

HW Class 6

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Function writing homework

Can you improve this analysis code?

```
library(bio3d)
# Line one of the function : s <- read.pdb (pdbfile)
s1 <- read.pdb("4AKE") # kinase with drug
```

Note: Accessing on-line PDB file

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

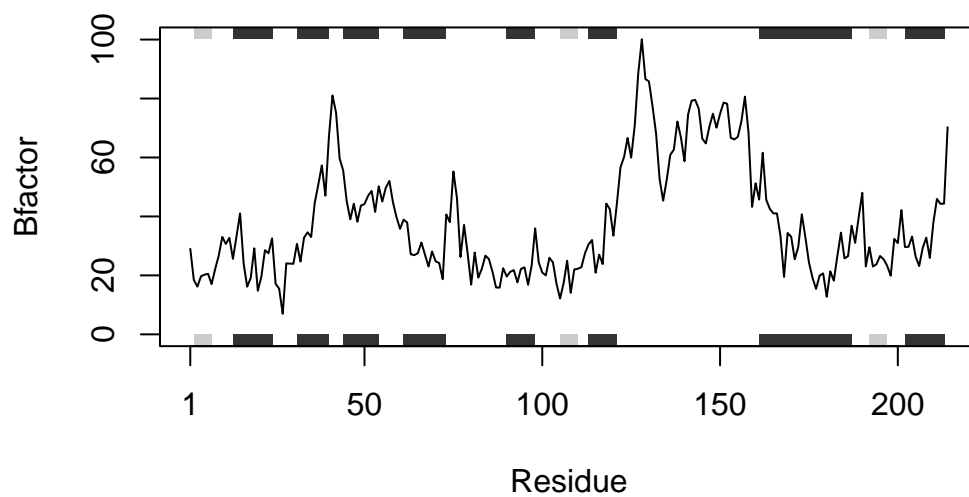
Note: Accessing on-line PDB file

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

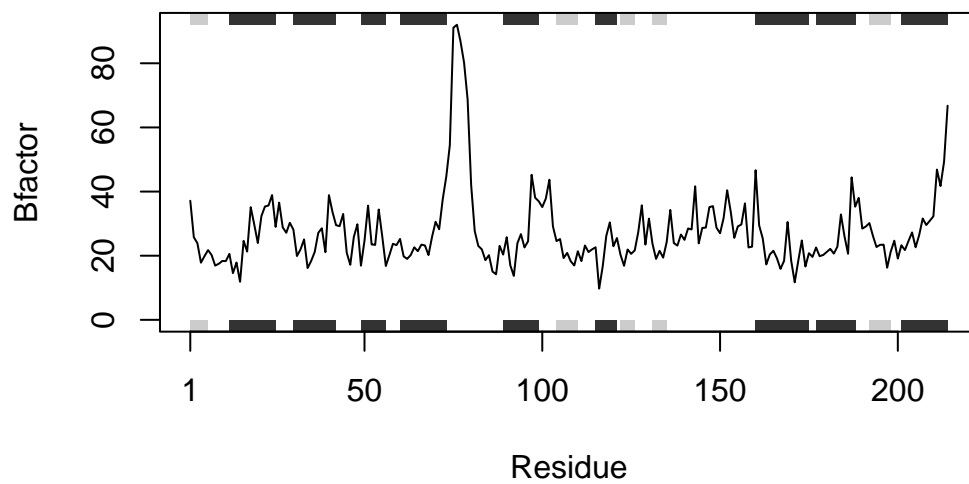
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

Note: Accessing on-line PDB file

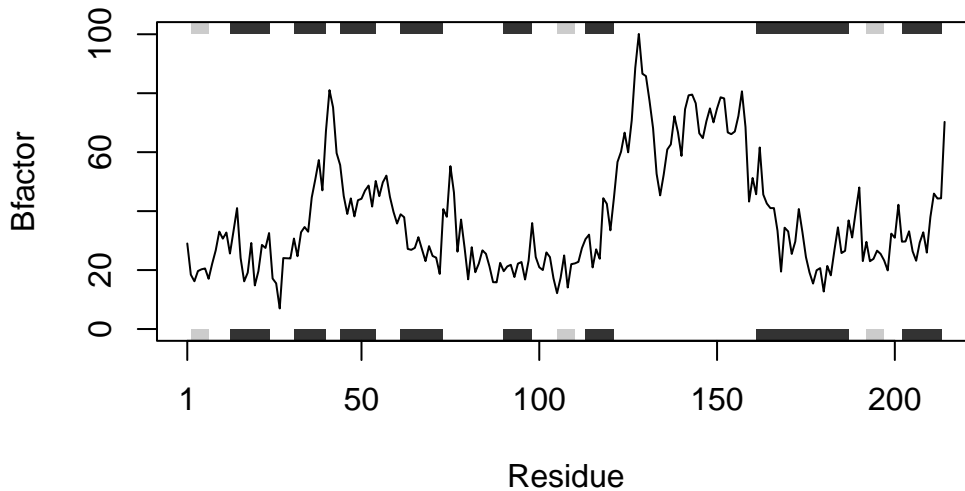
```
# Line two of the function : s.chain <- trim.pdb(s, chain = chainID, elety = "CA")
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")
# Line three of the function : b <- s.chain$atom$b
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
# Line four of the function : plotb3(b, sse = s.chain, typ = "l", ylab = "Bfactor")
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")
```

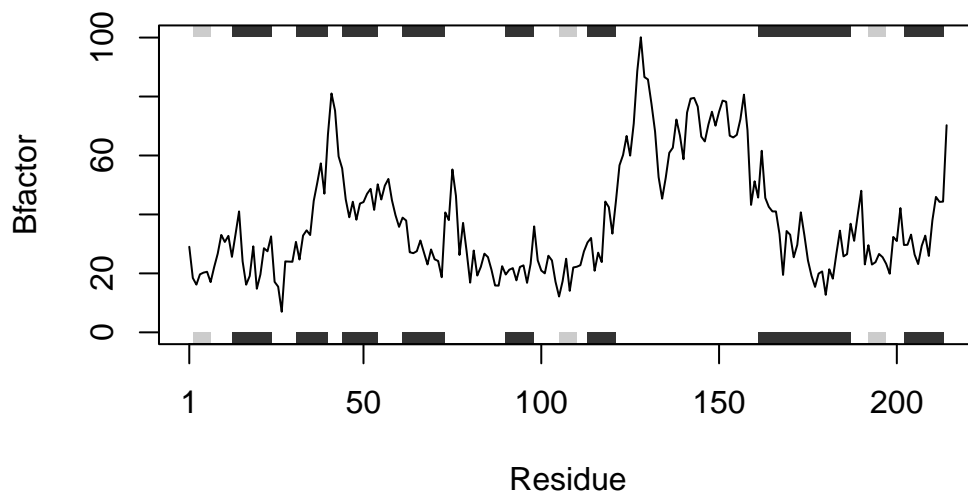


```
# Inputs to function: "pdbfile" like "4AKE" and "chainID" like "A"
# This function reads in a pdb file, trims to specified chain and CA atoms,
# The output of the function is a plot of B-factors for that chain.
plotchain <- function(pdbfile, chainID){
  library(bio3d)
  s <- read.pdb(pdbfile)
  s.chain <- trim.pdb(s, chain=chainID, elety="CA")
  s.b <- s.chain$atom$b
  plotb3(s.b, sse=s.chain, typ="l", ylab="Bfactor")
}

# Example usage:
plotchain("4AKE", "A")
```

Note: Accessing on-line PDB file

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/sj/hml9995936788r67rq_5blm00000gn/T/RtmpPNsisA/4AKE.pdb exists.
Skipping download
```

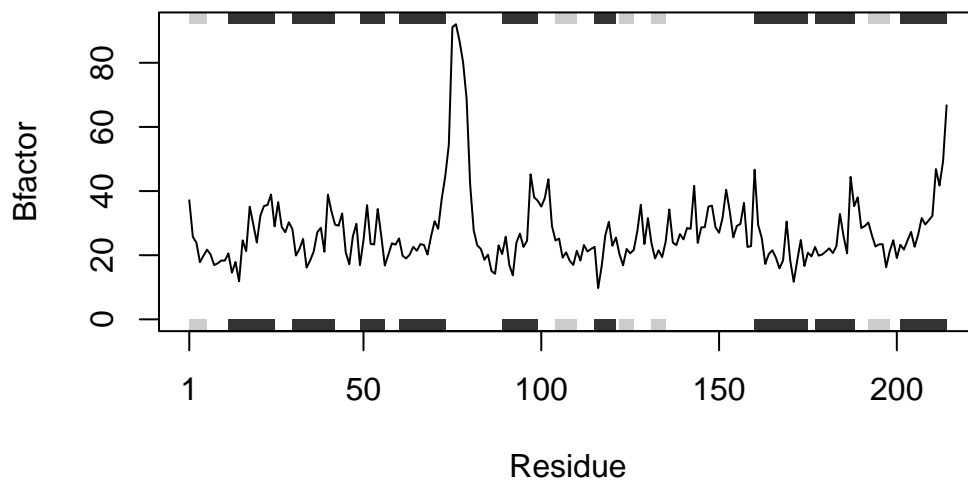


```
plotchain("1AKE", "A")
```

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/sj/hml9995936788r67rq_5blm00000gn/T/RtmpPNsisA/1AKE.pdb exists.
Skipping download

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



```
plotchain("1E4Y", "A")
```

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/sj/hml9995936788r67rq_5blm00000gn/T/RtmpPNsisA/1E4Y.pdb exists.
Skipping download

