

# Homework\_6

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```
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

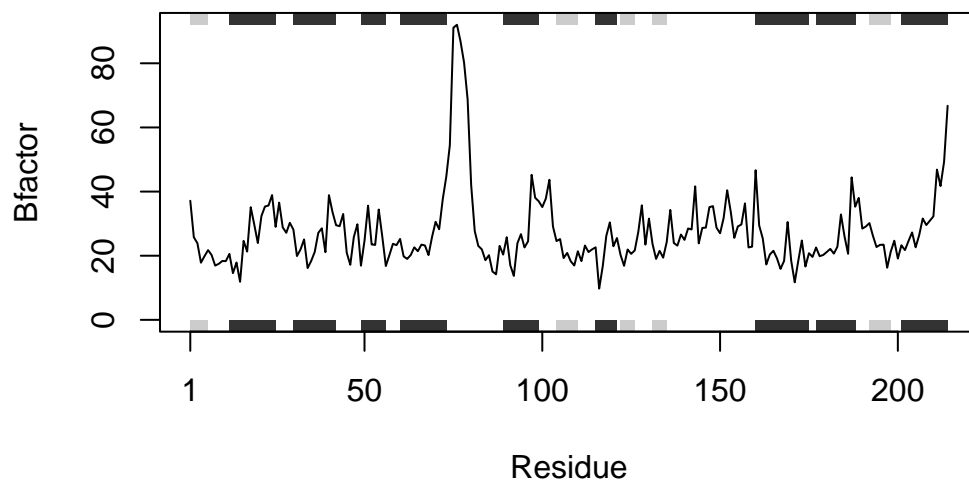
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

Note: Accessing on-line PDB file

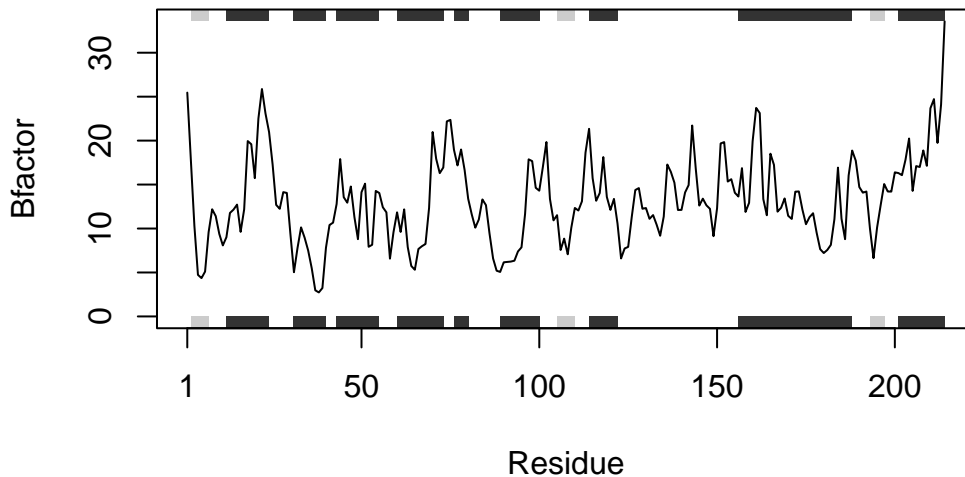
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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



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



## Use asuupy

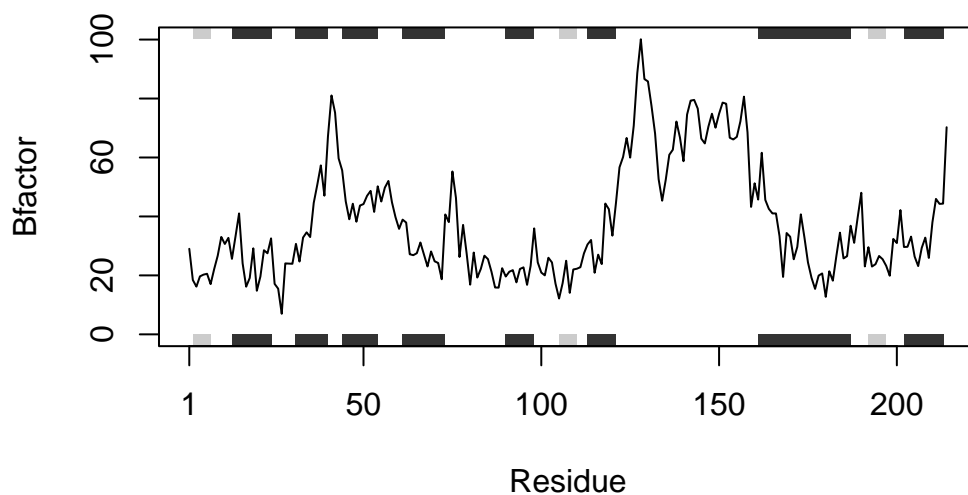
```
Drug_PI <- function(pdb) {  ## takes the pdb data point as the input
  s <- read.pdb(pdb)        ## reads the pdb file
  s_chain <- trim.pdb(s, chain="A", eley= "CA")  ## performs a specfic trim function of si

  s_b <- s_chain$atom$b      ## performs atom specfic on said chain
  plotb3(s_b, sse=s_chain, typ="l", ylab="Bfactor")  ## plots the accession site of said sp
}
```

```
Drug_PI("4AKE")
```

Note: Accessing on-line PDB file

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/_f/_c48_l_x09b103fx36xst2tr0000gn/T/RtmpijnQ0p/4AKE.pdb exists.
Skipping download
```

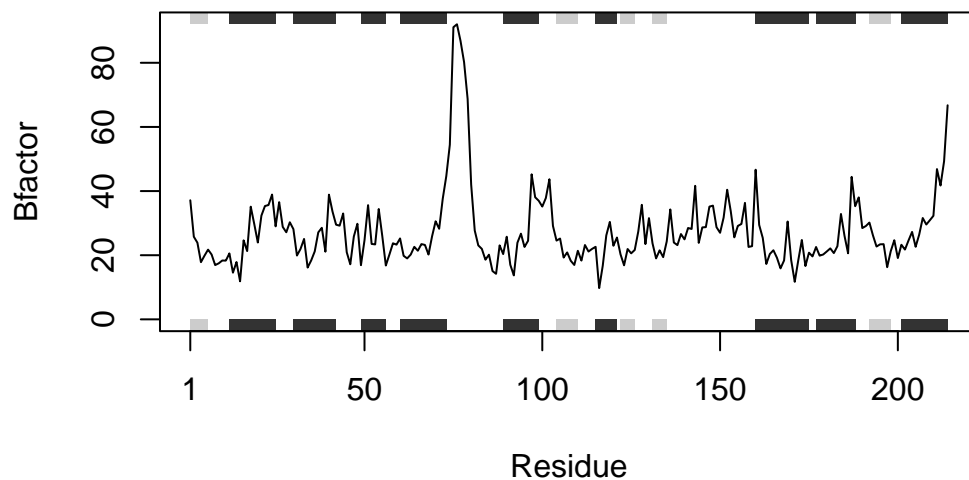


```
Drug_PI("1AKE")
```

Note: Accessing on-line PDB file

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):  
/var/folders/_f/_c48_l_x09b103fx36xst2tr0000gn/T/RtmpijnQ0p/1AKE.pdb exists.  
Skipping download
```

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



```
Drug_PI("1E4Y")
```

Note: Accessing on-line PDB file

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):  
/var/folders/_f/_c48_l_x09b103fx36xst2tr0000gn/T/RtmpijnQ0p/1E4Y.pdb exists.  
Skipping download
```

