

R-Functions-HW

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```
library(bio3d)
# Can you improve this analysis code? library(bio3d)
#including protein names
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

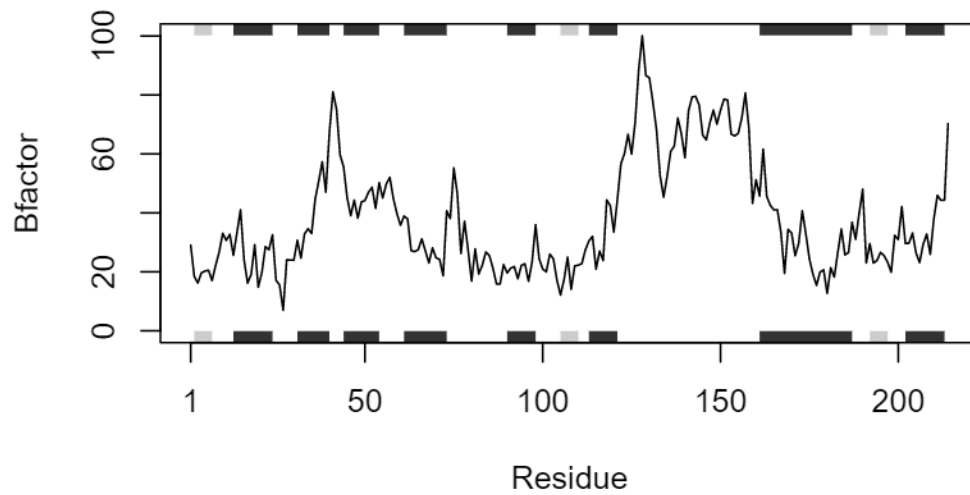
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

Note: Accessing on-line PDB file

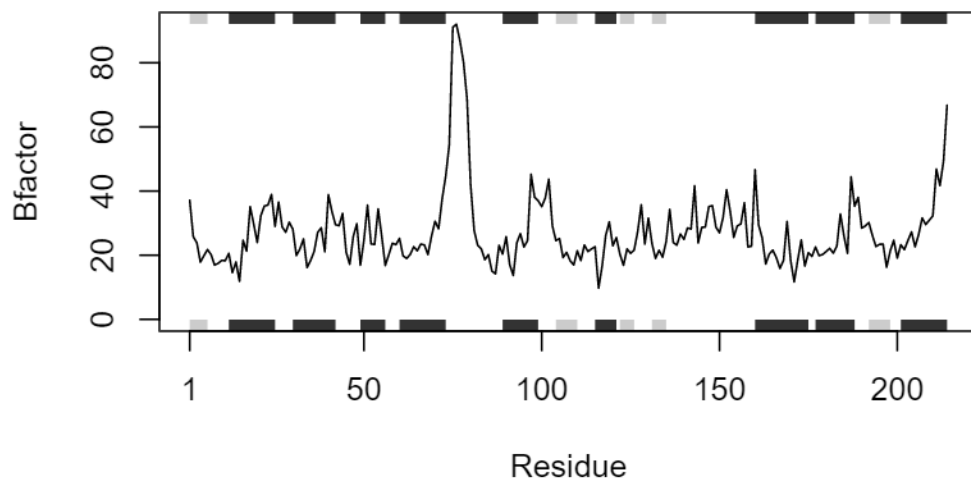
```
#extracting the A chain from each protein
s1.chainA <- trim.pdb(s1, chain="A", eley="CA")
s2.chainA <- trim.pdb(s2, chain="A", eley="CA")
s3.chainA <- trim.pdb(s1, chain="A", eley="CA")

#extracting atom b from the A chain
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
```

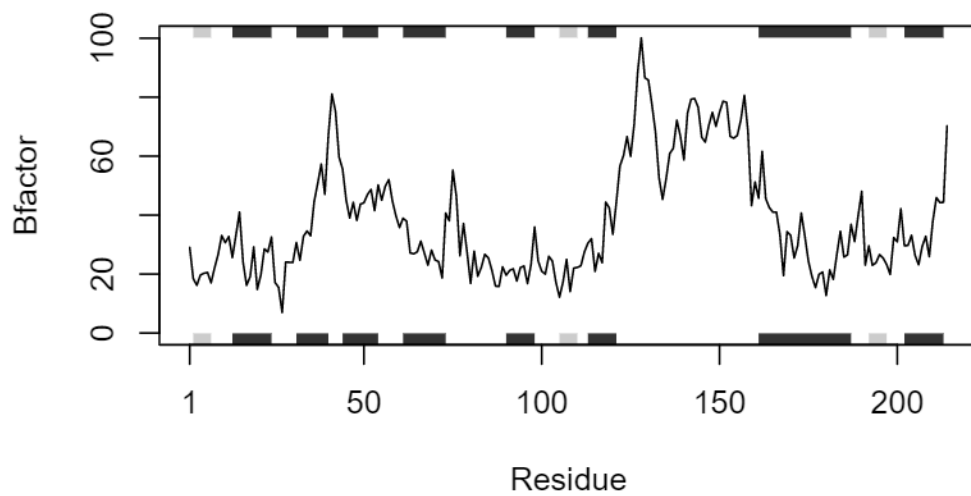
```
#plotting b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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



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



```

library(bio3d)
pdbplot <- function(x) {
  #read the pdb files
  x <- read.pdb(x)

  #extracting the A chain
  x_chainA <- trim.pdb(x, chain="A", elety="CA")

  #Extract the b atom
  x_b <- x_chainA$atom$b

  #plotting b #ylab means ylabel
  plotb3(x_b, sse=x_chainA, typ="l", ylab="Bfactor")
}

```

#This will work with any PDB ID #pdbplot("PDBID")