HW06

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Q1. What type of object is returned from the read.pdb() function? #typeof()

It is a list

Q2. What does the trim.pdb() function do?

It trims a PDB Object To A Subset of Atoms and produces a new smaller PDB object, containing a subset of atoms.

Q3. What input parameter would turn off the marginal black and grey rectangles in the plots and what do they represent in this case?

#top = FALSE, bot = FALSE

In this case, the black(gray20) rectangles represents alpha helices in the chainA of corresponding kinase, the gray(gray80) rectangles represents beta strands in the chainA of corresponding kinase.

Q4. What would be a better plot to compare across the different proteins?

To stack B Factor lines of different proteins to a single plot.

Q5. Which proteins are more similar to each other in their B-factor trends. How could you quantify this?

#hc <- hclust(dist(rbind(s1.b, s2.b, s3.b)))

#plot(hc)

"1AKE" and "1E4Y" are more similar to each other in their B-factor trends, which is shown in the Dendrogram. They share Height:250

Q6. How would you generalize the original code above to work with any set of input protein structures?

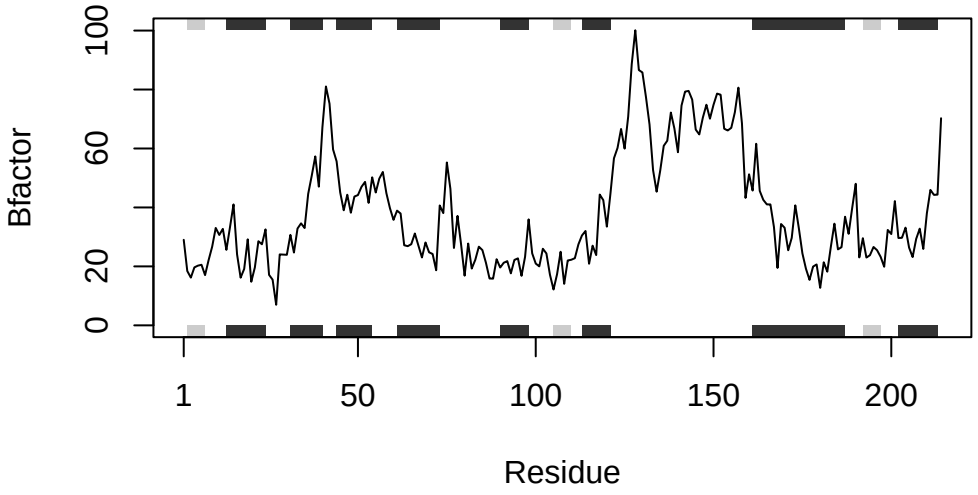
```
library(bio3d)

#PDB code to be analyzed are integrated to the 'vector_of_PDB_Code' vector
```

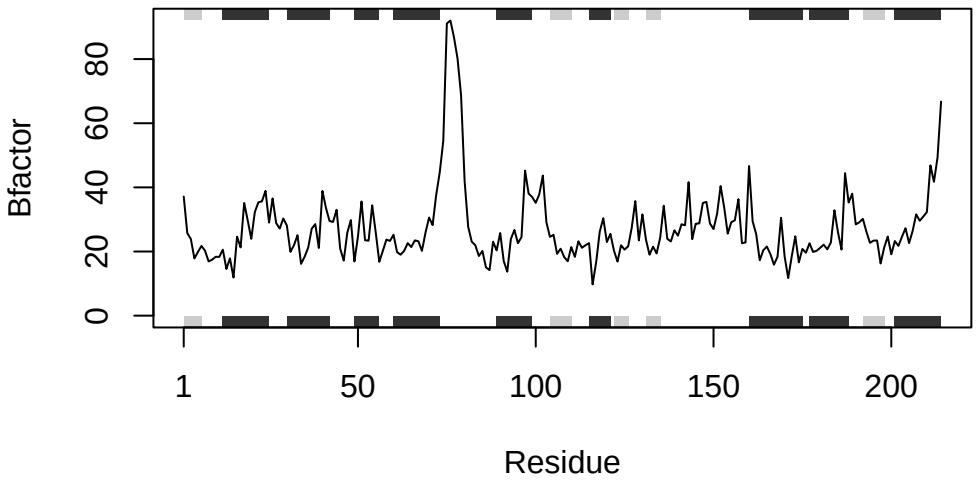
```
#Elements to be analyzed in input 'vector_of_PDB_Code'
#(new line)should be a (PDB_Code, Chain) vector
stru_analysis <- function(vector_of_PDB_Code){
  #Define a subfunction to analyze a single code
  analysis_of_one_Code <- function(Element_to_be_analyzed){
    s <- read.pdb(Element_to_be_analyzed[1])
    s.chain <- trim.pdb(s, chain= Element_to_be_analyzed[2], elety="CA")
    s.b <- s.chain$atom$b
    plotb3(s.b, sse=s.chain, typ="l", ylab="Bfactor")
  }
  #Analyze every PDB code in the vector_of_PDB_Code
  apply(matrix(vector_of_PDB_Code,nrow=2), 2, analysis_of_one_Code)
  #Below is to obtain the dendrogram plot
  #Define a subfunction to obtain the B Factor
  B_Factor <- function(Element_to_be_analyzed){
    s.b <- trim.pdb(read.pdb(Element_to_be_analyzed[1]),
                    chain= Element_to_be_analyzed[2],
                    elety="CA")$atom$b
  }
  transx <- apply(matrix(vector_of_PDB_Code,nrow=2), 2, B_Factor)
  #transx is also a matrix which is the transposition of
  #(new line)rbind(s1.b, s2.b, s3.b, ..., sn.b)
  hc <- hclust( dist( t(transx) ) )
  #dendrogram plot
  plot(hc)
  #The branch of dendrogram plot is numbered from 1 to n
  #(new line)corresponding to the sequence of input Element_to_be_analyzed
}
```

```
#Test the performance of function
vector_of_PDB_Code <- c(c("4AKE","A"), c("1AKE","A"), c("1E4Y","A"))
stru_analysis(vector_of_PDB_Code)
```

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

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Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\30396\AppData\Local\Temp\RtmpuOZokn/4AKE.pdb exists. Skipping download

  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\30396\AppData\Local\Temp\RtmpuOZokn/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):
C:\Users\30396\AppData\Local\Temp\RtmpuOZokn/1E4Y.pdb exists. Skipping download
```

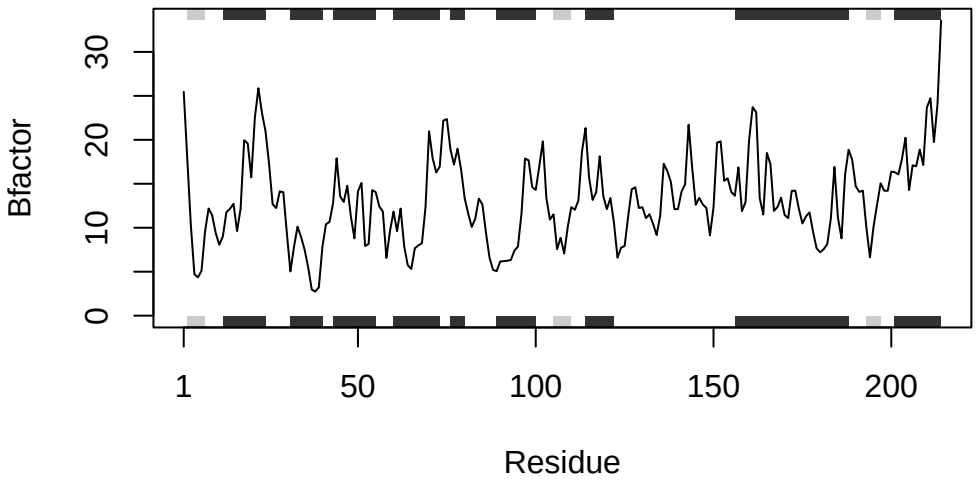

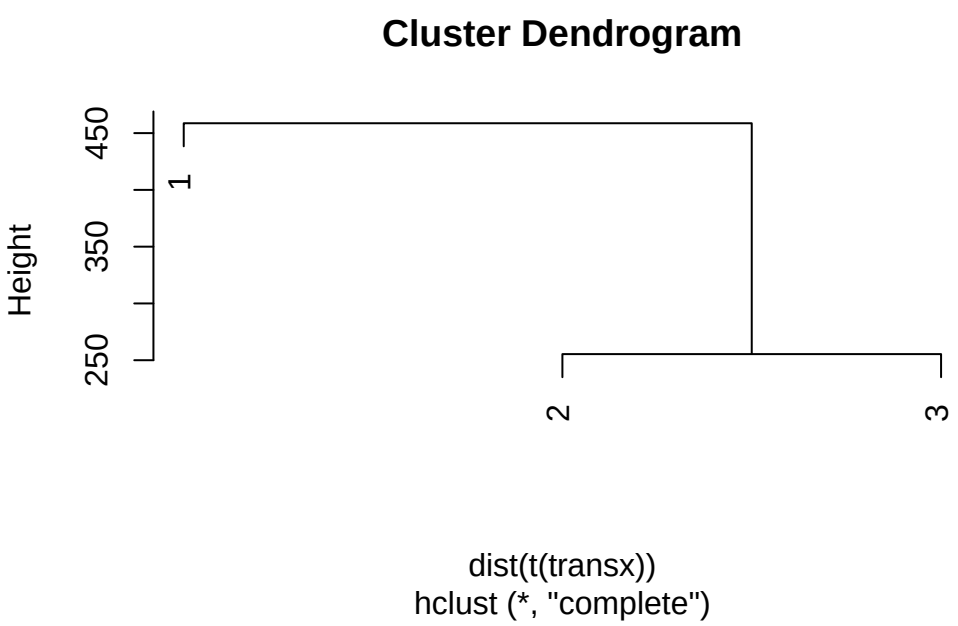
Cluster Dendrogram
Height
450
350
250
1
2
3
dist(t(transx))
hclust (*, "complete")