hw06

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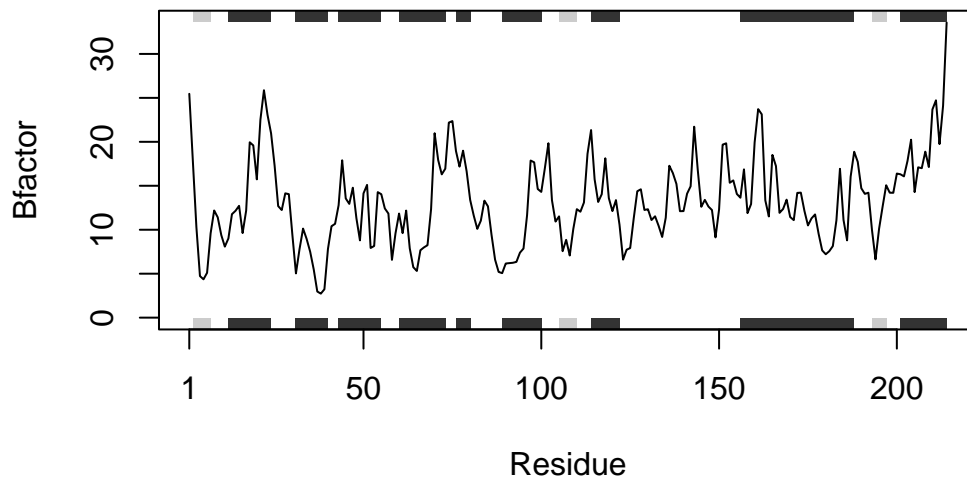
```
plotb3(s2.b, sse=s2.chainA, typ="l", ylab="Bfactor")
```

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


Above is the original coding and its outputs.

Q. How would you generalize the original code above to work with any set of input protein structures?

```
library(bio3d)

# 1. Read PDB file from ID
read_structure <- function(pdb_id) {
  read.pdb(pdb_id)
}

# 2. Extract only chain A and CA atoms
extract_chainA_CA <- function(pdb) {
  trim.pdb(pdb, chain = "A", elety = "CA")
}

# 3. Get B-factors from trimmed structure
get_bfactors <- function(trimmed) {
  trimmed$atom$b
}
```

```r
# 4. Plot B-factor line plot
plot_bfactor <- function(bfactors, trimmed, pdb_id) {
  plotb3(bfactors, sse = trimmed, typ = "l", ylab = "Bfactor", main = pdb_id)
}

# 5. General function to process a single PDB ID
process_pdb <- function(pdb_id) {
  pdb <- read_structure(pdb_id)
  trimmed <- extract_chainA_CA(pdb)
  b <- get_bfactors(trimmed)
  plot_bfactor(b, trimmed, pdb_id)
}

# 6. Apply to multiple PDB IDs
plot_multiple_bfactors <- function(pdb_ids) {
  lapply(pdb_ids, process_pdb)
}
```
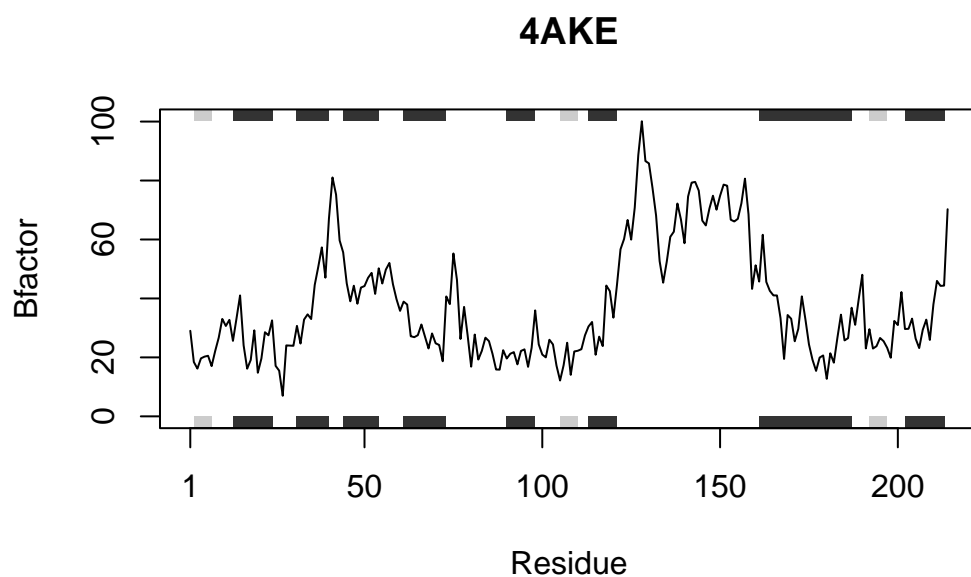
Now lets see if provides the desired output.

```r
plot_multiple_bfactors(c("4AKE", "1AKE", "1E4Y"))
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\anyol\AppData\Local\Temp\Rtmpi49Lsh/4AKE.pdb exists. Skipping download
```
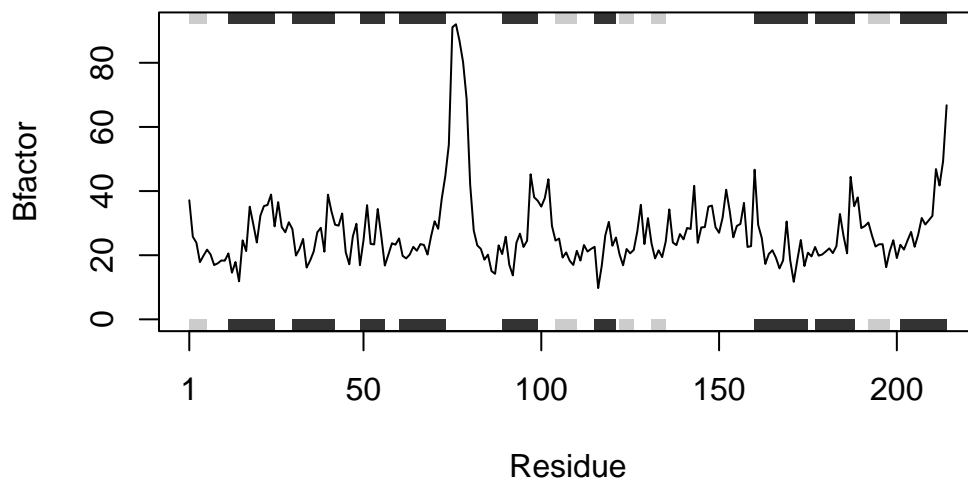
4AKE

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\anyol\AppData\Local\Temp\Rtmpi49Lsh/1AKE.pdb exists. Skipping download

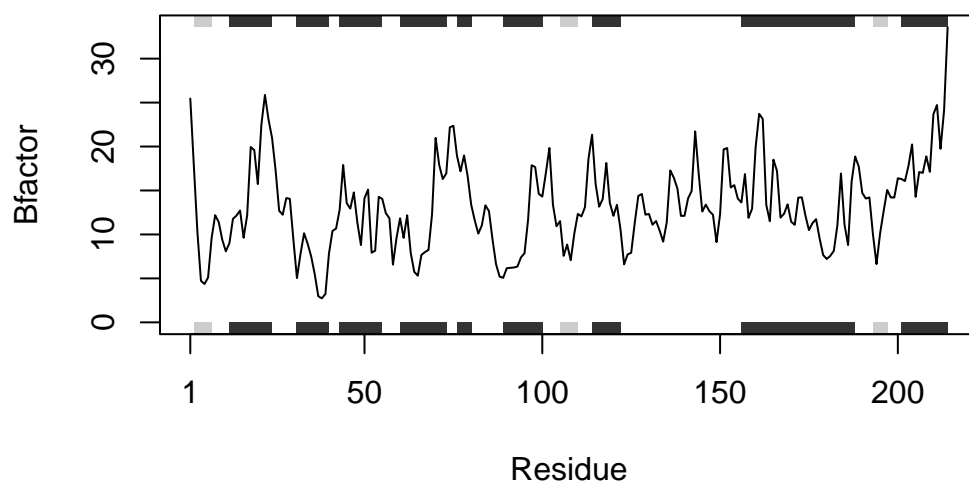PDB has ALT records, taking A only, rm.alt=TRUE

1AKE

Note: Accessing on-line PDB file

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\anyol\AppData\Local\Temp\Rtmpi49Lsh/1E4Y.pdb exists. Skipping download
```

1E4Y


```
[[1]]
NULL

[[2]]
NULL

[[3]]
NULL
```