Class 6 HW

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```
library(bio3d)
```

```
Warning: package 'bio3d' was built under R version 4.3.3
```

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

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

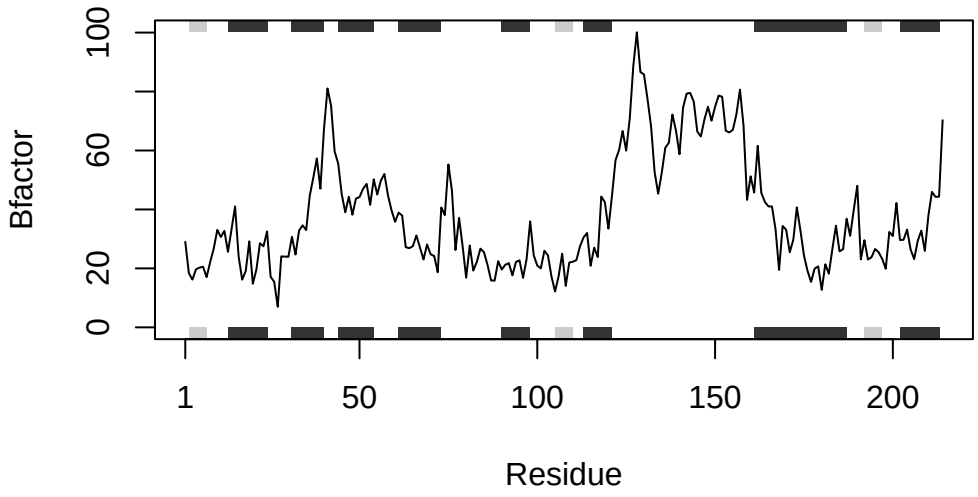
```
s2 <- read.pdb("1AKE") # kinase no drug
```

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

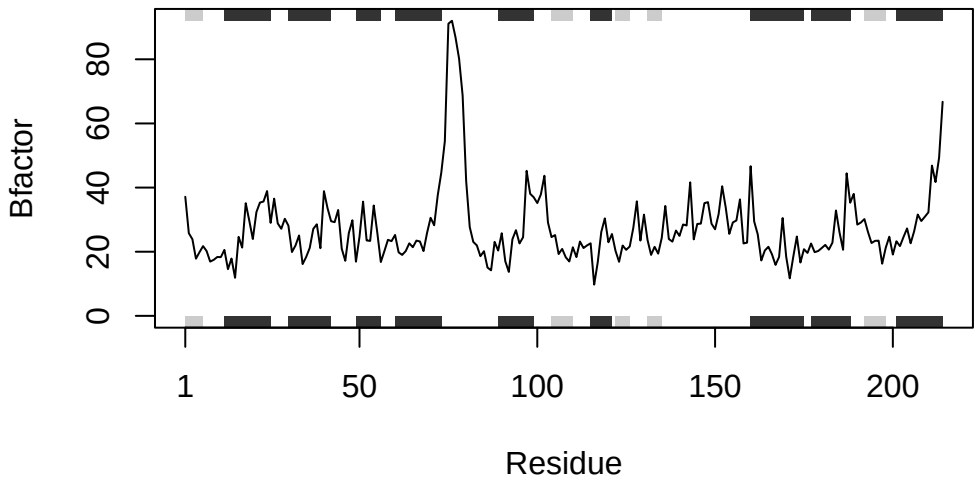
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

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

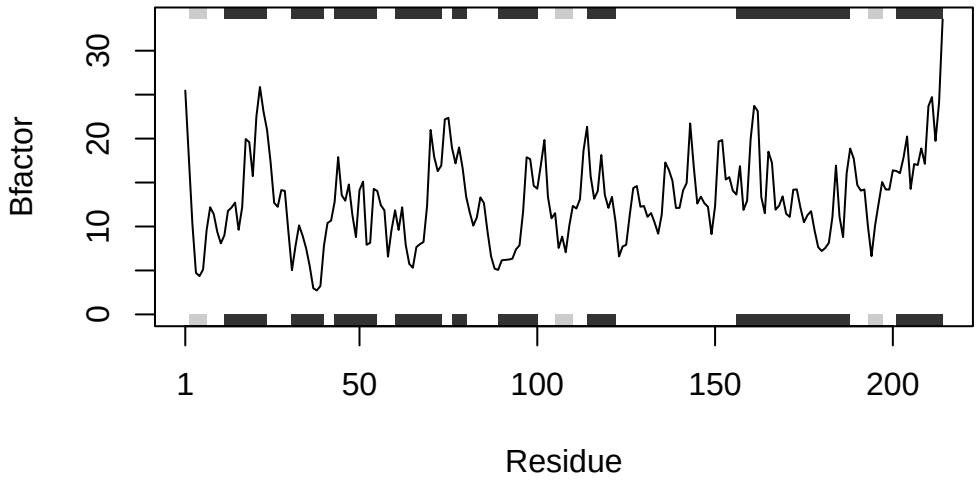
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")

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")
```



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

```
any_protein <- function(read.pdb) {
  s1 <-read.pdb("4AKE")
  s2 <-read.pdb("1AKE")
  s3 <-read.pdb("1E4Y")
  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")
  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")
}
read.pdb(c("4AKE"))
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\allen\AppData\Local\Temp\Rtmp2HryIh/4AKE.pdb exists. Skipping download
```

```
 Call:  read.pdb(file = c("4AKE"))

   Total Models#: 1
     Total Atoms#: 3459,  XYZs#: 10377  Chains#: 2  (values: A B)

     Protein Atoms#: 3312  (residues/Calpha atoms#: 428)
     Nucleic acid Atoms#: 0  (residues/phosphate atoms#: 0)

     Non-protein/nucleic Atoms#: 147  (residues: 147)
     Non-protein/nucleic resid values: [ HOH (147) ]

   Protein sequence:
      MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAAVKSGSELGKQAKDIMDAGKLVT
      DELVIALVKERIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVDRI
      VGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKDDQEETVRKRLVEYHQMTAPLIG
      YYSKEAEAGNTKYAKVDGTKPVAEVRADLEKILGMRIILLGAPGA...<cut>...KILG

+ attr: atom, xyz, seqres, helix, sheet,
        calpha, remark, call
```