

# Write\_a\_function

Hyeonseok Jang (PID# A59011126)

10/15/2021

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

My function—named **Bfactor**—receives any protein PDB data, and returns a plot for the specified protein. It receives the four-letter PDB identifier(PDBID) and a chain identifier(chainID) as its inputs, and creates the plot showing the temperature factors(B factors) of the backbone C-alpha atoms in a specified chain of the protein.

```
library(bio3d)
Bfactor <- function(PDBID, chainID){
  x <- read.pdb(PDBID)
  x.chain <- trim.pdb(x, chain=chainID, elety="CA")
  x.b <- x.chain$atom$b
  plotb3(x.b, sse=x.chain, typ="l", ylab="Bfactor")
}
```

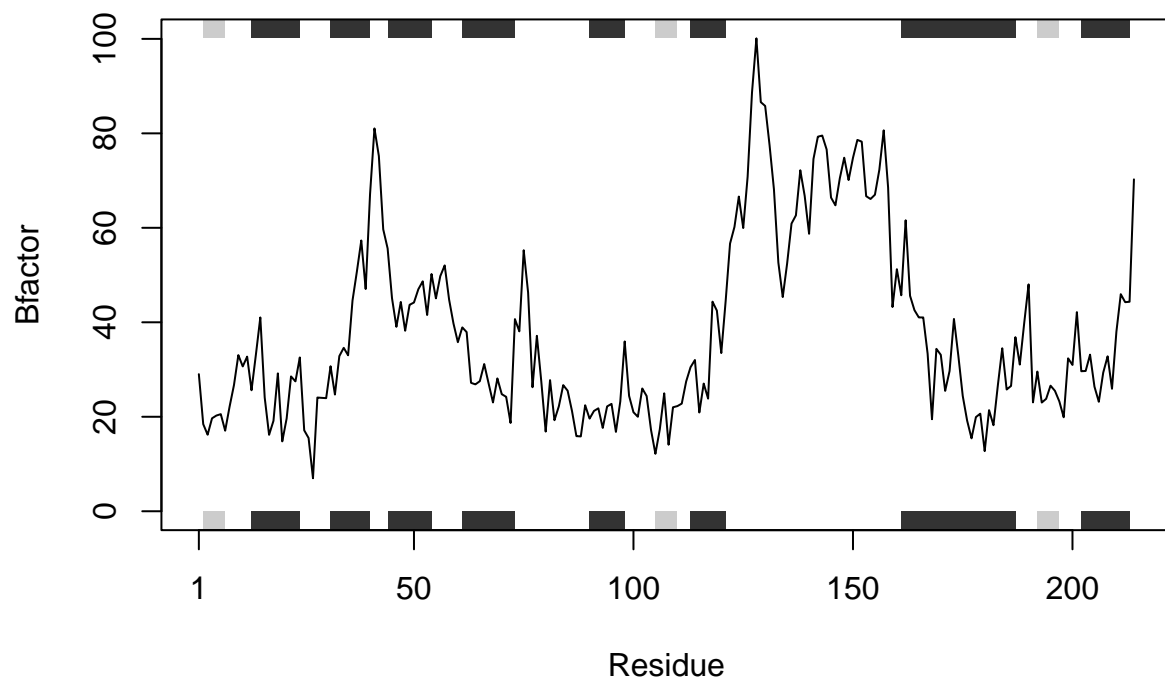
To use the function, you first have to install and load the bio3d package.

```
##install.packages("bio3d")
library(bio3d)
```

After then, you can enter the inputs following the order—PDBID, chainID.

```
Bfactor("4AKE", "A")
```

## Note: Accessing on-line PDB file

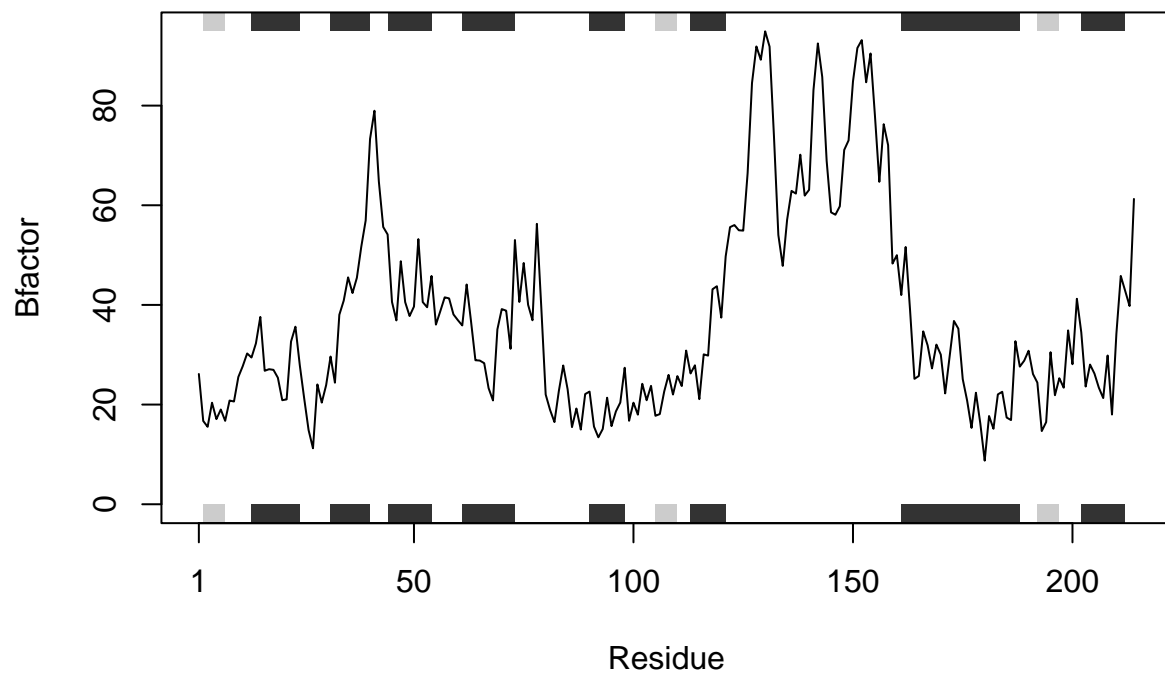


```
Bfactor("4AKE", "B")
```

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

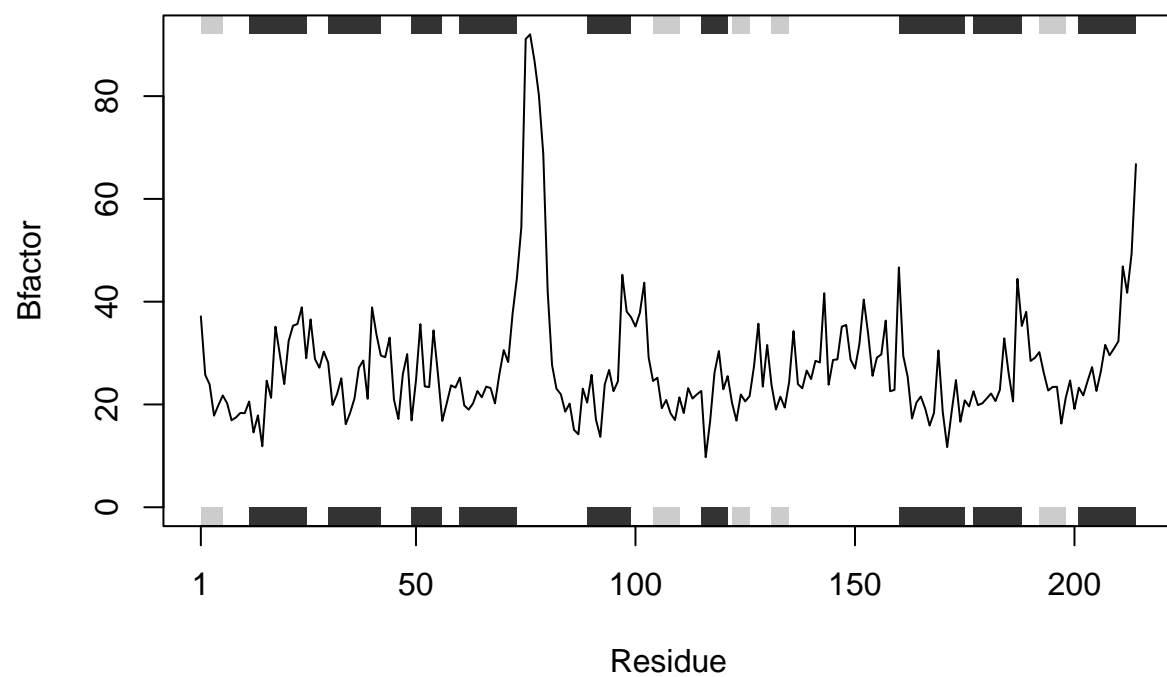
```
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE): C:
```

```
## \Users\HYEONS~1\AppData\Local\Temp\RtmpS8rCkP\4AKE.pdb exists. Skipping download
```



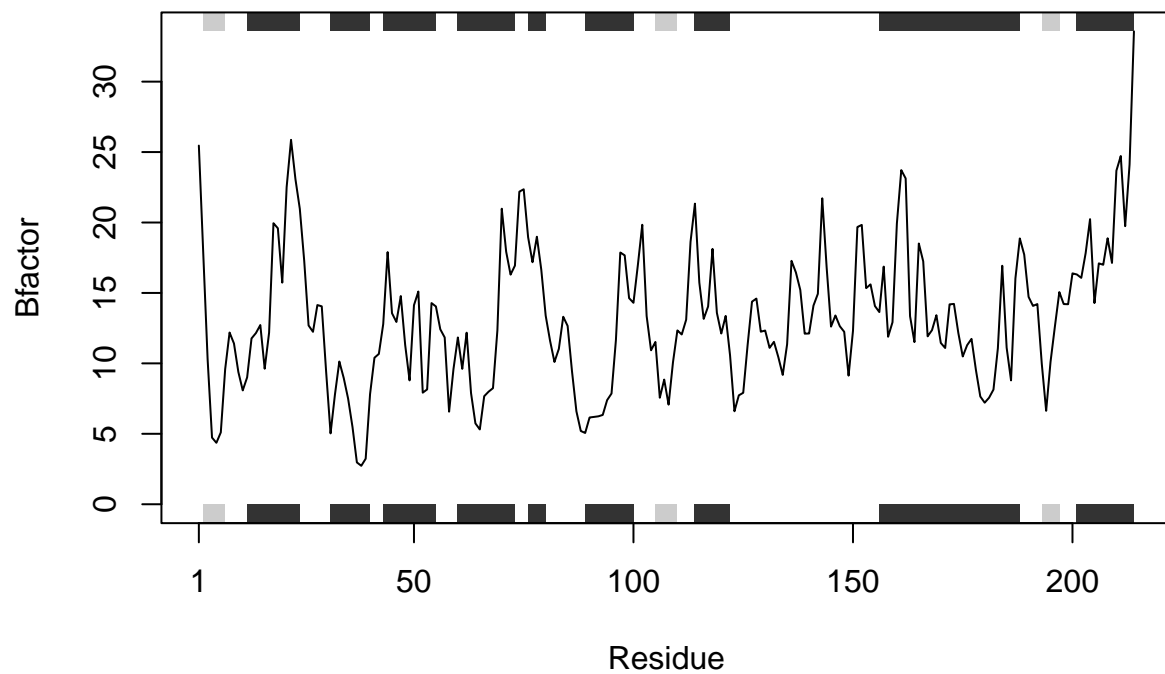
```
Bfactor("1AKE", "A")
```

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



```
Bfactor("1E4Y", "A")
```

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



The result is the line-type plot that has “Residue” and “Bfactor” as labels for its x-axis and y-axis, respectively. (The marginal black and grey rectangles in the plot represent alpha helices and beta strands, respectively.)