

Analysis of protein drug interactions

Jenny Zhou

2023-04-25

B-factor means “the attenuation of x-ray scattering or coherent neutron scattering caused by thermal motion”.

Reference: https://en.wikipedia.org/wiki/Debye%E2%80%93Waller_factor

This function is used to plot the value of B-factors of C-alpha atoms in the chain A of a specific protein.

```
#Loading the bio3d package before executing function
library(bio3d)

#Input of the function is the accession number (in the form of character) of protein on RCSB PDB
plot_bfactor <- function(x) {

  #Read pdb file from online database
  read <- read.pdb(x)

  #Select chainA dataset from the pdb file and select atom type to be C-alpha atoms found in protein re
  chainA <- trim.pdb(read, chain="A", elety="CA")

  #Plot the value of B-factors of C-alpha atoms against their protein residues
  plotb3(chainA$atom$b, sse=chainA, typ="l", ylab="Bfactor")
}
```

example:

```
#the input protein is MLK1 kinase domain with leucine zipper 1
library(bio3d)
plot_bfactor("4UY9")
```

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

