homework_for_pdb_analysis

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10/14/2022

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Ensure that you have performed `install.packages("bio3d")`

Example Code:

```
library(bio3d)
#Step one
s1 <- read.pdb("4AKE") # kinase with drug
```

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

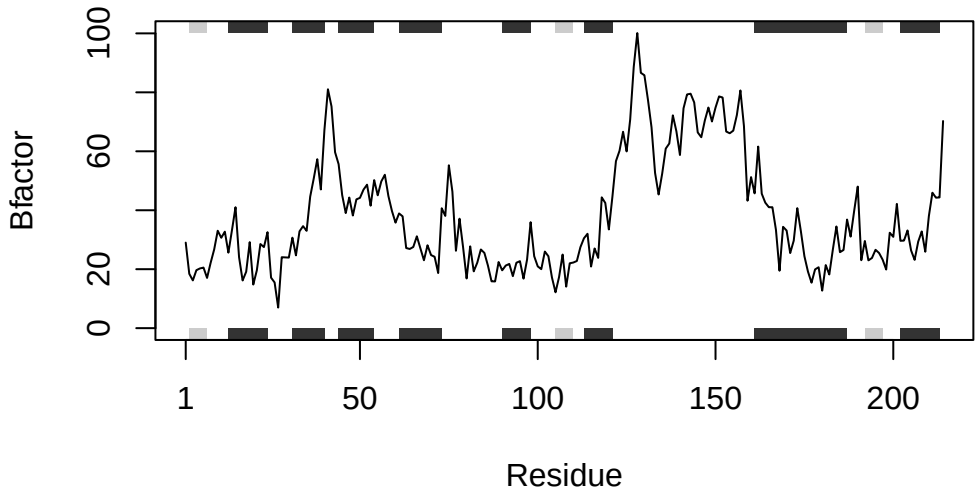
```
s2 <- read.pdb("1AKE") # kinase no drug
```

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

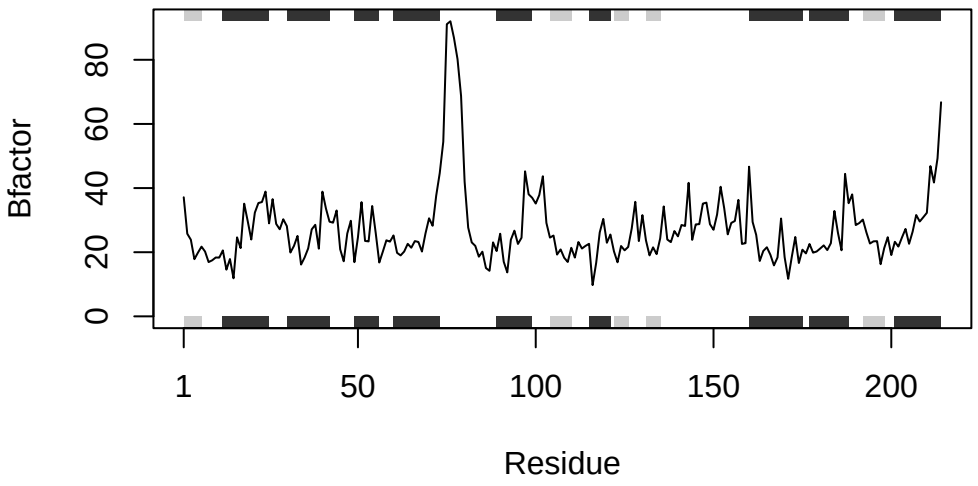
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

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

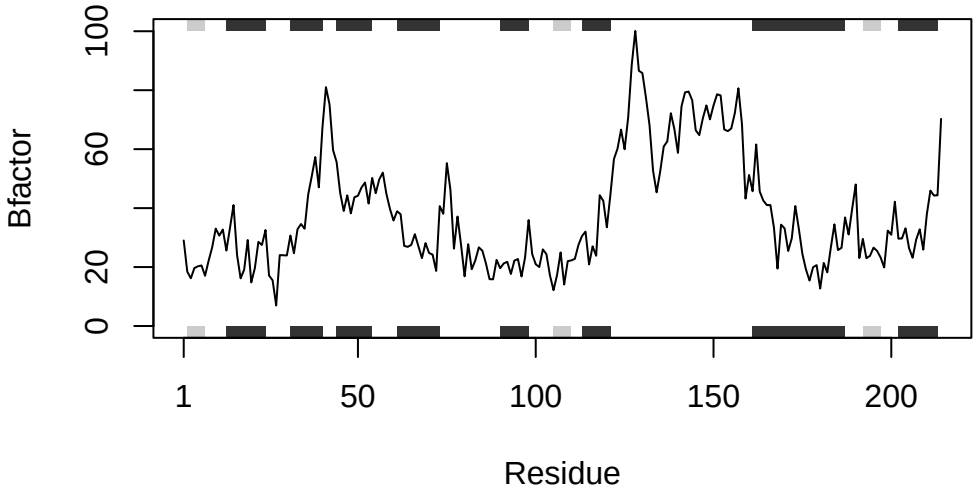
```
#Step two
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")
#Step 3
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
#Step 4
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```




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




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



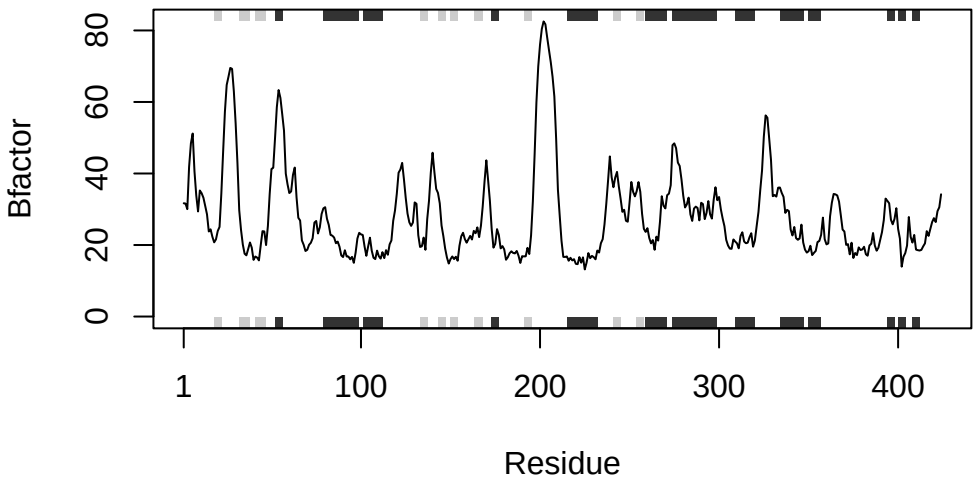
Question 6 How would you generalize the original code above to work with any set of input protein structures?

```
pdbfunction <- function(pdbname){
  pdbinfo <- read.pdb(pdbname)
  pdbinfo.chainA <- trim.pdb(pdbinfo, chain="A", elety="CA")
  pdbinfo.b <- pdbinfo.chainA$atom$b
  plotb3(pdbinfo.b,sse=pdbinfo.chainA,typ="l",ylab="Bfactor")
}
```

Now we want to call the function

```
pdbfunction("1xtg")
```

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

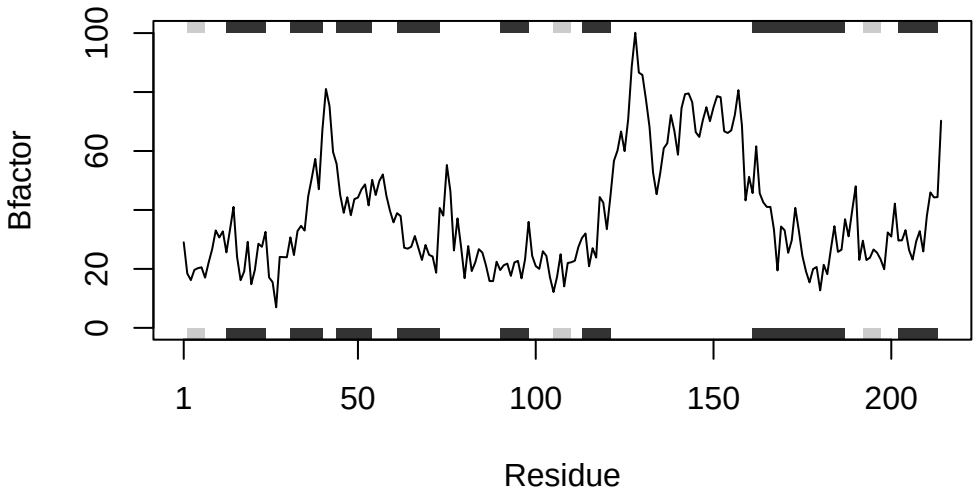



```
#Botulism Neurotox

pdbfunction("4AKE")#without
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/2x/
zrv7p34j78g85m6_r6jg3jrw0000gn/T//RtmpYay7Uc/4AKE.pdb exists. Skipping download
```

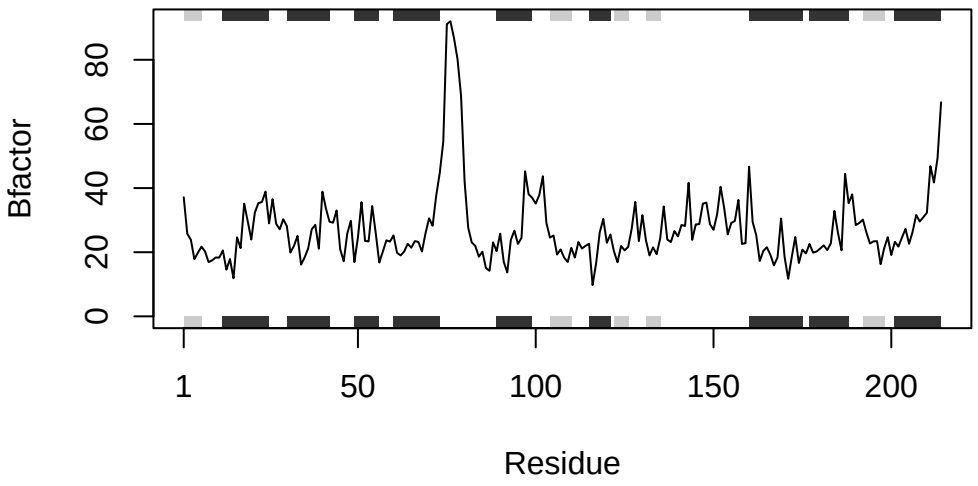



```
pdbfunction("1AKE")#with
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/2x/
zrv7p34j78g85m6_r6jg3jrw0000gn/T//RtmpYay7Uc/1AKE.pdb exists. Skipping download
```

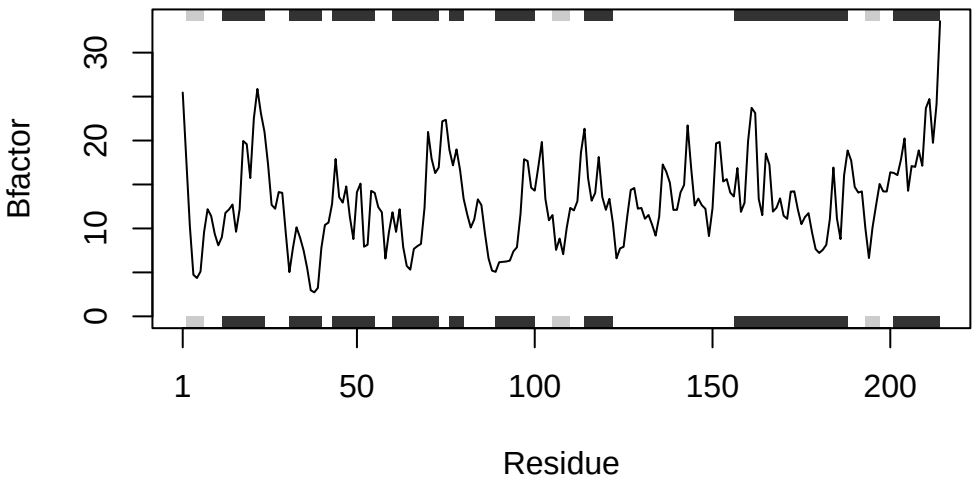
```
   PDB has ALT records, taking A only, rm.alt=TRUE
```




```
pdbfunction("1E4Y")
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/2x/
zrv7p34j78g85m6_r6jg3jrw0000gn/T//RtmpYay7Uc/1E4Y.pdb exists. Skipping download
```


Bfactor
0
10
20
30
1
50
100
150
200
Residue