The library values are obtained from over 60 small peptide or organic molecule crystal structures refined against ultra-high-resolution X-ray diffraction data. The library transfer is applied automatically in the MoPro software suite[2] to peptide and protein structures measured at atomic resolution. We are expanding the library from proteins to common chemical groups. A new automated strategy involving the algorithms for successive searching and matching the atom types in molecules has been recently developed[3]. The atom types are recognized on the basis of their chemical environment and local symmetry depending on the geometrical parameters (bonds, valence angles and planarity) of the considered atom. The local symmetry of the multipoles is imposed by the consistent use of optimal local axes systems and symmetry restraints/constraints.

The new atom types are added to the library every time when spotted during the refinement of new available charge density data. Further averaging is performed among the atom types within the same chemical context.


Keywords: experimental charge densities; multipole refinements; databases

With an increasing number of biomacromolecular crystal structures being measured to ultra-high resolution, it has become possible to extend to large systems experimental charge-density methods that are usually applied to small molecules. A library has been built of average multipole populations describing the electron density of chemical groups in all 20 amino acids found in proteins[1]. The library uses the Hansen & Coppens multipolar pseudo-atom model to derive molecular electron density and electrostatic potential distributions.

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