

Pex, Analytical Tools for PDB Structures

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Some Pex files can be downloaded from the CBMN site (<http://www.fsagx.ac.be/index.htm>).

Pex-files are handy output files in which PDB structures are described¹. In a single file numerous qualitative (secondary structures, main chain and side chain atom partners....) and quantitative (atomic distances, covalent and dihedral angles, accessible surface area, energies....) parameters of a 3D structure are listed in such a way that files can be easily filed up and compared.

In the last few years, we have been using Pex files¹ to revisit the main chain H-bond structures in proteins², to analyse the partial atomic charges of residues buried in proteins³, the accessible surface of residues in protein structures⁴, to analyse the aromatic pairing in protein structures⁵⁻⁸. Aside a description of structures, Pex are also handy to follow the course of calculations as the variations of structures during Monte Carlo dynamics, the insertion of proteins in membranes⁹⁻¹⁰. We shall present examples of Pex-derived possibilities.

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