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title: "HW Class 6 (R Function)"
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format: pdf

```{r}
# install.packages("bio3d")

```

```{r}
library(bio3d)

#--------------------------------------
# Function: plot_bfactors
#--------------------------------------
# Inputs:
#   pdb_ids – character vector of PDB IDs or file paths
#   chain   – which chain to analyze (default "A")
#   elety   – which atom type to analyze (default "CA")
#
# What it does:
#   For each structure, the function:
#     1. Reads the PDB file or downloads it.
#     2. Extracts the specified chain and atom type.
#     3. Retrieves the B-factors for those atoms.
#     4. Plots the B-factor profile for each structure.
#
# Output:
#   • A plot for each input structure showing B-factor vs. residue number.
#   • Invisibly returns a named list of B-factor vectors for later analysis.
#--------------------------------------

plot_bfactors <- function(pdb_ids, chain = "A", elety = "CA") {
  if (!is.character(pdb_ids)) stop("pdb_ids must be a character vector.")

  b_list <- list()

  for (id in pdb_ids) {
    # read PDB file (downloads automatically if only ID is provided)
    pdb <- read.pdb(id)

    # keep only one chain and atom type
    pdb_trim <- trim.pdb(pdb, chain = chain, elety = elety)

    # extract B-factors
    b_vals <- pdb_trim$atom$b
    b_list[[id]] <- b_vals

    # plot the B-factors
    plotb3(b_vals,
           sse = pdb_trim,
           typ = "l",
           ylab = "B-factor",
           main = paste("B-factor profile:", id))
  }

  invisible(b_list)
}

# Example use:
```

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