

# Class6 Homework

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

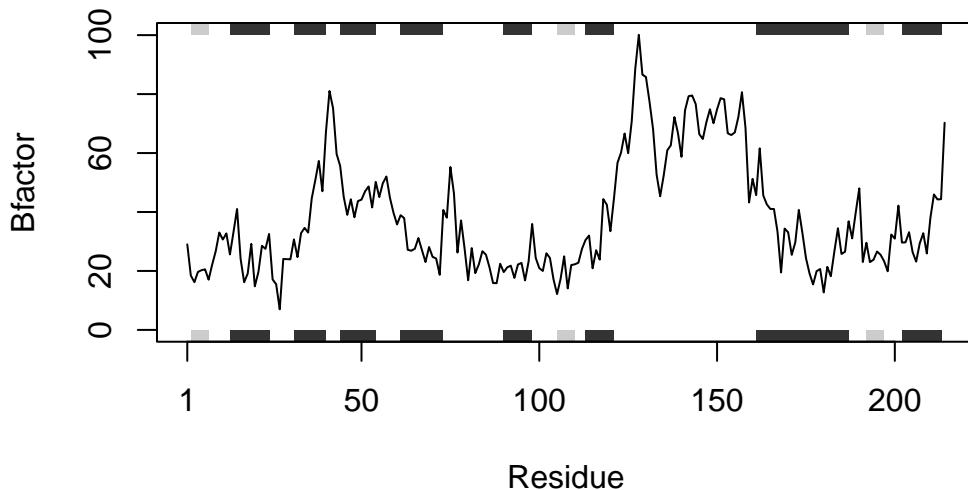
```
# This function analyzes protein B-factor trends by:  
# 1. Reading protein structure data from the Protein Data Bank (PDB)  
# 2. Extracting a specified chain and atom type  
# 3. Plotting B-factor values along the protein sequence  
  
#  
# Inputs:  
#   pdbid - PDB ID of the protein  
#   chain - 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

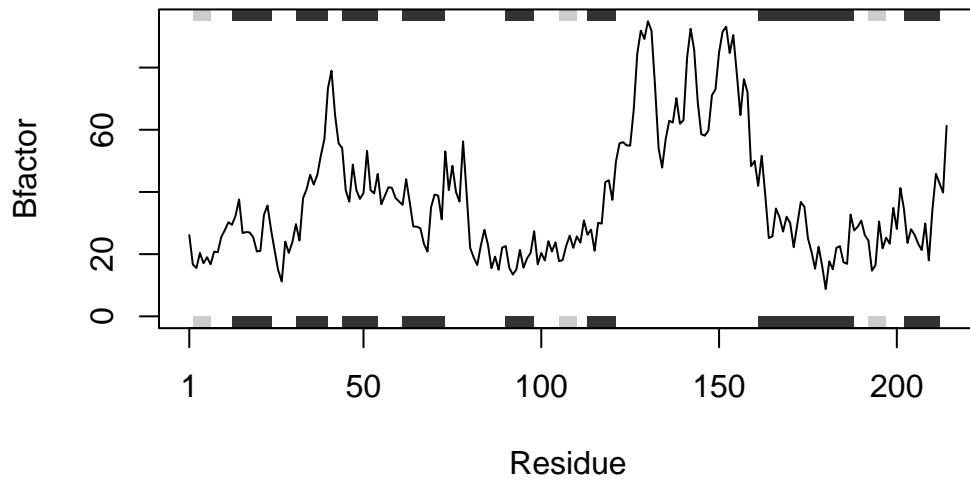


Test two with the ID 4AKE and chain B

```
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

