

Class06Q6

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10/23/2021

```
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

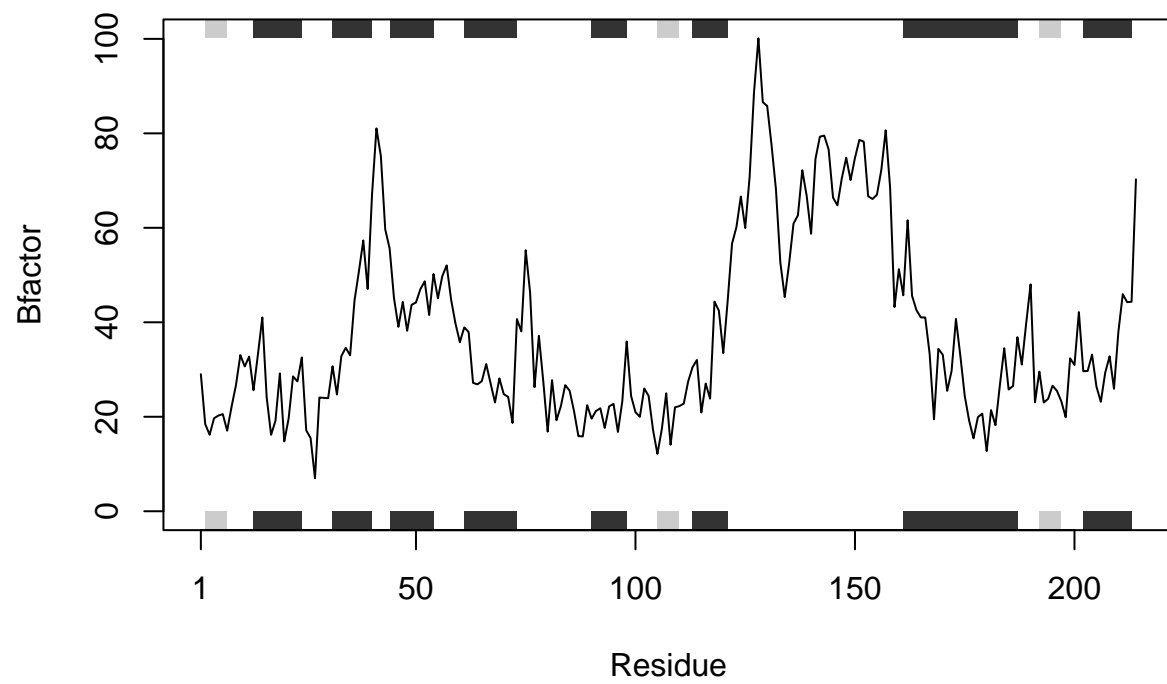
s3 <- read.pdb("1E4Y") # kinase with drug

## 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(s3, chain="A", elety="CA")

s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b

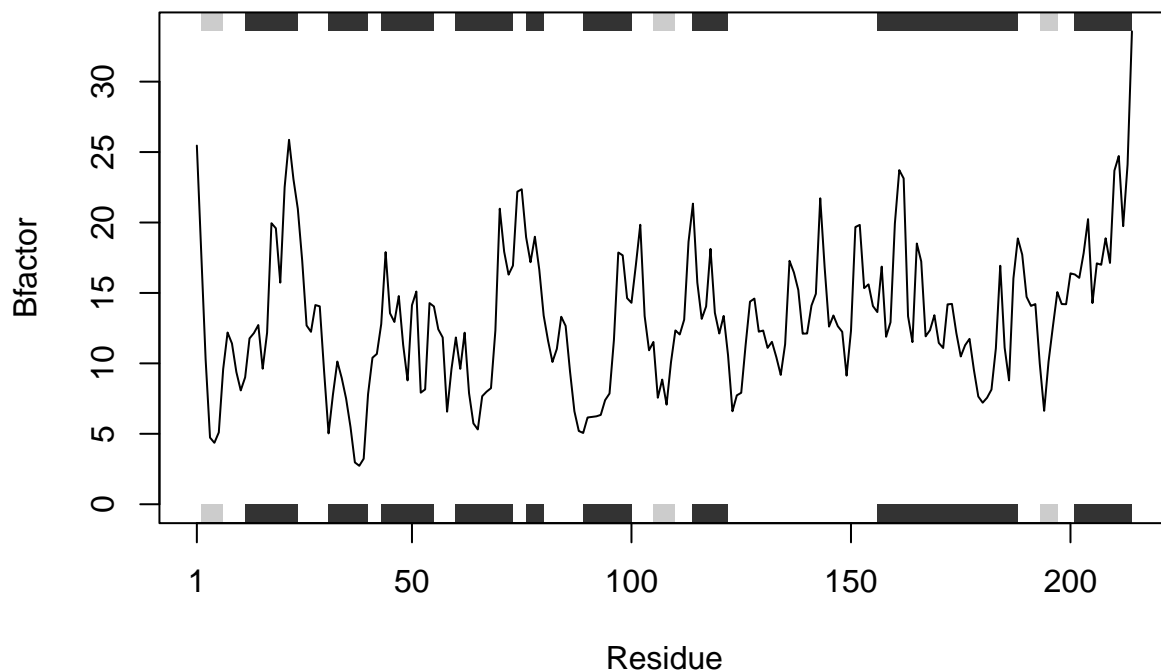
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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



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



A PDB file can be input in this function. This function first reads a PDB file and assigns it to a variable. Then, the PDB file is made into a smaller PDB object using `trim.pdb()` and assigned to a variable. Finally, the PDB file and previous variable that was assigned the smaller PDB object is input in `plotb3()` to create a plot. To use the function, you must write `make.a.b3.plot()` and input the variable containing the desired PDB file and add a `.b` at the end. # The output of the function is a line plot that contains secondary structure on the borders (top and bottom horizontal lines) of the graph.

```
make.a.b3.plot <- function(pdb, sse, typ, ylab) {
  s1 <- read.pdb("4AKE")
  s2 <- read.pdb("1AKE")
  s3 <- read.pdb("1E4Y")
  pdb.chainA <- trim.pdb(s1, chain="A", eley="CA")
  plotb3(pdb, sse=pdb.chainA, typ="l", ylab="Bfactor")
}
make.a.b3.plot(s1.b)
```

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

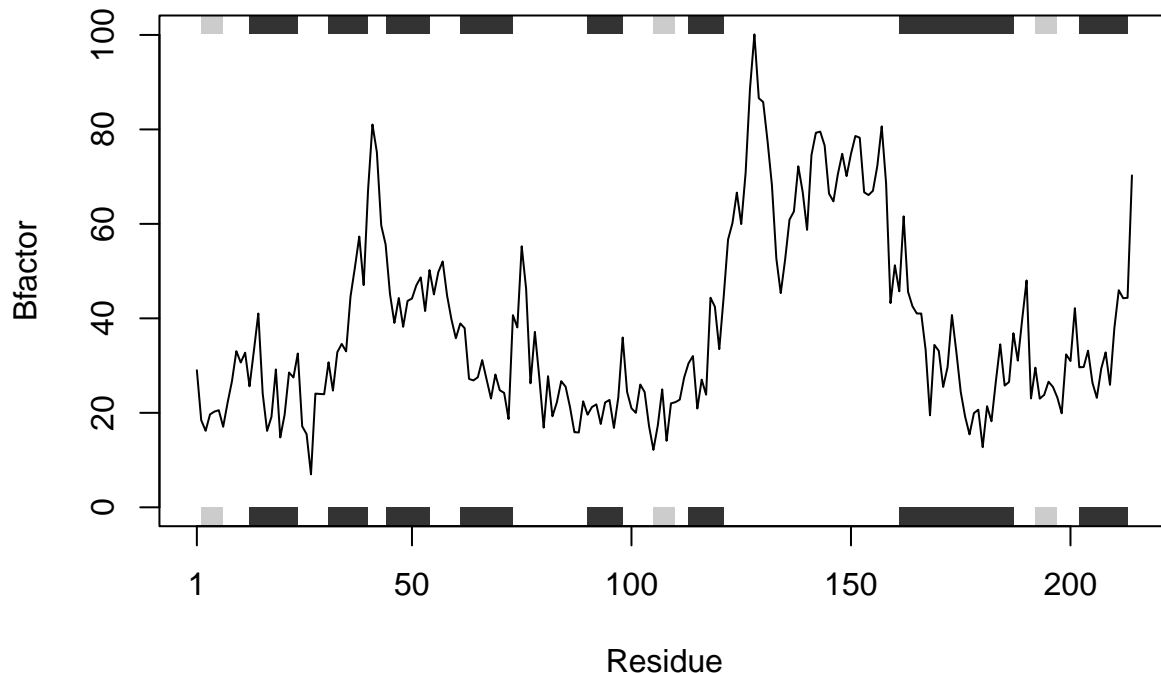
```
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/g7/
## wmlp_g173xghzg59nx8bg6w0000gn/T//RtmpU13xIY/4AKE.pdb exists. Skipping download
```

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

```
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/g7/
## wmlp_g173xghzg59nx8bg6w0000gn/T//RtmpU13xIY/1AKE.pdb exists. Skipping download
```

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

## Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/g7/
## wmlp_g173xghzg59nx8bg6w0000gn/T//RtmpU13xIY/1E4Y.pdb exists. Skipping download
```



```
make.a.b3.plot(s2.b)
```

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

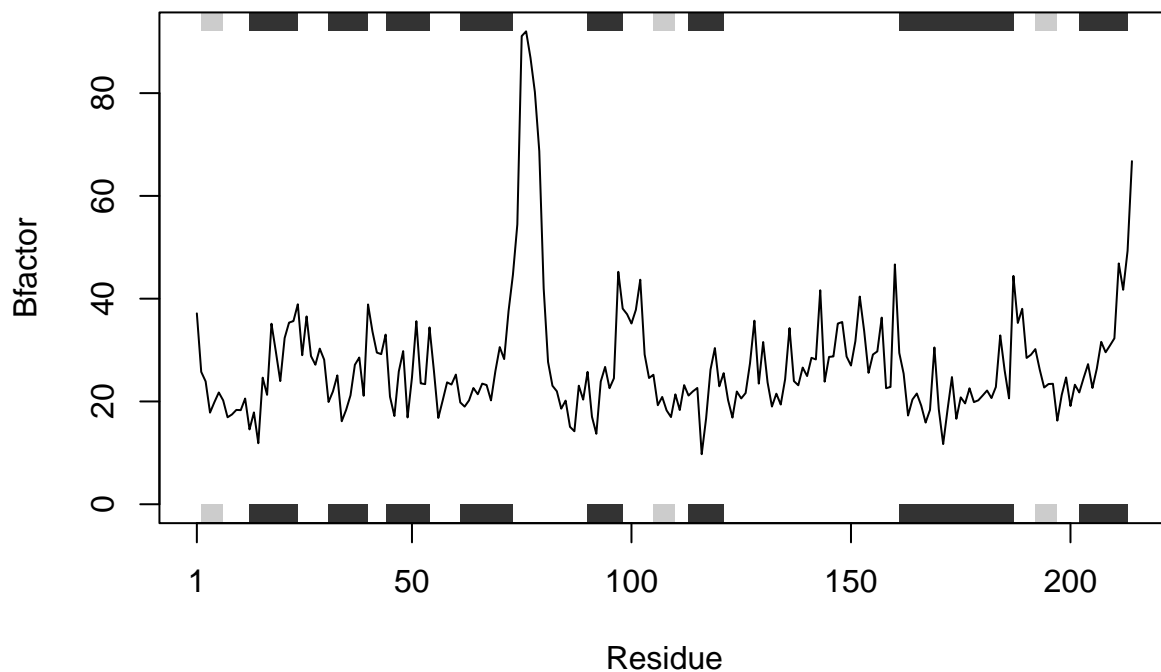
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/g7/
## wmlp_g173xghzg59nx8bg6w0000gn/T//RtmpU13xIY/4AKE.pdb exists. Skipping download

## Note: Accessing on-line PDB file

## Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/g7/
## wmlp_g173xghzg59nx8bg6w0000gn/T//RtmpU13xIY/1AKE.pdb exists. Skipping download

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

## Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/g7/
## wmlp_g173xghzg59nx8bg6w0000gn/T//RtmpU13xIY/1E4Y.pdb exists. Skipping download
```



```
make.a.b3.plot(s3.b)
```

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

```
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/g7/
## wmm1p_g173xghzg59nx8bg6w0000gn/T//RtmpU13xIY/4AKE.pdb exists. Skipping download
```

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

```
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/g7/
## wmm1p_g173xghzg59nx8bg6w0000gn/T//RtmpU13xIY/1AKE.pdb exists. Skipping download
```

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

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

```
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/g7/
## wmm1p_g173xghzg59nx8bg6w0000gn/T//RtmpU13xIY/1E4Y.pdb exists. Skipping download
```

