Class 6 function Homework

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Function Homework question 6:

Can you improve this analysis code?

library(bio3d) s1 <- read.pdb("4AKE") # kinase with drug s2 <- read.pdb("1AKE") # kinase no drug s3 <- read.pdb("1E4Y") # kinase with drug 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")

```
library(bio3d)
plot_kinase <- function(seq) {
  read.pdb(seq)
```

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

  Note: Accessing on-line PDB file

```
s2 <- read.pdb("1AKE") # kinase no drug
```
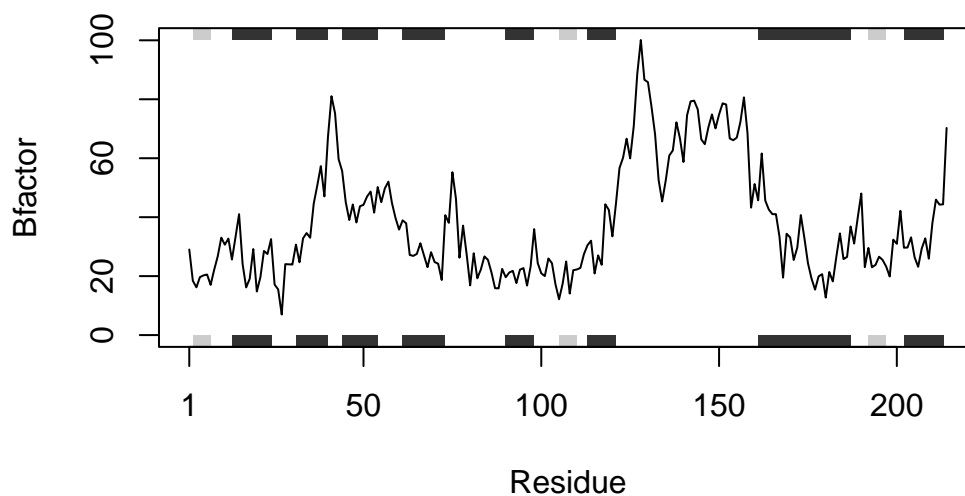
  Note: Accessing on-line PDB file
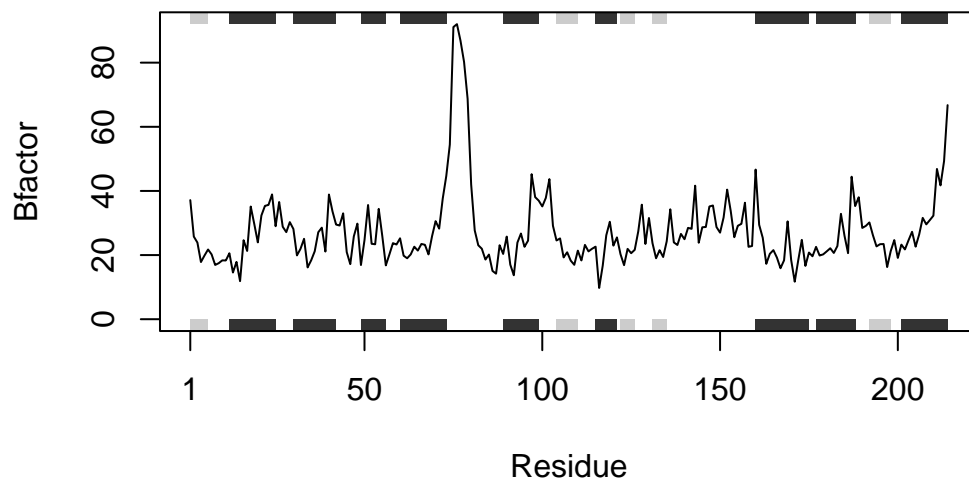   PDB has ALT records, taking A only, rm.alt=TRUE

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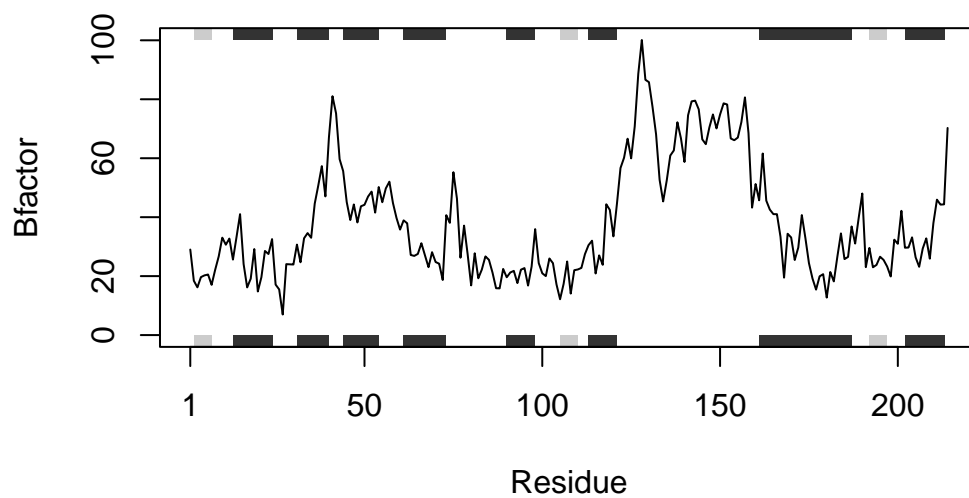
  Note: Accessing on-line PDB file

```
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")
```


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Step 1 Basic function that reads pdb based on reference.

```
library(bio3d)
plot_kinase <- function(pdb.id, chain= "A", elety="CA") {
  #PDB
  pdb <- read.pdb(pdb.id)
}
plot_kinase("4AKE")
```

    Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/hm/2q3nylms2wg32f2zn868mlgw0000gn/T//Rtmp5FPpJh/4AKE.pdb exists.
Skipping download

Step 2

Trim to selected chain and atom type

```
library(bio3d)
plot_kinase <- function(pdb.id, chain= "A", elety="CA") {
  #PDB
  pdb <- read.pdb(pdb.id)
   pdb_trim <- trim.pdb(pdb, chain = chain, elety = elety)
}
plot_kinase("4AKE")
```

    Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/hm/2q3nylms2wg32f2zn868mlgw0000gn/T//Rtmp5FPpJh/4AKE.pdb exists.
Skipping download

Step 3

Extract B-factors

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```r
library(bio3d)
plot_kinase <- function(pdb.id, chain= "A", elety="CA") {
  #PDB
  pdb <- read.pdb(pdb.id)
   pdb_trim <- trim.pdb(pdb, chain = chain, elety = elety)
    b_vals <- pdb_trim$atom$b
}
plot_kinase("4AKE")
```

   Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/hm/2q3nylms2wg32f2zn868mlgw0000gn/T//Rtmp5FPpJh/4AKE.pdb exists.
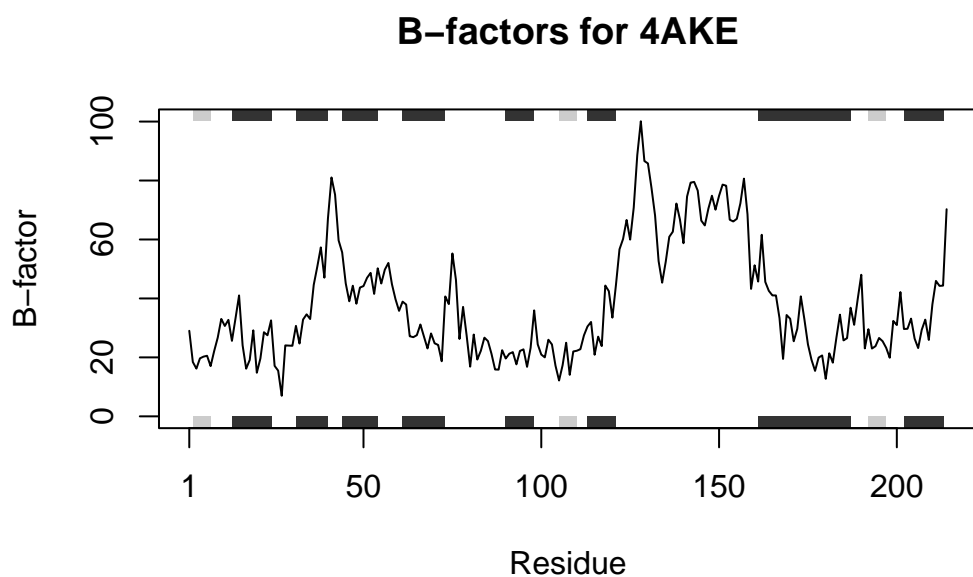Skipping download

Step 4

Plot function

```r
library(bio3d)
plot_kinase <- function(pdb.id, chain= "A", elety="CA") {
  #PDB
  pdb <- read.pdb(pdb.id)
   pdb_trim <- trim.pdb(pdb, chain = chain, elety = elety)
    b_vals <- pdb_trim$atom$b

      plotb3(b_vals,
          sse = pdb_trim,
          typ = "l",
          ylab = "B-factor",
          main = paste("B-factors for", pdb.id))

}
plot_kinase("4AKE")
```

   Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/hm/2q3nylms2wg32f2zn868mlgw0000gn/T//Rtmp5FPpJh/4AKE.pdb exists.
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B−factors for 4AKE


```
plot_kinase("1AKE")
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/hm/2q3nylms2wg32f2zn868mlgw0000gn/T//Rtmp5FPpJh/1AKE.pdb exists.
Skipping download
```
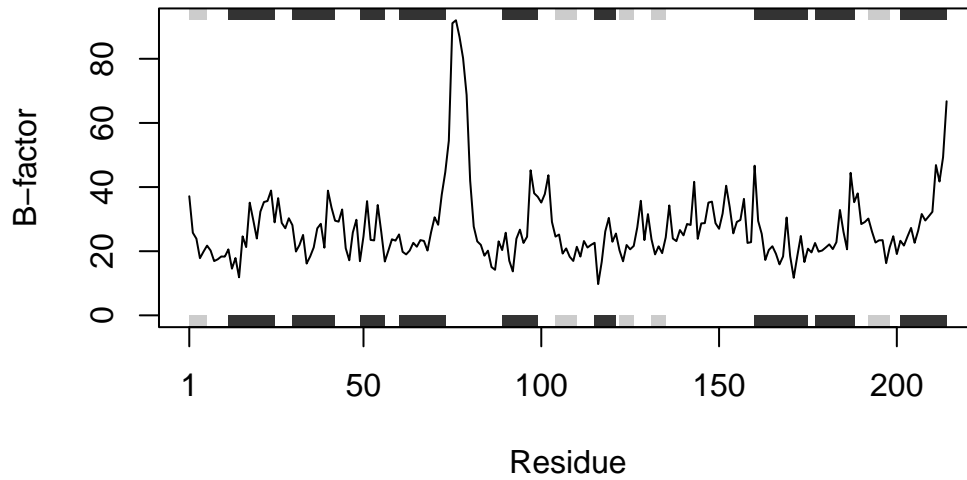
```
  PDB has ALT records, taking A only, rm.alt=TRUE
```

B−factors for 1AKE


```
plot_kinase("1E4Y")
```

  Note: Accessing on-line PDB file

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/hm/2q3nylms2wg32f2zn868mlgw0000gn/T//Rtmp5FPpJh/1E4Y.pdb exists.
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```

B−factors for 1E4Y