

lab6HW

Brad Hunter

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

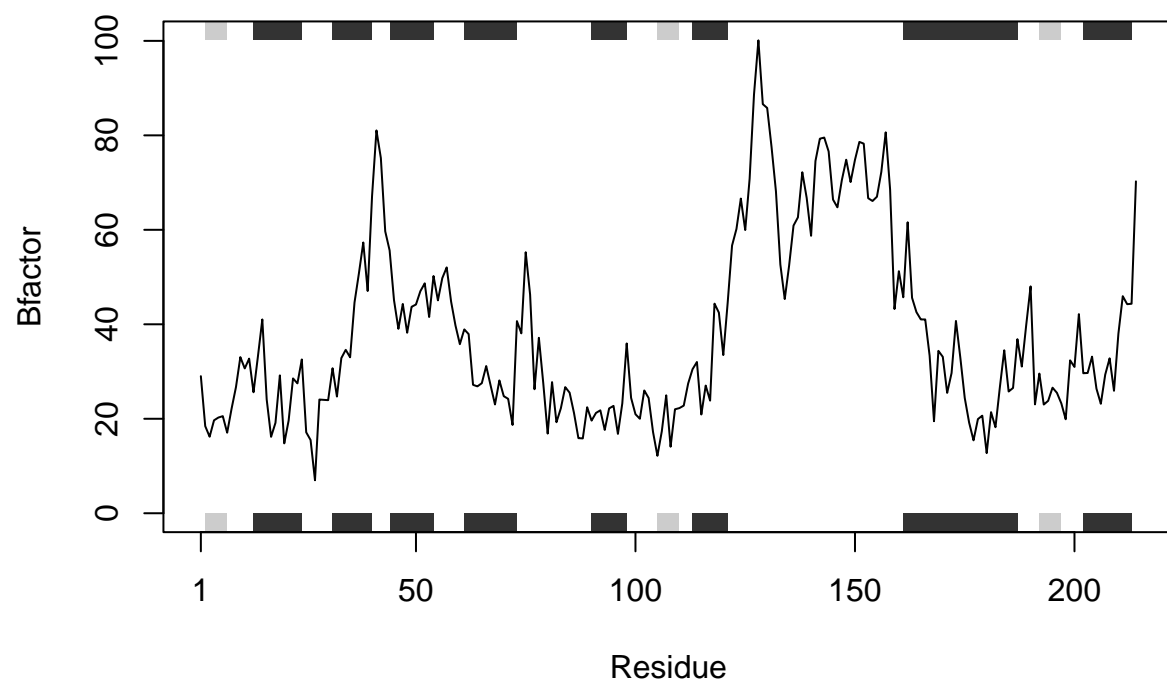
Original code

```
# Can you improve this analysis code?
library(bio3d)
s1 <- read.pdb("4AKE") # kinase with drug

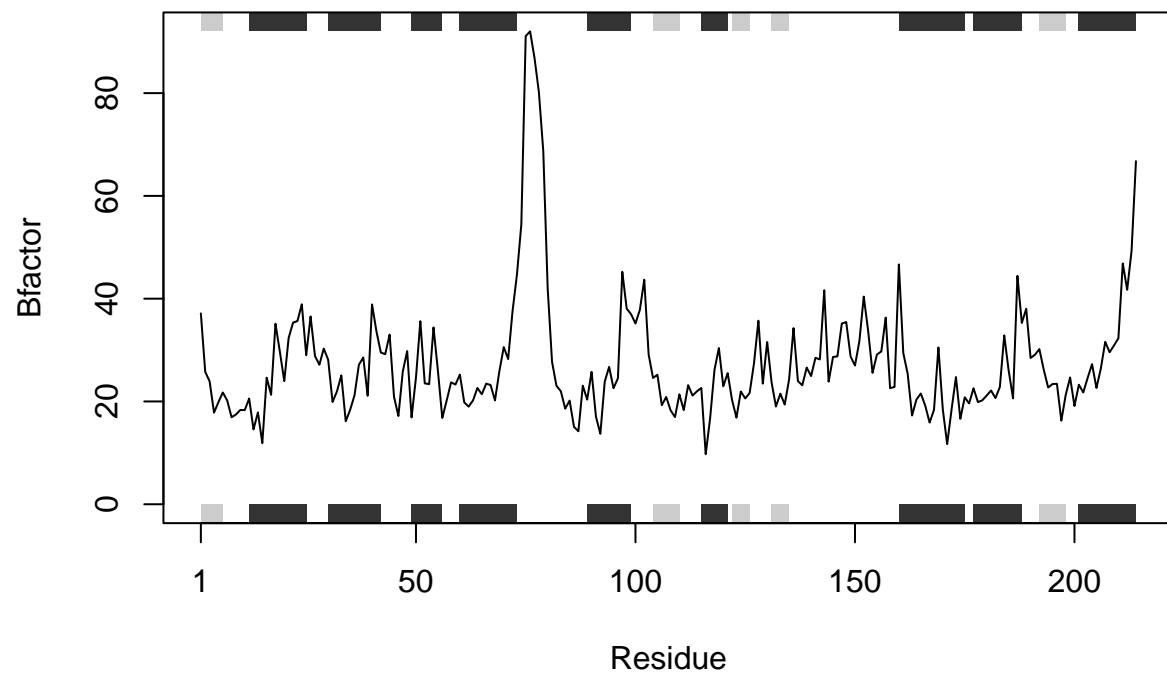
## Note: Accessing on-line PDB file
s2 <- read.pdb("1AKE") # kinase no drug

## Note: Accessing on-line PDB file
## PDB has ALT records, taking A only, rm.alt=TRUE
s3 <- read.pdb("1E4Y") # kinase with drug

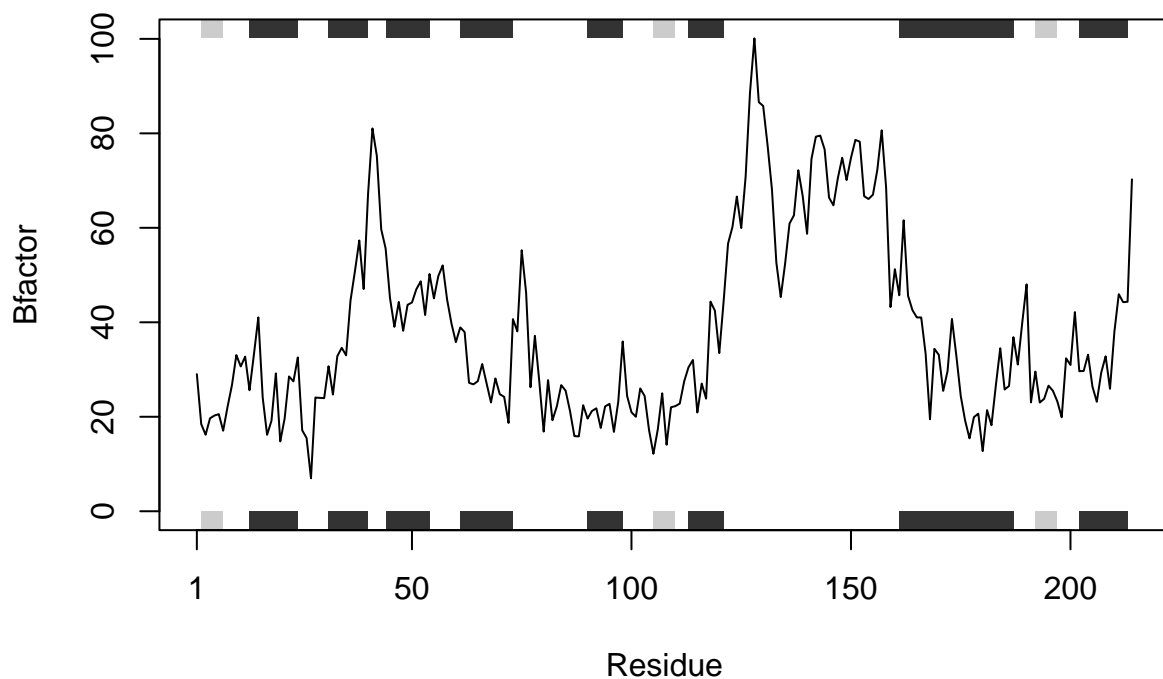
## Note: Accessing on-line PDB file
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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



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



Functionalized code

```
prot_analysis <- function(name){
  s <- read.pdb(name)
  s.chainA <- trim.pdb(s, chain="A", elety="CA")
  s.b <- s.chainA$atom$b
  plotb3(s.b, sse=s.chainA, typ="l", ylab="Bfactor")
}
```

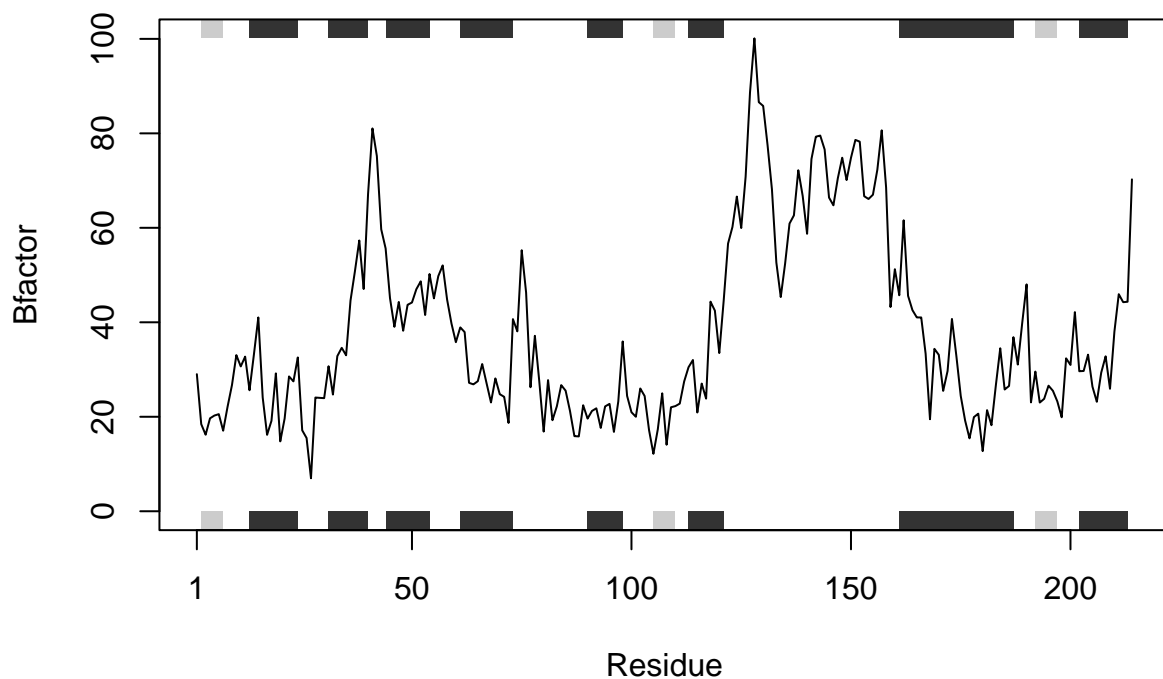
```
prot_analysis("4AKE")
```

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

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

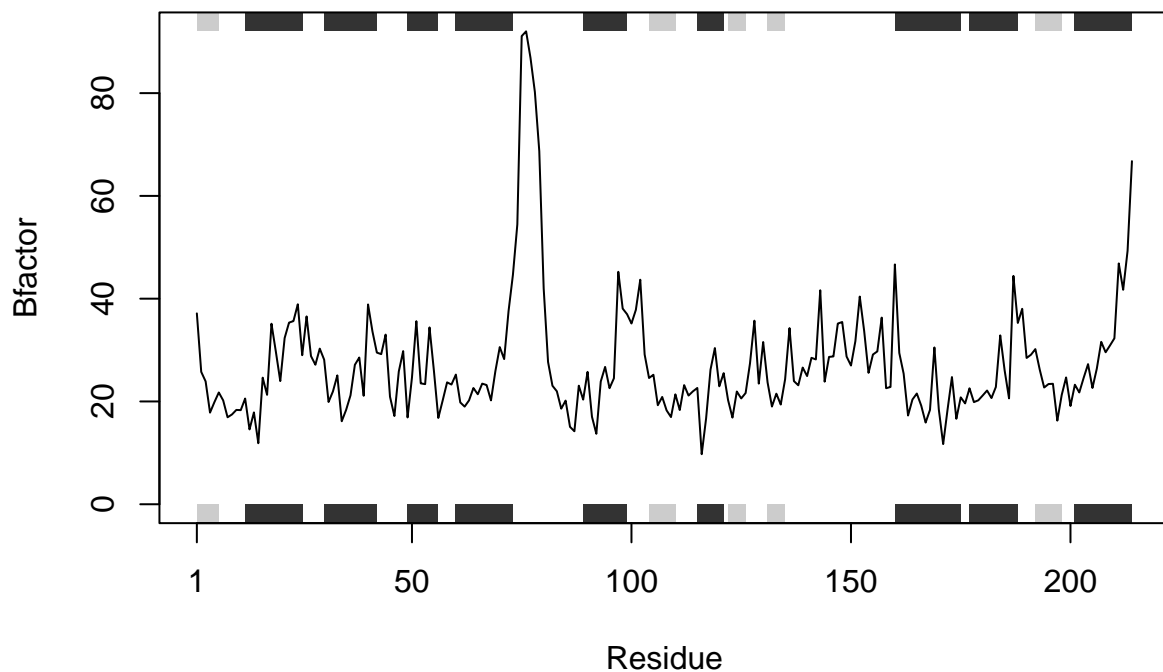
```
## /var/folders/vz/21nfbp357p110f67ysxl9w3m0000gn/T//RtmpNUwyvw/4AKE.pdb exists.
```

```
## Skipping download
```



```
prot_analysis("1AKE")
```

```
## Note: Accessing on-line PDB file
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
## /var/folders/vz/21nfbp357p110f67ysxl9w3m0000gn/T//RtmpNUwyvw/1AKE.pdb exists.
## Skipping download
## PDB has ALT records, taking A only, rm.alt=TRUE
```



```
prot_analysis("1E4Y")
```

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

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

```
## /var/folders/vz/21nfbp357p110f67ysxl9w3m0000gn/T//RtmpNUwyvw/1E4Y.pdb exists.
```

```
## Skipping download
```

