HW Class 6 (Q6 - Write a Function)

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Original Code:

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

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

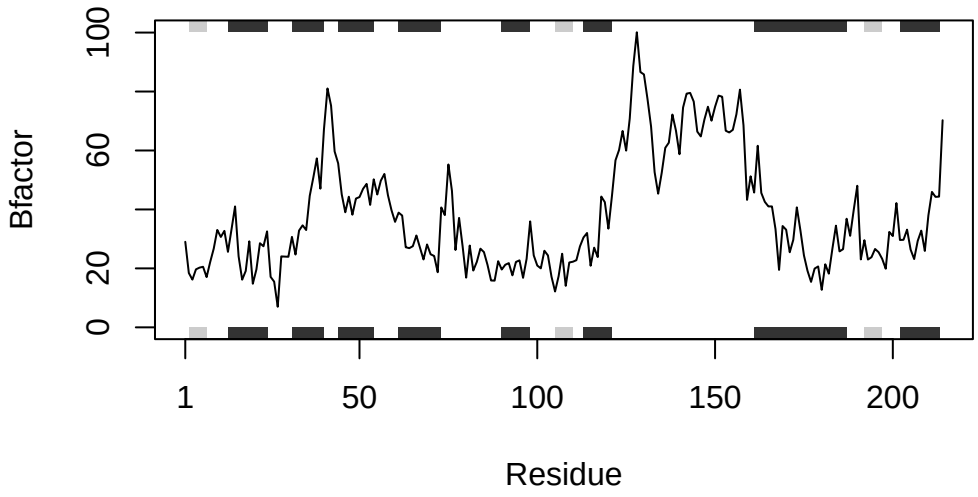
```
s2 <- read.pdb("1AKE")  # kinase no drug
```

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

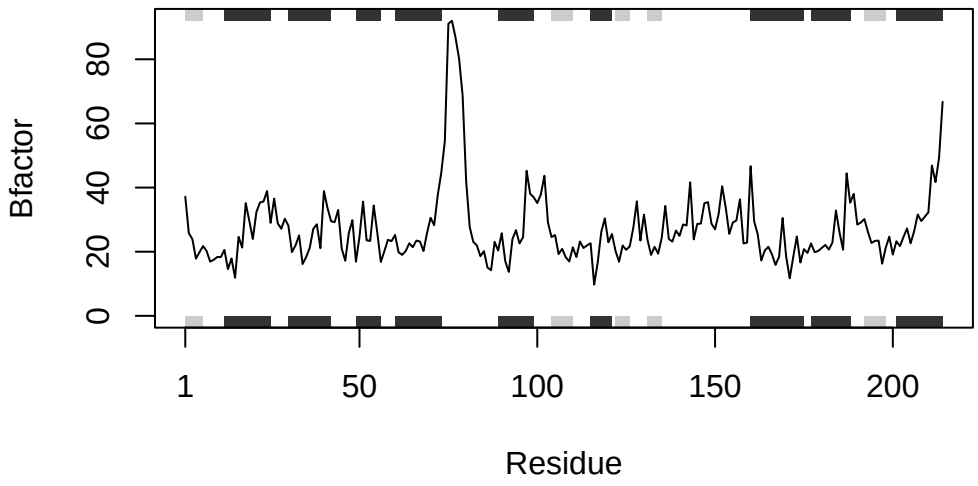
```
s3 <- read.pdb("1E4Y")  # kinase with drug
```

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

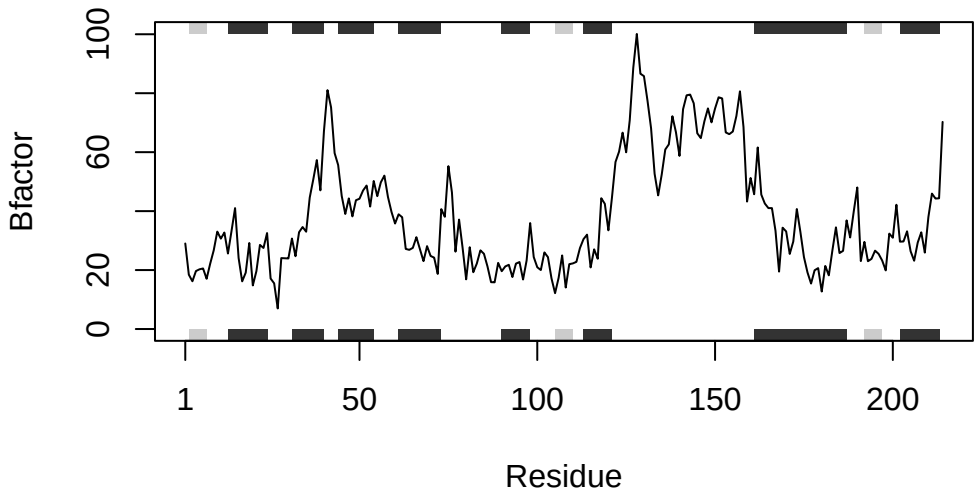
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```




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



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



Improved Code:

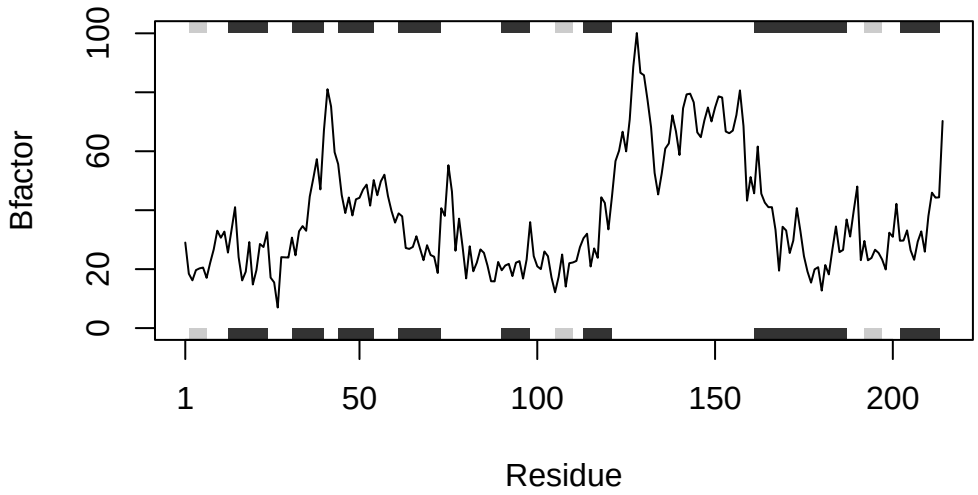
```
# Load bio3d
library(bio3d)

# Build function that takes PDB codes as strings for input
# This function will output b3 plots of the protein
new_function <- function(x) {
  y <- read.pdb(x)
  y.chainA <- trim.pdb(y, chain="A", elety="CA")
  y.b <- y.chainA$atom$b
  plotb3(y.b, sse=y.chainA, typ="l", ylab="Bfactor")
}

# Using sapply(), we can quickly generate all 3 plots
sapply(c("4AKE", "1AKE", "1E4Y"), new_function)
```

Note: Accessing on-line PDB file

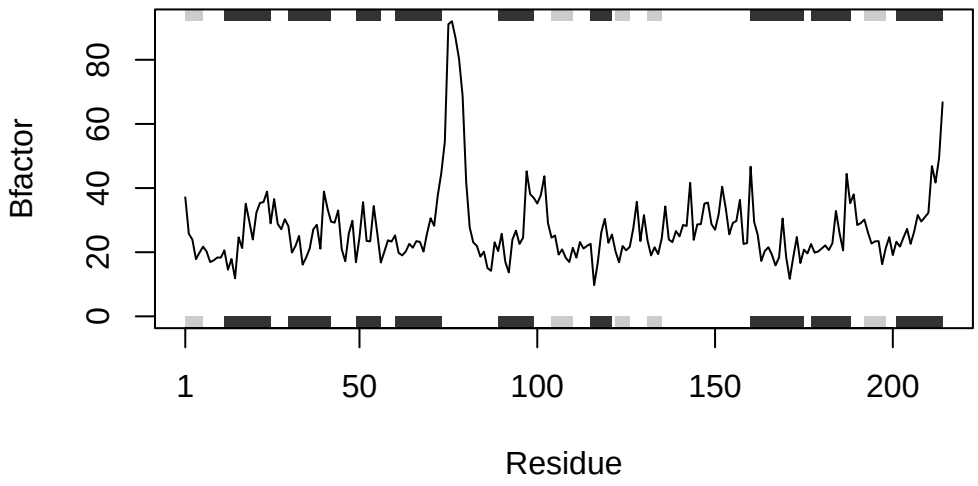
```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/d4/g6m2xsqs7kgd8953d7w3klc80000gn/T//RtmpUpM92g/4AKE.pdb exists.
Skipping download
```




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

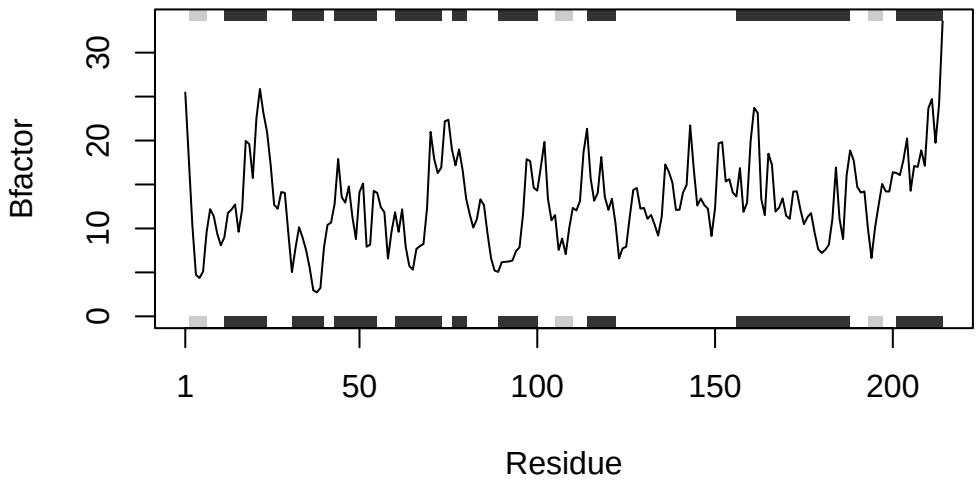
```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/d4/g6m2xsqs7kgd8953d7w3klc80000gn/T//RtmpUpM92g/1AKE.pdb exists.
Skipping download
```

```
   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/d4/g6m2xsqs7kgd8953d7w3klc80000gn/T//RtmpUpM92g/1E4Y.pdb exists.
Skipping download
```




```
$`4AKE`
NULL

$`1AKE`
NULL

$`1E4Y`
NULL
```

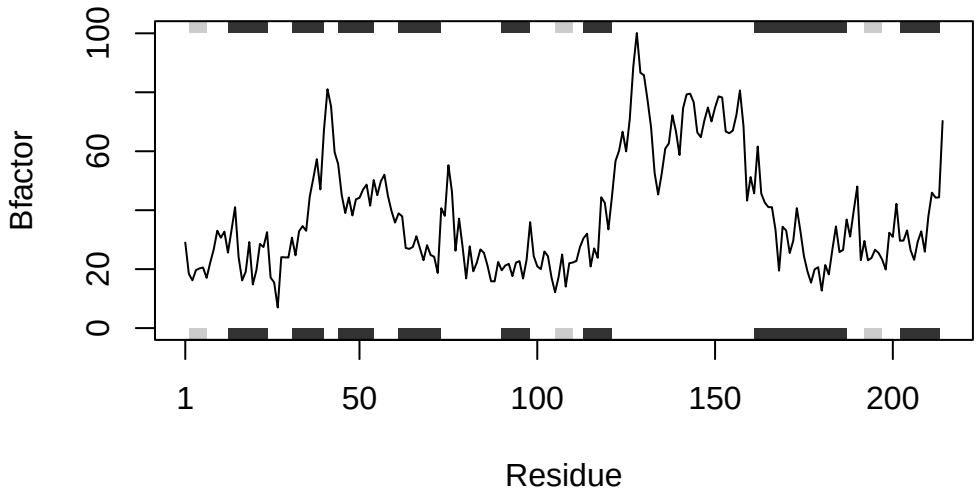
New Function Used in For-Loop:

```
# Create object of PDB codes
codes <- c("4AKE", "1AKE", "1E4Y")

for (i in codes) {
  new_function(i)
}
```

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

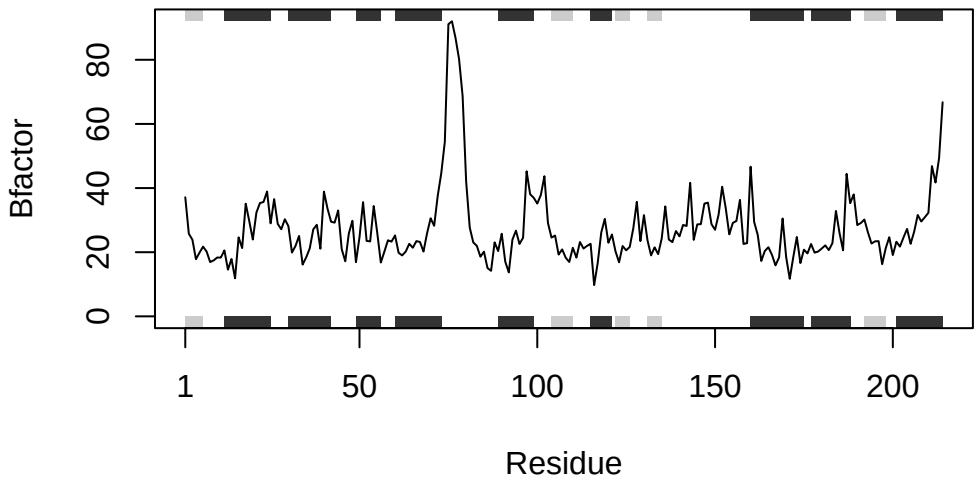
```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/d4/g6m2xsqs7kgd8953d7w3klc80000gn/T//RtmpUpM92g/4AKE.pdb exists.
Skipping download
```




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

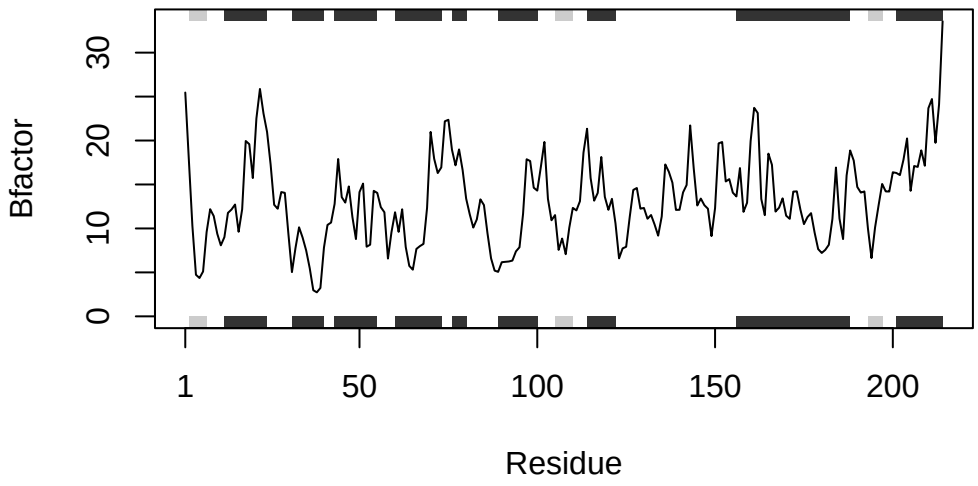
```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/d4/g6m2xsqs7kgd8953d7w3klc80000gn/T//RtmpUpM92g/1AKE.pdb exists.
Skipping download
```

```
   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/d4/g6m2xsqs7kgd8953d7w3klc80000gn/T//RtmpUpM92g/1E4Y.pdb exists.
Skipping download
```


Bfactor
0
10
20
30
1
50
100
150
200
Residue