

# Lab 6 Homework

Julia Ainsworth

## Table of contents

<b>Working through the problem</b>	<b>1</b>
Code given . . . . .	1
Breaking down code parts . . . . .	4

<b>Answer q6</b>	<b>5</b>
------------------	----------

Installed bio3d in the console and loaded it with library

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

## Working through the problem

### Code given

```
# 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
```

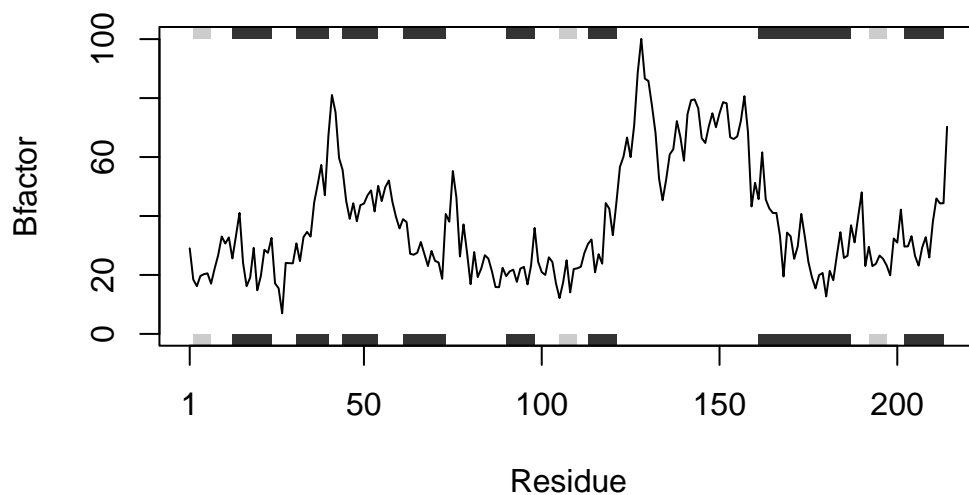
Note: Accessing on-line PDB file

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

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

Note: Accessing on-line PDB file

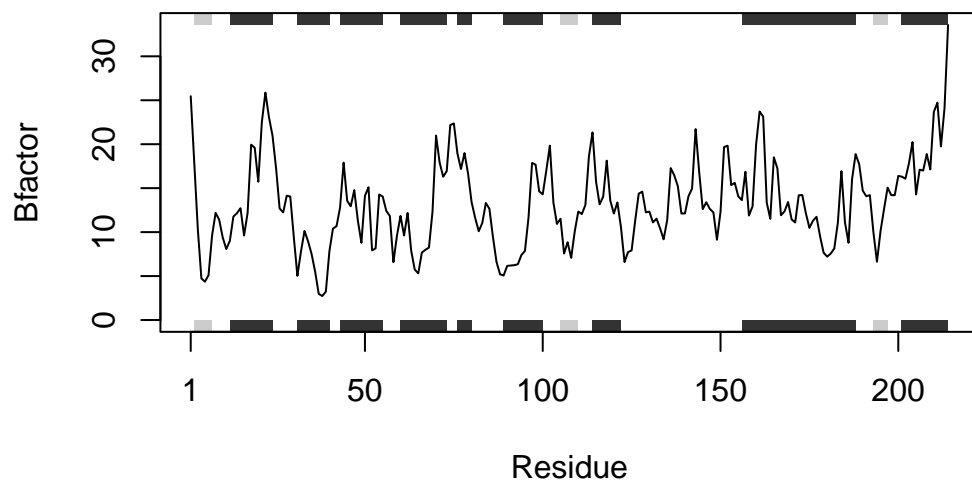
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")  
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")  
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")  
s1.b <- s1.chainA$atom$b  
s2.b <- s2.chainA$atom$b  
s3.b <- s3.chainA$atom$b  
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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



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



## Breaking down code parts

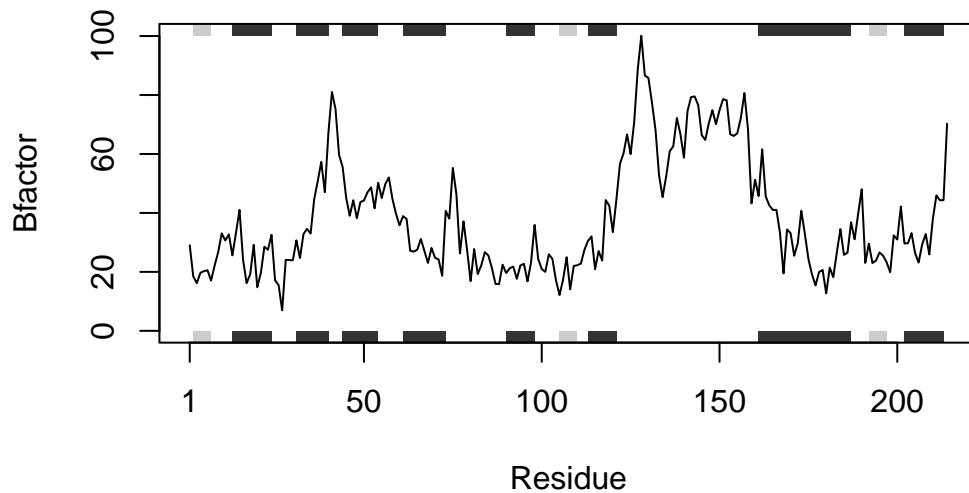
```
# Getting the information
#Trimming the information
s1.chainA <- trim.pdb(read.pdb("4AKE"), chain = "A", eley = "CA")
```

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/h3/q3d5vn\_j0sg0xqg1k5q0s8bw0000gp/T//RtmpLBXBZF/4AKE.pdb exists. Skipping download

```
#The first step (defining s1) can be combined with the second step

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



## Answer q6

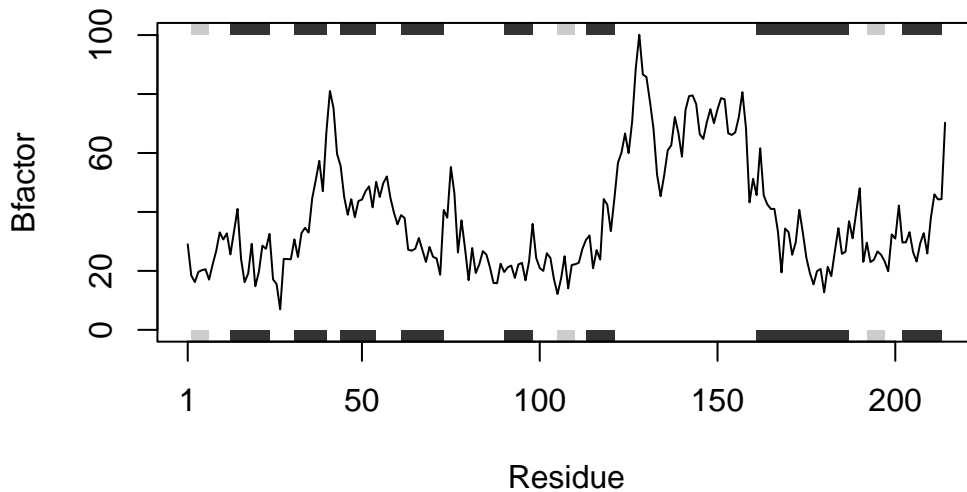
```
s.chain.A <- function(x) {  
  p <- (trim.pdb(read.pdb(x), chain = "A", elety = "CA"))  
  plotb3(p$atom$b, sse=p, type = "l", ylab = "Bfactor")  
}
```

#Input to the function has to be a pdb code in ""

```
#Testing it out  
s.chain.A("4AKE")
```

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/h3/q3d5vn\_j0sg0xqg1k5q0s8bw0000gp/T//RtmpLBXBZF/4AKE.pdb exists. Skipping download

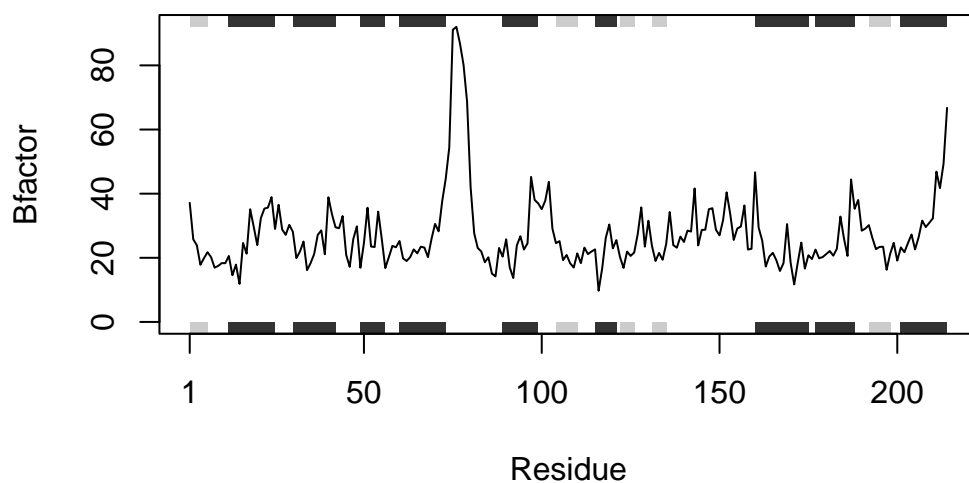


```
s.chain.A("1AKE")
```

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/h3/q3d5vn\_j0sg0xqg1k5q0s8bw0000gp/T//RtmpLBXBZF/1AKE.pdb exists. Skipping download

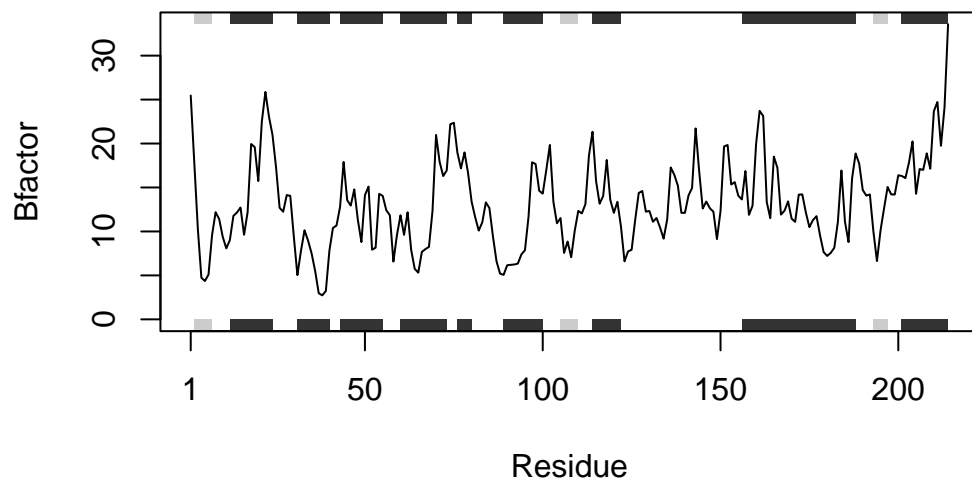
PDB has ALT records, taking A only, rm.alt=TRUE



```
s.chain.A("1E4Y")
```

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/h3/q3d5vn\_j0sg0xqg1k5q0s8bw0000gp/T//RtmpLBXBZF/1E4Y.pdb exists. Skipping download



The code returns the graphs that look the same as the (corrected) graphs from the original code.