R Functions

Xiaoyan Wang

2024-10-21

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

```
library(bio3d)
```

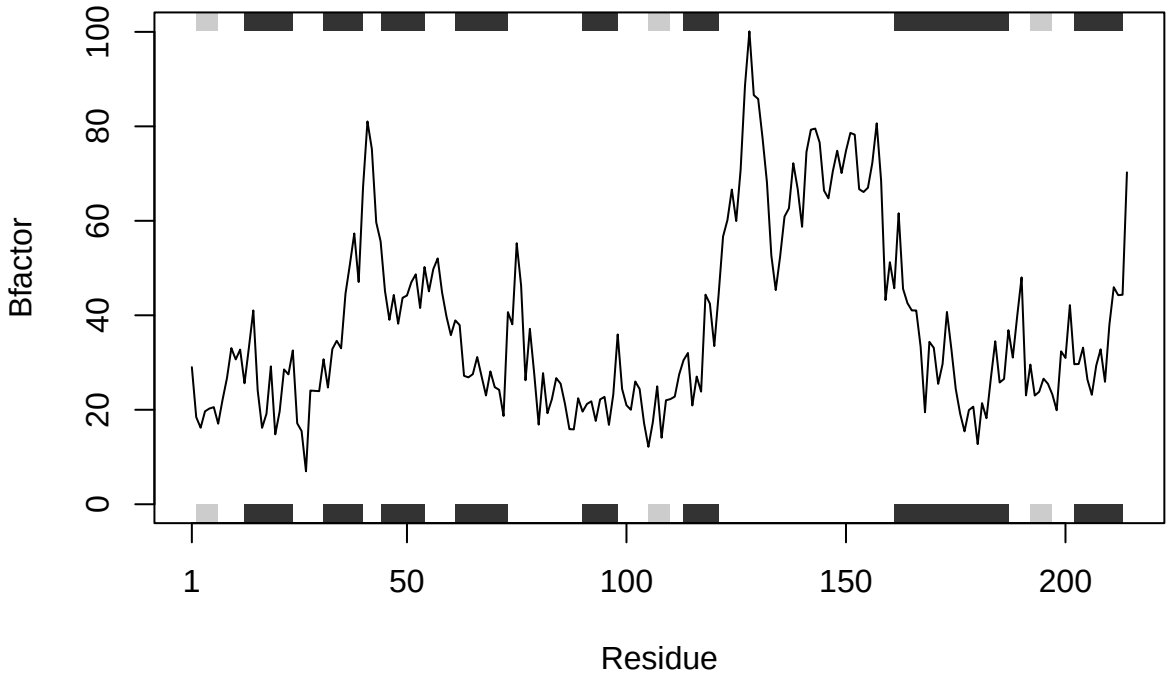
```
## Warning: package 'bio3d' was built under R version 4.3.3
```

```
#' Read protein's PDB data to plot a protein-drug interaction
#' plot indicating the relationship between protein
#' residue and bfactor.
#'
#'
#' @param x a string of 4 characters long PDB identification
#'  code/accession input is required. This code need to be
#'  valid on PDB.
#'
#' @return A plot
#' @export
#'
#' @examples
#' protein.interaction("4AKE")
#'
protein.interaction <- function(x) {
  # read pdb data from the protein code and store it in a variavle
  protein<-read.pdb(x)
  # trim the chain A from the pdb data
  chainA <- trim.pdb(protein, chain="A", elety="CA")
  # look at the atom b
  b <- chainA$atom$b
  #make the plot
  plotb3(b, sse=chainA, typ="l", ylab="Bfactor")
}
```

Demonstration

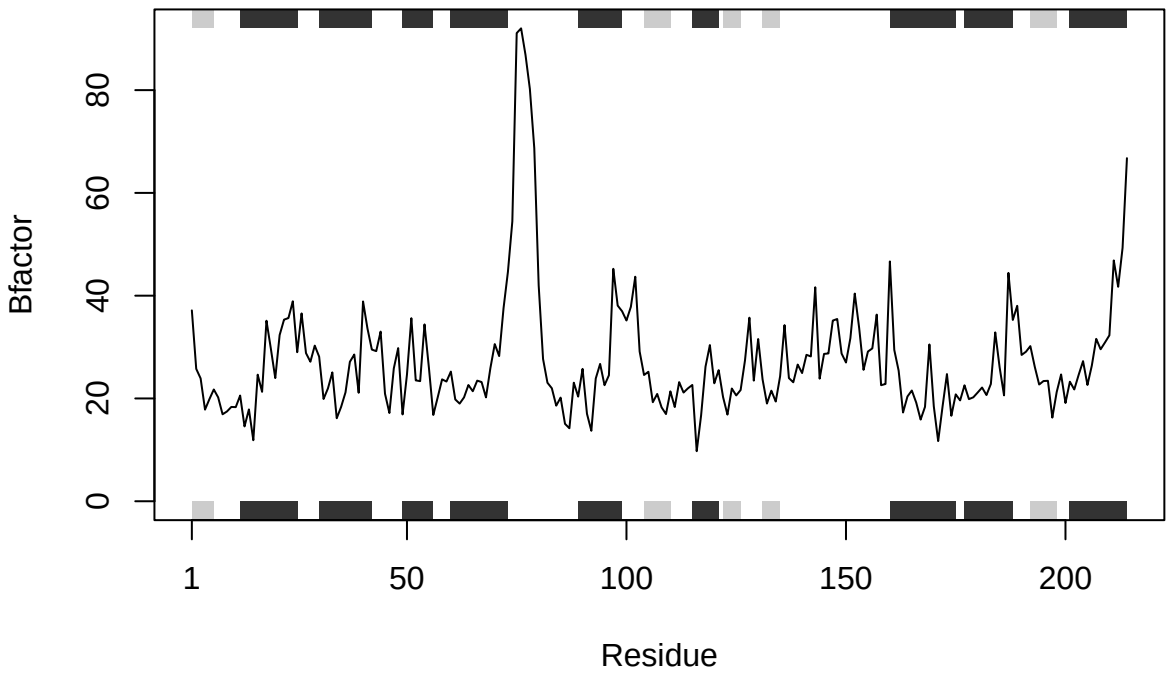
```
protein.interaction("4AKE")
```

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



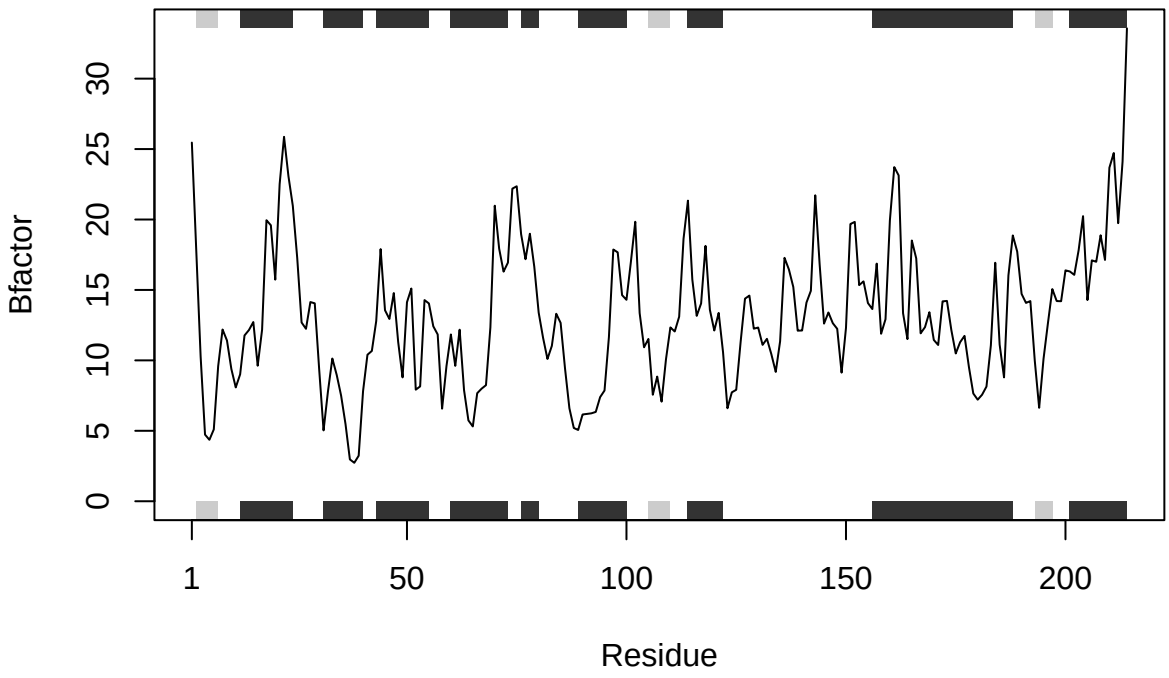

```
protein.interaction("1AKE")
```

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




```
protein.interaction("1E4Y")
```

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


Bfactor
0
5
10
15
20
25
30
1
50
100
150
200
Residue