

BIMM143 Class06 HW

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Q6. How would you generalize the original code above to work with any set of input protein structures? Write your own function starting from the code above that analyzes protein drug interactions by reading in any protein PDB data and outputs a plot for the specified protein. (See class lecture 9 for further details)

Original Provided 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

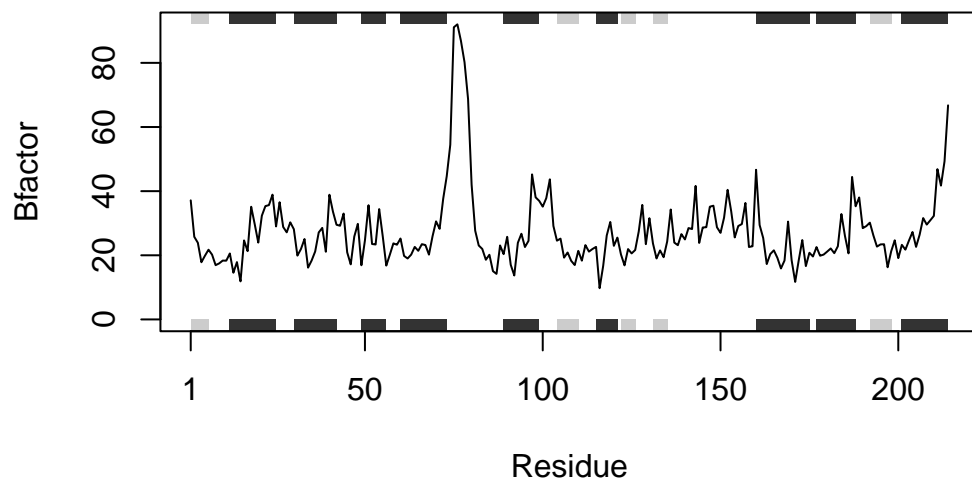
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

Note: Accessing on-line PDB file

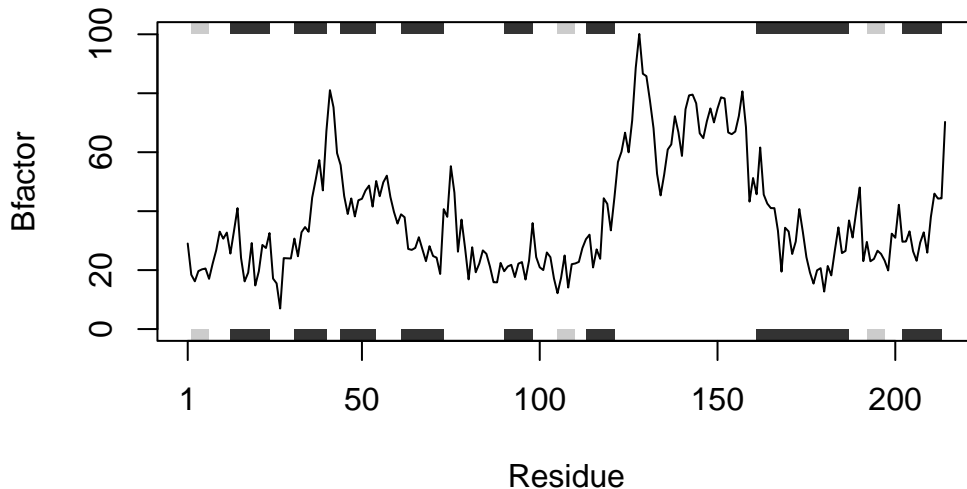
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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



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



Notes on the purpose/function of the provided code:

Used to define new more specific objects by trimming the pdb file: 1st term is the file, 2nd term defines chain A, third term is the atom type; CA is alpha carbons)

```
# s1.chainA <- trim.pdb(s1, chain="A", eley="CA")
```

This is selecting for the B factor of each atom that is included in the trimmed pdb structure; B factor is a measure of the flexibility of a residue: high b factor is more mobility

```
# s1.b <- s1.chainA$atom$b
```

The plotb3 function creates plots of 3d protein structures with their b factors The first argument is what contain the b factors, 2nd is for the secondary structure elements that can be displayed in the plot, in this case the sse should come from the trimmed pdb files; 3rd indicates that it should be a line plot; 4th indicates the label for the y axis

```
# plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```

My condensed function:

```

# the variable x is the input to the function, a pdb file
x <- "1AKE"
# I defined my function as plotpdb; gave it the input x (the pdb file)
plotpdb <- function(x) {
  s.chainA <- trim.pdb(read.pdb(x), chain="A", elety="CA")
  s.bfactor <- s.chainA$atom$b
  plotb3(s.bfactor, sse=s.chainA, typ="l", ylab="Bfactor")
}

#s.chainA: defines trimmed pdb file, with selection for chain A and alpha carbons, uses
#the pdb file x as the input
#s.bfactor: defines the b factor, takes the s.chainA variable previously defined as input
#plotb3: plots the b factor (first argument) against the protein structure from the
#trimmed pdb file (second argument)

#all together my function plotpdb reads and trims a pdb file, defines the b factor;
#and makes a plot output of b factor against protein structure from the input of a pdb file

plotpdb(x)

```

Note: Accessing on-line PDB file

```

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/6m/bxkzd5k95wvb_h3m4fx08vvm0000gn/T/Rtmpdhh64s/1AKE.pdb exists.
Skipping download

```

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

