

Class06HW

Dhruv

```
RUN <- function(x){ # x is a variable which specifies the PDB accession number

library(bio3d) #calling the package bio3d after installing the package

PDB_Read <- read.pdb(x) #calls and reads the PDB database and returns the information that

PDB_trim <- trim.pdb(PDB_Read, chain="A", eley="CA") #confines search to chain A, and CA :

add_b_factor <- PDB_trim$atom$b #Returns the b factor for each residue

plotb3(add_b_factor, sse = PDB_trim, typ="l", ylab="Bfactor") # plots residues on x axis as
return(x) #returns value for x, in this case the graph
}

RUN("1AKE") #if you want to only search for one PDB entry
```

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

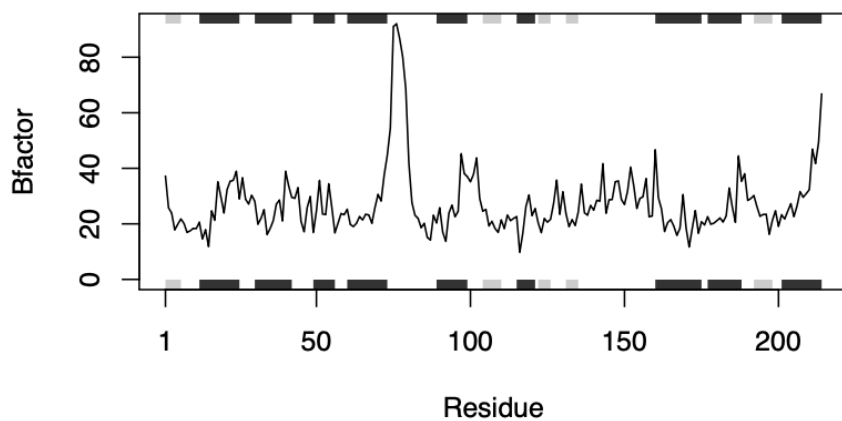
```
[1] "1AKE"
```

```
sapply(c("1AKE", "4AKE", "1E4Y"),RUN) # if you want to look for multiple PDB entries at once
```

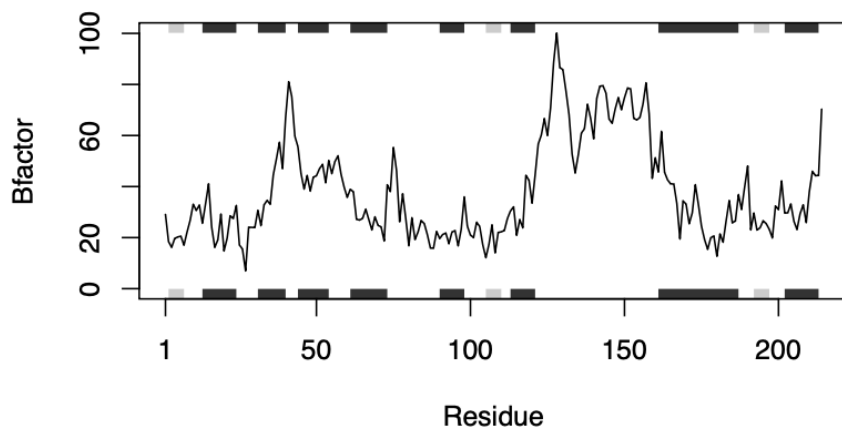
Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/lc/sgvmgnjn49q1m8n1ggfj8gz00000gn/T//RtmpUTMxDm/1AKE.pdb exists.
Skipping download

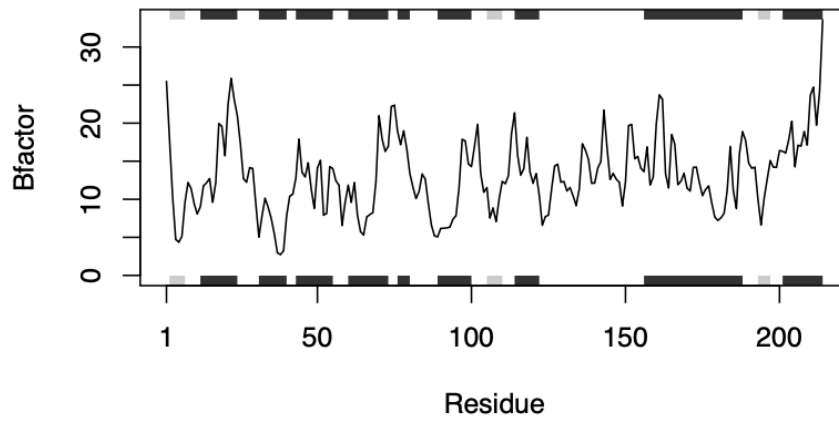
PDB has ALT records, taking A only, rm.alt=TRUE



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Note: Accessing on-line PDB file



1AKE 4AKE 1E4Y
"1AKE" "4AKE" "1E4Y"