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Assessment of Electron Density Refinement Quality Using Free-Rfactors and Restraints. Christian Jelsch[a], Slawomir Domagala[a], Bartosz Zarychta[a], Claude Lecomte[a], Benoît Guillot[a], Parthrapatim Munshi[a]. [a]*Laboratoire de Cristallographie, Résonance Magnétique et Modélisation. CNRS-Nancy Université, Vandoeuvre-lès-Nancy, France.*
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In the perspective of building an expanded electron density library [1] based on multipolar modelling for common chemical atom types, new consistent local axes systems are proposed in the software MoPro [2] . Optimal symmetry constraints can consequently be applied to atoms and a large number of multipole populations can be fixed to a zero value. The introduction of symmetry constraints in the multipolar refinement of small compounds allows the reduction of the number of multipolar parameters stored in the library and needed for the description of the atomic electron density. In a refinement, where the symmetry constraints are not applied, the use of optimal axes enables to highlight the deviations from the local pseudo-symmetry [3].
The application of symmetry constraints and/or restraints on the multipoles is more effective when the axes are in accordance with the local geometry of the atom and can lead to improved crystallographic R_{free} residuals. The systematic study of chemical equivalence and multipoles local symmetry with different restraints strengths is a valuable tool for assessing the quality of the diffraction data for a proper charge density refinement.

[1] Zarychta, B., Pichon-Pesme, V., Guillot, B., Lecomte, C. & Jelsch, C. **2007**. *Acta Cryst.* A63, 108-125. [2] Jelsch, C., Guillot, B., Lagoutte, A. & Lecomte, C. **2005**. *J. Appl. Cryst.* 38, 38-54. [3] Domagała S. & Jelsch C. **2008**. *J. Appl. Cryst*. 41, 1140-1149.

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Generalization of the Experimental Multipolar Pseudo-atom Library. Sławomir Domagała[a], Bartosz Zarychta[b], Benoît Guillot[a], Virginie Pichon-Pesme[a], Claude Lecomte[a], Christian Jelsch[a]. [a]*Laboratoire de Cristallographie, Résonance Magnétique et Modélisations Nancy Université, Vandoeuvre-lès-Nancy, France.* [b]*Opole University, Opole, Poland.*
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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.
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.

[1] Zarychta, B., Pichon-Pesme, V., Guillot, B., Lecomte, C. & Jelsch, C. **2007**. *Acta Cryst*. A63, 108-125. [2] Jelsch, C., Guillot, B., Lagoutte, A. & Lecomte, C. **2005**. *J. Appl. Cryst*. 38, 38-54. [3] Domagała S. & Jelsch C. **2008**. *J. Appl. Cryst.* 41, 1140-1149.

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