HW Class 6 (R Functions)

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```
# Q6. How would you generalize the original code above to work with any set of input protein
```

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

```
  Note: Accessing on-line PDB file
```

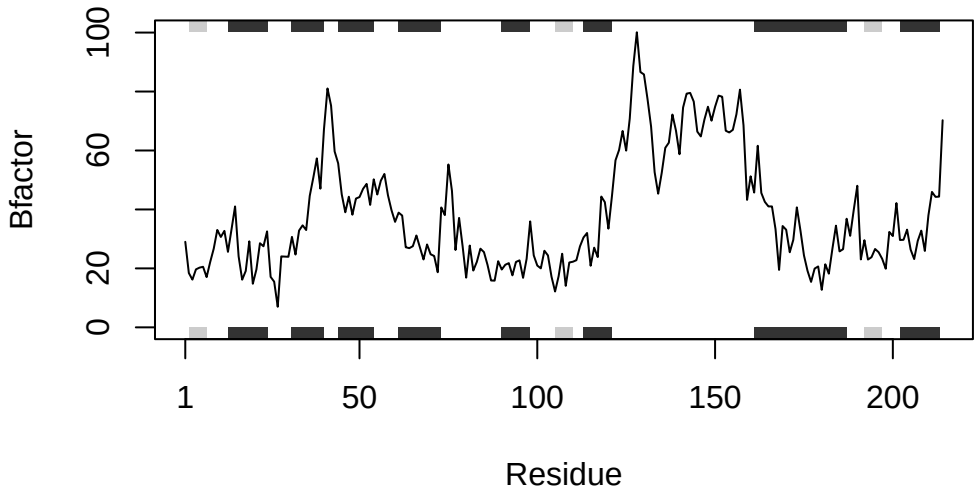
```
s2 <- read.pdb("1AKE") # kinase no drug
```

```
  Note: Accessing on-line PDB file
   PDB has ALT records, taking A only, rm.alt=TRUE
```

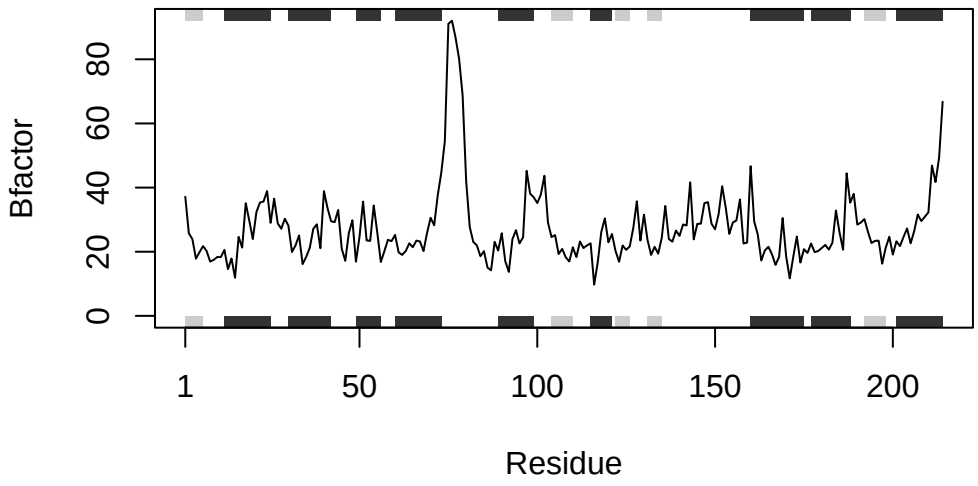
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

```
  Note: Accessing on-line PDB file
```

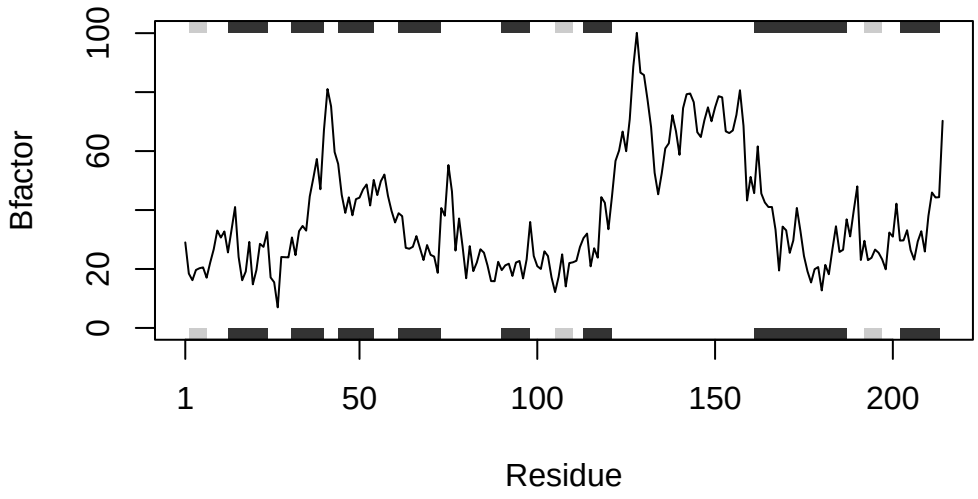
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```




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



```
plotb3(s3.b, sse=s3.chainA, typ="l", ylab="Bfactor")
```




```
# Make this into a function
# 1st get a simple working snippet
# make it as simple as possible
# reduce code duplication
# then turn it into a function
# test it and fix errors
```

```
# Beginning working function below:
```

```
# Install and Run necessary libraries containing protein structures data
# install.packages("bio3d")
```

```
library("bio3d")
```

```
# Analyzing b factors for protein data (PDB)
analyze_b_factors <- function(pdb_ids, chain="A", elety = "CA") {

  # List to store B-factors for each protein
   b_factors_list <- list()
```

```
  # Going through PDB ID
   for (pdb_id in pdb_ids) {

  # Read the PDB file
  protein <- read.pdb(pdb_id)

  # Trim to specified chain and atoms
    protein_chain <- trim.pdb(protein, chain=chain, elety=elety)

  # Store B-factors
  b_factors <- protein_chain$atom$b
  b_factors_list[[pdb_id]] <- b_factors

  # Plot B-factors
  plotb3(b_factors, sse = protein_chain, typ = "l", ylab= "B-factor",
  xlab = "Residue", main = paste("B-factor plot for PDB", pdb_id, "-Chain", chain))
   }

   #Output list of B-factors for pdb
   return(b_factors_list)

}
```