

Notes for authors 2008

1. Aims and scope

Acta Crystallographica Section F aims to respond to the need for rapid communication in crystallization and structural biology. The journal is electronic only, articles will be published online as soon as they are ready, and a streamlined route from database deposition to publication is provided.

Structures determined through structural genomics initiatives or from iterative studies such as those used in the pharmaceutical industry are particularly welcomed by the journal.

All communications benefit from unlimited free use of colour illustrations. The Editors are also keen to encourage articles with extended multimedia capabilities and these can be submitted in any of the following categories.

2. Categories of contributions

For the most part, articles which appear in *Acta Crystallographica Section F* will report structures or crystallizations. Authors should choose the most appropriate category for their communication. Contributions should conform to the general editorial style of the journal. To take best advantage of rapid publication, communications should not exceed three journal pages (about 2000 words) and structural communications should describe a single structure. Details of data requirements for structural communications can be found at <http://journals.iucr.org/f/services/structuralcommunications/>.

2.1. Protein Structure Communications

These articles describe the determination of biological structures. Structures of protein ligand complexes are among those suitable for this category.

2.2. Nucleic Acid Structure Communications

These articles describe the determination of nucleic acid structures.

2.3. Structural Genomics Communications

This category of structural papers provides rapid reporting of results from structural genomics research.

2.4. Crystallization Communications

Crystallization Communications should describe a coherent piece of work covering expression, purification and crystallization of a macromolecule, and the validation of crystal quality including a presentation of the diffraction data statistics. Authors should also take into account the evaluation criteria given at <http://journals.iucr.org/f/services/crystallization/>. If the structure of the macromolecule has been solved already, the PDB code and any publication references should be included in the paper.

2.5. Addenda and errata

These are short papers describing additions to, comments on, or errata to existing *Section F* publications and are not intended for

reports of work in progress. Addenda and errata should be submitted to the Co-editor of the original paper.

3. Submission and handling of manuscripts

Papers must be submitted electronically *via* the web at <http://journals.iucr.org/f/services/submitbdy.html>.

3.1. Submission

Full details of the submission procedure can be found at <http://journals.iucr.org/f/services/submitinstructions.html>. Authors of structural papers are encouraged to presubmit their data to the Protein Data Bank (PDB) and provide a PDB validation report on submission. Authors who presubmit to the PDB will be provided with a simplified route for the preparation of experimental tables using an mmCIF (see §6.3).

On initial submission, the article should be prepared as a single file (PDF, Word or RTF, PostScript, or encapsulated PostScript). Authors are encouraged to use the templates available from <http://journals.iucr.org/f/services/helpsubmit.html>. After acceptance, source files of the article (see §3.9) should be uploaded at the URL provided by the Co-editor.

3.2. Languages of publication

Acta Crystallographica Section F will publish papers in English, French, German and Russian.

3.3. Quality of writing

Papers should be clearly written and grammatically correct. If the Co-editor concludes that language problems would place an undue burden on the referees, the manuscript may be returned to the authors without review. Details of language-editing services can be found at <http://journals.iucr.org/services/languageervices.html>.

3.4. Handling of manuscripts

All contributions will be seen by referees (normally two) before they can be accepted for publication. The editor to whom the manuscript is assigned is responsible for the review process and for accepting or rejecting the paper. This responsibility includes decisions on the final form of the paper and interpretation of these Notes when necessary.

If changes to a manuscript requested by the Editor, Co-editor or the editorial staff are not received within **two months** of transmittal to the author, the submission will be considered as withdrawn. Should the manuscript require further revision, this would normally be expected to be completed within one month of the revision having been requested. If a manuscript is not acceptable after two revisions it will not be considered further. Any subsequent communication of the material will be treated as a new submission in the editorial process.

For accepted papers, it is the responsibility of the Managing Editor to prepare the paper for publication. This may involve correspondence with the authors and/or the responsible editor in order to

resolve ambiguities or to obtain satisfactory figures or tables. The date of acceptance that will appear on the published paper is the date on which the Managing Editor receives the last item required. Correspondence will be sent to the author who submitted the paper unless the Managing Editor is informed of some other suitable arrangement.

Papers will be made available on the web as soon as they are ready for publication. They will receive an online publication date when they appear, and each month new online papers will be collected and published as the next issue.

On rare occasions, an editor may consider that a paper is better suited to a section of *Acta Crystallographica* other than that specified by the author(s), to the *Journal of Applied Crystallography* or to the *Journal of Synchrotron Radiation*. Any change to the section or journal of publication will only be made after full discussion with the communicating author.

3.5. Author's warranty

The submission of a paper is taken as an implicit guarantee that the work is original, that it is the author(s) own work, that all authors concur with and are aware of the submission, that all workers involved in the study are listed as authors or given proper credit in the acknowledgements, that the manuscript has not already been published (in any language or medium), and that it is not being considered and will not be offered elsewhere while under consideration for an IUCr journal. The inclusion of material in an informal publication, e.g. a preprint server or a newsletter, does not preclude publication in an IUCr journal.

The co-authors of a paper should be all those persons who have made significant scientific contributions to the work reported, including the ideas and their execution, and who share responsibility and accountability for the results. Other contributions should be indicated in an 'Acknowledgments' section.

Important considerations related to publication have been given in the ethical guidelines published in *Acc. Chem. Res.* (2002), **35**, 74–76 and Graf *et al.* [*Int. J. Clin. Pract.* (2007), **61**(Suppl. 152), 1–26].

3.6. Copyright

Except as required otherwise by national laws, an author must sign and submit a copy of the Transfer of Copyright Agreement form for each manuscript before it can be accepted. Authors will be asked to transfer copyright during the electronic submission process.

3.7. Author grievance procedure

An author who believes that a paper has been unjustifiably treated by the Co-editor may appeal initially to the Section Editors for a new review and, finally, to the Editor-in-chief of *Acta Crystallographica* if the author is still aggrieved by the decision. The initial appeal must be made within three months of rejection of the paper. The decision of the Editor-in-chief is final. Any resubmission to another Co-editor will be forwarded to the Section Editors.

3.8. Contact e-mail address

The contact author must provide an e-mail address for editorial communications and despatch of electronic proofs.

3.9. File format for accepted papers

The files required after acceptance of the paper are: a single file in WORD, RTF or L^AT_EX format of the text, tables and figure captions of the article; a high-resolution graphics file (minimum 600 d.p.i.) in

TIFF, PostScript or encapsulated PostScript format for each figure and scheme; and files of any supplementary material not previously submitted.

3.10. File transfer for accepted papers

Files should be uploaded *via* the web at an address provided by the Co-editor. Full details of this procedure are given at <http://journals.iucr.org/f/services/submitbdy.html>.

4. Abstract and synopsis

All contributions must be accompanied by an English language *Abstract* and a one or two sentence *Synopsis* of the main findings of the paper for inclusion in the Table of Contents for the relevant issue. The *Abstract* should state as specifically and as quantitatively as possible the principal results obtained.

The *Abstract* should be suitable for reproduction by abstracting services without change in wording. It should not repeat information given in the title. Ordinarily 100 words suffice. It should make no reference to tables, diagrams, atom numbers or formulae contained in the paper. It should not contain footnotes. Numerical information given in the *Abstract* should not be repeated in the text. It should not include the use of 'we' or 'I'.

Literature references in an *Abstract* are discouraged. If a reference is unavoidable, it should be sufficiently full within the *Abstract* for unambiguous identification, e.g. [Terwilliger (1994). *Acta Cryst.* **D50**, 17–23].

5. Diagrams and photographs ('figures')

Figures should be prepared using one of the file formats listed in §3.9.

The choice of tables and figures should be optimized to produce the shortest paper consistent with clarity. Duplicate presentation of the same information in both tables and figures is to be avoided, as is redundancy with the text.

An illustration for the first page of the article and the contents pages may be included.

5.1. Quality

Electronic files in the formats listed in §3.9 are essential for high-quality reproduction. The resolution of bitmap graphics should be a minimum of 600 d.p.i.

5.2. Size

Diagrams will normally be sized so that the greatest width including lettering is less than the width of a column in the journal (8.8 cm).

5.3. Lettering and symbols

Fine-scale details and lettering must be large enough to be clearly legible (ideally 1.5–3 mm in height) after the whole diagram has been reduced to one column width.

Lettering should be kept to a minimum; descriptive matter should be placed in the caption.

5.4. Numbering and captions

Diagrams should be numbered in a single series in the order in which they are referred to in the text. A list of figure captions should be included in the manuscript.

5.5. Stereofigures

Atom labelling when included should be on both left and right views in stereo perspective. Both views should be incorporated into a single figure.

5.6. Colour figures

Figures in colour are accepted at **no cost to the author**. Authors preparing colour figures should consider how the figure would look if printed in greyscale and to readers who are colour-blind. It is very important that poor contrast (*e.g.* pale colours with a white background) be avoided.

5.7. Cover figure

The cover figure is normally a three-dimensional rotating structure. Authors who supply an mmCIF with their submission and/or use the interactive tool in described in §5.8 will be eligible for their structure to be considered for the cover.

5.8. Interactive figures

An online tool is available for authors to prepare standard and corresponding three-dimensional interactive structural diagrams. More details can be found at <http://journals.iucr.org/f/services/authorservices>.

6. Tables

Authors submitting in Word should use the Word table editor to prepare tables. Experimental tables can be prepared as in §6.3 below.

6.1. Use of tables

Extensive numerical information is generally most economically presented in tables. Text and diagrams should not be redundant with the tables.

6.2. Design, numbering and size

Tables should be numbered in a single series of arabic numerals in the order in which they are referred to in the text. They should be provided with a caption.

Tables should be carefully designed to occupy a minimum of space consistent with clarity.

6.3. Experimental tables

Experimental tables can be prepared using the mmCIF-to-RTF converter at <http://journals.iucr.org/services/cif/printmmcif.html>. The RTF obtained can then be incorporated into an article.

7. Mathematics and letter symbols

Authors submitting in Word should use the Word equation editor to prepare displayed mathematical equations.

The use of the stop (period) to denote multiplication should be avoided except in scalar products. Generally no sign is required but, when one is, a multiplication sign (\times) should be used.

Vectors should be in bold type and tensors should be in bold-italic type.

Greek letters should not be spelled out.

Care should be taken not to cause confusion by using the same letter symbol in two different meanings.

Gothic, script or other unusual lettering should be avoided. Another typeface may be substituted if that used by the author is not readily available.

Equations, including those in published Appendices, should be numbered in a single series.

8. Multimedia

Multimedia content (*e.g.* time-lapse sequences, three-dimensional structures) is welcomed.

9. Nomenclature

9.1. Crystallographic nomenclature

Authors should follow the general recommendations produced by the IUCr Commission on Crystallographic Nomenclature (see reports at <http://www.iucr.org/iucr-top/comm/cnom/>).

9.2. Nomenclature of compounds etc.

Formulae and nomenclature should conform to the rules of nomenclature established by the International Union of Pure and Applied Chemistry (IUPAC), the International Union of Biochemistry and Molecular Biology (IUBMB) and other appropriate bodies. As far as possible the crystallographic nomenclature should correspond to the systematic name.

9.3. Units

The International System of Units (SI) is used except that the ångström (symbol Å, defined as 10^{-10} m) is generally preferred to the nanometre (nm) or picometre (pm) as the appropriate unit of length. Recommended prefixes of decimal multiples should be used rather than ' $\times 10^n$ '.

10. References

References to published work must be indicated by giving the authors' names followed immediately by the year of publication, *e.g.* Neder & Schulz (1998) or (Neder & Schulz, 1998). Where there are three or more authors the reference in the text should be indicated in the form Smith *et al.* (1998) or (Smith *et al.*, 1998) *etc.* (all authors should be included in the full list).

In the reference list, entries for journals [abbreviated in the style of *Chemical Abstracts* (the abbreviations *Acta Cryst.*, *J. Appl. Cryst.* and *J. Synchrotron Rad.* are exceptions)], books, multi-author books, computer programs, personal communications and undated documents should be arranged alphabetically and conform with the following style:

- Brünger, A. T. (1992a). *X-PLOR. Version 3.1. A System for X-ray Crystallography and NMR*. Yale University, Connecticut, USA.
- Brünger, A. T. (1992b). *Nature (London)*, **355**, 472–474.
- Brünger, A. T., Adams, P. D., Clore, G. M., DeLano, W. L., Gros, P., Grosse-Kunstleve, R. W., Jiang, J.-S., Kuszewski, J., Nilges, M., Pannu, N. S., Read, R. J., Rice, L. M., Simonson, T. & Warren, G. L. (1998). *Acta Cryst.* **D54**, 905–921.
- Collaborative Computational Project, Number 4 (1994). *Acta Cryst.* **D50**, 760–763.
- Crowther, R. A. (1972). *The Molecular Replacement Method*, edited by M. G. Rossmann, pp. 173–178. New York: Gordon and Breach.
- International Union of Crystallography (2008). (*IUCr*) *Structural Biology and Crystallization Communications*, <http://journals.iucr.org/ft/journalhomepage.html>.

Jones, A. B. (2008). *Acta Cryst.* **F64**. In the press.
Kiser, P. D., Lodowski, D. T. & Palczewski, K. (2007). *Acta Cryst.* **F63**, doi:10.1107/S1744309107020295.
Schomaker, V. (1946). Unpublished work.

Note that **inclusive** page numbers must be given.

Identification of individual structures in the paper by use of database reference (identification) codes should be accompanied by a full citation of the original literature in the reference list. However, in tables containing more than ten such reference codes, citation in the reference list is not required.

References in the journal will be linked, where possible, to the original publication and also to appropriate bibliographic databases (e.g. Medline).

11. Evaluation criteria

11.1. Structural data

Evaluation criteria and data recommended for inclusion in structural communications can be found on the web at <http://journals.iucr.org/f/services/structuralcommunications/>.

11.2. Crystallization data

A list of data recommended for inclusion in *Crystallization Communications* can be found on the web at <http://journals.iucr.org/f/services/crystallization/>.

11.3. NMR data

Guidelines for publication of NMR data are available from <http://journals.iucr.org/f/services/structuralcommunications/>.

12. Supplementary content

12.1. Purpose and scope

All supplementary content will either be made available together with the article via **Crystallography Journals Online** or by links to the Protein Data Bank, the Nucleic Acid Database and the ICDD as appropriate.

12.2. Non-structural information

All non-structural supplementary content, which may include:
additional details of the experimental procedure;
details of mathematical derivations given only in outline in the main text and in mathematical Appendices;
lengthy discussion of points that are not of general interest or that do not lead to definite conclusions but that do have significant value;
and additional diagrams,

should be usually be supplied as a single file in one of the formats given in §3.9.

12.3. Macromolecular structures

Authors should follow the deposition recommendations of the IUCr Commission on Biological Macromolecules [*Acta Cryst.* (2000), **D56**, 2]. For all structural studies of macromolecules, coordinates and the related experimental data (structure-factor amplitudes/intensities) must be deposited at a member site of the Worldwide Protein Data Bank (<http://www.wwpdb.org>) if a total molecular structure has been reported. Authors are encouraged to deposit their data with the wwPDB in advance of submission to the journal and to provide an mmCIF and a wwPDB validation report on submission. Authors must supply the wwPDB reference codes before the paper can be published. For NMR structures, in addition to the coordinates, assigned chemical shifts and the restraint data used in the last round of refinement should be deposited with the wwPDB. It is recommended that the NOE peak list also be deposited.

Authors are encouraged to make arrangements for the diffraction data images for their structure to be archived.

13. Crystallography Journals Online

All IUCr journals are available on the web via **Crystallography Journals Online**; <http://journals.iucr.org/>. Full details of author services can be found at <http://journals.iucr.org/f/services/authorservices.html>.

13.1. Electronic status information

Authors may obtain information about the current status of their papers at <http://journals.iucr.org/services/status.html>.

13.2. Proofs

Proofs will be provided in portable document format (pdf). The correspondence author will be notified by e-mail when the proofs are ready for downloading.

13.3. Open access

At the proof stage, authors will be given the opportunity to make their papers 'open access' on **Crystallography Journals Online**.

13.4. Reprints

After publication, the correspondence author will be able to download the electronic reprint of the published article, free of charge.

**International Union of Crystallography
Transfer of Copyright Agreement**

Title of Article (*Please type or use capital letters*)

.....

Authors (*Please type or use capital letters*)

.....

Copyright to the above article is hereby transferred (except as otherwise required by national laws†) to the International Union of Crystallography (IUCr), effective if and when the article is accepted for publication in *Acta Crystallographica*, *Journal of Applied Crystallography* or *Journal of Synchrotron Radiation*. In addition to reproduction in conventional printed form your article will be stored electronically. Your assignment of Copyright signifies your agreement to the journal making arrangements to include your paper in document delivery services, CD-ROMs and electronic databases, etc., worldwide. This transfer of copyright also applies to data submitted in machine-readable form. However, the authors reserve the following:

- (1) All proprietary rights other than copyright, such as patent rights.
- (2) The right to use all or part of this article in future works prepared by or on the behalf of the author.
- (3) In the case of ‘work for hire’, the right of the employer to incorporate all or part of this article in future works.
- (4) The royalty-free right of the employer to make copies of this article, without further permission, for his or her own use but not for resale. Any identification or notice appearing on the pages to be reproduced must not be deleted.

Signature

Signature

Name and position, if not author

Name and position, if not author

.....

.....

Date

Date

This Transfer of Copyright Agreement must be signed by at least one of the authors (who agrees to inform the others, if any) and, as appropriate, by the employer (in the case of ‘work for hire’).

By signing this form you certify that your contribution is your original work, has not been published before (in any language or medium) and is not being considered for publication elsewhere; that you have obtained permission for and acknowledged the source of any excerpts from other copyright works; that to the best of your knowledge your paper contains no statements which are libellous, unlawful or in any way actionable; and, in the case of a multi-authored contribution, that you have obtained copyright assignment from all Co-authors and authorisation to enter this agreement on their behalf.

The signed statement must be received by the IUCr before the article can be accepted for publication. Requests for further information should be sent to the Executive Secretary of the Union.

† In this case please give further details overleaf.
 For use of the International Union of Crystallography only.

M. E. Reference	Coeditor No.	Issue	Journal
-----------------	--------------	-------	---------

This form may be photocopied.

The IUCr may store your name and contact details in electronic format in order to correspond with you about the publication of your contribution in the journal.