Lecture6_homework

need to install package `bio3d` with the function `install.packages()`.

Original Code

Running the original code snippet to understand the functions, inputs, and outputs. This code takes the pdb protein id, the chain, and the element type to isolate the B factors for this protein at that specific chain. It generates a plot for B-factor along with the chain of protein

```
library(bio3d)
s1 <- read.pdb("4AKE") # kinase with drug
```

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

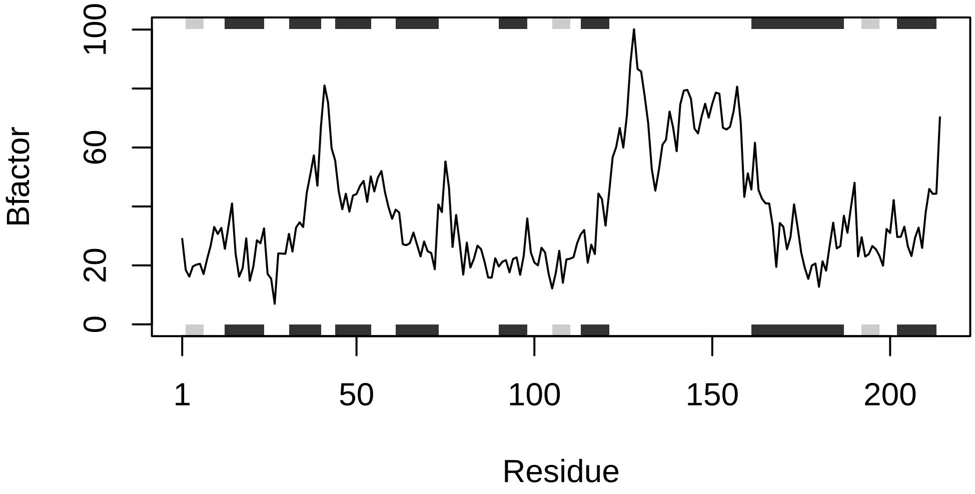
```
s2 <- read.pdb("1AKE") # kinase no drug
```

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

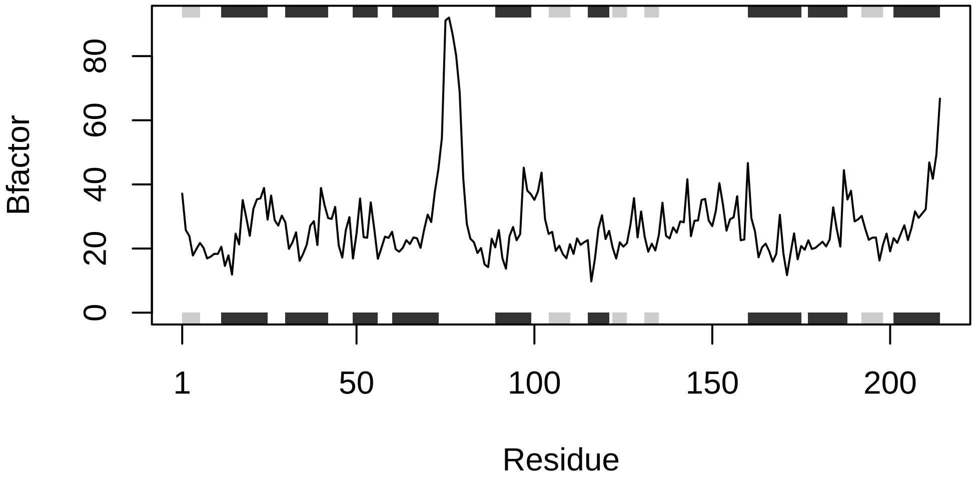
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

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

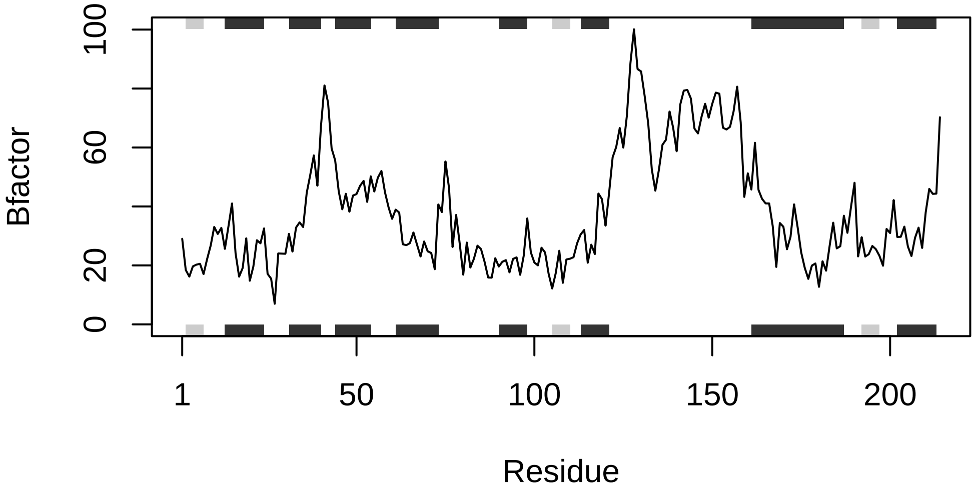
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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



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



Writing the Function

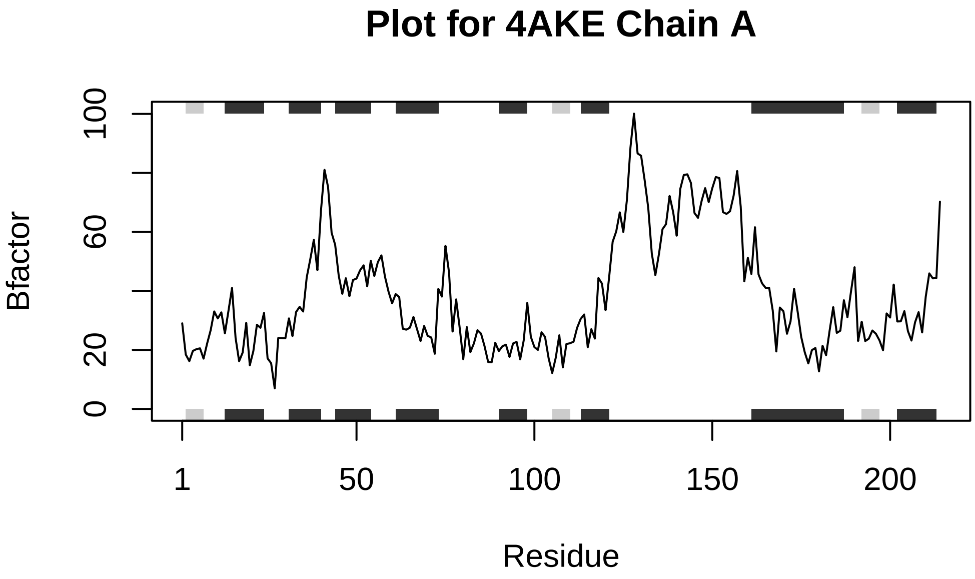
This code combines the steps from the previous code into a single function. The function takes three inputs: the protein PDB ID, the chain to focus on, and the element type. Similar to the previous approach, the function outputs a plot of B-factors. However, by using this function, we avoid repeating the same steps for each protein. Instead, we simply pass the relevant parameters for each protein to the function and get the desired plot.

```r
##Define function protein_analysis() that read the sequences and analyze their structure
protein_analysis <- function(pdb_id, chain_input="A", elety_input="CA"){

  ##read the protein sequence from PDB
  seq <- read.pdb(pdb_id)

  ##trim the sequence to focus on specific chain and element type
  seq.chainA <- trim.pdb(seq, chain = chain_input, elety = elety_input)

  ##isolate b-factors from chain A of sequence
  seq.b <- seq.chainA$atom$b

  ##plot b-factor vs. chainA
  plotb3(seq.b, sse=seq.chainA, typ="l", ylab="Bfactor", main=paste("Plot for", pdb_id, "Cha

}
```

Testing the function:

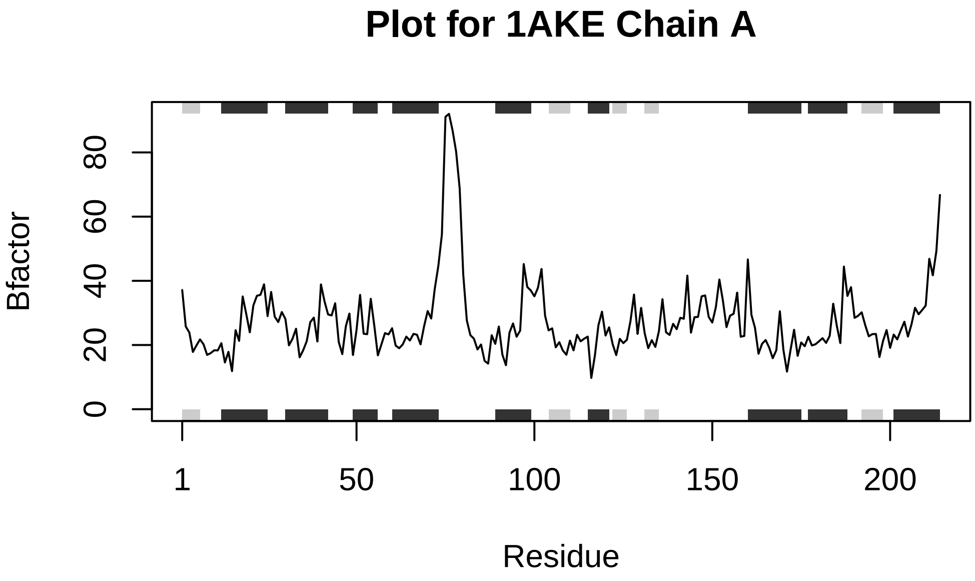
```r
protein_analysis("4AKE", chain_input = "A", elety_input = "CA")
```

```
  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/fr/phzdrrgx3wj4frmr82btkq2w0000gn/T//RtmpM8JsNu/4AKE.pdb exists.
Skipping download
```



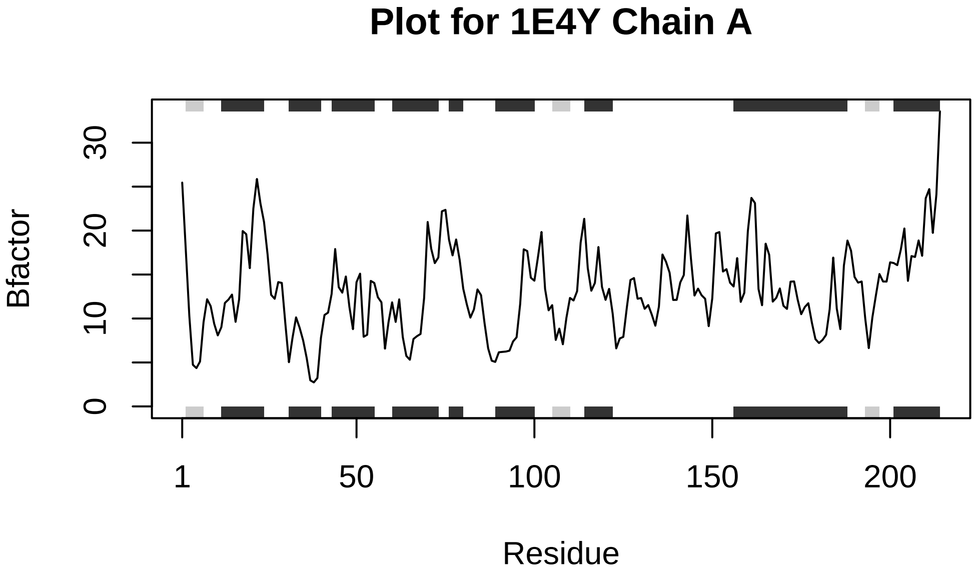
```r
protein_analysis("1AKE", "A", "CA")
```

```
  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/fr/phzdrrgx3wj4frmr82btkq2w0000gn/T//RtmpM8JsNu/1AKE.pdb exists.
Skipping download

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



```
protein_analysis("1E4Y")
```

```
  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/fr/phzdrrgx3wj4frmr82btkq2w0000gn/T//RtmpM8JsNu/1E4Y.pdb exists.
Skipping download
```


Plot for 1E4Y Chain A
Bfactor
Residue