HW 6

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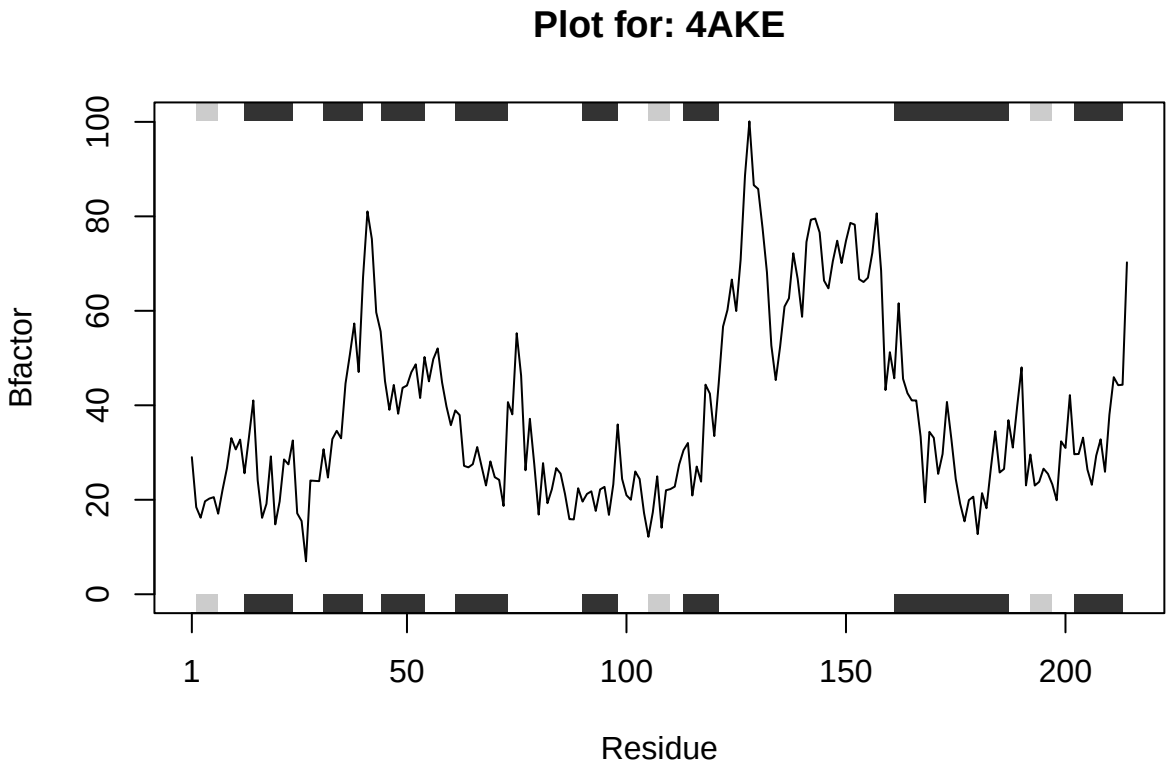
```
library(bio3d)
```

```
## Warning: package 'bio3d' was built under R version 4.2.3
```

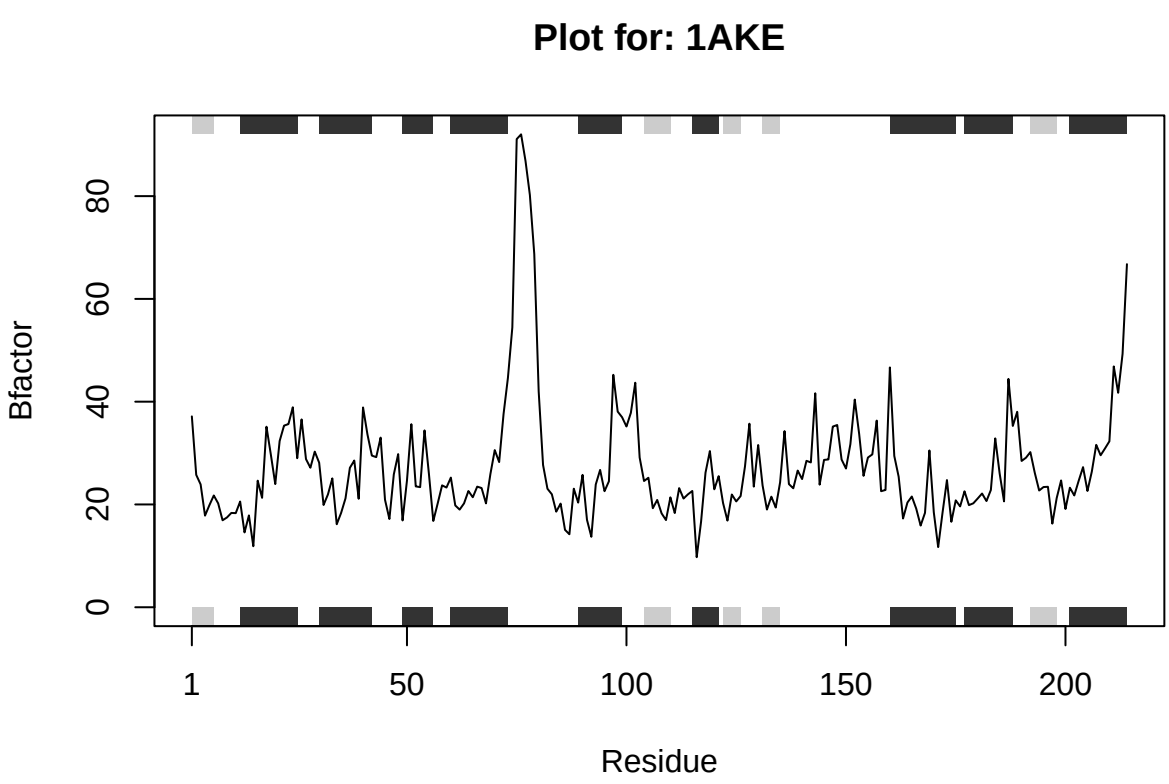
```
# Creating function to analyze protein drug interactions by reading in protein PDB data
# The function takes in a PDB ID as input
# The function outputs a plot of B-factor values vs residue for the specified protein
# The function reads in a protein structure from its PDB ID, trims it to get the CA atoms from chain A,
analyze_protein_interaction <- function(pdb_id) {
  # Reads PDB ID
  s <- read.pdb(pdb_id)

  # Gets CA atoms from chain A
  s.chainA <- trim.pdb(s, chain='A', elety='CA')

  # Gets B-factors
  s.b <- s.chainA$atom$b

  # Plots B-factors
  plotb3(s.b, sse=s.chainA, typ='l', ylab='Bfactor', main = paste("Plot for:", pdb_id))
}
```

```
pdb_ids <- c("4AKE", "1AKE", "1E4Y")

# Iterating through list of ids and calling analyze_pdb function on each PDB ID
for (id in pdb_ids) {
  analyze_protein_interaction(id)
}
```

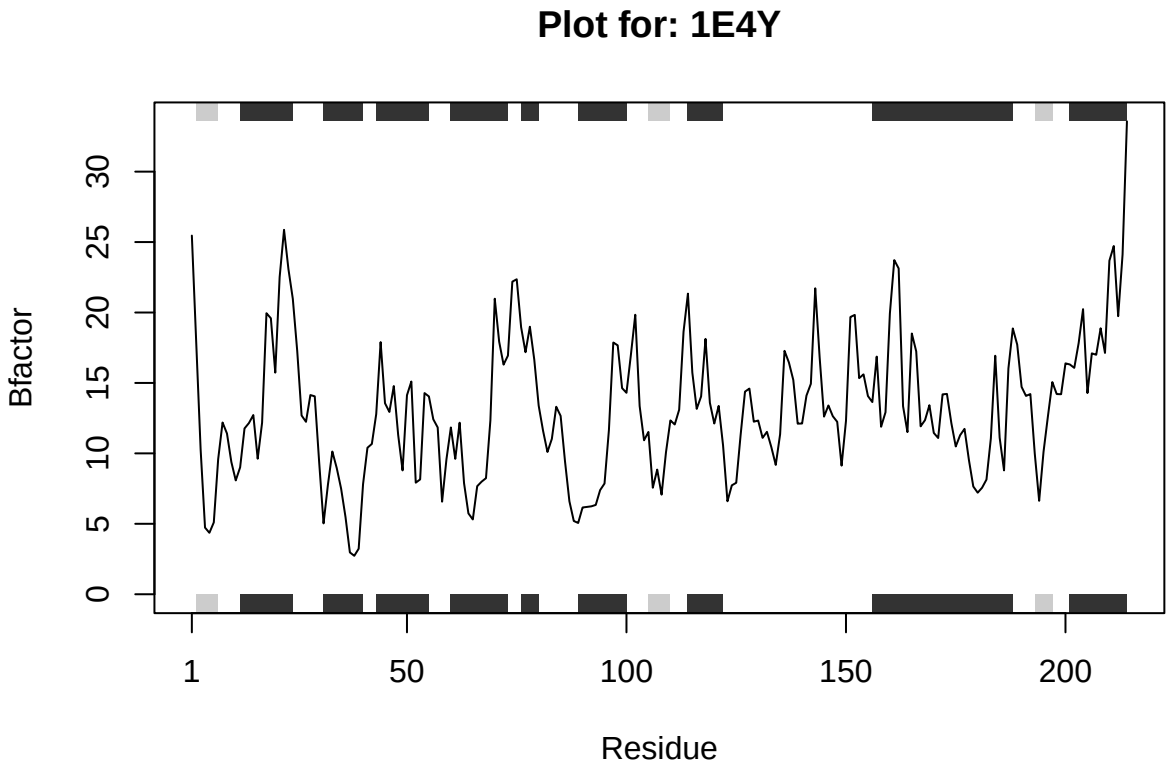
```
##   Note: Accessing on-line PDB file
```




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




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


Plot for: 1E4Y
Bfactor
0
5
10
15
20
25
30
1
50
100
150
200
Residue