Acta Crystallographica Section D
Biological Crystallography
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Notes for authors 2006

1. Scientific scope

Section D of *Acta Crystallographica* welcomes the submission of papers covering any aspect of structural biology, with a particular emphasis on the structures of biological macromolecules and the methods used to determine them. Reports on new protein structures are particularly encouraged, as are structure–function papers that could include crystallographic binding studies, or structural analysis of mutants or other modified forms of a known protein structure. The key criterion is that such papers should present new insights into biology, chemistry or structure. Papers on crystallographic methods should be oriented towards biological crystallography, and may include new approaches to any aspect of structure determination or analysis. Papers on the crystallization of biological molecules will be accepted providing that these focus on new methods or other features that are of general importance or applicability. Those that report routine crystallization results will not be accepted and should be submitted instead to *Acta Crystallographica Section F*. For all structural papers, sufficient information should be provided to convince the referees that the interpretations of the diffraction data and electron-density maps are correct, within the resolution of the analysis.

2. Categories of contributions

Contributions should conform to the general editorial style of the journal.

2.1. Research Papers

Full-length *Research Papers* should not normally exceed 15 journal pages (about 15 000 words).

2.2. Short Communications

Short Communications are intended for the presentation of topics of limited scope, or for preliminary announcements of novel research findings. They are not intended for interim reports of work in progress, and must report results that are of scientific value in their own right.

Short Communications should not exceed two journal pages (about 1500 words). A maximum of two figures and two tables of appropriate size are permitted.

2.3. Lead Articles

Lead Articles are authoritative, comprehensive and forward-looking reviews of major areas of research interest. They are always **commissioned by the Section Editors**, on the advice of the Editorial Board. Suggestions for suitable topics and of potential author(s) are welcomed by the **Section Editors** for discussion with the Board.

The Section Editors will discuss the treatment of the topic, the length of the *Article* and the delivery date of the manuscript with invited author(s); *Lead Articles* will be refereed in the normal manner; they will be made open access on publication.

2.4. Feature Articles

A *Feature Article* is a focused survey covering recent advances in an area of current research. It should not aim to be comprehensive, but a brief introduction should provide historical perspective and a brief conclusion should indicate likely future directions. Inclusion of relevant new results is appropriate.

Feature Articles will be about ten journal pages (10 000 words). Shorter articles on rapidly evolving areas are also actively encouraged. They will be **commissioned by the Section Editors** either personally, **or following a formal proposal by prospective author(s)**. *Feature Articles* will be refereed in the normal way; they will be made open access on publication.

2.5. Letters to the Editor

These may deal with non-technical aspects of crystallography, its role, its propagation, the proper function of its Societies *etc*., or may make a technical 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 *Acta Crystallographica* only.

2.6. 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.

2.7. Meeting Reports

These are normally invited. Prospective authors interested in writing such items should first contact the Section Editors.

2.8. New Commercial Products

Announcements of new commercial products are published free of charge. The descriptions, up to 300 words or the equivalent if a figure is included, should give the manufacturer's full address.

2.9. Obituaries

These will be **commissioned by the Section Editors**.

3. Submission and handling of manuscripts

3.1. Submission

Full details of the submission procedure can be found at **http://journals.iucr.org/d/services/submitbdy.html**. 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/d/services/helpsubmit.html**. Full instructions for submitting a paper are given at **http://journals.iucr.org/d/services/submitinstructions.html**. After acceptance, source files of the article (see §3.9) should be uploaded.

In the case of Addenda or Errata to published papers, the article should be submitted to the Co-editor of the original paper.

3.2. Languages of publication

Acta Crystallographica Section D 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 referee(s), the manuscript may be returned to the authors without review.

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 choosing referees 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 Section Editors, 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 printing. 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.

The journal is partnered by *Acta Crystallographica Section F: Structural Biology and Crystallization Communications*. In general, *Section D* publishes detailed papers on biological structures and on crystallographic methods and theory including novel methods related to crystallization; *Section F* publishes short articles on structural biology and crystallization. In some cases, the editors may recommend that a paper submitted to *Section D* is better suited for publication in *Section F*. 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. All authors will be required to sign off the final version of the paper.

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.

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 procedure.

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 3 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 LaTeX 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/d/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. 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 200 words suffice for *Abstracts* of *Research Papers*, *Lead Articles* and *Feature Articles*, and 100 words for shorter contributions. 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.* D**50**, 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 printed 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.

Authors of protein structure papers are requested to submit a picture of the Cα chain trace. This will be helpful for referees and may be deposited. In addition, a diagram of the fit of a side chain is helpful to the reader in terms of assessing the resolution and map quality.

Fibre data should contain appropriate information such as a photograph of the data. As primary diffraction data cannot be satisfactorily extracted from such figures, the basic digital diffraction data should be deposited.

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 should be as small as possible consistent with legibility. They will normally be sized so that the greatest width including lettering is less than the width of a column in the journal.

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; grids and shadings should be avoided where they are not required to improve clarity. Descriptive matter should be placed in the legend.

5.4. Numbering and legends

Diagrams should be numbered in a single series in the order in which they are referred to in the text. A list of the legends ('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** provided that the editor agrees that they improve the understanding of the paper. Poor contrast (*e.g.* pale colours with a white background) should be avoided. At the editor's discretion, figures printed in black and white may appear in colour in **Crystallography Journals Online.**

6. Tables

Authors submitting in Word should use the Word table editor to prepare tables.

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.

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.

Make sure only scalar variables and non-standard functions appear in italic font.

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 additions to a paper (*e.g.* time-lapse sequences, three-dimensional structures) are welcomed; they will be made available *via* **Crystallography Journals Online**.

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/**).

Atoms of the same chemical species within an asymmetric unit should be distinguished by an appended arabic numeral. **Chemical and crystallographic numbering should be in agreement wherever possible.** When it is necessary to distinguish crystallographically equivalent atoms in different asymmetric units the distinction should be made by lower-case roman numeral superscripts (*i.e.* i, ii, iii *etc.*) to the original atom labels.

Space groups should be designated by the Hermann–Mauguin symbols. Standard cell settings, as listed in Volume A of *International Tables for Crystallography*, should be used unless objective reasons to the contrary are stated. When a non-standard setting is used, the list of equivalent positions should be given. Hermann–Mauguin symbols should also be used for designating point groups and molecular symmetry. It is helpful if the origin used is stated explicitly where there is a choice.

The choice of axes should normally follow the recommendations of the Commission on Crystallographic Data [Kennard *et al.* (1967). *Acta Cryst.* **22**, 445–449].

A symbol such as 123 or *hkl* without brackets is understood to be a reflection, (123) or (*hkl*) a plane or set of planes, [123] or [*uvw*] a direction, {*hkl*} a form and ⟨*uvw*⟩ all crystallographically equivalent

directions of the type [*uvw*]. Other bracket notations should be explicitly defined.

9.2. Nomenclature of chemical compounds *etc*.

Chemical 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), the International Mineralogical Association 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.

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. (1992*a*). *X-PLOR. Version 3.1. A System for X-ray Crystallography and NMR*. Yale University, Connecticut, USA.

Brünger, A. T. (1992*b*). *Nature (London)*, **355**, 472–474.

Collaborative Computational Project, Number 4 (1994). *Acta Cryst.* D**50**, 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 (1999). *(IUCr) Crystallography Journals Online*, http://journals.iucr.org.

International Union of Crystallography (2005). *(IUCr) Structural Biology and Crystallization Communications*, http://journals.iucr.org/f/journalhomepage.html.

Sheldrick, G. M. (2006). *Acta Cryst.* D**62**. In the press.

Yariv, J. (1983). Personal communication.

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.

11. Evaluation criteria

Authors are strongly encouraged to provide evaluation criteria along the following lines.

11.1. Resolution

The effective resolution should be described clearly. Values of the internal agreement of the data, $R_{\rm merge}$, together with the multiplicity, the mean value of I/σ and the percentage completeness of the data are required for the overall data set and the highest resolution shell together with the limits of that shell in Å. For high-quality data obtained with synchrotron radiation, values of $R_{\rm merge} < 20\%$, completeness $> 93\%$ and observable data $> 70\%$ should be achievable for the highest resolution shell. A complete table listing the above criteria as a function of resolution should also be submitted, but will normally be included in the supplementary material, see §13.

11.2. Refined structures

It is expected that structures submitted to *Section D* will have been refined crystallographically. The data required depend on the effective resolution of the analysis and the following information should be included.

A final Ramachandran plot is important and should be provided for review purposes. The paper should include a brief statement of the percentage of amino acids in allowed, additionally allowed and disallowed regions of the plot.

Details of any restraints on *B* factors should be included.

The crystallographic *R* index should be tabulated as a function of resolution and $R_{\rm free}$ should also be included.

Adequate details should be provided regarding the steps followed in constructing the model and refining the structure. Also requested are: the number of solvent atoms; solvent *B* values; the history and salient details of the refinement methods employed, including the resolution ranges that were used at various stages of refinement; the restraints used; a description of how the thermal parameters were treated; and how the solvent sites were selected and handled during refinement. It should be clear if van der Waals distances were restrained.

Hydrogen-bonding patterns within the protein should be described including the number of hydrogen-bond donors not involved in hydrogen bonding and any unsatisfied buried main-chain hydrogen bonds.

Any structural features that are considered somewhat unusual should be described. Examples include *cis* peptide bonds; unoccupied volume inside the protein, buried charge groups that are not involved in salt bridges or reasonable hydrogen-bonding environments; unusual locations of glycine and proline residues; unusual distributions of polar and hydrophobic groups within the molecule; and unusual bond lengths, bond angles, planes, intra- and intermolecular contacts.

Any unexplained electron density that is not accounted for by the current model, or whose interpretation is ambiguous, should be discussed.

12. Small-molecule structure determinations

Papers that report the results of crystal structure determinations of small molecules must report the associated experimental data as required in Notes for Authors for *Section C* of *Acta Crystallographica*. These data should be supplied as a single electronic file in CIF format. The CIF will be checked in the Editorial Office in Chester for internal consistency.

13. Supplementary publication procedure (deposition)

13.1. Purpose and scope

Parts of some papers are of interest to only a small number of readers, and the cost of printing these parts is not warranted. Arrangements have therefore been made for such material to be made available from the IUCr electronic archive *via* **Crystallography Journals Online** or to be deposited with the Protein Data Bank, the Nucleic Acid Database and the ICDD as appropriate.

13.2. IUCr electronic archive

All material for deposition in the IUCr electronic archive should be supplied electronically.

Non-structural information, which may include:

details of the experimental procedure;
details of the stages of structure refinement;
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 usually be supplied as a single file in one of the formats given in §3.9.

Structural information (for small-molecule structures) should be supplied in CIF format; structure factors should be supplied as .fcf files.

13.3. Macromolecular structures

Authors should follow the deposition recommendations of the IUCr Commission on Biological Macromolecules [*Acta Cryst.* (2000), D**56**, 2]. For all structural studies of macromolecules, coordinates and structure factors must be deposited with the Protein Data Bank or the Nucleic Acid Database if a total molecular structure has been reported. Authors must supply the Protein Data Bank/Nucleic Acid Database reference codes before the paper can be published.

14. Powder diffraction data

Authors of powder diffraction papers should consult the notes provided at (**http://journals.iucr.org/services/cif/powder.html**). For papers that present the results of powder diffraction profile fitting or refinement (Rietveld) methods, the primary diffraction data, *i.e.* the numerical intensity of each measured point on the profile as a function of scattering angle, should be deposited.

15. 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/d/services/authorservices.html.**

15.1. Electronic status information

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

15.2. 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.

15.3. Open access

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

15.4. Reprints

After publication, the correspondence author will be able to download the electronic reprint of the published article, free of charge. Authors will also be able to order printed reprints at the proof stage.

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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.

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