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Enhancements in *Acta Crystallographica Section C*

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Acta Crystallographica Section C continues to specialize in the rapid dissemination of high-quality studies of novel and challenging crystal and molecular structures in papers that provide a detailed discussion of the structures. The journal also accepts reports of difficult or challenging structures not meeting all validation criteria when the presented structures are correct and the difficulties and strategies used to treat them are scientifically discussed and properly documented. Such structures might display features such as twinning, severe disorder, or diffuse solvent regions.

The journal is striving to offer authors additional ways to increase the impact and visibility of their papers. One feature introduced a couple of years ago is the ability to generate additional enhanced crystallographic diagrams online at the time of submission. Such diagrams are dynamic in the online version of the journal, thereby allowing readers to rotate and view the image from various directions.

A new initiative planned for the latter part of 2011 is the introduction of virtual issues of the journal. As the journal specializes in the rapid publication of papers, it does not lend itself easily to the production of special issues for which long lead times or the holding over of relevant submissions is required. Nevertheless, online publishing readily facilitates the creation of virtual issues, which can be used to bring together and highlight papers on specific topics that had been published over the preceding several months. The contents page of the virtual issue then provides suitable links to the original papers. Such virtual issues may focus on topics of current interest, such as twinned structures, polymorphs, metal–organic frameworks, particular classes of chemical compounds, and so on. The virtual issue makes it easier for readers to find papers relevant to their field of interest, thus increasing the visibility and impact of those papers.

The first virtual issue will focus on polymorphism. Authors interested in contributing papers for this virtual issue only need to submit their papers to *Section C* in the usual way in the coming months. These will be published shortly after they are accepted, as normal, and then collated into the virtual issue towards the end of the year. Papers published in the 12 months prior to September 30, 2011, will be considered for inclusion. Authors do not need to make any special request to have their paper included. Announcements of upcoming future virtual issues will be made on the journal's home page.

Recent discussions about validation and *checkCIF* have indicated that there are still misconceptions in some quarters about the purpose and wisdom of validation. The validation software is intended to be a tool for crystallographers and alerts are provided as an information guide to give the user a 'heads-up' about aspects of the analysis that perhaps they had not noticed, possible errors to be checked, or unusual features or outliers. *checkCIF* also encourages best practice by suggesting certain standards be aimed for whenever possible. *checkCIF* is designed to be an aid to publication, not an obstacle to it.

Two aspects of *checkCIF* are important for authors and referees alike. Firstly, alerts in a validation report do not always mean a structure is wrong and/or unacceptable. Severe alerts usually suggest remedial attention is required, but not always. Validation criteria should not be seen as inviolable rules. Alerts do not have to be eliminated if the cause or reason for making a particular choice is well understood, the experiment and model development has been conducted as well as possible, and there has not been a mistake or oversight. In any case, unusual aspects of a structure or non-routine experimental procedures should always be properly documented either in the experimental section of a paper or in the special details fields of a CIF, so only minimal additional effort should then be needed to explain alerts that are considered unavoidable or inapplicable to the case in hand.

Secondly, a clean validation report does not always guarantee the structure is correct or free of errors. Not all problems or errors in a structure are detectable by validation software, either because it is not viable to devise and program such a test, or because no-one has yet thought to implement it. One should not rely solely on *checkCIF*; additional checking of the results is always advisable, *e.g.* by looking critically at displacement ellipsoid plots, refinement output files, *etc*.

It may also be advantageous to address validation alerts at the completion of a structure determination, when things are fresh in the mind, rather than trying to deal with the issues immediately prior to publication. It is certainly inappropriate to manually change entries in a CIF simply to make validation alerts disappear. Where improper manipulations of CIF data are detected in submissions to this journal, the submission will not be considered further. Validation alerts can be indicative of something unusual, but not necessarily wrong: it would indeed be a pity if a really interesting unusual feature of a structure was overlooked because of attempts to suppress alerts. Sometimes people ask why *checkCIF* occasionally produces apparently trivial alerts for a quite routine and correct structure and whether such tests are really needed. Our experience is typically that there are cases where the same validation tests do detect serious issues with a reported structure, so the test is indeed warranted.

It is a pleasure to welcome Andrew Bond (University of Southern Denmark), Eugene Cheung (Amgen Inc., Cambridge, USA), Maria Teresa Duarte (Instituto Superior Tecnico, Lisbon), Alan Kennedy (University of Strathclyde), Allen Oliver (University of Notre Dame), Bernard Santarsiero (University of Illinois at Chicago), Amber Thompson (Chemical Crystallography, Department of Chemistry, University of Oxford), Jonathan White (The University of Melbourne), Glenn Yap (University of Delaware) and Dmitry Yufit (University of Durham) as new members of the *Section C* editorial board. I warmly thank Len Barbour and Joel Barbier, two Co-editors who have recently retired, for their services to the journal and the crystallography community. I would also like to take this opportunity to thank all the current *Section C* Co-editors (listed on the inside front cover) and the Chester Editorial Office staff for their support and for their continued commitment and dedication to the journal.