portfolio_view

PDB to Average B-Factors per residue

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Public access: https://github.com/Eddy-Barraud/PDB2AvgBFactors

Requirements : numpy pandas matplotlib seaborn biopython

This script is extracting B-Factor values of every PDB file in the same folder. It will generate two files per PDB file :

- filename.resbfactors.txt : average B-Factors per residue (# RES AvgValue)
- filename.resbfactors.png : plot of the calculated data

The python script behind the app is using Seaborn and BioPython libraries.

Instructions

- Copy b-factor.convert.all.PDB.exe on your working directory, containing PDB file(s).
- Run b-factor.convert.all.PDB.exe and it will extract B-Factors from all PDB in the current directory.