Class6: BGGN

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Quarto

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Running Code

My first function

```
add <- function(x, y) {
  x + y
  }
```

Can I just use it?

```
add(1,1)
```

```
[1] 2
```

```
add(x=1, y=100)
```

```
[1] 101
```

```
add(c(100,1,100),1)
```

```
[1] 101   2 101
```

```
add(x=c(100,1,100), y=1)
```

```
[1] 101   2 101
```

```
#add(10) #Missing argument Y
```

My second function. So if I next time don’t give Y argument, it will still work

```
add <- function(x, y=1) {
  x + y
  }
```

```
#add(10)
#add(10,10) #you can still overwrite the y=1 of the original function

#add(1,1,1)
#add(1,1, z=1) #same error, you use an unused argument, you can modify your funct
```

Let's write a function to generate a random nucleotide sequence of any length.

```
bases <- c("A", "C", "T", "G")

sample(bases, size = 2)
```

```
[1] "C" "G"
```

```
#sample(bases, size = 5) #this gives error because you cannot take a sample large
sample(bases, size = 100, replace = TRUE)
```

```
  [1] "G" "A" "A" "G" "A" "C" "T" "C" "G" "G" "C" "A" "A" "G" "C" "A" "A" "C"
 [19] "C" "G" "T" "G" "G" "A" "C" "A" "A" "T" "T" "A" "G" "C" "T" "T" "A" "T"
 [37] "C" "A" "C" "T" "C" "A" "C" "G" "G" "G" "T" "C" "C" "C" "T" "C" "C" "G"
 [55] "A" "G" "T" "C" "C" "G" "C" "C" "C" "T" "T" "T" "A" "C" "G" "C" "T" "C"
 [73] "A" "A" "C" "A" "A" "G" "T" "T" "T" "G" "C" "G" "A" "G" "C" "A" "G" "G"
 [91] "C" "G" "C" "C" "C" "T" "T" "G" "A" "G"
```

```
sequence <- sample(bases, size = 100, replace = TRUE)
```

That is my wee working snipet now I can make it into a function

```
generate_dna <- function(length) {
  bases <- c("A", "C", "T", "G")
  sequence <- sample(bases, size = length, replace = TRUE)
  return(sequence) #to get your answer
}
```

```
generate_dna(10)
```

```
 [1] "G" "G" "T" "A" "T" "A" "T" "C" "A" "C"
```

```
generate_dna(length = 10)
```

```
 [1] "A" "C" "T" "G" "A" "A" "T" "G" "G" "C"
```

```
# Install the bio3d package
#install.packages("bio3d")

# Load the bio3d library
```

```r
#library(bio3d)

# Check the version of the bio3d package
#package_version("bio3d")

bio3d::aa.table #all what we want is the 3 letter code
```

```
    aa3 aa1    mass      formula                             name
ALA ALA   A  71.078    C3 H5 N O1                          Alanine
ARG ARG   R 157.194  C6 H13 N4 O1                         Arginine
ASN ASN   N 114.103   C4 H6 N2 O2                       Asparagine
ASP ASP   D 114.079    C4 H4 N O3                    Aspartic Acid
CYS CYS   C 103.143  C3 H5 N O1 S                          Cystein
GLN GLN   Q 117.126   C4 H9 N2 O2                        Glutamine
GLU GLU   E 128.106    C5 H6 N O3                    Glutamic Acid
GLY GLY   G  57.051    C2 H3 N O1                          Glycine
HIS HIS   H 137.139   C6 H7 N3 O1                        Histidine
ILE ILE   I 113.158   C6 H11 N O1                       Isoleucine
LEU LEU   L 113.158   C6 H11 N O1                          Leucine
LYS LYS   K 129.180  C6 H13 N2 O1                           Lysine
MET MET   M 131.196  C5 H9 N O1 S                       Methionine
PHE PHE   F 147.174    C9 H9 N O1                    Phenylalanine
PRO PRO   P  97.115    C5 H7 N O1                          Proline
SER SER   S  87.077    C3 H5 N O2                           Serine
THR THR   T 101.104    C4 H7 N O2                        Threonine
TRP TRP   W 186.210 C11 H10 N2 O1                       Tryptophan
TYR TYR   Y 163.173    C9 H9 N O2                         Tyrosine
VAL VAL   V  99.131    C5 H9 N O1                           Valine
ABA ABA   X  85.104   C4 H7 N1 O1          alpha-aminobutyric acid
ASH ASH   D 115.087    C4 H5 N O3            Aspartic acid Neutral
CIR CIR   R 157.170  C6 H11 N3 O2                       citrulline
CME CME   C 179.260 C5 H9 N O2 S2 s,s-(2-hydroxyethyl)thiocysteine
CMT CMT   C 115.154  C4 H5 N O1 S                 o-methylcysteine
CSD CSD   C 134.134  C3 H4 N O3 S          s-cysteinesulfinic acid
CSO CSO   C 119.142  C3 H5 N O2 S                s-hydroxycysteine
CSW CSW   C 135.142  C3 H5 N O3 S               cysteine-s-dioxide
CSX CSX   C 119.142  C3 H5 N O2 S                   s-oxy cysteine
CYM CYM   C 102.135  C3 H4 N O1 S                 Cystein Negative
CYX CYX   C 102.135  C3 H4 N O1 S                   Cystein SSbond
DDE DDE   H 280.346 C13 H22 N5 O2                      diphthamide
GLH GLH   E 129.114    C5 H7 N O3           Glutatmic acid Neutral
HID HID   H 137.139   C6 H7 N3 O1                        Histidine
HIE HIE   H 137.139   C6 H7 N3 O1                        Histidine
HIP HIP   H 138.147   C6 H8 N3 O1               Histidine Positive
HSD HSD   H 137.139   C6 H7 N3 O1                        Histidine
HSE HSE   H 137.139   C6 H7 N3 O1                        Histidine
HSP HSP   H 138.147   C6 H8 N3 O1               Histidine Positive
IAS IAS   D 115.087    C4 H5 N O3                    beta-aspartyl
KCX KCX   K 172.182  C7 H12 N2 O3        lysine nz-carboxylic acid
LYN LYN   K 129.180  C6 H13 N2 O1                   Lysine Neutral
```

```
MHO MHO   M 147.195  C5 H9 N O2 S               s-oxymethionine
MLY MLY   K 156.225  C8 H16 N2 O1               n-dimethyl-lysine
MSE MSE   M 178.091 C5 H9 N O1 SE               selenomethionine
OCS OCS   C 151.141  C3 H5 N O4 S          cysteinesulfonic acid
PFF PFF   F 165.164  C9 H8 F N O1        4-fluoro-l-phenylalanine
PTR PTR   Y 243.153 C9 H10 N O5 P              o-phosphotyrosine
SEP SEP   S 167.057  C3 H6 N O5 P                  phosphoserine
TPO TPO   T 181.084  C4 H8 N O5 P                phosphothreonine
```

```
bio3d::aa.table$aa1 #all what we want is the 3 letter code
```

```
 [1] "A" "R" "N" "D" "C" "Q" "E" "G" "H" "I" "L" "K" "M" "F" "P" "S" "T" "W" "Y"
[20] "V" "X" "D" "R" "C" "C" "C" "C" "C" "C" "C" "C" "H" "E" "H" "H" "H" "H" "H"
[39] "H" "D" "K" "K" "M" "K" "M" "C" "F" "Y" "S" "T"
```

```
unique(bio3d::aa.table$aa1)[1:20]
```

```
 [1] "A" "R" "N" "D" "C" "Q" "E" "G" "H" "I" "L" "K" "M" "F" "P" "S" "T" "W" "Y"
[20] "V"
```

```
aa <- unique(bio3d::aa.table$aa1)[1:20]
```

Generate random protein sequence of length 6-13

```
generate_protein <- function(length) {
  aa <- unique(bio3d::aa.table$aa1)[1:20]
  sequence <- sample(aa, size = length, replace = TRUE)
  return(sequence) #to get your answer
}
```

```
generate_protein(10)
```

```
 [1] "E" "R" "A" "L" "N" "E" "T" "Q" "S" "W"
```

```
generate_protein(length = 10)
```

```
 [1] "L" "Q" "G" "E" "Q" "G" "R" "T" "Y" "K"
```

```
generate_protein(6)
```

```
[1] "V" "Y" "A" "L" "P" "Y"
```

```
generate_protein(7)
```

```
[1] "P" "D" "Y" "H" "K" "C" "K"
```

To get sequences one by one is boring. So generate random protein sequences of length 6 to 12

```
#sapply(vector, function)
sapply(6:12, generate_protein) #you can not easy paste this somewhere because of
```

```
[[1]]
[1] "K" "F" "I" "M" "P" "M"

[[2]]
[1] "Y" "L" "E" "P" "T" "I" "N"

[[3]]
[1] "Q" "T" "R" "T" "T" "M" "Y" "L"

[[4]]
[1] "H" "P" "A" "P" "N" "W" "L" "E" "G"

[[5]]
 [1] "N" "G" "Y" "T" "A" "W" "A" "E" "S" "H"

[[6]]
 [1] "L" "R" "L" "G" "K" "Y" "L" "C" "T" "A" "T"

[[7]]
 [1] "T" "Y" "M" "T" "H" "S" "P" "V" "K" "Y" "C" "Q"
```

```
paste(c("barry", "alice"), "loves R", sep = "-")
```

```
[1] "barry-loves R" "alice-loves R"
```

```
paste(c("barry", "alice"), "loves R", sep = "")
```

```
[1] "barryloves R" "aliceloves R"
```

```
paste(c("barry", "alice"), "loves R")
```

```
[1] "barry loves R" "alice loves R"
```

```
generate_protein <- function(length) {
  aa <- unique(bio3d::aa.table$aa1)[1:20]
  sequence <- sample(aa, size = length, replace = TRUE)
  sequence <- paste(sequence, collapse = "")
  return(sequence) #to get your answer
}

sapply(6:12, generate_protein)
```

```
[1] "WFNDNV"       "YNKVHCC"      "DCLVVLWN"     "SNSRPKAHP"    "GWYQVKPDMN"  
[6] "DYAGQCTRTTQ"  "LTVYFETHKPYT"
```

```r
answer <- sapply(6:12, generate_protein)
answer
```

```
[1] "TFLTFC"       "YMSNDQY"      "HDDWMVWI"     "PATQMRKIH"    "NPCCEGSDGM"  
[6] "FVRGHFDSNKR"  "SDAIVCHQSFMW"
```

FASTA formatting

```r
paste(">id.",6:12) #we don't want spaces
```

```
[1] ">id. 6"  ">id. 7"  ">id. 8"  ">id. 9"  ">id. 10" ">id. 11" ">id. 12"
```

```r
paste(">id.",6:12, sep = "")
```

```
[1] ">id.6"  ">id.7"  ">id.8"  ">id.9"  ">id.10" ">id.11" ">id.12"
```

```r
paste(">id.",6:12, answer, sep = "") #but now we want everything on new line
```

```
[1] ">id.6TFLTFC"       ">id.7YMSNDQY"      ">id.8HDDWMVWI"    
[4] ">id.9PATQMRKIH"    ">id.10NPCCEGSDGM"  ">id.11FVRGHFDSNKR"
[7] ">id.12SDAIVCHQSFMW"
```

```r
paste(">id.", 6:12, "\n", answer, sep = "")
```

```
[1] ">id.6\nTFLTFC"        ">id.7\nYMSNDQY"       ">id.8\nHDDWMVWI"     
[4] ">id.9\nPATQMRKIH"     ">id.10\nNPCCEGSDGM"   ">id.11\nFVRGHFDSNKR"
[7] ">id.12\nSDAIVCHQSFMW"
```

```r
cat(paste(">id.", 6:12, "\n", answer, sep = "")) #but we want to look like fasta
```

```
>id.6
TFLTFC >id.7
YMSNDQY >id.8
HDDWMVWI >id.9
PATQMRKIH >id.10
NPCCEGSDGM >id.11
FVRGHFDSNKR >id.12
SDAIVCHQSFMW
```

```r
cat(paste(">id.", 6:12, "\n", answer, sep = ""), sep="\n")
```

```
>id.6
TFLTFC
>id.7
YMSNDQY
>id.8
HDDWMVWI
```

```
>id.9
PATQMRKIH
>id.10
NPCCEGSDGM
>id.11
FVRGHFDSNKR
>id.12
SDAIVCHQSFMW
```

HOMEWORK:

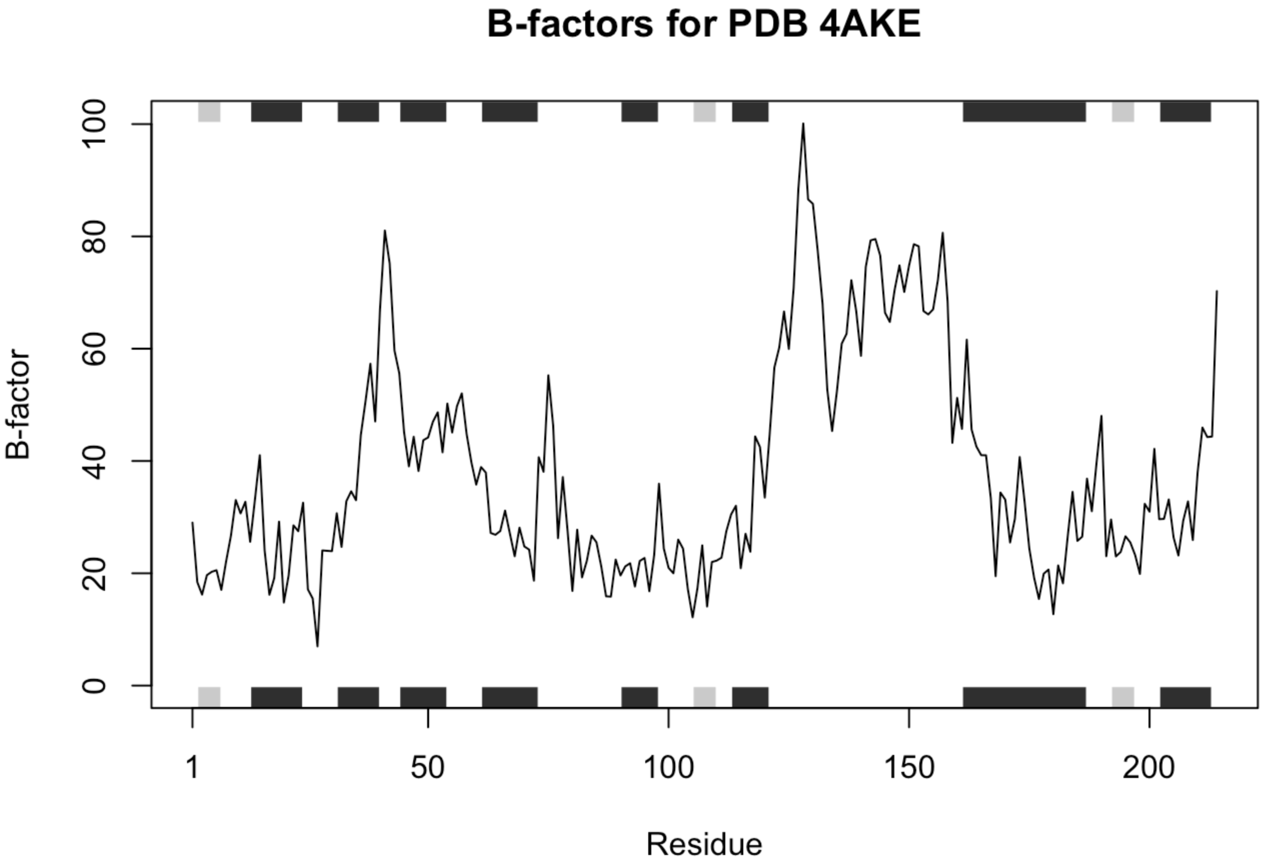
```r
# How would you generalize the original code above to work with any set of input
library(bio3d)
bio3d::aa.table
```

```
    aa3 aa1    mass       formula                             name
ALA ALA   A  71.078    C3 H5 N O1                          Alanine
ARG ARG   R 157.194  C6 H13 N4 O1                         Arginine
ASN ASN   N 114.103   C4 H6 N2 O2                       Asparagine
ASP ASP   D 114.079    C4 H4 N O3                    Aspartic Acid
CYS CYS   C 103.143  C3 H5 N O1 S                          Cystein
GLN GLN   Q 117.126   C4 H9 N2 O2                        Glutamine
GLU GLU   E 128.106    C5 H6 N O3                    Glutamic Acid
GLY GLY   G  57.051    C2 H3 N O1                          Glycine
HIS HIS   H 137.139   C6 H7 N3 O1                        Histidine
ILE ILE   I 113.158   C6 H11 N O1                       Isoleucine
LEU LEU   L 113.158   C6 H11 N O1                          Leucine
LYS LYS   K 129.180  C6 H13 N2 O1                           Lysine
MET MET   M 131.196  C5 H9 N O1 S                       Methionine
PHE PHE   F 147.174    C9 H9 N O1                    Phenylalanine
PRO PRO   P  97.115    C5 H7 N O1                          Proline
SER SER   S  87.077    C3 H5 N O2                           Serine
THR THR   T 101.104    C4 H7 N O2                        Threonine
TRP TRP   W 186.210 C11 H10 N2 O1                       Tryptophan
TYR TYR   Y 163.173    C9 H9 N O2                         Tyrosine
VAL VAL   V  99.131    C5 H9 N O1                           Valine
ABA ABA   X  85.104   C4 H7 N1 O1          alpha-aminobutyric acid
ASH ASH   D 115.087    C4 H5 N O3            Aspartic acid Neutral
CIR CIR   R 157.170  C6 H11 N3 O2                       citrulline
CME CME   C 179.260 C5 H9 N O2 S2 s,s-(2-hydroxyethyl)thiocysteine
CMT CMT   C 115.154  C4 H5 N O1 S                 o-methylcysteine
CSD CSD   C 134.134  C3 H4 N O3 S          s-cysteinesulfinic acid
CSO CSO   C 119.142  C3 H5 N O2 S                s-hydroxycysteine
CSW CSW   C 135.142  C3 H5 N O3 S               cysteine-s-dioxide
CSX CSX   C 119.142  C3 H5 N O2 S                   s-oxy cysteine
CYM CYM   C 102.135  C3 H4 N O1 S                 Cystein Negative
CYX CYX   C 102.135  C3 H4 N O1 S                   Cystein SSbond
DDE DDE   H 280.346 C13 H22 N5 O2                      diphthamide
GLH GLH   E 129.114    C5 H7 N O3           Glutatmic acid Neutral
```

```
HID HID   H 137.139   C6 H7 N3 O1                        Histidine
HIE HIE   H 137.139   C6 H7 N3 O1                        Histidine
HIP HIP   H 138.147   C6 H8 N3 O1               Histidine Positive
HSD HSD   H 137.139   C6 H7 N3 O1                        Histidine
HSE HSE   H 137.139   C6 H7 N3 O1                        Histidine
HSP HSP   H 138.147   C6 H8 N3 O1               Histidine Positive
IAS IAS   D 115.087    C4 H5 N O3                    beta-aspartyl
KCX KCX   K 172.182  C7 H12 N2 O3        lysine nz-carboxylic acid
LYN LYN   K 129.180  C6 H13 N2 O1                   Lysine Neutral
MHO MHO   M 147.195  C5 H9 N O2 S                  s-oxymethionine
MLY MLY   K 156.225  C8 H16 N2 O1                n-dimethyl-lysine
MSE MSE   M 178.091 C5 H9 N O1 SE                 selenomethionine
OCS OCS   C 151.141  C3 H5 N O4 S            cysteinesulfonic acid
PFF PFF   F 165.164  C9 H8 F N O1         4-fluoro-l-phenylalanine
PTR PTR   Y 243.153 C9 H10 N O5 P                o-phosphotyrosine
SEP SEP   S 167.057  C3 H6 N O5 P                    phosphoserine
TPO TPO   T 181.084  C4 H8 N O5 P                 phosphothreonine
```

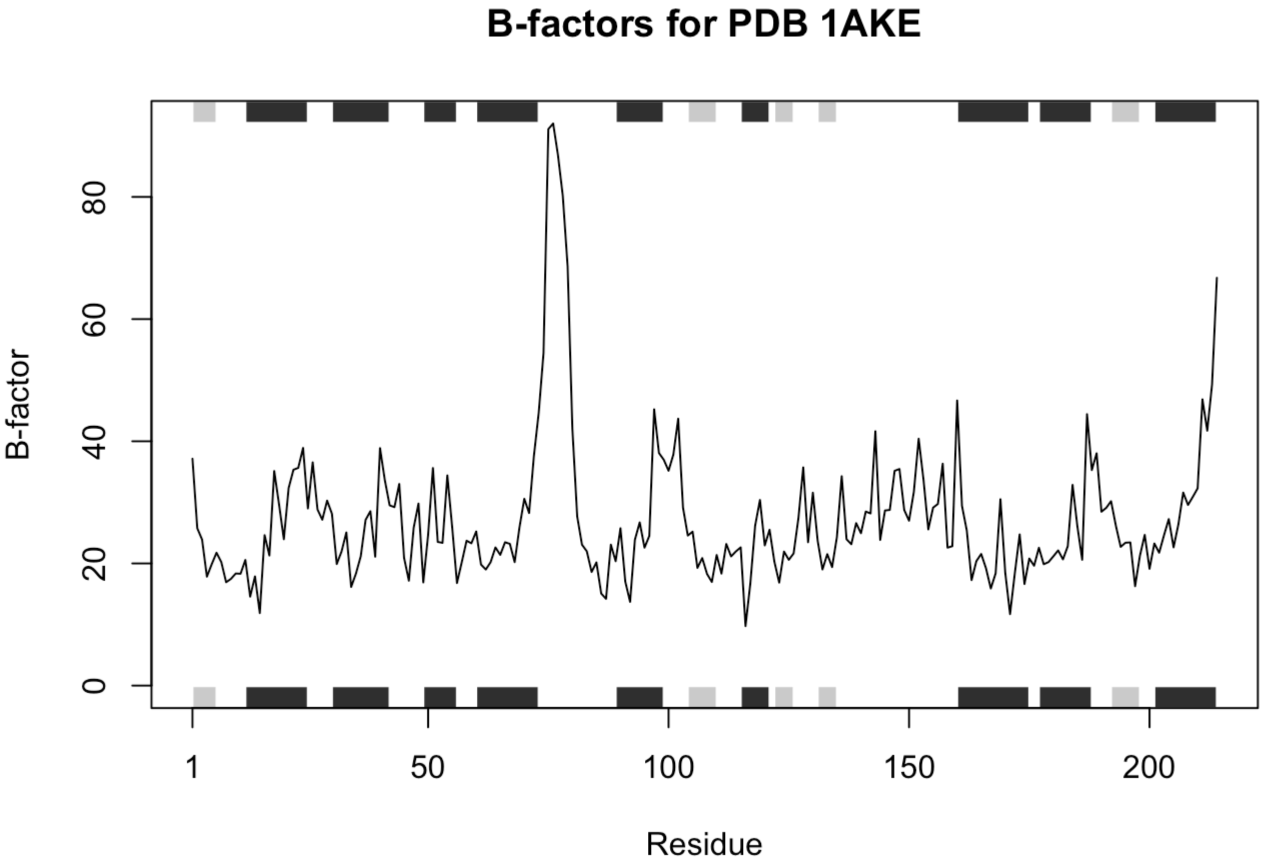
```r
b_factors_for_pdb <- function(pdb_id, chain = "A", elety = "CA") {
  # Read and trim the PDB file
  chain_data <- trim.pdb(read.pdb(pdb_id), chain = chain, elety = elety)
  # Extract B-factors
  extractB <- chain_data$atom$b
  # Plot B-factors
  plotb3(extractB, sse = chain_data, typ = "l", ylab = "B-factor",
         main = paste("B-factors for PDB", pdb_id))
}

b_factors_for_pdb("4AKE")
```

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



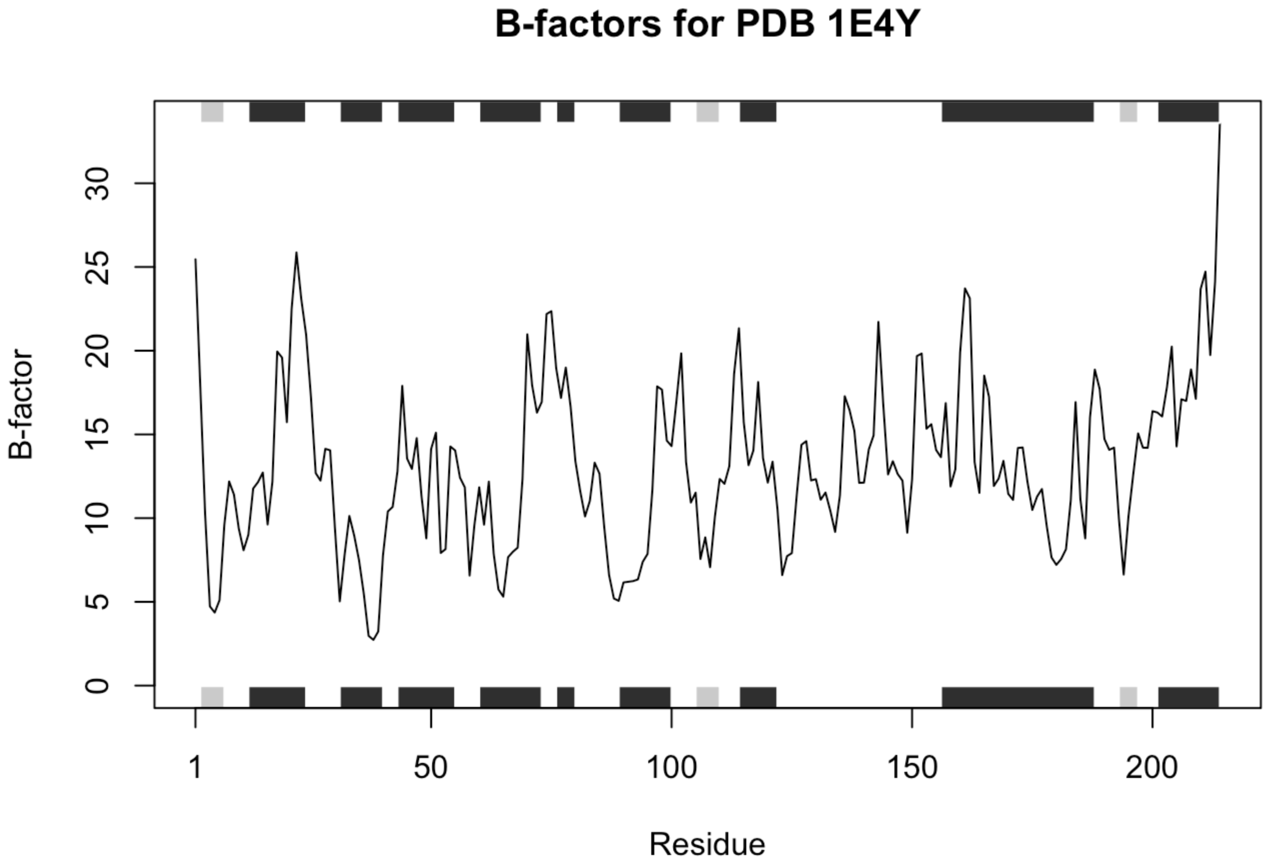
```
b_factors_for_pdb("1AKE")
```

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



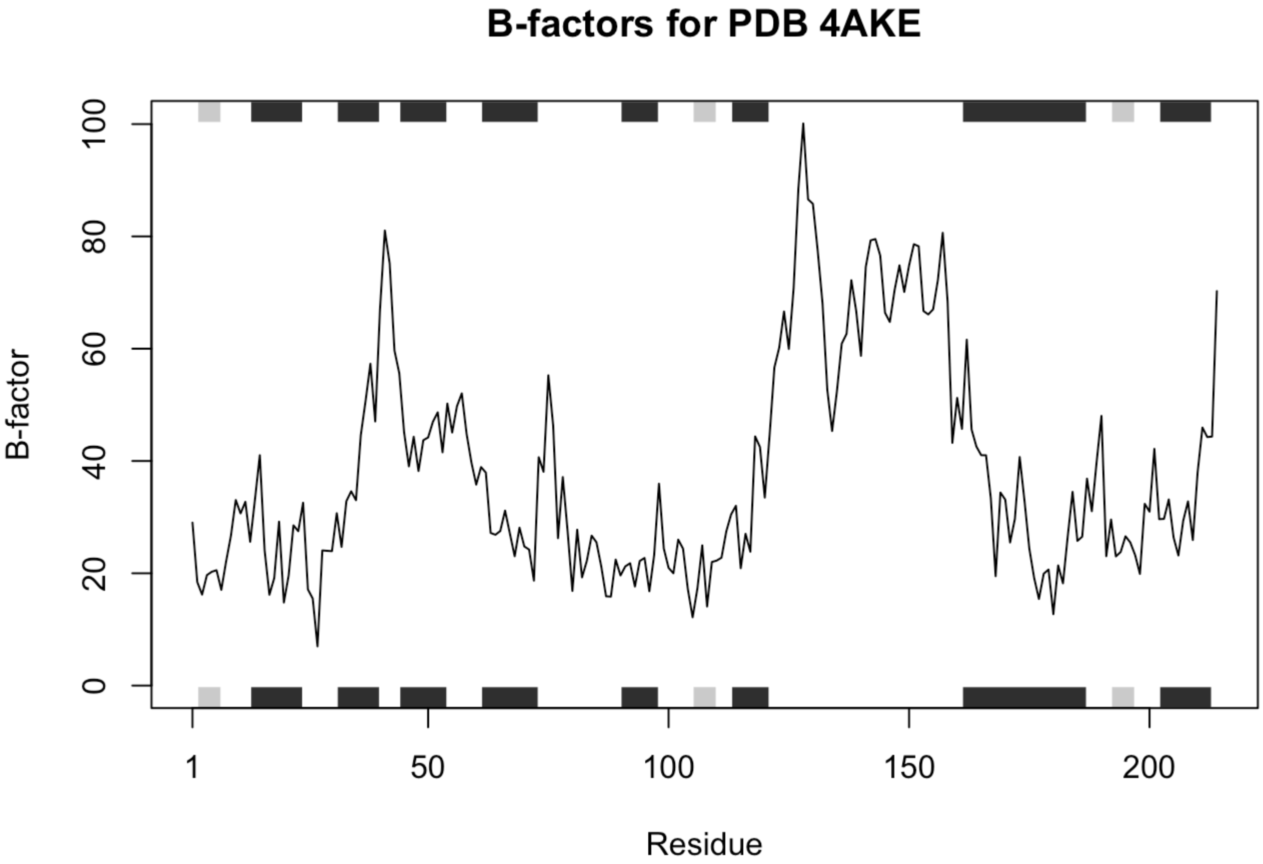
```
b_factors_for_pdb("1E4Y")
```

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

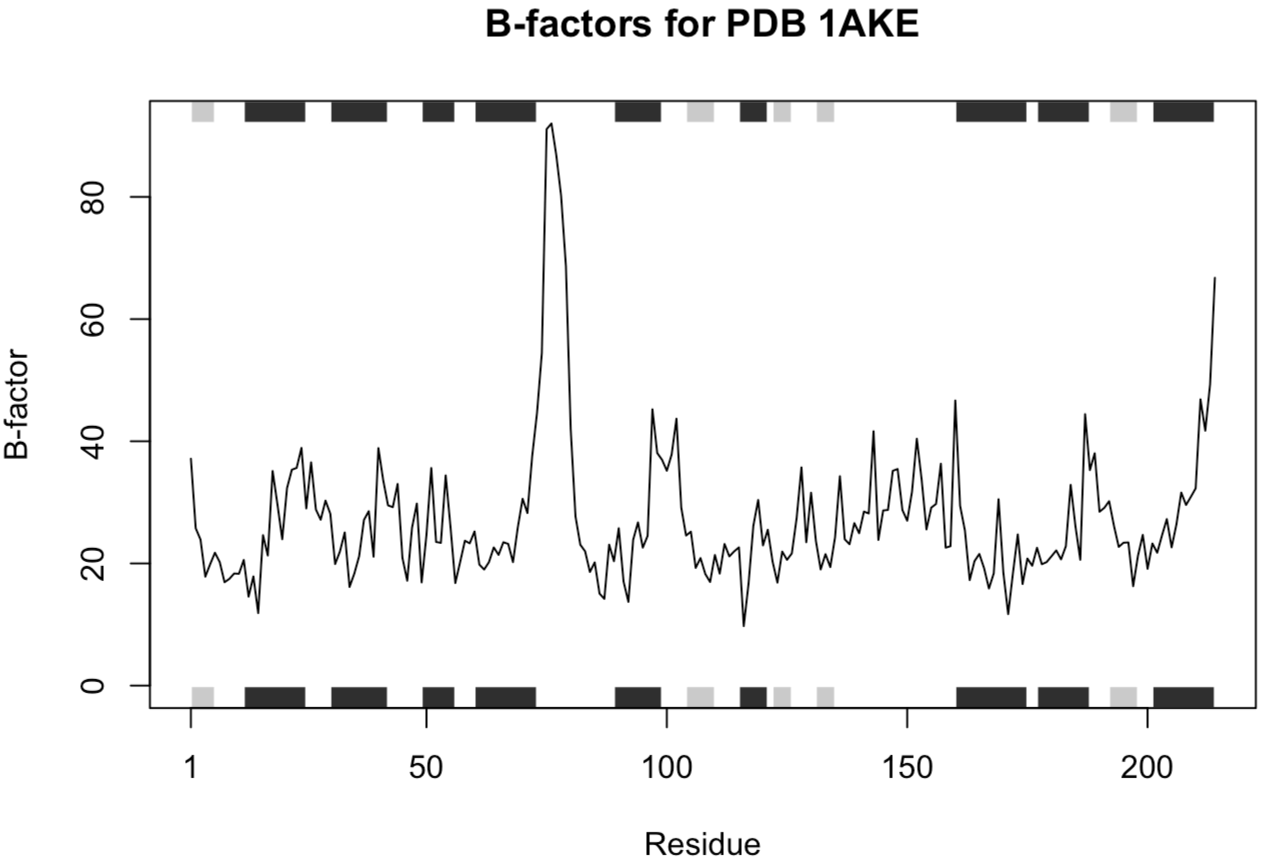


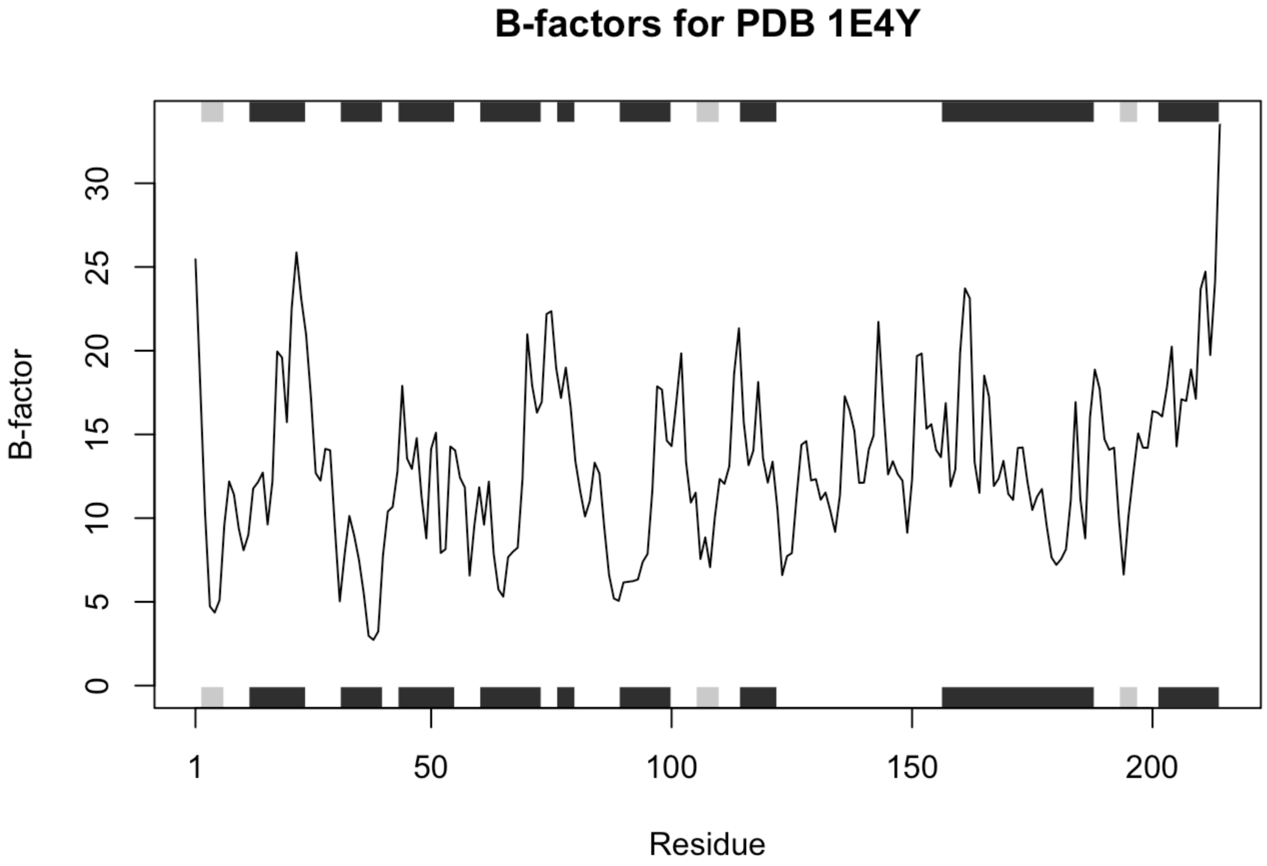
```
#Or make it all in 1 line
sapply(c("4AKE", "1AKE", "1E4Y"), b_factors_for_pdb)
```

```
  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/wc/y60y10bj5jz0zzxkrq739z580000gn/T//RtmpGq8EYr/4AKE.pdb exists.
Skipping download

  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/wc/y60y10bj5jz0zzxkrq739z580000gn/T//RtmpGq8EYr/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/wc/y60y10bj5jz0zzxkrq739z580000gn/T//RtmpGq8EYr/1E4Y.pdb exists.
Skipping download
```


B-factors for PDB 1AKE
B-factor
0
20
40
60
80
1
50
100
150
200
Residue



```
$`4AKE`
NULL

$`1AKE`
NULL

$`1E4Y`
NULL
```