HW Class 6 (R Functions)

Ruth Barnes: A16747659

2025-01-23

HW Class 6 (R Functions)

Q6. How would you generalize the original code below to work with any set of input protein structures?

```r
library(bio3d)

#read in pdb structures
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
```
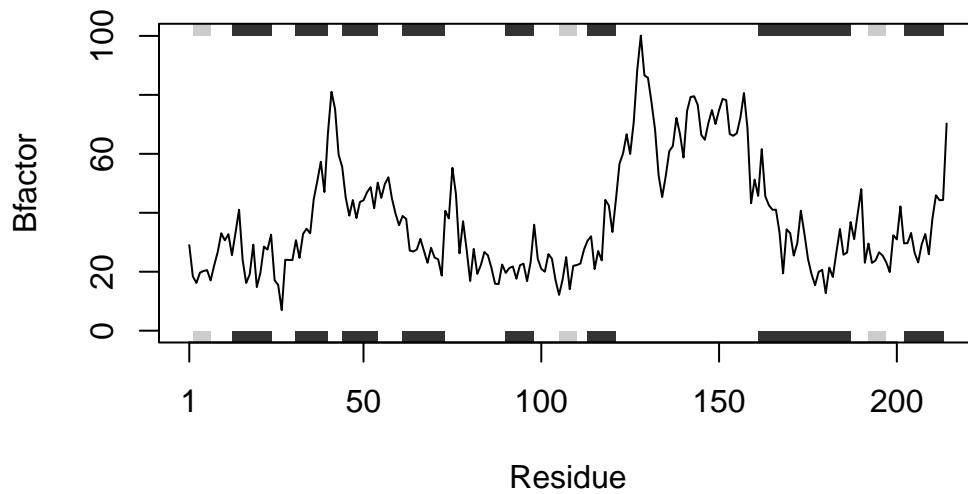
```
  Note: Accessing on-line PDB file
```

```r
#trimming the PDB structures to a smaller subset of atoms
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")

#selecting atom b
```
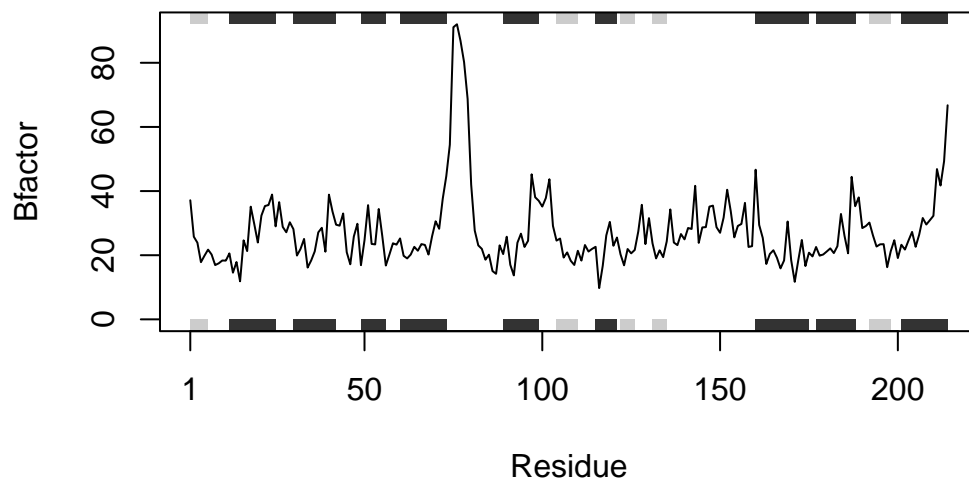
```
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b

#plot atom b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```
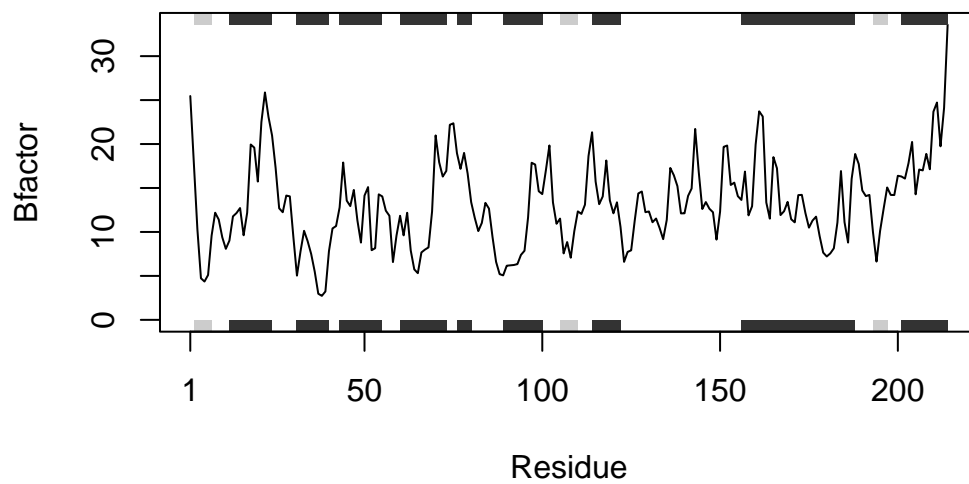


```
plotb3(s2.b, sse=s2.chainA, typ="l", ylab="Bfactor")
```

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

Write function to improve above code

```r
library(bio3d)

plot_PDB_protein <- function(pdb_code){

  #read in pdb code using the function read.pdb(), with input being pdb_code

  s <- read.pdb(pdb_code)

  #trimming the PDB structures to a smaller subset of atoms using trim.pdb(), with input bei

  s.chainA <- trim.pdb(s, chain = "A", elety = "CA")

  #selecting beta factor for atom

  s.b <- s.chainA$atom$b

  #plot the beta factor, with input being s.b, sse=s.chainA, type = "l", and ylab = "Bfactor"

  plotb3(x = s.b, sse=s.chainA, type = "l", ylab = "Bfactor")

}
```
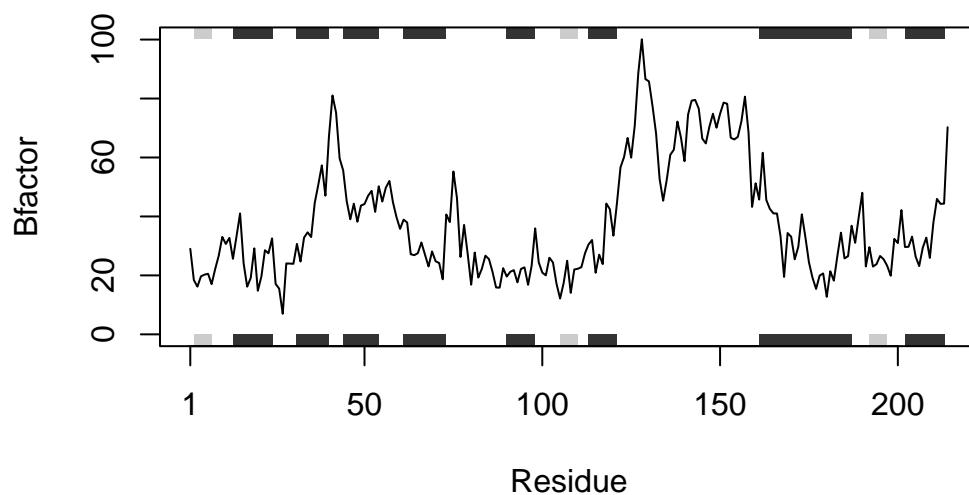
Use/test the written function

```r
#apply the function to the three proteins to output plots

sapply(X = c("4AKE", "1AKE", "1E4Y"), FUN = plot_PDB_protein)
```
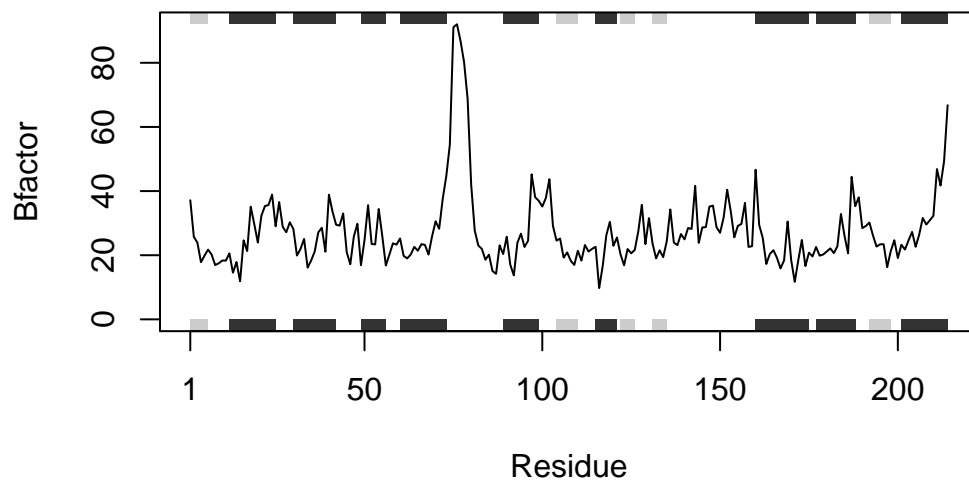
```
  Note: Accessing on-line PDB file
```

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/1b/n1k79swd0sq2jc0hpnx3ybjr0000gn/T//RtmppCveWT/4AKE.pdb exists.
Skipping download
```
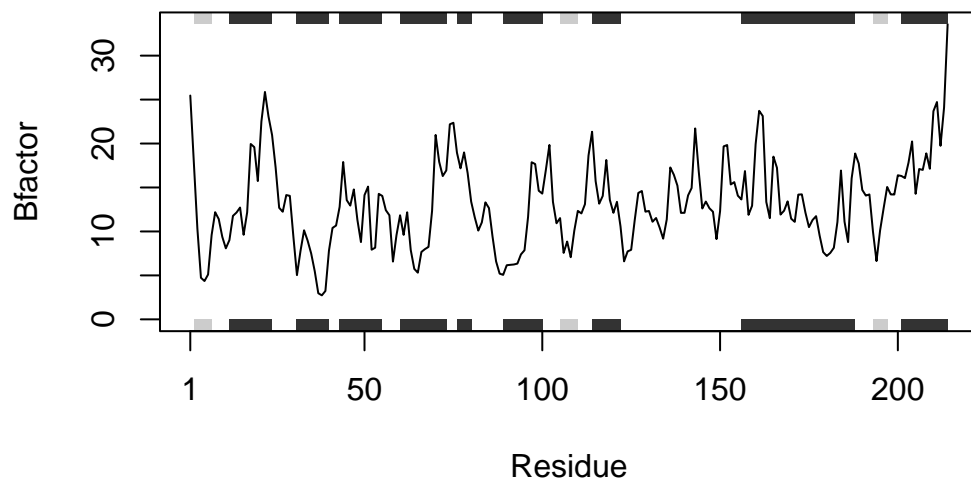
```
Note: Accessing on-line PDB file
```

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/1b/n1k79swd0sq2jc0hpnx3ybjr0000gn/T//RtmppCveWT/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/1b/n1k79swd0sq2jc0hpnx3ybjr0000gn/T//RtmppCveWT/1E4Y.pdb exists.
Skipping download
```

6

```
$`4AKE`
NULL

$`1AKE`
NULL

$`1E4Y`
NULL
```