

# Class06 HW

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Write a function from the following code

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

Note: Accessing on-line PDB file

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

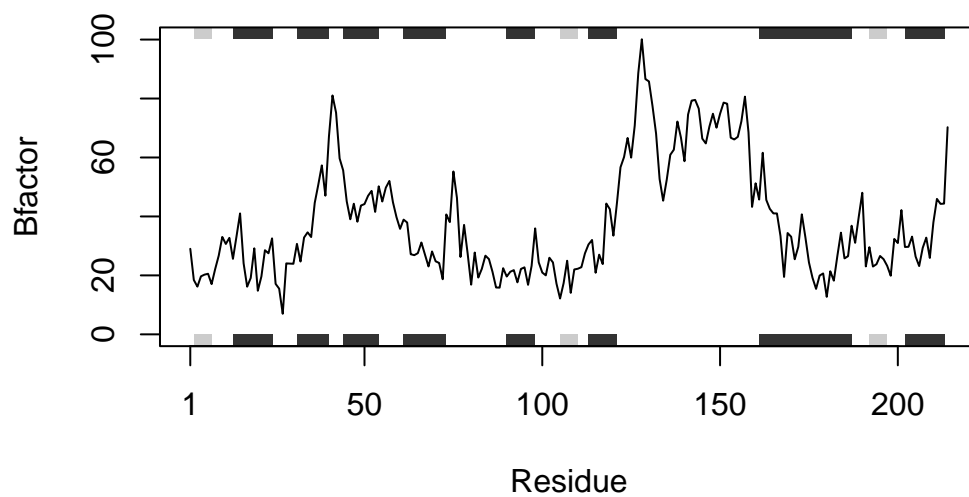
Note: Accessing on-line PDB file

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

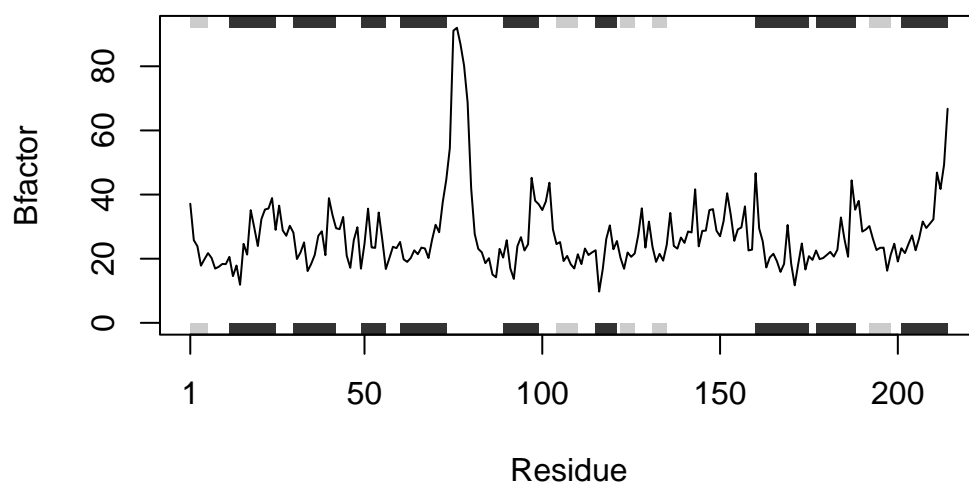
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

Note: Accessing on-line PDB file

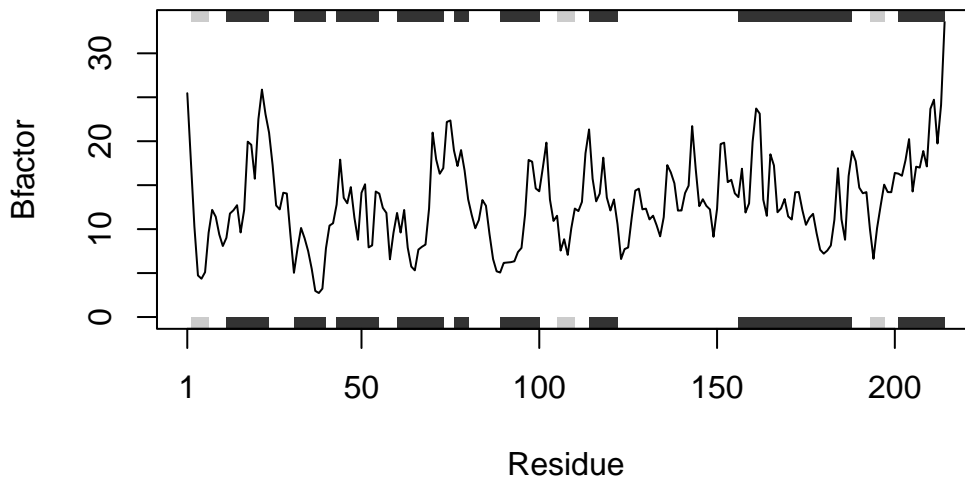
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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



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



```
library(bio3d) #Access bio3d.
graph <- function(n,k)
#n:number of total kinase inputs;
#k:a vector including n kinase PDB IDs.
{
  for(i in 1:n) #A loop goes through n inputs.
  {
    #Get the structure data of kinase k[i] from PDB.
    s <- read.pdb(k[i])
    #Focus on chain A and Ca atoms of kinase k[i].
    s.chainA <- trim.pdb(s,chain="A",elety="CA")
    #Get the B factor value for Ca atoms in chain A of kinase k[i].
    s.b <- s.chainA$atom$b
    #Print out the input PDB ID of kinase k[i]
    cat(k[i])
    #Output the plot showing Bfactor value of Ca vs.
    #residue position in chain A of kinase k[i].
    plotb3(s.b,sse=s.chainA,typ="l",ylab="Bfactor")
  }
}
```

### Input format:

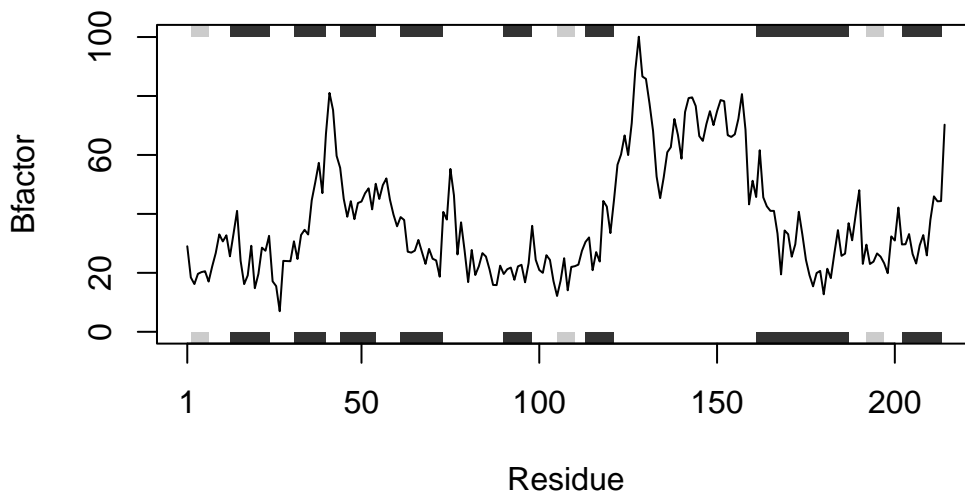
```
graph(number of inputs, c("input 1","input 2",...,"input n"))
```

```
graph(3,c("4AKE","1AKE","1E4Y"))
```

Note: Accessing on-line PDB file

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):  
/var/folders/xx/15z5d5l56hg_8s2365q0dxnm0000gn/T//RtmpeJtlyu/4AKE.pdb exists.  
Skipping download
```

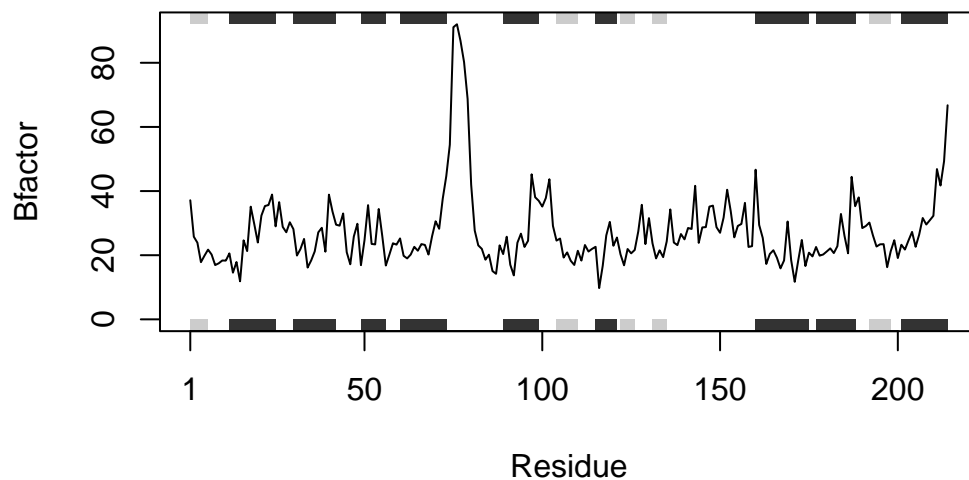
4AKE



Note: Accessing on-line PDB file

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):  
/var/folders/xx/15z5d5l56hg_8s2365q0dxnm0000gn/T//RtmpeJtlyu/1AKE.pdb exists.  
Skipping download
```

```
PDB has ALT records, taking A only, rm.alt=TRUE  
1AKE
```



Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):  
/var/folders/xx/15z5d5l56hg\_8s2365q0dxnm0000gn/T//RtmpeJtlyu/1E4Y.pdb exists.  
Skipping download

1E4Y

