HW for Class 6

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Prior to rendering Quarto document, a CRAN mirror error popped up. To troubleshoot, set a CRAN mirror before installing packages to R base.

```
options(repos = c(CRAN = "http://cran.rstudio.com"))
```

Install bio3d package.

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

```
The downloaded binary packages are in
    /var/folders/4h/mpp5b0bd1p70msy2wwpvtkm00000gn/T//RtmpuIwnv1/downloaded_packages
```

Pasted code from the online document.

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

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

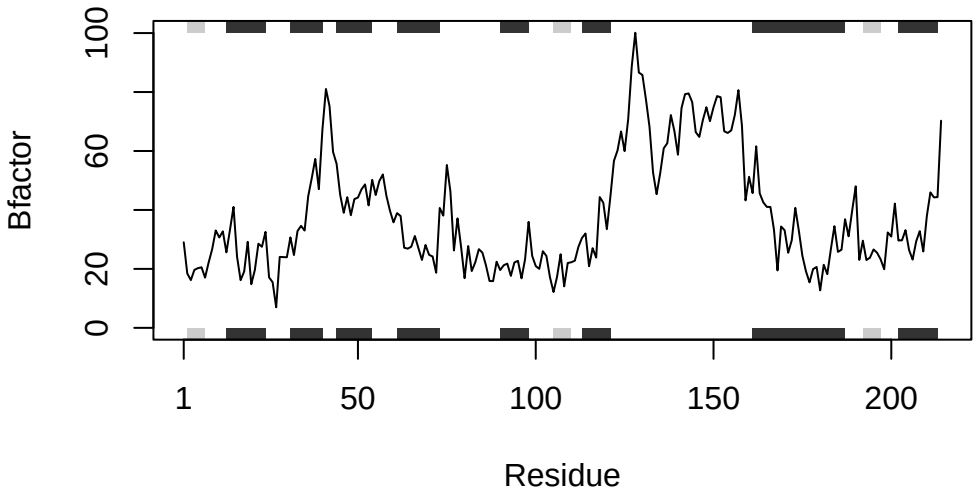
```
s2 <- read.pdb("1AKE")  # kinase no drug
```

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

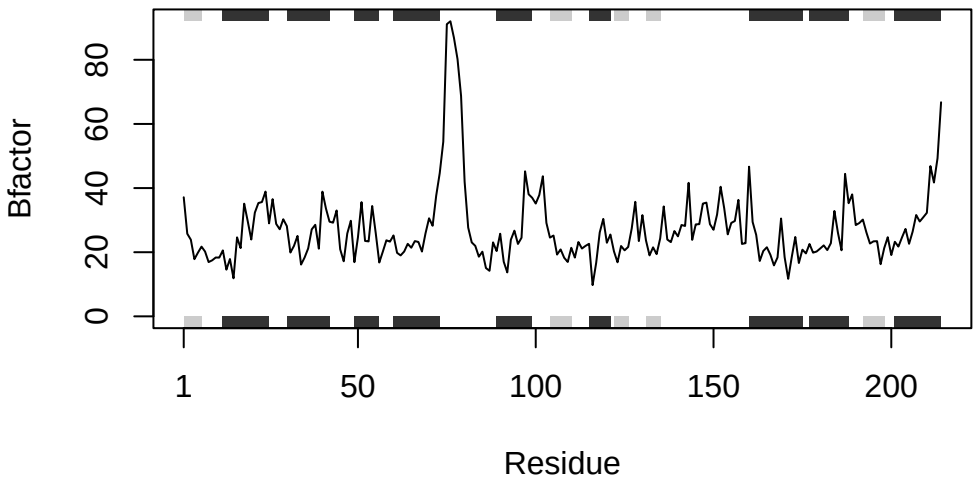
```
s3 <- read.pdb("1E4Y")  # kinase with drug
```

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

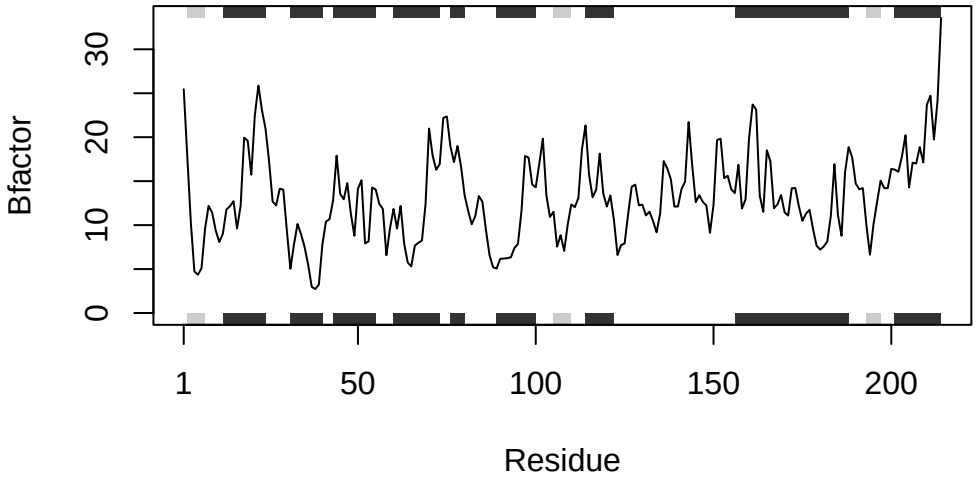
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```




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




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



Load the bio3d, and ggplot2 packages by using the `library` function.

```
library(bio3d)
library(ggplot2)
```

Run the codes above, except for the `plotb3` functions.

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

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/4h/mpp5b0bd1p70msy2wwpvtkm00000gn/T//RtmpuIwnv1/4AKE.pdb exists.
Skipping download
```

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

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/4h/mpp5b0bd1p70msy2wwpvtkm00000gn/T//RtmpuIwnv1/1AKE.pdb exists.
Skipping download
```

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

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

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/4h/mpp5b0bd1p70msy2wwpvtkm00000gn/T//RtmpuIwnv1/1E4Y.pdb exists.
Skipping download
```

```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")
```

```
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
```

Combine the s1,s2,s3 PDB files into one vector 'pdb_files'. Then use `read.pdb` to read the PDB files and `lapply` function to store it in a list.

```
pdb_files <- c("4AKE", "1AKE", "1E4Y")
pdb <- lapply(pdb_files, read.pdb)
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/4h/mpp5b0bd1p70msy2wwpvtkm00000gn/T//RtmpuIwnv1/4AKE.pdb exists.
Skipping download
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/4h/mpp5b0bd1p70msy2wwpvtkm00000gn/T//RtmpuIwnv1/1AKE.pdb exists.
Skipping download
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/4h/mpp5b0bd1p70msy2wwpvtkm00000gn/T//RtmpuIwnv1/1E4Y.pdb exists.
Skipping download
```

```
pdb
```

```
[[1]]

 Call:  FUN(file = X[[i]])

   Total Models#: 1
     Total Atoms#: 3459,  XYZs#: 10377  Chains#: 2  (values: A B)
```

```
     Protein Atoms#: 3312  (residues/Calpha atoms#: 428)
     Nucleic acid Atoms#: 0  (residues/phosphate atoms#: 0)

     Non-protein/nucleic Atoms#: 147  (residues: 147)
     Non-protein/nucleic resid values: [ HOH (147) ]

   Protein sequence:
      MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAAVKSGSELGKQAKDIMDAGKLVT
      DELVIALVKERIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVDRI
      VGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKDDQEETVRKRLVEYHQMTAPLIG
      YYSKEAEAGNTKYAKVDGTKPVAEVRADLEKILGMRIILLGAPGA...<cut>...KILG

+ attr: atom, xyz, seqres, helix, sheet,
        calpha, remark, call

[[2]]

 Call:  FUN(file = X[[i]])

   Total Models#: 1
     Total Atoms#: 3804,  XYZs#: 11412  Chains#: 2  (values: A B)

     Protein Atoms#: 3312  (residues/Calpha atoms#: 428)
     Nucleic acid Atoms#: 0  (residues/phosphate atoms#: 0)

     Non-protein/nucleic Atoms#: 492  (residues: 380)
     Non-protein/nucleic resid values: [ AP5 (2), HOH (378) ]

   Protein sequence:
      MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAAVKSGSELGKQAKDIMDAGKLVT
      DELVIALVKERIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVDRI
      VGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKDDQEETVRKRLVEYHQMTAPLIG
      YYSKEAEAGNTKYAKVDGTKPVAEVRADLEKILGMRIILLGAPGA...<cut>...KILG

+ attr: atom, xyz, seqres, helix, sheet,
        calpha, remark, call

[[3]]

 Call:  FUN(file = X[[i]])

   Total Models#: 1
     Total Atoms#: 3428,  XYZs#: 10284  Chains#: 2  (values: A B)
```

```
     Protein Atoms#: 3314  (residues/Calpha atoms#: 428)
     Nucleic acid Atoms#: 0  (residues/phosphate atoms#: 0)

     Non-protein/nucleic Atoms#: 114  (residues: 2)
     Non-protein/nucleic resid values: [ AP5 (2) ]

   Protein sequence:
      MRIILLGALVAGKGTQAQFIMEKYGIPQISTGDMLRAAVKSGSELGKQAKDIMDAGKLVT
      DELVIALVKERIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVDRI
      VGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKDDQEETVRKRLVEYHQMTAPLIG
      YYSKEAEAGNTKYAKVDGTKPVAEVRADLEKILGMRIILLGALVA...<cut>...KILG

+ attr: atom, xyz, seqres, helix, sheet,
        calpha, remark, call
```

Use the `lapply` function again to trim the PDB files, and only extract the b-factors.

```
pdb_trim <- lapply(pdb, function(x) trim.pdb(x, chain="A", elety="CA"))
b_factors <- lapply(pdb_trim, function(x) x$atom$b)
pdb_trim
```

```
[[1]]

 Call:  trim.pdb(pdb = x, chain = "A", elety = "CA")

   Total Models#: 1
     Total Atoms#: 214,  XYZs#: 642  Chains#: 1  (values: A)

     Protein Atoms#: 214  (residues/Calpha atoms#: 214)
     Nucleic acid Atoms#: 0  (residues/phosphate atoms#: 0)

     Non-protein/nucleic Atoms#: 0  (residues: 0)
     Non-protein/nucleic resid values: [ none ]

   Protein sequence:
      MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAAVKSGSELGKQAKDIMDAGKLVT
      DELVIALVKERIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVDRI
      VGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKDDQEETVRKRLVEYHQMTAPLIG
      YYSKEAEAGNTKYAKVDGTKPVAEVRADLEKILG

+ attr: atom, helix, sheet, seqres, xyz,
```

```
        calpha, call

[[2]]

 Call:  trim.pdb(pdb = x, chain = "A", elety = "CA")

   Total Models#: 1
     Total Atoms#: 214,  XYZs#: 642  Chains#: 1  (values: A)

     Protein Atoms#: 214  (residues/Calpha atoms#: 214)
     Nucleic acid Atoms#: 0  (residues/phosphate atoms#: 0)

     Non-protein/nucleic Atoms#: 0  (residues: 0)
     Non-protein/nucleic resid values: [ none ]

   Protein sequence:
      MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAAVKSGSELGKQAKDIMDAGKLVT
      DELVIALVKERIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVDRI
      VGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKDDQEETVRKRLVEYHQMTAPLIG
      YYSKEAEAGNTKYAKVDGTKPVAEVRADLEKILG

+ attr: atom, helix, sheet, seqres, xyz,
        calpha, call

[[3]]

 Call:  trim.pdb(pdb = x, chain = "A", elety = "CA")

   Total Models#: 1
     Total Atoms#: 214,  XYZs#: 642  Chains#: 1  (values: A)

     Protein Atoms#: 214  (residues/Calpha atoms#: 214)
     Nucleic acid Atoms#: 0  (residues/phosphate atoms#: 0)

     Non-protein/nucleic Atoms#: 0  (residues: 0)
     Non-protein/nucleic resid values: [ none ]

   Protein sequence:
      MRIILLGALVAGKGTQAQFIMEKYGIPQISTGDMLRAAVKSGSELGKQAKDIMDAGKLVT
      DELVIALVKERIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVDRI
      VGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKDDQEETVRKRLVEYHQMTAPLIG
      YYSKEAEAGNTKYAKVDGTKPVAEVRADLEKILG
```

```
+ attr: atom, helix, sheet, seqres, xyz,
        calpha, call
```

```
b_factors
```

```
[[1]]
  [1]  29.02  18.44  16.20  19.67  20.26  20.55  17.05  22.13  26.71  33.05
 [11]  30.66  32.73  25.61  33.19  41.03  24.09  16.18  19.14  29.19  14.79
 [21]  19.63  28.54  27.49  32.56  17.13  15.50   6.98  24.07  24.00  23.94
 [31]  30.70  24.70  32.84  34.60  33.01  44.60  50.74  57.32  47.04  67.13
 [41]  81.04  75.20  59.68  55.63  45.12  39.04  44.31  38.21  43.70  44.19
 [51]  47.00  48.67  41.54  50.22  45.07  49.77  52.04  44.82  39.75  35.79
 [61]  38.92  37.93  27.18  26.86  27.53  31.16  27.08  23.03  28.12  24.78
 [71]  24.22  18.69  40.67  38.08  55.26  46.29  26.25  37.14  27.50  16.86
 [81]  27.76  19.27  22.22  26.70  25.52  21.22  15.90  15.84  22.44  19.61
 [91]  21.23  21.79  17.64  22.19  22.73  16.80  23.25  35.95  24.42  20.96
[101]  20.00  25.99  24.39  17.19  12.16  17.35  24.97  14.08  22.01  22.26
[111]  22.78  27.47  30.49  32.02  20.90  27.03  23.84  44.37  42.47  33.48
[121]  44.56  56.67  60.18  66.62  59.95  70.81  88.63 100.11  86.60  85.80
[131]  77.48  68.13  52.66  45.34  52.43  60.90  62.64  72.19  66.75  58.73
[141]  74.57  79.29  79.53  76.58  66.40  64.76  70.48  74.84  70.11  74.82
[151]  78.61  78.24  66.70  66.10  67.01  72.28  80.64  68.54  43.23  51.24
[161]  45.72  61.60  45.61  42.57  41.03  41.02  33.34  19.48  34.38  33.11
[171]  25.48  29.68  40.71  32.91  24.41  19.20  15.43  19.93  20.66  12.72
[181]  21.40  18.21  26.68  34.50  25.77  26.52  36.85  31.05  39.84  48.03
[191]  23.04  29.57  23.00  23.80  26.59  25.49  23.25  19.89  32.37  30.97
[201]  42.16  29.64  29.69  33.15  26.38  23.17  29.35  32.80  25.92  38.01
[211]  45.95  44.26  44.35  70.26

[[2]]
  [1] 37.14 25.76 23.90 17.83 19.86 21.75 20.21 16.92 17.47 18.35 18.31 20.57
 [13] 14.56 17.87 11.87 24.63 21.29 35.13 29.68 23.96 32.34 35.34 35.64 38.91
 [25] 29.00 36.55 28.83 27.15 30.28 28.13 19.90 21.95 25.07 16.15 18.35 21.19
 [37] 27.13 28.55 21.10 38.88 33.63 29.51 29.21 33.01 20.92 17.17 25.84 29.80
 [49] 16.89 24.66 35.62 23.52 23.37 34.41 25.96 16.79 20.20 23.72 23.29 25.23
 [61] 19.81 19.00 20.21 22.62 21.40 23.47 23.20 20.21 25.90 30.58 28.25 37.60
 [73] 44.66 54.46 91.10 92.02 86.85 80.21 68.72 42.01 27.69 23.06 21.98 18.60
 [85] 20.17 15.06 14.20 23.07 20.36 25.76 17.02 13.71 23.88 26.72 22.58 24.51
 [97] 45.23 38.07 36.97 35.17 37.83 43.69 29.14 24.56 25.20 19.27 20.88 18.27
[109] 16.96 21.38 18.33 23.18 21.15 21.97 22.63  9.74 16.71 26.18 30.39 22.95
[121] 25.51 20.28 16.86 21.94 20.59 21.64 27.42 35.72 23.47 31.57 23.71 19.01
```

```
[133] 21.52 19.40 24.32 34.28 23.96 23.14 26.60 24.94 28.49 28.18 41.64 23.85
[145] 28.67 28.76 35.16 35.46 28.74 26.99 31.74 40.41 33.73 25.57 29.13 29.74
[157] 36.32 22.58 22.82 46.67 29.44 25.40 17.27 20.38 21.55 19.19 15.89 18.37
[169] 30.51 18.47 11.70 18.45 24.75 16.63 20.80 19.62 22.56 19.87 20.22 21.16
[181] 22.13 20.66 22.82 32.86 26.04 20.60 44.44 35.28 38.03 28.46 29.10 30.19
[193] 26.17 22.71 23.39 23.44 16.27 21.26 24.67 19.12 23.26 21.75 24.59 27.26
[205] 22.63 26.40 31.60 29.57 30.90 32.29 46.86 41.73 49.31 66.76

[[3]]
  [1] 25.46 17.86 10.28  4.73  4.36  5.10  9.59 12.19 11.41  9.39  8.08  9.01
 [13] 11.77 12.15 12.72  9.62 12.18 19.95 19.59 15.73 22.51 25.87 23.08 20.97
 [25] 17.28 12.69 12.24 14.14 14.05  9.38  5.03  7.78 10.13  8.96  7.50  5.48
 [37]  2.97  2.73  3.23  7.81 10.40 10.67 12.79 17.90 13.56 12.94 14.78 11.31
 [49]  8.79 14.13 15.10  7.92  8.15 14.28 14.04 12.42 11.84  6.57  9.59 11.84
 [61]  9.61 12.18  7.89  5.74  5.31  7.67  7.99  8.24 12.34 20.98 17.93 16.30
 [73] 16.94 22.19 22.36 18.96 17.18 18.99 16.65 13.39 11.61 10.10 11.03 13.31
 [85] 12.66  9.44  6.60  5.20  5.06  6.16  6.20  6.24  6.34  7.39  7.86 11.66
 [97] 17.87 17.67 14.63 14.30 16.98 19.84 13.36 10.93 11.52  7.56  8.85  7.07
[109] 10.08 12.34 12.05 13.10 18.63 21.34 15.73 13.16 14.04 18.13 13.59 12.12
[121] 13.37 10.57  6.60  7.73  7.91 11.31 14.38 14.60 12.25 12.33 11.10 11.53
[133] 10.44  9.18 11.36 17.28 16.45 15.21 12.11 12.12 14.10 14.94 21.72 16.82
[145] 12.61 13.40 12.64 12.24  9.13 12.31 19.68 19.83 15.34 15.61 14.07 13.64
[157] 16.87 11.89 12.92 19.93 23.72 23.13 13.35 11.51 18.51 17.24 11.92 12.36
[169] 13.42 11.45 11.09 14.19 14.22 12.15 10.49 11.29 11.74  9.53  7.65  7.21
[181]  7.56  8.14 11.07 16.93 11.12  8.79 16.03 18.87 17.72 14.72 14.08 14.21
[193]  9.99  6.63 10.11 12.64 15.06 14.21 14.20 16.39 16.31 16.07 17.83 20.24
[205] 14.28 17.10 17.00 18.88 17.13 23.68 24.72 19.74 24.12 33.57
```

Use the `data.frame` function to create a date frame for each structure. Where `seq_along` is a function that creates an integer sequence corresponding to the vector length.

```
df1 <- data.frame(x = seq_along(s1.b), y = s1.b, structure = "s1")
df2 <- data.frame(x = seq_along(s2.b), y = s2.b, structure = "s2")
df3 <- data.frame(x = seq_along(s3.b), y = s3.b, structure = "s3")
```

Combine the data frames into one `data.frame` function.

```
df <- rbind(df1, df2, df3)
```

Use `ggplot2` to create a single plot containing all protein structures

```
ggplot(df, aes(x = x, y = y, color = structure)) +
  geom_line() +
  labs(x = "Residue", y = "Bfactor")
```

Define a function to work for the protein structures provided by copy and pasting all of the above codes.

```
b3_plots <- function(pdb) {

  # Read PDB files
  pdb_files <- c("4AKE", "1AKE", "1E4Y")
  pdb <- lapply(pdb_files, read.pdb)

  # Trim PDB files and extract b factors
  pdb_trim <- lapply(pdb, function(x) trim.pdb(x, chain="A", elety="CA"))
  b_factors <- lapply(pdb_trim, function(x) x$atom$b)

  # Create a 'data.frame' for each structure
  df1 <- data.frame(x = seq_along(s1.b), y = s1.b, structure = "s1")
  df2 <- data.frame(x = seq_along(s2.b), y = s2.b, structure = "s2")
  df3 <- data.frame(x = seq_along(s3.b), y = s3.b, structure = "s3")
```

```
  # Combine the data frames
  df <- rbind(df1, df2, df3)

  # Use 'ggplot2' to plot all structures on one plot.
  ggplot(df, aes(x = x, y = y, color = structure)) +
  geom_line() +
  labs(x = "Residue", y = "Bfactor")
  }
```

Use the defined `b3_plots` function to plot the protein structures provided in the original code.

```
b3_plots(c("4AKE", "1AKE", "1E4Y"))
```

```
  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/4h/mpp5b0bd1p70msy2wwpvtkm00000gn/T//RtmpuIwnv1/4AKE.pdb exists.
Skipping download

  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/4h/mpp5b0bd1p70msy2wwpvtkm00000gn/T//RtmpuIwnv1/1AKE.pdb exists.
Skipping download

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

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/4h/mpp5b0bd1p70msy2wwpvtkm00000gn/T//RtmpuIwnv1/1E4Y.pdb exists.
Skipping download
```

Generalize the above code to work with any protein.

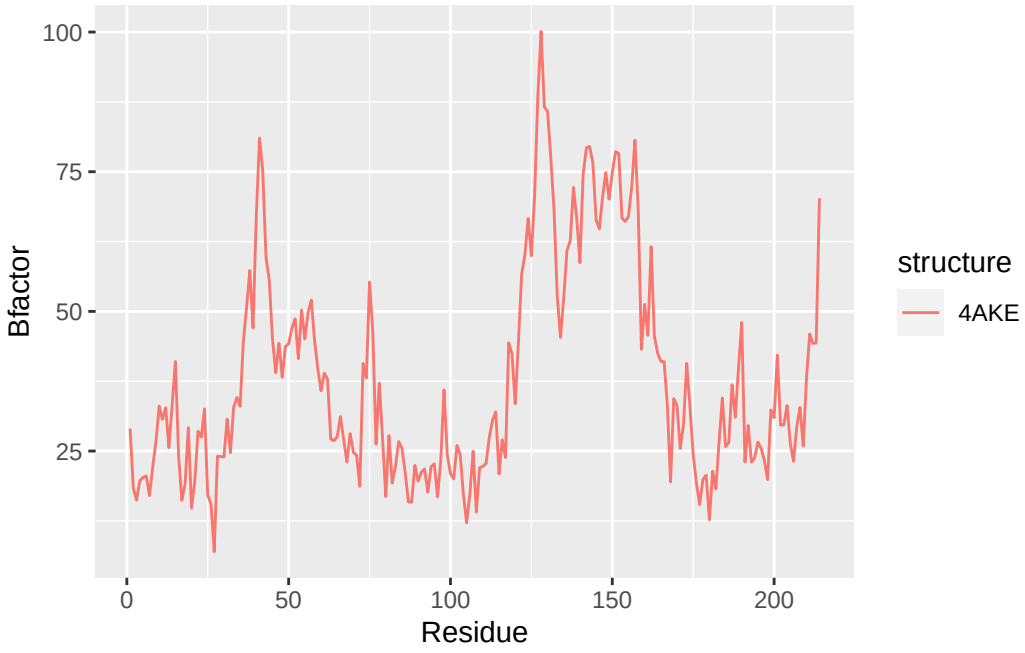
```
any_plots <- function(pdb_id) {

  # Read PDB file
  pdb <- read.pdb(pdb_id)

  # Trim PDB file and extract b factors
  pdb_trim <- trim.pdb(pdb, chain="A", elety="CA")
  b_factors <- pdb_trim$atom$b

  # Create a 'data.frame' for the structure
  df <- data.frame(x = seq_along(b_factors),
                   y = b_factors,
                   structure = pdb_id)

  # Use ggplot2 to plot the protein structure
  ggplot(df, aes(x = x, y = y, color = structure)) +
  geom_line() +
  labs(x = "Residue", y = "Bfactor")
}
```

Now the function `any_plots` can be used to plot any protein structure.

```
any_plots("4AKE")
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/4h/mpp5b0bd1p70msy2wwpvtkm00000gn/T//RtmpuIwnv1/4AKE.pdb exists.
Skipping download
```

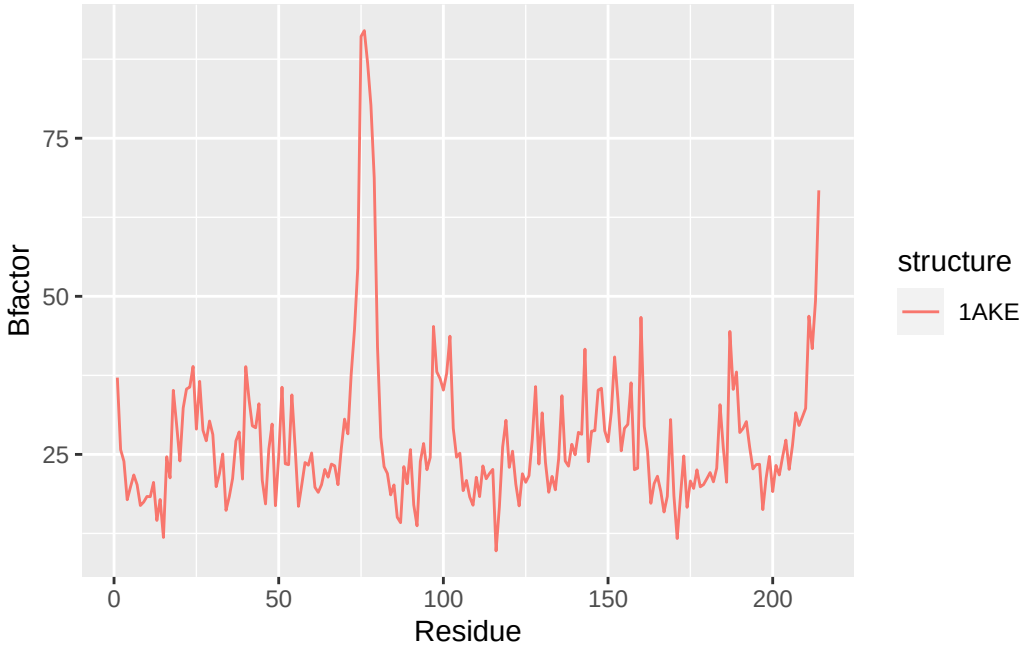



```
any_plots("1AKE")
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/4h/mpp5b0bd1p70msy2wwpvtkm00000gn/T//RtmpuIwnv1/1AKE.pdb exists.
Skipping download
```

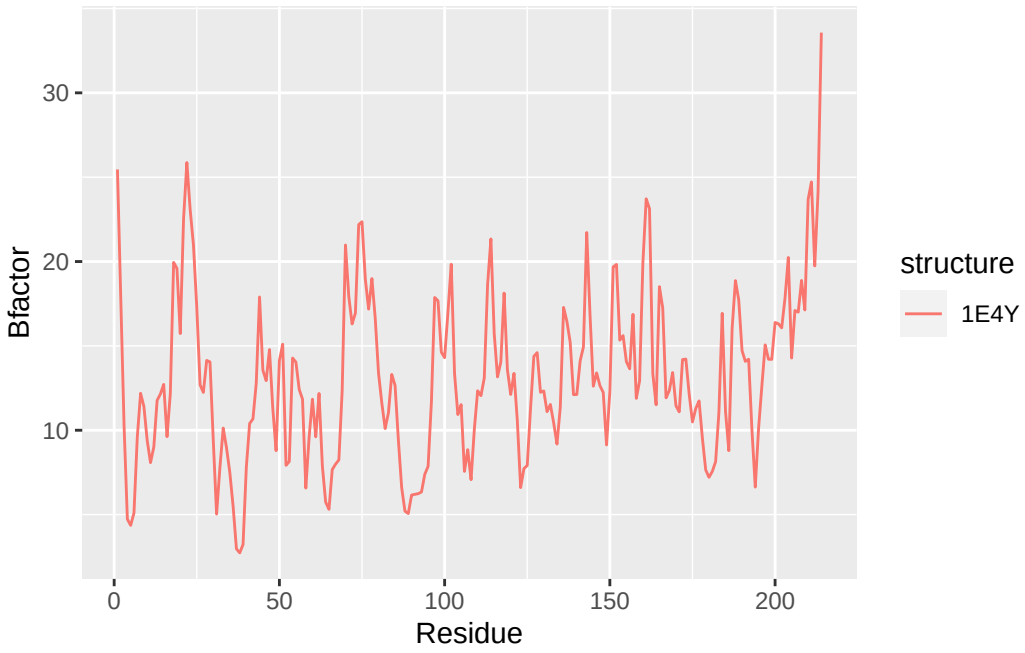
```
   PDB has ALT records, taking A only, rm.alt=TRUE
```




```
any_plots("1E4Y")
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/4h/mpp5b0bd1p70msy2wwpvtkm00000gn/T//RtmpuIwnv1/1E4Y.pdb exists.
Skipping download
```


30
20
10
Bfactor
0
50
100
150
200
Residue
structure
1E4Y