

# Class 6 - HW

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```
library(bio3d)
```

Warning: package 'bio3d' was built under R version 4.4.1

```
s1 <- read.pdb("4AKE") # kinase with drug
```

Note: Accessing on-line PDB file

```
s2 <- read.pdb("1AKE") # kinase no drug
```

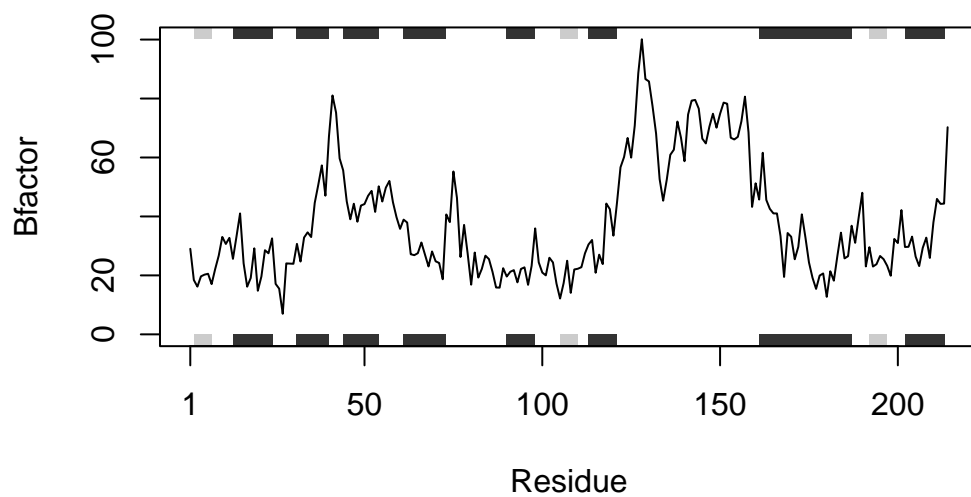
Note: Accessing on-line PDB file

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

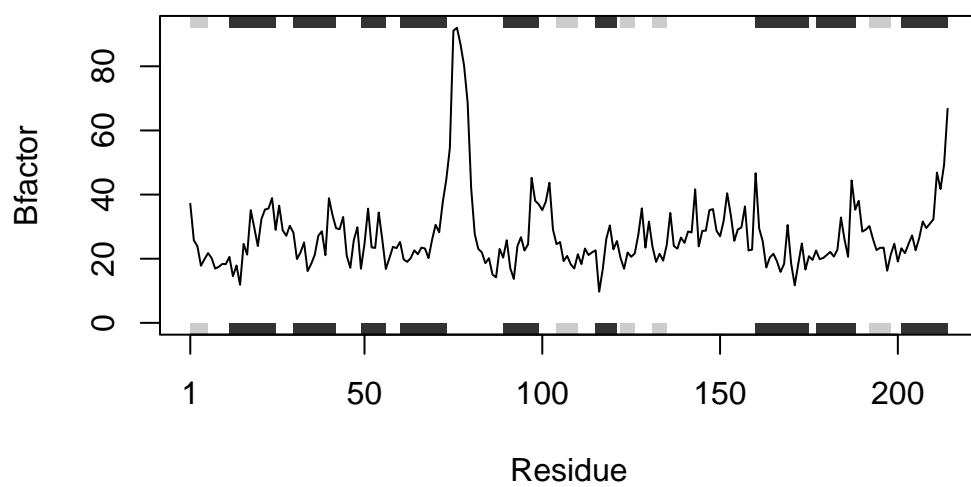
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

Note: Accessing on-line PDB file

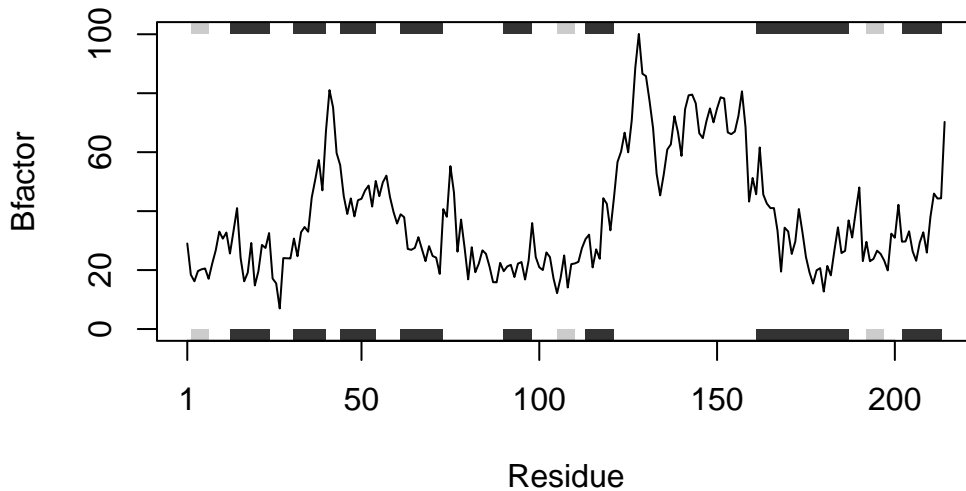
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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



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



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

```
# load in bio3d package
library(bio3d)

compare_bfactor <- function(kinase_input, chain_input="A", elety_input="CA") {
  # input is a 4 character protein code (e.g. "4AKE"), name of a chain (e.g. "A"), and elety
  # output is a line graph depicting the B factor trends of the kinase

  # load in protein database dataframe of inputed kinase
  pdb_df <- read.pdb(kinase_input)

  # select the chain
  pdb_df.chain <- trim.pdb(pdb_df, chain=chain_input, elety=elety_input)

  # select the B factor of the chain
  pdb_df.b <- pdb_df.chain$atom$b

  # plot the Bfactor of the kinase
```

```

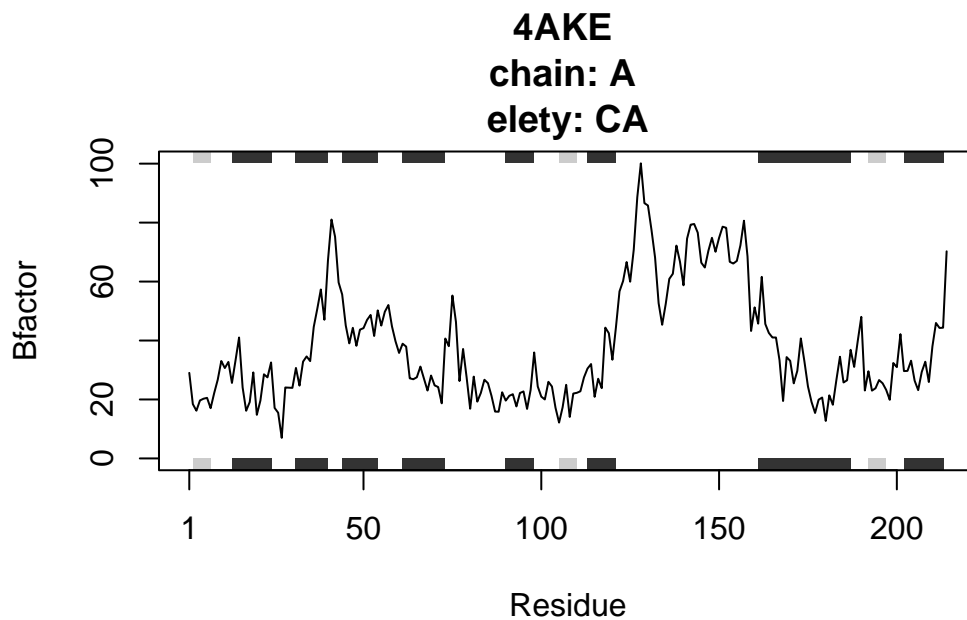
plotb3(pdb_df.b, sse=pdb_df.chain, typ="l", ylab="Bfactor", main=paste(kinase_input, "\nchain: A", "\nelely: CA"))
}

# confirm that it works
default_plot <- compare_bfactor("4AKE")

```

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):  
/var/folders/hz/3cdf12jj3qv7fyz\_dbg0rc2r0000gn/T//Rtmpe0760m/4AKE.pdb exists.  
Skipping download



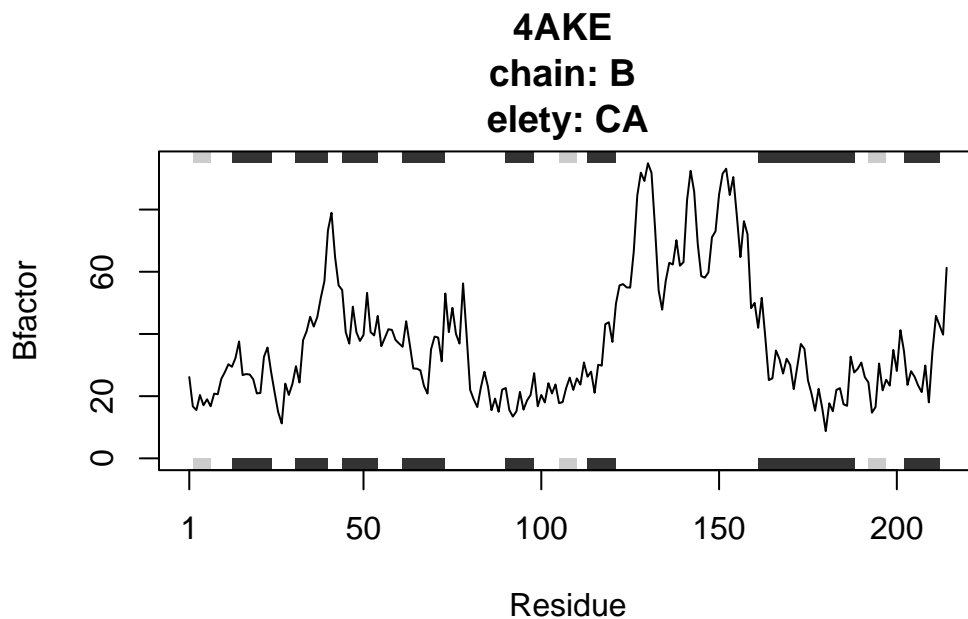
```

chain_diff_plot <- compare_bfactor("4AKE", chain_input="B")

```

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):  
/var/folders/hz/3cdf12jj3qv7fyz\_dbg0rc2r0000gn/T//Rtmpe0760m/4AKE.pdb exists.  
Skipping download



```
elety_diff_plot <- compare_bfactor("4AKE", elety_input = "CB")
```

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):  
/var/folders/hz/3cdf12jj3qv7fyz\_dbg0rc2r0000gn/T/Rtmpe0760m/4AKE.pdb exists.  
Skipping download

Warning in pdb2sse(sse): No helix and sheet defined in input 'sse' PDB object:  
try using dssp()

Warning in plotb3(pdb\_df.b, sse = pdb\_df.chain, typ = "l", ylab = "Bfactor", :  
Length of input 'sse' does not equal the length of input 'x'; Ignoring 'sse'

**4AKE**  
**chain: A**  
**elety: CB**

