

Lab6_HW

AUTHOR

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Lab 6 HW

First, I'm going to install the bio3d package and call the library.

Then I'm going to call in the pdf files and name them s1-3

```
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

`trim.pdb` produces a smaller PDB object that contains a subset of atoms from the larger object. Here, we're grabbing chain A from each protein and naming them in correlation with the new subset.

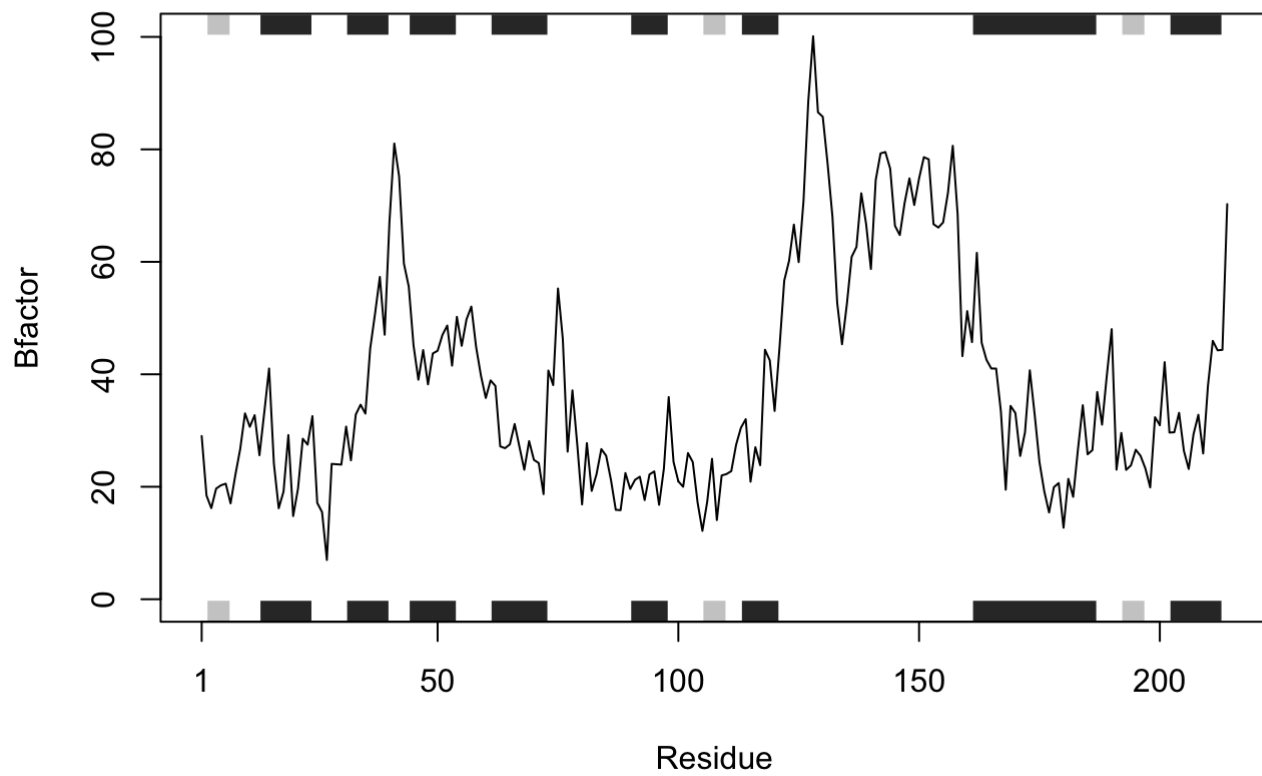
```
s1.chainA <- trim.pdb(s1, chain="A", eley="CA")
s2.chainA <- trim.pdb(s2, chain="A", eley="CA")
s3.chainA <- trim.pdb(s3, chain="A", eley="CA")
```

Creating and naming more specific subsets

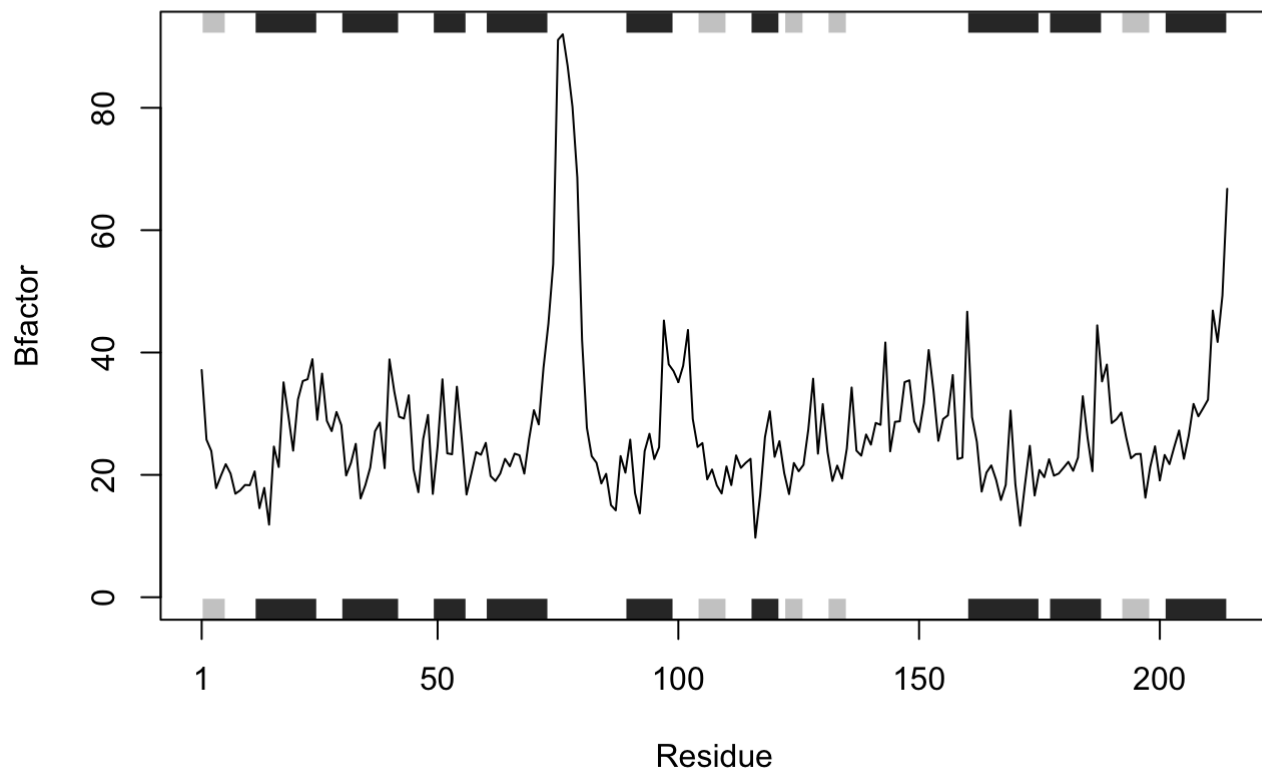
```
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
```

`plotb3` is going to create a scatter plot (here with a line aesthetic) with the option to add secondary structures in the marginal regions that should correlate with the protein (ie "sse=" should match protein)

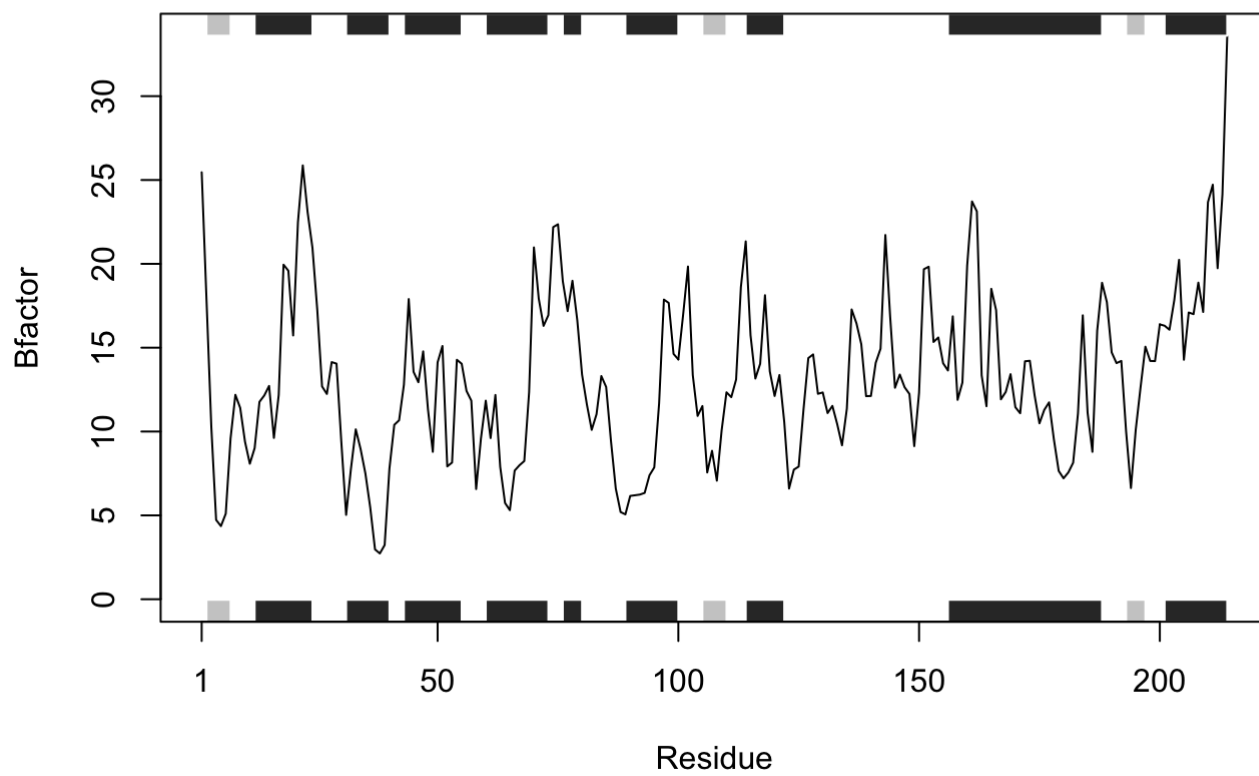
```
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



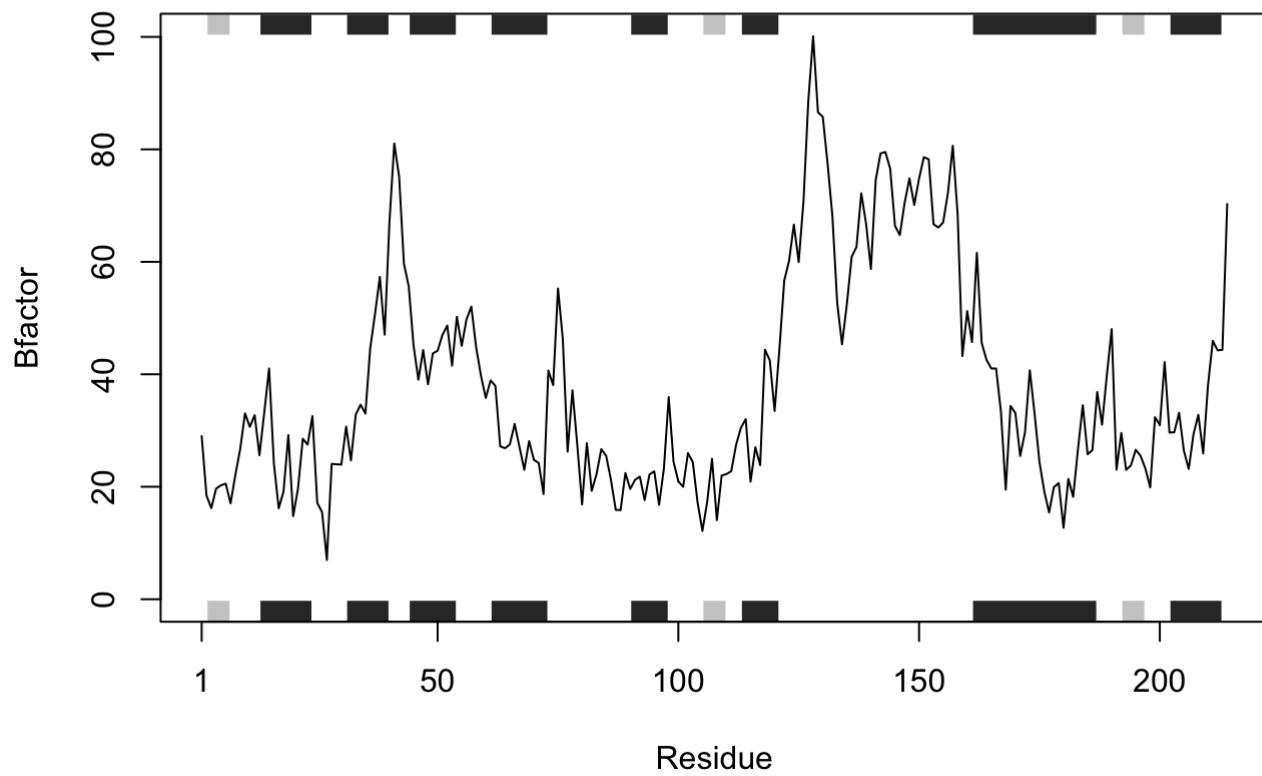
```
plotb3(s2.b, sse=s2.chainA, typ="l", ylab="Bfactor")
```



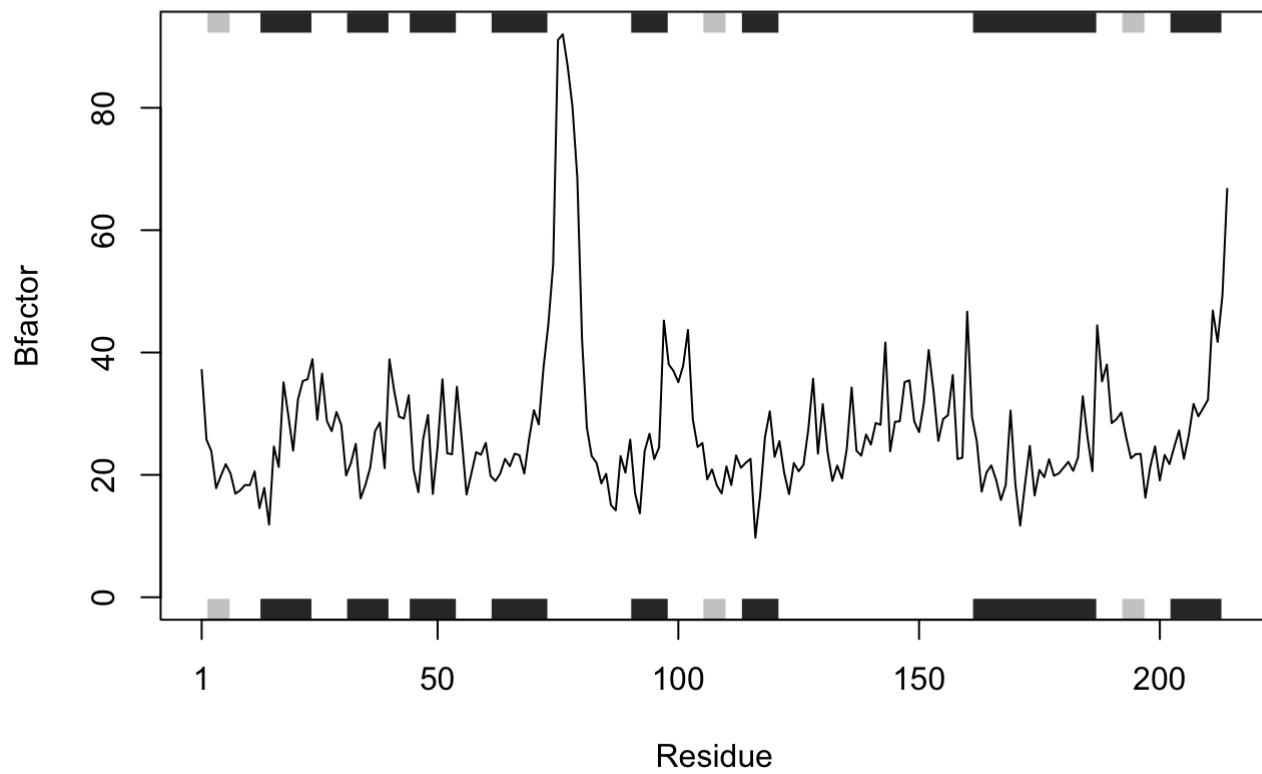
```
plotb3(s3.b, sse=s3.chainA, typ="l", ylab="Bfactor")
```



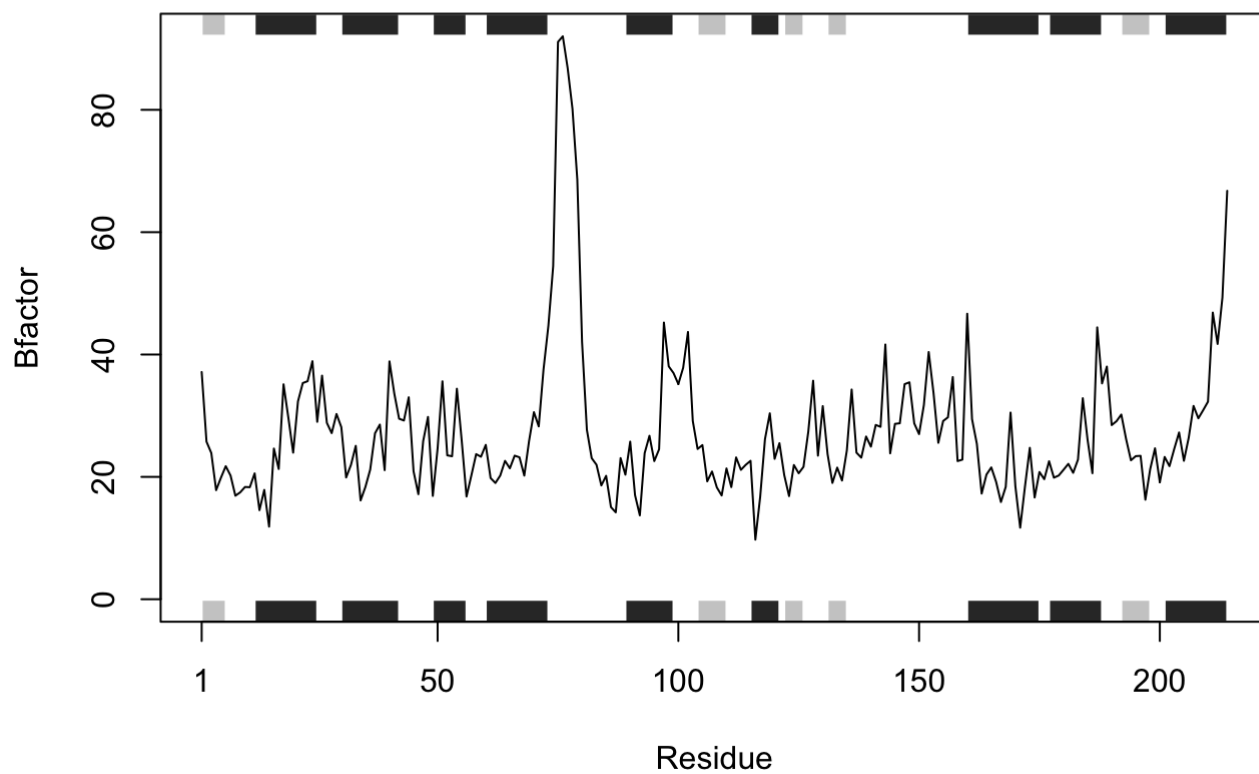
```
x <- s1.b  
plotb3(x, sse=s1.chainA, typ="l", ylab="Bfactor")
```



```
x <- s2.b  
plotb3(x, sse=s1.chainA, typ="l", ylab="Bfactor")
```

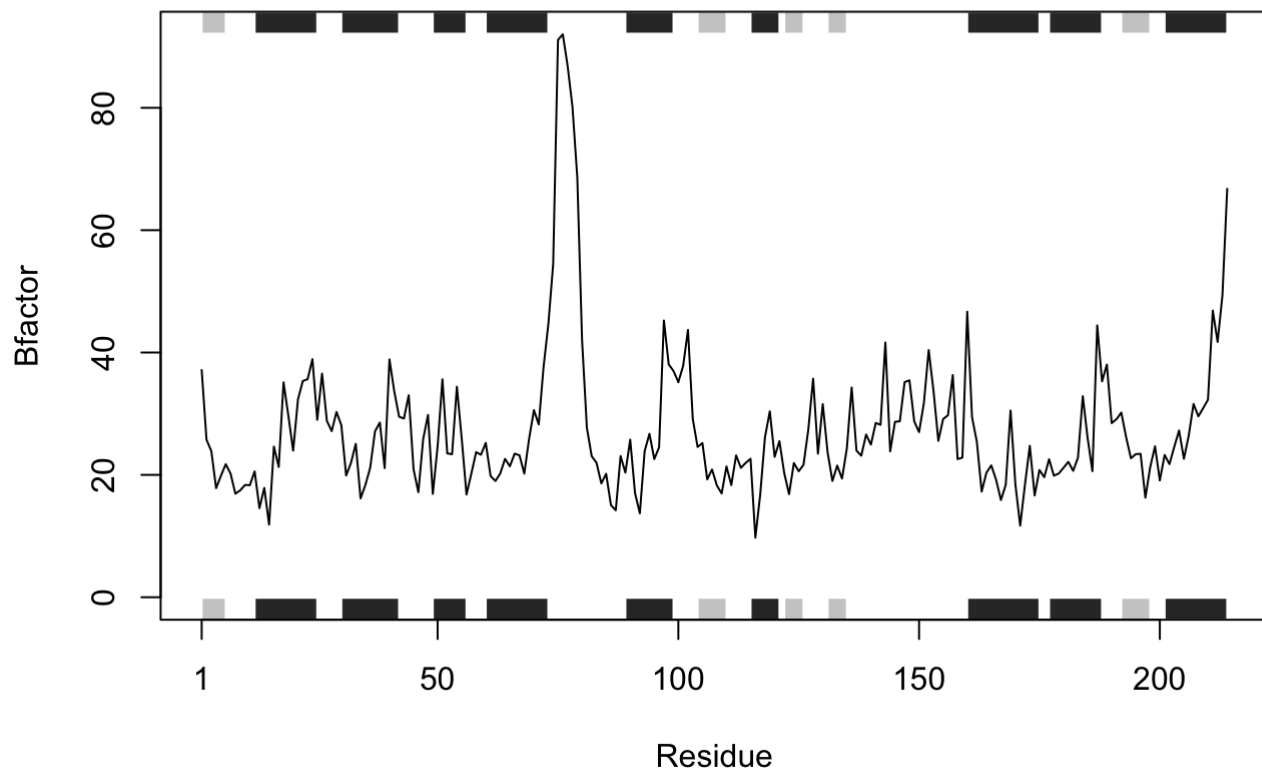


```
x <- s2.b  
plotb3(x, sse=s2.chainA, typ="l", ylab="Bfactor")
```

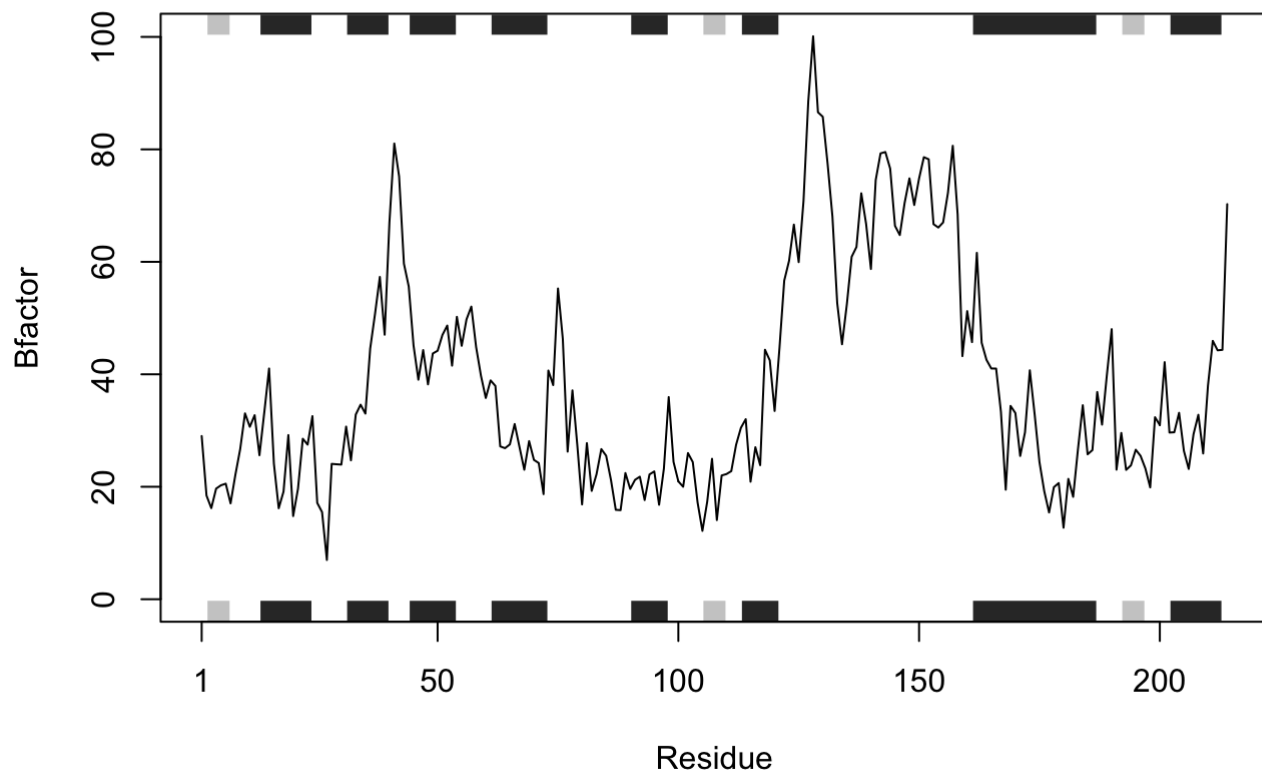


#need to figure out how to make the "sse=" part interchangeable with the protein subset n

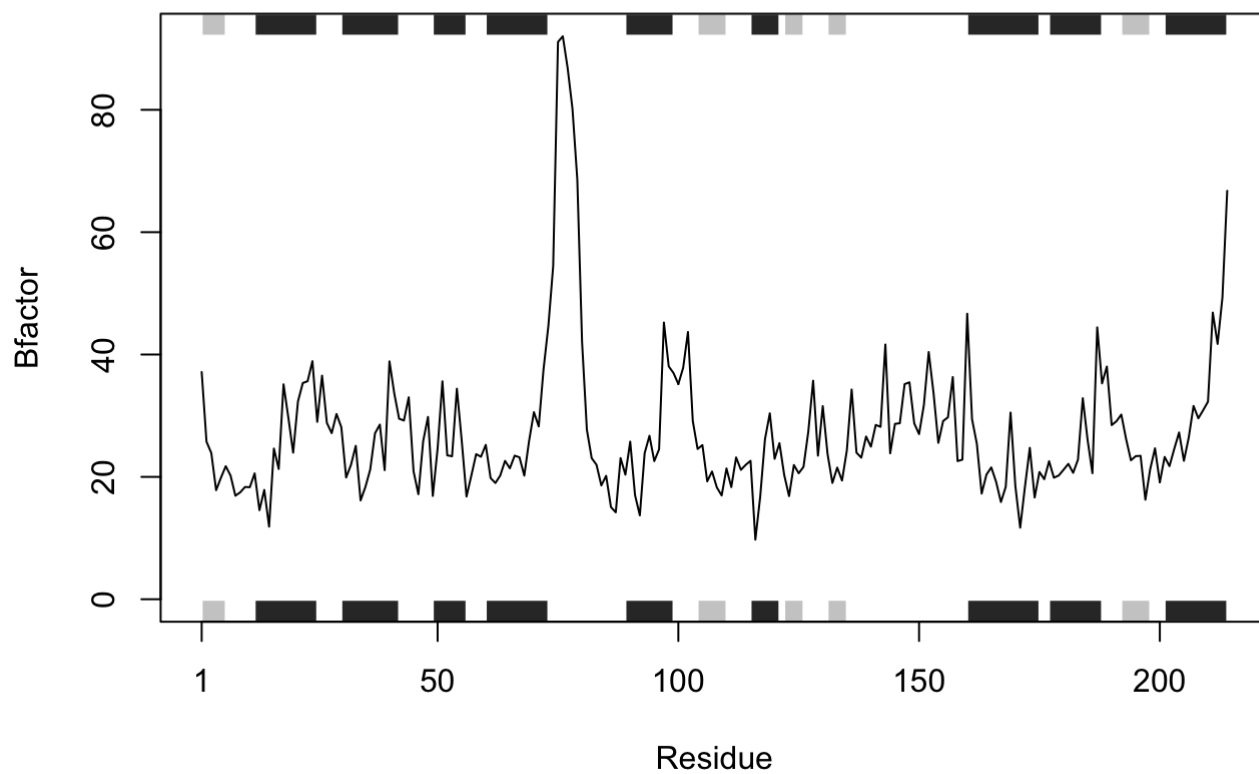
```
y <- s2.chainA  
  
x <- s2.b  
plotb3(x, sse=y, typ="l", ylab="Bfactor")
```



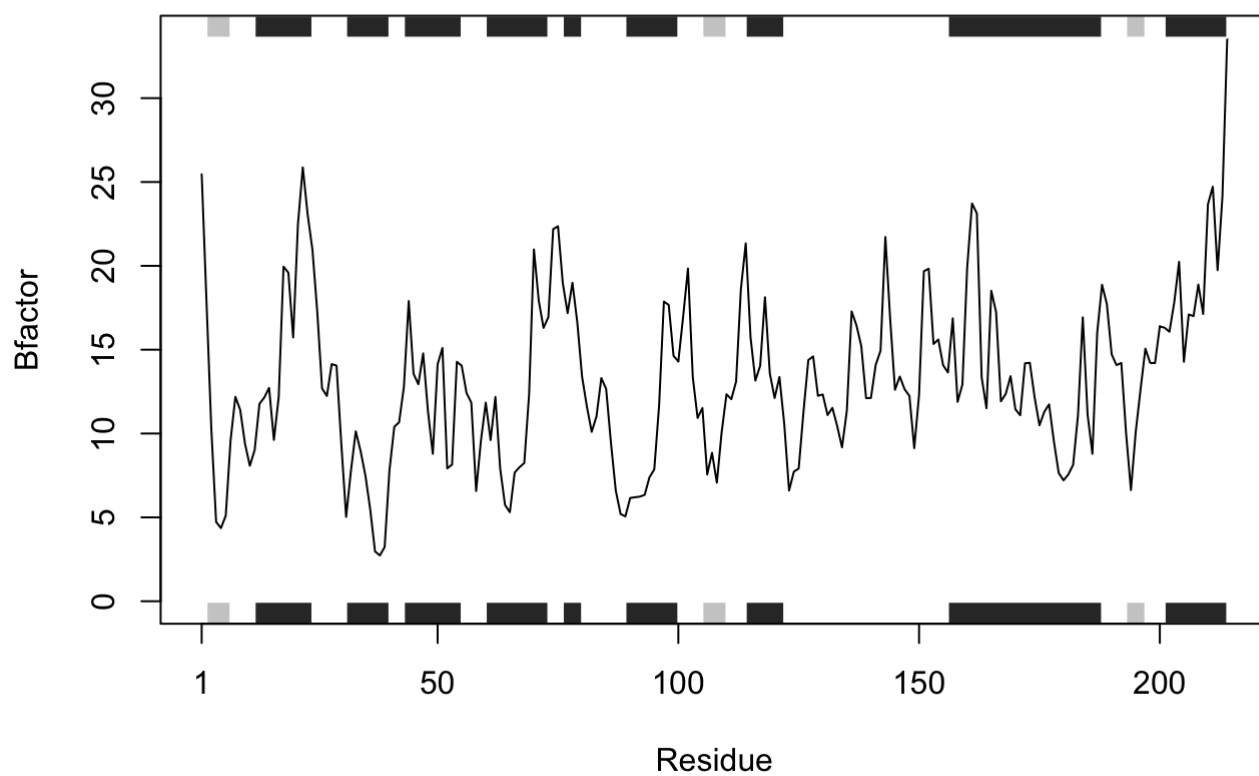
```
x <- s1.b  
y <- s1.chainA  
plotb3(x, sse=y, typ="l", ylab="Bfactor")
```

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

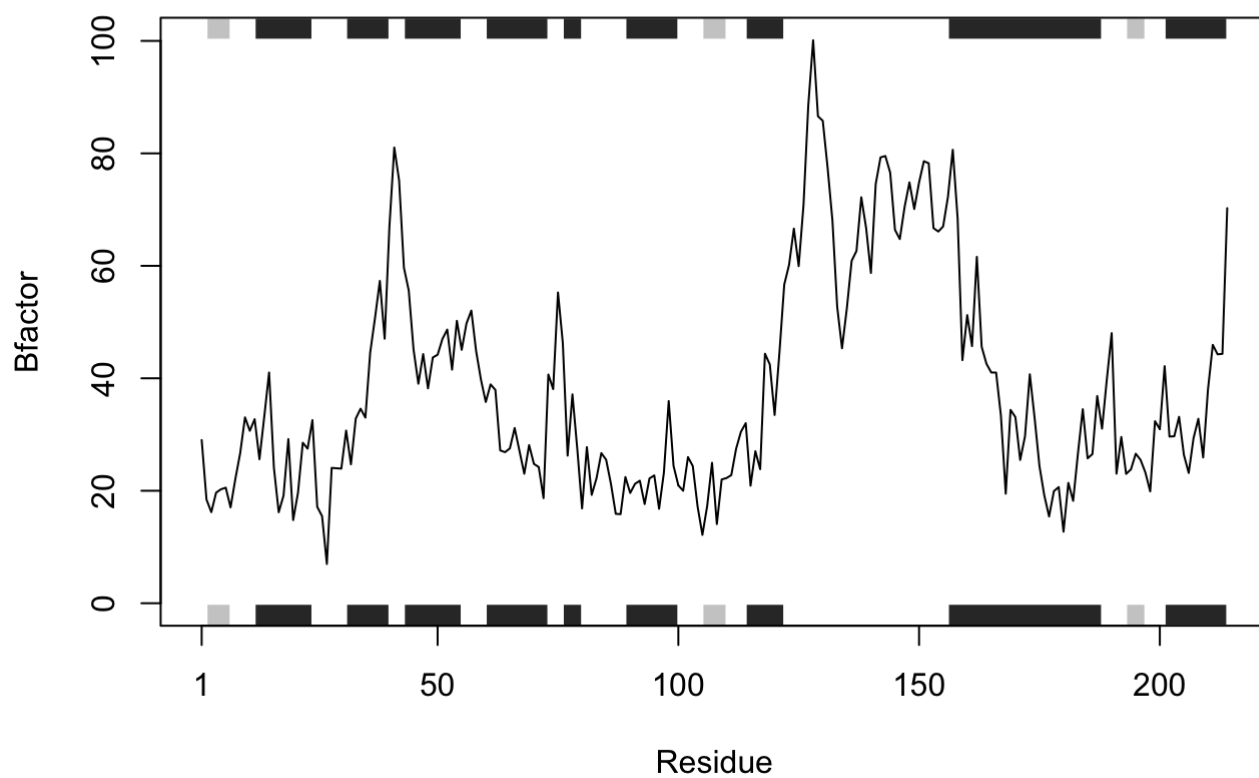


```
x <- s3.b  
y <- s3.chainA  
plotb3(x, sse=y, typ="l", ylab="Bfactor")
```

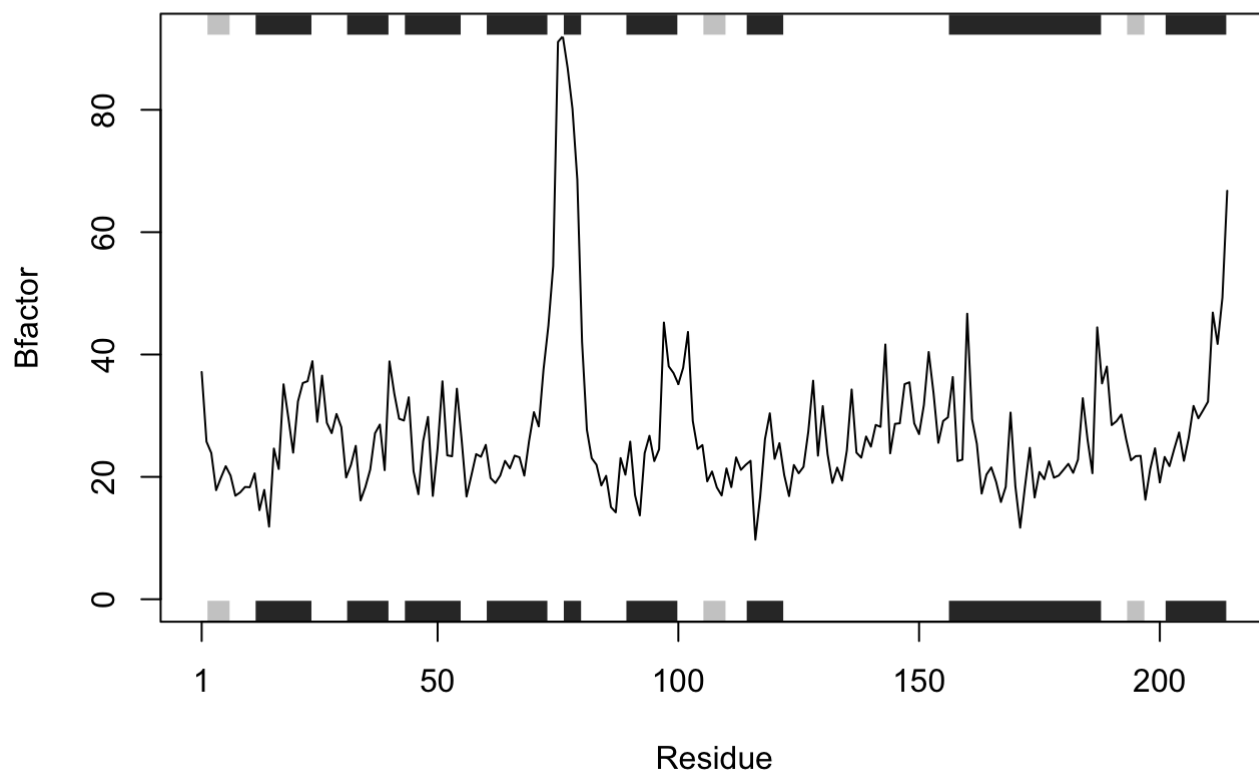


now to put everything together

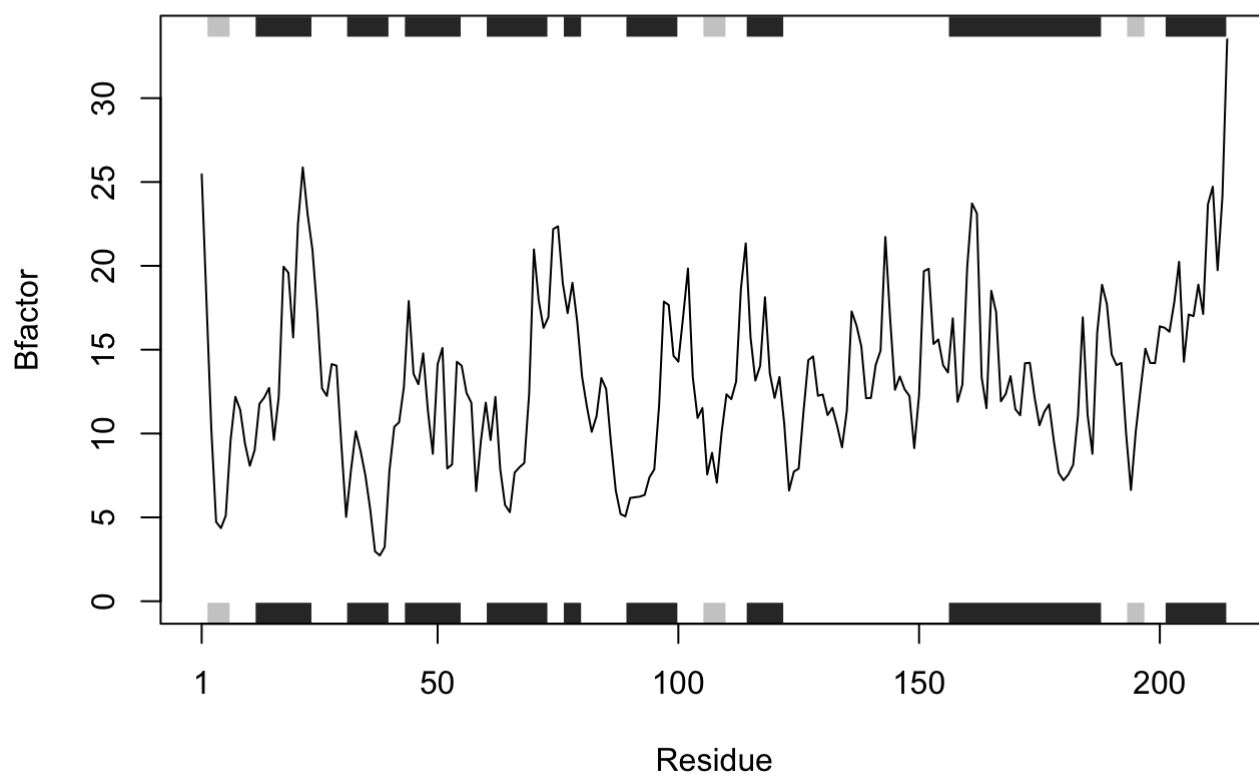
```
visualplot <- function(x) {  
  plotb3(x, sse=y,  
    typ="l", ylab="Bfactor")  
}  
  
visualplot(s1.b)
```



```
visualplot(s2.b)
```



```
visualplot(s3.b)
```



I think I'm getting closer but the margins are not right :/