

Use of mmCIF in the Publication of Macromolecular Crystallography Communications

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Acta Crystallographica Section F: Structural Biology and Crystallization Communications was launched by the IUCr in 2005 as a rapid-publication electronic-only journal for communications on the crystallization and structure determination of biological macromolecules. Structure reports are expected to come initially from structural genomics and protein–ligand studies. For such reports, the IUCr is collaborating with the Protein Data Bank (PDB) to facilitate the deposition and publication procedures by extracting as much information as possible from program output files and capturing additional information in a standard exchange mechanism. The mechanism that is used is the macromolecular crystallographic information file (mmCIF). Authors may send the mmCIF generated during the PDB deposition process directly to the journal office, where automated scripts use it for preparation of validation reports for scrutiny by the referees, and for generation of summary tables of information, suitable for embedding within the article, about the structure determination and refinement. Details of these procedures will be given. Further work will be undertaken to refine the mmCIF dictionary and facilitate its use for publication purposes.

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