

Notes for authors

1. Aims and scope

Acta Crystallographica Section F is a rapid structural biology communications journal.

Articles on any aspect of the crystallization and structure determination of biological macromolecules, including those determined using high-throughput methods or from iterative studies such as those used in the pharmaceutical industry, are welcomed by the journal.

The journal offers the option of open access, and all communications benefit from unlimited free use of colour illustrations and no page charges. Authors are encouraged to submit multimedia content for publication with their articles.

Acta Cryst. F has a dedicated online tool called *publBio* that is designed to make the preparation and submission of articles easier for authors.

2. Categories of contributions

Contributions should conform to the general editorial style of the journal. Articles should not exceed four journal pages (about 3000 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. Details of data requirements for structural communications can be found at <http://journals.iucr.org/f/services/evaluationcriteria/>. *publBio* templates are available for this type of article (see §3.1).

2.2. Crystallization Communications

Crystallization Communications should describe a coherent study covering expression, purification and crystallization of a macromolecule, and the validation of crystal quality including a presentation of the diffraction data statistics. If the structure of the macromolecule has been solved already, the PDB code and any publication references should be included in the article. **Special submission instructions apply to this type of article (see §3.2).**

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.

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. Special issues

Acta Cryst. F also publishes special sections and issues devoted to the work of groups focusing on specific areas of structural biology. For more information, contact actaf@iucr.org.

3. Submission and handling of articles

3.1. Submission

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

Full details of the submission procedure, instructions for submitting an article and details of the files required are given at <http://journals.iucr.org/f/services/submitinstructions.html>. All authors are encouraged to use the *publBio* publication tool to prepare and submit their article (see <http://journals.iucr.org/f/services/publbiobiosubmission.html>). Alternatively, authors may use the Word or OpenOffice templates available from <http://journals.iucr.org/services/docxtemplate/>.

Authors of structural articles are required to provide a wwPDB validation report on submission.

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

3.2. Crystallization Communications

Crystallization Communications must be prepared using *publBio* or the *publBio* tools within the IUCr Word template. Full details of how to submit *Crystallization Communications* using *publBio* can be found at <http://journals.iucr.org/f/services/publbiobiosubmission.html>.

3.3. File format

For articles not produced using *publBio*, the text, tables and figure captions should be supplied as a single file in Word or OpenOffice format. For all articles, each figure or scheme should be provided as a high-resolution graphics file (minimum 600 d.p.i.) in TIFF, PostScript, encapsulated PostScript or PNG format; files of any supporting information should be provided in one of the formats listed at <http://journals.iucr.org/services/filetypes.html>.

3.4. Handling of articles

Each article is handled by an editor chosen by the author from a list of those available at the time of submission. Authors should choose an editor whose area of expertise most closely matches the subject of the article. Details of the current Editorial Board can be found at <http://journals.iucr.org/f/services/editors.html>.

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. Further information on the peer review process can be found at <http://journals.iucr.org/f/services/peerreview.html>.

Changes to an article requested by the Section Editors, Co-editor or the editorial staff should be received within **one month** of transmittal to the author, otherwise the submission will be considered as withdrawn. If an article 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.

After initial submission, any revised or new files should be uploaded **only** in response to a specific request from an editor.

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 contact author who submitted the article unless the Managing Editor is informed of some other suitable arrangement. Contact details for the Managing Editor of *Section F* can be found at <http://journals.iucr.org/services/contactus.html>.

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 *IUCrJ*, *Journal of Applied Crystallography* or to *Journal of Synchrotron Radiation*. Any change to the section or journal of publication will only be made after full discussion with the contact author.

Articles will be checked for plagiarism using the CrossCheck service.

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 article 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.

The IUCr is a member of COPE (Committee on Publication Ethics) and endorses its recommendations, including the Code of Conduct for Editors, which are available at <http://www.publicationethics.org/>. 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. 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.

3.7. Copyright

Except as required otherwise by national laws, an author will be required to agree to the transfer of copyright before an article can be accepted. Authors selecting open access do not need to transfer copyright. Details of author rights can be found at <http://journals.iucr.org/services/authorrights.html>.

3.8. Open access

Authors are 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 (CC-BY) Licence. Further details can be found at <http://journals.iucr.org/services/openaccess.html>.

3.9. Publication fees

There are no fees for colour figures or electronic reprints. If authors require open access or printed reprints there is a charge and details will be given at the proof stage.

4. Article preparation

4.1. General information

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 available at http://journals.iucr.org/f/sample_issue.html.

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. Authors should also supply at least five keywords.

The Abstract should state as specifically and as quantitatively as possible the principal results obtained. It should be suitable for reproduction by abstracting services without a change in wording and should not repeat information given in the title. It should make no reference to tables, diagrams, atom numbers or formulae contained in the article. It should not contain footnotes and should not include the use of 'we' or 'I'.

The main body of the article should normally be divided into the following sections: introduction, experimental (including materials and methods), results, discussion, acknowledgements and references.

4.2. 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>.

4.3. 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 §3.3.

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 §6).

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

4.3.1. Quality. Electronic files in the formats listed in §3.3 are essential for high-quality reproduction. The resolution of bitmap graphics should be a minimum of 600 d.p.i.

4.3.2. 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).

4.3.3. 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.

4.3.4. Numbering and captions. Diagrams should be numbered in a single series in the order in which they are referred to in the text. Each figure should be accompanied by a caption.

4.3.5. 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. The type of stereoview used (cross-eyed or wall-eyed) should be given in the caption.

4.3.6. 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.

4.3.7. 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 §4.3.8 will be eligible for their structure to be considered for the cover.

4.3.8. 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>.

4.4. Tables

Authors submitting in Word should use the Word table editor to prepare tables. Experimental tables should be prepared as in §4.4.3 below.

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

4.4.2. 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.

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

4.5. Video and multimedia content

Multimedia content (*e.g.* time-lapse sequences, three-dimensional structures) is welcomed. For details of how to prepare enhanced three-dimensional figures, see §4.3.8. The preferred file formats for multimedia are given at <http://journals.iucr.org/services/filetypes.html>.

4.6. 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.

4.7. Nomenclature

4.7.1. 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 ' $\times 10^n$ '.

4.7.2. Biochemical nomenclature. The recommendations of the Nomenclature Committee of IUBMB and the IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (see <http://www.chem.qmul.ac.uk/iubmb/>) should be followed as far as practicable. The recommendations of the latest edition of *Enzyme Nomenclature* (1992, San Diego: Academic Press; and its supplements) should be followed as far as possible (see <http://www.chem.qmul.ac.uk/iubmb/enzyme>). This includes the quoting of EC numbers. It is recommended that authors use the new nomenclature for restriction enzymes, DNA, methyltransferases, homing endonucleases (and their genes) that has been proposed by Roberts *et al.* [(2003), *Nucleic Acids Res.* **31**, 1805–1812].

4.7.3. 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.

4.7.4. Nomenclature of chemical compounds etc. Formulae and nomenclature should conform to the rules of nomenclature established by the International Union of Pure and Applied Chemistry (IUPAC) and other appropriate bodies. As far as possible the crystallographic nomenclature should correspond to the systematic name.

Any accepted trivial or non-systematic name may be retained, but the corresponding systematic (IUPAC) name should also be given.

4.8. 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.*

The reference list 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 (2014). *IUCr Structural Biology Communications*. <http://journals.iucr.org/ff/journalhomepage.html>.
- Jones, A. B. (2014). *Acta Cryst.* **F70**. 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.

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

Citations in supporting information should appear in the main body of the article or be given in a related literature section.

4.8.1. References to structures. 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)'.

5. Evaluation criteria

5.1. Structural data

Evaluation criteria and data recommended for inclusion in *Structural Communications* can be found at <http://journals.iucr.org/ff/services/evaluationcriteria/>.

5.2. Crystallization data

A list of data recommended for inclusion in *Crystallization Communications* can be found at <http://journals.iucr.org/ff/services/evaluationcriteria/>. *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.

5.3. NMR data

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

5.4. 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.

5.5. 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 required.

5.6. 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.

6. Supporting information

6.1. Purpose and scope

Supporting information (such as experimental data, additional figures and multimedia content) that may be of use or interest to some readers but does not form part of the article itself will be made available from the IUCr archive. Arrangements have also been made for such information to be deposited, where appropriate, with other relevant databases.

6.2. IUCr archive

All material for deposition in the IUCr archive should be supplied in one of the formats described at <http://journals.iucr.org/services/filetypes.html>.

6.3. 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.

7. Author information and services

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

7.1. Author tools

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

Authors are encouraged to use *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.

Alternatively, Word and OpenOffice templates can be downloaded from <http://journals.iucr.org/services/helpsubmit.html>.

Table tools within the Word template can be used to prepare experimental tables from an mmCIF file or from a structure in the PDB.

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

7.2. Status information

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

7.3. 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.

7.4. Reprints

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

7.5. Open-access articles

The final published version of each IUCr open-access article is deposited with PubMed Central on behalf of the authors.

7.6. Publicising your article

There are many ways in which the IUCr promotes and raises awareness of articles published in its journals. More information on this and suggestions on how to publicise your articles can be found at <http://journals.iucr.org/f/services/articlepublicity.html>.

7.7. Crystallography Journals Online

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