

Abstract

We developed a software framework that allows the analysis of ligand-free (apo) and ligand-bound (holo) forms of proteins that are accessible in PDB. The software downloads the current version of the PDB, divides the structures into groups of the same molecules, and these into apo and holo forms. Finally, it is possible to analyze pairs of apo and holo structures with respect to their different structural characteristics. In addition to the software work itself, we present the results of selected analyses of the current version of the data in the PDB. We also verify the results against previous work.