

# Hw6

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## HW 6

Can you improve this analysis code?

```
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

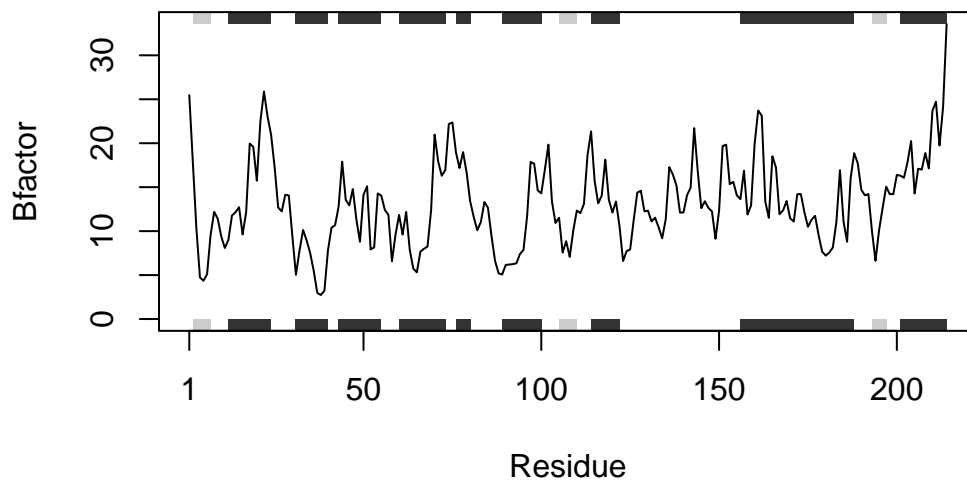
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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



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



Step 1

```
# x <- read.pdb('name')
```

Step 2

```
# x.chainA <- trim.pdb(x, chain = "A", elety = "CA")
```

step 3

```
# x.b <- x.chainA$atom$b
```

step 4

```
# plotx(x.b, sse=x.chainA, typ="l", ylab="Bfactor")
```

combine

```

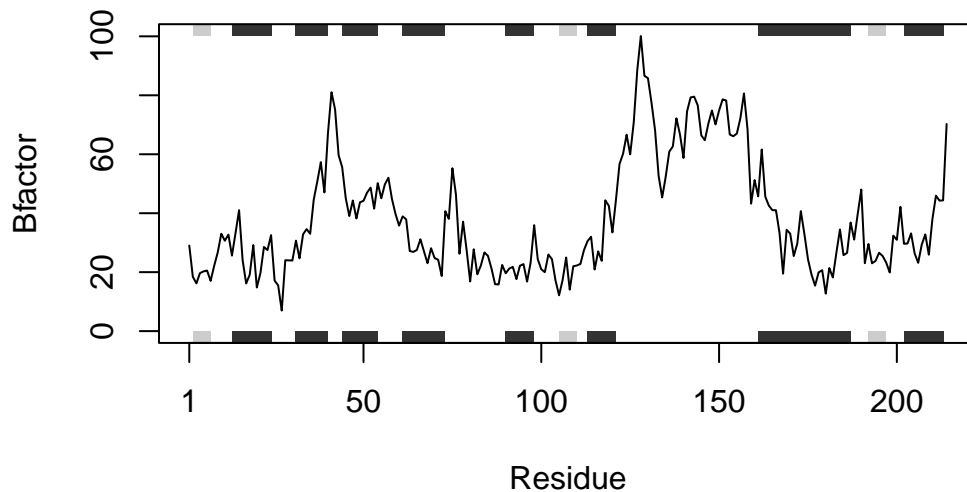
plotfunc <- function(name){
  x.chainA <- trim.pdb(read.pdb(name), chain = "A", eley = "CA")
  x.b <- x.chainA$atom$b
  plotx <- plotb3(x.b, sse=x.chainA, typ="l", ylab="Bfactor")
  return(plotx)}

```

```
plotfunc("4AKE")
```

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):  
/var/folders/17/k395p2f11z34yz15\_fk6m6\_w0000gn/T//Rtmpxnb9fp/4AKE.pdb exists.  
Skipping download



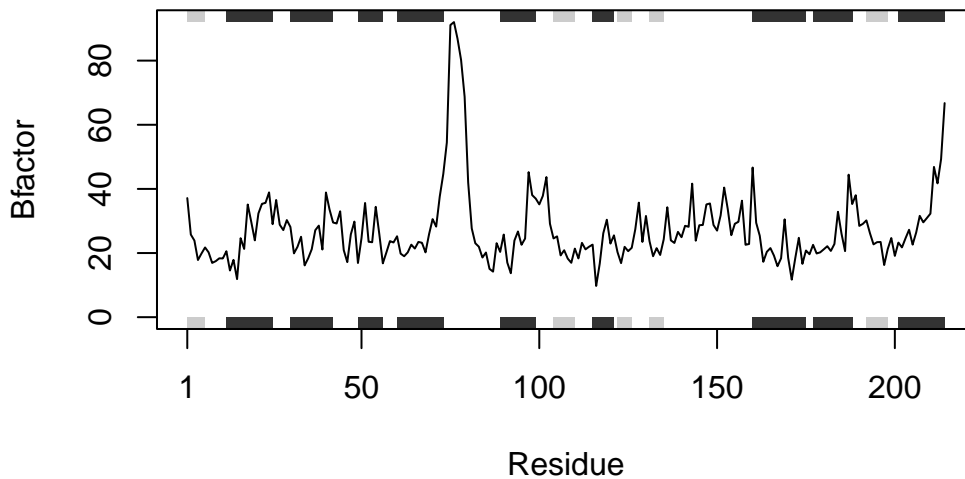
NULL

```
plotfunc("1AKE")
```

Note: Accessing on-line PDB file

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):  
/var/folders/17/k395p2f11z34yzl5_fk6m6_w0000gn/T//RtmpxnB9fp/1AKE.pdb exists.  
Skipping download
```

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

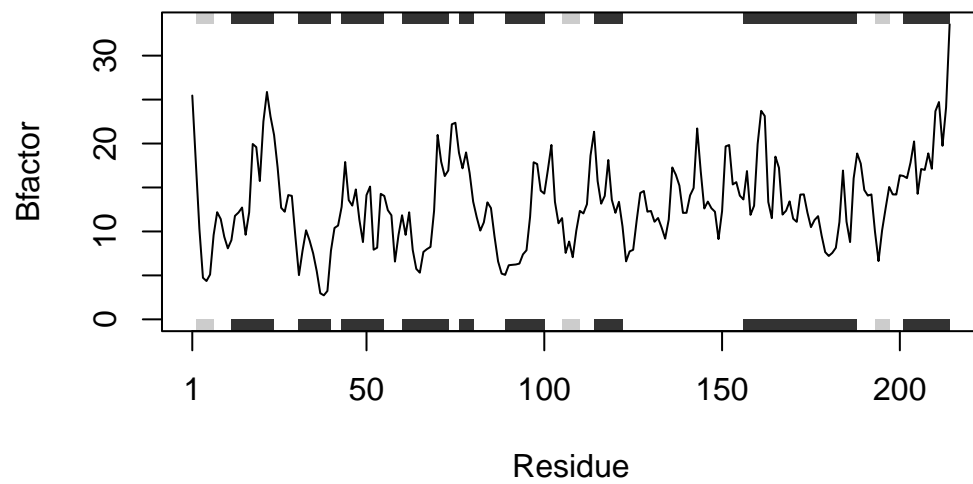


NULL

```
plotfunc("1E4Y")
```

Note: Accessing on-line PDB file

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):  
/var/folders/17/k395p2f11z34yzl5_fk6m6_w0000gn/T//RtmpxnB9fp/1E4Y.pdb exists.  
Skipping download
```



NULL