HW_Class06

Mari Williams (PID: A15858833)

Q6 function

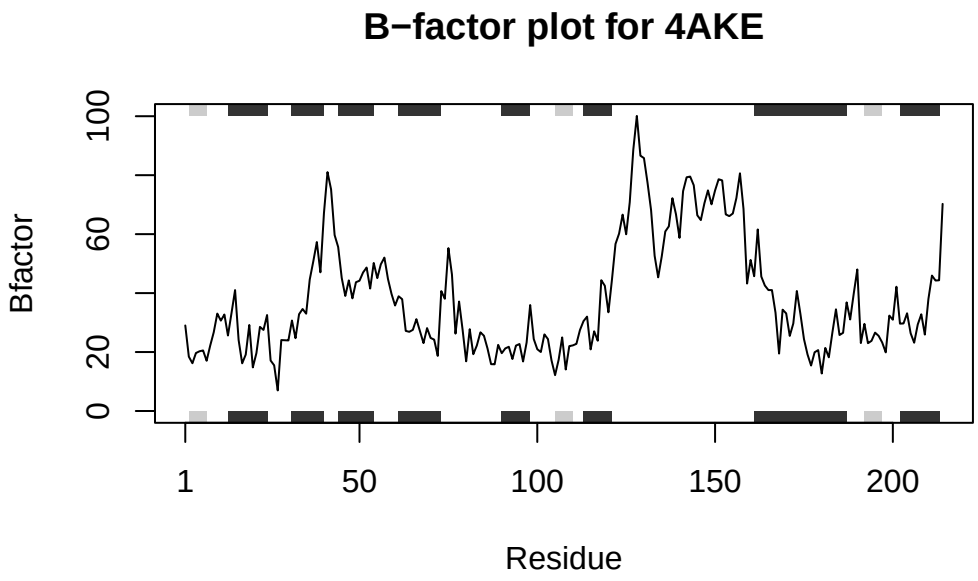
```
library(bio3d)
```

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

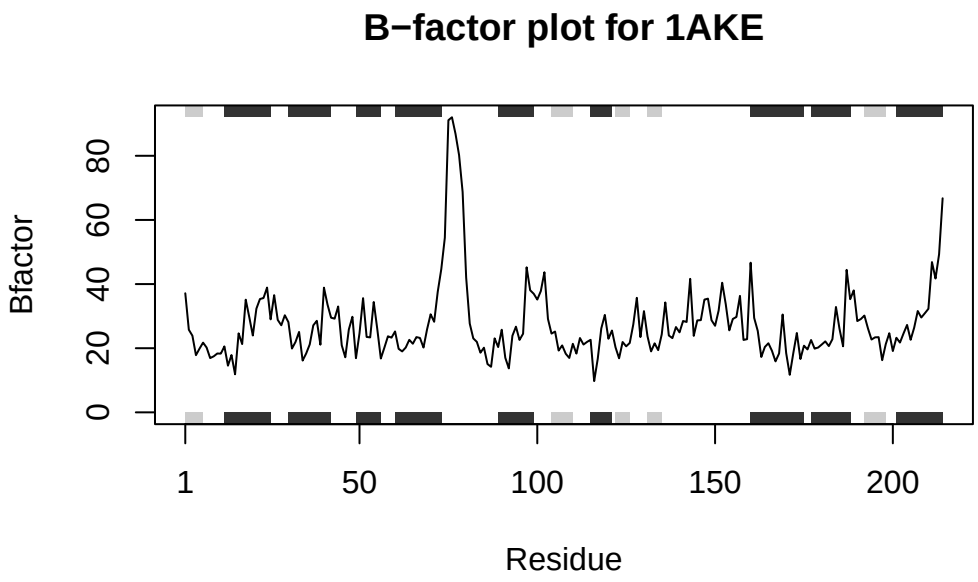
```
#This function will load in the PDB data and create
#plots of the B-factor values of the the Chain A alpha carbons

#Define function with one input, the pdb code we want to analyse
pro <- function(pdb_code){

  #loads in pdb data from the input code
  s <- read.pdb(pdb_code)

  #Filters the pdb data to only include the atoms we want,
  #in this case the alpha carbon atoms in chain A
  s.chainA <- trim.pdb(s, chain ="A", elety="CA")

  #extracts the B-factor, which measures disorder/flexibility
  s.b <-s.chainA$atom$b

  #Plots the b factors as a line plot, visualizing regions that
  #are more disordered than others
  plotb3(s.b, sse=s.chainA,
         typ="l",
         ylab="Bfactor",
         main = paste("B-factor plot for", pdb_code) )
```

```
}
#call function invisibly to suppress R console response
invisible(sapply(c("4AKE", "1AKE", "1E4Y"), pro))
```

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




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




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