HW Class 6 (R Functions) Question 6

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> Q6. How would you generalize the original code above to work with any set of input protein structures?

Get bio3d function

```
# install.packages('bio3d')
library(bio3d)
```

Description

Takes in a pdb file of a protein and creates a line plot of the Bfactor over residues while adding the secondary structure elements as marginal black and grey rectangles.

Arguments

x: a `character` object depicting the specific protein

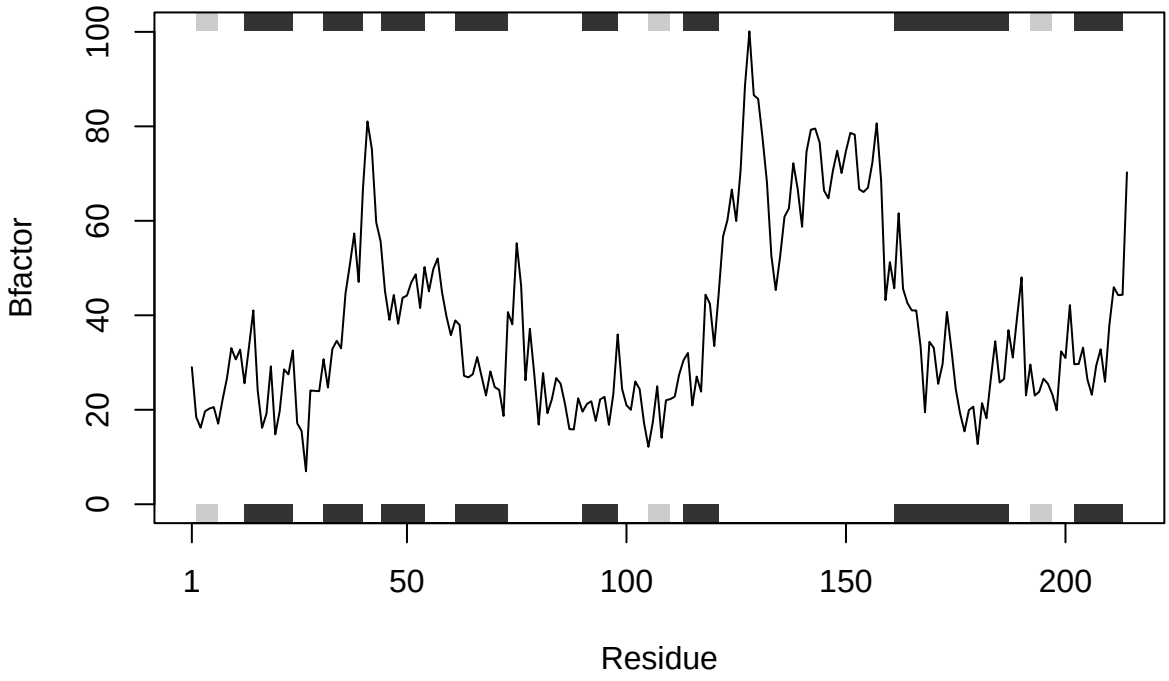
Function

```
plot_protein  <- function(x){

  # Reads the specific pdb file from the bio3d library
  s.x <- read.pdb(x)

  # Trims the read pdb file and extracts alpha carbon atoms from chain A
  s.x.chainA <- trim.pdb(s.x, chain="A", elety="CA")

  # Retrieves the B factor from the atom column
  s.x.b <- s.x.chainA$atom$b

  # Returns a plot of the new pdb file on a line graph based on Bfactor and includes the sse's taken fr
  plotb3(s.x.b, sse=s.x.chainA, typ='l', ylab='Bfactor')

}
```

Examples:

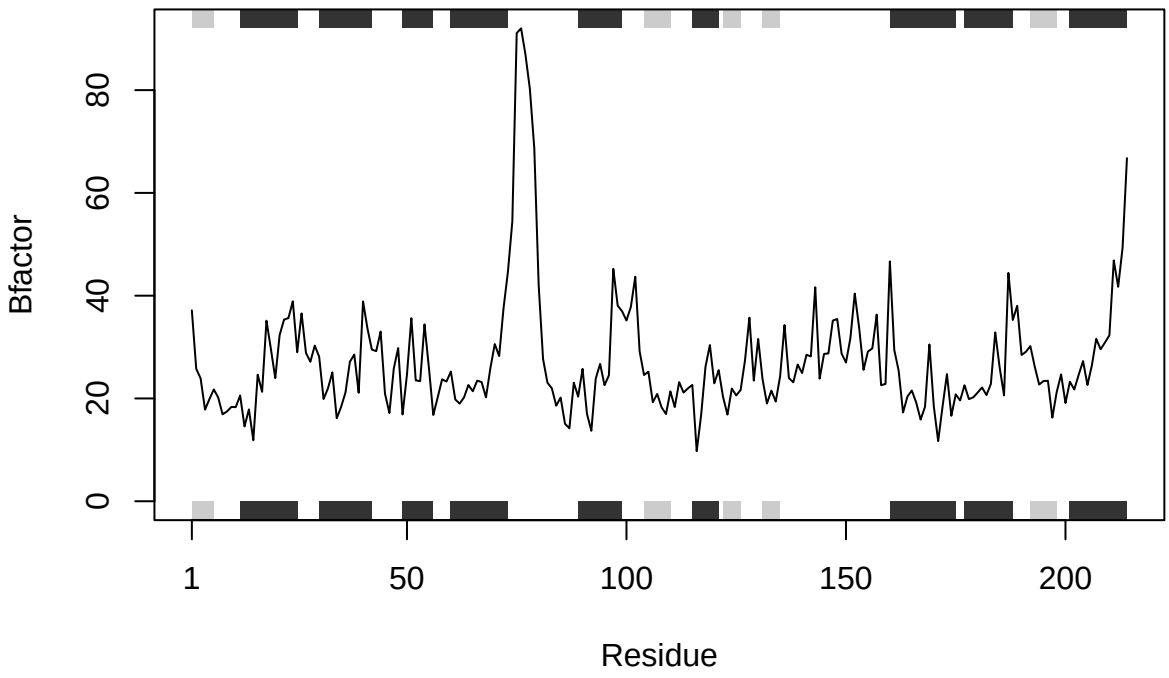
```
plot_protein('4AKE')
```

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



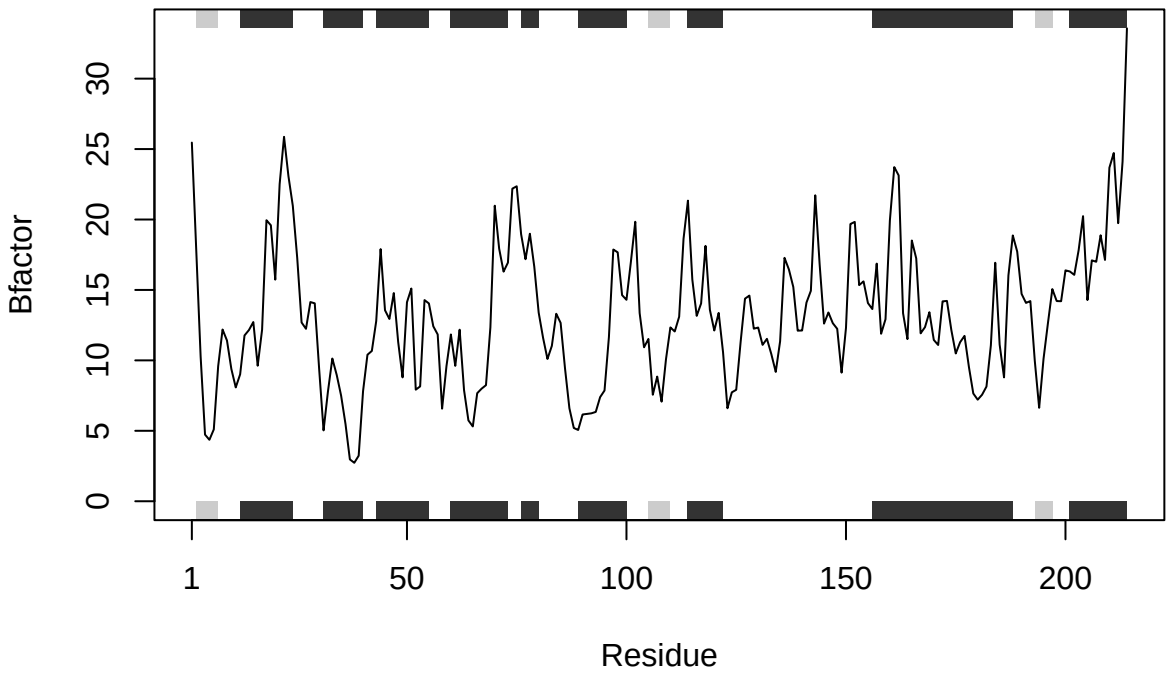

```
plot_protein('1AKE')
```

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




```
plot_protein('1E4Y')
```

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


Bfactor
0
5
10
15
20
25
30
1
50
100
150
200
Residue