

Class6

Mudit

```
#Input: function takes the PDB ID character sequence as an input
#function plots chain A flexibility of the protein (whose pdb ID is given as an argument).
#output: It plots the B-factor vs residue position
```

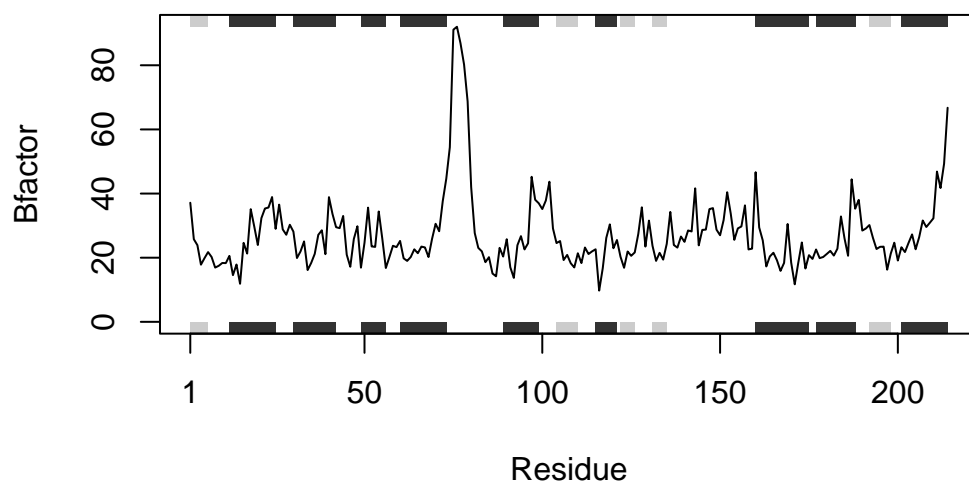
```
func_x <- function(pdbID){
  #calling the bio3d library
  library(bio3d)
  # Reading the pdb ID and assigning it to object 's'
  s <- read.pdb(pdbID)
  #trims the structure and include chain A's alpha carbon atoms
  s.chainA <- trim.pdb(s, chain="A", elety="CA")
  #extracts the B-factors from the trimmed structure
  s.b <- s.chainA$atom$b
  #plotting secondary structure elements against b factors
  plotb3(s.b, sse=s.chainA, typ="l", ylab="Bfactor")
}
```

```
#| warning: false
#vector of pdbIDs
seq_vec <- c("4AKE", "1AKE", "1E4Y")
#looping over
sapply(seq_vec, func_x)
```

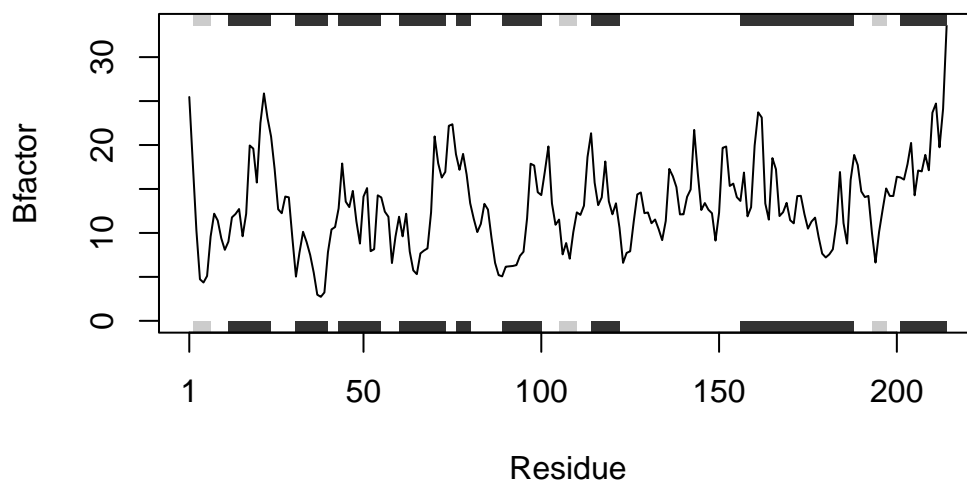
Note: Accessing on-line PDB file



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



Note: Accessing on-line PDB file



```
$`4AKE`
```

```
NULL
```

```
$`1AKE`
```

```
NULL
```

```
$`1E4Y`
```

```
NULL
```

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

Note: Accessing on-line PDB file

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):  
/var/folders/pq/n_hbs121309bf8n2d4n71v100000gn/T//RtmpQgkve/4AKE.pdb exists.  
Skipping download
```

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

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/pq/n_hbs121309bf8n2d4n71v100000gn/T//RtmppQgkve/1AKE.pdb exists.
Skipping download

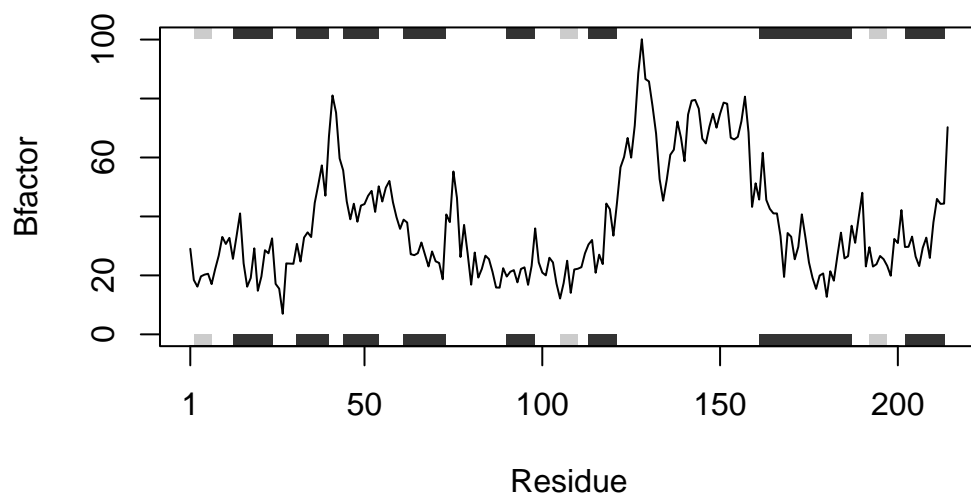
PDB has ALT records, taking A only, rm.alt=TRUE

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

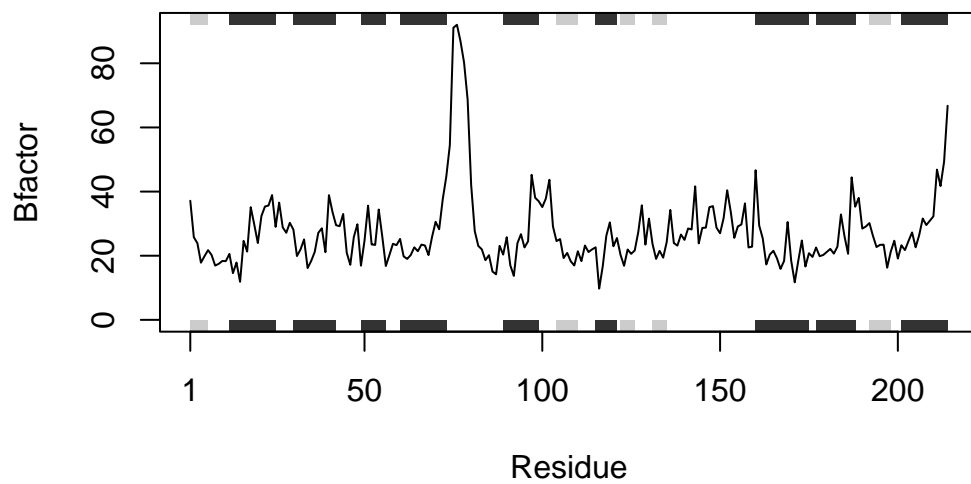
Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/pq/n_hbs121309bf8n2d4n71v100000gn/T//RtmppQgkve/1E4Y.pdb exists.
Skipping download

```
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")
```

