Acta Crystallographica Section D
**Biological Crystallography**
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# Notes for authors

## 1. Scientific scope

*Section D* of *Acta Crystallographica* welcomes the submission of papers covering any aspect of biological crystallography, particularly structures of biological macromolecules. In addition to new structural determinations, preliminary data on unit-cell dimensions and space groups will be considered for publication, provided suitable diffraction photographs (or their equivalent), together with an estimate of resolution, are included. Also, articles on crystal growth of biological macromolecules are welcomed, and refinements of known structures may be published if the information content warrants it. For all structural papers, sufficient evidence 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. Crystallization Papers

These are short papers which report the crystallization of novel, important or difficult-to-crystallize biological macromolecules, or new crystallization techniques. *Crystallization Papers* should not normally exceed two journal pages (about 1500 words).

### 2.4. Lead Articles

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

The Editor will discuss the treatment of the topic, the length of the *Article* and the delivery date of the manuscript with invited author(s); manuscripts will be refereed in the normal manner.

### 2.5. Topical Reviews

A *Topical Review* is a short, highly focused survey covering a relatively narrow area of current research interest. It should not aim to be comprehensive, but a brief introduction should provide historical perspective and a brief conclusion should indicate likely future directions.

*Topical Reviews* will be limited to about ten journal pages (10 000 words) except in special agreed circumstances. Shorter reviews on rapidly evolving areas are also actively encouraged. They will be **commissioned by the Section Editor** either personally, **or following a formal proposal by prospective author(s)**. *Topical Reviews* will be refereed in the normal way.

### 2.6. 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 sent to the **Section Editor** or to the **Editor-in-Chief** of *Acta Crystallographica* only.

### 2.7. 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.

### 2.8. Obituaries

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

## 3. Submission and handling of manuscripts

### 3.1. Submission

Manuscripts and figures should be prepared using the file formats listed in §3.8. Three paper copies and the electronic file(s) should be submitted; authors are reminded to keep an exact copy of the submission for later editorial adjustments and for checking proofs. Unless stated otherwise in §2, the submission should be sent to the Section Editor or any of the Co-editors taking into account their areas of expertise. On acceptance, an electronic version of the final manuscript will be required by the Editorial Office.

Contact details for the editors are available at **http://journals.iucr.org/d/services/editors.html**.

### 3.2. Languages of publication

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

### 3.3. 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 sent 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 editorial staff or the Co-editor are not received within **two months** of transmittal to the author, the submission will automatically be withdrawn. 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 signed the letter of submission unless the Managing Editor is informed of some other suitable arrangement.

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.

### 3.4. 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 acknowledegments, 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. For these reasons, all authors will be required to sign off the final version of the paper.

### 3.5. 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.

### 3.6. Author grievance procedure

An author who believes that a paper has been unjustifiably treated by the Co-editor may appeal initially to the **Section Editor** and then to the Editor-in-Chief if still aggrieved by the decision.

### 3.7. Contact e-mail address

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

### 3.8. File format, naming and transfer

The manuscript should be prepared using TEX, LATEX or Word. Authors are encouraged to use the templates available from the Editorial Office by e-mail (**med@iucr.org**) or by ftp (from the 'templates' directory). All Word submissions should be accompanied by an RTF (rich text format) file.

Figures may be sent in PostScript, encapsulated PostScript or TIFF formats. The resolution of bitmap graphics should be a minimum of 1200 d.p.i.

All files need to be given a filename constructed from the *reference number* supplied by the Co-editor. Files containing text in TEX or LATEX should be given the extension `.tex`, Word files should be given the extension `.doc` and RTF files `.rtf`. Illustrations in PostScript, encapsulated PostScript or TIFF format should be given the extensions `.ps`, `.eps` or `.tif`, respectively. Multiple files for the same submission should be identified by filenames constructed as `ref.id.ext` where `id` indicates the contents, *e.g.* `xz1087.fig1.ps` and `xz1087.fig2.ps`.

After acceptance, the final version of the paper should be sent to the Editorial Office by e-mail (med@iucr.org), on diskette or (for files larger than 70K bytes) by ftp as described below.

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|---|---|
| (i) On your workstation enter: | **ftp ftp.iucr.org** |
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| (v) Transfer a file from your account (*e.g.* j29.ps) as an identifiable name (*e.g.* ja0325.ps): | **put j29.ps ja0325.ps** |
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| (vii) Finish off the ftp session by entering: | **bye** |
| (viii) Send an e-mail to Chester (**med@iucr.org**) with a list of the files transferred by ftp | |

## 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 200 words suffice for *Abstracts* of *Research Papers*, *Lead Articles* and *Topical Reviews*, 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 §3.8. Hard-copy figures must be provided in all cases.

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 C$\alpha$ 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

Hard-copy greyscale or colour images should be provided as glossy prints; laser printer or photocopier output will generally be unsatisfactory for reproduction of such diagrams. High-resolution laser printer output is satisfactory for line drawings.

### 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; 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.

## 6. Tables

Tables produced in Word should be prepared using the Word table editor.

### 6.1. Economy in use of tables

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.

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 Commision 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 $\langle uvw \rangle$ 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).

At the end of the paper a list giving full details of all references should be appended separately. 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.

Veerapandian, P. (2000). *Acta Cryst.* D**56**. In the press.

Yariv, J. (1983). Personal communication.

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

## 11. Evaluation criteria

The criteria by which papers are evaluated are based on recommendations of the Commission on Biological Macromolecules.

### 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 (*i.e.* the average number of measurements for each reflection from which $R_{\rm merge}$ is calculated), the percentage of data with $I > 3\sigma(I)$ and 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. Unrefined structures

Adequate experimental details should be provided to convince referees that the interpretation is correct, within the resolution of the analysis. If heavy-atom derivatives were used, sufficient data should be provided for evaluation of the quality of those derivatives. The fit of the model to the electron-density maps used to determine the structure should be shown or described by quantitative indicators, such as real-space residuals.

### 11.3. Refined structures

For refined structures the data required depend on the effective resolution of the analysis. The following 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.

The r.m.s. deviations in $B$ values within each residue's main-chain and side-chain atoms 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.

## 12. Small-molecule structure determinations

Papers which report the results of crystal structure determinations of small molecules should report the associated numerical data as required in Notes for Authors for *Section C* of *Acta Crystallographica*. These data must be supplied as an electronic file in CIF format. All numerical data will be checked 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 deposited with the IUCr electronic archive, 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;
additional diagrams,

should be supplied in one of the formats given in §3.8.

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 [Commission on Biological Macromolecules (2000). *Acta Cryst.* 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. *Crystallography Journals Online*

Full details of author services can be found at http://journals.iucr.org/d/services/authorservices.html.

### 14.1. Electronic status information

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

### 14.2. 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.

### 14.3. 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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