Lopez_Lab6_hw

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Section 1 of lab 6

##Example

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

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

```r
s2 <- read.pdb("1AKE") # kinase w/out drug
```

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

```r
s3 <- read.pdb("1E4Y") # kinase w/ drug
```
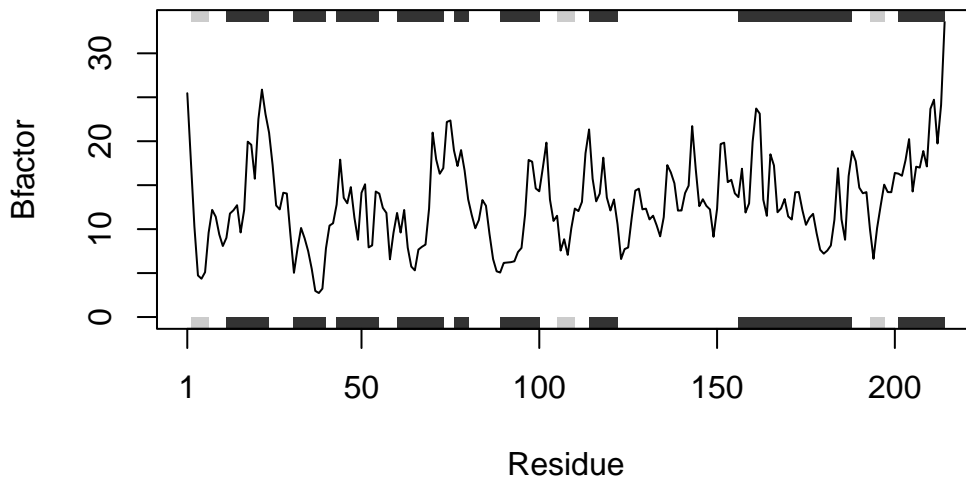
```
Note: Accessing on-line PDB file
```

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


Optimized code:

```
protein_analysis <- function(x) {
  #f load bio3d library
  library(bio3d)
  # read.pdb to load the protein data bank file for the protein name in the query (x)
  read <- read.pdb(x)
  # trim.pdb to clean pdb file, will remove the protein structures and only keeping the seque
  trim <- trim.pdb(read, chain = "A", elety="CA")
  #isolate sequence of b row in  atom column
  choose_atom <- trim$atom$b
  #blot  B factor and residue number
  graph <- plotb3(choose_atom, sse=trim, typ="l", ylab="Bfactor")
  return(protein_analysis)
}
#apply  function to several queries in a vector
sapply(c("4AKE", "1AKE", "1E4Y"), protein_analysis)
```
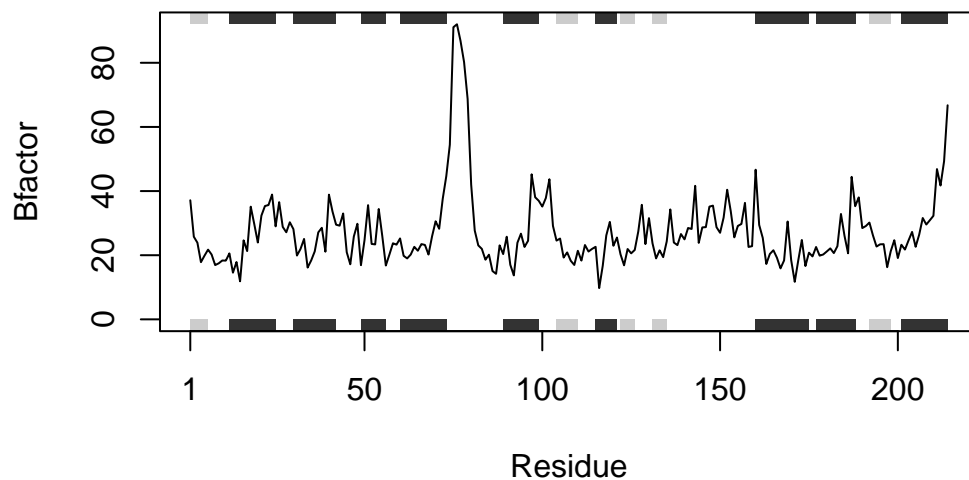
```
Note: Accessing on-line PDB file
```

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/k9/64p05h751k797np7vrhm0lg40000gn/T//RtmpPyNzYz/4AKE.pdb exists.
Skipping download
```
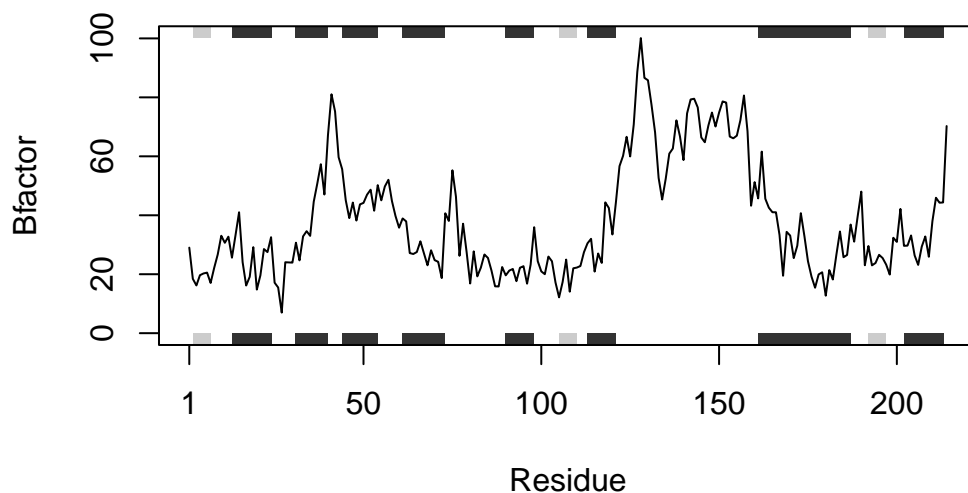


```
  Note: Accessing on-line PDB file
```

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/k9/64p05h751k797np7vrhm0lg40000gn/T//RtmpPyNzYz/1AKE.pdb exists.
Skipping download
```

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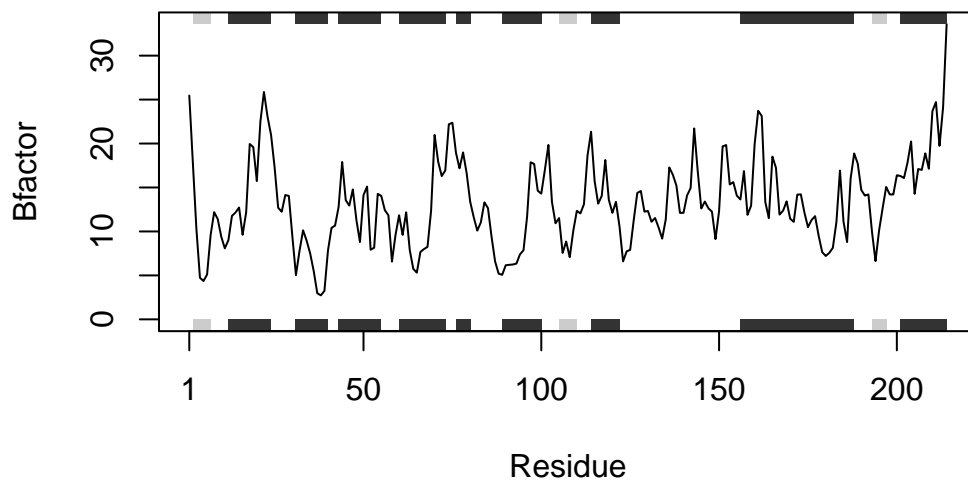
Note: Accessing on-line PDB file

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/k9/64p05h751k797np7vrhm0lg40000gn/T//RtmpPyNzYz/1E4Y.pdb exists.
Skipping download
```

```
$`4AKE`
function (x)
{
    library(bio3d)
    read <- read.pdb(x)
    trim <- trim.pdb(read, chain = "A", elety = "CA")
    choose_atom <- trim$atom$b
    graph <- plotb3(choose_atom, sse = trim, typ = "l", ylab = "Bfactor")
    return(protein_analysis)
}
<bytecode: 0x10e1bc0e0>

$`1AKE`
function (x)
{
    library(bio3d)
    read <- read.pdb(x)
    trim <- trim.pdb(read, chain = "A", elety = "CA")
    choose_atom <- trim$atom$b
    graph <- plotb3(choose_atom, sse = trim, typ = "l", ylab = "Bfactor")
    return(protein_analysis)
}
<bytecode: 0x10e1bc0e0>
```

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```
$`1E4Y`
function (x)
{
    library(bio3d)
    read <- read.pdb(x)
    trim <- trim.pdb(read, chain = "A", elety = "CA")
    choose_atom <- trim$atom$b
    graph <- plotb3(choose_atom, sse = trim, typ = "l", ylab = "Bfactor")
    return(protein_analysis)
}
<bytecode: 0x10e1bc0e0>
```