HW06

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2025-10-17

Contents

Generalize the following protein analysis code to work for any protein sequence

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

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

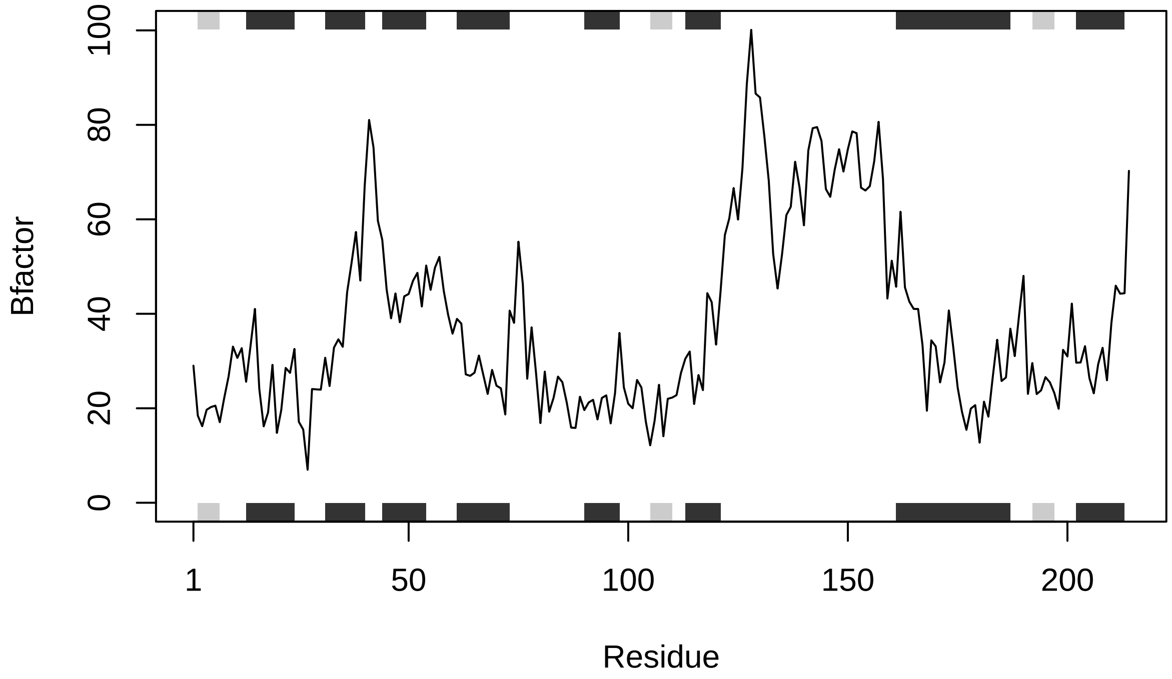
```r
s2 <- read.pdb("1AKE") # kinase no drug
```

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

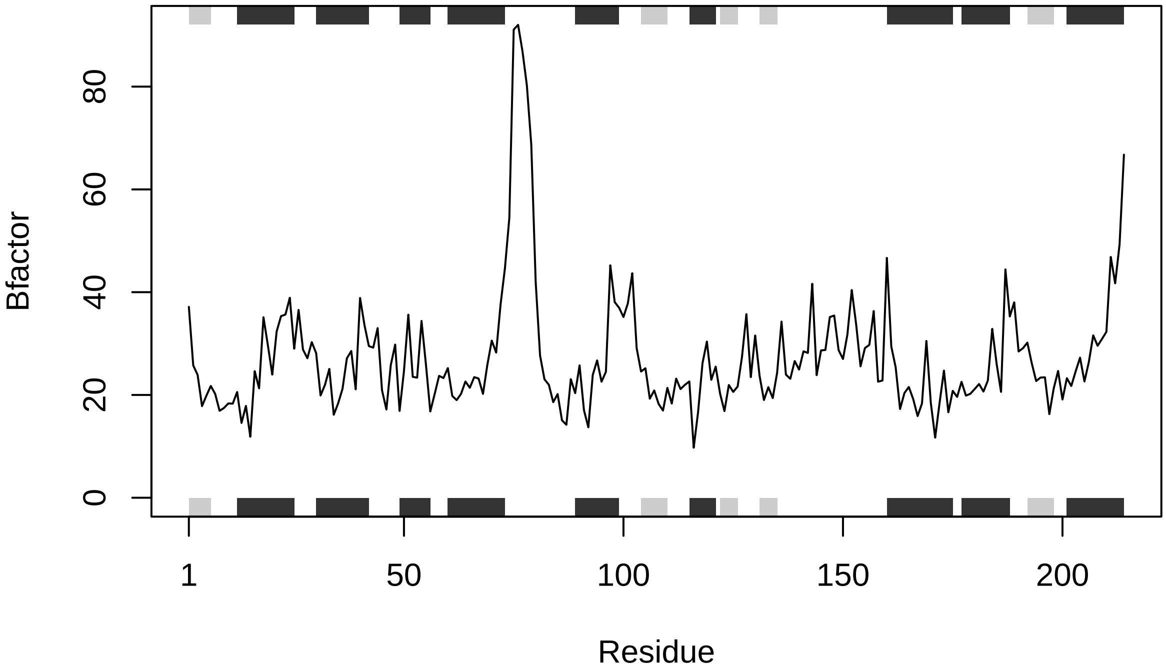
```r
s3 <- read.pdb("1E4Y") # kinase with drug
```

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

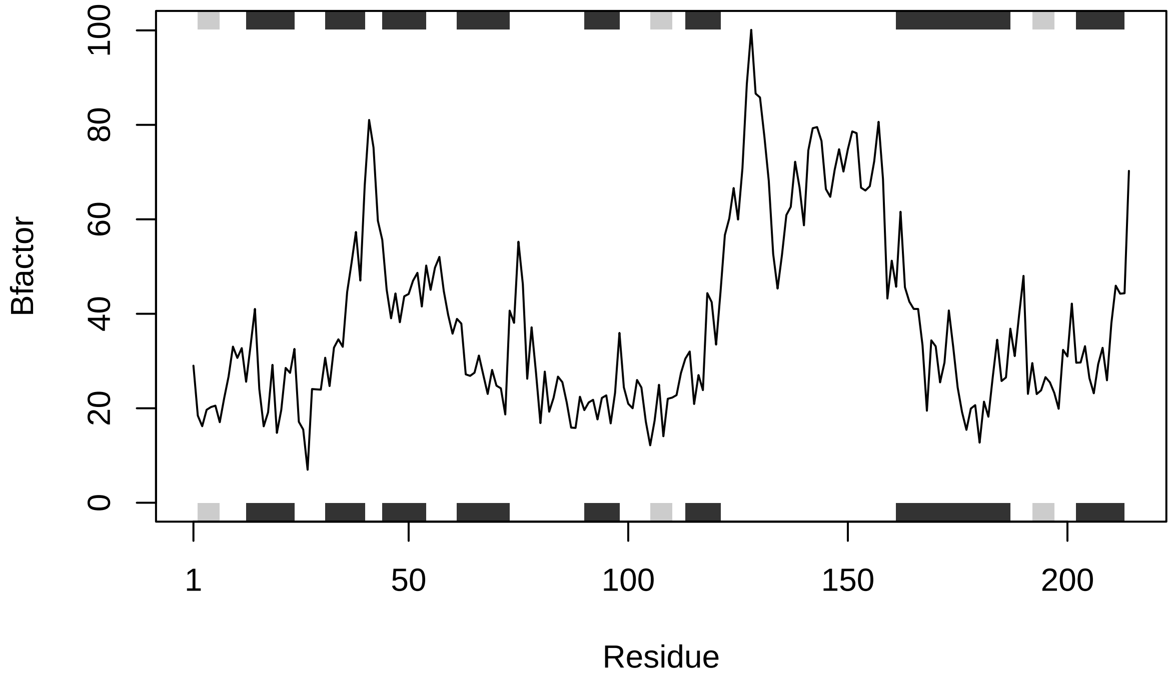
```r
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")

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")
```



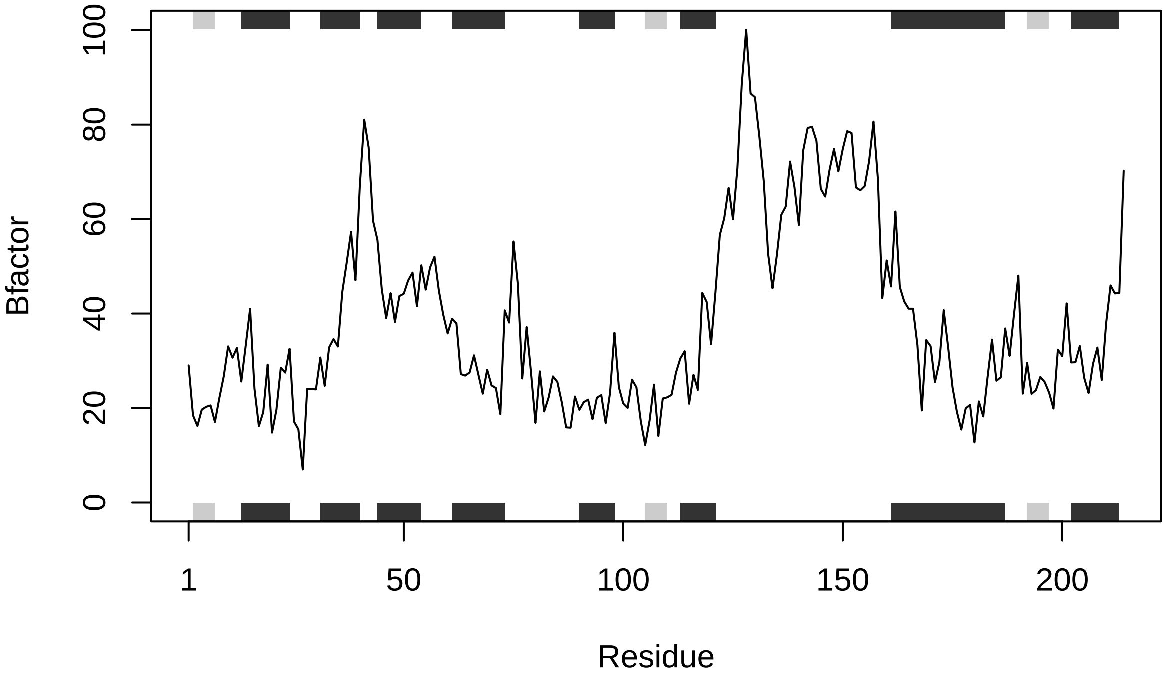
Q6. How would you generalize the original code above to work with any set of input protein structures?

Converting the general code above into a more generalized version

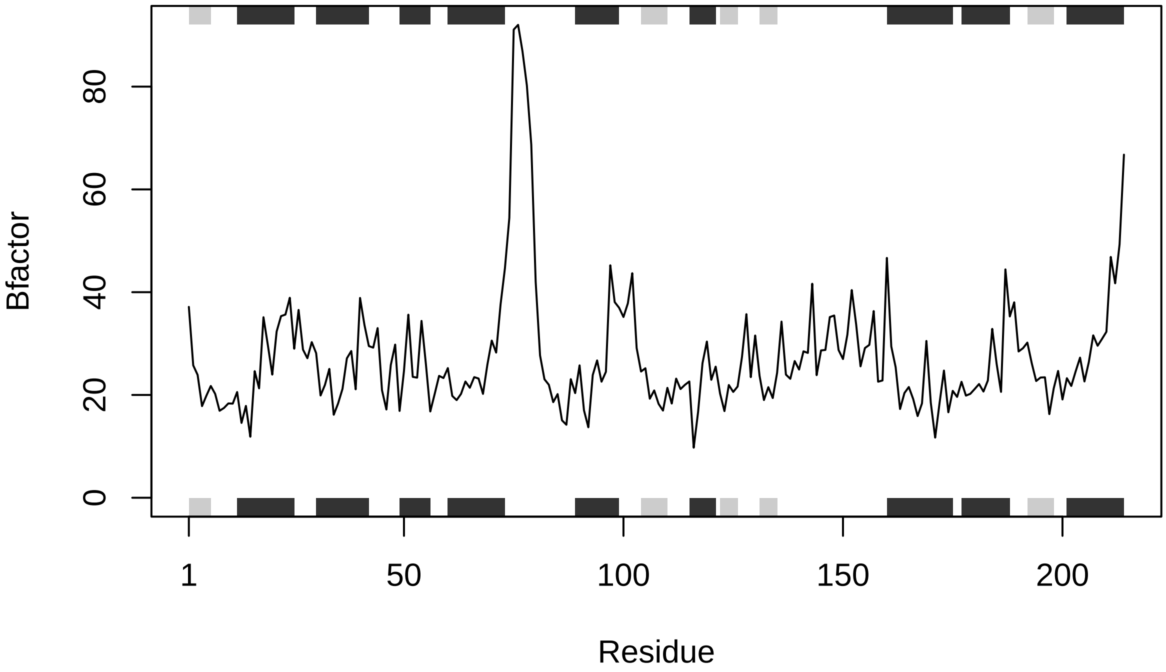
```
inputProteins = c("4AKE", "1AKE", "1E4Y")

#generating a for loop that takes a list of PDB protein ID's and analyzes each one individually as show

for (i in inputProteins) {
  s <- read.pdb(i)
  s.chainA <- trim.pdb(s, chain="A", elety="CA")
  s.b <- s.chainA$atom$b
  plotb3(s.b, sse=s.chainA, typ="l", ylab="Bfactor")
}
```

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

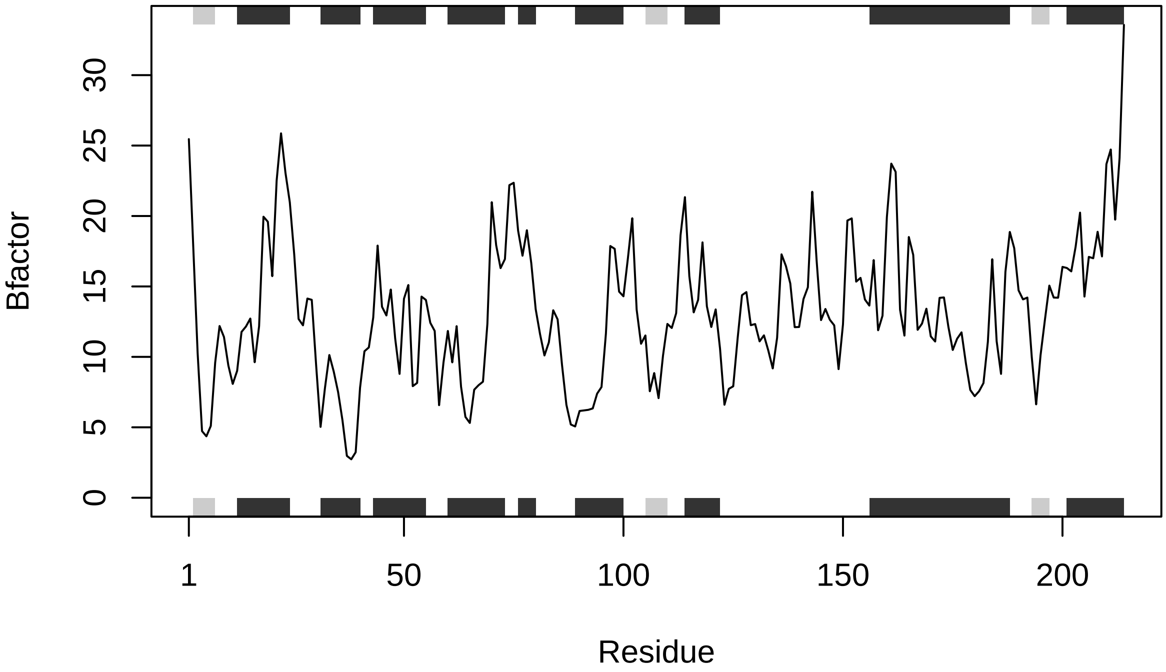
```
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
## C:\Users\eashl\AppData\Local\Temp\Rtmpw5aLRZ/4AKE.pdb exists. Skipping download
```



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

## Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
## C:\Users\eashl\AppData\Local\Temp\Rtmpw5aLRZ/1AKE.pdb exists. Skipping download

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



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

## Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
## C:\Users\eashl\AppData\Local\Temp\Rtmpw5aLRZ/1E4Y.pdb exists. Skipping download
```



Converting the generalized code into a function that can be applied to any list of sequences

```
#This function accepts a list of PDB protein ID's and analyzes each one individually as shown above. ma

analyzeProteins <- function(seqs) {
  for (i in inputProteins) {
    s <- read.pdb(i)
    s.chainA <- trim.pdb(s, chain="A", elety="CA")
    s.b <- s.chainA$atom$b
        plotb3(s.b, sse=s.chainA, typ="l", ylab="Bfactor", main=i)
  }
}
```

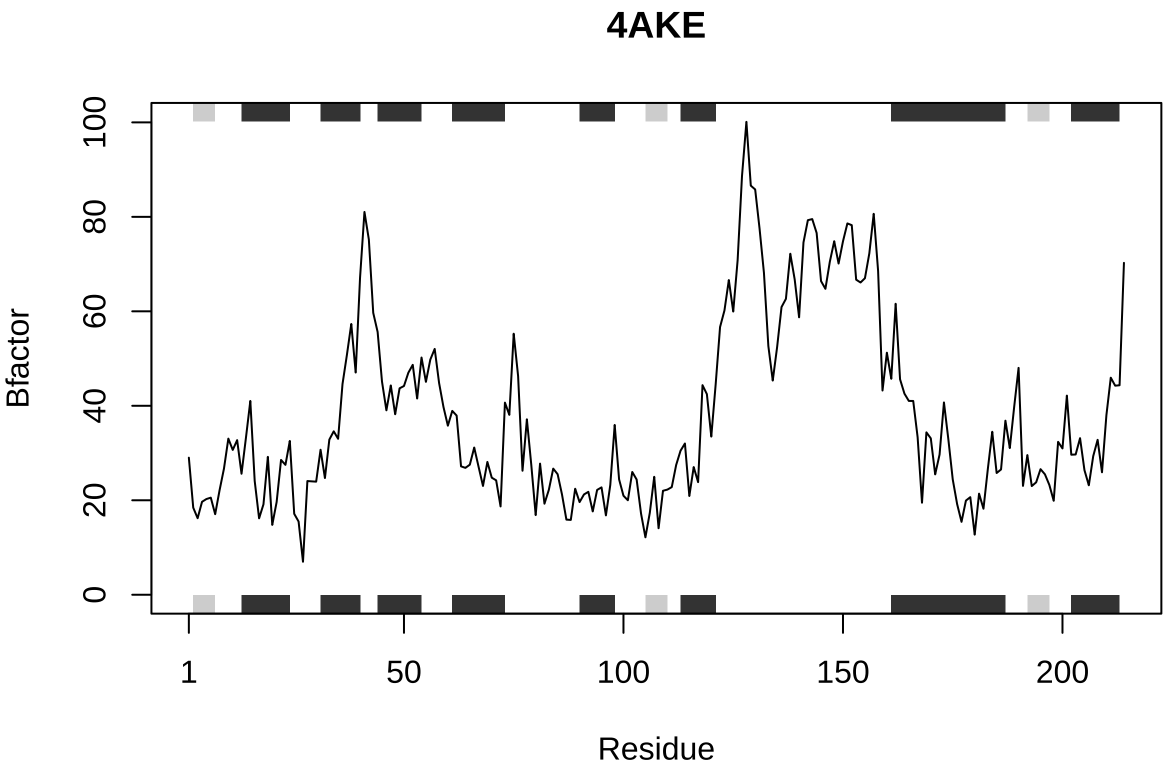
This function accepts a list of PDB protein ID's and analyzes each one individually as shown above generating a plot of the residue position vs. the B factor

Testing new function on the provided list of sequences

```
analyzeProteins(inputProteins)
```

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

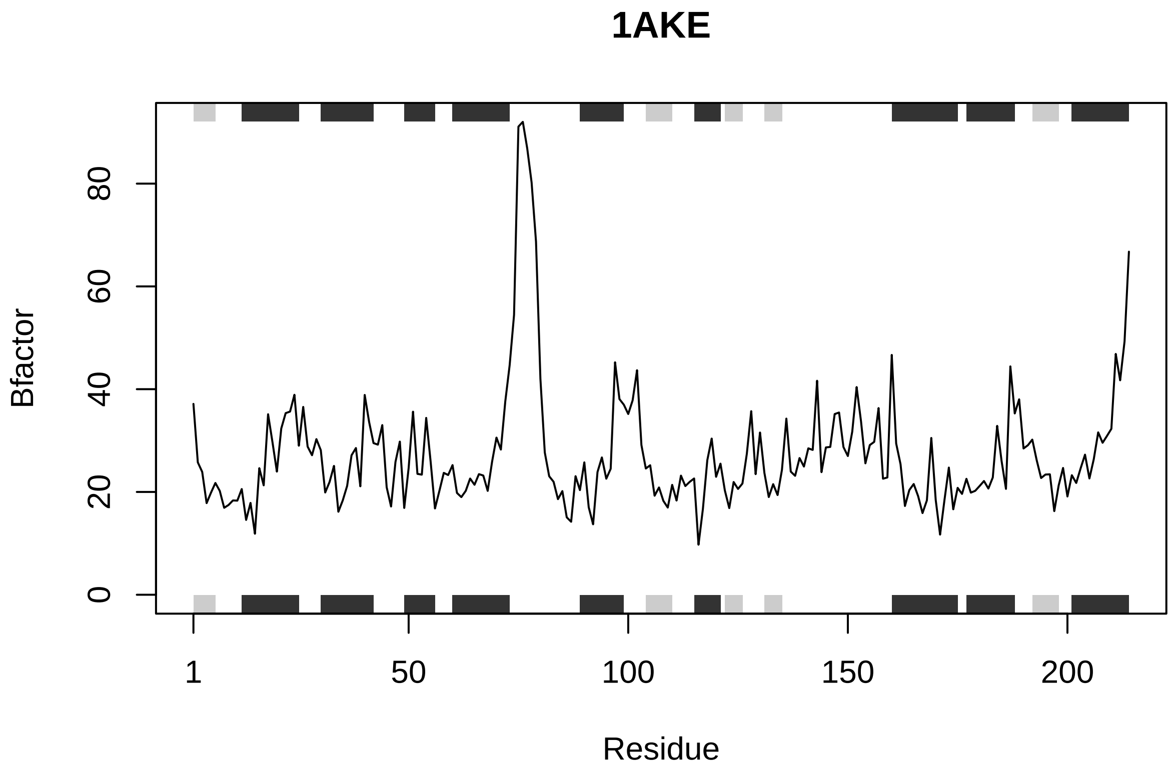
```
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
## C:\Users\eashl\AppData\Local\Temp\Rtmpw5aLRZ/4AKE.pdb exists. Skipping download
```



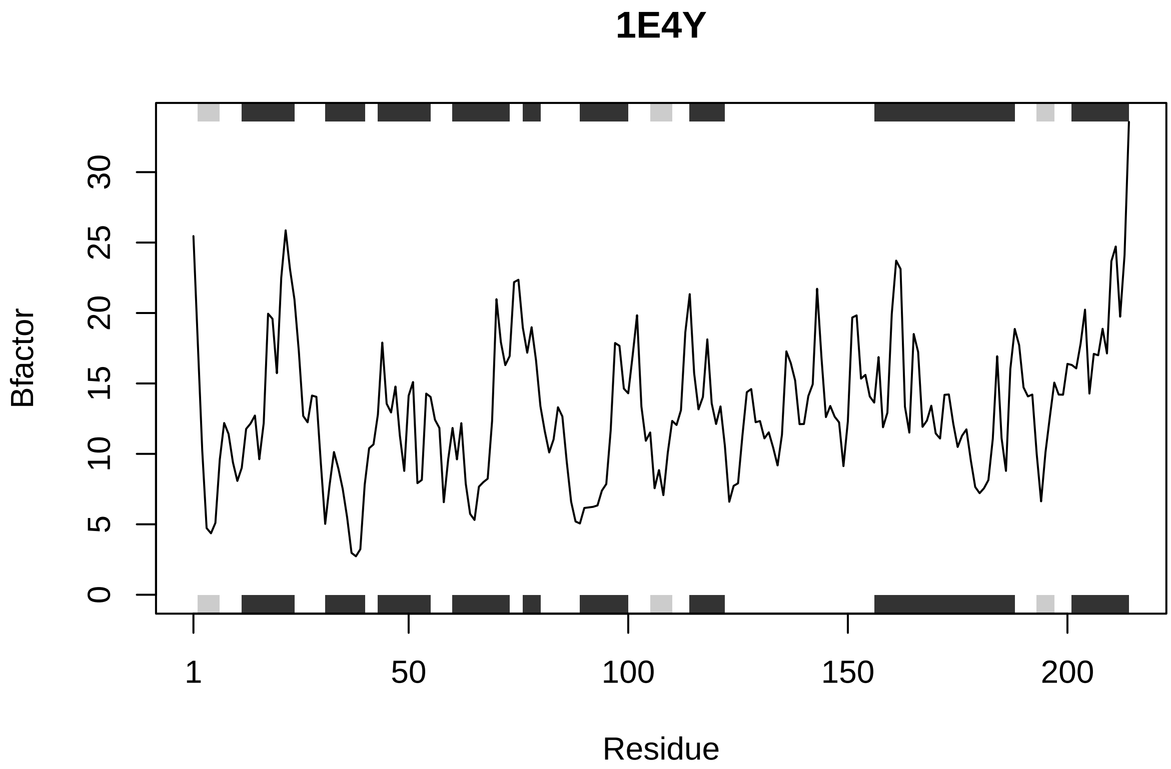
```
##   Note: Accessing on-line PDB file
```

```
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
## C:\Users\eashl\AppData\Local\Temp\Rtmpw5aLRZ/1AKE.pdb exists. Skipping download
```

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



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

## Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
## C:\Users\eashl\AppData\Local\Temp\Rtmpw5aLRZ/1E4Y.pdb exists. Skipping download
```



Testing with sapply()

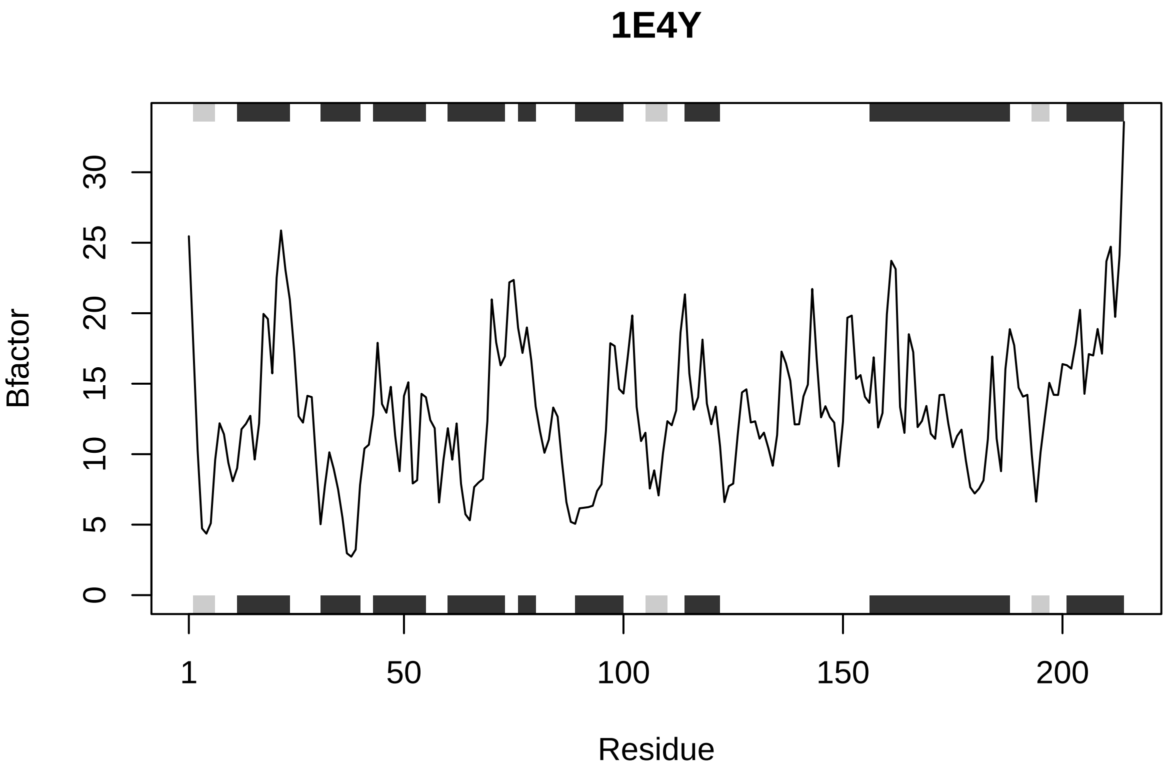
Making the function even more generalized so that it can be utilized with sapply(). It accepts a single PDB ID at a time but can be vectorized with sapply() to achieve the same output as previously

```
analyzeProteins <- function(seqs) {
    s <- read.pdb(i)
    s.chainA <- trim.pdb(s, chain="A", elety="CA")
    s.b <- s.chainA$atom$b
    plotb3(s.b, sse=s.chainA, typ="l", ylab="Bfactor", , main=i)
}
```

```
sapply(inputProteins, analyzeProteins)
```

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

```
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
## C:\Users\eashl\AppData\Local\Temp\Rtmpw5aLRZ/1E4Y.pdb exists. Skipping download
```



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

## Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
## C:\Users\eashl\AppData\Local\Temp\Rtmpw5aLRZ/1E4Y.pdb exists. Skipping download

##   Note: Accessing on-line PDB file

## Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
## C:\Users\eashl\AppData\Local\Temp\Rtmpw5aLRZ/1E4Y.pdb exists. Skipping download

## $‘4AKE‘
## NULL
##
## $‘1AKE‘
## NULL
##
## $‘1E4Y‘
## NULL
```