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Validation of macromolecular structures: updating standards for publication of NMR structures in an IUCr journal

We are pleased to announce that a set of guidelines which supplement the International Union of Pure and Applied Chemistry's (IUPAC) Recommendations for the Presentation of NMR Structures of Proteins and Nucleic Acids [J. L. Markley *et al.* (1998), *J. Mol. Biol.* **280**, 933–952] are now available from our web pages at <http://journals.iucr.org/f/services/structuralcommunications/>. The guidelines will be used by the referees and editors of *Acta Crystallographica Section F* to evaluate future submissions of structure reports determined by use of NMR spectroscopy until such time as a more comprehensive review of standards is reported. These guidelines for NMR data are mentioned in the 2008 Notes for authors which appear in this issue, and in the coming weeks they will be expanded and annotated with examples of good publication practice.

'Where are the submissions of structure reports which have been determined by use of NMR?' you may ask. In reply, we point to our editorial in June 2006, which announced the publication in that issue of *Solution structure of Arabidopsis thaliana protein At5g39720.1, a member of the AIG2-like protein family* [B. L. Lytle *et al.* (2006), *Acta Cryst. F* **62**, 490–493]. Publication of NMR structure reports in *Acta Cryst. F* underscores the journal's commitment to serve the structural genomics community and we look forward to other submissions in the future. At the same time, the journals of the International Union of Crystallography (IUCr) continue to hold to the highest standards of review and reproducibility in its crystallographic papers and this update expresses the commitment that those same high standards be maintained for its NMR papers as well.

The guidelines were drafted on 21 July 2007 at a workshop, whose title we chose for this editorial, which was held as part of the program of the American Crystallographic Association (ACA) meeting in Salt Lake City, Utah. The workshop was sponsored by the IUCr with additional support from Bruker BioSpin Corp., Cambridge Isotope Labs and Varian, Inc. Representatives from the NMR structure community, IUCr Journals, the relevant databases, Worldwide Protein Data Bank (wwPDB) and Biological Magnetic Resonance Data Bank (BMRB), and NMR instrumentation participated. We thank the ACA and the meeting organizers for hosting this productive workshop, the IUCr and the NMR support companies for their generous financial support and the participants, who worked together so congenially and productively to produce this important result.

The workshop it seems has anticipated an emergent effort of the NMR community itself to update the 1998 IUPAC standards in order to reflect progress in technical developments and best practices. It is an effort of the NMR Task Force, which is an advisory body of the wwPDB that provides advice and recommendations on standards for submission of NMR-derived biomolecular structures and supporting data. Over the years, the aims and goals of the PDB and the journals serving structural biology have coalesced around a number of issues of mutual concern and they have worked together to good effect on behalf of the structural biology community. The work the NMR Task Force has undertaken is another example of the continuing good service the PDB and its leadership have provided structural biology in anticipating its needs and undertaking to satisfy them. We await with interest the report of the NMR Task Force and wish them success in their deliberations. If we have been in some way helpful to their effort, we are pleased to have done so.