

# HW Class 6 (R Functions)

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```
# Can you improve this analysis 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

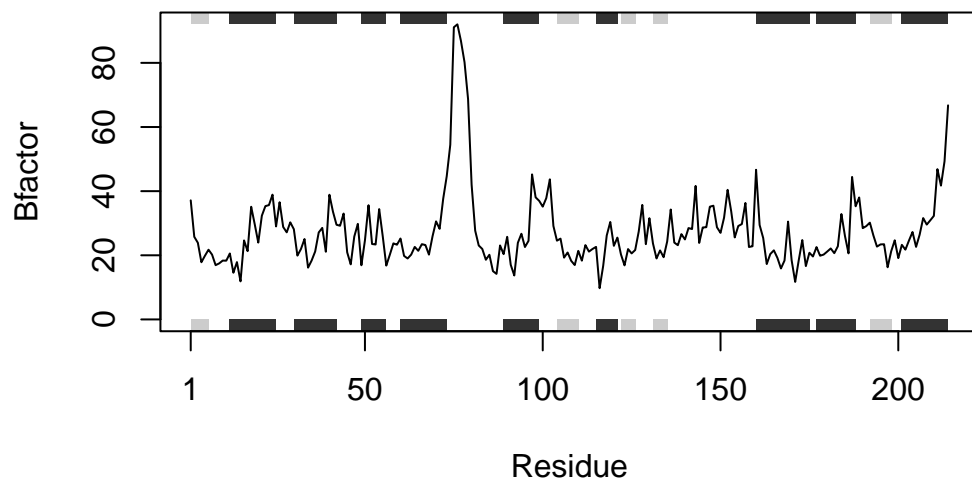
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

Note: Accessing on-line PDB file

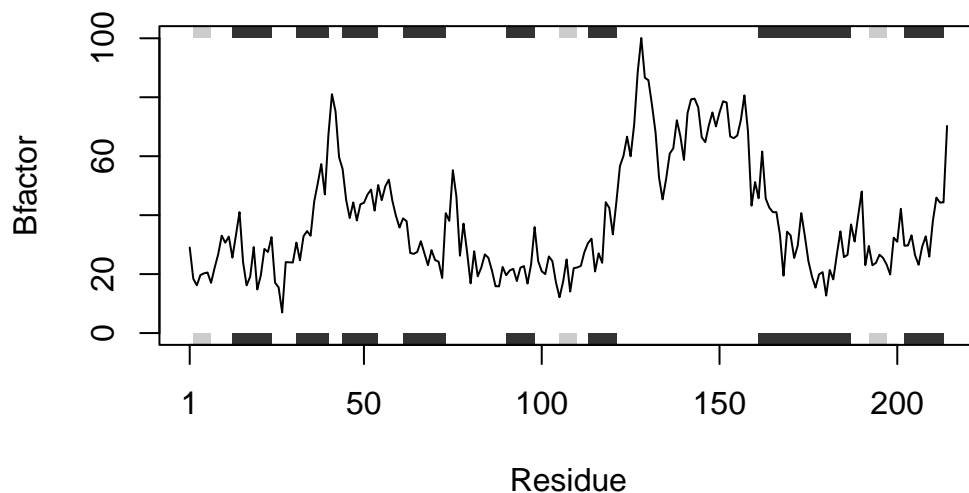
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")  
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")  
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")  
s1.b <- s1.chainA$atom$b  
s2.b <- s2.chainA$atom$b  
s3.b <- s3.chainA$atom$b  
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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



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



Let's write a function that accepts the PDB identifier as an argument and returns Bfactor vs. Residue plots:

```
prot_analysis <- function(x) {

  #load the protein data as a PDB object
  s <- read.pdb(x)

  #produce a PDB object only containing chain A data
  chain <- trim.pdb(s, chain="A", eley="CA")

  #plot each atom's Bfactor
  plotb3(chain$atom$b, sse=chain, typ="l", ylab="Bfactor")

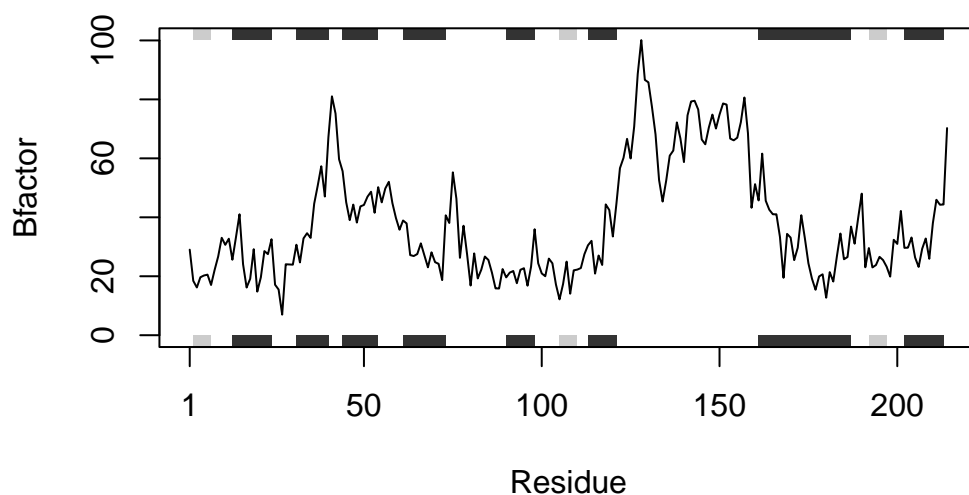
}
```

And use it to do the analysis

```
library(bio3d) #load the bio3d package
prot_analysis("4AKE") # kinase with drug
```

Note: Accessing on-line PDB file

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

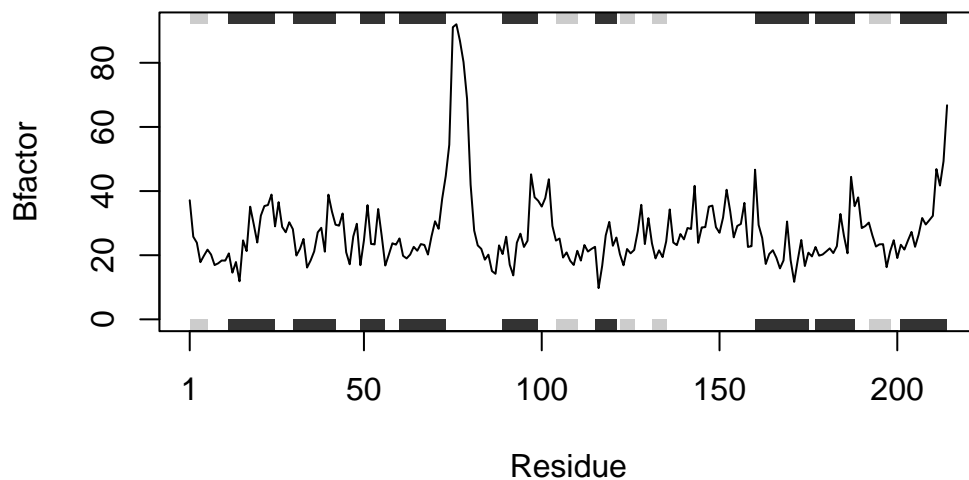


```
prot_analysis("1AKE") # kinase no drug
```

Note: Accessing on-line PDB file

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

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



```
prot_analysis("1E4Y") # kinase with drug
```

Note: Accessing on-line PDB file

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

