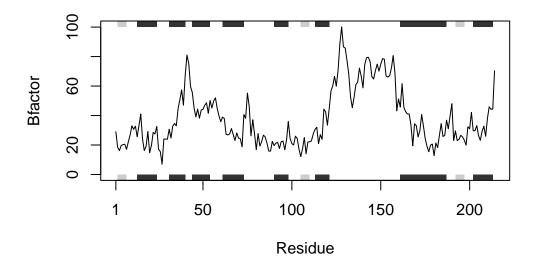
Class06_Extension

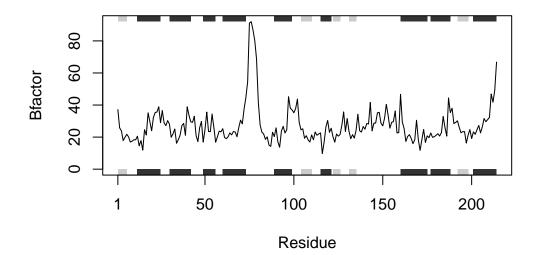
Hailey Wheeler (A13312713)

```
# Can you improve this analysis code?
library(bio3d)
\# Inserting PDB structure file for a specific protein "" - generating vector
s1 <- read.pdb("4AKE") # kinase with drug</pre>
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
# Create data.frame based on selected file: chain identifier, and atom type = elety
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")</pre>
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")</pre>
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")</pre>
# select character matrix containing all atomic coordinate data - create row per atom and
s1.b <- s1.chainA$atom$b</pre>
s2.b <- s2.chainA$atom$b</pre>
s3.b <- s3.chainA$atom$b
```

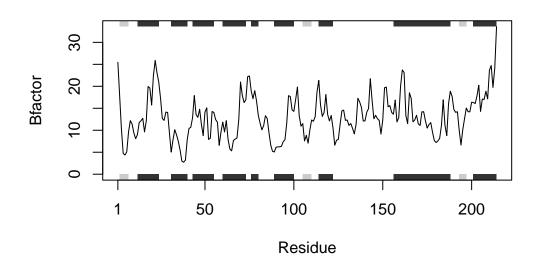
```
# Plot data with x = 1 and y = Bfactor
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



plotb3(s2.b, sse=s2.chainA, typ="1", ylab="Bfactor")



plotb3(s3.b, sse=s3.chainA, typ="1", ylab="Bfactor")



hierarchical cluster analysis on the dissimilarities between the chain associated with the \leftarrow hclust(dist(rbind(s1.b, s2.b, s3.b))) plot(hc)

Cluster Dendrogram



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

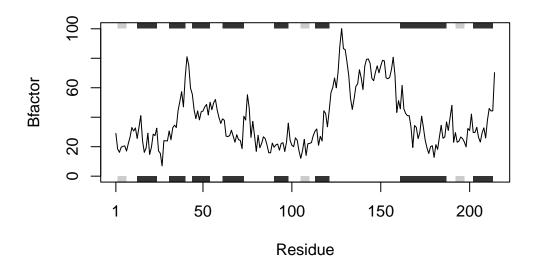
lbio3d()

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"aa2index"	"aa2mass"	"aa321"
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[265] "summary.cna" "summary.cnapath" "summary.pdb" [268] "torsion.pdb" "torsion.xyz" "transducin" [271] "trim" "trim.mol2" "trim.pdb" [274] "trim.pdbs" "trim.xyz" "unbound" [277] "uniprot" "var.pdbs" "var.xyz" [280] "vec2resno" "vmd" "vmd_colors" [283] "vmd.cna" "vmd.cnapath" "vmd.ecna" [286] "vmd.ecnapath" "wrap.tor" "write.crd" [289] "write.fasta" "write.mol2" "write.ncdf" [292] "write.pdb" "write.pir" "write.pqr"	[259]	"sip.enma"	"sip.nma"	"sse.bridges"
[268] "torsion.pdb" "torsion.xyz" "transducin" [271] "trim" "trim.mol2" "trim.pdb" [274] "trim.pdbs" "trim.xyz" "unbound" [277] "uniprot" "var.pdbs" "var.xyz" [280] "vec2resno" "vmd" "vmd_colors" [283] "vmd.cna" "vmd.cnapath" "vmd.ecna" [286] "vmd.ecnapath" "wrap.tor" "write.crd" [289] "write.fasta" "write.mol2" "write.ncdf" [292] "write.pdb" "write.pir" "write.pqr"		"store.atom"	"stride"	"struct.aln"
[271] "trim" "trim.mol2" "trim.pdb" [274] "trim.pdbs" "trim.xyz" "unbound" [277] "uniprot" "var.pdbs" "var.xyz" [280] "vec2resno" "vmd" "vmd_colors" [283] "vmd.cna" "vmd.cnapath" "vmd.ecna" [286] "vmd.ecnapath" "wrap.tor" "write.crd" [289] "write.fasta" "write.mol2" "write.ncdf" [292] "write.pdb" "write.pir" "write.pqr"		•	"summary.cnapath"	"summary.pdb"
[274] "trim.pdbs" "trim.xyz" "unbound" [277] "uniprot" "var.pdbs" "var.xyz" [280] "vec2resno" "vmd" "vmd_colors" [283] "vmd.cna" "vmd.cnapath" "vmd.ecna" [286] "vmd.ecnapath" "wrap.tor" "write.crd" [289] "write.fasta" "write.mol2" "write.ncdf" [292] "write.pdb" "write.pir" "write.pqr"		_	•	"transducin"
[277] "uniprot" "var.pdbs" "var.xyz" [280] "vec2resno" "vmd" "vmd_colors" [283] "vmd.cna" "vmd.cnapath" "vmd.ecna" [286] "vmd.ecnapath" "wrap.tor" "write.crd" [289] "write.fasta" "write.mol2" "write.ncdf" [292] "write.pdb" "write.pir" "write.pqr"	[271]		"trim.mol2"	"trim.pdb"
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[283] "vmd.cna" "vmd.cnapath" "vmd.ecna" [286] "vmd.ecnapath" "wrap.tor" "write.crd" [289] "write.fasta" "write.mol2" "write.ncdf" [292] "write.pdb" "write.pir" "write.pqr"		_		-
[286] "vmd.ecnapath" "wrap.tor" "write.crd" [289] "write.fasta" "write.mol2" "write.ncdf" [292] "write.pdb" "write.pir" "write.pqr"			"vmd"	"vmd_colors"
[289] "write.fasta" "write.mol2" "write.ncdf" [292] "write.pdb" "write.pir" "write.pqr"	[283]	"vmd.cna"	_	"vmd.ecna"
[292] "write.pdb" "write.pir" "write.pqr"		_		"write.crd"
[295] "xyz2atom" "xyz2z nca" "z2xyz nca"			_	
22Ay2.pca 22Ay2.pca	[295]	"xyz2atom"	"xyz2z.pca"	"z2xyz.pca"

```
help(bio3d)
  ## Install Bio3D package on Quarto
  library(bio3d)
  ## Call your function(x)
  protein <- function(x){</pre>
    # call protein file and establish as "x"
    x <- read.pdb(x)
    # create a new PDB object based on pdb selection of backbone atoms (selecting for Chain
    x.chainA <- trim.pdb(x, chain = "A", elety = "CA")</pre>
    # select character matrix containing all atomic coordinate data (create row per atom and
    # Plot residue temperature factor by secondary structure element of Chain A, using x = 1
    plot.bio3d(x.chainA$atom$b, sse=x.chainA, type="1", ylab ="Bfactor")
  }
  # sse = secondary structure element
  # Bfactor = residue temperature factors
  # trim.pdb() = create a new PDB object based on our selection of backbone atoms
  # Call created function 'protein' and apply that to a pdb object to analyze B-factor vs. R
  protein("4AKE")
  Note: Accessing on-line PDB file
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/cs/673kvc2j4yn7dpx3wvpdlh8c0000gn/T//RtmpWvwj9S/4AKE.pdb exists.
Skipping download
```

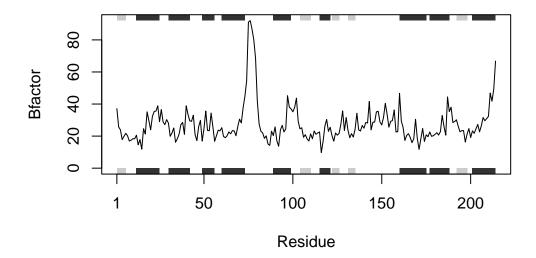


protein("1AKE")

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/cs/673kvc2j4yn7dpx3wvpdlh8c0000gn/T//RtmpWvwj9S/1AKE.pdb exists.
Skipping download

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



protein("1E4Y")

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/cs/673kvc2j4yn7dpx3wvpdlh8c0000gn/T//RtmpWvwj9S/1E4Y.pdb exists.
Skipping download

