class06hw

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The provided code that we want to improve and adapt to be more general.

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

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

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

```
Note: Accessing on-line PDB file
 PDB has ALT records, taking A only, rm.alt=TRUE
```
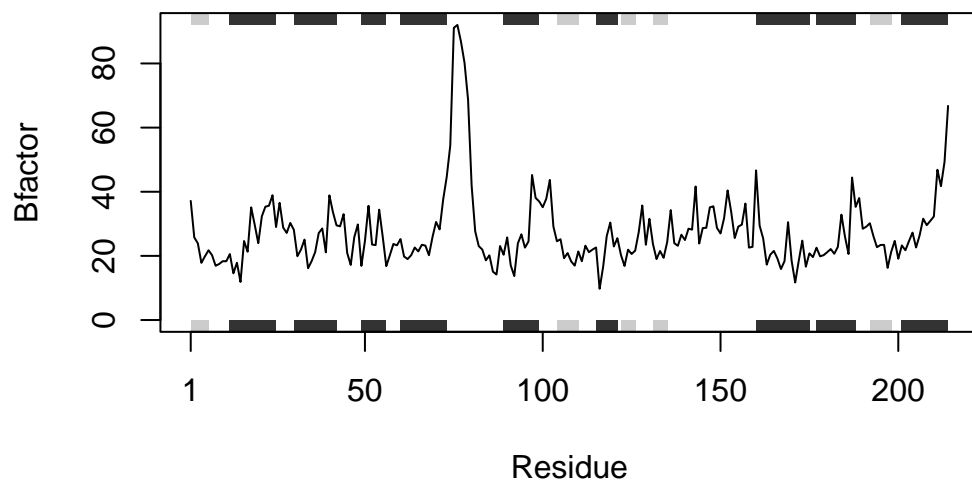
```r
s3 <- read.pdb("1E4Y")  # kinase with drug
```
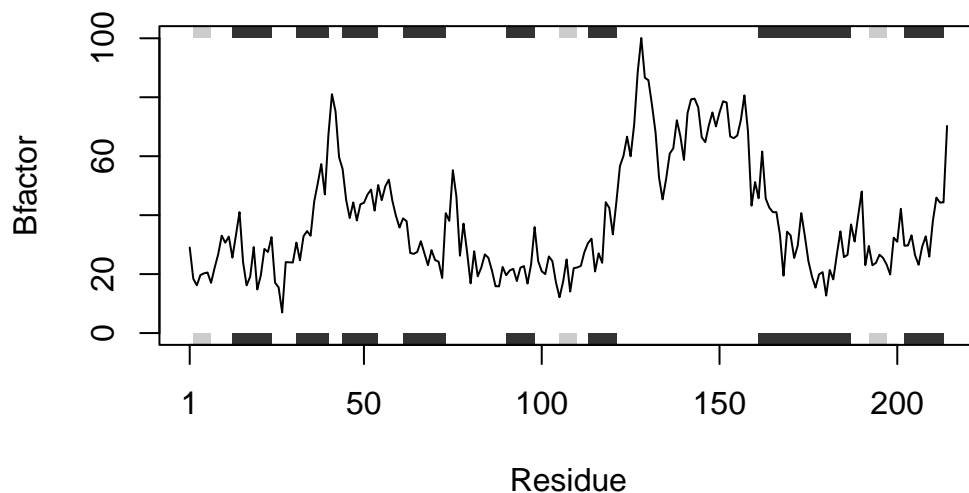
```
Note: Accessing on-line PDB file
```

```r
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")
```


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



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

  Note: Accessing on-line PDB file

```
Warning in get.pdb(file, path = tempdir(), verbose =
FALSE): /var/folders/mh/k7ynyddj67b1vsydwxlwgqwh0000gn/T//RtmpsiTtMI/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/mh/k7ynyddj67b1vsydwxlwgqwh0000gn/T//RtmpsiTtMI/1AKE.pdb
exists. Skipping download
```
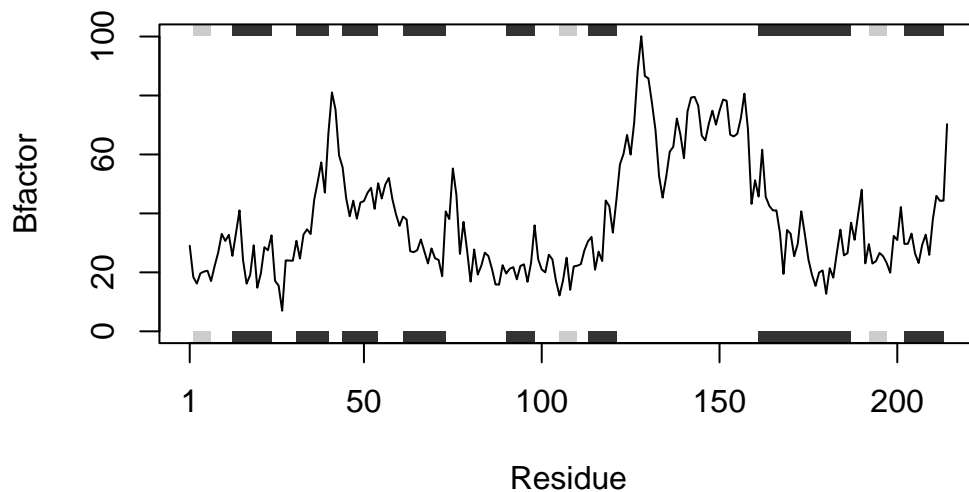
```
  PDB has ALT records, taking A only, rm.alt=TRUE
```

```
  s3 <- read.pdb("1E4Y")   # kinase with drug
```
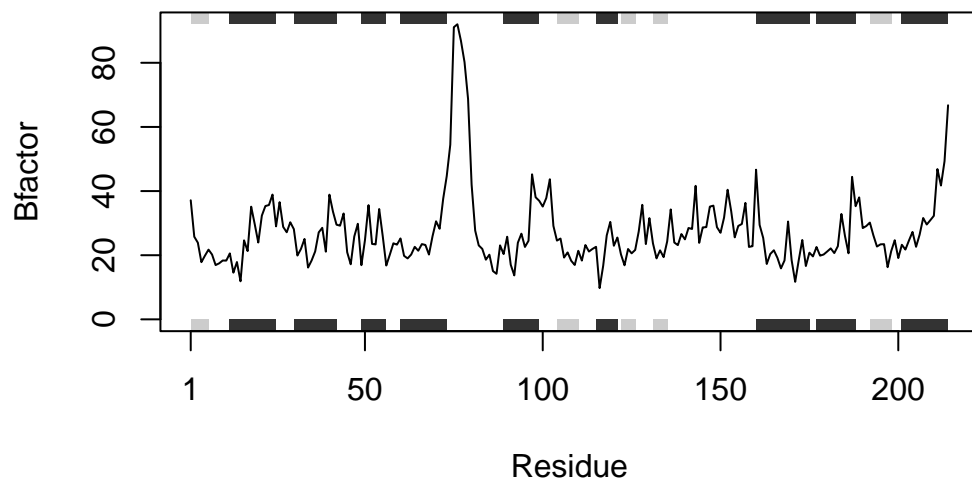
```
  Note: Accessing on-line PDB file
```

```
Warning in get.pdb(file, path = tempdir(), verbose =
FALSE): /var/folders/mh/k7ynyddj67b1vsydwxlwgqwh0000gn/T//RtmpsiTtMI/1E4Y.pdb
exists. Skipping download
```
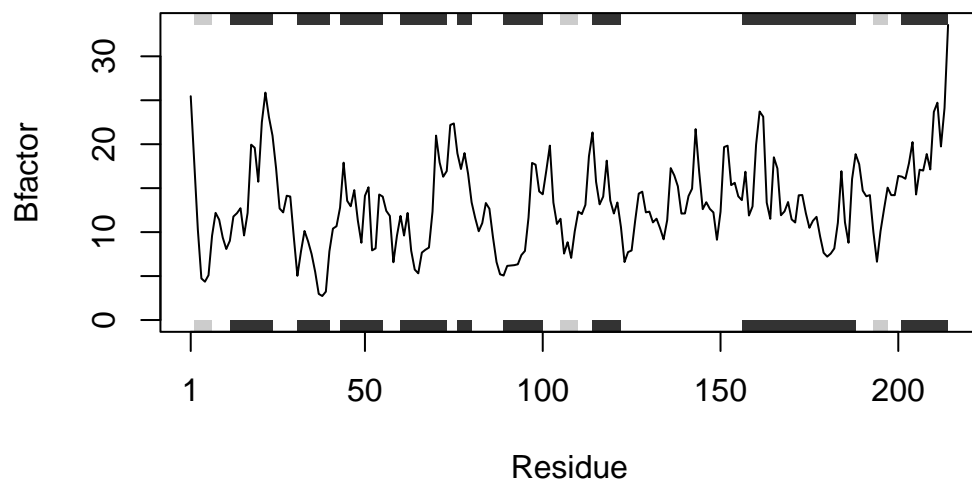
```
  s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
  s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
  s3.chainA <- trim.pdb(s3, chain="A", elety="CA")
  s1.b <- s1.chainA$atom$b
  s2.b <- s2.chainA$atom$b
  s3.b <- s3.chainA$atom$b
  plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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

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


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```r
library(bio3d)
plot_pdb <- function(id) {
  #Read the input PDB file
  pdb <- read.pdb(id)
  #Extract a subset of chain A
  chain <- trim.pdb(pdb, chain="A", elety="CA")

  plotb3(chain$atom$b, sse=chain, typ="l", ylab="Bfactor")
}
```

Code - extract function (with function code highlighted)

```r
plot_pdb("4AKE")
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose =
FALSE): /var/folders/mh/k7ynyddj67b1vsydwxlwgqwh0000gn/T//RtmpsiTtMI/4AKE.pdb
exists. Skipping download
```