Class 6 Homework'

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title: "Class 6 Homework"' author: "Janie Chang-Weinberg (PID: A69037446)" format: pdf editor: visual

10/18/24 Homework (Class 6)

What hath been bestowed upon us:

```r
# Can you improve this analysis code?
library(bio3d)
s1 <- read.pdb("4AKE") # kinase with drug
```

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

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

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

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

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

```r
s1.chainA <- trim.pdb(s1, chain="A", elety="CA") #elety means "element type"
s2.chainA <- trim.pdb(s2, chain="A", elety="CA") #CA means "alpha carbon"
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")
```


2

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


Residue
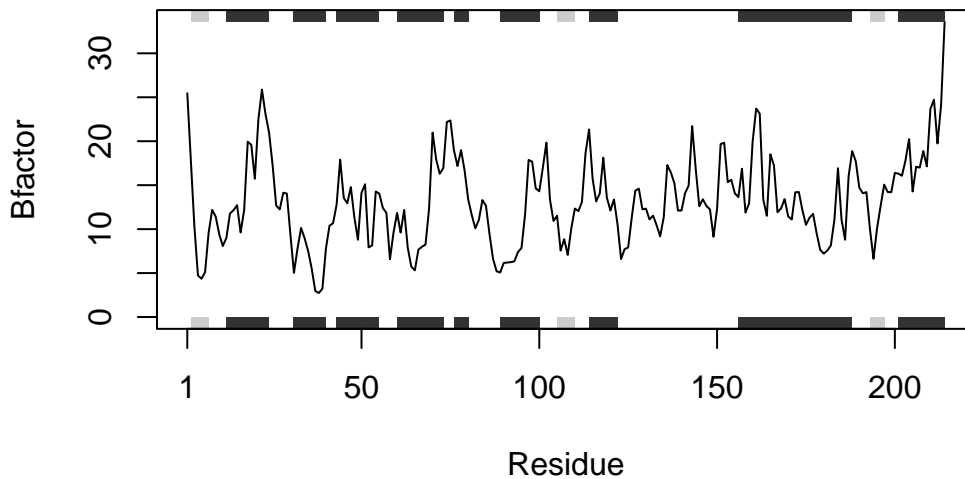
My attempt:

```
pleppy <- function(pepseq){ #pepseq is whatever peptide name you want to look for
  library(bio3d) #loads the bio3d library

  s <- read.pdb(pepseq) #will search the db for whatever pepseq you want, assigned    to varia

  s.chainA <- trim.pdb(s, chain="A", elety="CA") #this narrows your search to just    the "A"

  s.b <- s.chainA$atom$b #further narrows your search to the "B-factor" of the        protein

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

}
```
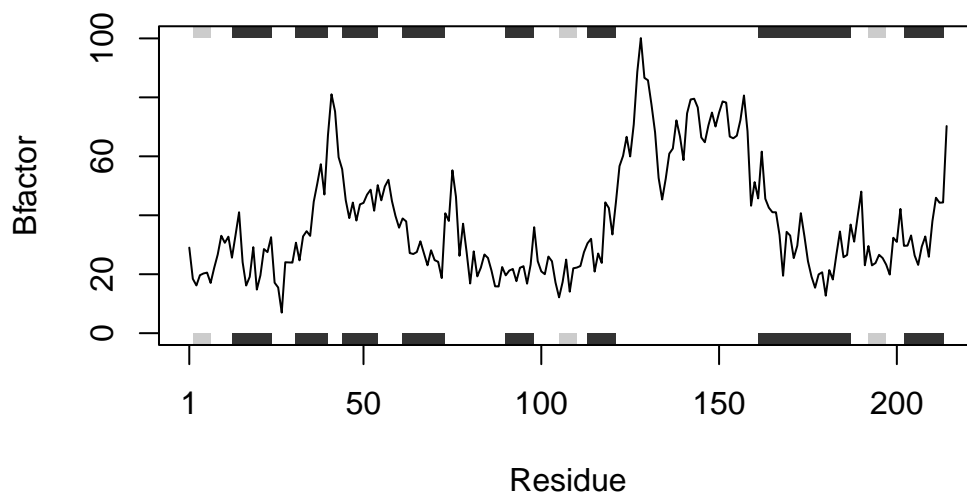
Now plot all 3 peptides

```
test_peps <- c("4AKE", "1AKE", "1E4Y")
sapply(test_peps, pleppy)
```
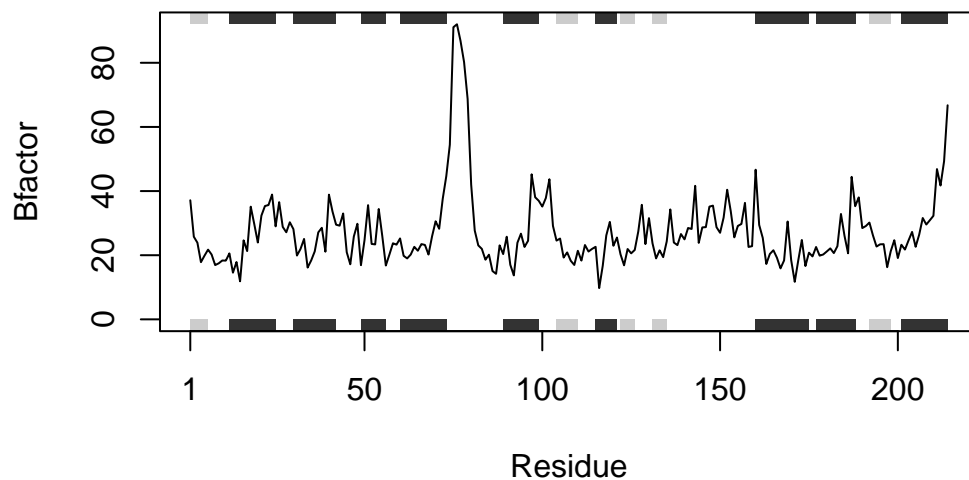
```
Note: Accessing on-line PDB file
```

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/f_/cyy9xbr92bvbqb1y55vkxd5h0000gn/T//RtmpAvUI3y/4AKE.pdb exists.
Skipping download
```
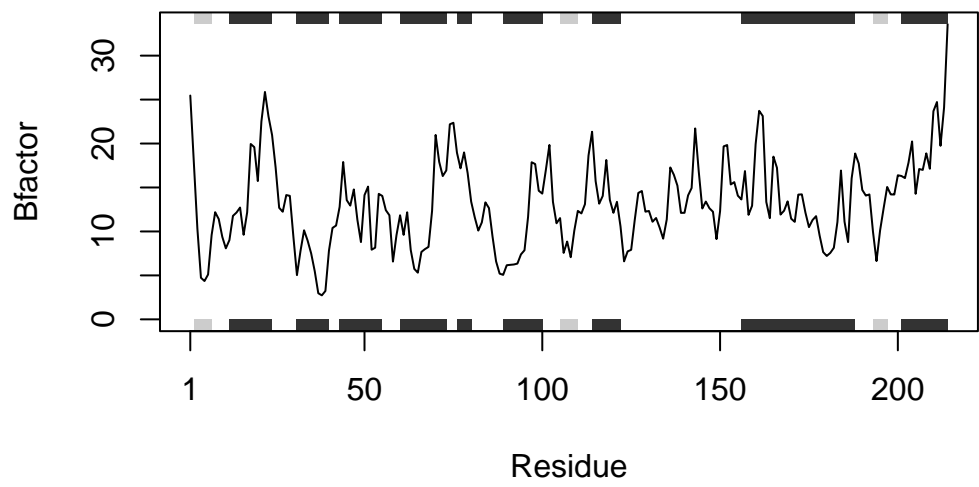


```
Note: Accessing on-line PDB file
```

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/f_/cyy9xbr92bvbqb1y55vkxd5h0000gn/T//RtmpAvUI3y/1AKE.pdb exists.
Skipping download
```

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

Note: Accessing on-line PDB file

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/f_/cyy9xbr92bvbqb1y55vkxd5h0000gn/T//RtmpAvUI3y/1E4Y.pdb exists.
Skipping download
```

```
$`4AKE`
NULL

$`1AKE`
NULL

$`1E4Y`
NULL
```