

Notes for authors 2012

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

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. Typical articles may be viewed by going to http://journals.iucr.org/f/sample_issue.html.

2.1. Structural Communications

These articles describe the determination of biological structures. This category provides rapid reporting of results including those from structural genomics research. Structures of protein ligand complexes or of nucleic acids are also suitable for this category. Details of data requirements for structural communications can be found at <http://journals.iucr.org/f/services/structuralcommunications/>. Templates are available for this type of article (see §13.1).

2.2. 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 article. Templates are available for this type of article (see §13.1).

2.3. Laboratory Communications

These are brief descriptions of special methods, equipment modifications, techniques for accomplishing certain tasks *etc.* and can be related to crystallization or other fields of structural biology.

2.4. Letters to the Editor

These may deal with any aspect of crystallography, its role, its propagation or the proper function of its Societies *etc.* They may also deal with a technical or scientific observation that would usefully be

brought to a wider audience. Letters should be submitted to one of the Section Editors or to the Editor-in-chief of IUCr Journals.

2.5. Scientific Comment

Comments of general scientific interest to the readership are welcomed. These should not normally exceed two journal pages and should be submitted as in §3.

2.6. Addenda and errata

These are short articles 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 article.

2.7. Special issues

Acta Crystallographica Section F also publishes special sections and issues devoted to the work of groups focusing on structural genomics and specific thematic areas. For more information, contact med@iucr.org.

3. Submission and handling of manuscripts

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

3.1. Submission

Full details of the submission procedure can be found at <http://journals.iucr.org/f/services/submitbdy.html>. Full instructions for submitting an article and details of the files required are given at <http://journals.iucr.org/f/services/submitinstructions.html>. Authors are encouraged to use the *publBio* publication tool available at <http://publbio.iucr.org/> to prepare and submit their article. Authors of structural articles are required to provide a validation report on submission. Articles will be checked for plagiarism using the Cross-Check service.

3.2. Languages of publication

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

3.3. Quality of writing

Articles 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 article. This responsibility includes decisions on the final form of the article 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 **one month** 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. An article that has been rejected must not be resubmitted to any IUCr journal unless the reasons given for the rejection have been fully addressed in the revised version.

For accepted articles, it is the responsibility of the Managing Editor to prepare the article 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 article is the date on which the Managing Editor receives the last item required. Correspondence will be sent to the author who submitted the article unless the Managing Editor is informed of some other suitable arrangement.

Articles 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 articles will be collected and published as the next issue.

On rare occasions, an editor may consider that an article 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 contact author.

3.5. Author's warranty

The submission of an article is taken as an implicit guarantee that the work is original, that it is the author(s) own work, that all authors are aware of and concur with 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 an article 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 the acknowledgments. Changes to the list of authors will normally require the agreement of the editor and all authors.

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]. Authors are expected to comply with these guidelines.

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. Details

of author rights can be found at <http://journals.iucr.org/services/authorrights.html>. See §13.4 for information on the licensing of open-access articles.

3.7. Author grievance procedure

An author who believes that an article 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 article. 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

The source files required for an article are: a single file in Word, OpenOffice 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. These should be uploaded as described in the **online submission instructions**. Alternatively, authors may use the new version of *publBio* to prepare and submit their article directly.

3.10. Revisions

After initial submission, any revised or new files should be uploaded *via* the web interface **only** in response to a specific request from a Co-editor; these files should be uploaded at the web address provided by the Co-editor.

4. Format of articles

Before preparing articles, authors should consult a current issue of the journal to make themselves familiar with the general format, such as the use of headings, layout of tables and citation of references. A sample issue is also available at http://journals.iucr.org/sample_issue.html.

The title should be concise but informative. Articles should also be headed by the authors' names and by the name and full postal address of the institution(s) where the work was carried out.

All contributions must be accompanied by an English language *Abstract* and a one or two sentence *Synopsis* of the main findings of the article 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 article. 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].

The main body of the article should normally be divided into the following sections: introduction; experimental, including materials

and methods; results; discussion; acknowledgements; references; and tables and figures.

5. Diagrams and photographs ('figures')

A set of guidelines for preparing figures is available from <http://journals.iucr.org/ff/services/help/artwork/guide.html>. Figures should be prepared using one of the file formats listed in §3.9.

The choice of figures should be optimized to produce the shortest article consistent with clarity. Duplicate presentation of the same information in both figures and tables is to be avoided, as is redundancy with the text. Supplementary figures may be deposited (see §12).

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 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. Enhanced figures

An online tool for authors to prepare standard and corresponding three-dimensional interactive structural diagrams is available from <http://submission.iucr.org/jtkf>.

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

Each Crystallization or Structural Communication will normally include a standard experimental details table. Authors are advised to use *publBio* to generate this table. The tool and an example table can be found at <http://publbio.iucr.org>. Alternatively, a standard experimental table may be generated using the table tools option within the Word template available from <http://journals.iucr.org/services/docxtemplate/>.

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.

Scalar variables and non-standard functions should appear in italic type.

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.

All displayed 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. For details of how to prepare enhanced three-dimensional figures, see §5.8.

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/commissions/cnom.html>). Quality indicators should be given as defined in H. M. Einspahr & M. S. Weiss (2011). *International Tables for Crystallography*, Vol. F, ch. 2.2, pp. 64–74.

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 '× 10ⁿ'.

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.*

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 and personal communications 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.
- 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/ijournalhomepage.html>.
- Jones, A. B. (2012). *Acta Cryst.* **F68**. In the press.
- Schomaker, V. (1946). Personal communication.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Weiss, M. S., Einspahr, H., Baker, E. N., Dauter, Z., Kaysser-Pyzalla, A., Kostorz, G. & Larsen, S. (2010). *Acta Cryst.* **F66**, doi:10.1107/S1744309110041825.
- Winn, M. D., Ballard, C. C., Cowtan, K. D., Dodson, E. J., Emsley, P., Evans, P. R., Keegan, R. M., Krissinel, E. B., Leslie, A. G. W., McCoy, A., McNicholas, S. J., Murshudov, G. N., Pannu, N. S., Potterton, E. A., Powell, H. R., Read, R. J., Vagin, A. & Wilson, K. S. (2011). *Acta Cryst.* **D67**, 235–242.

Note that all authors and **inclusive** page numbers must be given.

Identification of individual structures in the article by use of database reference (identification) codes should be accompanied by a full citation of the original literature in the reference list. In such cases, the citation in the text should take the form '... the structure of amicyanin (PDB code 1aac, Cunane *et al.*, 1996)'.

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

Citations in supplementary material should also appear in the main body of the article.

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/ff/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/ff/services/crystallization/>. Crystallization communications will typically contain no information about phase determination. However, if a statement is made which requires the determination of phases, the relevant statistics, such as the number of heavy-atom sites, phasing power, estimated phase error *etc.*, in the case of experimental phasing, and some combination of initial rigid-body R_{work} and R_{free} , the correlation coefficient, or Z score, in the case of phasing by molecular replacement, need to be provided.

11.3. NMR data

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

11.4. Neutron data

In articles reporting neutron data, preliminary nuclear density maps should not be included unless the relevant statistics of R , R_{free} , correlation coefficient and error estimates are provided.

11.5. Small-angle scattering data

Guidelines for articles reporting structural modelling of small-angle scattering may be found at <http://journals.iucr.org/services/sas/>. For articles that present experimental SAS data, the deposition of an ASCII file representing the background-corrected scattering profile(s) with errors is recommended.

11.6. Validation reports

Authors of structural articles are required to provide a validation report on submission. Authors are encouraged to presubmit their data to the wwPDB and obtain a validation report for their structure. Further information about validation reports can be found in the online submission instructions.

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 appropriate structural databases.

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;
additional diagrams;
and multimedia content,
should be supplied in one of the formats described at <http://journals.iucr.org/services/filetypes.html>.

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 which will be required on submission. Further information about mmCIFs and validation reports can be found in the online submission instructions. Authors must supply the wwPDB reference codes before the article can be published and the data must be released upon publication.

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 and available on request.

13. Author information and services

An author services page is available at <http://journals.iucr.org//services/authorservices.html>.

13.1. Author tools

A number of tools are available to help with the preparation of articles.

Word, OpenOffice and L^AT_EX templates can be downloaded from the author services page.

Table tools within the Word template may be used to prepare experimental tables from an mmCIF file.

A toolkit for preparing enhanced figures is available at <http://submission.iucr.org/jtk>.

Authors are encouraged to use the new version of *publBio* available at <http://publbio.iucr.org>. This web service provides a quick and easy route to prepare and submit an article, and helps to ensure that all items necessary for publication are included.

13.2. Electronic status information

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

13.3. Proofs

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

13.4. Open access

At the proof stage, authors will be given the opportunity to make their articles 'open access' on **Crystallography Journals Online**. Authors of open-access articles will not be asked to transfer copyright to the IUCr, but will instead be asked to agree to an open-access licence. This licence is identical to the Creative Commons Attribution Licence.

13.5. Reprints

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

13.6. Crystallography Journals Online

All IUCr journals are available on the web via **Crystallography Journals Online**; <http://journals.iucr.org/>.