



Commission on Journals 2011

Submission to publication

Introduction

Crystallography
Journals
Online



Journal publishing activities

8 Journals in crystallography and related areas

- Approximately 170 Editors and Co-editors
- Provide peer review service to more than 7000 articles (2010)
- Publish 5000+ articles
- *Acta Crystallographica*, 60 issues
- *Journal of Applied Crystallography*, 6 issues
- *Journal of Synchrotron Radiation*, 6 issues
- 13000 pages

Crystallography Journals Online



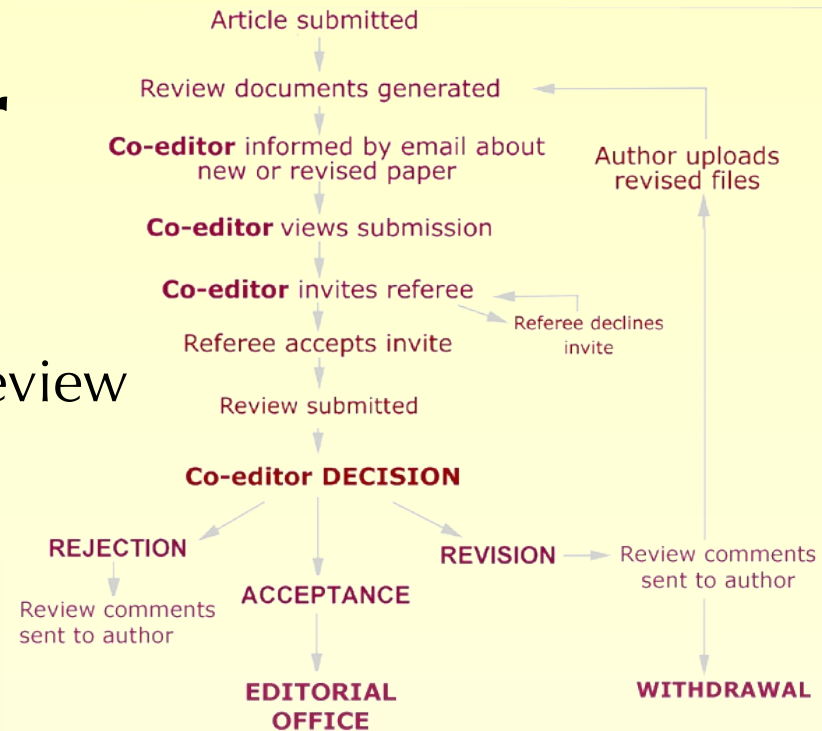
17 editorial, production
and R&D staff work in Chester
Staff trained as scientists to degree or PhD level



Today's speakers

What we intend to cover

- Authoring and submission
- Handling of submissions and article review
- Technical editing and production
- Typesetting and proofreading
- Journal printing
- Putting the journals online
- Distribution of online content and metadata



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IUCr templates and tools

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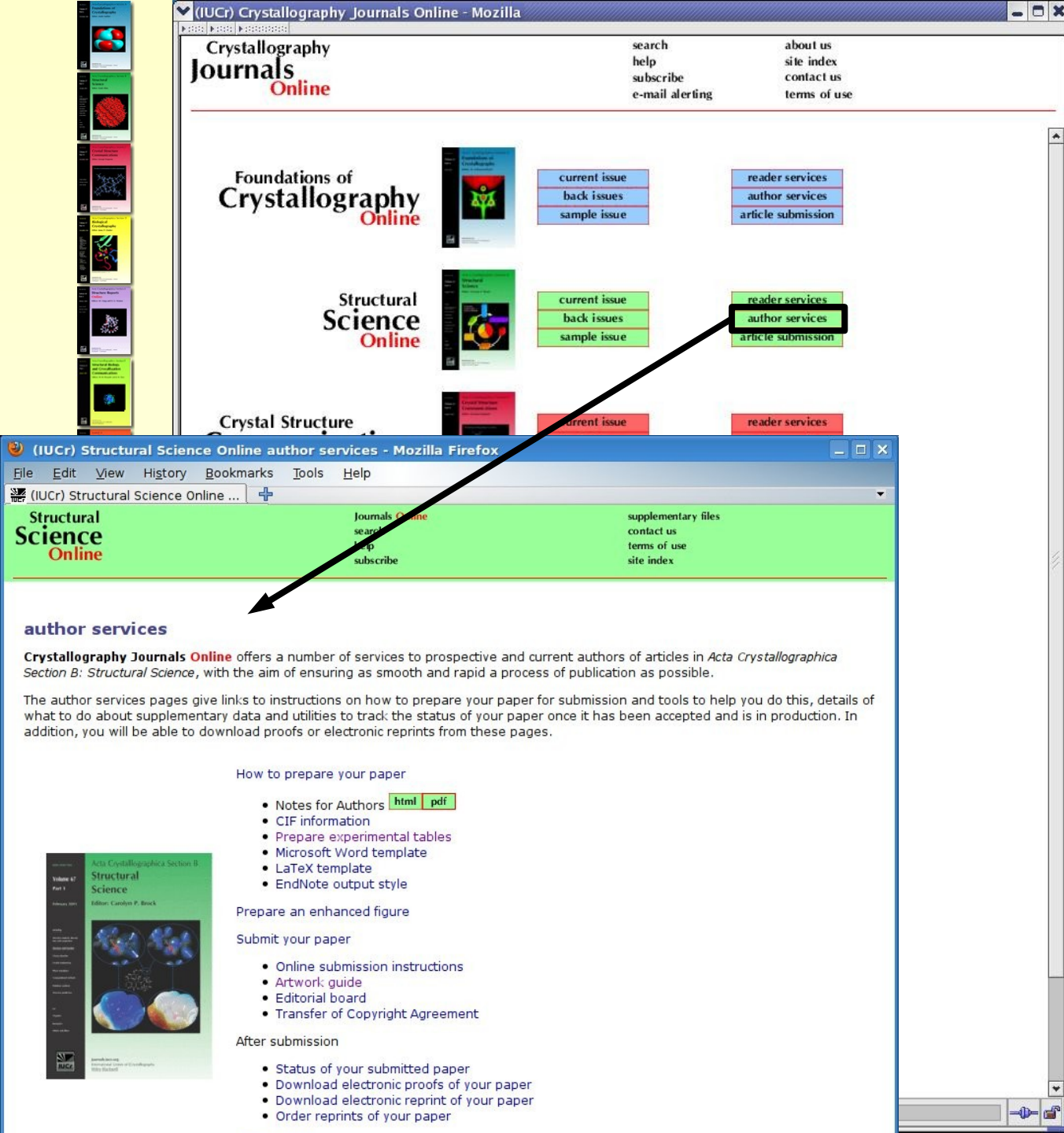
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- journals.iucr.org
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Crystallography Journals Online



- Links include
- WORD template
 - LaTeX template
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 - How to prepare experimental tables from CIF
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- Provide a structured way of capturing articles
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Current template

This template is packaged with a number of tools, including tools that allow tables of experimental data to be prepared easily.

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Author: All journals: volume: page:

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The IUCr is a scientific union serving the interests of crystallographers and other scientists employing crystallographic methods.

Done

- Template for WORD 2007 and 2010
- Utilizes content management features of WORD
- Older templates also available

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IUCr

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Select paper type _____

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Correspondence email:

Keywords: semicolon-separated list

Synopsis

One or two sentences appropriate for the journal's contents listing

Abstract

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Page: 1 of 2 Words: 272 English (U.K.) 100%

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- Articles can be written in the template or quickly imported and marked up

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IUCr

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Acta Crystallographica Section A
Acta Crystallographica Section B
Acta Crystallographica Section D
Acta Crystallographica Section F
Journal of Applied Crystallography
Journal of Synchrotron Radiation

Correspondence email:

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- Use drop-down menu lists to select journal

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IUCr

Acta Crystallographica Section B

Select paper type
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- Styles also available from IUCr ribbon

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Figure 1 Each figure caption should be a single paragraph (style: IUCr figure caption; this style applies the figure numbering).

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A1.1. Third level appendix heading (style: IUCr appendix heading 3)

IUCr body text

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- Tables should be prepared using WORD's table editor with styles applied to caption, headnotes and footnotes

- Experimental tables can be prepared using **Table tools**

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Tools: Author details, Check styles, Table tools

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A1. Second level appendix heading (style: IUCr appendix heading 2)

IUCr body text

A1.1. Third level appendix heading (style: IUCr appendix heading 3)

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- Use **Table tools** to prepare experimental tables from a CIF for small molecule structures

- For macromolecular structures use PDB code to import mmCIF to create table of experimental details

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Figure 1 Each figure applies the figure

Appendix A. First IUCr body text

A1. Second level IUCr body text

A1.1. Third level IUCr body text

Add to document Options... Save CIF Geometry tables

Experimental details

For all structures: monoclinic, $P2_1/c$. Experiments were carried out at 180 K with Mo λ radiation. Refinement was with 0 restraints.

| | Id425_180k_22apr2011.int4 | Id489 | Id473 |
|---------------------------|---|--|--|
| Crystal data | | | |
| Chemical formula | $C_{13}H_{14}N_2O_3$ | $C_{13}H_{15}F_3N_2O_2$ | $C_{17}H_{19}F_3N_2O$ |
| M_r | 246.26 | 312.29 | 324.34 |
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| β (°) | 103.559 (6) | 102.537 (3) | 93.4529 (11) |
| V (Å ³) | 2339.0 (16) | 1423.44 (14) | 1581.43 (9) |
| Z | 8 | 4 | 4 |
| μ (mm ⁻¹) | 0.10 | 0.12 | 0.11 |
| Crystal size (mm) | 0.55 × 0.26 × 0.12 | 0.42 × 0.22 × 0.14 | 0.32 × 0.16 × 0.12 |
| Data collection | | | |
| Diffractometer | Rigaku CrystalClear-SM Expert 2.0 f4 diffractometer | KappaCCD diffractometer | KappaCCD diffractometer |
| Absorption correction | Multi-scan Higashi, 1995 | Multi-scan from symmetry-related measurements, SORTA V (Blessing 1997) | Multi-scan from symmetry-related measurements, SORTA V (Blessing 1997) |

Page: 2 of 2 Words: 274 English (U.K.) 100%

Each datablock from the CIF appears as column in table

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Author details Check styles Table tools

<keywords> <synopsis> <abstract>

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h3 <heading 3 style>

ack <acknowledgements>

ref <reference>

fig <figure caption>

th <table heading>

<table headnote> <table text> <table footnote>

<Appendix heading 1> <Appendix heading 2> <Appendix heading 3>

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Current style: IUCr table caption

References

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Table 1 This is a table head

IUCr table text

IUCr table text

This is a table foot

Figure 1 Each figure applies the figure

Appendix A. First IUCr body text

A1. Second level IUCr body text

A1.1. Third level IUCr body text

Rebuild table

Column heads: Datablock_name

Data blocks:

- Id425_180k_22apr2011int4
- Id489
- Id473

The following items are **not** usually published, but may be included if of special interest

- F000
- Specimen_density
- Cell_measurement_reflections
- Cell_measurement_theta_range
- Crystal_shape
- Specimen_colour
- Radiation_source
- Monochromator
- Detector_resolution
- Scan_method
- Reflection_theta_range
- hkl_range
- Structure_factor_coefficient
- Weighting_scheme
- refine ls shift/su max

'Options...' include changing the order of structures in this table and including extra items.

| Id489 | Id473 |
|--------------------------------------|--|
| $C_{15}H_{19}F_3N_2O_2$ | $C_{17}H_{19}F_3N_2O$ |
| 312.29 | 324.34 |
| 8.9941 (5), 11.2954 (6), 14.3596 (9) | 12.1853 (5), 12.2242 (4), 10.6361 (3) |
| 102.597 (3) | 99.4529 (11) |
| 1423.44 (14) | 1581.43 (9) |
| 4 | 4 |
| 0.12 | 0.11 |
| 0.42 × 0.22 × 0.14 | 0.32 × 0.16 × 0.12 |
| KappaCCD diffractometer | KappaCCD diffractometer |
| Absorption correction | Multi-scan Higashi, 1995 |
| | Multi-scan from symmetry-related measurement, SORTAV (Blessing 1997) |
| | Multi-scan from symmetry-related measurement, SORTAV (Blessing 1997) |

Page: 2 of 2 Words: 274 English (U.K.) 100%

- Extra “non-standard” items present in the CIF can be added to table

- Datablocks can be selected for inclusion or exclusion

- Several types of column headings can be selected

- Small molecule, powder and incommensurate CIFs handled

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Tools: Author details, Check styles, Table tools

Styles: <keywords>, <synopsis>, <abstract>, txt, h1, h2, h3, ack, ref, fig, th, <table headnote>, <table text>, <table footnote>, <Appendix heading 1>, <Appendix heading 2>, <Appendix heading 3>

References

This is Word's reference management system, but if you usually use a different citation manager, please apply the IUCr references style to each reference.

Table 1 This is a table head
IUCr table text
IUCr table text
This is a table foot

Figure 1 Each figure applies the figure style

Appendix A. First IUCr body text

A1. Second level IUCr body text

A1.1. Third level IUCr body text

Experimental details

For all structures: monoclinic, $P2_1/c$. Experiments were carried out at 180 K with Mo $K\alpha$ radiation. Refinement was with 0 restraints.

| | 18425_180k_22apr2011int4 | 18489 | 18473 |
|---------------------------|---|---|---|
| Crystal data | | | |
| Chemical formula | $C_{13}H_{14}N_2O_3$ | $C_{13}H_{13}F_3N_2O_2$ | $C_{17}H_{19}F_3N_2O$ |
| M_r | 246.26 | 312.29 | 324.34 |
| a, b, c (Å) | 7.059 (3), 24.497 (10), 13.914 (6) | 8.9941 (5), 11.2954 (6), 14.3536 (9) | 12.1853 (5), 12.2242 (4), 10.6361 (3) |
| β (°) | 103.559 (6) | 102.537 (3) | 99.4529 (11) |
| V (Å ³) | 2339.0 (16) | 1423.44 (14) | 1581.43 (9) |
| Z | 8 | 4 | 4 |
| μ (mm ⁻¹) | 0.10 | 0.12 | 0.11 |
| Crystal size (mm) | 0.55 × 0.26 × 0.12 | 0.42 × 0.22 × 0.14 | 0.32 × 0.16 × 0.12 |
| Data collection | | | |
| Diffractometer | Rigaku CrystalClear-SM Expert 2.0 θ diffractometer | KappaCCD diffractometer | KappaCCD diffractometer |
| Absorption correction | Multi-scan Higashi, 1995 | Multi-scan multi-scan from symmetry-related measurement, SORTAV (Blessing 1997) | Multi-scan multi-scan from symmetry-related measurement, SORTAV (Blessing 1997) |

Page: 2 of 2 | Words: 274 | English (U.K.) | 100%

Once all items have been selected, the experimental table can be added to the document

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h2 <heading 2 style>

h3 <heading 3 style>

ack <acknowledgements>

ref <reference>

fig <figure caption>

th <table heading>

<table headnote> <table text> <table footnote>

<Appendix heading 1> <Appendix heading 2> <Appendix heading 3>

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Current style: IUCr table caption

References

This is Word's reference management system, but if you usually use a different citation manager, please apply the IUCr references style to each reference.

Table 1 This is a table head IUCr table text IUCr table text This is a table foot

Figure 1 Each figure applies the figure IUCr body text

Appendix A. First IUCr body text

A1. Second level IUCr body text

A1.1. Third level IUCr body text

Selection of geometric parameters prior to creation of tables

Select/deselect a single parameter by clicking it; select/deselect a group of parameters by dragging the mouse over them.

Move a single parameter by dragging its icon

Move a group of parameters that have the same selection state by holding down the SHIFT key before dragging the icon of the first parameter in the group.

Move a structure block by dragging its icon

Bonds Angles

| 3d425_180k_22apr2011.int4 | 3d489 | 3d473 |
|---------------------------|--------------------|-------|
| ○ O1—C8* 1.379(2) | ○ O1—C7 1.378(2) | |
| ○ O1—C2* 1.386(2) | ○ O1—C1 1.3821(19) | |
| ○ O1—C8 1.380(2) | ○ N1—C7 1.315(2) | |
| ○ O1—C2 1.380(2) | ○ N1—C6 1.344(2) | |
| ○ O2—C2* 1.216(2) | ○ C7—C8 1.390(2) | |
| ○ O2—C2 1.209(2) | ○ O2—C1 1.215(2) | |
| ○ C3—C4* 1.343(3) | ○ C4—C5 1.366(2) | |
| ○ C3—C2* 1.435(3) | ○ C4—C8 1.416(2) | |
| ○ C3—H3* 0.97(2) | ○ C4—H4 0.9500 | |
| ○ C9—C8* 1.389(3) | ○ F1—C15 1.327(2) | |
| ○ C9—C5* 1.394(3) | ○ C6—N2 1.357(2) | |
| ○ C9—C4* 1.450(3) | ○ C6—C5 1.433(2) | |
| ○ N1—C8* 1.323(2) | ○ F3—C15 1.331(2) | |
| ○ N1—C7* 1.349(2) | ○ C8—C3 1.435(2) | |
| ○ C3—C4 1.348(3) | ○ C2—C3 1.355(2) | |

Page: 2 of 2 Words: 274 English (U.K.) 100%

• Can also create geometry tables from CIF

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Author details Check styles Table tools

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h3 <heading 3 style>

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Current style: IUCr table caption

References

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Table 1 This is a table head

IUCr table text

IUCr table text

This is a table foot

Figure 1 Each figure applies the figure

Appendix A. First IUCr body text

A1. Second level IUCr body text

A1.1. Third level IUCr body text

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Select/deselect a single parameter by clicking it; select/deselect a group of parameters by dragging the mouse over them.

Move a single parameter by dragging its icon

Move a group of parameters that have the same selection state by holding down the SHIFT key before dragging the icon of the first parameter in the group.

Move a structure block by dragging its icon

Bonds Angles

| 3d425_180k_22apr2011.tnt4 | 3d489 | 3d473 |
|---------------------------|----------------------|-------|
| Select... | Select... | |
| ⊙C8—O1—C2* 121.04(14) | ⊙C7—O1—C1 122.18(13) | |
| ⊙C8—O1—C2 121.43(14) | ⊙C7—N1—O6 117.72(14) | |
| ⊙C4—C3—C2* 122.71(17) | ⊙N1—C7—O1 112.50(14) | |
| ⊙C4—C3—H3* 123.1(12) | ⊙N1—C7—C8 126.52(15) | |
| ⊙C2—C3—H3* 114.2(11) | ⊙O1—C7—C8 120.98(14) | |
| ⊙C8—C9—C5* 115.18(17) | ⊙C5—C4—C8 121.77(15) | |
| ⊙C8—C9—C4* 119.15(17) | ⊙C5—C4—H4 119.1 | |
| ⊙C5—C9—C4* 125.66(17) | ⊙C8—C4—H4 119.1 | |
| ⊙C8—N1—C7* 116.81(16) | ⊙N1—C6—N2 116.34(15) | |
| ⊙C4—C3—C2 122.67(17) | ⊙N1—C6—C5 122.03(15) | |
| ⊙C4—C3—H2 122.1(13) | ⊙N2—C6—C5 121.63(15) | |
| ⊙C2—C3—H2 115.1(13) | ⊙C7—C8—C4 114.64(15) | |
| ⊙C3—C4—C9 118.65(17) | ⊙C7—C8—C3 117.61(15) | |
| ⊙C3—C4—C1 121.59(17) | ⊙C4—C8—C3 127.74(15) | |
| ⊙C9—C4—C1 119.75(16) | ⊙C3—C2—O1 120.91(16) | |

Page: 2 of 2 Words: 274 English (U.K.) 100%

- Can also create geometry tables from CIF

- Can select which bonds and angles to include in table

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Author details Check styles Table tools

<keywords> <body text style> <synopsis> <abstract>

txt h1 h2 h3 ack ref fig th

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<Appendix heading 1> <Appendix heading 2> <Appendix heading 3>

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Current style: IUCr table caption

References

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Table 1 This is a table head

IUCr table text

IUCr table text

This is a table foot

Figure 1 Each figure applies the figure

Appendix A. First IUCr body text

A1. Second level IUCr body text

A1.1. Third level IUCr body text

Create tables Select... Hide non-selected geometry Change layout

If there is more than one structure, the layout can be switched between a 'side-by-side' view and a 'top-to-bottom' view.

Selection of geometric parameters prior to creation of tables

Select/deselect a single parameter by clicking it; select/deselect a group of parameters by dragging the mouse over them.

Move a single parameter by dragging its icon

Move a group of parameters that have the same selection state by holding down the SHIFT key before dragging the icon of the first parameter in the group.

Move a structure block by dragging its icon

Bonds Angles

| Structure | Parameter | Value |
|---------------------------|-----------|------------|
| Jd425_180k_22apr2011.int4 | ∠O1'-C8* | 1.379(2) |
| | ∠O1'-C2' | 1.386(2) |
| | ∠O1-C8 | 1.380(2) |
| | ∠O1-C2 | 1.380(2) |
| | ∠O2'-C2' | 1.216(2) |
| | ∠O2-C2 | 1.209(2) |
| | ∠C3'-C4* | 1.343(3) |
| | ∠C3'-C2' | 1.435(3) |
| | ∠C3'-H3' | 0.97(2) |
| | ∠O9'-C8* | 1.389(3) |
| | ∠O9'-C5' | 1.394(3) |
| | ∠O9'-C4' | 1.450(3) |
| ∠N1'-C8* | 1.323(2) | |
| ∠N1'-C7' | 1.349(2) | |
| ∠C3-C4 | 1.348(3) | |
| Jd489 | ∠O1-C7 | 1.378(2) |
| | ∠O1-C1 | 1.3821(19) |
| | ∠N1-C7 | 1.315(2) |
| | ∠N1-C6 | 1.344(2) |
| | ∠C7-C8 | 1.390(2) |
| | ∠O2-C1 | 1.215(2) |
| | ∠C4-C5 | 1.366(2) |
| | ∠C4-C8 | 1.416(2) |
| | ∠C4-H4 | 0.9500 |
| | ∠F1-C15 | 1.327(2) |
| ∠C6-N2 | 1.357(2) | |
| ∠C6-C5 | 1.433(2) | |
| ∠F3-C15 | 1.331(2) | |
| ∠C8-C3 | 1.435(2) | |
| ∠C2-C3 | 1.355(2) | |
| Jd473 | | |

Page: 2 of 2 Words: 274 English (U.K.) 100%

- Can also create geometry tables from CIF

- Can select which bonds and angles to include in table

- Layout can be changed to accommodate comparison tables

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Author details Check styles Table tools

< keywords > < synopsis > < abstract >

txt h1 h2 h3 ack ref fig th

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< Appendix heading 1 > < Appendix heading 2 > < Appendix heading 3 >

Help Info SGML Sgml Toggle highlights Misc

Current style: Heading 3

Table 2 Data collection and refinement statistics

| Data collection | |
|---|------------------------------------|
| Resolution range (Å) | 49.43-2.9 (3.06-2.9) ^a |
| Unit cell | |
| (Å) | 132.5, 196.7, 170.8 |
| (°) | 90.0, 92.8, 90.0 |
| Space group | <i>P</i> 2 ₁ |
| Redundancy | 4.2 (4.2) |
| Reflections | 805846 |
| Unique reflections | 193013 |
| Completeness (%) | 100 (99.9) |
| <i>R</i> _{merge} (%) | 12.0 (56.6) |
| <i>I</i> / <i>σ</i> _{<i>I</i>} | 10.7 (2.5) |
| Refinement | |
| Range (Å) | 20.0-2.9 |
| Reflections used | 191418 |
| $\frac{1}{2}R_{\text{free}}$ | 19.0/22.3 |
| No. of atoms in the asymmetric unit | |
| Protein | 63129 |
| Ligand | 645 |
| Solvent | 65 |
| Rms deviations | |
| Bond lengths (Å) | 0.014 |
| Bond angles (°) | 1.47 |
| Average B | 45.04 |
| MolProbity validation | |
| Clashscore (all atom contacts) | 4.2 (100 th percentile) |
| Poor rotamers (%) | 3.91 |
| Ramachandran (%) | |
| Favoured | 96.28 |
| Allowed | 3.59 |
| Disallowed | 0.13 |
| C ^β deviations > 0.25 Å | 18 |
| MolProbity score | 1.90 (99 th percentile) |

Use a CIF or mmCIF to create tables

Load CIF

Load a structure from the PDB archives to create tables

Fetch PDB CIF PDB code: 2xq1

Page: 16 of 17 Words: 4,993 English (U.K.) 130%

For macromolecular papers the PDB reference code can be used to upload an mmCIF

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Author details Check styles Table tools

<keywords> <synopsis> <abstract>

txt h1 h2 h3 ack ref fig th <table headnote> <table text> <table footnote> <Appendix heading 1> <Appendix heading 2> <Appendix heading 3>

Tools

Current style: Heading 3

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Table 2 Data collection and refinement statistics

Data collection

| | |
|------------------------|-----------------------------------|
| Resolution range (Å) | 49.43-2.9 (3.06-2.9) ^a |
| Unit cell | |
| (Å) | 132.5, 196.7, 170.8 |
| (°) | 90.0, 92.8, 90.0 |
| Space group | |
| Redundancy | |
| Reflections | |
| Unique reflections | |
| Completeness (%) | |
| R_{merge} (%) | |
| $I/\sigma I$ | |

Refinement

| | |
|-------------------------------------|------------------------------------|
| Range (Å) | |
| Reflections used | |
| R_{free} | |
| No. of atoms in the asymmetric unit | |
| Protein | |
| Ligand | |
| Solvent | |
| Rms deviations | |
| Bond lengths (Å) | |
| Bond angles (°) | |
| Average B | |
| MolProbity validation | |
| Clashscore (all atom contacts) | |
| Poor rotamers (%) | |
| Ramachandran (%) | |
| Favoured | 96.28 |
| Allowed | 3.59 |
| Disallowed | 0.13 |
| C β deviations > 0.25 Å | 18 |
| MolProbity score | 1.90 (99 th percentile) |

Add following table to document

Sample information

| | |
|---|--|
| Macromolecule details | |
| Database code(s) | PDB code: 2XQ1; UNP code: CATA_PICAN |
| Component molecules | Peroxisomal catalase (EC number: 1.11.1.6), protoporphyrin IX containing Fe, water |
| Macromolecular assembly | |
| Mass (Da) | |
| Source organism | FICHTIA ANGUSTA |
| Crystallization and crystal data | |
| Crystallization method | . |
| Temperature (K) | . |
| Apparatus | . |
| Atmosphere | . |
| Pressure (kPa) | . |
| Crystal growth time | . |
| Seeding | . |
| Additional details | . 0.2 M magnesium formate, 20% (W/V) PBG 3350 |
| Crystallization solutions | |
| Crystal data | |

Page: 16 of 17 Words: 4,993 English (U.K.) 130%

Tables generated containing

- Sample information

Crystallography
Journals
Online

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Author details Check styles Table tools

< keywords > < synopsis > < abstract >

txt h1 h2 h3 ack ref fig th

< body text style > < heading 1 style > < heading 2 style > < heading 3 style > < acknowl- edgements > < reference > < figure caption > < table heading > < table footnote >

< Appendix heading 1 > < Appendix heading 2 > < Appendix heading 3 >

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Current style: Heading 3

Table 2 Data collection and refinement statistics

Data collection

| | |
|------------------------|-----------------------------------|
| Resolution range (Å) | 49.43-2.9 (3.06-2.9) ^a |
| Unit cell | |
| (Å) | 132.5, 196.7, 170.8 |
| (°) | 90.0, 92.8, 90.0 |
| Space group | |
| Redundancy | |
| Reflections | |
| Unique reflections | |
| Completeness (%) | |
| R_{merge} (%) | |
| $I/\sigma I$ | |

Refinement

| | |
|-------------------------------------|------------------------------------|
| Range (Å) | |
| Reflections used | |
| R_{refined} | |
| No. of atoms in the asymmetric unit | |
| Protein | |
| Ligand | |
| Solvent | |
| Rms deviations | |
| Bond lengths (Å) | |
| Bond angles (°) | |
| Average B | |
| MolProbability validation | |
| Clashscore (all atom contacts) | |
| Poor rotamers (%) | |
| Ramachandran (%) | |
| Favoured | 96.28 |
| Allowed | 3.59 |
| Disallowed | 0.13 |
| C β deviations > 0.25 Å | 18 |
| MolProbability score | 1.90 (99 th percentile) |

Crystal data

| | |
|--|------------------------|
| Crystal shape | NONB |
| Crystal size (mm) | 7 x 7 x 7 mm |
| Matthews coefficient, V_M (Å ³ Da ⁻¹) | 2.49 |
| Solvent content (%) | 50.14 |
| Unit-cell data | |
| Crystal system, space group | $P2_1$ |
| a, b, c (Å) | 132.52, 196.68, 170.85 |
| α, β, γ (°) | 90, 92.85, 90 |
| No. of molecules in unit cell, Z | |

Add all tables to document

Add following table to document

Data collection and structure solution statistics

Values for the outer shell are given in parentheses.

| | |
|----------------------|-----------------------------------|
| Diffraction source | Synchrotron; ESRF beamline ID14-1 |
| X-ray beam size | . |
| Sampling protocol | |
| Diffraction protocol | Single wavelength |
| Monochromator | Diamond (111), Ge(220) |
| Collimation | . |

Page: 16 of 17 Words: 4,993 English (U.K.) 130%

Tables generated containing

- Sample information
- Data collection and structure solution statistics

Crystallography
Journals
Online

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Author details Check styles Table tools

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< Appendix heading 1 > < Appendix heading 2 > < Appendix heading 3 >

Help Info SGML Sgml Toggle highlights Misc

Current style: Heading 3

Table 2 Data collection and refinement statistics

Data collection

| | |
|-------------------------------------|------------------------------------|
| Resolution range (Å) | 49.43-2.9 (3.06-2.9) [#] |
| Unit cell | |
| (Å) | 132.5, 196.7, 170.8 |
| (°) | 90.0, 92.8, 90.0 |
| Space group | |
| Redundancy | |
| Reflections | |
| Unique reflections | |
| Completeness (%) | |
| <i>R</i> _{average} (%) | |
| <i>I</i> / <i>σ</i> | |
| Refinement | |
| Range (Å) | |
| Reflections used | |
| <i>R</i> _{free} | |
| No. of atoms in the asymmetric unit | |
| Protein | |
| Ligand | |
| Solvent | |
| Rms deviations | |
| Bond lengths (Å) | |
| Bond angles (°) | |
| Average B | |
| MolProbity validation | |
| Clashscore (all atom contacts) | |
| Poor rotamers (%) | |
| Ramachandran (%) | |
| Favoured | 96.28 |
| Allowed | 3.59 |
| Disallowed | 0.13 |
| C ^α deviations > 0.25 Å | 18 |
| MolProbity score | 1.90 (99 th percentile) |

Structure refinement and model validation

Values for the outer shell are given in parentheses.

| | |
|--|--------------------------|
| Refinement software | REFMAC 5.5.0109 |
| Refinement on | |
| σ cutoff | |
| Resolution range (Å) | 20.00-2.90 (2.974-2.900) |
| No. of reflections used in refinement | (13850) |
| No. of reflections above σ cutoff in final cycle | 191418 |
| Final overall R factor | 0.191 |
| Atomic displacement model | |
| Overall average B factor (Å ²) | 42.5 |
| No. of protein atoms | 63129 |
| No. of ligand atoms | 645 |
| No. of solvent atoms | 65 |
| Total No. of atoms | 63839 |
| No. of refined parameters | |
| Non-crystallographic symmetry restraints | |
| Bulk solvent model | MASK |
| Final R _{work} | 0.19059 (0.298) |
| No. of reflections for R _{work} | 976 (69) |

Page: 16 of 17 Words: 4,993 English (U.K.) 130%

Tables generated containing

- Sample information
- Data collection and structure solution statistics
- Structure refinement and model validation

Crystallography
Journals
Online

Document1 - Microsoft Word

Home Insert Page Layout References Mailings Review View MathType Developer Add-Ins IUCr template EndNote X2 Acrobat IUCr Design Layout

Tools: Author details, Check styles, Table tools

Styles: <keywords>, <synopsis>, <abstract>, txt, h1, h2, h3, ack, ref, fig, th, <table headnote>, <table text>, <table footnote>, <Appendix heading 1>, <Appendix heading 2>, <Appendix heading 3>

Current style: IUCr table text

References

This is Word's reference management system, but if you usually use a different citation manager, please apply the IUCr references style to each reference.

Table 1 This is a table heading (style: IUCr table caption; this style applies table numbering)

This is a table headnote (style: IUCr table headnote)

| | | | |
|-----------------|-----------------|-----------------|-----------------|
| IUCr table text | IUCr table text | IUCr table text | IUCr table text |
| IUCr table text | IUCr table text | IUCr table text | IUCr table text |

This is a table footnote (style: IUCr table footnote)

Figure 1 Each figure caption should be a single paragraph (style: IUCr figure caption; this style applies the figure numbering).

Appendix A. First level appendix heading (style: IUCr appendix heading 1)

IUCr body text

A1. Second level appendix heading (style: IUCr appendix heading 2)

IUCr body text

A1.1. Third level appendix heading (style: IUCr appendix heading 3)

IUCr body text

Page: 2 of 2 | Words: 274 | English (U.K.) | 100%

- Figure captions should be listed
- Insert appendices if appropriate
- Headings, tables, figure captions etc. are automatically numbered in journal style

Document1 - Microsoft Word

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Author details Check styles Table tools

< keywords > < synopsis > < abstract >

txt < body text style >

h1 < heading 1 style >

h2 < heading 2 style >

h3 < heading 3 style >

ack < acknowl- edgements >

ref < reference >

fig < figure caption >

th < table heading >

< table headnote > < table text > < table footnote >

< Appendix heading 1 > < Appendix heading 2 > < Appendix heading 3 >

Help Info SGML Sgml Toggle highlights Misc

Current style: IUCr references

Update Citations and Bibliography

Built-In Bibliography

Bibliography

Chen, J. (2003). *Citations and References*. New York: Cortoso Press.
 Haas, J. (2005). *Creating a Formal Publication*. Boston: Proseware, Inc.
 Kramer, J. D. (2006). *How to Write Bibliographies*. Chicago: Adventure Works Press.

Works Cited

Works Cited

Chen, J. (2003). *Citations and References*. New York: Cortoso Press.
 Haas, J. (2005). *Creating a Formal Publication*. Boston: Proseware, Inc.
 Kramer, J. D. (2006). *How to Write Bibliographies*. Chicago: Adventure Works Press.

IUCr sections

IUCr references

References

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Convert bibliography to static text

Filter Languages

a different citation manager.

able numbering)

IUCr table text

IUCr table text

IUCr figure caption; this style applies the figure numbering).

Appendix A. First level appendix heading (style: IUCr appendix heading 1)

IUCr body text

A1. Second level appendix heading (style: IUCr appendix heading 2)

IUCr body text

A1.1. Third level appendix heading (style: IUCr appendix heading 3)

IUCr body text

Page: 2 of 2 Words: 272 English (U.K.) 100%

- References added using Microsoft citation manager or EndNote recognised

Document1 - Microsoft Word

Home Insert Page Layout References Mailings Review View MathType Developer Add-Ins IUCr template EndNote X2 Acrobat IUCr

Author details Check styles Table tools

< keywords > < synopsis > < abstract >

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h1 < heading 1 style >

h2 < heading 2 style >

h3 < heading 3 style >

ack < acknowl- edgements >

ref < reference >

fig < figure caption >

th < table heading >

< table headnote > < table text > < table footnote >

< Appendix heading 1 > < Appendix heading 2 > < Appendix heading 3 >

Help Info SGML Sgml Toggle highlights Misc

Current style: IUCr references

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Built-In Bibliography

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Kramer, J. D. (2006). *How to Write Bibliographies*. Chicago: Adventure Works Press.

IUCr sections

IUCr references

a different citation manager.

IUCr table text

IUCr table text

IUCr figure caption; this style

yle: IUCr appendix heading 1)

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EndNote output style files are available

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author services

Crystallography Journals Online offers a number of services to prospective and current authors of articles in *Acta Crystallographica Section B: Structural Science*, with the aim of ensuring as smooth and rapid a process of publication as possible.

The author services pages give links to instructions on how to prepare your paper for submission and tools to help you do this, details of what to do about supplementary data and utilities to track the status of your paper once it has been accepted and is in production. In addition, you will be able to download proofs or electronic reprints from these pages.

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Paul P. Ewald, *Acta Crystallographica*

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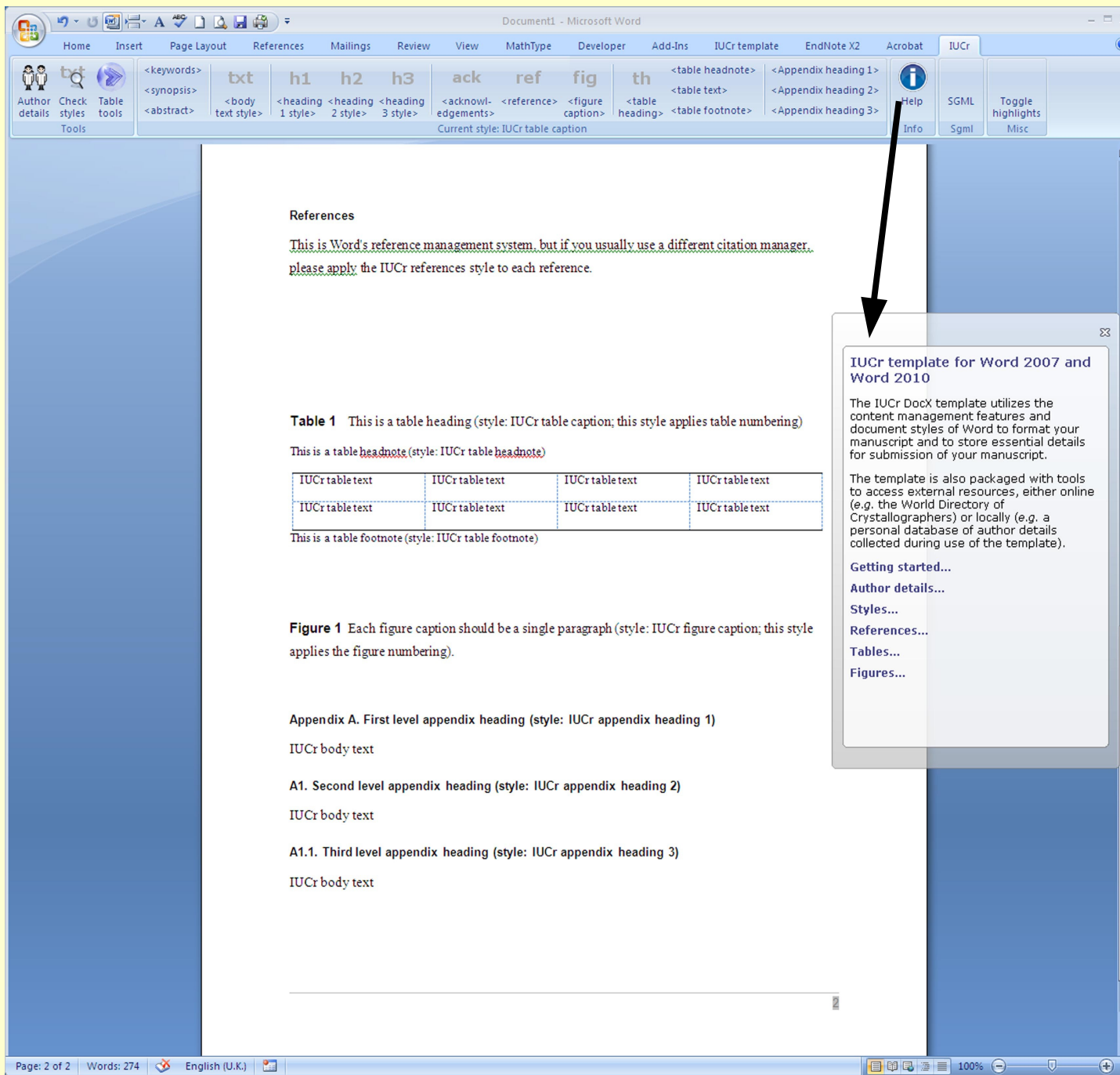
EndNote output style

EndNote output style files are available for *Acta Crystallographica*, *Journal of Applied Crystallography* and *Journal of Synchrotron Radiation*.

To download use the right mouse button or use "Save As..."

- Acta Crystallographica* style
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- Help accessible at any time
- But the template is designed to be easy to use and to save time for authors
- Mac version to be available in autumn
- Simple OpenOffice template also available



LaTeX template



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LaTeX style file and templates

Authors who use **LaTeX** may prepare their papers for submission with a set of customised macros. The macros allow an author to structure a manuscript in the style of the journal, and to present mathematical equations in a portable form. A LyX template is also available for users of this LaTeX-compatible graphical document editor.

prerequisites

1. LaTeX2e, version 1997/12/01 or later.
2. The *iucr* macro package.
3. Optionally, BibTeX for citation handling.

See *availability* below for sources.

general notes on the use of the *iucr* package

A paper prepared in LaTeX format should declare a document of class *iucr*; that is, the first non-comment line of the file should be of the form

```
\documentclass{iucr}
```

Additional options will normally be specified with this command. The most common option is preprint, to produce a single double-spaced version of the paper suitable for review purposes. Use this option for the hard-copy version of the paper. The Co-editor:

```
\documentclass[preprint]{iucr}
```

Since the journals are not typeset directly from LaTeX (but from another language, SGML, into which the LaTeX file is translated), it is usually appropriate to prepare the manuscript **solely** in this 'preprint' mode.

For camera-ready conference papers the preprint option may be omitted, and the paper should be made up according to the style of the journal, including the proper placement of figures and tables. See the specific instructions for preparing a camera-ready copy in such cases

For papers containing long mathematical equations, it is helpful if the author processes the paper without the preprint option, so that the equations may be adjusted to fit properly into the narrow columns of the journal.

special instructions for Acta Crystallographica Section B

A submission to Acta Crystallographica Section B often comprises one or more sets of crystal structure data in CIF format for the body of the manuscript. For such papers the following applies:

1. Standard experimental tables (*i.e.* those containing data that can be encoded in a CIF - experimental details, geometry, displacement parameters) will be typeset from the CIF.
2. All other parts of the paper including non-standard tabular information may be presented in LaTeX format. Manuscripts should be prepared for submission to a Coeditor with the document class invocation:


```
\documentclass[preprint]{iucr}
\journalcode{B}
```
3. Authors should provide a preprint version to the Coeditor for review. This has double line spacing and one column. They should also send hard-copy versions of the figures, and the CIF file (by email or on diskette). When the preprint is accepted the author will be asked to send final electronic versions to the editorial office in Chester.
4. Electronic versions of the figures should preferably be PostScript files, with one figure per page. However, there is an option for calling figures into the LaTeX file so that they can be printed in the hard-copy review manuscript.

When accepted for publication, the final version to be submitted to the editorial office should be prepared with the invocation

```
\documentclass[dj]{iucr}
\journalcode{B}
```

• LaTeX template instructions and files (**template** and **IUCr class file**) from author services page

Mozilla Firefox

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ftp://ftp.iucr.org/te...es/latex/template.ltx

Most Visited Journals Online (IUCr) International U... (International Tables)... (IUCr) submission sys... Index of /cjo/pete/css

```

%-----
% Template file for the submission of papers to IUCr journals in LaTeX2e
% using the iucr document class
% Copyright 1999-2011 International Union of Crystallography
% Version 1.4a (17 April 2011)
%-----
\documentclass{iucr}          % DO NOT DELETE THIS LINE

%-----
% Information about the type of paper
%-----
\paperprodcode{a000000}      % Replace with production code if known
\paperref{xx9999}           % Replace xx9999 with reference code if known
\papertype{FA}              % Indicate type of article
                             % FA - research papers (full article)
                             % SC - short communications
                             % LA - lead article
                             % FE - feature articles
                             % ST - structural communications
                             % XC - crystallization communications
                             % (Following categories rarely in LaTeX)
                             % AA - abstracts
                             % AD - addenda and errata
                             % BC - books received
                             % BR - book reviews
                             % CA - cif applications
                             % CE - current events
                             % CI - inorganic compounds
                             % CM - metal-organic compounds
                             % CN - cryocrystallography papers
                             % CO - organic compounds
                             % CP - computer programs
                             % CR - crystallographers
                             % CS - scientific comment
                             % ED - editorial
                             % EI - inorganic compounds
                             % EM - metal-organic compounds
                             % EO - organic compounds

```



```
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% Version 1.4a (17 April 2011)
%-----

\documentclass(iucr)           % DO NOT DELETE THIS LINE

%-----
% Information about the type of paper
%-----
\paperprocode{a000000}        % Replace with production code if known
\paperref{xx9999}             % Replace xx9999 with reference code if known
\papertype{FA}                % Indicate type of article
% FA - research papers (full article)
% SC - short communications
% LA - lead article
% FE - feature articles
% ST - structural communications
% XC - crystallization communications
% (Following categories rarely in LaTeX)
% AA - abstracts
% AD - addenda and errata
% BC - books received
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% CI - inorganic compounds
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% CR - crystallographers
% CS - scientific comment
% ED - editorial
% EI - inorganic compounds
% EM - metal-organic compounds
% EO - organic compounds
% FI - inorganic compounds
% FM - metal-organic compounds
% FO - organic compounds
% IP - issue preface
% IU - iucr
% LE - letters to the editor
% LN - laboratory notes
% ME - forthcoming meetings/short courses
% MR - meeting reports
% NN - notes and news
% NP - new commercial products
% OB - obituaries
% SR - software reviews
% TE - teaching and education

\paperlang(english)          % Can be english, french, german or russian
%-----
% Information about journal to which submitted
%
```

LaTeX

- Easy to create complex mathematical equations
- Indicates structure of document which is useful in translating for production
- However, authors can essentially redefine any command, sometimes making the use of LaTeX challenging within submission and production systems

LaTeX templates

- Authors strongly encouraged to use IUCr template (in **preprint mode**) – will closely match target sgml file for production
- Other styles (e.g. REVTeX) can be handled but more editorial intervention needed to create effective sgml translation

```
Mozilla Firefox
File Edit View History Bookmarks Tools Help
ftp://ftp.iucr.org/te...es/latex/template.ltx x +
ftp://ftp.iucr.org/templates/latex/template.ltx
Most Visited Journals Online (IUCr) International U... (International Tables)... (IUCr) submission sys... Index of /cio/pete/css

%-----
% Template file for the submission of papers to IUCr journals in LaTeX2e
% using the iucr document class
% Copyright 1999-2011 International Union of Crystallography
% Version 1.4a (17 April 2011)
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% MR - meeting reports
% NN - notes and news
% NP - new commercial products
% OB - obituaries
% SR - software reviews
% TE - teaching and education

\paperlang(english)          % Can be english, french, german or russian
%-----
% Information about journal to which submitted
%
```

BibTeX

```
1 :
2 @Book{          knuth84,
3   author       = "Donald E. Knuth",
4   title        = "The \TeX{}book",
5   publisher    = {Addison-Wesley},
6   year        = 1984
7 }
8
9 @Book{          lamport86,
10  author       = "Leslie Lamport",
11  title        = "{\LaTeX{}} A Document Preparation System",
12  publisher    = {Addison-Wesley},
13  year        = 1986
14 }
15
16 @Book{          NocedalWright2000,
17  author       = "Nocedal, J., and Wright, S.",
18  title        = "Numerical Optimization",
19  address     = "New York",
20  publisher    = {Springer},
21  year        = 2000
22 }
23
24 @book(Saad-book2,
25   author="Y. Saad", title={Iterative Methods for
26   Sparse Linear Systems, 2nd edition},
27   Publisher="SIAM", address="Philadelphia, PA", year="2003")
28
29
30 @Article{       pauling89,
31  author       = {Pauling, L.},
32  title        = {},
33  journal      = {Proc. Natl Acad. Sci},
34  volume      = {86},
35  pages       = "8595--8599",
36  year        = 1989
37 }
38
39 @Article{       crambin95,
40  author       = {Stec, B., and Zhou, B., and Teeter, M. M.},
41  title        = {},
42  journal      = {Acta Cryst.},
43  volume      = {D51},
44  pages       = "663--681",
45  year        = 1995
46 }
47
48 @Article{       kabsch93,
49  author       = {Kabsch, W.},
50  title        = {},
51  journal      = {J. Appl. Cryst.},
52  volume      = {26},
53  pages       = "795--800",
54  year        = 1993
55 }
56
57 @Article{       kabsch2010,
```

- LaTeX submissions usually have an associated bibliography (BibTeX) file
- BibTeX files contain structured information and allow references to be automatically formatted in journal style (provided the quality of information in the BibTeX file is reasonable)



publBio



Crystallography
Journals
Online

The screenshot shows a web browser window displaying the IUCr website. The address bar shows the URL http://scripts.iucr.org/cgi-bin/chub_login. The page header includes the IUCr logo and navigation links for journals, books, news, education, people, and resources. The main content area is titled "IUCr Online services" and contains a login form with fields for "IUCr ID*" (containing "IUCr3019") and "Password*" (masked with dots), and a "Login" button. To the right of the login form is a "Register" section with a "Create a new entry" button and a link for forgotten passwords. Below the login form is an "About publBio" section with a bulleted list of features and a "Hopefully, you will find that the route from laboratory data to publication becomes more streamlined through the use of publBio." footer. The bottom of the page features a navigation bar with links for home, advanced search, contact us, site index, and journals, along with the IUCr copyright notice.

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http://scripts.iucr.org/cgi-bin/chub_login Google

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IUCr Online services

Please sign in here to access **publBio** and other IUCr Online services (e.g. World Directory of Crystallographers, e-mail alerting).

IUCr ID*

Password*

Login

About publBio

publBio offers you tools to prepare the text, experimental data tables, and figures for a structural biology or crystallization communication, along with personal web space in which to use them.

Your personal web space gives you the freedom to use these tools to whatever extent suits you, ranging from simply obtaining a document 'template' for completion using a word processor and submission in the conventional manner, to preparing your entire paper 'online' and then submitting on the click of a button.

However you use it, we hope that publBio will make preparation of your paper a little easier:

- With or without a starting data source, the tools for experimental data tables should ensure that your paper contains the items appropriate for submission.
- A growing number of data resources and validation procedures should help to ensure that your data are presented according to current standards.
- Use of established formatting routines should relieve some of the tedium of trying to conform to journal style.
- Use of your personal web space should provide 'added value': you will be able to build up your own data resources for use in future projects (e.g. easy access to databases of names and addresses, standard laboratory protocols, instrumentation, etc., for inclusion in new papers).
- By exploiting publBio to the full, you will be able to avoid the time-consuming process of re-entering data at the point of submission, and realise the benefits of preparing your paper using an application tailored to online submission.

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Done

PublBio is a first attempt to provide an online authoring tool for authors in the “cloud”

It is currently available to authors of Sections D and F

A quick tour of publBio follows

publBio requires a login and simple registration

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http://publbio.iucr.org/publbio/publbio.php?&login_id=87e79827ede5ba94

publBio – tools for writing structural biology and crystallization communications

Welcome Peter R. Strickland
 Preferences | Log out

Acta Cryst. D | Acta Cryst. F
 Personal home page

You have the following projects

Current Submitted

| | |
|-----------------------------------|---|
| 3ee9 (modified 10 Mar 09 15:37) | Submit to Acta Cryst. D Submit to Acta Cryst. F |
| 2e39 (modified 06 Apr 09 12:40) | Submit to Acta Cryst. D Submit to Acta Cryst. F |
| 2hqq (modified 07 Apr 09 13:31) | Submit to Acta Cryst. D Submit to Acta Cryst. F |
| dz5146 (modified 07 Apr 09 13:31) | Submit to Acta Cryst. D Submit to Acta Cryst. F |

Start a new project

Start a new project without a data source
 Or enter a PDB code
 Or upload an mmCIF

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Hopefully, you will find that the route from laboratory data to publication becomes more streamlined through the use of publBio.

Notes on this version

Although this is a 'beta' version, we encourage you to use it to the full, safe in the knowledge that any changes to publBio will only be enhancements, i.e. they will not adversely affect any projects you may have started. When using this version, please consider the following when making any suggestions/comments (which are most welcome):

- An equation editor plugin for the WYSIWYG editors is being developed.
- The Jmol tool will be enhanced.
- Previous request/suggestions regarding the original version of the experimental tables have been gratefully received and are being reviewed.
- 'One-click submission' is not yet implemented.
- The speed of some of the data processing operations is a known issue, and will be improved.

Done zotero

your publBio home page shows all your projects

The screenshot shows the pubBio website interface. At the top, there is a navigation bar with 'File', 'Edit', 'View', 'History', 'Bookmarks', 'Tools', and 'Help'. The address bar shows the URL 'http://publbio.iucr.org/publbio/publbio.php?&login_id=87e79827ede5ba94'. The main header reads 'pubBio – tools for writing structural biology and crystallization communications'. Below this, a user is logged in as 'Peter R. Strickland' with options for 'Preferences' and 'Log out'. A section titled 'You have the following projects' lists four projects with their IDs (3ee9, 2e39, 2hqq, dz5146) and modification dates. Each project has icons for 'Current' and 'Submitted' status and buttons to 'Submit to Acta Cryst. D' and 'Acta Cryst. F'. Below this is a 'Start a new project' section with three options: 'Start a new project without a data source', 'Or enter a PDB code' (with an input field), and 'Or upload an mmCIF' (with a 'Browse...' button). The bottom section contains 'About pubBio' and 'Notes on this version' text, along with a list of updates.

start from scratch

or

enter a PDB code

or

upload an mmCIF

starting a project is simple

pubBio – tools for writing structural biology and crystallization communications

Welcome Peter R. Strickland
 Preferences | Log out

Acta Cryst. D | Acta Cryst. F
 Personal home page

You have the following projects

| Current | Submitted |
|-----------------------------------|---|
| 3ee9 (modified 10 Mar 09 15:37) | Submit to Acta Cryst. D Submit to Acta Cryst. F |
| 2e39 (modified 06 Apr 09 12:40) | Submit to Acta Cryst. D Submit to Acta Cryst. F |
| 2hqq (modified 07 Apr 09 13:31) | Submit to Acta Cryst. D Submit to Acta Cryst. F |
| dz5146 (modified 07 Apr 09 13:31) | Submit to Acta Cryst. D Submit to Acta Cryst. F |

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- Use of established formatting routines should relieve some of the tedium of trying to conform to journal style.
- Use of your personal web space should provide 'added value': you will be able to build up your own data resources for use in future projects (e.g. easy access to databases of names and addresses, standard laboratory protocols, instrumentation, etc., for inclusion in new papers).
- By exploiting pubBio to the full, you will be able to avoid the time-consuming process of re-entering data at the point of submission, and realise the benefits of preparing your paper using an application tailored to online submission.

Hopefully, you will find that the route from laboratory data to publication becomes more streamlined through the use of pubBio.

Notes on this version

Although this is a 'beta' version, we encourage you to use it to the full, safe in the knowledge that any changes to pubBio will only be enhancements, i.e. they will not adversely affect any projects you may have started. When using this version, please consider the following when making any suggestions/comments (which are most welcome):

- An equation editor plugin for the WYSIWYG editors is being developed.
- The Jmol tool will be enhanced.
- Previous request/suggestions regarding the original version of the experimental tables have been gratefully received and are being reviewed.
- 'One-click submission' is not yet implemented.
- The speed of some of the data processing operations is a known issue, and will be improved.

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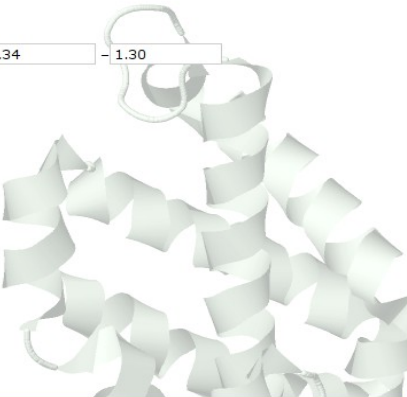
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Macromolecule details, crystallization, data collection, phasing and refinement

Please navigate using the tabs below and fill out as many fields as possible (items labelled in grey are not essential, but you are encouraged to provide them where possible).

Macromolecule | Crystallization | Crystal data | Data collection | Data-collection statistics | Phasing | Refinement

Resolution range (Å) (e.g. 30.0–1.68) 20 – 1.3 Outer shell 1.34 – 1.30
 No. of unique reflections 78519 Outer shell 6815
 No. of observed reflections 78519 Criterion
 Completeness (%) 99.300 Outer shell
 Redundancy (%) 8.900 Outer shell 6.8
 $\langle I/\sigma(I) \rangle$ overall Outer shell: all reflections
 OR observed reflections
 $R_{\text{merge}}(F)$ for all reflections Outer shell
 OR for observed relections Outer shell
 $R_{\text{merge}}(I)$ for all reflections Outer shell
 OR for observed relections 0.066 Outer shell
 Data-processing software
 more...



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data can be reported for structural studies

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Macromolecule details, crystallization and data collection

Please navigate using the tabs below and fill out as many fields as possible (items labelled in grey are not essential, but you are encouraged to provide them where possible).

Macromolecule Crystallization Crystal data Data collection Data-collection statistics

i

Resolution range (Å) (e.g. 30.0–1.68) 20 – 1.3 Outer shell 1.34 – 1.30

No. of unique reflections 78519 Outer shell 6815

No. of observed reflections 78519 Criterion

Completeness (%) 99.300 Outer shell

Redundancy (%) 8.900 Outer shell 6.8

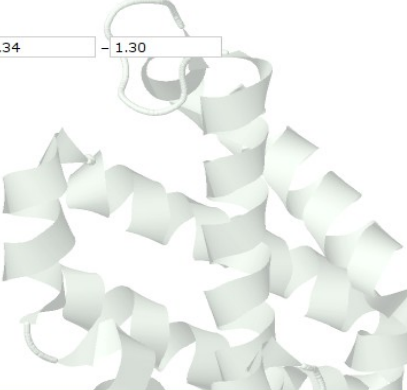
$\langle I/\sigma(I) \rangle$ overall Outer shell: all reflections
OR observed reflections

$R_{\text{merge}}(F)$ for all reflections Outer shell
OR for observed relections Outer shell

$R_{\text{merge}}(I)$ for all reflections Outer shell
OR for observed relections 0.066 Outer shell

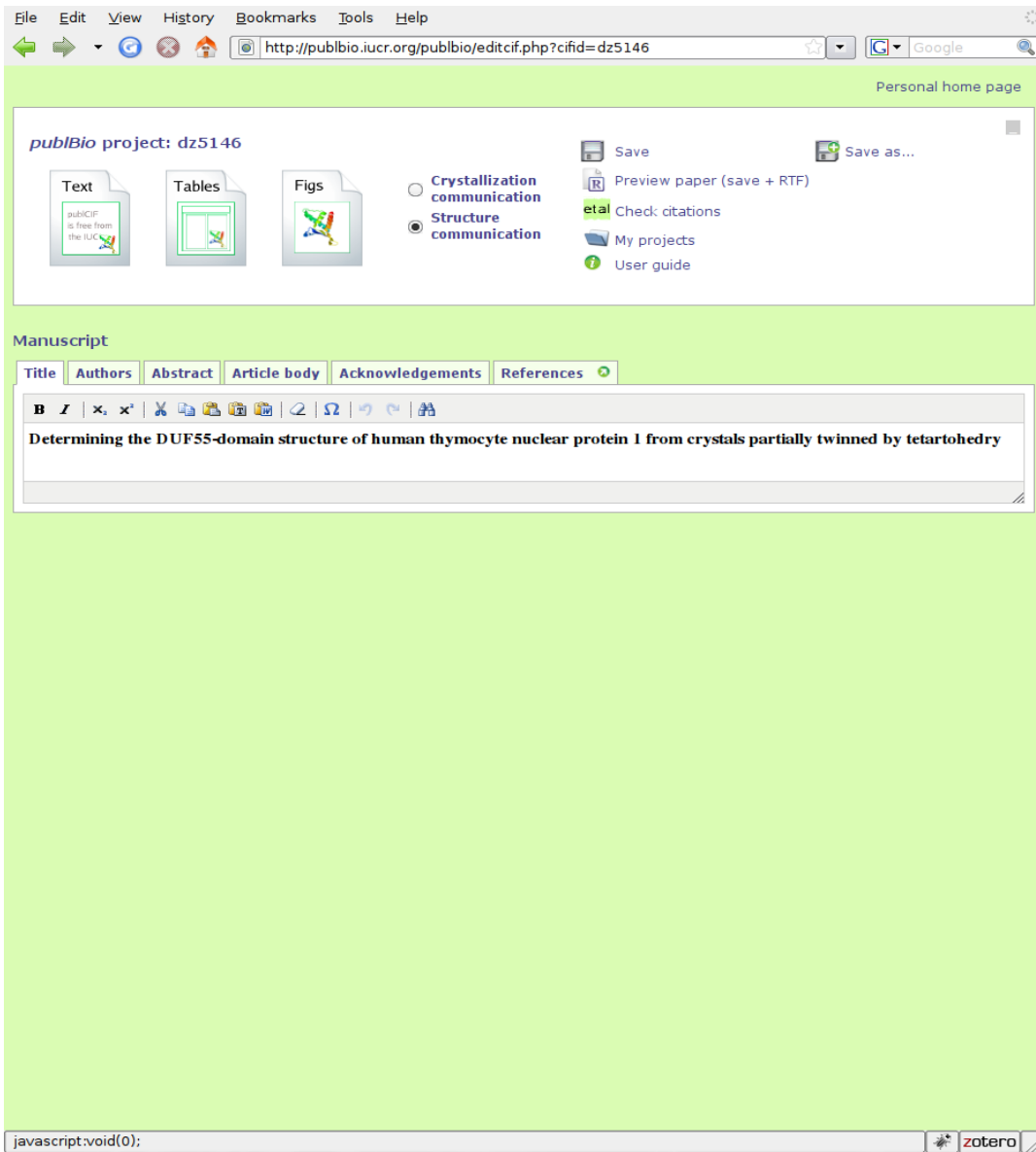
Data-processing software

more...



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or just for crystallization studies



The text tab consists of six tabs

title

authors

abstract

article body

acknowledgements

references

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The "Manuscript" section is active, showing tabs for "Title", "Authors", "Abstract", "Article body", "Acknowledgements", and "References". Below the tabs, there are instructions: "Add another author: before the active tab; after the active tab" and "Move active author tab: to the left; to the right". A list of authors is shown: Song, Yu, Xu, Sun, Li, Tang, Yu, Yeates, Hu, He. The "Yu" author is selected.

The author details form for "Yu" includes:

- Click: here to remove this author
- Use author details from previous projects: [dropdown menu]
- Name**
 - Forename(s): Feng
 - Surname: Yu [Search button]
 - Qualifier (e.g. Jr, III): [text input]
 - E-mail: [text input]
 - Correspondence author:
- Address**
 - Use same address as: [dropdown menu]
 - Department: Shanghai Institute of Applied Physics
 - Organization: Chinese Academy of Sciences
 - Street/PO box: [text input]
 - City: [text input]
 - State/province/county: [text input]
 - Post/zip code: [text input]
 - Country: People's Republic of China [dropdown menu]
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- Address**
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 - Department: [text input]

A 3D ribbon diagram of a protein structure is visible on the right side of the page. The browser status bar at the bottom shows "Done" and a "zotero" icon.

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Song Yu Xu Sun Li Tang Yu Yeates Hu He

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Name

Forename(s) Todd O.

Surname Yeates

Qualifier (e.g. Jr, III)

E-mail

Correspondence author

Address

Use same address as

Department Department of Chemistry and Biochemistry

Organization University of California

Street/PO box

City

State/province/county

Post/zip code

Country USA

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authors may be added by searching

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The "Manuscript" section is active, showing tabs for "Title", "Authors", "Abstract", "Article body", "Acknowledgements", and "References". Below the tabs, there are instructions: "Add another author: before the active tab; after the active tab" and "Move active author tab: to the left; to the right". A row of author names is displayed: Song, Yu, Xu, Sun, Li, Tang, Yu, Yeates, Hu, He. The "Yeates" tab is selected.

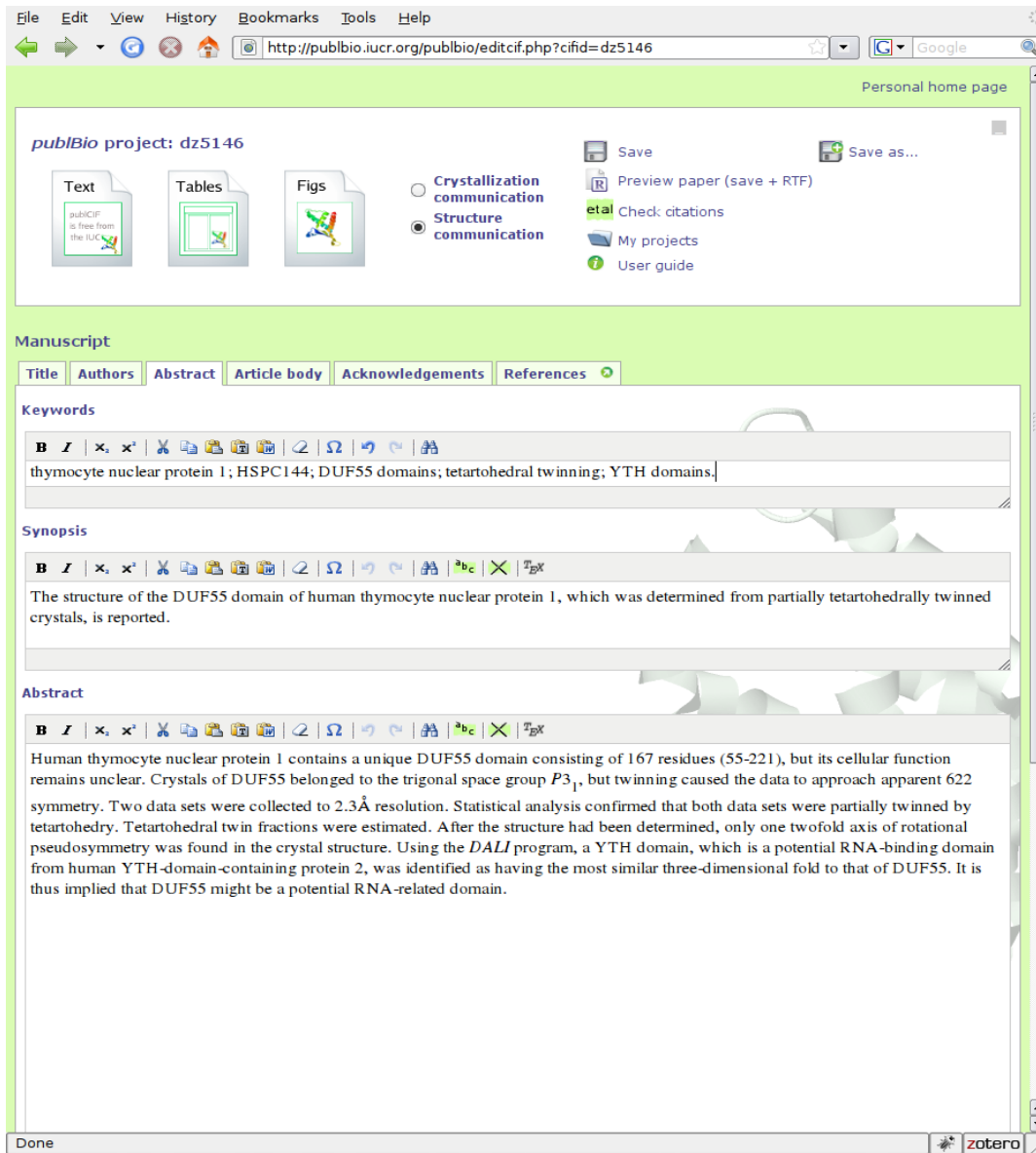
Below the author names, there is a form for adding an author. It includes a link to "remove this author" and a dropdown menu for "Use author details from previous projects". The form fields are: Name (Forename(s): Todd O., Surname: Yeates, Qualifier: [empty], E-mail: [empty], Correspondence author: [checkbox]), Address (Use same address as: [empty], Department: Department of Chemistry, Organization: University of California, Street/PO box: [empty], City: [empty], State/province/county: [empty], Post/zip code: [empty], Country: USA), and links to "remove this address" and "add a further address".

A 3D ribbon diagram of a protein structure is visible on the right side of the page. The browser status bar at the bottom shows "Done" and a Zotero icon.

pubBio maintains a record of author details used in previous projects

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authors may be added from previous projects



the abstract tab contains
the following fields

keywords

synopsis

abstract

text fields have a WYSIWYG interface

The screenshot shows a web browser window displaying the 'pubBio project: dz5146' editor. The interface includes a top navigation bar with 'File', 'Edit', 'View', 'History', 'Bookmarks', 'Tools', and 'Help'. Below this is a 'Personal home page' section with icons for 'Text', 'Tables', and 'Figs', and a list of actions: 'Save', 'Save as...', 'Preview paper (save + RTF)', 'Check citations', 'My projects', and 'User guide'. The 'Structure communication' option is selected. The main area is titled 'Manuscript' and contains tabs for 'Title', 'Authors', 'Abstract', 'Article body', 'Acknowledgements', and 'References'. The 'Article body' tab is active, showing a text editor with a toolbar and a document containing sections like '2.1 Protein expression and purification', '2.2 Protein crystallization', '2.3 Data collection', and '2.4 Data analysis and molecular replacement'. A 'Select custom character - Mozilla Firefox' dialog box is open over the text, displaying a grid of various characters and symbols. The dialog box also shows the URL 'http://publbio.iucr.org/publbio/javascript/tiny_mce/scripts/tiny_mce/themes/ar...' and the character 'Ä' selected. The status bar at the bottom of the browser shows 'Done' and a 'zotero' icon.

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Crystallization communication Structure communication

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Protein expression and purification

DUF55 was expressed and purified as described previously (Song *et al.*, 2005). Briefly, the DUF55 DNA sequence (residues 55-221) was cloned into plasmid pET22b, and subheadings is a C-terminally His-tagged protein. DUF55 was purified using metal-chelating chromatography, SP cation-exchange chromatography (Amersham) and gel filtration on Amersham HiLoad Superdex 75. Finally, the protein was concentrated in a buffer consisting of 20mM HEPES pH 7.2, 150mM NaCl, 5% glycerol and 2mM DTT.

2.1 . Protein crystallization

DUF55 at a concentration of 10mgml⁻¹ was crystallized using the hanging-drop vapour-diffusion method at 291 or 277K. After screening numerous conditions, the following crystallization condition was identified: a hanging drop containing 1μl protein solution, 1μl reservoir solution (0.1M sodium acetate pH 4.0-4.8, 28% PEG 2000 MME, 200mM ammonium sulfate) and 0.2μl 30% 1,6-diaminohexane as an additive (1,6-diaminohexane is a basic reagent, so that the actual pH is about 10.9). After a week, fan-like crystals appeared. The dimensions of the crystals obtained at 291K (0.45 × 0.15 × 0.08mm) were notably larger than those obtained at 277K (0.30 × 0.07 × 0.02mm). The crystals were soaked in a cryoprotectant solution (0.1M sodium acetate pH 4.0-4.8, 42% PEG 2000 MME, 75mM ammonium sulfate, 75mM NaCl, 15% glycerol, 3% 1,6-diaminohexane) and flash-frozen in liquid nitrogen.

2.2 . Data collection

The diffraction of the DUF55 crystals was too weak for the collection of usable data sets using a rotating-anode X-ray generator. Two data sets (named data set 1 and data set 2) were collected to 2.3Å resolution on beamline 3W1A at the Beijing Synchrotron Radiation Facility and processed using *MOSFLM* (Leslie, 2006) and *SCALA* (Collaborative Computational Project, Number 4, 1994).

2.3 . Data analysis and molecular replacement

Initially, the data sets were processed in space group *P*_{6₂22/*P*_{6₄22} according to the self-rotation function plots (Fig. 1) and the detected systematic absences. However, crystal twinning was indicated by an impossibly low value of the Matthews coefficient in this symmetry (1.16Å³ Da⁻¹ for one molecule per asymmetric unit). The presence of twinning was confirmed by examination of the cumulative intensity distribution (Fig. 2) and Padilla-Yeates local intensity statistics (Fig. 3). Plausible lower symmetry space groups included *P*_{3₁}, *P*_{3₂}, *P*_{3₁12}/*P*_{3₂12}, *P*_{3₁21}/*P*_{3₂21} and *P*_{6₃}/*P*_{6₄}. Molecular-replacement searches were therefore carried out under all}

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tabs form the main headings

subheadings are inserted by the WYSIWYG editor

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Check that references in the reference list are in the text

references in the text can be checked

The screenshot shows a web browser window with the URL <http://publinfo.iucr.org/publinfo/editcif.php?cifid=dz5146>. The page is titled "Manuscript" and has tabs for "Title", "Authors", "Abstract", "Article body", and "Acknowledgements". The "Article body" tab is active, showing a text editor with a rich text toolbar. The text in the editor discusses crystal twinning and the Matthews coefficient. A "References" panel is open on the right, displaying a list of citations. Some citations are highlighted in green, indicating they are confidently identified. A "References" report is also visible, showing the number of citations identified in different sections of the manuscript.

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according to the self-rotation function plots (Fig. 1) and the detected systematic absences. However, crystal twinning was indicated by an impossibly low value of the Matthews coefficient in this symmetry ($1.16\text{\AA}^3\text{Da}^{-1}$ for one molecule per asymmetric unit). The presence of twinning was confirmed by examination of the cumulative intensity distribution (Fig. 2) and Padilla-Yeates local intensity statistics (Fig. 3). Plausible lower symmetry space groups included $P3_1$, $P3_2$, $P3_12/P3_212$, $P3_21/P3_21$ and $P6_2/P6_4$. Molecular-replacement searches were therefore carried out under all possible symmetries using the program *Phaser* (McCoy *et al.*, 2007) and data set 1. The search model was PDB entry 2ar1, which had 43% sequence identity (Arakaki *et al.*, 2006). Although potential molecular-replacement solutions were found in $P3_12$, $P3_21$ and $P6_4$, they were judged to be unreliable because of low log-likelihood gain (LLG) values (13, 49 and 5, respectively). A more reliable solution was found in $P3_1$, with an LLG value of 182. We tested out all four solutions in *CNS* (Brünger *et al.*, 1998) and after one cycle of hemihedral/tetartohedral twinning refinement only the solution in $P3_1$ led to improved R_{work} and R_{free} values simultaneously (Table 1); the others led to a poorer R_{free} although R_{work} clearly decreased. The true space group was therefore assigned as $P3_1$, implying that the DUF55 crystals were tetartohedrally twinned. Similar results were obtained using data set 2 (data not shown).

2.5. Estimation of tetartohedral twin fractions

Overall intensity statistics were evaluated in order to test for high or perfect twinning (Yeates, 1997) and the results confirmed severe twinning (Table 2). In order to identify the twin operator and estimate the twin fraction, the data (reduced in $P3_1$) were evaluated using the *H*-test (Yeates, 1988) under the three possible twin operators in $P3_1$. The results (Table 2) suggested that data set 1 was partially twinned by tetartohedry and that data set 2 might be nearly perfectly twinned by tetartohedry. We therefore attempted to refine the structure against data set 2 using *CNS* and available scripts (Barends *et al.*, 2005). However, it was not possible to obtain a satisfactory refinement. One possible explanation was that data set 2 was

References

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Anand, K., Schulte, A., Fujinaga, K., Scheffzek, K. & Geyer, M. (2007). *J. Mol. Biol.* **370**, 826–836.

Arakaki, T., Le Trong, I., Phizicky, E., Quartley, E., DeTitta, G., Luft, J., Lauricella, A., Anderson, L., Kalyuzhnyi, O., Worthey, E., Myler, P. J., Kim, D., Baker, D., Hol, W. G. J. & Merritt, E. A. (2006). *Acta Cryst.* **F62**, 175–179.

Barends, T. R. M., de Jong, R. M., van Straaten, K. E., Thunnissen, A.-M. W. H. & Dijkstra, B. W. (2005). *Acta Cryst.* **D61**, 613–621.

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.

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Compton, M. M., Thomson, J. M. & Icard, A. H. (2001). *Apoptosis*, **6**, 299–314.

Dauter, Z. (2003). *Acta Cryst.* **D59**, 2004–2016.

Dauter, Z., Botos, I., LaRonde-LeBlanc, N. & Wlodawer, A. (2005). *Acta Cryst.* **D61**, 967–975.

Emsley, P. & Cowtan, K. (2004). *Acta Cryst.* **D60**, 2126–2132.

Finn, R. D., Mistry, J., Schuster-Bockler, B., Griffiths-

Any uncertainties in the references are highlighted (double-click a highlighted uncertainty for more information).

No citations identified in Abstract

33 citation(s) confidently identified in § 1. Introduction

14 citation(s) confidently identified in § 2. Materials and methods

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confidently identified references are checked in green

possible citation problems are highlighted

a reference checking report is provided

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The main text area contains a paragraph about tetartohedrally twinned crystals and twin fractions. A mathematical equation editor is open over the text, showing a complex equation with subscripts and Greek letters. The equation is:
$$\begin{cases} \alpha_1 I_1 + \alpha_2 I_2 + \alpha_3 I_3 + \alpha_4 I_4 = J_1 \\ \alpha_1 I_2 + \alpha_2 I_1 + \alpha_3 I_4 + \alpha_4 I_3 = J_2 \\ \alpha_1 I_3 + \alpha_2 I_4 + \alpha_3 I_1 + \alpha_4 I_2 = J_3 \\ \alpha_1 I_4 + \alpha_2 I_3 + \alpha_3 I_2 + \alpha_4 I_1 = J_4 \end{cases}$$
The editor includes a toolbar with various symbols and a preview window showing the rendered equation. The text in the background discusses the assignment of subscripts to twin operations and the determination of twin fractions.

complex mathematics can be handled

mathematics may be input with an equation editor or as TeX

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satisfactory refinement. One possible explanation was that data set 2 was also partially (but not perfectly) tetartohedrally twinned and that the correct twin fractions therefore needed to be incorporated into the refinement. To this end, a new method for estimating tetartohedral twin fractions (Yeates & Yu, 2008) was applied. Two unique and equally plausible solutions for the four twin-fraction values were obtained from this method; the correct so... The potential solutions for the twin fractions for data sets 1 and 2 are shown in Table... In the case of tetartohedral twinning, the observed intensity... object_0_text... intensities (I_k) as follows:

Spell check complete

Any spelling uncertainties are highlighted (double-click: a highlighted uncertainty for more information).

The assignment of subscripts to twin operations is arbitrary. $-h, -l$ and I_4 refers to $I(-h, -k, l)$, according to the three then the intensities can be detwinned (i.e. one can solve for the true intensities, arbitrarily setting $I_{true} = I_1$). If the data have been detwinned successfully, then the resulting intensities should obey exponential statistics (Wilson, 1949). On the other hand, if an incorrect solution for the twin fractions has been chosen then the detwinned intensities may not follow the correct distribution. In this way, it is possible to distinguish between correct and incorrect solutions for the twin fractions (Yeates & Yu, 2008). This approach was used to analyze the potential twin-fraction solutions for data sets 1 and 2 (Fig. 4). In the case of data set 1, the detwinned data calculated under solution 1 followed a somewhat more ideal distribution than those calculated under solution 2. In the case of data set 2, solution 2 was much better.

It is important to note here that for each solution for the twin-fraction values there are four different permutations of the four twin fractions which are equally correct (Yeates & Yu, 2008); different permutations simply correspond to exchanging the assignments of I_1, I_2, I_3 and I_4 in (2). The permutation of the twin fractions that is chosen is therefore arbitrary, unless it is necessary to obtain agreement with a previously defined set of intensities. This was the case here, as a molecular-replacement model (and its calculated intensities) had already been obtained (i.e. prior to detwinning). In this work, therefore, detwinning under all four allowed permutations of the twin-fraction solution was performed and the correct solution was decided by the behaviour of atomic refinement and by the inspection of electron-density maps. For completeness, the four permutations of the alternate (less plausible) solution for the twin fractions were also tested. The same procedure was applied to data set 2. Thus, eight separate preliminary refinements were conducted using each of the two data sets (the results for data set 1 are shown in Table 3). Solution 1 for data set 1 was (0.424, 0.300, 0.134, 0.142), with the alternate orderings (0.300, 0.424, 0.142, 0.134), (0.134, 0.142, 0.424, 0.300) and (0.142, 0.134, 0.300, 0.424) being equally possible. It was verified that solution 1 of data set 1 (0.424, 0.300, 0.134, 0.142) and solution 2 of data set 2 (0.291, 0.276, 0.151, 0.282) were correct. This was consistent with the previous examination of detwinned intensity statistics (Fig. 4).

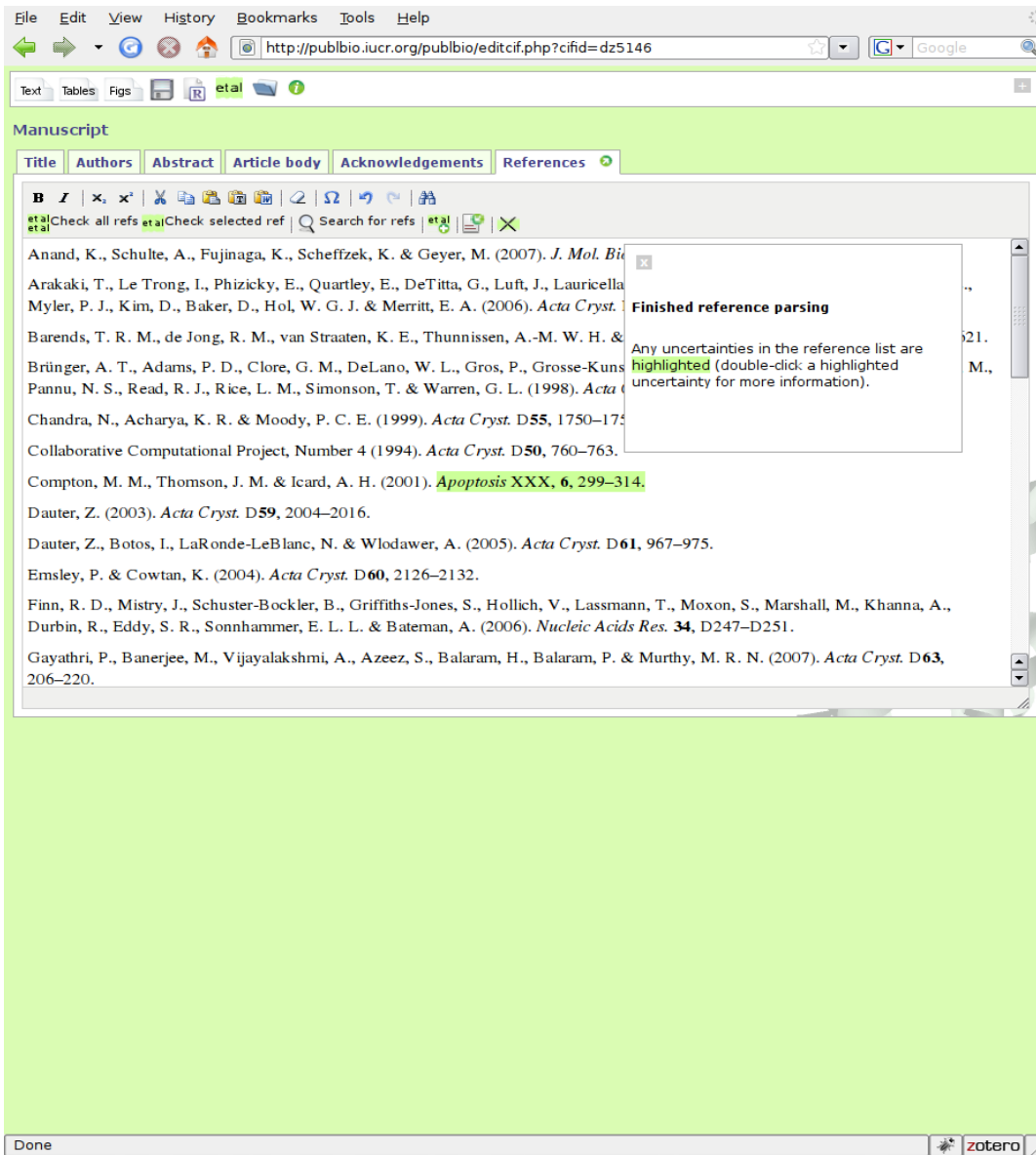
2.6 . Refinement under partial tetartohedral twinning

Because all four twin-related reflections must be observed for detwinning to be carried out (2), data completeness is important for detwinning. We therefore refined the structure using data set 1. An atomic model was rebuilt using *Coot* (Emsley & Cowtan, 2004)

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possible spelling problems are highlighted

spell checking is also available



possible problems with reference list formatting are highlighted

reference list formatting may be checked

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- Search citation databases:** IUCr PubMed
- personal
- Search for
- Author(s)
- Journal
- Volume Year First page
-

Below the search fields, a note reads: "Please note: enhancements to the citation manager are under development". The background text of the manuscript includes citations such as: "Anand, K., Schulte, A., Fujinaga, K., Scheffzek, K. & Geyer, M. (2007). *J. Mol. Biol.* **370**, 826–836." and "Arakaki, T., Le Trong, I., Phizicky, E., Quartley, E., DeTitta, G., Luft, J., Lauricella, A., Anderson, L., Kalyuzhniy, O., Worthey, E., Myler, P. J., Kim, D., Baker, D., Hol, W. G. J. & Merritt, E. A. (2006). *Acta Cryst.* **F62**, 175–179."

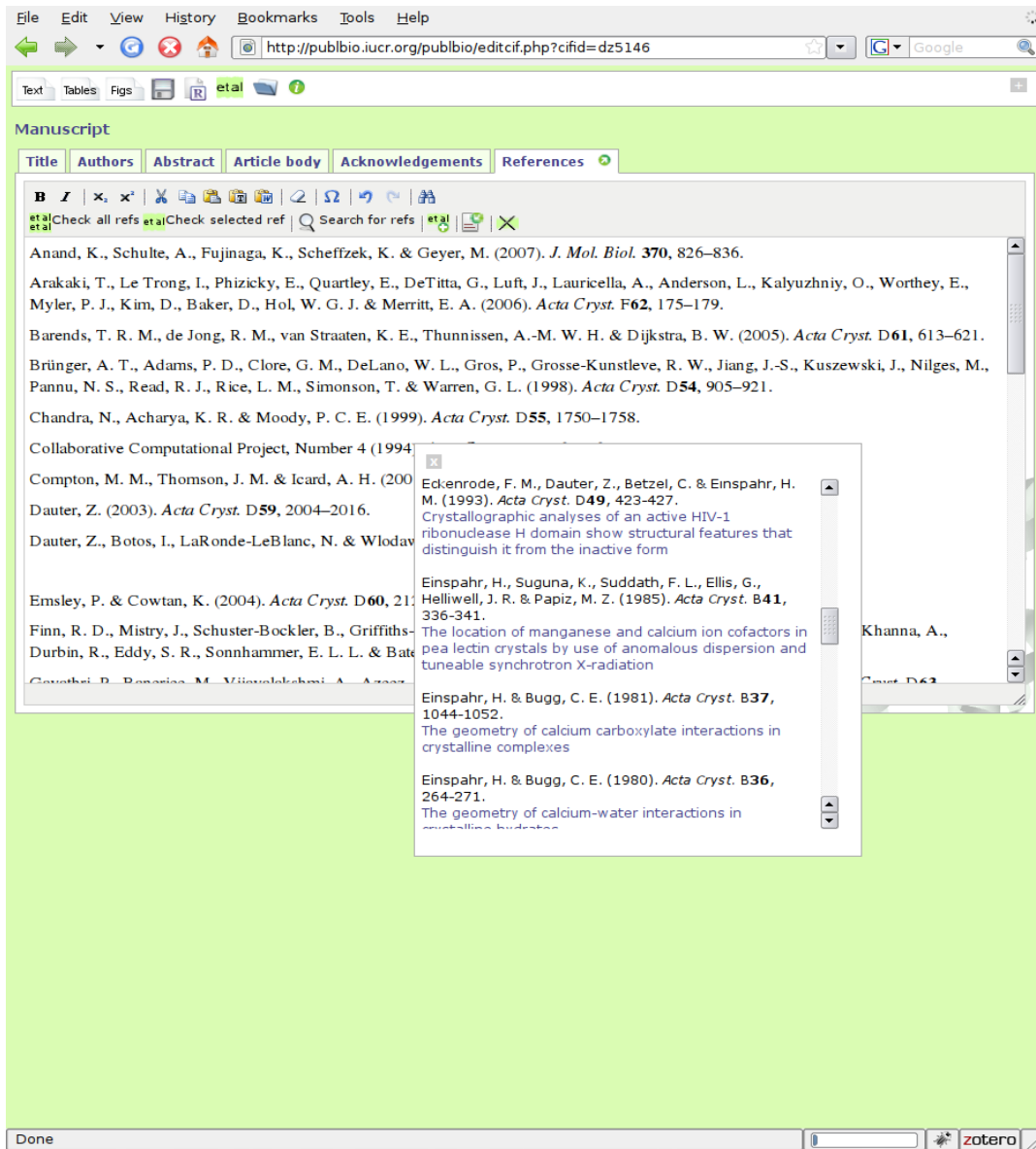
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Component molecules (entities) Macromolecular assembly

Details (such as chemical composition, name and source) of the component molecules (entities) that are present in the crystallographic structure

Click here to add data for another component molecule (entity) of this macromolecule

Entity 1

Click here to remove this entity

Entity description

Description: Human thymocyte nuclear protein 1

Mutation(s)

Modification(s)

EC number

Entity source

Source type

Entity production

Select appropriate production protocol(s)

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The tables tab consists of a number of tabs

macromolecule

crystallization

crystal data

data collection

data-collection statistics

phasing

refinement

experimental data can be edited in the tables tabs

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http://publbio.iucr.org/publbio/editcif.php?cifid=dz5146

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Text Tables Figs

Crystallization communication
Structure communication

Save
Preview paper (save + RTF)
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Save as...

Macromolecule details, crystallization, data collection, phasing and refinement

Please navigate using the tabs below and fill out as many fields as possible (items labelled in grey are not essential, but you are encouraged to provide them where possible).

Macromolecule Crystallization Crystal data Data collection Data-collection statistics Phasing Refinement

Click: here to add data for another crystal of this macromolecule

Crystal 1

Click: here to remove this set of crystal data

Crystal growth

Method: vapor diffusion

Apparatus: Hanging-drop vapour diffusion
Sitting-drop vapour diffusion
Free interface diffusion/counterdiffusion

Temperature (K): Microbatch
Microdialysis

Seeding protocol

Growth time

Additional details

more...

Crystallization solutions

Click: here to access a database of crystallization screens (which may help when listing the solution components)

Macromolecule solution

Volume Volume units pH



Done zotero

data from previous projects are remembered

standard descriptions of methods are also offered

input forms suggest possible wording

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Text Tables Figs

Crystallization communication
Structure communication

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Preview paper (save + RTF)
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User guide

Macromolecule details, crystallization, data collection, phasing and refinement

Please navigate using the tabs below and fill out as many fields as possible (items labelled in grey are not essential, but you are encouraged to provide them where possible).

Macromolecule Crystallization Crystal data Data collection Data-collection statistics Phasing Refinement

Click: here to add data for another crystal of this macromolecule

Crystal 1

Click: here to remove this set of crystal data

Crystal growth

Method vapor diffusion

Apparatus

Temperature (K) 291

Atmosphere

Seeding protocol

Growth time

Additional details

more...

Crystallization solutions

Click: here to access a database of crystallization screens (wh

Macromolecule solution

Volume Volume units pH

Done

zotero

Crystallization screens
(data kindly provided by Rigaku)

Vendor Hampton Research

Screen Crystal Screen Cryo

Well number 4

tris hydrochloride (0.075 M, pH 8.5)
ammonium sulfate (1.5 M)
glycerol (25 v/v)

Click: any of the above components to add them to your table [the 'target' input box: will be highlighted when you hover over the above items - click in any of the component fields (Name, Concentration...) to change the 'target']

standard commercial crystallization screens can be looked up

crystallization conditions can be added from a database

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http://publbio.iucr.org/publbio/editcif.php?cifid=dz5146

Growth time

Additional details

more...

Crystallization solutions

Click: [here](#) to access a database of crystallization screens (which may help when listing the solution components)

Macromolecule solution

Volume Volume units pH

Components of the macromolecule solution

| Macromolecule | Concentration OR concentration range in the macromolecule solution | Concentration units | pH |
|--|--|----------------------|----------------------|
| <input type="text"/> | <input type="text"/> | <input type="text"/> | <input type="text"/> |
| Other components | | | |
| <input type="text"/> | <input type="text"/> | <input type="text"/> | <input type="text"/> |
| <input type="checkbox"/> ammonium acetate | | | |
| <input type="checkbox"/> ammonium bromide | | | |
| <input type="checkbox"/> ammonium chloride | | | |
| <input type="checkbox"/> Ammoniumchlorid | | | |
| <input type="checkbox"/> ammonium citrate - ammonium hydroxide | | | |
| <input type="checkbox"/> ammonium citrate - citric acid | | | |
| <input type="checkbox"/> ammonium dihydrogen phosphate | | | |
| <input type="checkbox"/> ammonium phosphate (monobasic) | | | |
| <input type="checkbox"/> ammonium phosphate monobasic | | | |
| <input type="checkbox"/> ammonium phosphate, monobasic | | | |
| <input type="checkbox"/> ammonium fluoride | | <input type="text"/> | <input type="text"/> |
| <input type="checkbox"/> ammonium formate | | | |
| <input type="checkbox"/> ammonium iodide | | | |
| <input type="checkbox"/> ammonium nitrate | | | |
| <input type="checkbox"/> ammonium selenate | | | |
| <input type="checkbox"/> ammonium sulfate | | | |
| <input type="checkbox"/> Ammoniumsulfate | | | |
| <input type="checkbox"/> ammonium sulphate | | | |
| <input type="checkbox"/> ammonium sulphate | | | |
| <input type="checkbox"/> ammonium sulfite | | | |
| <input type="checkbox"/> ammonium sulphite | | | |
| <input type="checkbox"/> ammonium citrate (dibasic) | | | |
| <input type="checkbox"/> ammonium citrate dibasic | | | |
| <input type="checkbox"/> ammonium citrate, dibasic | | | |
| <input type="checkbox"/> ammonium monohydrogen citrate | | | |
| <input type="checkbox"/> ammonium monohydrogen phosphate | | | |
| <input type="checkbox"/> ammonium phosphate (dibasic) | | | |
| <input type="checkbox"/> ammonium phosphate dibasic | | | |
| <input type="checkbox"/> ammonium phosphate, dibasic | | | |

Concentration OR concentration range in the precipitant solution

Concentration units

Concentration OR concentration range in the reservoir solution

Concentration units

Done

zotero

the software predicts the names of standard crystallization components

crystallization conditions can be added manually

File Edit View History Bookmarks Tools Help

http://publbio.iucr.org/publbio/editcif.php?cifid=2e39

publBio data collection (IUCr) Data for structural an...

Figures

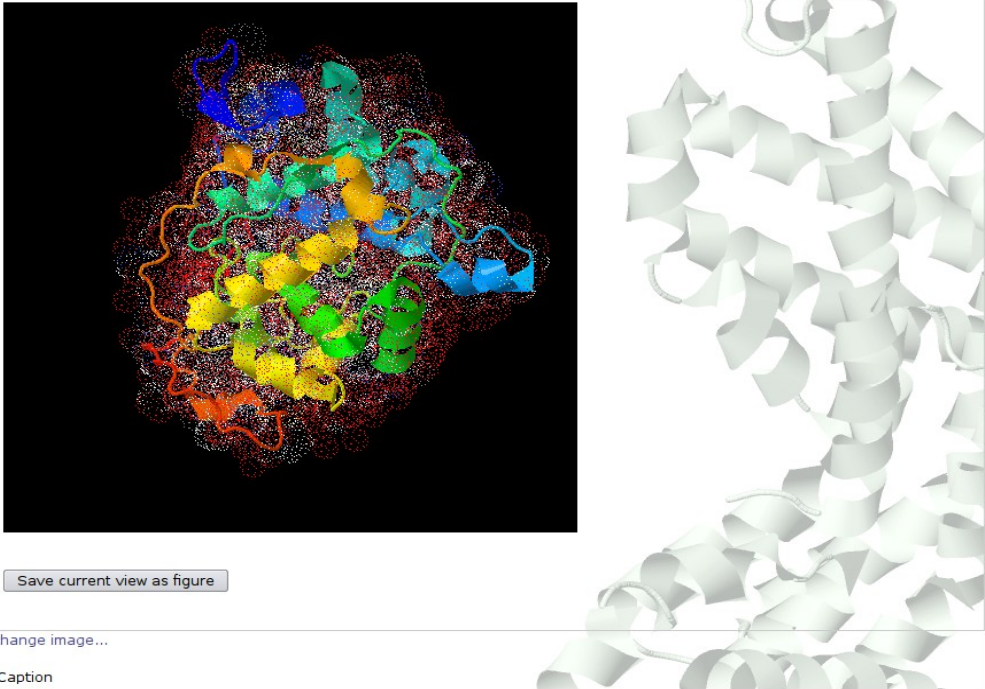
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Fig. 1 Fig. 2 Fig. 3 Fig. 4 Fig. 5 Fig. 6

Click here to remove this figure



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change image...

Caption

B *I* × × |  **et al** | ***b**c |  π σ

View of the structure with surface.

Jmol script terminated zotero

or can be created as interactive Jmol figures

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http://publbio.iucr.org/publbio/editcif.php?cifid=2e39

publBio data collection (IUCr) Data for structural an...

Figures

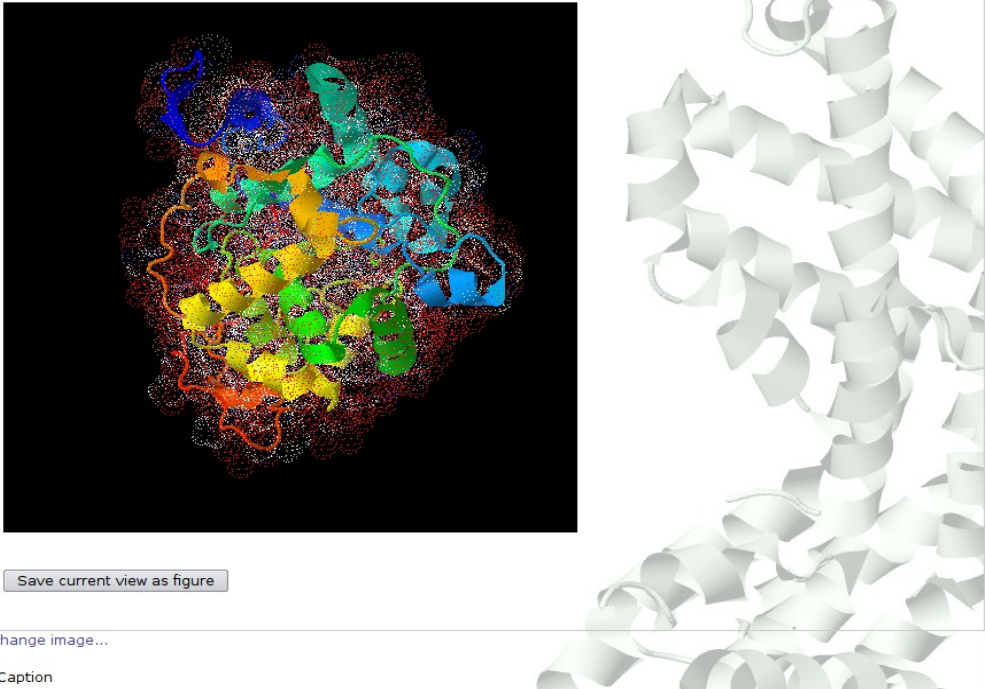
Add another figure: before the active tab; after the active tab

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Fig. 1 Fig. 2 Fig. 3 Fig. 4 Fig. 5 Fig. 6

Click here to remove this figure












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



Save current view as figure


change image...

Caption

B *I* × × |           

etal | **b**c |  

View of the structure with surface.

Jmol script terminated  zotero

or can be created as interactive Jmol figures



Other tools (ask for a demonstration)

publCIF

- Standalone tool for editing CIFs and previewing them in journal style
- Used mainly for submissions to Sections C and E
- publCIF engine underlies WORD template and publBio
- Popular, well established and widely distributed; used by most C and E Co-editors

Enhanced figure toolkit

- Available as a standalone tool or within the submission system
- Creates standard figures for inclusion in the “archived” journal and corresponding 3D interactive figures
- Easy to use, but not yet adopted by the majority of authors
- Interactive figures can be created from small molecule and macromolecular CIFs

Chemistry toolkit

Work is in progress on a chemistry toolkit, to allow chemical connectivity information and diagrams to be created from CIFs on a routine basis

Other toolkits

What else should we be working on?



Commission on Journals 2011

Submission to publication

Figure preparation

Crystallography
Journals
Online



(IUCr) Artwork guide - Mozilla Firefox

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(IUCr) Artwork guide

artwork guide

The aim of this guide is to help you prepare your electronic artwork for submission to IUCr journals. By following the recommendations in this guide, you will be helping us to achieve the highest possible standards of reproduction.

1. General points to consider
2. Preferred file formats
3. Figure sizing
4. Composite images
5. Fonts, labelling
6. Number formats
7. Colour
8. Cropping
9. Notes on particular types of figures
10. General guide to digital images
11. Checklist
12. Useful resources
13. FAQs

1. General points to consider

All figures should be submitted electronically via the submission system. Figures should be numbered sequentially in the order in which they are referred to in the text. Captions to figures should be provided separately in the manuscript file. Please submit one file per figure.

Please aim to keep lettering on figures to a minimum, and ensure you use SI units (*e.g.* K) throughout.

Only those figures that are necessary to illustrate the techniques or results described will be published; any others will be deposited.

For any figures that have been published previously, please ensure you obtain permission from the copyright holder prior to submitting your article to us. Please also forward a copy of the permission letter to the IUCr.

[Back to contents](#)

2. Preferred file formats

The IUCr recommends that only the following file formats are used for electronic artwork submission:

- EPS (Encapsulated PostScript, .eps), PS (PostScript, .ps)
- TIFF (Tagged Image File Format, .tif)
- HPGL (Hewlett Packard Graphics Language, .hpg)

We recommend that you **do not use** the following file formats, because they may result in lower standards of reproduction:

- JPEG (Joint Photographic Expert Group Image File, .jpg)
- GIF (Graphic Image File, .gif)
- PDF (Portable Document File, .pdf)
- MS Office (Word, Excel, PowerPoint) (.doc, .rtf, .xls, .ppt)

EPS, PS (resolution independent unless there is an embedded bitmap/halftone)

Line weights should be between 0.35 and 1.5pt at final size. Please ensure that fonts are embedded. For embedded images, please follow the guidelines for TIFF below.

TIFF

Colour images should have a resolution of at least 400 d.p.i. (dots per inch) at final size.

Monochrome images (black line art on a white background) and greyscale images should have a minimum resolution of 600 d.p.i.

Done

- Online artwork guide available from author services page

Figures – general

- All figures submitted electronically, ideally at start of submission
- All figures have caption; schemes do not
- Figures numbered in order they are cited in the text
- Grids and shadings to be avoided (and coloured backgrounds)
- Specialised symbols (e.g. open circles, closed triangles) should either be avoided in the caption or given as words
- Consider how final figure will appear in print – should fit one page
- Any special instructions for figure handling should be sent to the Editorial Office on acceptance

Image formats

- Recommended formats in Notes for Authors
 - Encapsulated Postscript or PostScript (.eps, .ps) (resolution independent unless there is an embedded bitmap, in which case minimum 600 d.p.i.)
 - Tiff (.tif, minimum resolution 600 d.p.i. final size)
 - HPGL (.hpg) (resolution independent)
 -
- Less recommended
 - MS Office (WORD, Powerpoint, Excel) (.doc, .rtf, .ppt, .xls) (potential loss of image quality; loss of fonts, movement of labelling)
 - PDF (.pdf) (potential loss of image quality)
 - JPEG (.jpg) (uses lossy compression methods – loss of features, ghost effects)
 - GIF (low resolution and limited to 256 colours)
 - PNG (limited colour range in certain circumstances)
- However, PDF and PNG may be necessary for certain LaTeX distributions

Resolution and image formats

This one
is saved
as an EPS
file

vector format
EPS file

This is an
example of
a 600-dpi
image

600 dpi
TIFF file

This is an
example of
a 72-dpi
image

72 dpi
TIFF file

This is an
example of
a 72-dpi
image

72 dpi
JPEG file
(medium quality)

Black and white line images should be a minimum of 600 d.p.i. at final size

Resolution and image formats



400 dpi
TIFF file

72 dpi
TIFF file

72 dpi
JPEG file
(medium quality)

Greyscale and colour images should be a minimum of 400 d.p.i. at final size

What is considered to be a figure, table or scheme?

Table 2. Calculated apatite lattice parameters.

| Sample | $a(\text{\AA})$ | $c(\text{\AA})$ |
|---------|-----------------|-----------------|
| GI744/1 | 9.376(3) | 6.888(4) |
| GI744/2 | 9.382(7) | 6.889(0) |
| SAR1 | 9.369(4) | 6.886(9) |
| HAI08 | 9.385(0) | 6.884(3) |
| 988 | 9.446(7) | 6.884(9) |
| LI95 | 9.443(9) | 6.884(2) |
| LI95A | 9.430(2) | 6.883(3) |
| ELISH | 9.449(5) | 6.883(6) |
| ELISH2 | 9.448(3) | 6.884(5) |
| HAI03 | 9.404(0) | 6.877(9) |
| C57 | 9.438(8) | 6.879(3) |
| KH1 | 9.449(8) | 6.872(3) |

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| HAI08 | 9.385 (1) | 6.884 (3) |
| 988 | 9.446 (7) | 6.884 (9) |
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FIGURE OR TABLE?

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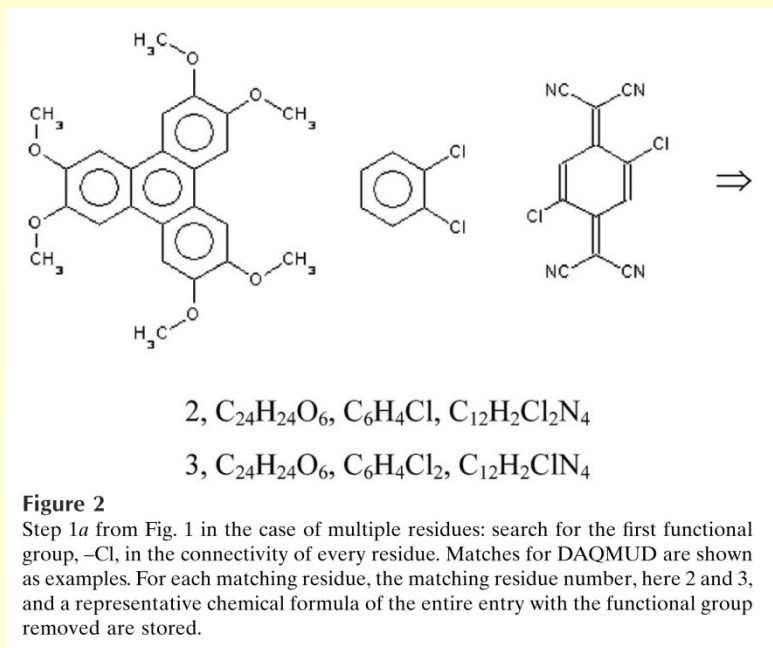
Table 2. Calculated apatite lattice parameters.

| Sample | $a(\text{\AA})$ | $c(\text{\AA})$ |
|---------|-----------------|-----------------|
| GI744/1 | 9.376(3) | 6.888(4) |
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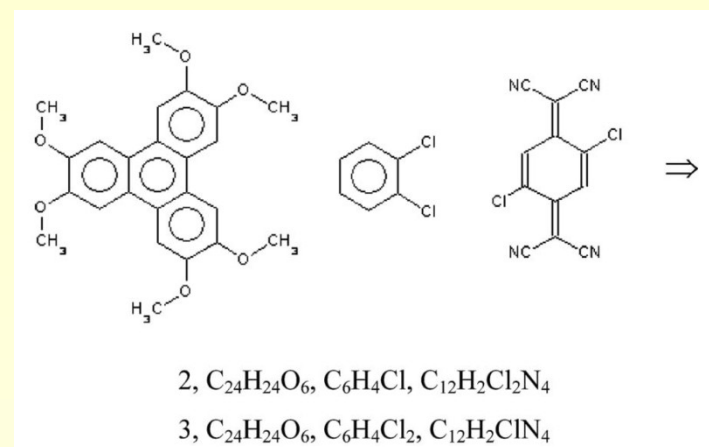
FIGURE OR TABLE

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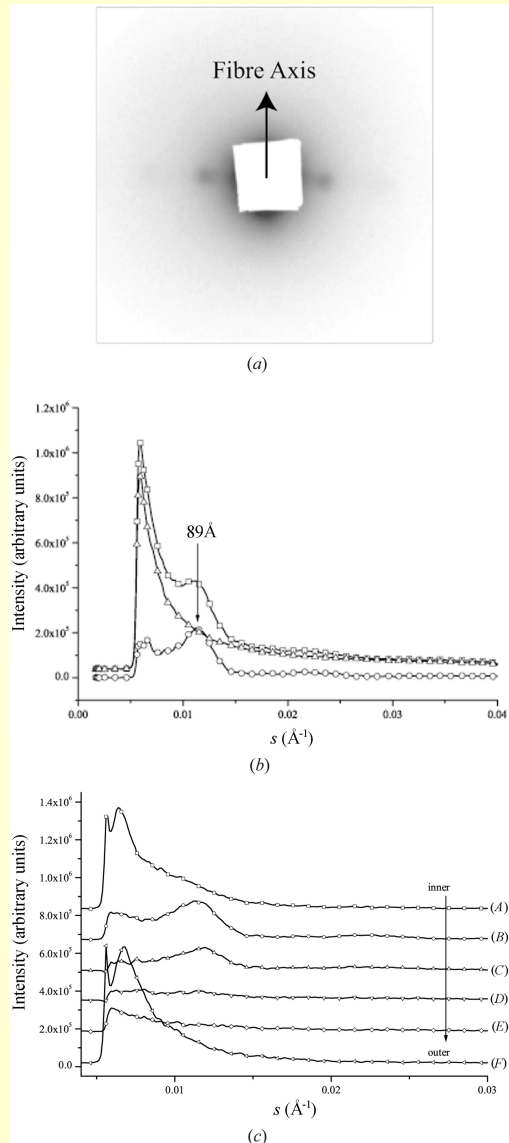


FIGURE



SCHEME

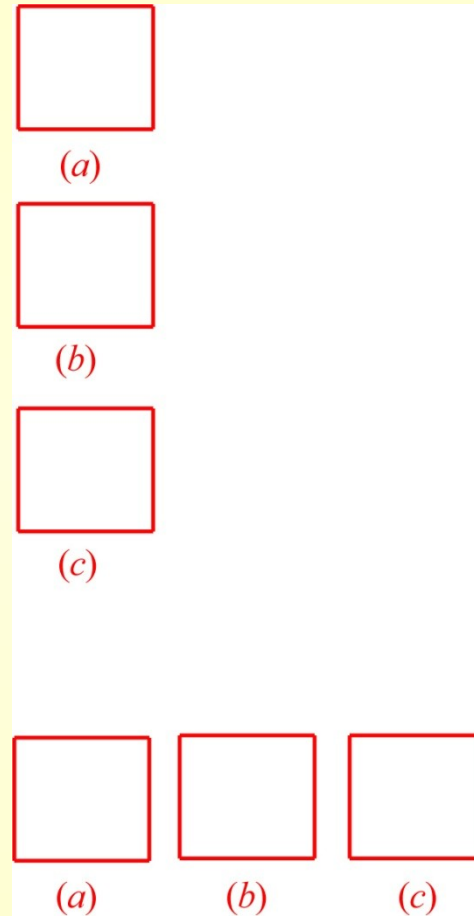
Composite figures



- Parts of figures (a), (b) etc.; labelling should be in 8pt Times and Times Italic at final size
- Ask authors to revise figures if labelling too small

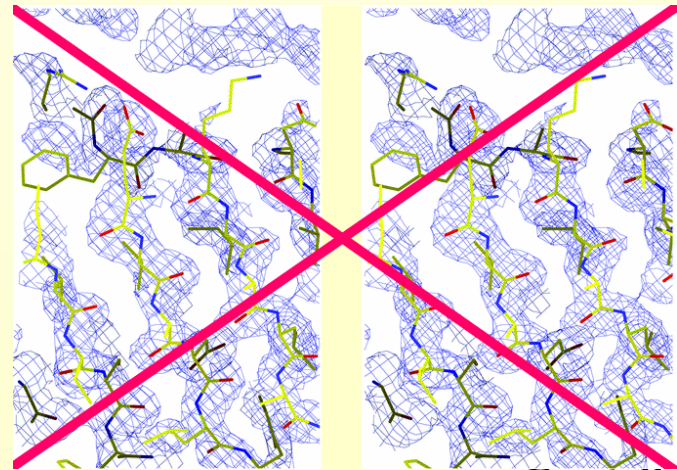
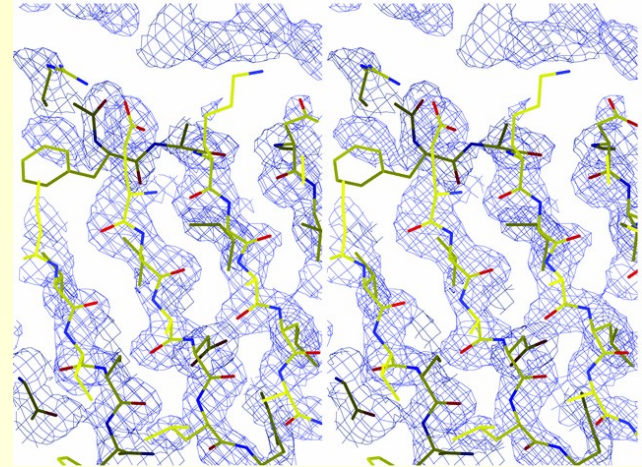
Arrangement of composite figures

- Vertical or horizontal arrangements are OK
- The overall width and height of the journal page should be considered
- Composite figures (together with their caption) should fit on one page – if more space is needed, ask authors to split figure into two
- Large amounts of white space should be avoided



Stereoviews

- Left and right views should be within a single figure
- Atom labelling should be on both left and right views in stereo perspective

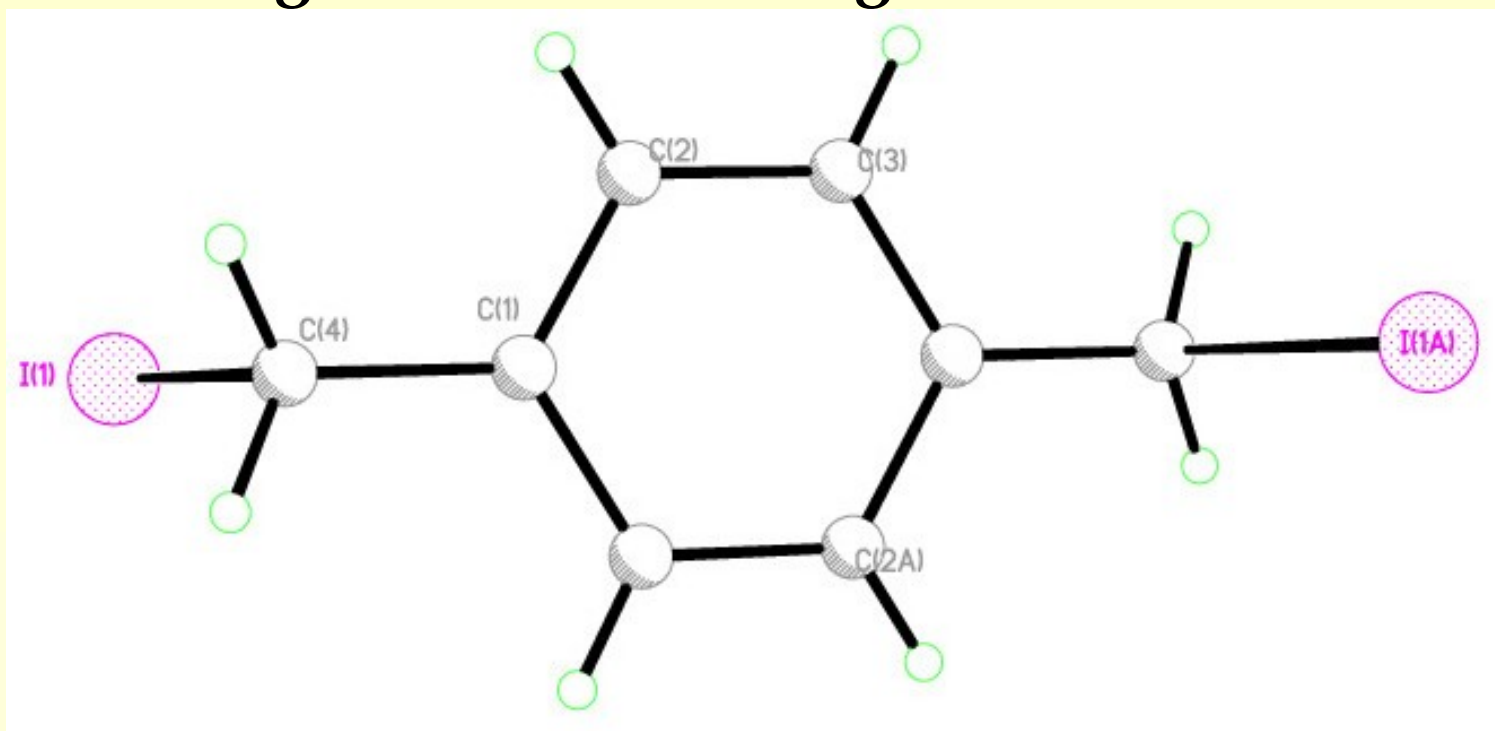





Cropping images

- Images should be cropped before submission
- Information such as 'Figure 1' that will not be part of the final figure should be omitted
- Images should not be boxed
- Labels for parts of a figure should ideally be centred below the figure

Labelling of structural diagrams



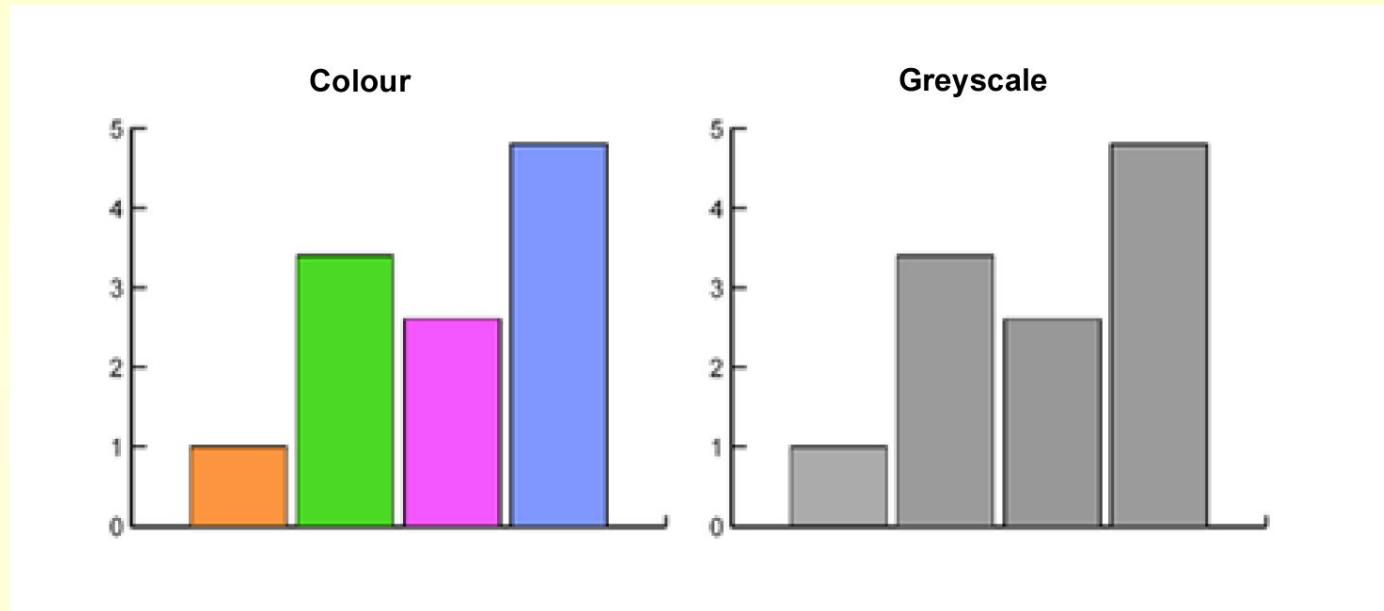
- Atoms should be shown as ellipsoids not spheres
- Atom numbers should usually not be in parentheses
- Atom labels should not intersect with bonds or ellipsoids



Sizing of artwork

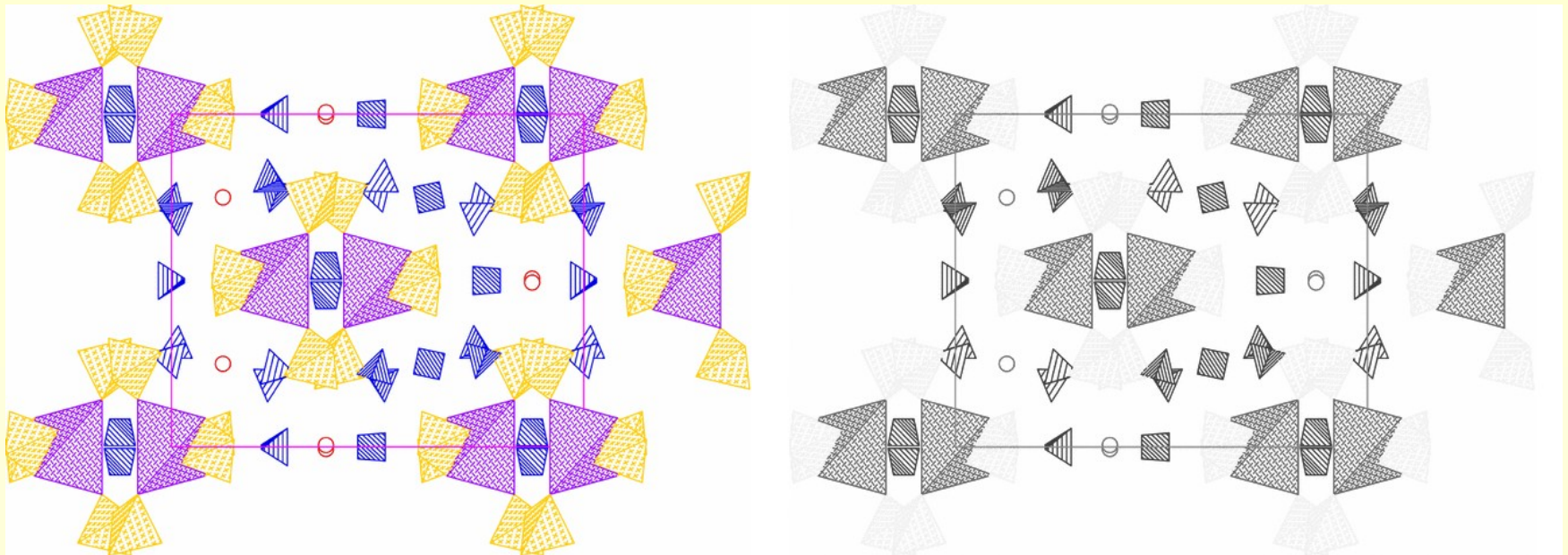
- Most artwork will be sized to fit a single column which is 21.5 picas (8.85 cm) wide
- In exceptional circumstances diagrams will be sized to fit 1.5 columns (12 cm) or double column width (18 cm)
- Submitted artwork should generally be the same size or larger than the published size

Colour and greyscale



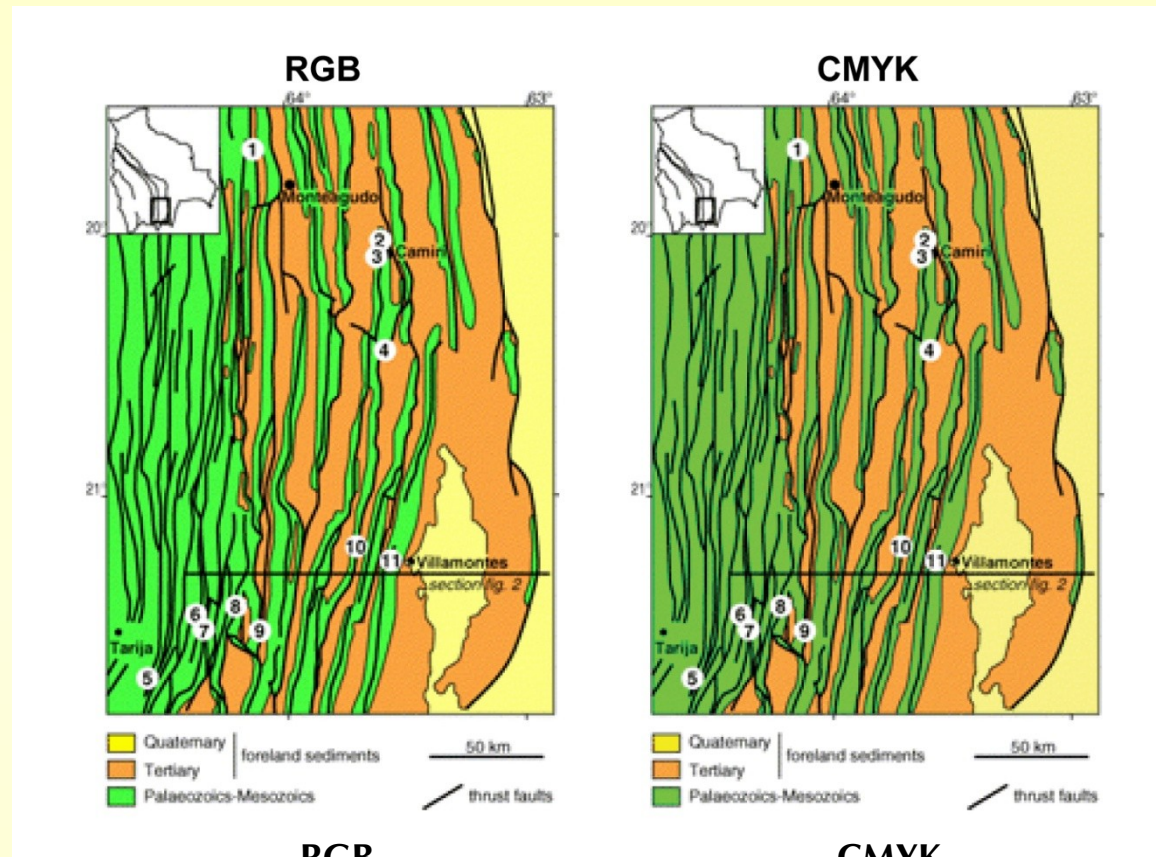
- In the printed journal colour figures may be printed as greyscale, but appear in colour online
- Colours should be distinct when converted

Colour and greyscale



Colours should not disappear when converted – authors to revise figures where pale colours are used

RGB and CMYK colour

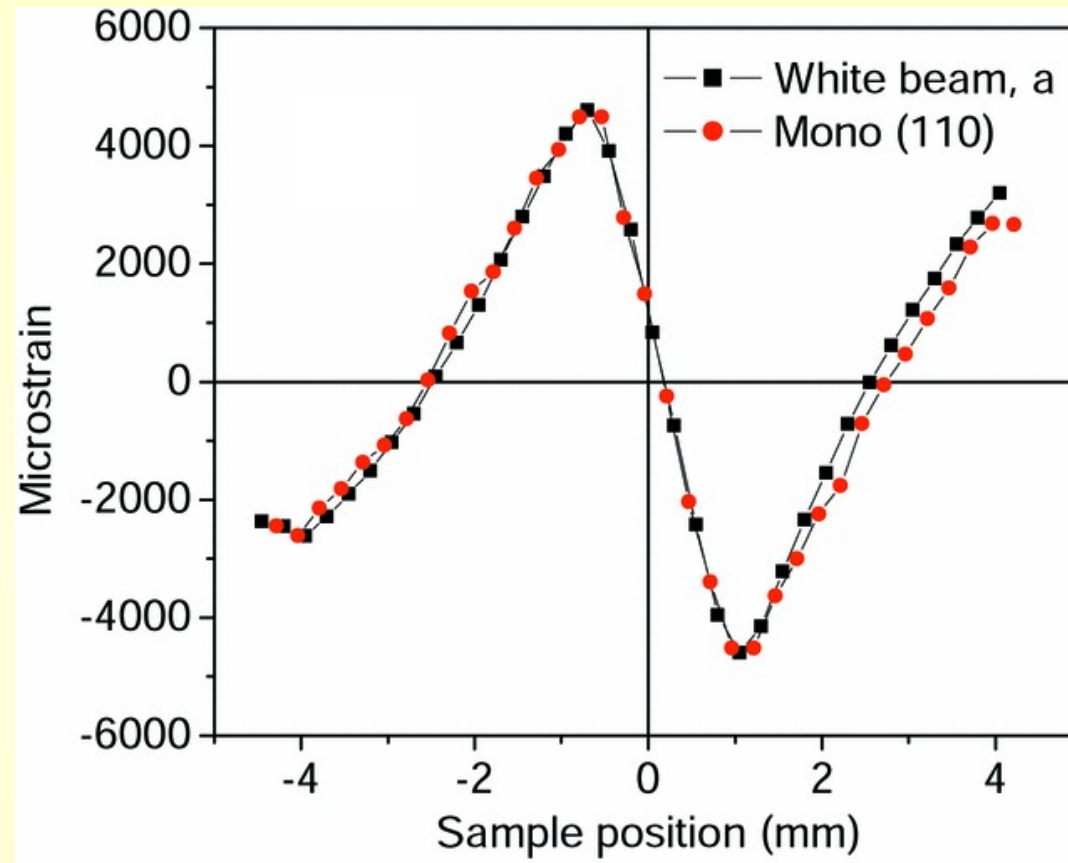


RGB
Red, Green, Blue

CMYK
Cyan, Magenta, Yellow (and Black)

- Colour figures are converted to CMYK for printing
- If accurate colour reproduction is required, figures should be submitted as CMYK

Use of colour



- Colour is expensive to print
- Colour to be used only when absolutely necessary
- Figure captions to be colour independent



Commission on Journals 2011

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| Crystal Structure Communications Online | | current issue back issues sample issue | reader services author services article submission |
| Biological Crystallography Online | | current issue back issues sample issue | reader services author services article submission |
| Structure Reports Online | | current issue back issues sample issue | reader services author services article submission |
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If you have not used this service before, please first read the detailed [online submission instructions](#). Context-sensitive help is available by holding your mouse over underlined text in the submission forms or by clicking on the help icons

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Done

Full submission instructions are available

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submissions home page

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- the text of your article as a single file
- your full contact details
- details of your article
- details of the authors of your article (surnames, forenames and e-mail addresses of all authors)
- high-resolution graphics files for each figure and chemical scheme, and supplementary data (including a CIF and structure factor or Rietveld data files for structural papers), together with any other supplementary files you wish to submit

If you have not used this service before, please first read the detailed [online submission instructions](#). Context-sensitive help is available by holding your mouse over underlined text in the submission forms or by clicking on the help icons

Submission tips can be found by holding your mouse over underlined text [submit your article](#)

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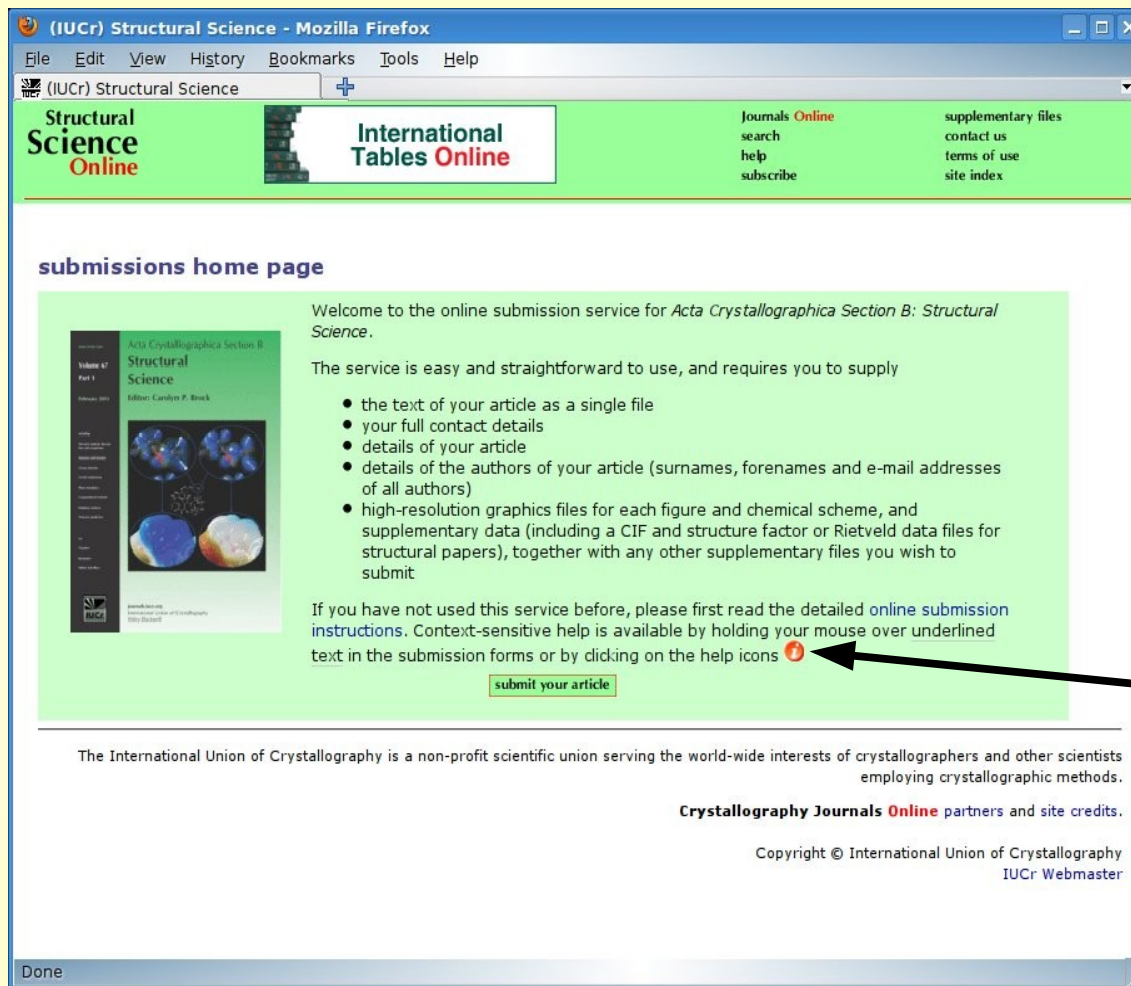
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- Full submission instructions are available
- Submission tips are also available

Getting started



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submissions home page

Welcome to the online submission service for *Acta Crystallographica Section B: Structural Science*.

The service is easy and straightforward to use, and requires you to supply

- the text of your article as a single file
- your full contact details
- details of your article
- details of the authors of your article (surnames, forenames and e-mail addresses of all authors)
- high-resolution graphics files for each figure and chemical scheme, and supplementary data (including a CIF and structure factor or Rietveld data files for structural papers), together with any other supplementary files you wish to submit

If you have not used this service before, please first read the detailed [online submission instructions](#). Context-sensitive help is available by holding your mouse over underlined text in the submission forms or by clicking on the help icons 

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Done

- Full submission instructions are available
- Submission tips are also available
- As is context-sensitive help

What needs to be ready before submission?

- Article text prepared as a single file
- Figures and schemes as separate graphics files
- A CIF for articles reporting a crystal structure
- Structure factor/powder data file for each datablock in the CIF
- Any other supplementary data as separate file
- Full contact details (e-mail address, mailing address, telephone and fax numbers)
- Details of all the authors, including e-mail addresses
- Other details (article title, article category)
- Comments and suggestions for reviewers
- Validation report/mmCIF for macromolecular submissions



Types of files for submission

- WORD or OpenOffice file preferably created using **IUCr template**
- LaTeX (using **IUCr template**)
- Figures as PostScript, encapsulated PostScript or TIFF files, but other formats are supported
- Valid CIF/validation report/mmCIF (for structural papers)
- Structure factor/powder data files in CIF format
- Any other supplementary files

Stage 1

- Contact e-mail address
- Article title
- Category
- **Structural paper?**
- Upload main article text

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http://submissiontest.iucr.org:8600/submit/b

new submission

Stage - 1 - 2 - 3 - 4 - 5 - 6 - 7 - 8
New submission

New submission details

E-mail address*

Repeat e-mail address*

Article title*

Article category

Does your article report a crystal structure?

Upload your article

NB: Do not attempt to upload the same file more than once.
If you experience problems during the file upload please contact support@iucr.org for advice.

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Submission and review

What kinds of file may I submit?

For **submission and refereeing** we require the word processing and other source files for your article to be submitted. The files should be prepared according to the Notes for Authors. You may submit either (a) **WORD** or **OpenOffice** files, or (b) **LaTeX** files.

WORD or OpenOffice submissions:

At **Stage 1**, we require a **WORD** or **OpenOffice** file of the text, tables and figure captions of your article to be uploaded. Note that figures should not be included in this file.

At **Stage 3**, we request you to provide the following source files:

- A high-resolution graphics file in TIFF, PostScript or encapsulated PostScript format for each figure and scheme
- Files of any supplementary material that should accompany your publication

For each source file you will be asked to

- Select the role of the file, its number and part number as applicable
- Locate the file on your local system
- Upload the file

You may overwrite an incorrectly uploaded file by uploading a replacement file with the same role, number and part number.

Once you have uploaded all your files, you should CONTINUE to the next stage. All files, including graphics files, will be automatically converted into a **PDF review document** by the submission system. If for any reason the submission system is unable to convert your source files to PDF, you may be asked to upload a PDF at the end of **Stage 3**.

LaTeX submissions

(IUCr) Notes for authors 2010 - Mozilla Firefox

international union of crystallography

Notes for authors 2010

Keywords: Notes for authors.

1. Scientific scope

Section B of *Acta Crystallographica* publishes papers in which structure is the primary focus of the work reported. The central themes of *Section B* are the acquisition of structural knowledge from novel experimental observations or from existing data, the correlation of structural knowledge with physico-chemical and other properties, and the application of this knowledge to solve problems in the structural domain. *Section B* has broad chemical coverage, encompassing metals and alloys, inorganics and minerals, metal-organics and purely organic compounds. Biological, particularly macromolecular, structural science is covered by *Sections D and F*. A more complete definition of scientific scope is given in an Editorial [*Acta Cryst.* (1994), B50, 1-3].

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

Stage 2

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article details

Your file has been received.

Stage - 1 - **2** - 3 - 4 - 5 - 6 - 7

Article details

1. Contact author details

E-mail address*

Repeat e-mail address*

Title

First name(s)*

Surname*

Name qualifier (e.g. Jr, III)

Department

Organization

Street/PO Box*

City*

State/province /country

Post/zip code

Country*

Telephone*

Fax*

2. Details of the article

Article title*

Authors (one per line, in article order; please indicate the contact author)

What does the overall submission and review procedure involve?

The overall procedure involves six stages:

- **Stage 1**
You will be asked to provide your e-mail details and the article title, and to select your article also be asked to upload a **single** file of the text of your article. Details of the file required are
 - **Stage 2**
You will be asked to give further details of your article (see [above](#)).
 - **Stage 3**
You will be asked to upload graphics files and supplementary data for your article (see [below](#)) should only click on the **CONTINUE** button when you have uploaded all relevant files and have a **review document**.
 - **Stage 4**
You will be invited to select a Co-editor, from a list of those available, to coordinate the review. Comments concerning your article and details of possible referees should be typed into the sp
 - **Stage 5**
A PDF review document is generated from the file(s) you submit and you will be provided with accessing and viewing this document.
- Once your review document is created, the system will assign a Co-editor to your article. You contact details of this Co-editor and a **Co-editor reference code**. The reference code has two digits (e.g. au0165) and should be quoted in all subsequent communications with the Co-editor Office. **You should keep a record of the web address for viewing your article and the Co-editor article.**
- The Co-editor will arrange for the review of your article and will inform you by e-mail of the ou review. You may be asked to submit revised versions of your article (see [below](#)). **Please note should only be submitted at the request of the Co-editor handling your article.**
- **Stage 6**
Your submission is now complete and you will be returned to the home page for your article. If you submit a covering letter at this stage, it may be uploaded using the **contact co-editor** tab.

[Back to contents](#)

Done

Confirmation of receipt of file

Stage 2

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article details

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Stage - 1 - **2** - 3 - 4 - 5 - 6 - 7

Article details

1. Contact author details

E-mail address*

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- **Stage 1**
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- **Stage 2**
You will be asked to give further details of your article (see above).
- **Stage 3**
You will be asked to upload graphics files and supplementary data for your article (see below) should only click on the **CONTINUE** button when you have uploaded all relevant files and have a **review document**.
- **Stage 4**
You will be invited to select a Co-editor, from a list of those available, to coordinate the review. Comments concerning your article and details of possible referees should be typed into the space provided.
- **Stage 5**
A PDF review document is generated from the file(s) you submit and you will be provided with a link to access and view this document.
- **Stage 6**
Your submission is now complete and you will be returned to the home page for your article. If you submit a covering letter at this stage, it may be uploaded using the **contact co-editor** tab.

Once your review document is created, the system will assign a Co-editor to your article. You will be provided with the contact details of this Co-editor and a **Co-editor reference code**. The reference code has two digits (e.g. au0165) and should be quoted in all subsequent communications with the Co-editor. **You should keep a record of the web address for viewing your article and the Co-editor reference code.**

The Co-editor will arrange for the review of your article and will inform you by e-mail of the progress of the review. You may be asked to submit revised versions of your article (see below). **Please note that revised articles should only be submitted at the request of the Co-editor handling your article.**

Back to contents

Done

- Confirmation of receipt of file
- E-mail sent to author confirming receipt of file
- Tracking number quoted

paper details - Mozilla Firefox <2>

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paper details

forward reply

To: jmc61@cam.ac.uk
From: jb@iucr.org
Subject: Receipt of your submission to Acta Crystallographica Section B
Date: 2011-06-09 16:48:07 +0100
*** RECEIPT OF SUBMISSION TO ACTA CRYSTALLOGRAPHICA SECTION B ***

9 June 2011

Dear Author

Thank you for submitting your article entitled:
Molecular origins of commercial laser dye functionality in azacoumarins and quinolones: LD 425, LD 489 and LD 473
for publication in Acta Crystallographica Section B. It has been assigned the following web address:
http://submission.iucr.org/submit/b/review_address/X1Q8fOIFme3Ps44_/t065344

IMPORTANT - Please make a careful note of this web address, as you will need it throughout the review process.

To complete your submission (if you have not already done so), please fill out the additional details and upload any source files including a CIF if this is a structural paper. The files should include

(a) a single file in Word, RTF or LaTeX format of the text, tables and figure captions of your article,
(b) a high-resolution graphics file in TIFF, PostScript or encapsulated PostScript format for each figure and scheme, and

Potential problems

- Title and main article text file are checked against previous submissions in our database
- For journals other than Sections C and E, an **exact duplication** of the title or main article text file with one previously submitted will cause the system to ask the author to contact support rather than continuing with the submission
- Software is used to check all uploaded file types - this can occasionally not identify a file type correctly (e.g. where the file starts with comments) resulting in problems uploading files

Stage 2, continued

- Enter article details
- Enter e-mail address for each author
- Enter abstract

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(IUCr) article details

Stage - 1 - **2** - 3 - 4 - 5 - 6 - 7 - Article details

1. Contact author details

E-mail address*

Repeat e-mail address*

Title

First name(s)*

Surname*

Name qualifier (e.g. Jr, III)

Department

Organization

Street/PO Box*

City*

State/province /county

Post/zip code

Country*

Telephone*

Fax*

2. Details of the article

Article title*

Authors (one per line, in article order; please indicate the contact author)

| Contact author* | First name(s) | Surname* | E-mail address |
|----------------------------------|---------------|----------|-----------------|
| <input checked="" type="radio"/> | Carolyn P. | Brock | cpbrock@uky.edu |
| <input type="radio"/> | Xiaogang | Liu | xl316@cam.ac.uk |
| <input type="radio"/> | Jacqueline | Cole | jmc61@cam.ac.uk |
| <input type="radio"/> | Paul G. | Waddell | pgw27@cam.ac.uk |
| <input type="radio"/> | | | |
| <input type="radio"/> | | | |
| <input type="radio"/> | | | |
| <input type="radio"/> | | | |
| <input type="radio"/> | | | |
| <input type="radio"/> | | | |

Add more authors

Language

Abstract (please paste your abstract into the form below)

The molecular structures of three compounds, LD 425 (C13H14N(C15H15F3N2O2) and LD 473 (C17H19F3N2O), are determined by single-crystal X-ray diffraction. LD 425 and LD 489 possess para-quinoidal bond distance patterns in the benzene rings due to inter-ring charge transfer (IRCT) from these rings to the adjoining ring. The chemical substitution of the coumarin single-bonded O with N, to form a quinolone, results in the suppression of this IRCT effect. Instead, intra-ring charge transfer is shown to become more

Continue

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What should I do if I do not have the e-mail address of a co-author?

During submission you will be asked to provide e-mail addresses for all authors. These addresses will be used to inform your co-authors that the article has been submitted. In some cases, e.g. where a co-author is a student who is no longer at your institution, it may be difficult to provide an e-mail address. If you are unable to find an address for a coauthor, you may substitute your e-mail address when filling out the form at Stage 2 of the submission.

[Back to contents](#)

What should I do if I get stuck?

You will find detailed help links throughout the submission pages, and you can use any of these links without stopping the submission. If you are having more serious problems, you should contact support@iucr.org.

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Stage 2, continued

- Must complete fields marked with asterisks

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(IUCr) article details

article details

Error: Please supply your street address or PO Box number!
Please try again

Stage - 1 - **2** - 3 - 4 - 5 - 6 - 7 - 8
Article details

1. Contact author details

E-mail address*

Repeat e-mail address*

Title

First name(s)*

Surname*

Name qualifier (e.g. Jr, III)

Department

Organization

Street/PO Box*

City*

State/province /county

Post/zip code

Country*

Telephone*

Fax*

2. Details of the article

Article title*

Authors (one per line, in article order; please indicate the contact author)

| Contact author* | First name(s) | Surname* | E-mail address |
|----------------------------------|---|--------------------------------------|--|
| <input checked="" type="radio"/> | <input type="text" value="Carolyn P."/> | <input type="text" value="Brock"/> | <input type="text" value="cpbrock@uky.edu"/> |
| <input type="radio"/> | <input type="text" value="Xiaogang"/> | <input type="text" value="Liu"/> | <input type="text" value="xl316@cam.ac.uk"/> |
| <input type="radio"/> | <input type="text" value="Jacqueline"/> | <input type="text" value="Cole"/> | <input type="text" value="jmc61@cam.ac.uk"/> |
| <input type="radio"/> | <input type="text" value="Paul G."/> | <input type="text" value="Waddell"/> | <input type="text" value="pgw27@cam.ac.uk"/> |

Language

Abstract (please paste your abstract into the form below)

The molecular structures of three compounds, LD 425 (C13H14N2O3), LD 489 (C15H15F3N2O2) and LD 473 (C17H19F3N2O), are determined by single-crystal X-ray diffraction at 180 K. Azacoumarins LD 425 and LD 489 possess para-quinoidal bond distance patterns in their benzene rings due to inter-ring charge transfer (IRCT) from these rings to the adjoining ring. In contrast, chemical substitution of the coumarin single-bonded O with N, to form a quinolone, results in the suppression of this IRCT effect. Instead, intra-ring charge transfer is shown to become more pronounced. Such

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Stage -1-2-**3**-4-5-6-7-8
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Molecular origins of commercial laser dye functionality in azacoumarins and quinolones

Carolyn P. Brock*, Xiaogang Liu, Jacqueline Cole and Paul G. Waddell [Modify these details](#)

upload submission | **upload enhanced figure**

Current version 26 July 2011 10:25:41 BST [Upload source files](#)

Review document (PDF) Tue Jul 26 10:49:45 2011

Abstract More...

The following files have been deposited for this submission

| Name | Component | Size | Upload time |
|---------------------|--------------|--------|---|
| t050607_source.docx | Article body | 114744 | Tue Jul 26 10:25:41 2011 Delete |

Upload your source files for this submission ⓘ

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3. Click on the 'Upload file' button

revised Word file
 figure Figure number
 scheme Scheme number
 cif
 supplementary material ⓘ

File name on your local filesystem:

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Stage 3

- All other files (e.g. Figures, Schemes, structural and supplementary data) can now be uploaded

FIGURE UPLOAD

- Click on figure
- Choose figure number and part
- Select file on your system to upload
- Click on upload file

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Stage - 1 - 2 - 3 - 4 - 5 - 6 - 7 - 8
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Molecular origins of commercial laser dye functionality in azacoumarins and quinolones

Carolyn P. Brod*, Xiaogang Liu, Jacqueline Cole and Paul G. Waddell [Modify these details](#)

upload submission | **upload enhanced figure**

Create an enhanced figure

Figure number:

Type of structure:

Use structural CIF already uploaded: (check to select this option)

or upload CIF from your local filesystem:

or upload external entry: (supply PDB or other database code)

or transfer enhanced figure from presubmission:
(paste presubmission URL)

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File Edit View History Bookmarks Tools Help

(IUCr) Jmol enhanced figure toolkit

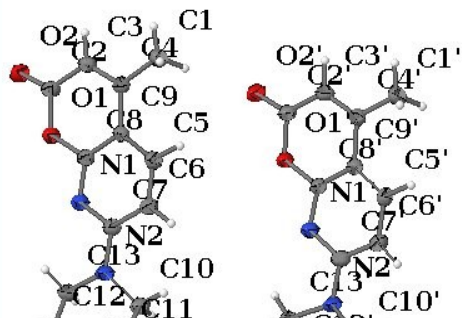
oolkit 1.0 beta2: **Figure 10** [Return to submission page](#) Powered by Jmol

preview | model | select/label | scripts | captions | about

Enhanced figure

These buttons (and one to show the static image) will always appear on your enhanced figure. Your additional scripts will be listed below.

The three-dimensional structure may be explored in this enhanced view.



Stage 3, continued

ENHANCED FIGURES

- Toolkit allows easy creation and editing of interactive Jmol figures
- Generate from CIF associated with article
- Upload a new CIF
- Supply a database code
- Import a previously prepared enhanced figure

Stage 3, continued

CORRECTING MISTAKES

- If wrong file uploaded just reupload and file will be overwritten
- Only use delete to remove no longer required files
- Figure ordering can be corrected

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Abstract More...

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| Name | Component | Size | Upload time |
|-------------------------------------|--------------|----------|---------------------------------|
| t050607_source.docx | Article body | 114744 | Tue Jul 26 10:25:41 Delete 2011 |
| t050607fig1.ps | Figure | 16448 | Tue Jul 26 10:53:04 Delete 2011 |
| t050607fig2.ps | Figure | 10807510 | Tue Jul 26 10:54:26 Delete 2011 |
| t050607fig3.ps | Figure | 12181330 | Tue Jul 26 10:55:20 Delete 2011 |
| t050607fig4.ps | Figure | 12593502 | Tue Jul 26 10:56:35 Delete 2011 |
| t050607fig5.ps | Figure | 62880 | Tue Jul 26 10:57:50 Delete 2011 |
| t050607fig6.ps | Figure | 21167 | Tue Jul 26 10:58:21 Delete 2011 |
| t050607fig7.ps | Figure | 7985884 | Tue Jul 26 10:59:04 Delete 2011 |
| t050607fig8.ps | Figure | 33479 | Tue Jul 26 11:01:36 Delete 2011 |
| t050607fig9.ps | Figure | 25455 | Tue Jul 26 11:02:06 Delete 2011 |

Upload your source files for this submission ⓘ

For each file you wish to upload,

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Done

Stage 3, continued

CORRECTING MISTAKES

- If wrong file uploaded just reupload and file will be overwritten
- Only use delete to remove no longer required files
- Figure ordering can be corrected

The screenshot displays the IUCr online submission interface. At the top, a browser window titled '(IUCr) Upload source files - Mozilla Firefox' shows the 'Current version' section with a 'Review document (PDF)' button. Below this, a 'change figure order' dialog box is open, showing a table of graphical files available for the submission. The table has columns for Name, Component, Image number, and New Figure number. The files listed are t050611fig1.ps, t050611fig2.ps, and t050611fig3.ps. The dialog box also includes a 'Change ordering of figures' button and a 'Cancel' button. In the background, the main submission page is visible, showing a list of uploaded files with columns for Name, Component, Image number, and Upload time. The files listed are t050607fig8.ps and t050607fig9.ps. The 'Change ordering of figures' button on the main page is circled in red. Below the file list, there is a section titled 'Upload your source files for this submission' with instructions for uploading files.

| Name | Component | Image number | New Figure number | New Figure part |
|----------------|-----------|--------------|-------------------|-----------------|
| t050611fig1.ps | Figure | 1 | 1 | |
| t050611fig2.ps | Figure | 2 | 2 | |
| t050611fig3.ps | Figure | 3 | 3 | |

| Name | Component | Image number | Upload time |
|----------------|-----------|--------------|---------------------|
| t050607fig8.ps | Figure | 33479 | Tue Jul 26 11:01:36 |
| t050607fig9.ps | Figure | 33455 | Tue Jul 26 11:02:06 |

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For each file you wish to upload,

1. Select the role of the file, its number and part number as applicable
2. Locate the file on your local system using the 'Browse' button
3. Click on the 'Upload file' button

Stage 3, continued

**STRUCTURAL PAPER =
yes (small molecule
structures)**

- You will be requested to upload a CIF
- CIF will not upload if file does not pass syntax checks

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File Edit View History Bookmarks Tools Help

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| | | | | | |
|--|-----------------------|--------|----------|--------------------------|--------|
| | t050607fig4.ps | Figure | 12593502 | Tue Jul 26 10:56:35 2011 | Delete |
| | t050607fig5.ps | Figure | 62880 | Tue Jul 26 10:57:50 2011 | Delete |
| | t050607fig6.ps | Figure | 21167 | Tue Jul 26 10:58:21 2011 | Delete |
| | t050607fig7.ps | Figure | 7985884 | Tue Jul 26 10:59:04 2011 | Delete |
| | t050607fig8.ps | Figure | 33479 | Tue Jul 26 11:01:36 2011 | Delete |
| | t050607fig9.ps | Figure | 25455 | Tue Jul 26 11:02:06 2011 | Delete |

Change ordering of figures

Upload your source files for this submission ⓘ

For each file you wish to upload,

1. Select the role of the file, its number and part number as applicable
2. Locate the file on your local system using the 'Browse' button
3. Click on the 'Upload file' button

revised Word file

figure

scheme

cif

supplementary material ⓘ

Figure number Part

Scheme number

File name on your local filesystem: Browse

Upload file

I have uploaded all my files - CONTINUE to next stage

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Should I submit supplementary data?

If your article describes a crystal structure study, a CIF (Crystallographic Information File) containing the crystallographic data for all the reported structures will be required for the review process. You will be asked to upload your CIF during the submission procedure. You should ensure that at least a **basic structural check** is run on the final version of your CIF prior to submission. Also, a separate structure factor or Rietveld data file in CIF format should be submitted for each structure reported. Other supplementary materials (e.g. videos) may be submitted; for a full list of allowed file types, click [here](#).

Supplementary material which is for "review only" can be uploaded in the same way as regular supplementary material but it should be made clear on the first page of the material that it is for review only and not for publication.

[Back to contents](#)

What do I need to do about copyright?

When your article has been successfully uploaded, a Co-editor reference code assigned and a PDF review document created, you will be sent an e-mail to confirm that your article has entered the review stage. You will also be sent a **Transfer of Copyright agreement**. You should complete and sign this agreement and return it to the Editorial Office by e-mail (copyright@iucr.org). The e-mail should include the Co-editor reference code in the Subject line.

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(IUCr) Upload source files

| Thumbnail | Filename | Type | ID | Date | Action |
|-----------|----------------|--------|----------|--------------------------|--------|
| | t050607fig4.ps | Figure | 12593502 | Tue Jul 26 10:56:35 2011 | Delete |
| | t050607fig5.ps | Figure | 62880 | Tue Jul 26 10:57:50 2011 | Delete |
| | t050607fig6.ps | Figure | 21167 | Tue Jul 26 10:58:21 2011 | Delete |
| | t050607fig7.ps | Figure | 7985884 | Tue Jul 26 10:59:04 2011 | Delete |
| | t050607fig8.ps | Figure | 33479 | Tue Jul 26 11:01:36 2011 | Delete |
| | t050607fig9.ps | Figure | 25455 | Tue Jul 26 11:02:06 2011 | Delete |

Change ordering of figures

Upload your source files for this submission

For each file you wish to upload,

1. Select the role of the file, its number and part number as applicable
2. Locate the file on your local system using the 'Browse' button
3. Click on the 'Upload file' button

revised Word file
 figure
 scheme
 cif
 structure factors
 powder diffraction data
 other supplementary material

Structure factors, powder diffraction data and other supplementary material may also be uploaded.

Datablock: Id473

Figure number: Part:
 Scheme number:

File name on your local filesystem:

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Done

Stage 3, continued

**STRUCTURAL PAPER =
yes (small molecule
structures)**

- Structure-factor files should be uploaded for each datablock in the CIF
- Datablocks from CIF are listed to allow selection when uploading structure factors or powder data files

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Molecular origins of commercial laser dye functionality in azacoumarins and quinolones

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0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check
  
```

Datablock: ld473

Bond precision: C-C = 0.0022 Å Wavelength=0.71073
 Cell: a=12.1853(5) b=12.2242(4) c=10.6361(3)
 alpha=90 beta=93.4529(11) gamma=90
 Temperature: 180 K

| | Calculated | Reported |
|------------------------|-----------------|-----------------|
| Volume | 1581.43(9) | 1581.43(9) |
| Space group | P 21/c | P2(1)/c |
| Hall group | -P 2ybc | -P 2ybc |
| Moiety formula | C17 H19 F3 N2 O | C17 H19 F3 N2 O |
| Sum formula | C17 H19 F3 N2 O | C17 H19 F3 N2 O |
| Mr | 324.34 | 324.34 |
| Dx, g cm ⁻³ | 1.362 | 1.362 |
| Z | 4 | 4 |
| Mu (mm ⁻¹) | 0.110 | 0.110 |
| F000 | 680.0 | 680.0 |
| F000' | 680.41 | |
| h,k,lmax | 15,15,13 | 15,15,13 |
| Nref | 3617 | 3601 |
| Tmin,Tmax | 0.979,0.987 | 0.943,0.989 |
| Tmin' | 0.965 | |

Correction method= MULTI-SCAN
 Data completeness= 0.996
 Theta(max)= 27.460
 R(reflections)= 0.0482(2179) wR2(reflections)= 0.1230(3601)
 S = 0.996 Npar= 284

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database duplication summary

Datablock: Id425_180k_22apr2011int4

- Chemical name = LD 425
- R factor = 0.061
- Space group = P2(1)/c
- Formula = C13 H14 N2 O3
- a=7.059 b=24.497 c=13.914
- alpha=90 beta=103.559 gamma=90

Datablock: Id473

- Chemical name = LD 473
- R factor = 0.048
- Space group = P2(1)/c
- Formula = C17 H19 F3 N2 O
- a=12.1853 b=12.2242 c=10.6361
- alpha=90 beta=93.4529 gamma=90

Datablock: Id489

- Chemical name = LD 489
- R factor = 0.049
- Space group = P_21/c
- Formula = C15 H15 F3 N2 O2
- a=8.9941 b=11.2954 c=14.3536
- alpha=90 beta=102.537 gamma=90

DATABLOCK: Id473

- Chinnakali, K., Sivakumar, K., Natarajan, S., McGuire, N. K. & Clearfield, A. (1991). *Acta Cryst. C* **47**, 561-563 [details](#)
- [Cell: 10.694,12.216,12.356(90,94.24,90) R=4.4 T=Room Temp.(283-303)]

Datablock Id425_180k_22apr2011int4 - ellipsoid plot

76 Y

NOMOVE FORCED

Prob = 50
Temp = 180

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Datablock ld473 - ellipsoid plot

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PLATON-Aug 2 09:30:40 2011 - (180711)

Z -52 ld473 P2(1)/c R = 0.05 RES= 0 -176 X

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STRUCTURAL PAPER =
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EDS summary for PDB entry 2xq1.

The following statistics were obtained using the structure factors deposited for your PDB entry, using a customised version of the Uppsala Electron Density Server (EDS) running at PDBe. More information about EDS and the output presented here can be found on the original EDS site (<http://eds.bmc.uu.se>).

| | |
|---|--|
| Resolution | |
| Resolution from map-calculations (low) | 19.99Å |
| Resolution from map-calculations (high) | 2.90Å |
| Resolution from PDB header | 2.90Å |
| R-factors | |
| R-factor for map | 0.188 |
| R-factor from PDB header | 0.191 |
| Free R-factor from PDB header | 0.223 |
| Structure quality | |
| Average Real space R-factor (Deviation) | 0.163 (0.061) |
| Average Real-space correlation coefficient (Deviation) | 0.947 (0.041) |
| Average Occupancy-weighted avg temperature factor (Deviation) | 43.0Å ² (15.3Å ²) |
| Padilla-Yeates statistics | |
| Padilla-Yeates < L > | 0.457 |
| Padilla-Yeates <L ² > | 0.283 |
| Wilson statistics | |

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| | Microsoft Word (DOC) file | application/msword | |
| | Microsoft Word (DOCX) file | application/vnd.openxmlformats-officedocument.wordprocessingml.document | |
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






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Professor E.V. BOLDYREVA (high pressures; organic solids; hydrogen bonds; crystal engineering; low temperatures; reactivity of solids)

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Dr D.L. DORSET (electron crystallography; linear chain assemblies (waxes, polymers,lipids); zeoform materials)

Suggestions for referees

Referees (one per line)

| First name(s) | Surname* | E-mail address |
|----------------------|----------------------|----------------------|
| Jillian | Bradshaw | jb@iucr.org |
| Peter | Strickland | ps@iucr.org |
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Molecular origins of commercial laser dye functionality in azacoumarins and quinolones: LD 425, LD 489 and LD 473

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This is to inform you as a Co-author that the following article:

Title: Molecular origins of commercial laser dye functionality in azacoumarins and quinolones: LD 425, LD 489 and LD 473
 Author(s): Xiaogang Liu, Jacqueline M Cole* and Paul G Waddell
 Contact author: Professor Jacqueline Cole
 Contact e-mail: jmc61@cam.ac.uk
 Reference: BK5105

Abstract: The molecular structures of three compounds, LD 425 (C₁₃H₁₄N₂O₃), LD 489 (C₁₅H₁₅F₃N₂O₂) and LD 473 (C₁₇H₁₉F₃N₂O), are determined by single-crystal X-ray diffraction at 180 K. Azacoumarins LD 425 and LD 489 possess para-quinoidal bond distance patterns in their benzene rings due to inter-ring charge transfer (IRCT) from these rings to the adjoining ring. In contrast, chemical substitution of the coumarin single-bonded O with N, to form a quinolone, results in the suppression of this IRCT effect. Instead, intra-ring charge transfer is shown to become more pronounced. Such charge transfer trends are present in many quinolones including LD 473. Resonance theory is used to explain these bond pattern changes and assisted spectral blue shifts in relation to their coumarin analogues. The application of this theory offers an effective and intuitive understanding of the structure-property relationship in azacoumarins and quinolones. Such understanding is important for recognising the reaction mechanisms in these compounds such that new laser dyes can be designed with desired spectral shifts.

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The article (reference: BK5105)

Molecular origins of commercial laser dye functionality in azacoumarins and quinolones: LD 425, LD 489 and LD 473

Author(s): Xiaogang Liu, Jacqueline M Cole* and Paul G Waddell
Contact author: Professor Jacqueline Cole
Contact e-mail: jmc61@cam.ac.uk
Paper type: research papers
Received: Thu 9 June 17:14:23 2011

has been submitted to Acta Crystallographica Section B and is now available from the IUCr web server for review.

The author has indicated that this article includes a crystal structure report; the CIF and a ched.CIF report are also available from the web address below.

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Jill Bradshaw
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Gyöngyi Wang*, Jian Li, Robert D. Hart, Arie van Riessen and Robbie McDonald

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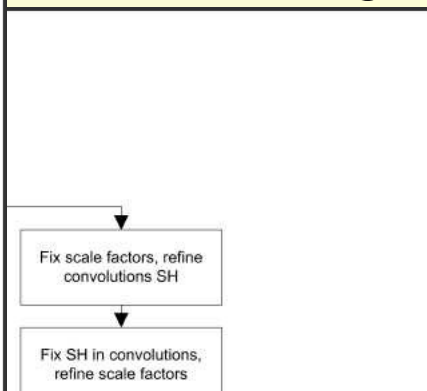
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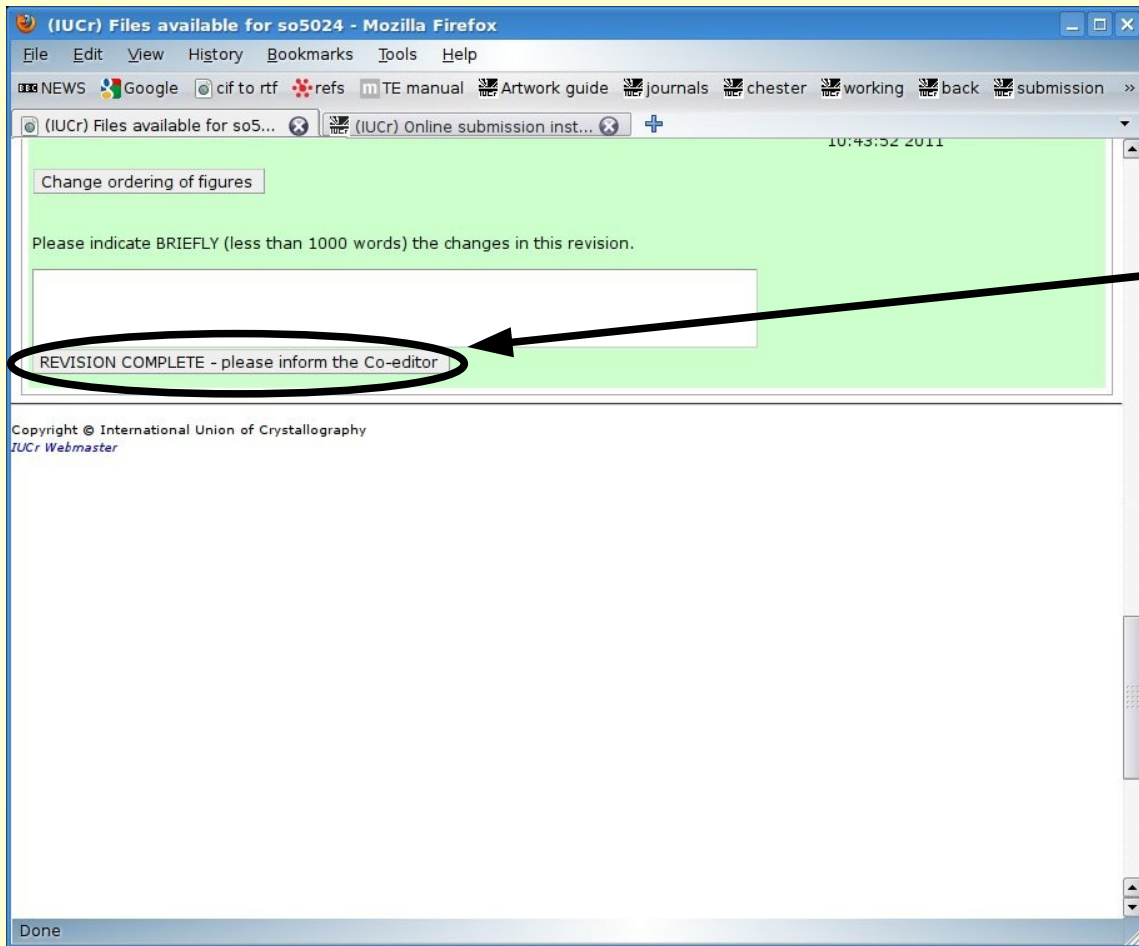
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Author revisions

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contact the co-editor

Stage -1-2-3-4-5-6-7- Article review page

Molecular origins of commercial laser dye functionality in azacoumarins and quinolones

Carolyn P. Brock*, Xiaogang Liu, Jacqueline Cole and Paul G. Waddell

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Dear Dr Dorset,

I am writing to you concerning my paper (dr5023).

Best wishes

Professor Carolyn P. Brock

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E-mail address* cpbrock@uky.edu

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Title Professor

First name(s)* Carolyn P.

Surname* Brock

Name qualifier (e.g. Jr, III)

Department Department of Chemistry

Organization University of Kentucky

Street/PO Box* Lexington

City* Kentucky

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Post/zip code 40506-0055

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