HWclass6

Jordan Prych (A17080226)

2025-01-24

HW in R Markdown

Output of original code:

```r
#access bio3d database
library(bio3d)

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

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

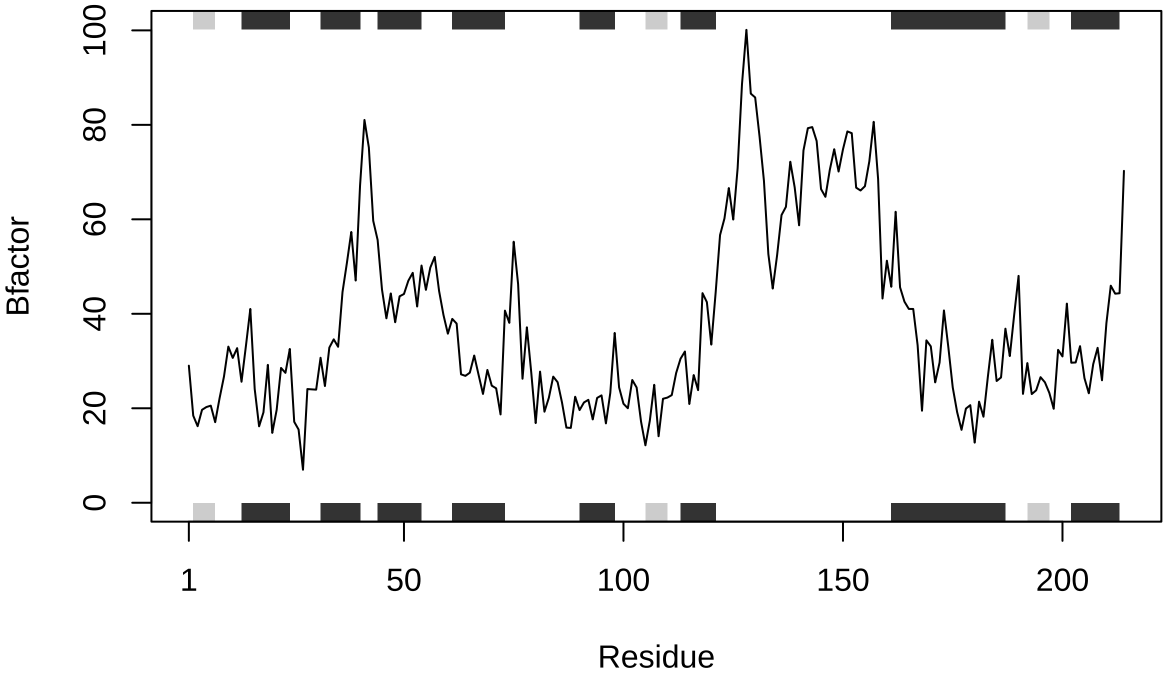
```r
 s2 <- read.pdb("1AKE")  # kinase no drug
```

```
##   Note: Accessing on-line PDB file
##    PDB has ALT records, taking A only, rm.alt=TRUE
```

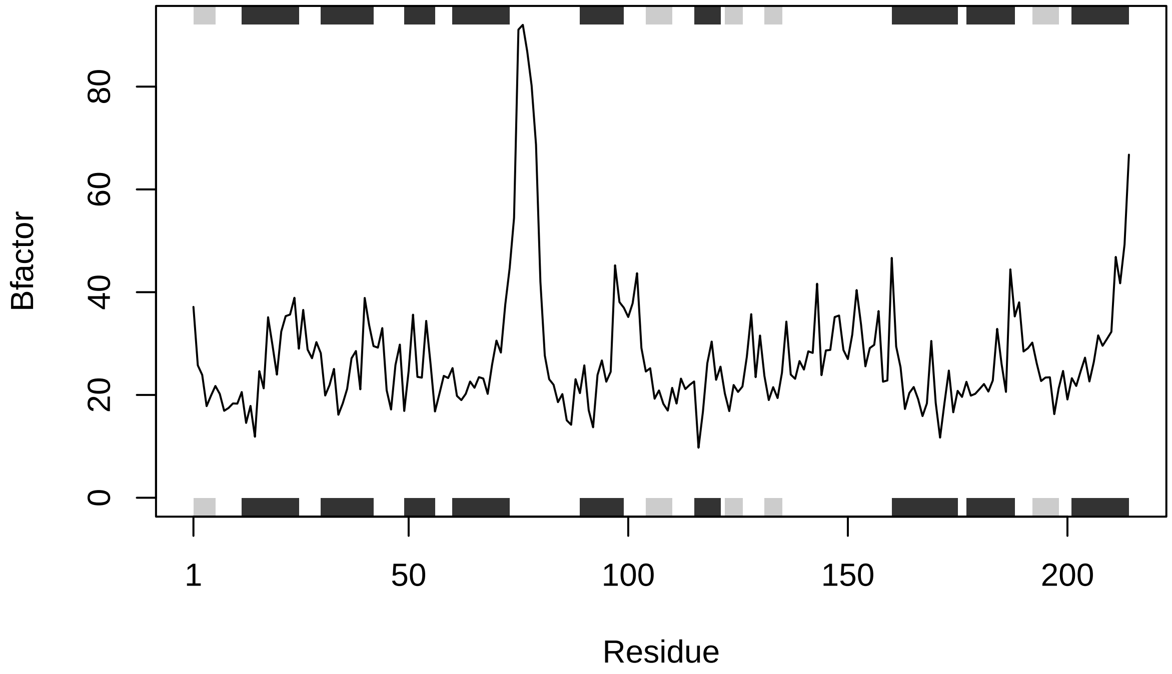
```r
 s3 <- read.pdb("1E4Y")  # kinase with drug
```

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

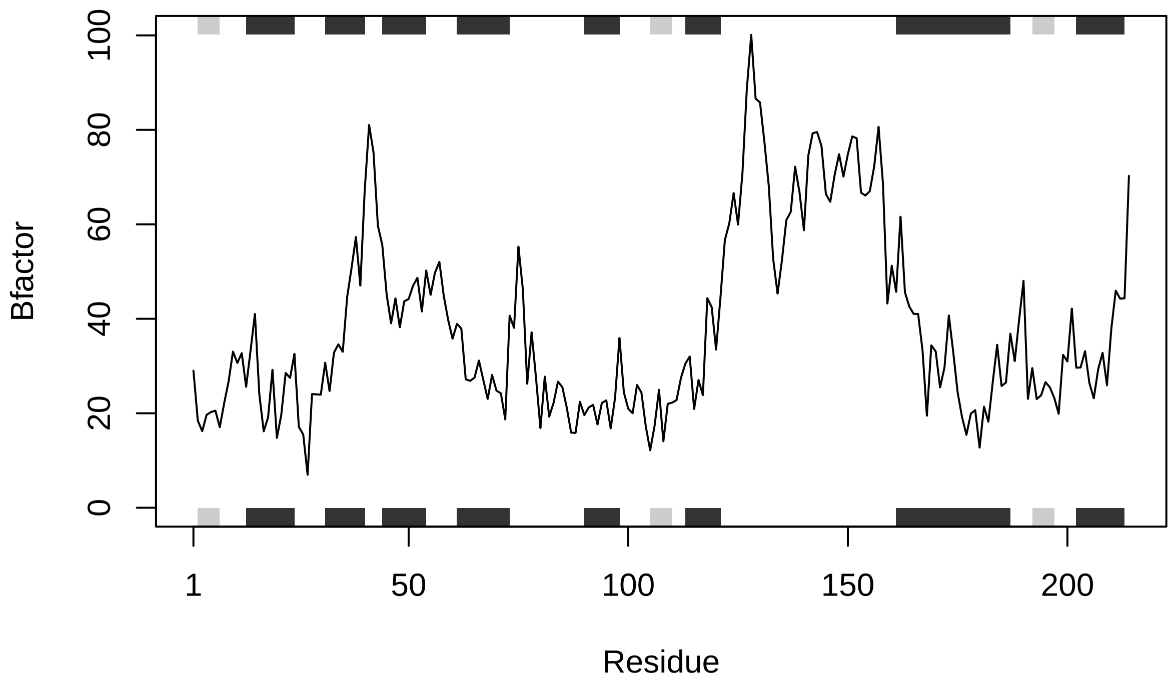
```r
#takes the input of previous PDB structure and trims the file to a smaller subset of atoms, by sleectin
 s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
 s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
 s3.chainA <- trim.pdb(s1, chain="A", elety="CA")

 #select for atom "b" from "atom" column (selecting beta factor from atom)
 s1.b <- s1.chainA$atom$b
 s2.b <- s2.chainA$atom$b
 s3.b <- s3.chainA$atom$b

#plotting beta factor
 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")
```



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

-Step 1 - read PDB code using `read.pdb()`. This function will read the file in PBD structures. The output accesses an-online PBD file and reads atom, seqres, helix, sheet, chain, and other variables pertaining to this protein.

-Step 2 - trim PDB structure to a smaller subset of atoms using `trim.pdb()`. This function outputs a trimmed PBD file regarded specified information from the arguments(chain and elety)

-Step 3 - select for atom "b" in chain A from "atom" column. This will select all "b" values in the "atom" column and output these values.

-Step 4 - plot values using `plotb3()` function. This will generate a scatter plot of the beta factor.

```
#access bio3d database
library(bio3d)
#input to function is protein PDB file to read
plot.pdb <- function(pdb.protein) {
#read in PDB structures
   s <- read.pdb(pdb.protein)
#takes the input of previous PDB structure and trims the file to a smaller subset of atoms, by selectin
  s.chainA <- trim.pdb(s, chain="A", elety="CA")
#select for atom "b" from "atom" column (selecting beta factor from atom)
  s.b <- s.chainA$atom$b
#plotting beta factor
  plotb3(s.b, sse=s.chainA, typ="l", ylab="Bfactor")
}
```

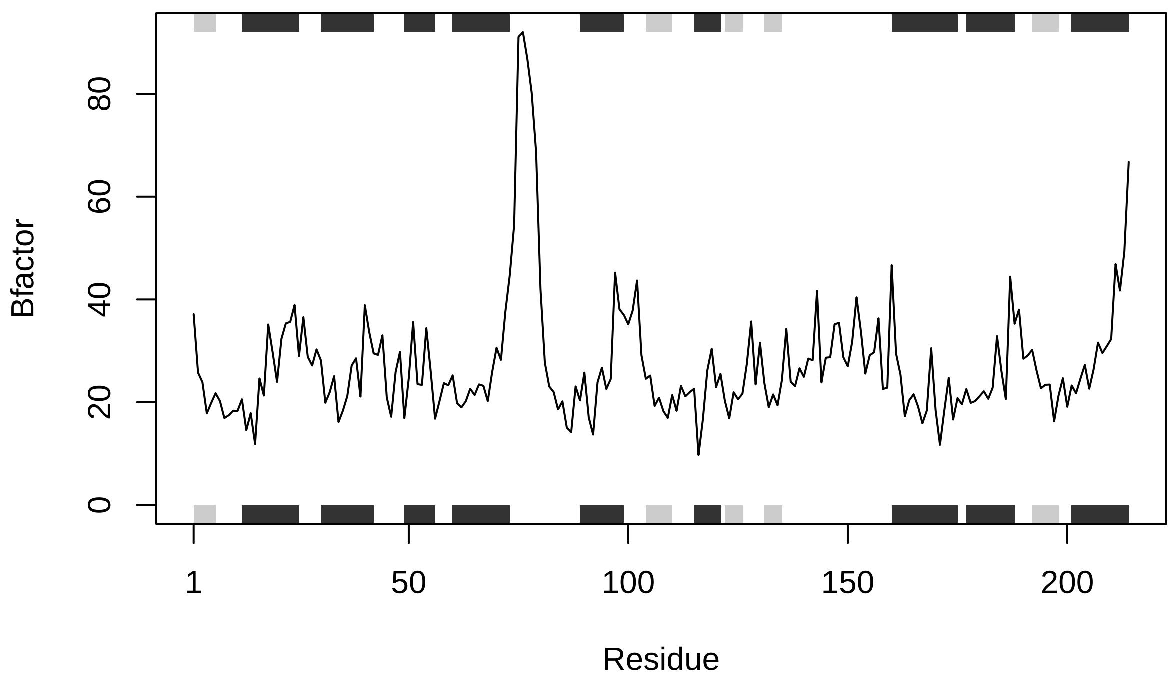
Testing generated function:

```
plot.pdb("1AKE")
```

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

```
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
## C:\Users\joelp\AppData\Local\Temp\RtmpYp5bXE/1AKE.pdb exists. Skipping download
```

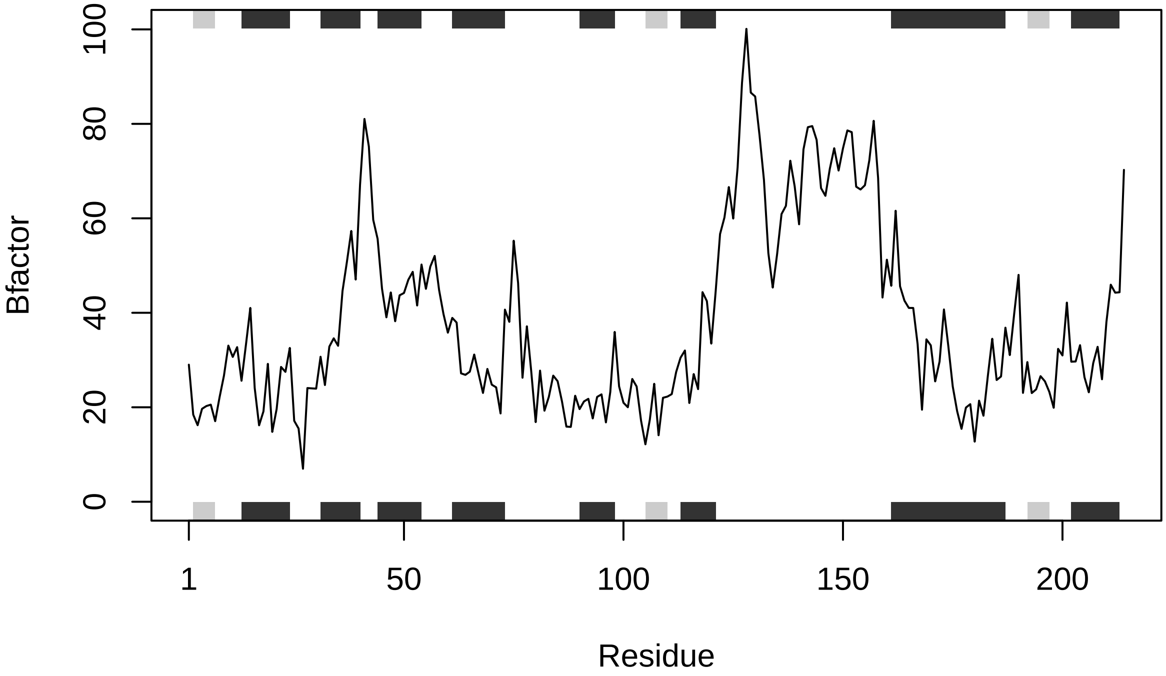
```
##    PDB has ALT records, taking A only, rm.alt=TRUE
```



```
plot.pdb("4AKE")
```

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

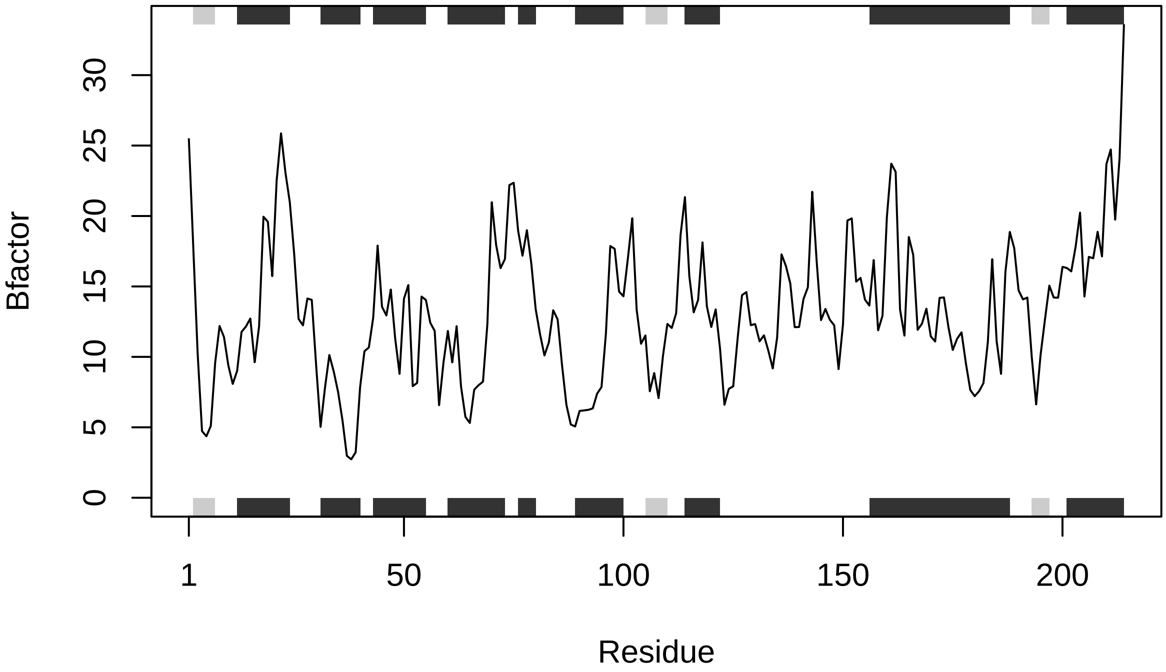
```
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
## C:\Users\joelp\AppData\Local\Temp\RtmpYp5bXE/4AKE.pdb exists. Skipping download
```



```
plot.pdb("1E4Y")
```

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

```
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
## C:\Users\joelp\AppData\Local\Temp\RtmpYp5bXE/1E4Y.pdb exists. Skipping download
```


Bfactor
0
5
10
15
20
25
30
Residue
1
50
100
150
200