

Class6 Homework

Yuntian Zhu (PID: A17816597)

I want to condense the codes in the supplement file to a function that can be easily called

```
# This function analyzes protein B-factor trends by:
# 1. Reading protein structure data from the Protein Data Bank (PDB)
# 2. Extracting a specified chain and atom type
# 3. Plotting B-factor values along the protein sequence
#
# Inputs:
#   pdbid - PDB ID of the protein
#   chain - chain identifier to analyze (the default chain is "A")
#   elety - atom type to analyze (the default elety is "CA")
#
# Output: A plot showing B-factor trends with secondary structure annotations

plot_pdb_bfactor <- function (pdbid, chain = "A", elety = "CA"){

  #load the bio3d package
  library(bio3d)

  #read the structures in PDB with the PDB ID
  structure <- read.pdb(pdbid)

  #extract one particular chain and the alpha carbon atoms
  structure.chain <- trim.pdb(structure, chain = chain, elety = elety)

  #extract the B factors
  structure.bfactor <- structure.chain$atom$b

  #plot B factors along the sequence and return the plot
  return(
    plotb3(structure.bfactor,
```

```

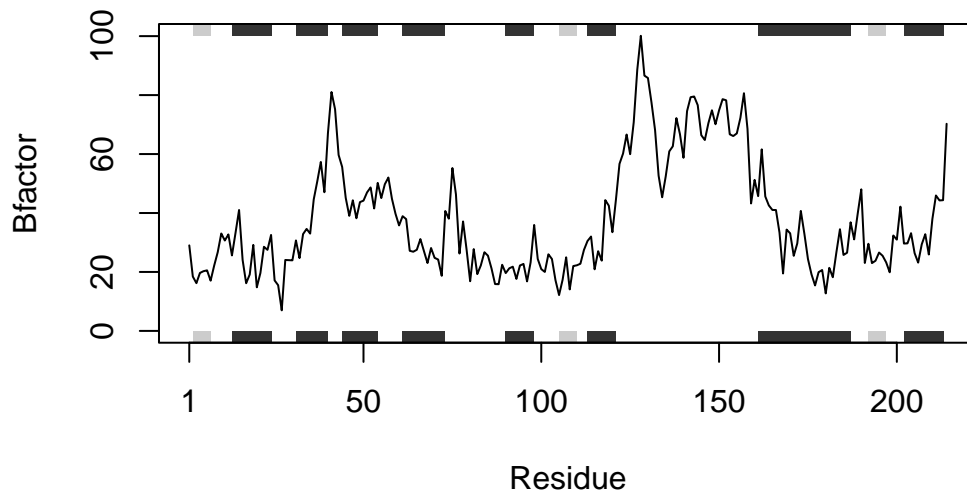
    sse = structure.chain,
    typ = "l",
    ylab = "Bfactor")
)
}

```

Test one with the ID 4AKE

```
plot_pdb_bfactor("4AKE")
```

Note: Accessing on-line PDB file

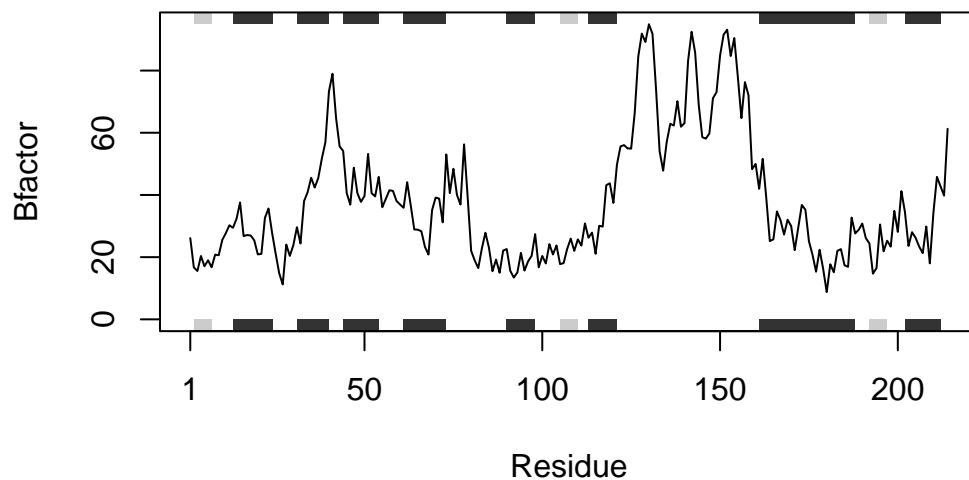


Test two with the ID 4AKE and chain B

```
plot_pdb_bfactor("4AKE", chain = "B")
```

Note: Accessing on-line PDB file

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/j9/c6jg3wlj0wx7jw6ws7j7znnw0000gn/T/RtmpcXfuof/4AKE.pdb exists.
Skipping download
```



Test three with the ID 1AKE

```
plot_pdb_bfactor("1AKE")
```

Note: Accessing on-line PDB file

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

