

ProteinAnalysisFunction

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This is the original code

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

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

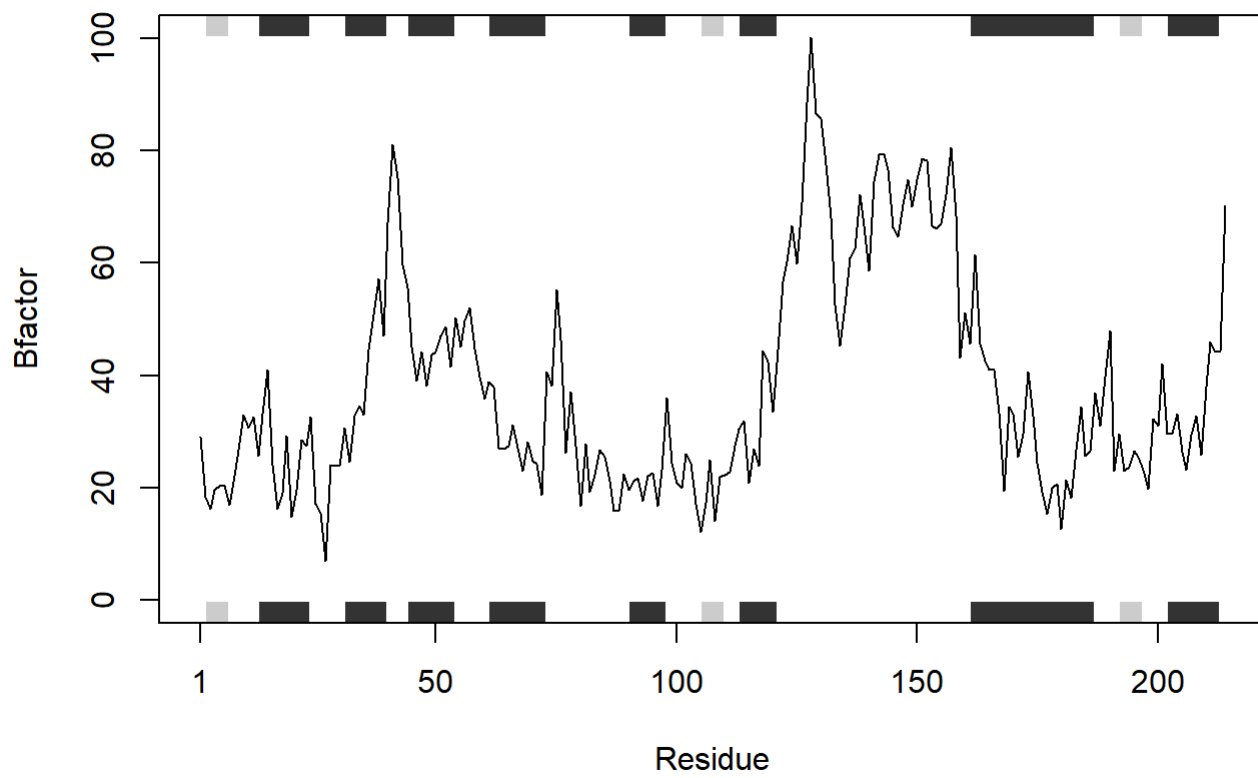
```
s2 <- read.pdb("1AKE") # kinase no drug
```

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

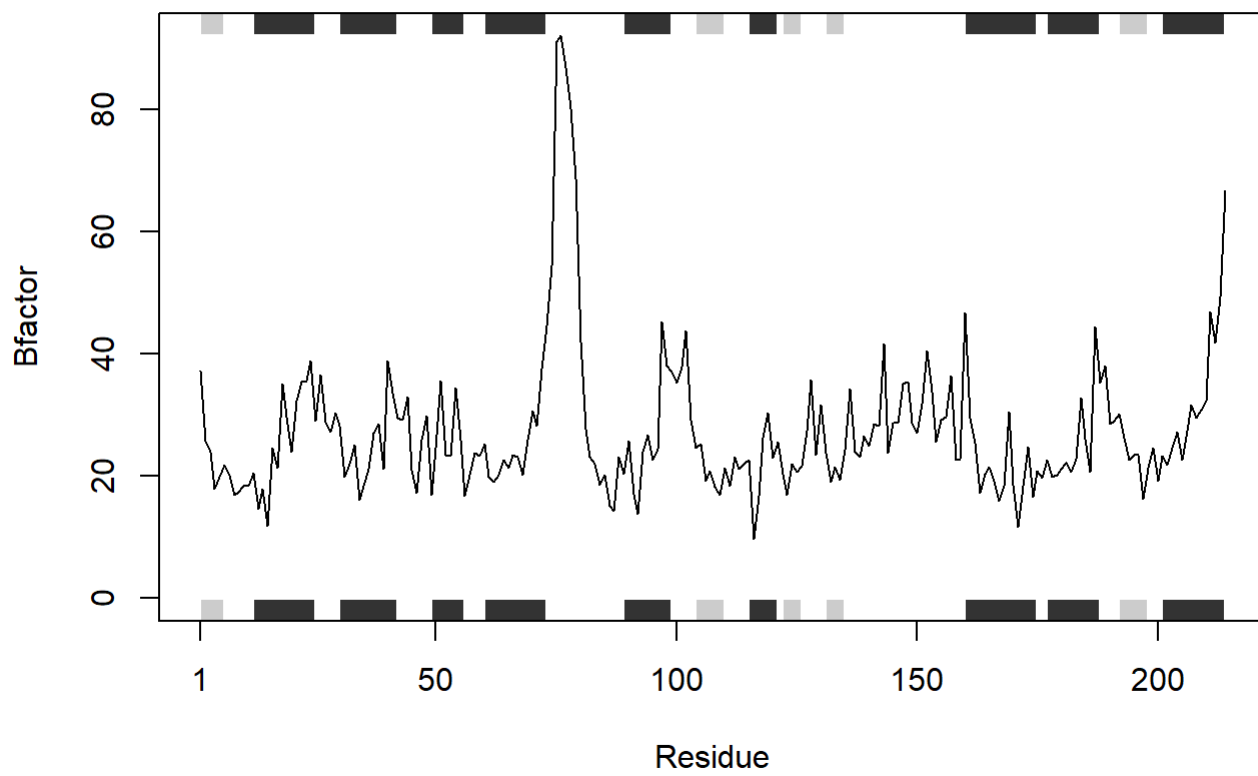
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

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

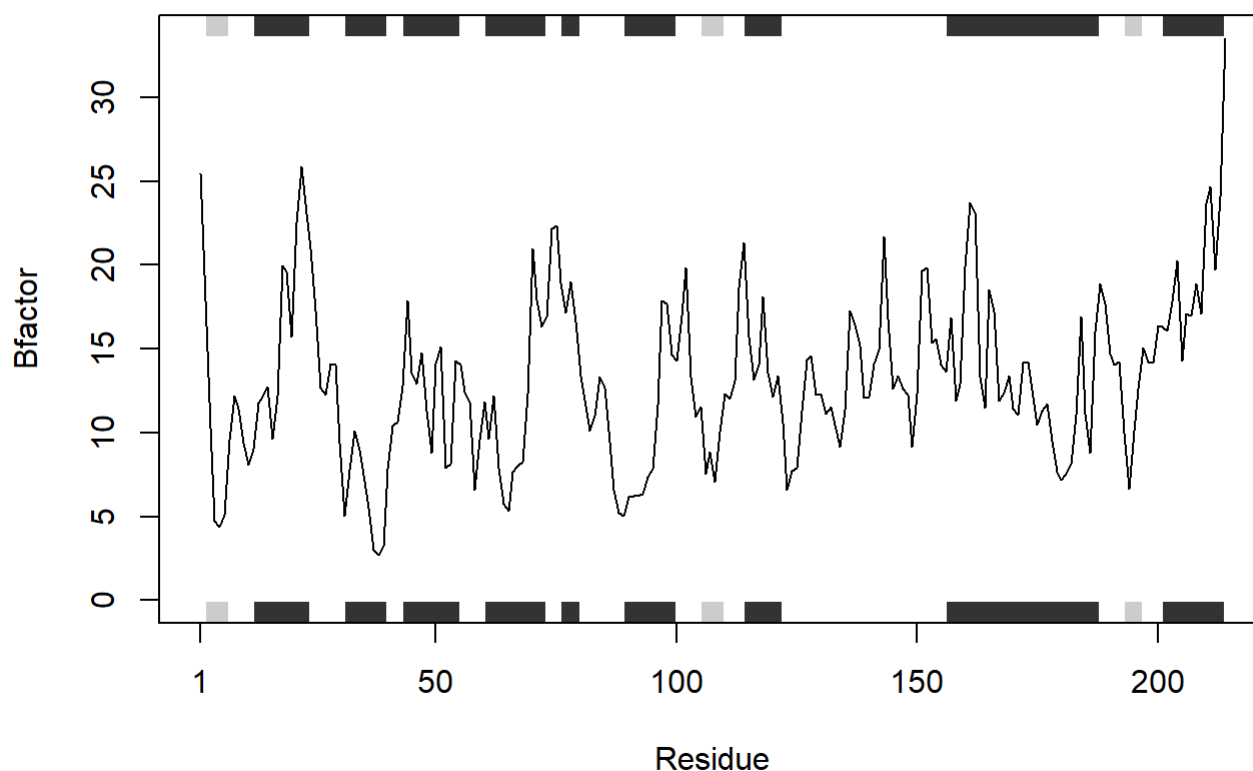
```
s1.chainA <- trim.pdb(s1, chain="A", eley="CA")
s2.chainA <- trim.pdb(s2, chain="A", eley="CA")
s3.chainA <- trim.pdb(s3, chain="A", eley="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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



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



The assignment is to make a function that can be used to analyze any protein.

The input of this function is x, which is the protein name ("4AKE", etc).

When you use the function `anaylzeprotein()`, it will make a plot that maps the Bfactor of the protein in relation to its residue. You use it by typing `anaylzeprotein("x")`, where x is the code name for the protein you want to analyze.

The output of the function is `analyzeprotein`, which will make a plot of the protein you inputted.

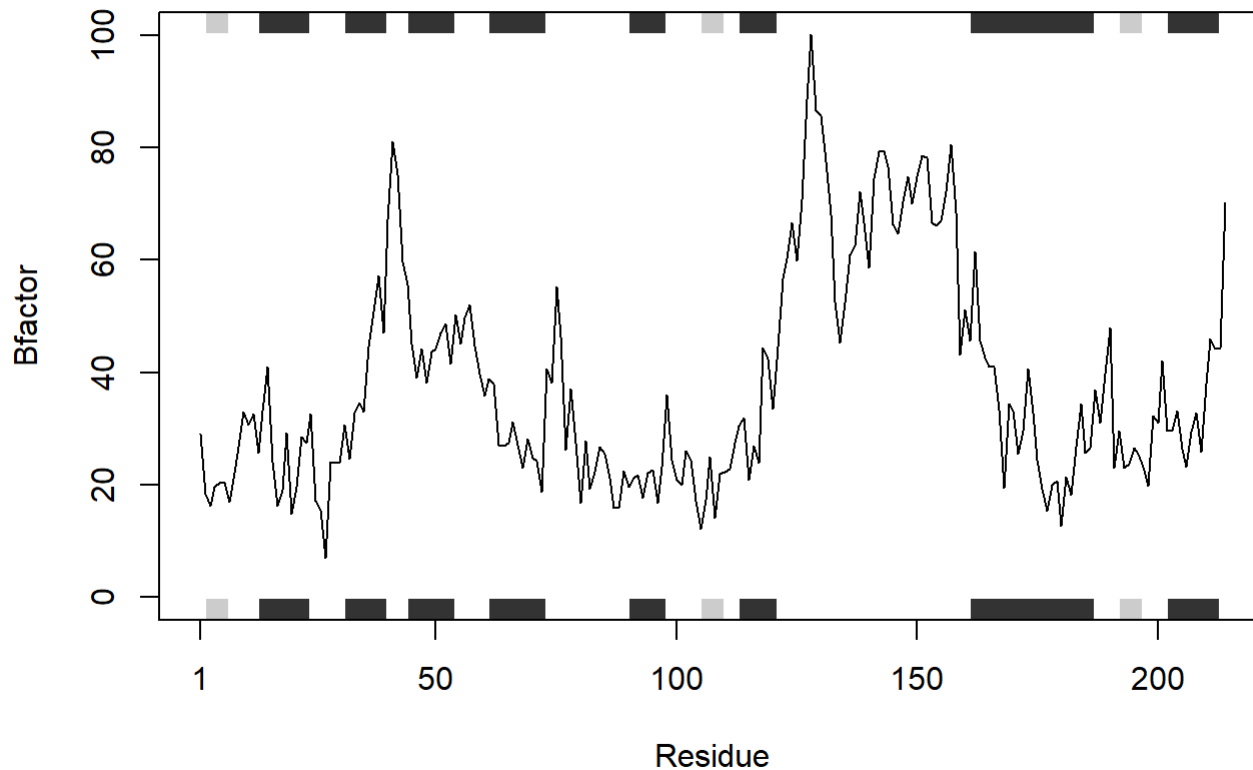
```
library(bio3d)
analyzeprotein <- function(x) {
  s1 <- read.pdb(x)
  s1.chainA <- trim.pdb(s1, chain = "A", elety= "CA")
  s1.b <- s1.chainA$atom$b
  plotb3(s1.b, sse=s1.chainA, typ= "l", ylab= "Bfactor")
}
```

Testing out to see if we get the same results.

```
analyzeprotein("4AKE")
```

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

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

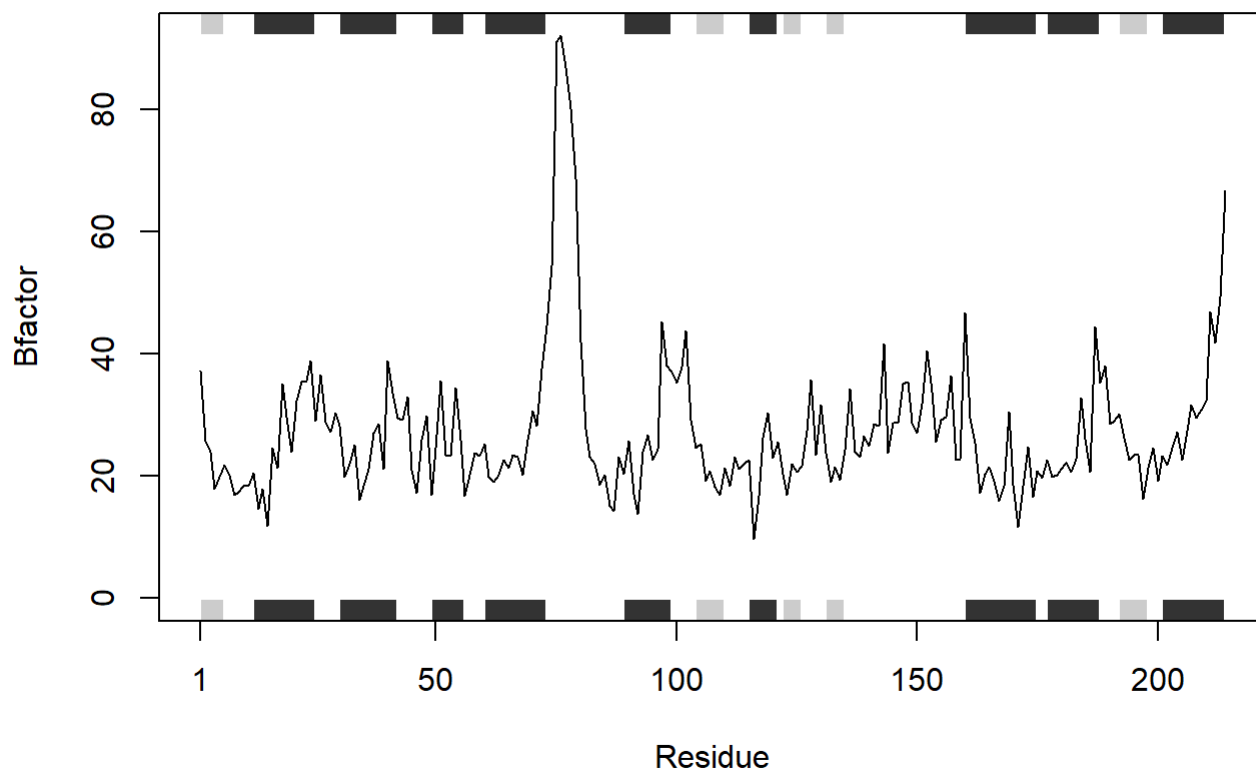


```
analyzeprotein("1AKE")
```

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

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

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



```
analyzeprotein("1E4Y")
```

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

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

