Class 06 Homework

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```
library(bio3d)
```

Can you improve this code?

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

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

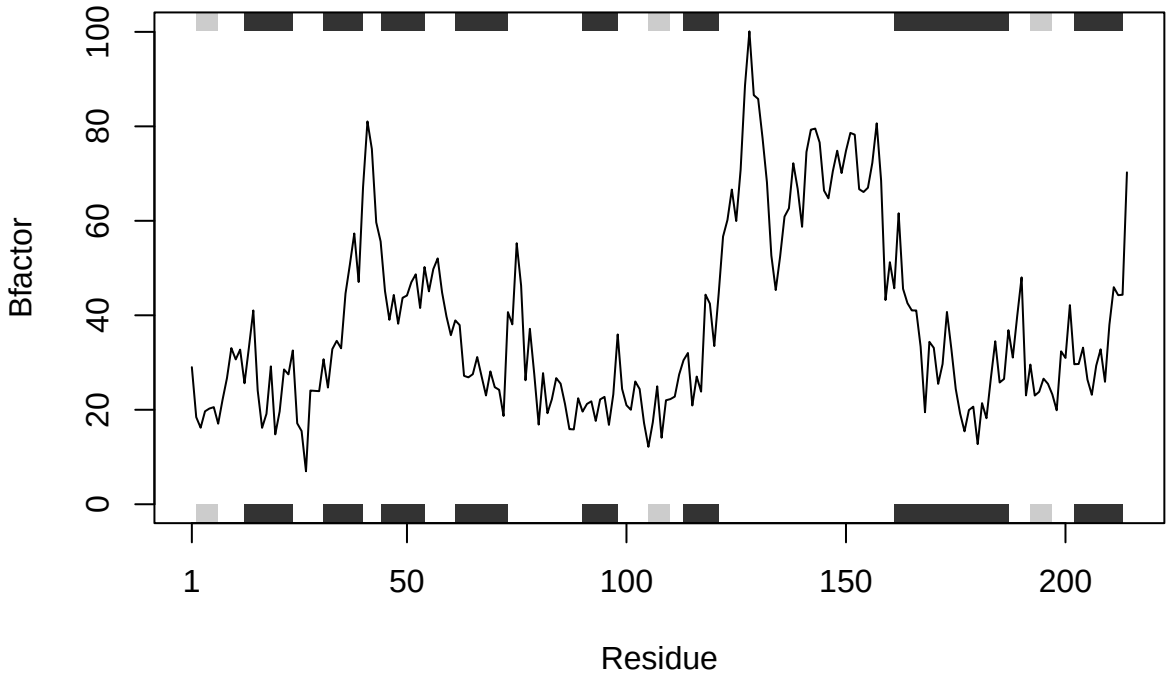
```
s2 <- read.pdb("1AKE") # kinase no drug
```

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

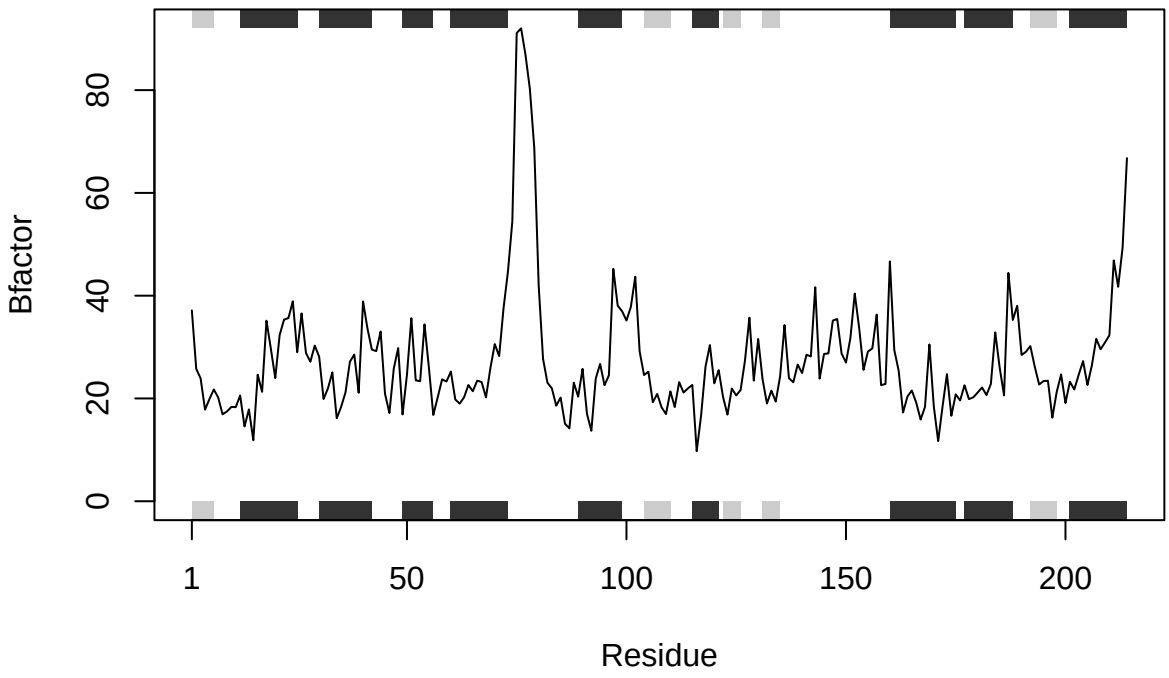
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

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

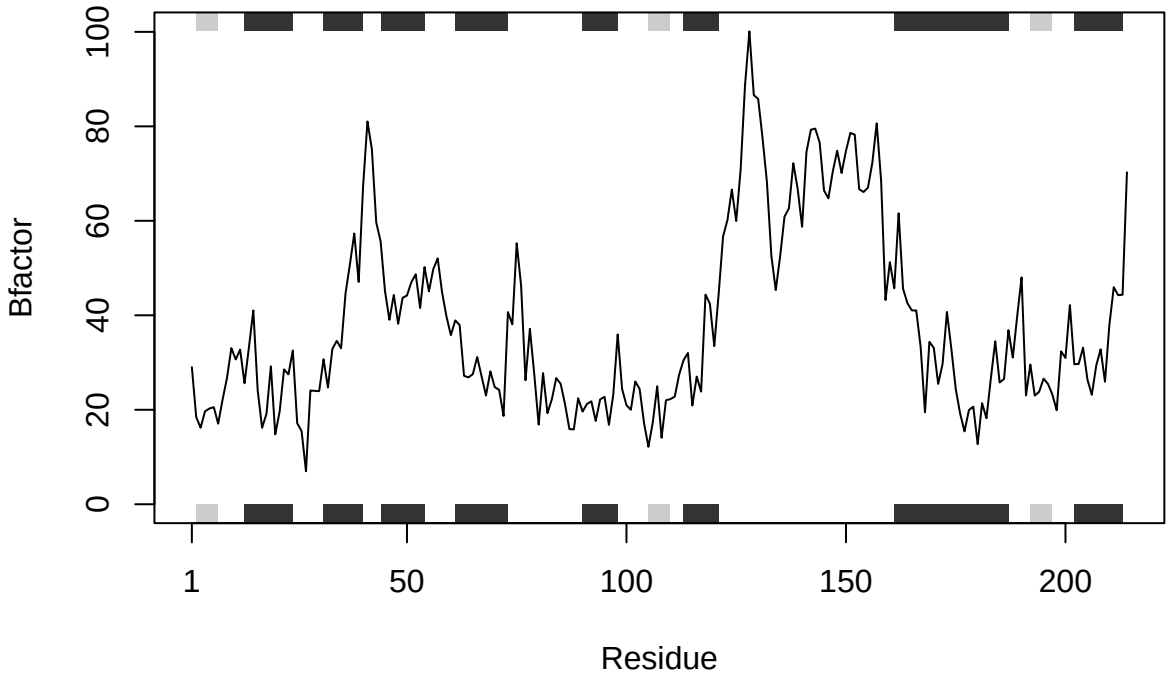
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")

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")
```



Fixing copy/paste errors

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

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

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

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

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

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

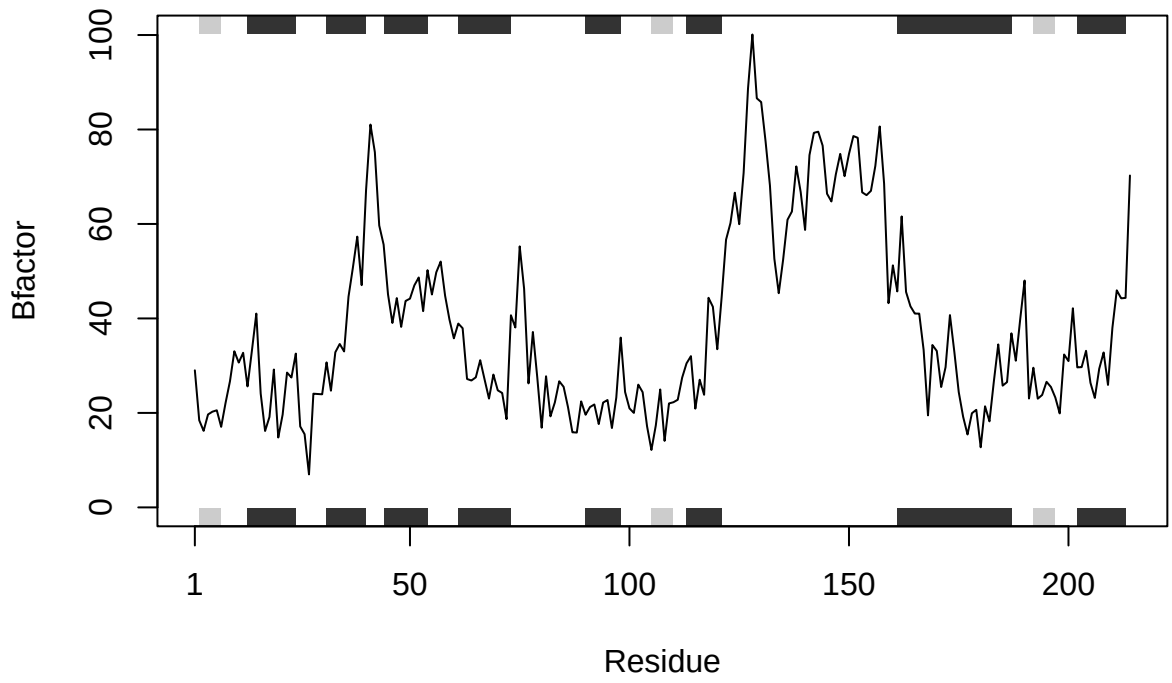
```
##    PDB has ALT records, taking A only, rm.alt=TRUE
```

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

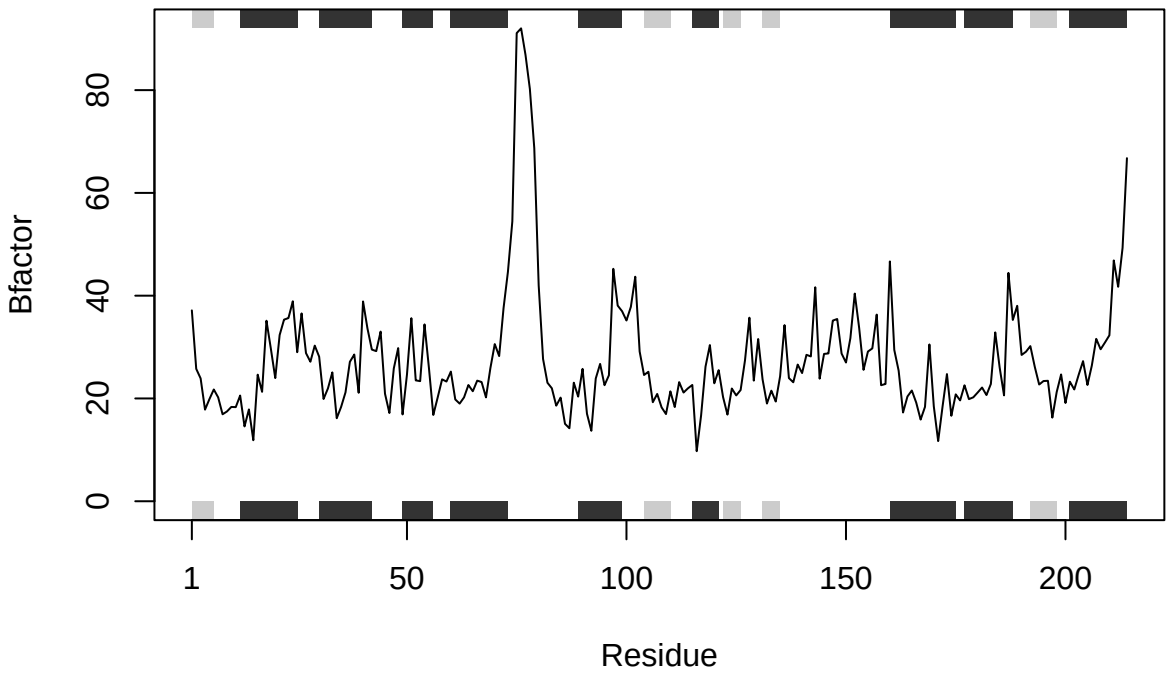
```
##   Note: Accessing on-line PDB file
```

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

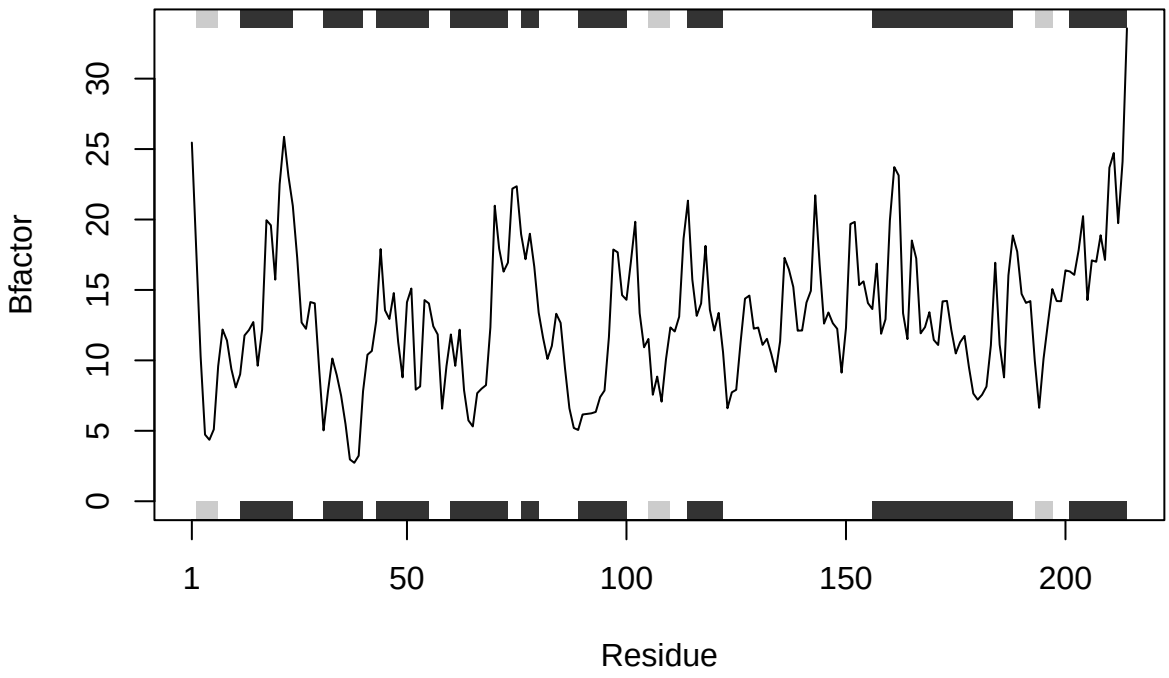
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")

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")
```

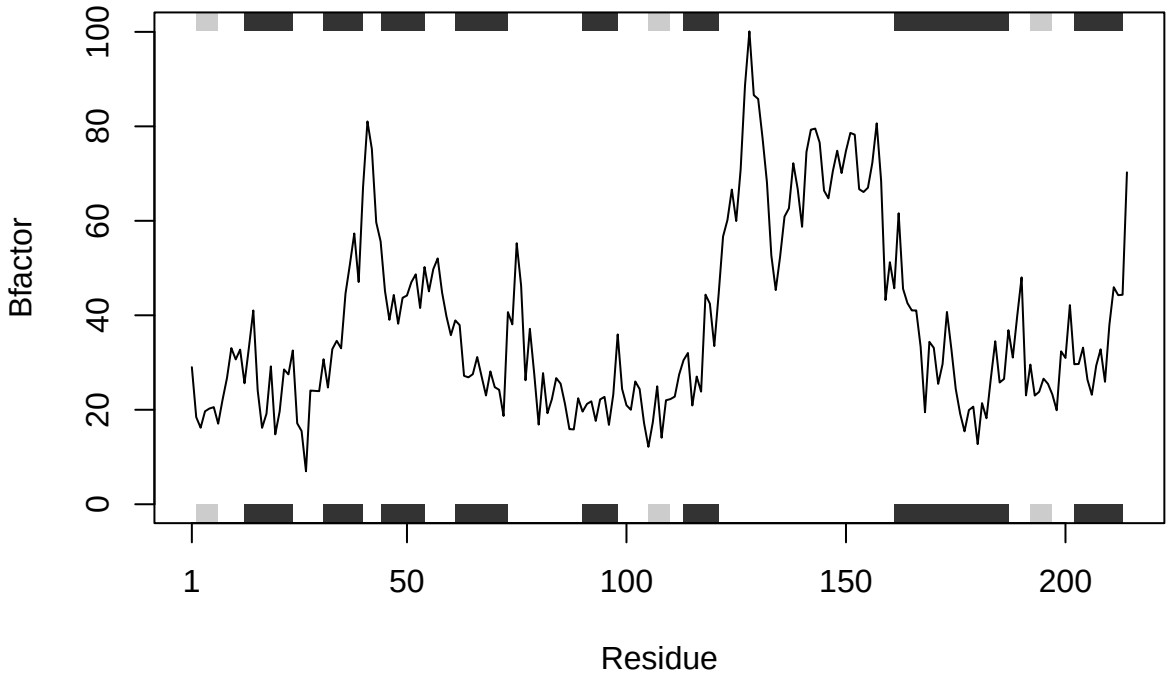


Simplifying the core code snippet

```
x <- read.pdb("4AKE")
```

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

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

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



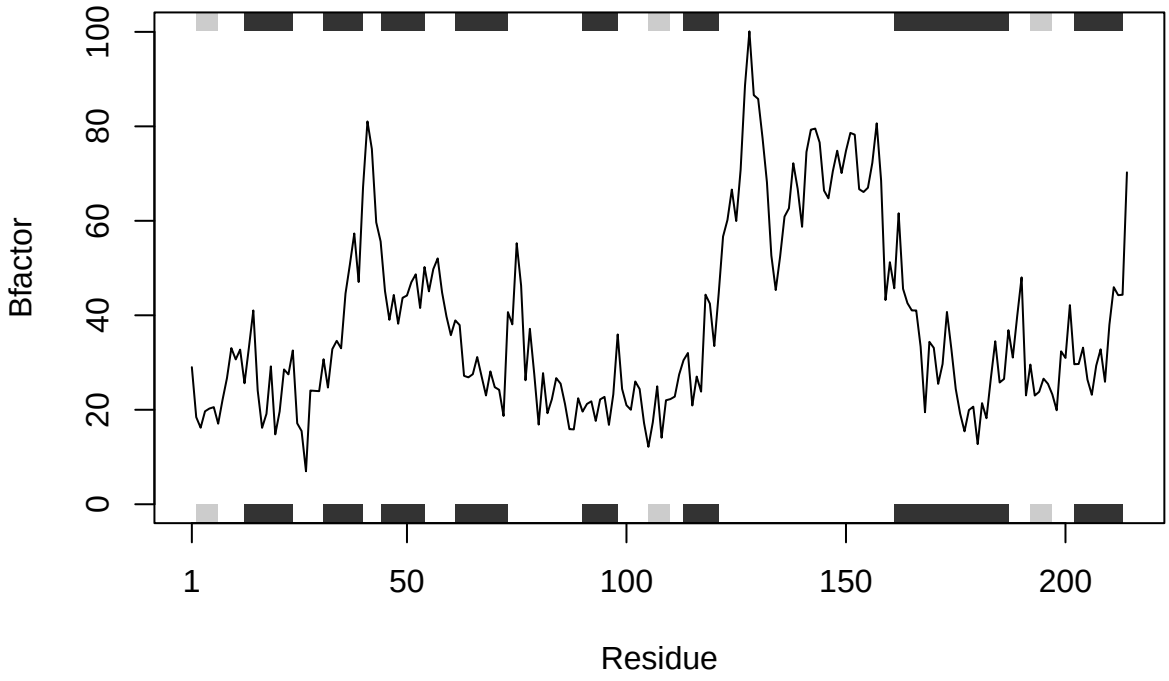
Making a function out of the simplified snippet

```
protein <- function(file) {
  x <- read.pdb(file)
  x.chainA <- trim.pdb(x, chain="A", elety="CA")
  x.atomb <- x.chainA$atom$b
  plotb3(x.atomb, sse=x.chainA, typ = "l", ylab = "Bfactor")
}
```

Testing the new function

```
protein("4AKE")
```

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

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

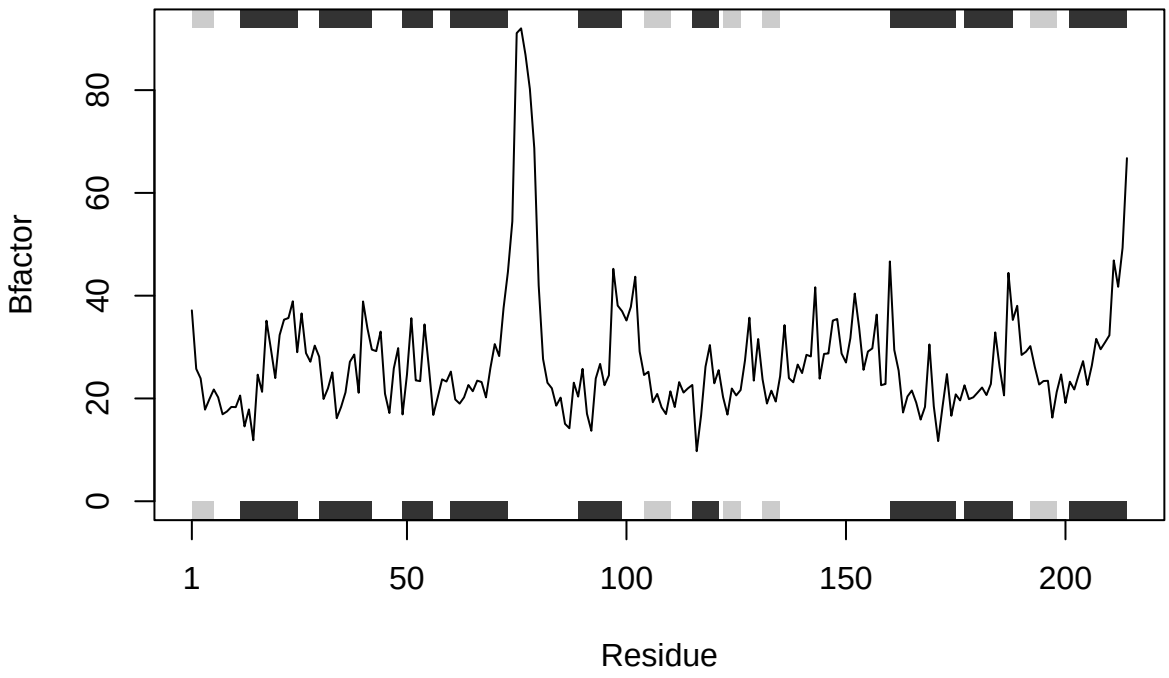



```
protein("1AKE")
```

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

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

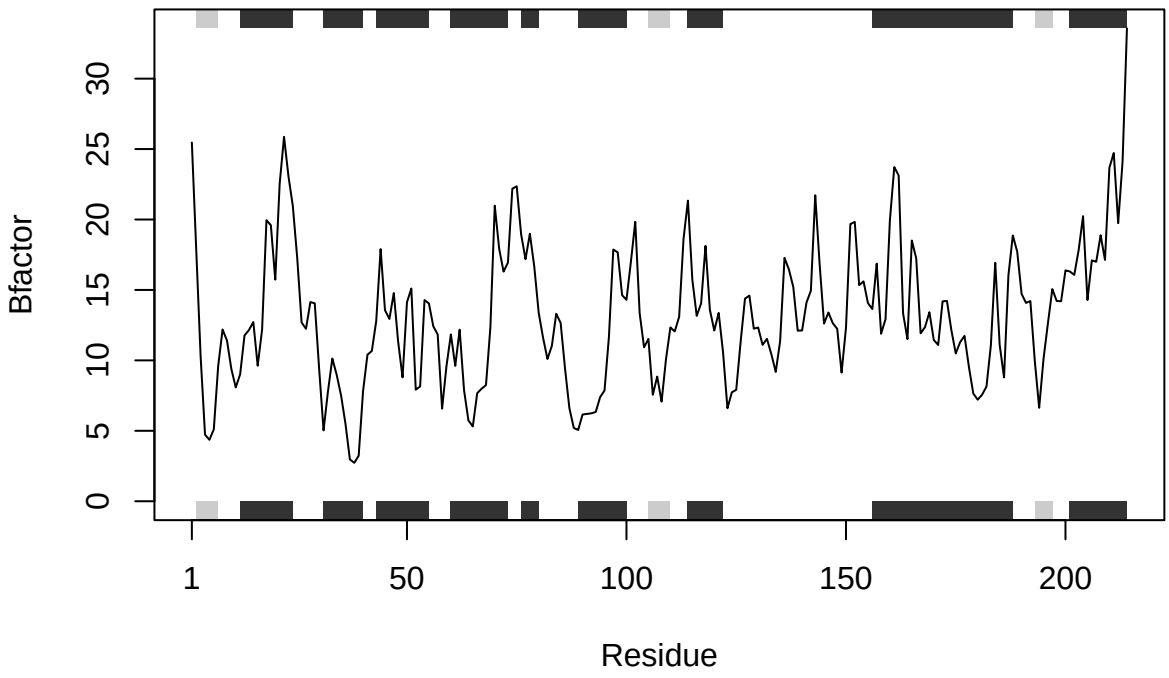
```
##    PDB has ALT records, taking A only, rm.alt=TRUE
```




```
protein("1E4Y")
```

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

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



Adding annotations

First exploring plotb3() to understand the plot better

```
help(plotb3)
```

```
## starting httpd help server ... done
```

Annotations

```
#' Line Plot of Protein Drug Interactions
#'
#' @param x A .pdb file
#'
#' @return plot of chain A of a protein drug interaction
#' @export
#'
#' @examples
protein <- function(file) {
  x <- read.pdb(file)
  x.chainA <- trim.pdb(x, chain="A", elety="CA")
  x.atomb <- x.chainA$atom$b
  plotb3(x.atomb, sse=x.chainA, typ = "l", ylab = "Bfactor")
}
```

```
protein("4AKE")
```

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

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