

Homework 6

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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

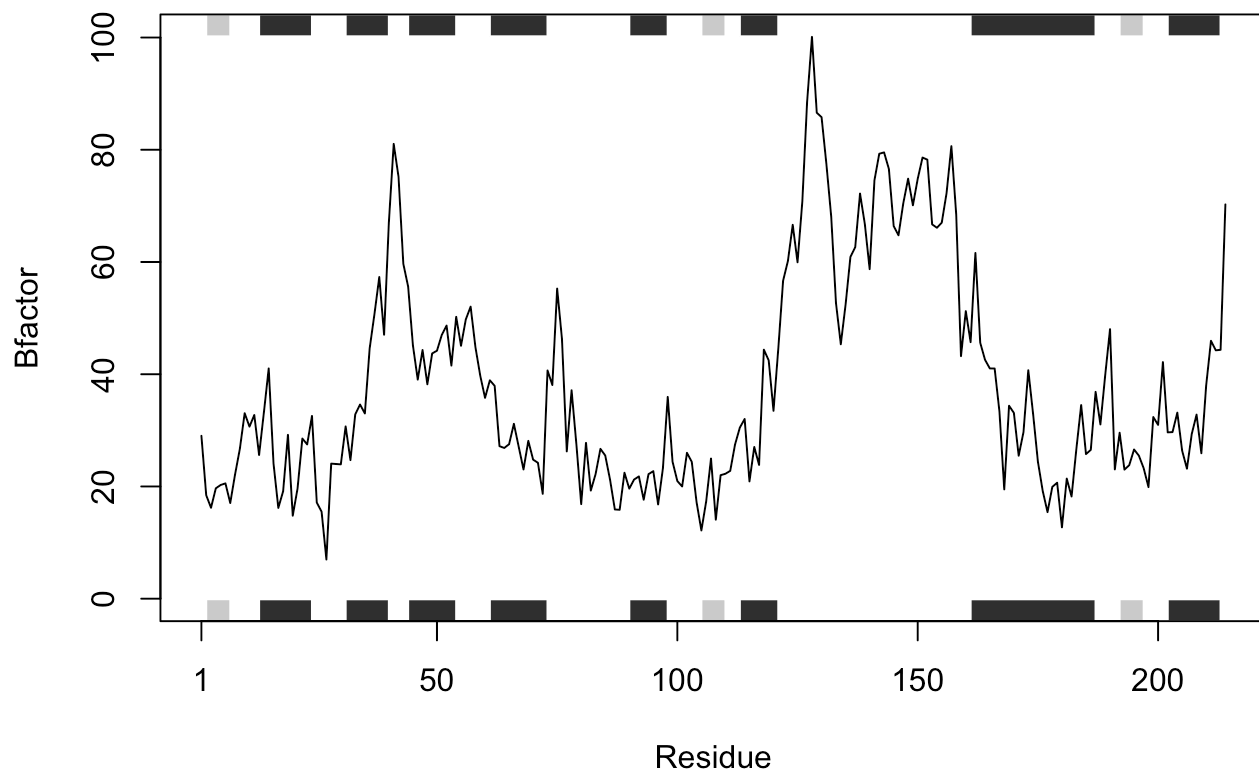
```
s2 <- read.pdb("1AKE") # kinase no drug
```

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

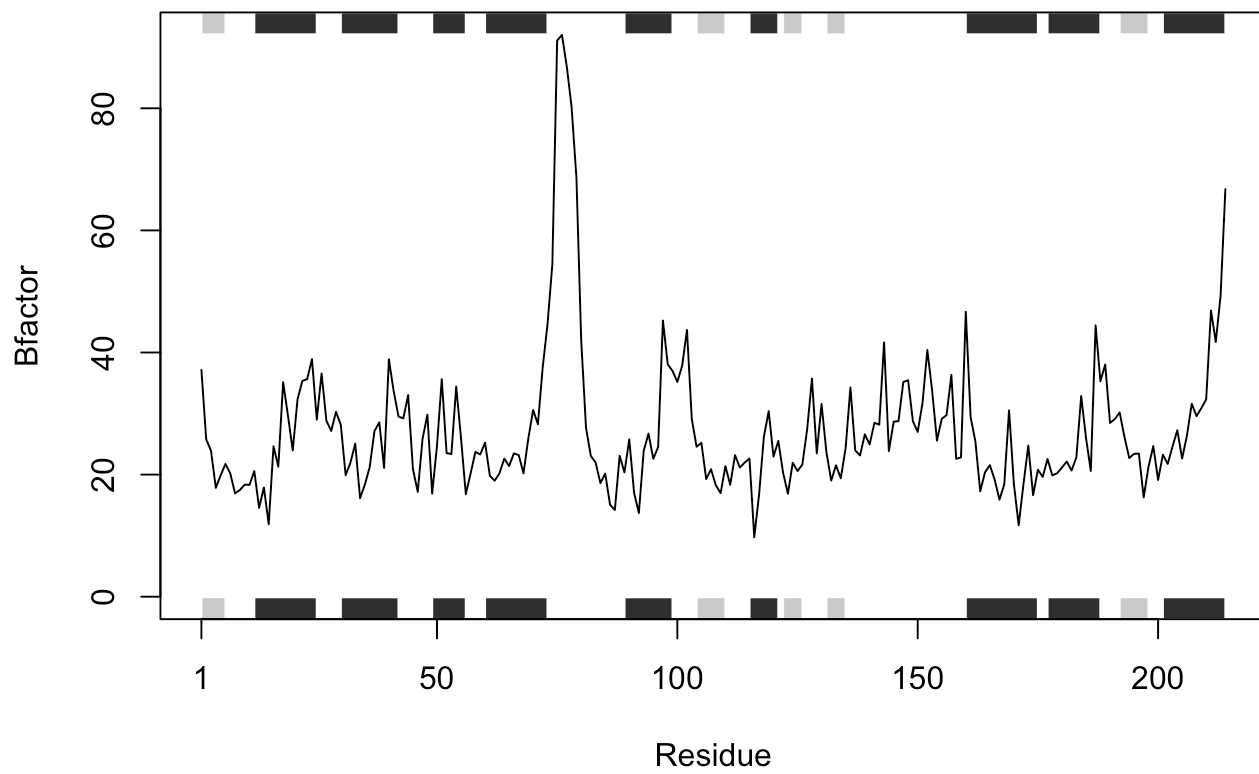
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

Note: Accessing on-line PDB file

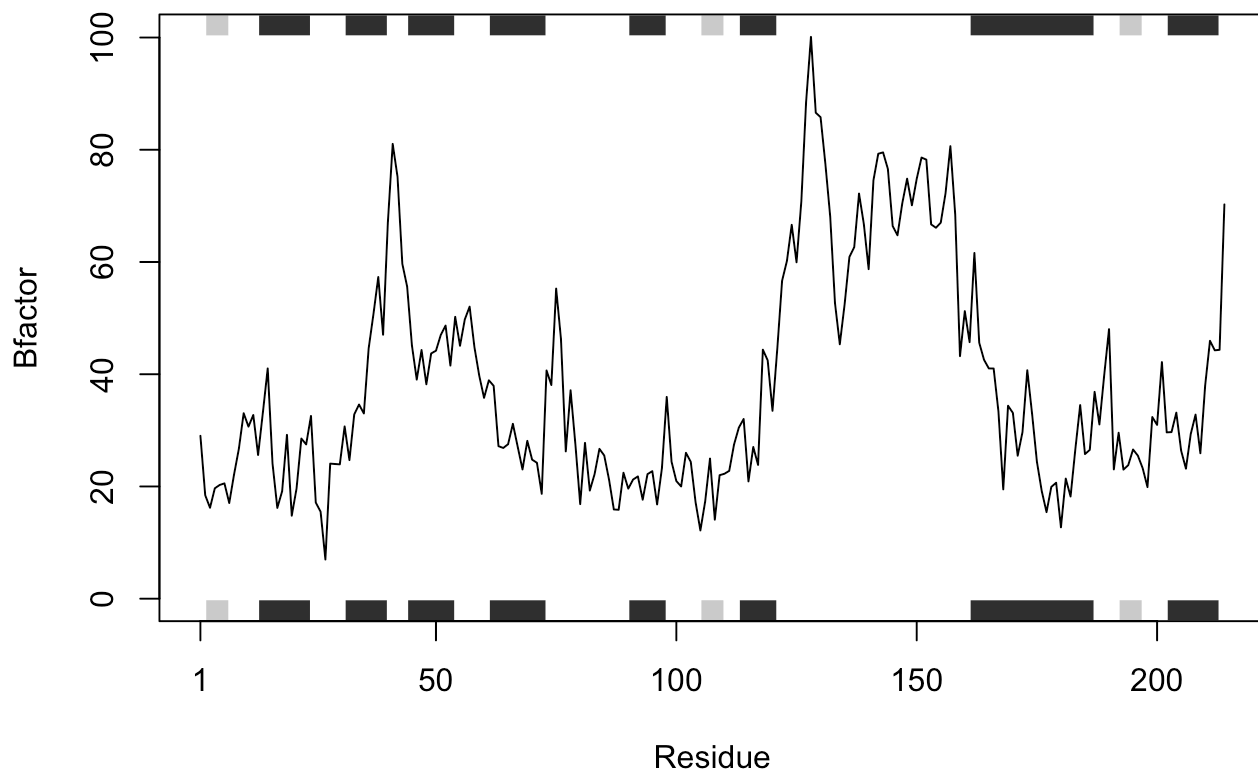
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")  
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")  
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")  
s1.b <- s1.chainA$atom$b  
s2.b <- s2.chainA$atom$b  
s3.b <- s3.chainA$atom$b  
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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



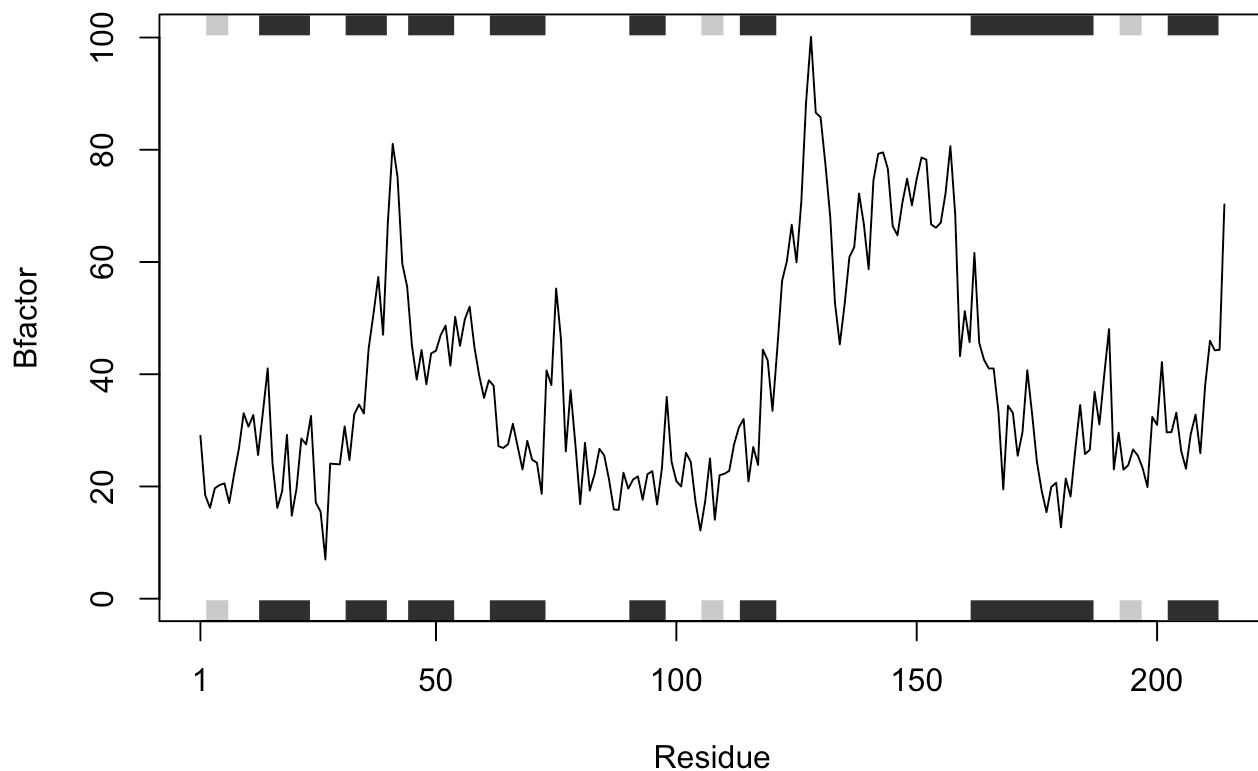
```
plotb3(s3.b, sse=s3.chainA, typ="l", ylab="Bfactor")
```



```
# Inputs: A list of PDB file identifiers (e.g., "4AKE", "1AKE", "1E4Y") to be analyzed.
library(bio3d); lapply(list("4AKE", "1AKE", "1E4Y"), function(pdb) {
  protein <- read.pdb(pdb)
  food <- trim.pdb(protein, chain="A", elety="CA")
  cookie <- food$atom$b
  plotb3(cookie, sse=food, typ="l", ylab="Bfactor")
  cat("Serve sushi ", pdb, "with pasta ")
})
```

Note: Accessing on-line PDB file

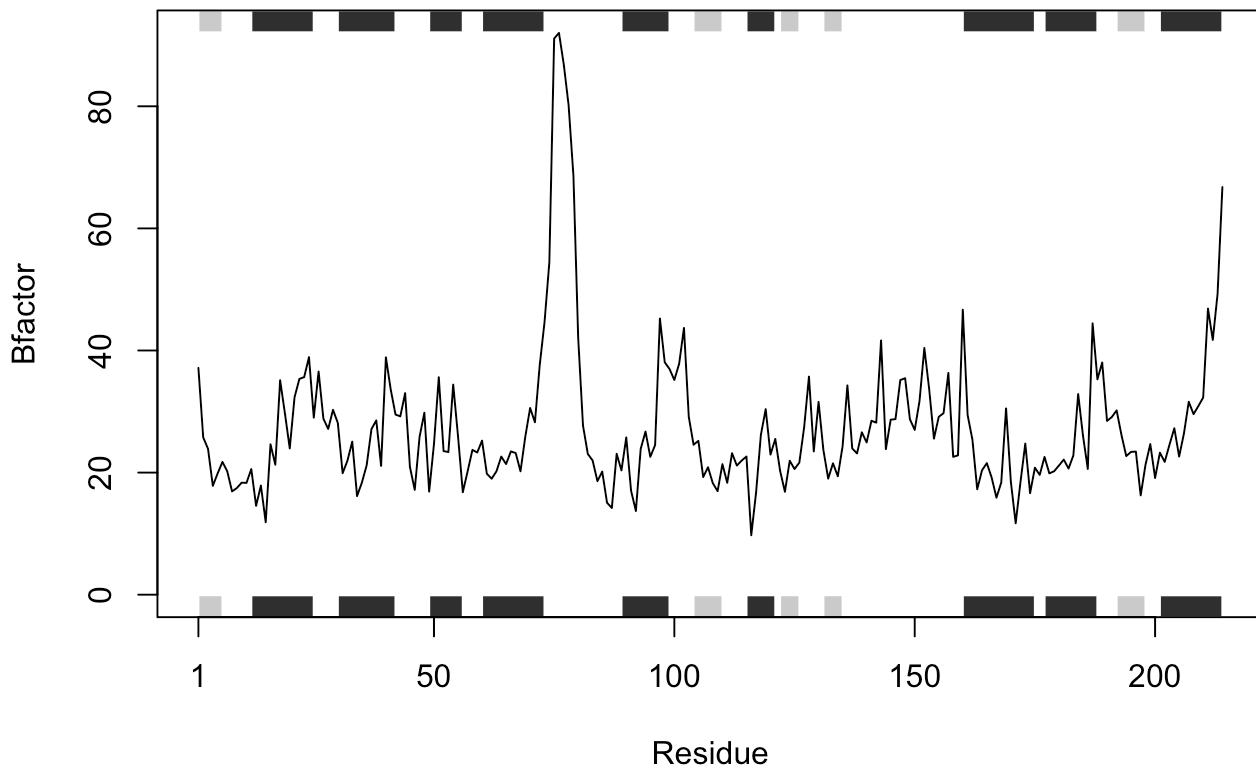
```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/8v/ljcn64zd6bs7yszj9yy3lnc80000gn/T//RtmpjHKOY1/4AKE.pdb exists.
Skipping download
```



Serve sushi 4AKE with pasta Note: Accessing on-line PDB file

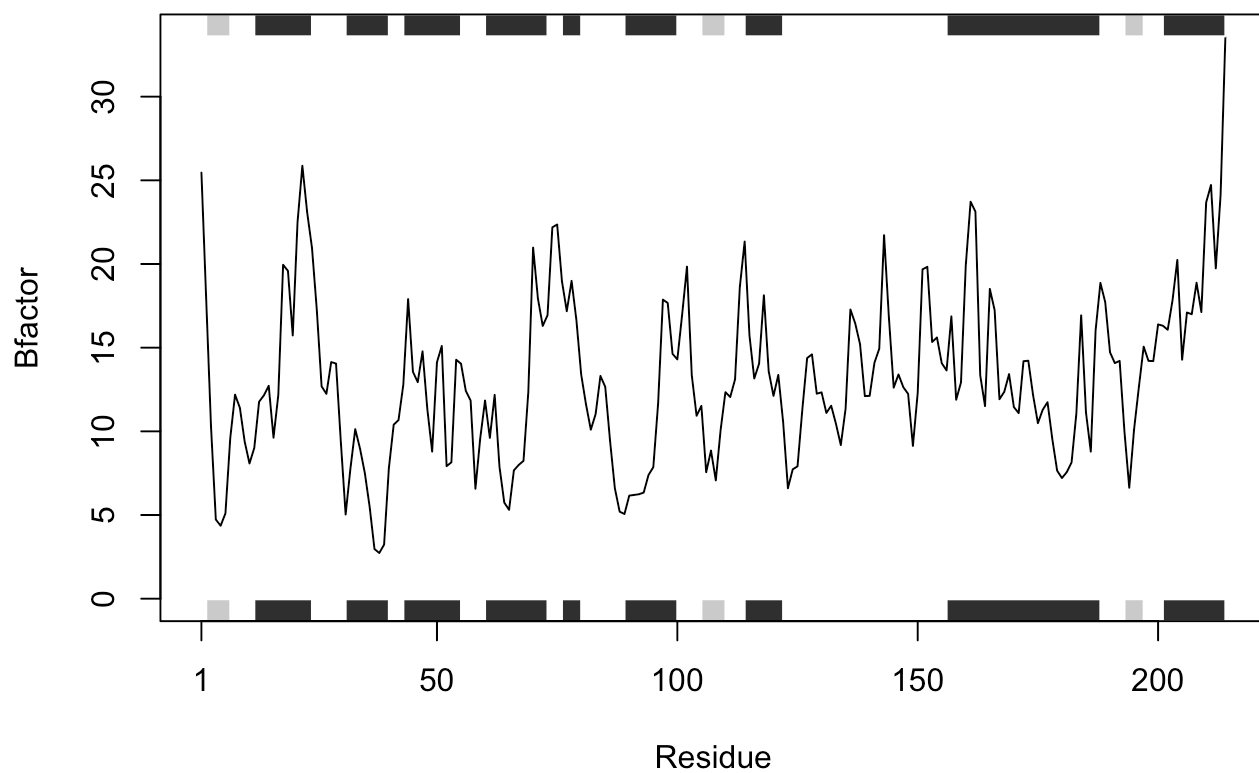
```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):  
/var/folders/8v/ljcn64zd6bs7yszej9yy3lnc80000gn/T/RtmpjHKoY1/1AKE.pdb exists.  
Skipping download
```

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



Serve sushi 1AKE with pasta Note: Accessing on-line PDB file

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):  
/var/folders/8v/ljcn64zd6bs7yszj9yy3lnc80000gn/T//RtmpjHKoY1/1E4Y.pdb exists.  
Skipping download
```



Serve sushi 1E4Y with pasta

[[1]]

NULL

[[2]]

NULL

[[3]]

NULL