

Homework 6: Write a Function

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Load packages:

```
library(bio3d)
```

Generalize the example code by writing a function

Example code:

```
s1 <- read.pdb("4AKE")
```

Note: Accessing on-line PDB file

```
s2 <- read.pdb("1AKE")
```

Note: Accessing on-line PDB file

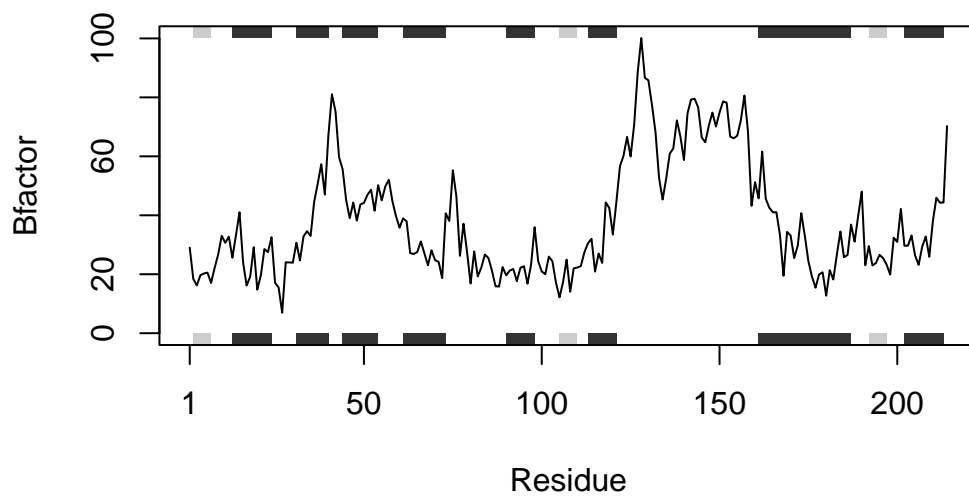
PDB has ALT records, taking A only, rm.alt=TRUE

```
s3 <- read.pdb("1E4Y")
```

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(s3, chain="A", elety="CA") # corrected error  
s1.b <- s1.chainA$atom$b  
s2.b <- s2.chainA$atom$b
```

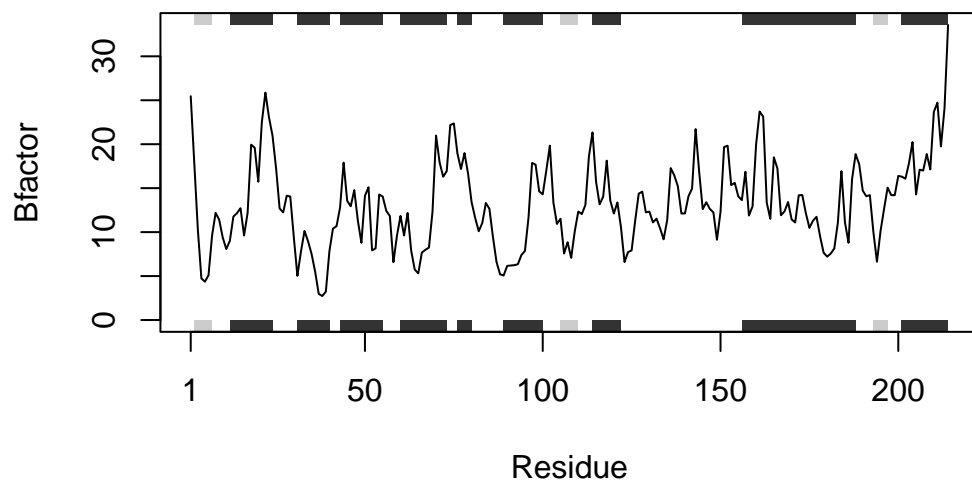
```
s3.b <- s3.chainA$atom$b  
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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



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



My function:

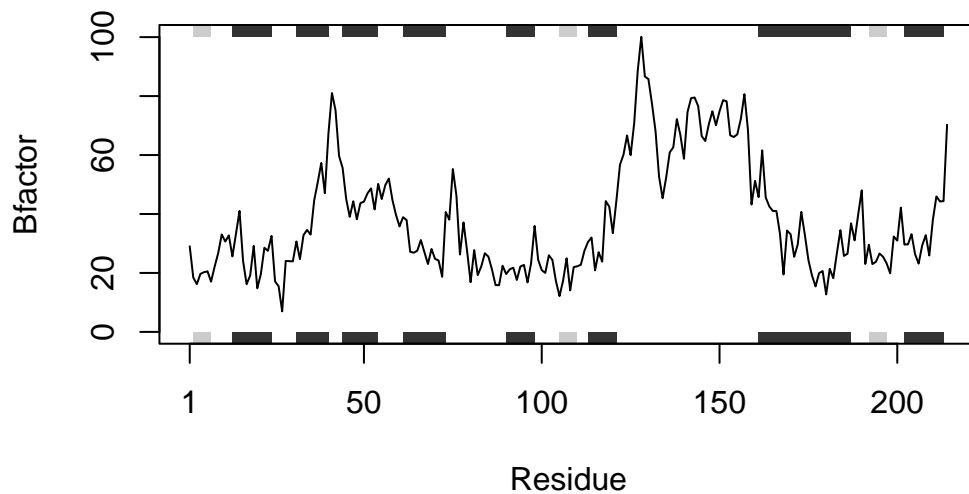
```
protein <- function(x){ # input = PDB accession code
  s <- read.pdb(x) # read PDB coordinate file
  s.chainA <- trim.pdb(s, chain = "A", eley="CA") # trim to a subset of atoms
  s.b <- s.chainA$atom$b # select one vector ("b") from the list
  plotb3(s.b, sse=s.chainA, typ="l", ylab="Bfactor") # generate a scatter plot
}
```

Test my function:

```
# compare to output from example code
protein("4AKE")
```

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/kw/y425qndd13sg9ys06ggcw67h0000gn/T/RtmppTJJs0/4AKE.pdb exists.
Skipping download

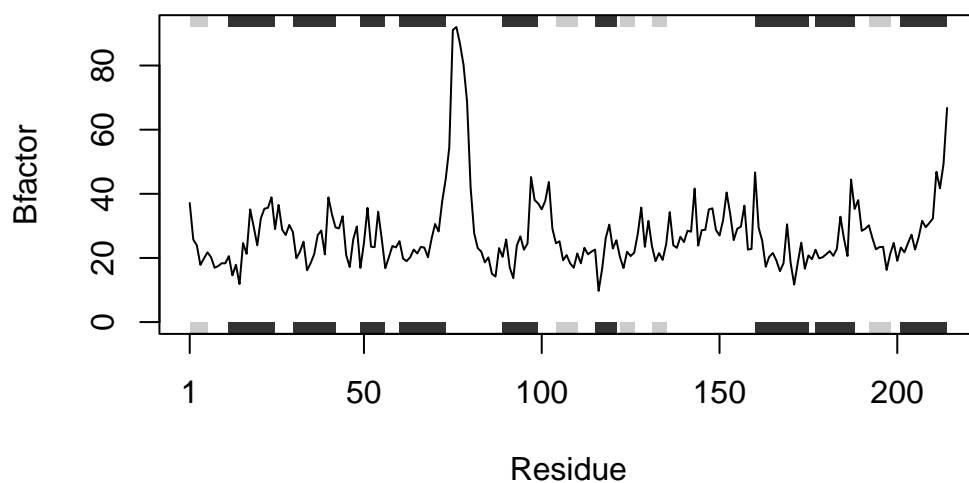


```
protein("1AKE")
```

Note: Accessing on-line PDB file

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):  
/var/folders/kw/y425qndd13sg9ys06ggcw67h0000gn/T//RtmppTJJs0/1AKE.pdb exists.  
Skipping download
```

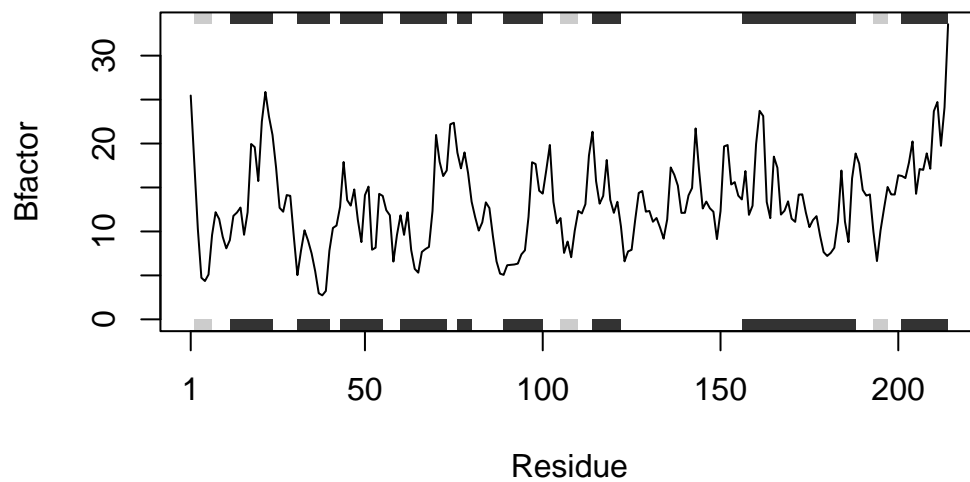
PDB has ALT records, taking A only, rm.alt=TRUE



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

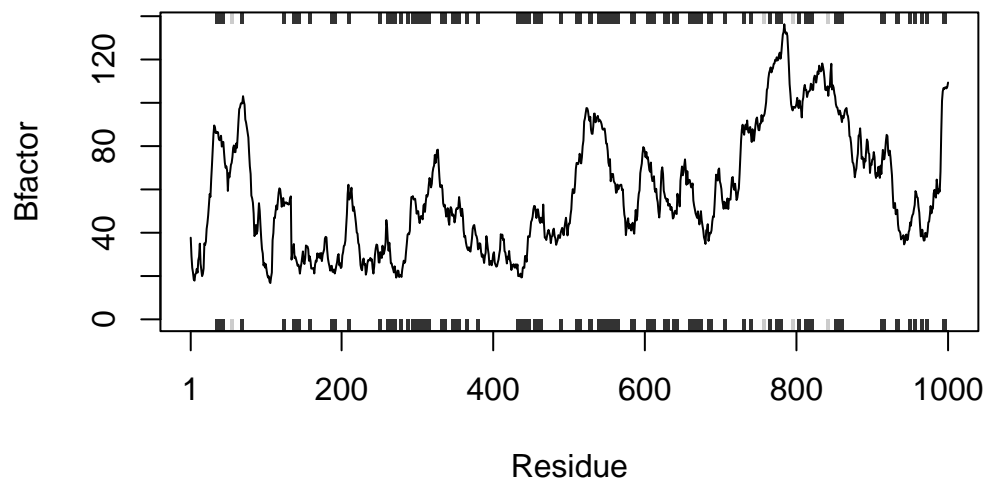
Note: Accessing on-line PDB file

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):  
/var/folders/kw/y425qndd13sg9ys06ggcw67h0000gn/T//RtmppTJJs0/1E4Y.pdb exists.  
Skipping download
```



```
# test a new accession code  
protein("6DRD")
```

Note: Accessing on-line PDB file



My function: `protein()`

Description: Analyzes protein drug interactions by reading in any protein PDB data and outputs a plot for the specified protein.

Usage: `protein("x")`, x = PDB accession code.