

HW Class 06

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```
library(bio3d)
s1 <- read.pdb("4AKE") # kinase with drug
```

Note: Accessing on-line PDB file

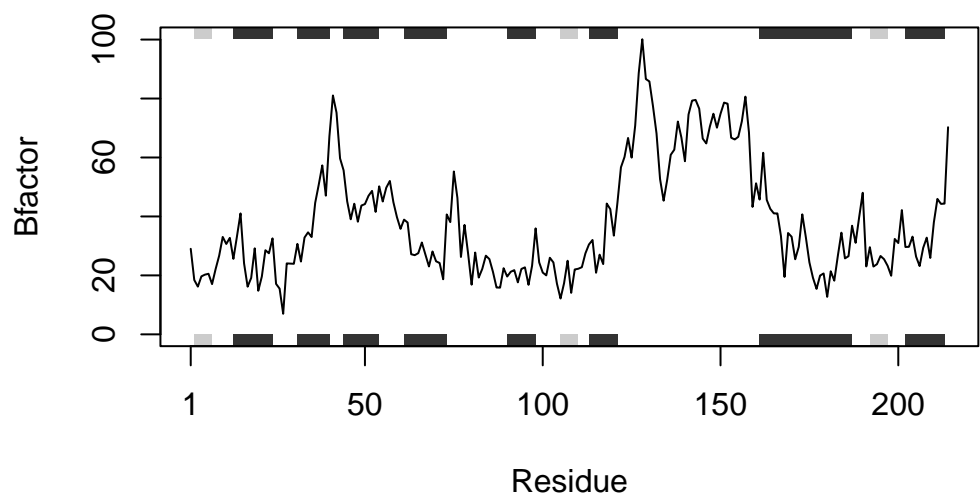
```
s2 <- read.pdb("1AKE") # kinase no drug
```

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

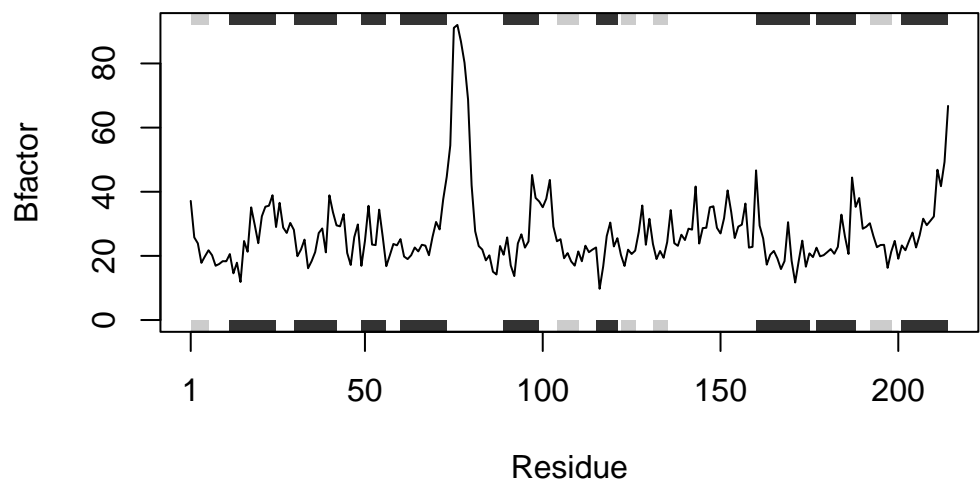
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

Note: Accessing on-line PDB file

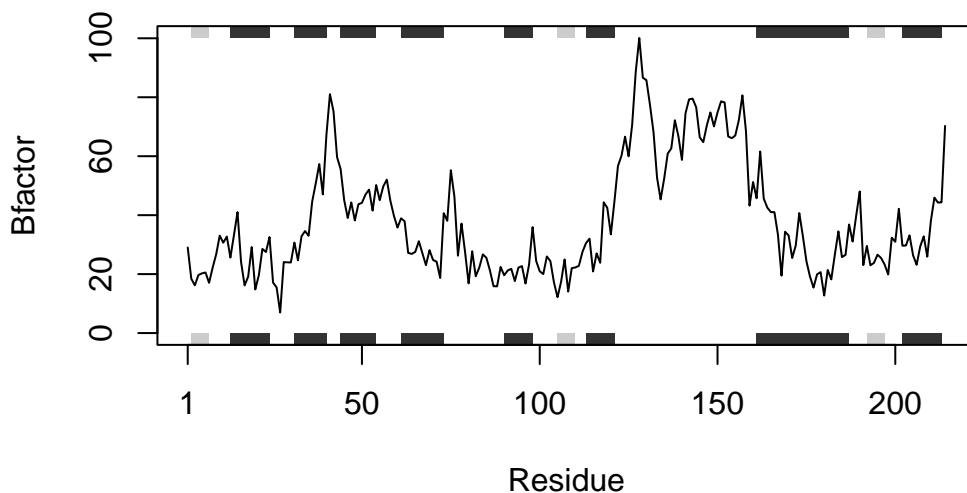
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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



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



```
prot_drug_plot <- function(file, chain, elmnt, fctr)
#the prot_drug_plot function sets parameters and applies them to each set of data. It the
s1 <- read.pdb("4AKE") # kinase with drug
s2 <- read.pdb("1AKE") # kinase no drug
```

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/2p/bdscffkd58n94sw6ccdsy6t80000gn/T//RtmpxQjncb/1AKE.pdb exists. Skipping download

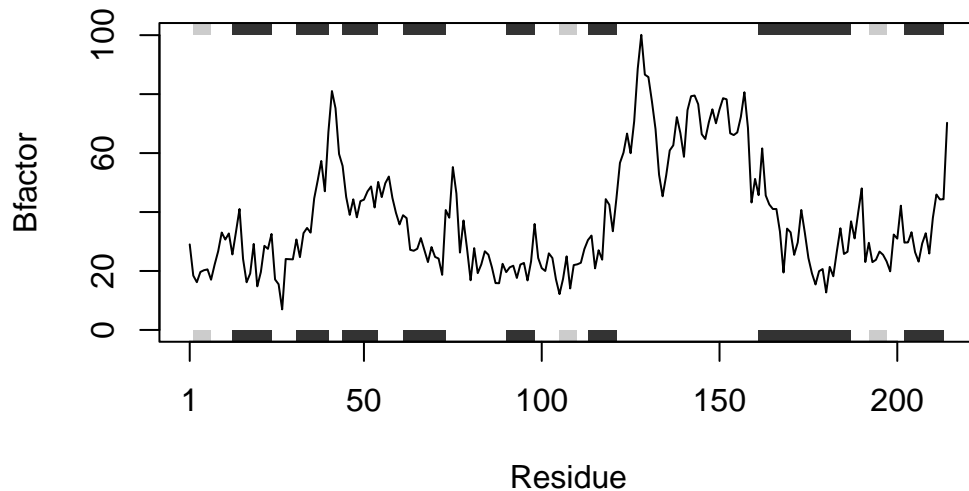
PDB has ALT records, taking A only, rm.alt=TRUE

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

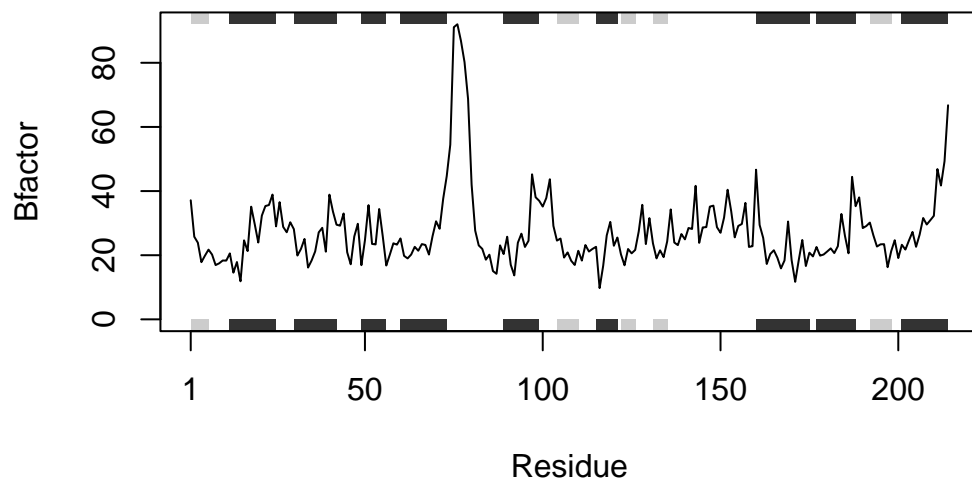
Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/2p/bdscffkd58n94sw6ccdsy6t80000gn/T//RtmpxQjncb/1E4Y.pdb exists. Skipping download

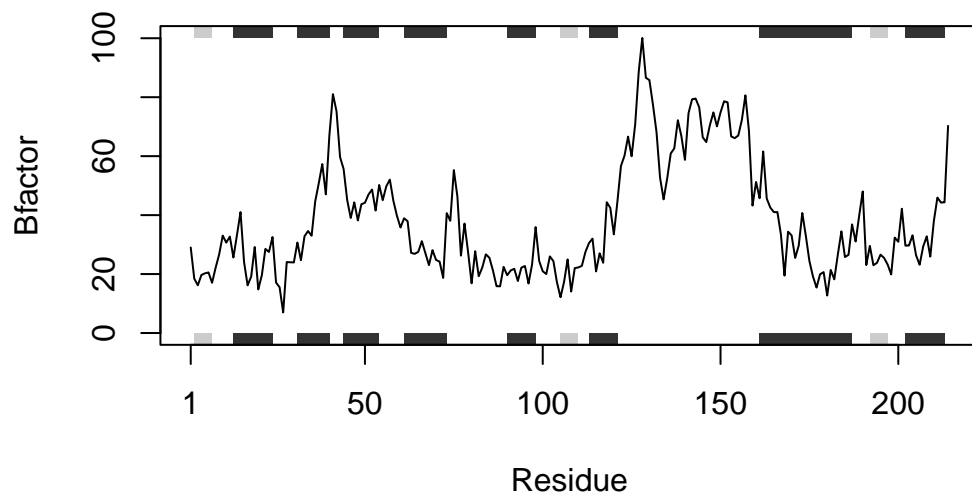
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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



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



```
prot_drug_plot(c("4AKE", "1AKE", "1E4Y"), "A", "CA", "b")
```

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose =
FALSE): /var/folders/2p/bdscffkd58n94sw6ccdsy6t80000gn/T//RtmpxQjncb/4AKE.pdb
exists. Skipping download