HW Class 6

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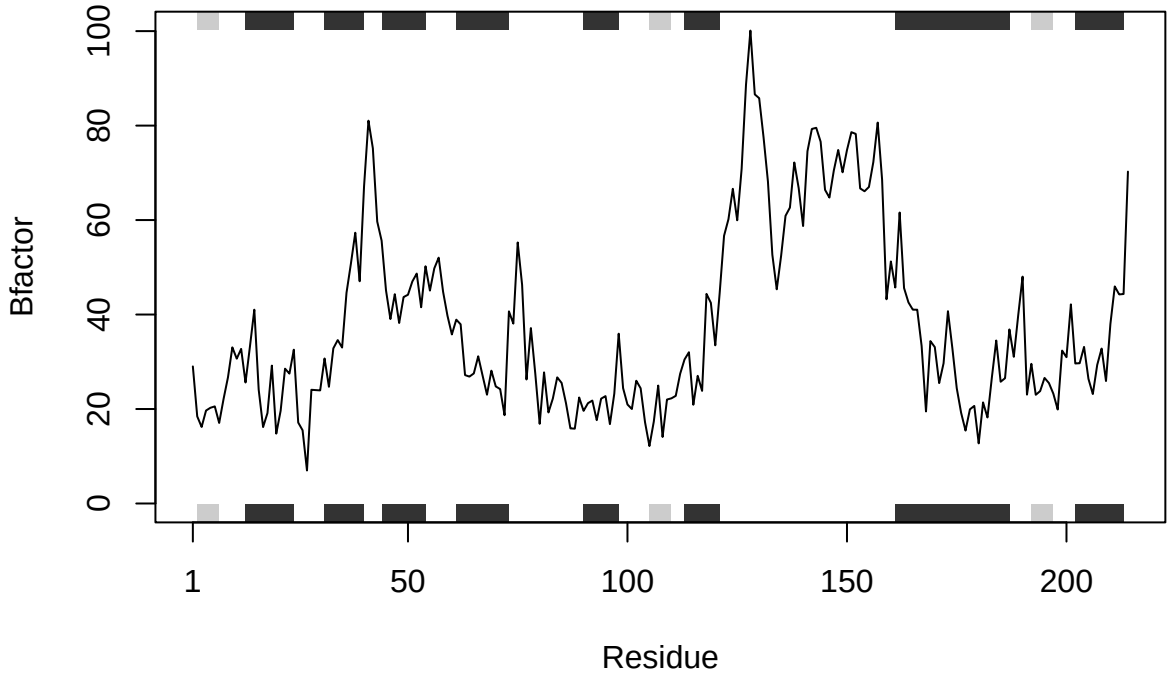
Q. How would you generalize the original code above to work with any set of input protein structures?

```
library(bio3d)
protein_drug_int <- function(x, y, z) {

s <- read.pdb(x)
s.chain <- trim.pdb(s, chain=y, elety=z)
s.b <- s.chain$atom$b
plotb3(s.b, sse=s.chain, typ="l", ylab="Bfactor")
}
```

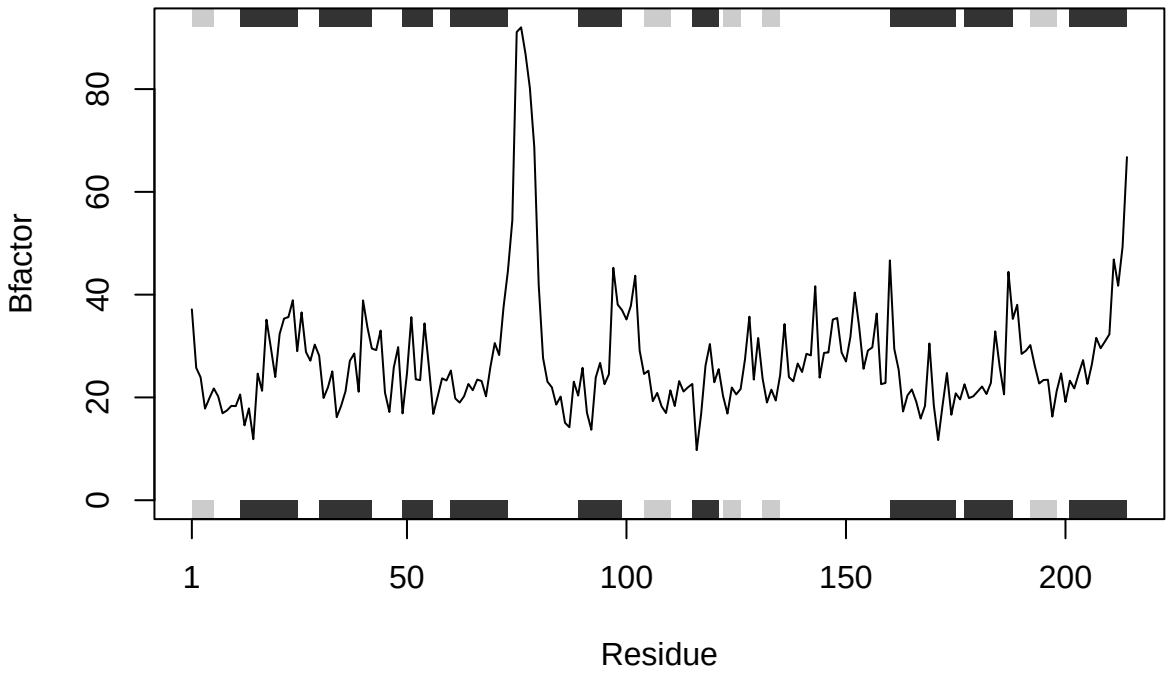
```
protein_drug_int("4AKE", 'A', 'CA')
```

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



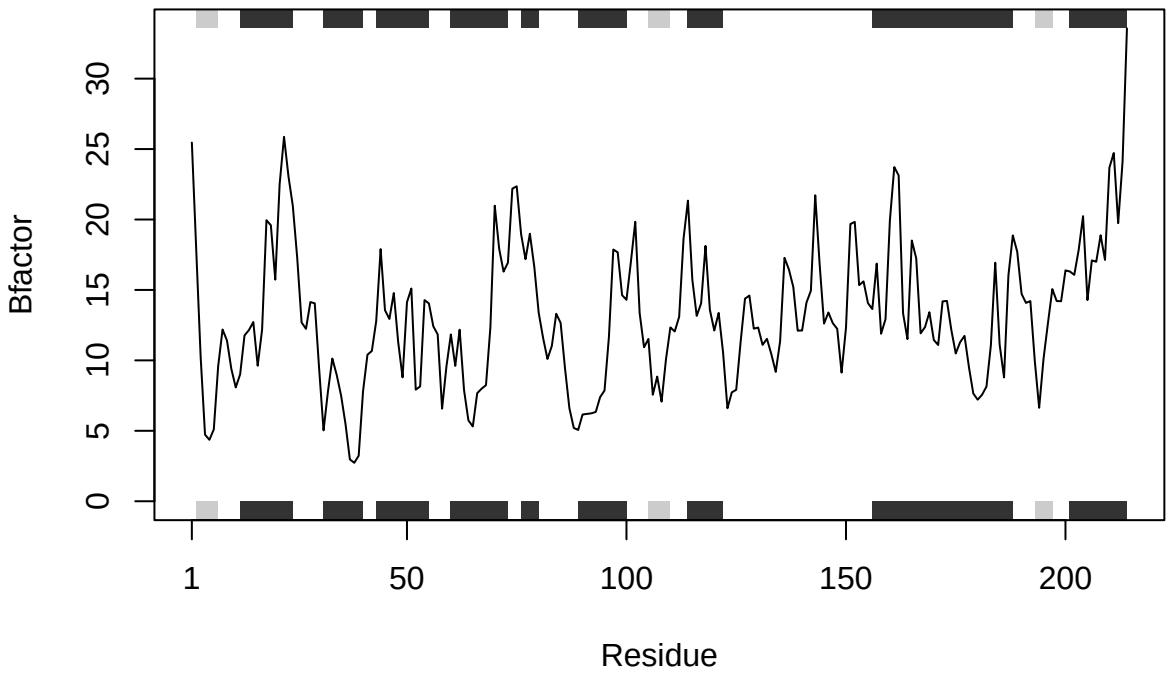
```
protein_drug_int("1AKE", 'A', 'CA')
```

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




```
protein_drug_int("1E4Y", 'A', 'CA')
```

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



The inputs to this function is the PDB file that corresponds to a respective protein structure, the specific protein chain of the protein that was read, and the element type of the PDB structure.

The function will read the PDB file that correlates with a specific protein structure, provide a subset from the PDB file that was read (specific to the chain and element type), and retrieves the B factor of the atoms from the chain.

The output of the function is a plot that demonstrates the relationship between Bfactor and residue for a specific protein structure.