

# HW6

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## Initial code for PDB Data

First the bio3d package was installed:

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

Sample code to improve and transform into a function:

```
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

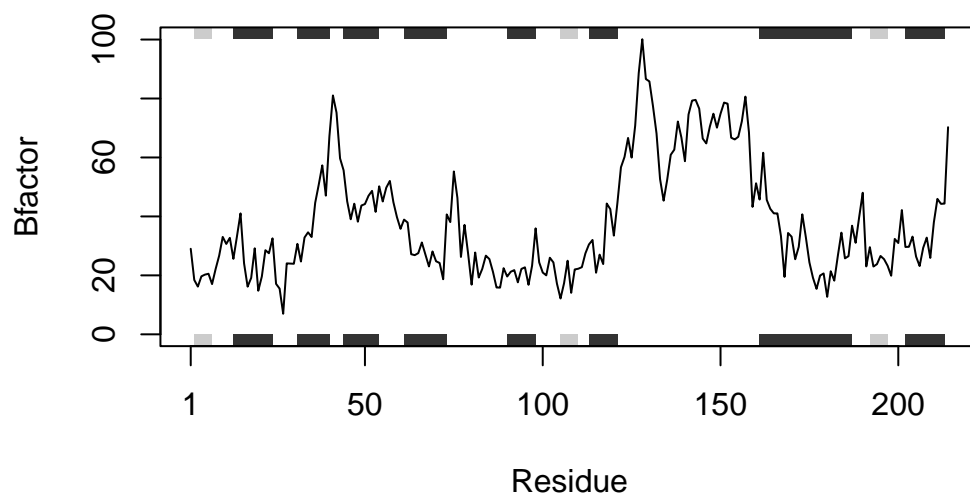
PDB has ALT records, taking A only, rm.alt=TRUE

```
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
```

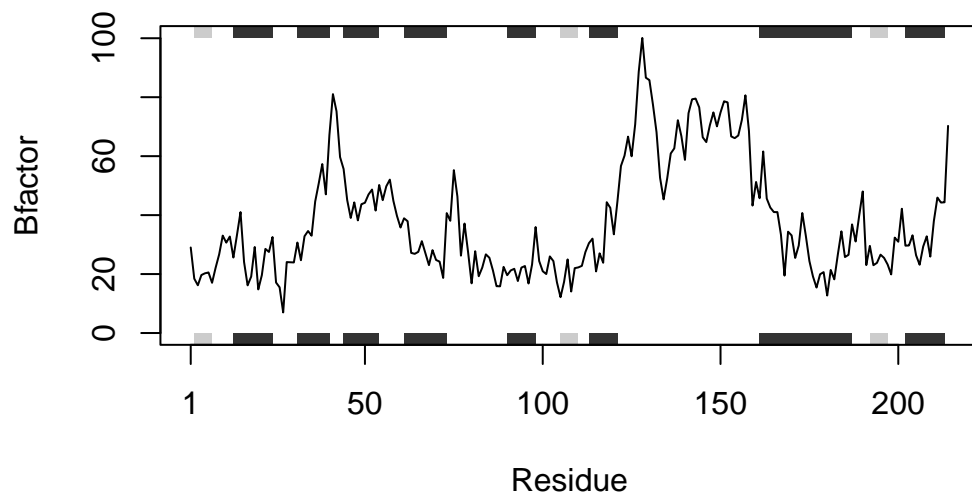
```
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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

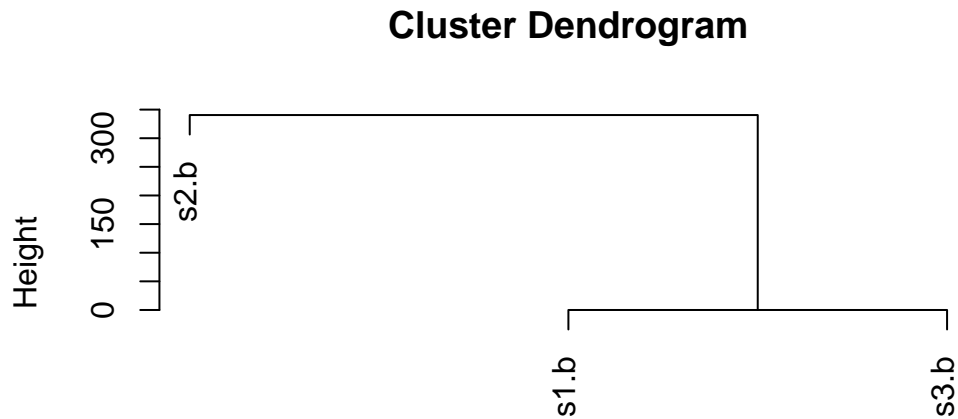


```
plotb3(s3.b, sse=s3.chainA, typ="l", ylab="Bfactor")
```



A sample dendrogram plot was provided to compare protein trends:

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



```
dist(rbind(s1.b, s2.b, s3.b))  
hclust (*, "complete")
```

## New Function for any PDB input

```
library(bio3d)  
  
# This function reads in 3D structures of protein kinases, trims them, and plots its B-factors  
plot_bfactors <- function(pdb_id) {  
  
  # Read in PDB structure based on ID number  
  pdb <- read.pdb(pdb_id)  
  
  # Trim the protein to only contain chain A  
  pdb.chainA <- trim.pdb(pdb, chain="A", elety="CA")  
  
  # Extract B-factors from the chain  
  pdb.b <- pdb.chainA$atom$b
```

```

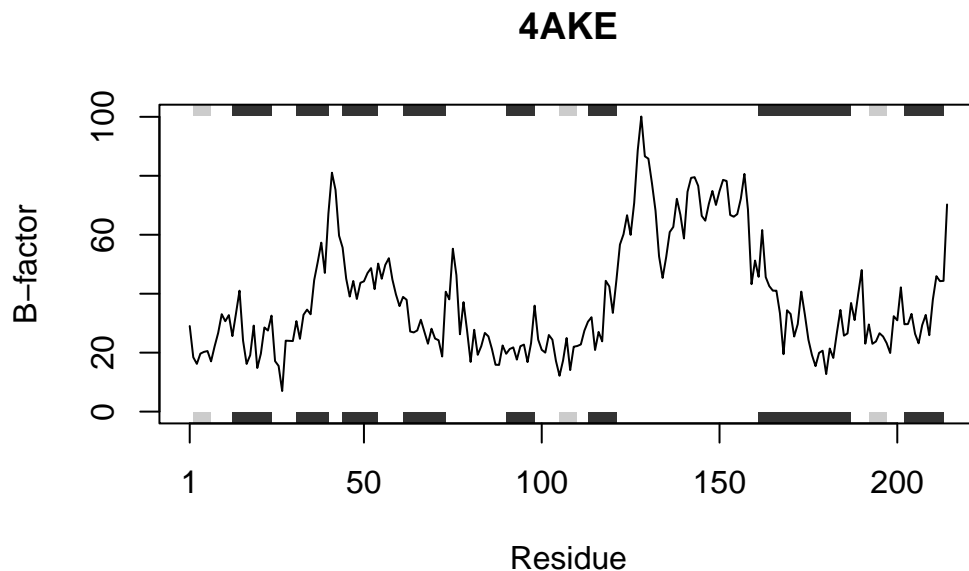
# Plot B-factors in a line graph for visualizing trends
plotb3(pdb.b, sse=pdb.chainA, typ="l", ylab="B-factor", main = (pdb_id))
}

# Call function with PDB ID
plot_bfactors("4AKE")

```

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):  
/var/folders/cm/8l7g\_491105c3slwzpmk4bkc0000gn/T//RtmpCqxyBC/4AKE.pdb exists.  
Skipping download



Trials with different inputs:

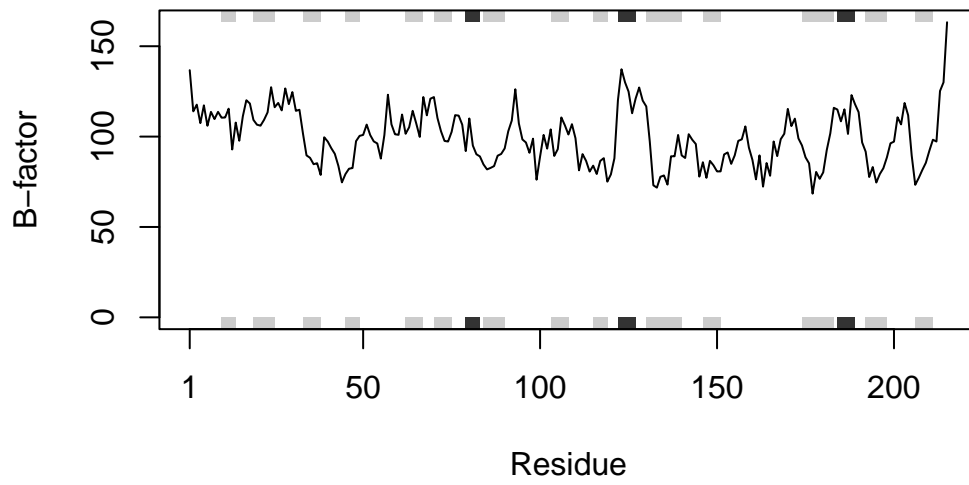
```

plot_bfactors("7Y0W")

```

Note: Accessing on-line PDB file

## 7YOW



```
plot_bfactors("8HBH")
```

Note: Accessing on-line PDB file

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

# 8HBH

