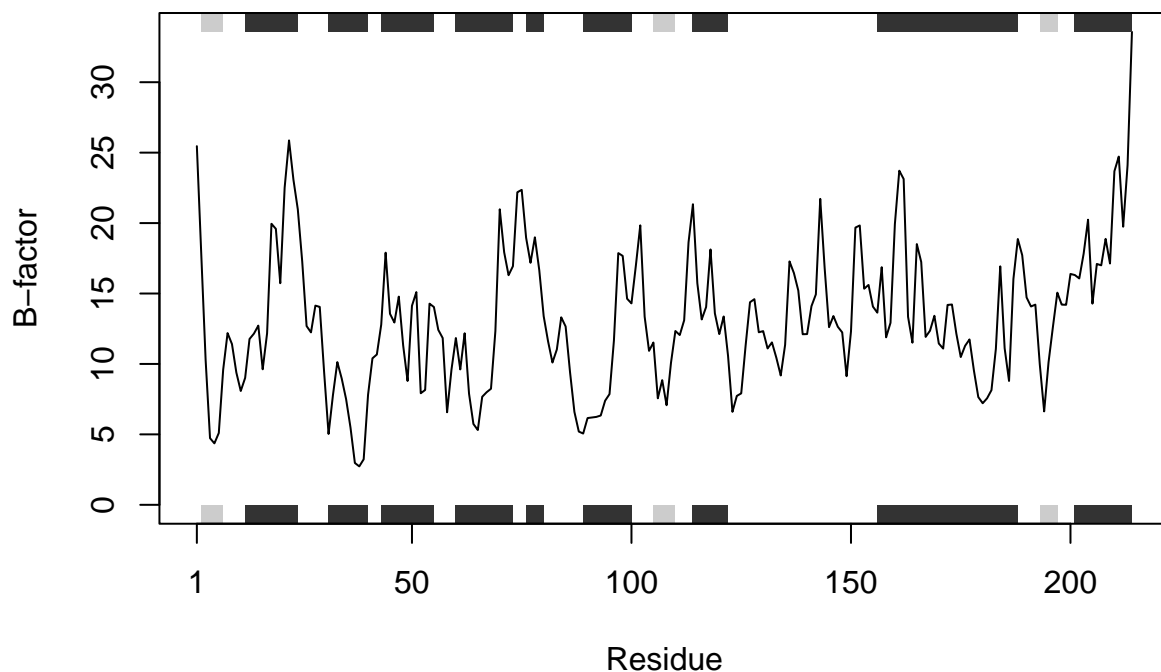
# Example 1: Use the function to analyze and plot the B-factors for the protein "1E4Y"
# The plot will display the B-factor plot for protein "1E4Y" for chain "A"
b_factors_4AKE <- plot_bfactor_interaction("1E4Y", chain = "A", plot_type = "1")

## Note: Accessing on-line PDB file

## Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
## /var/folders/vk/tzsk8t154q3czvryhl3wyc_80000gn/T//Rtmpfnpe9o/1E4Y.pdb exists.
## Skipping download

```

B-factor Plot for 1E4Y



```

# Example 2: Use the function to analyze and plot the B-factors for the protein "1AKE"
# The plot will display the B-factor plot for protein "1AKE" for chain "A"
b_factors_1AKE <- plot_bfactor_interaction("1AKE", chain = "A", plot_type = "1")

## Note: Accessing on-line PDB file

## Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
## /var/folders/vk/tzsk8t154q3czvryhl3wyc_80000gn/T//Rtmpfnpe9o/1AKE.pdb exists.
## Skipping download

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

```

B-factor Plot for 1AKE

