

HWFunction

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Simplier function for similar repetitive units

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

Note: Accessing on-line PDB file

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

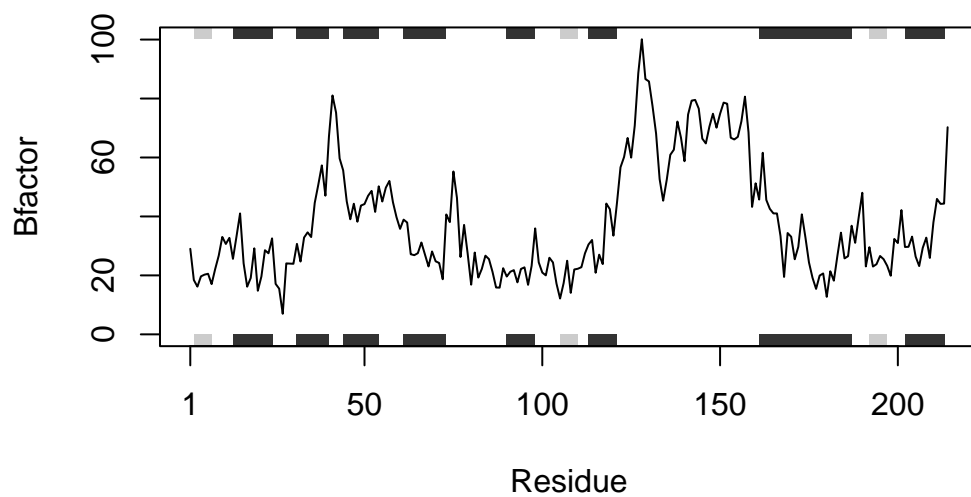
Note: Accessing on-line PDB file

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

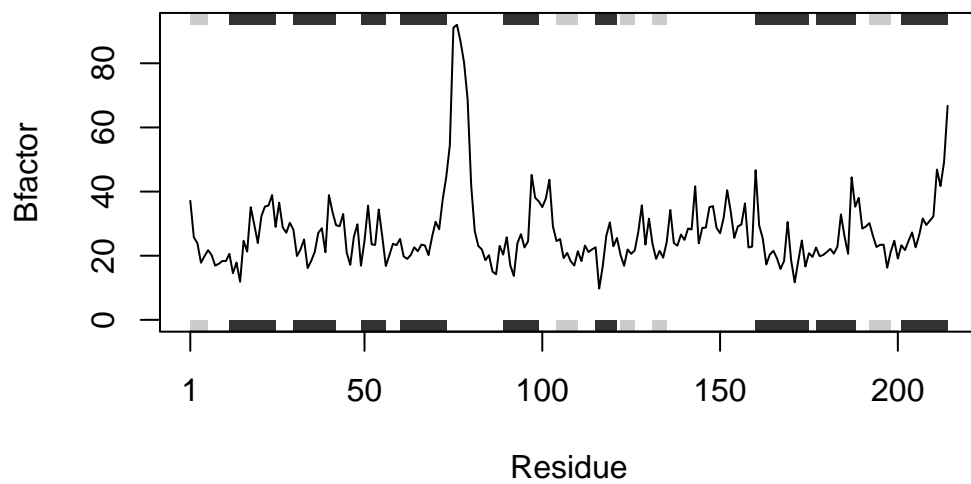
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

Note: Accessing on-line PDB file

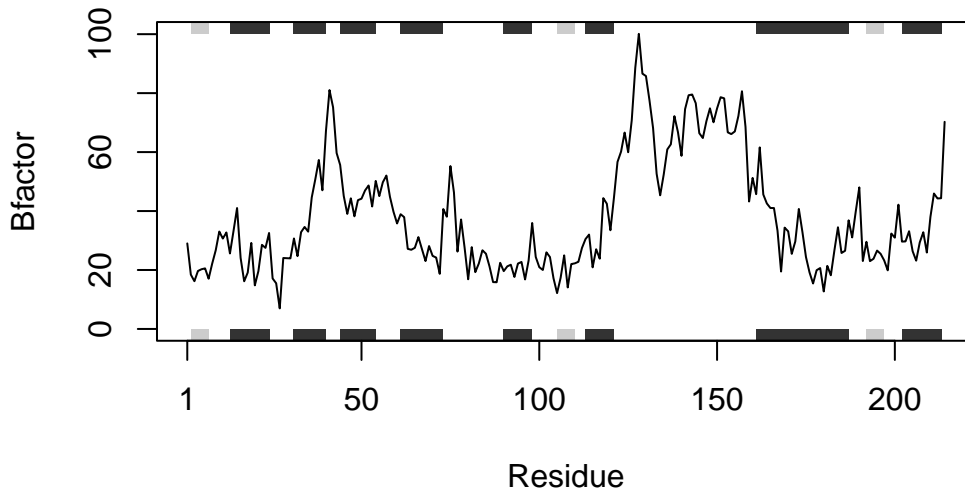
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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



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



```
#Generating a general function for repetitive sequences
mypdb <- function(x) {
  spdb <- read.pdb(x)
  #Generating function called mypdbchain
  mypdbchain <- trim.pdb(spdb, chain="A", elety="CA")

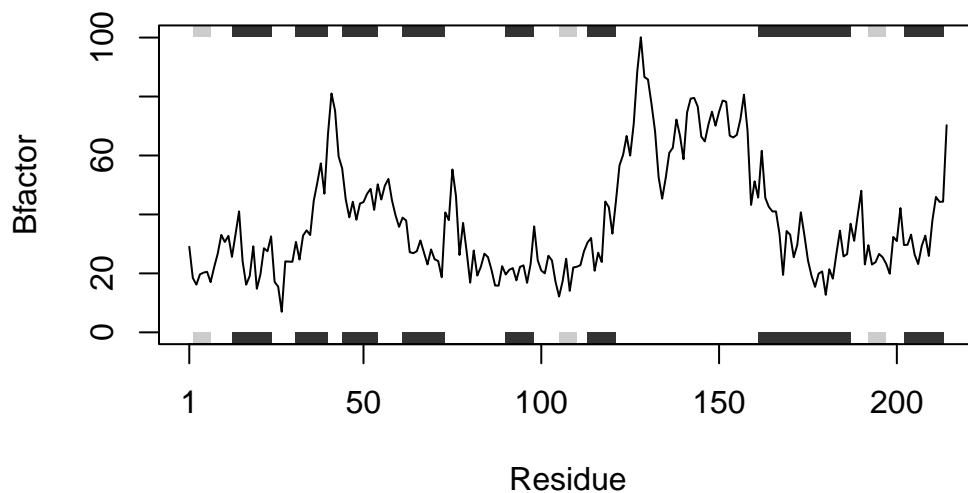
  #Generating a function called chainatoms
  chainatoms <- mypdbchain$atom$b

  plotb3(chainatoms, sse=mypdbchain, typ="l", ylab="Bfactor")
}
```

```
#Running Function
mypdb("4AKE")
```

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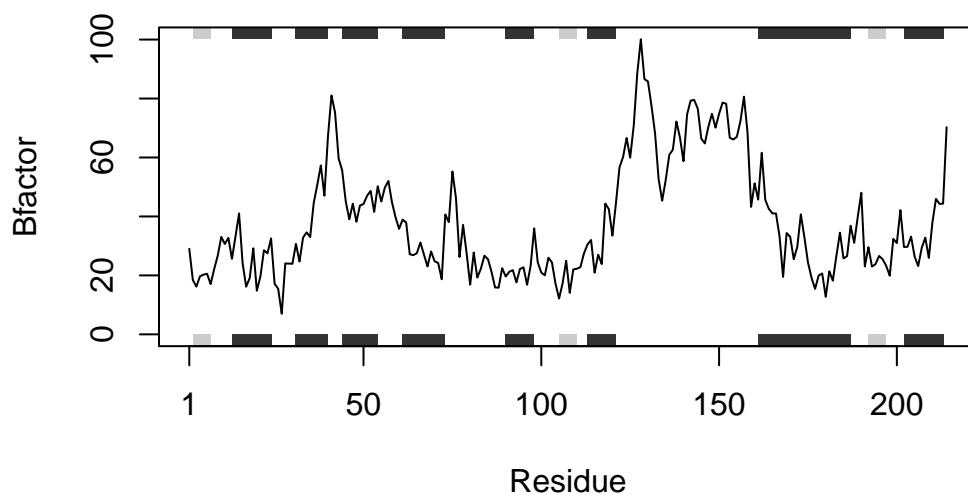
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
 /var/folders/sy/_fr9v5r51nxc7bzp4h_683nh0000gn/T/Rtmp16T3K6/4AKE.pdb exists.
 Skipping download



```
#Generating Multiple plots  
sapply (c("4AKE", "1AKE", "1E4Y"), mypdb)
```

Note: Accessing on-line PDB file

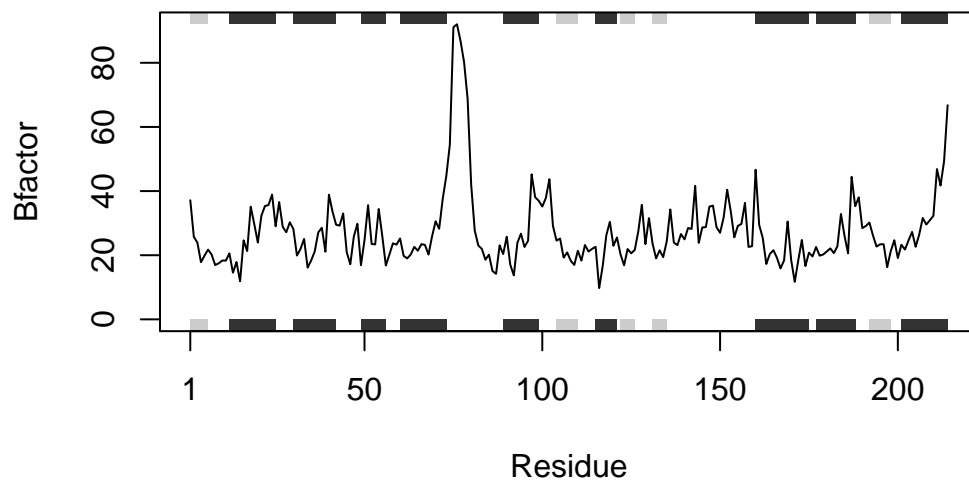
```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):  
/var/folders/sy/_fr9v5r51nxc7bzp4h_683nh0000gn/T/Rtmp16T3K6/4AKE.pdb exists.  
Skipping download
```



Note: Accessing on-line PDB file

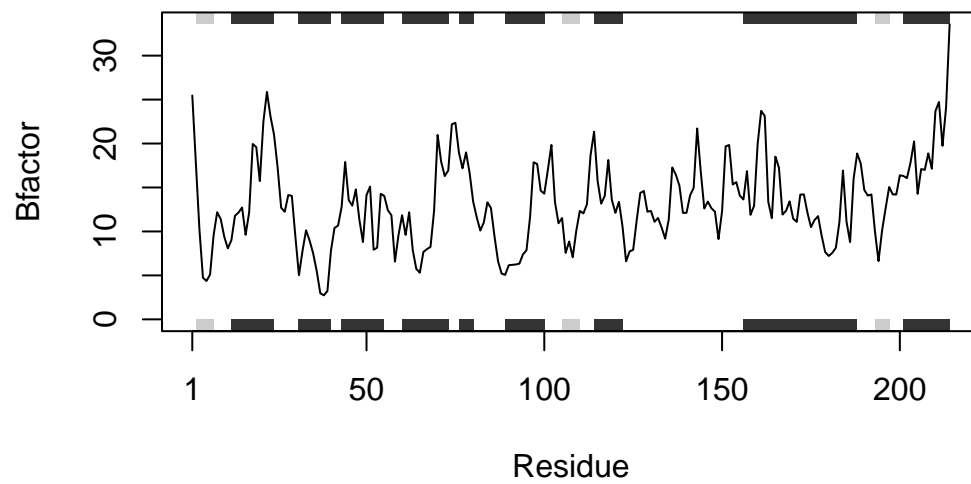
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/sy/_fr9v5r51nxc7bzp4h_683nh0000gn/T//Rtmp16T3K6/1AKE.pdb exists.
Skipping download

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/sy/_fr9v5r51nxc7bzp4h_683nh0000gn/T//Rtmp16T3K6/1E4Y.pdb exists.  
Skipping download
```



\$`4AKE`
NULL

\$`1AKE`
NULL

\$`1E4Y`
NULL