2013
international year of crystallography

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

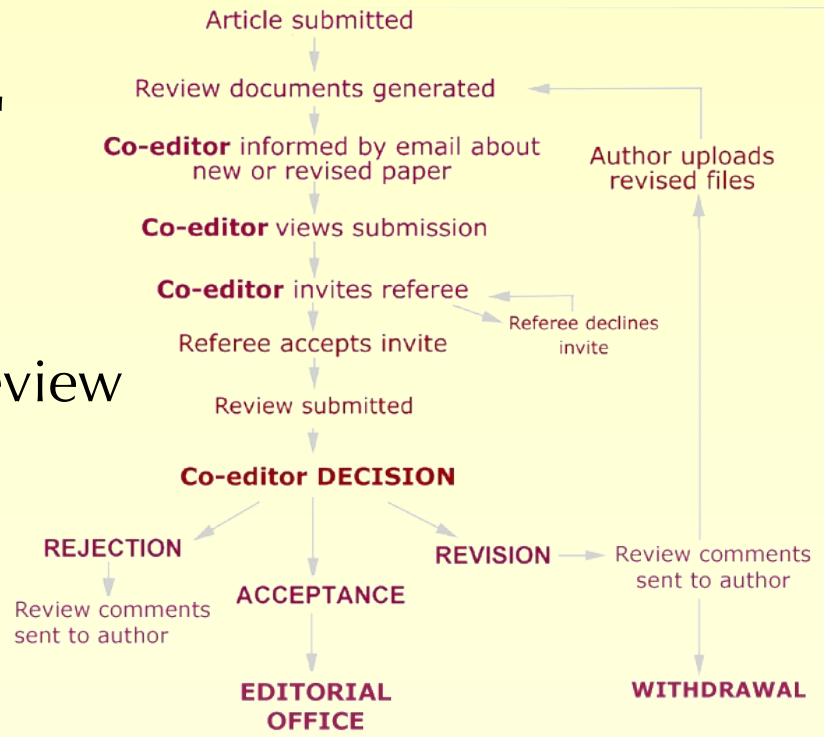
17 editorial, production
and R&D staff work in Chester

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



PLEASE ASK QUESTIONS THROUGHOUT

Crystallography Journals Online

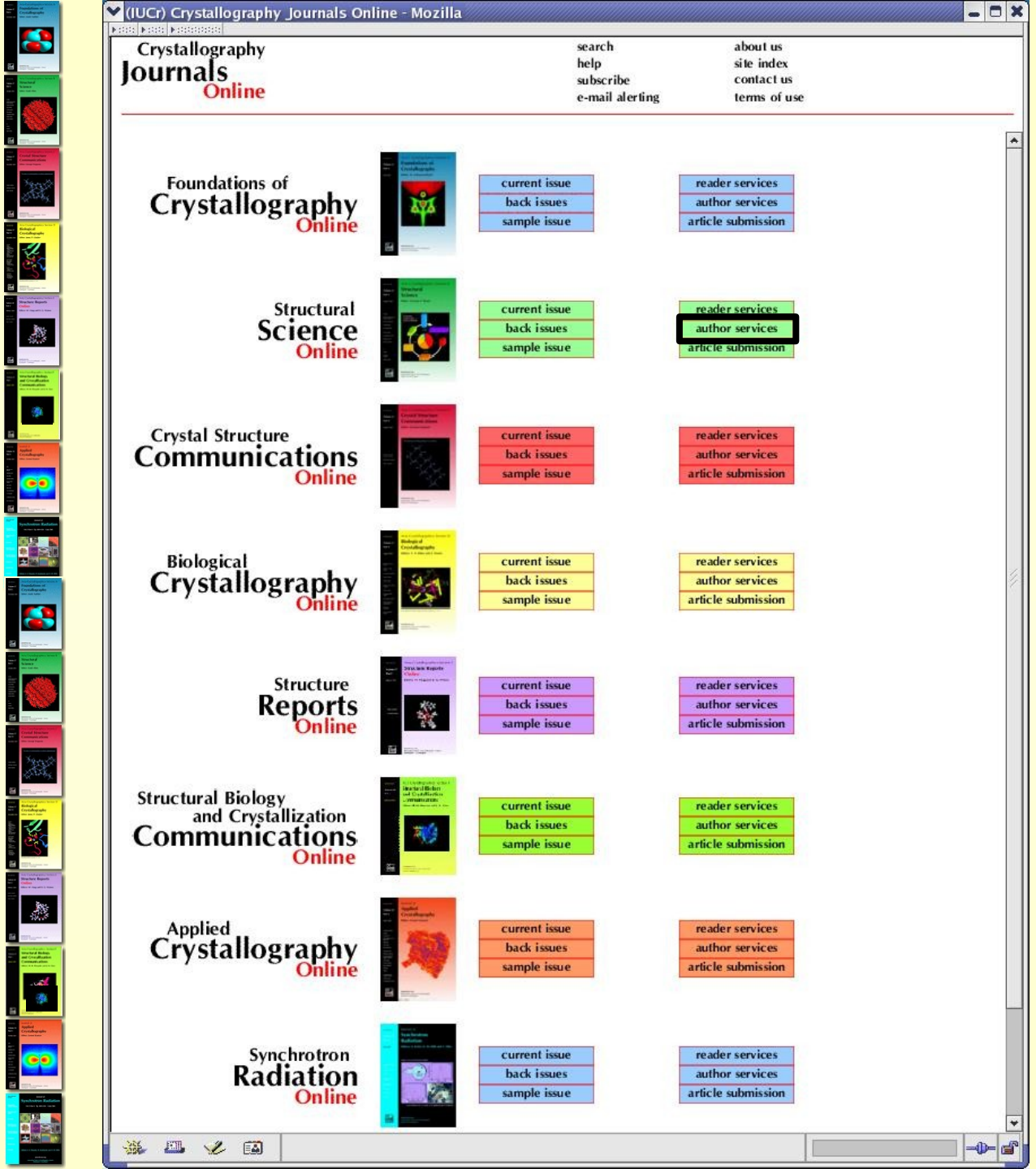
2013
international year of crystallography

Commission on Journals 2011

Submission to publication

IUCr templates and tools

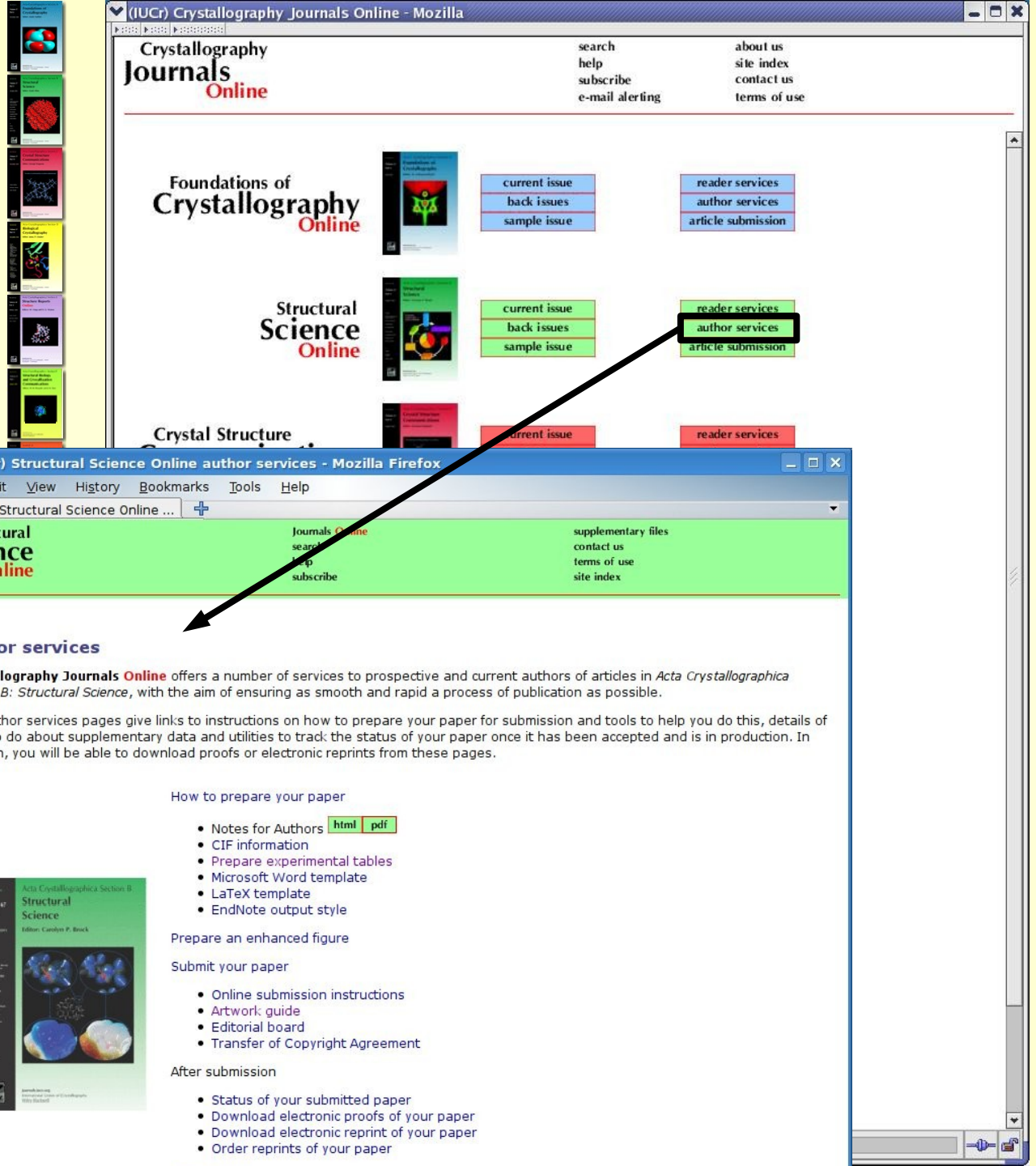
Crystallography Journals Online



Tools and author information available from

- journals.iucr.org
- author services

Crystallography Journals Online



Links include

- WORD template
- LaTeX template
- CIF information
- How to prepare experimental tables from CIF
- publBio

Crystallography Journals Online

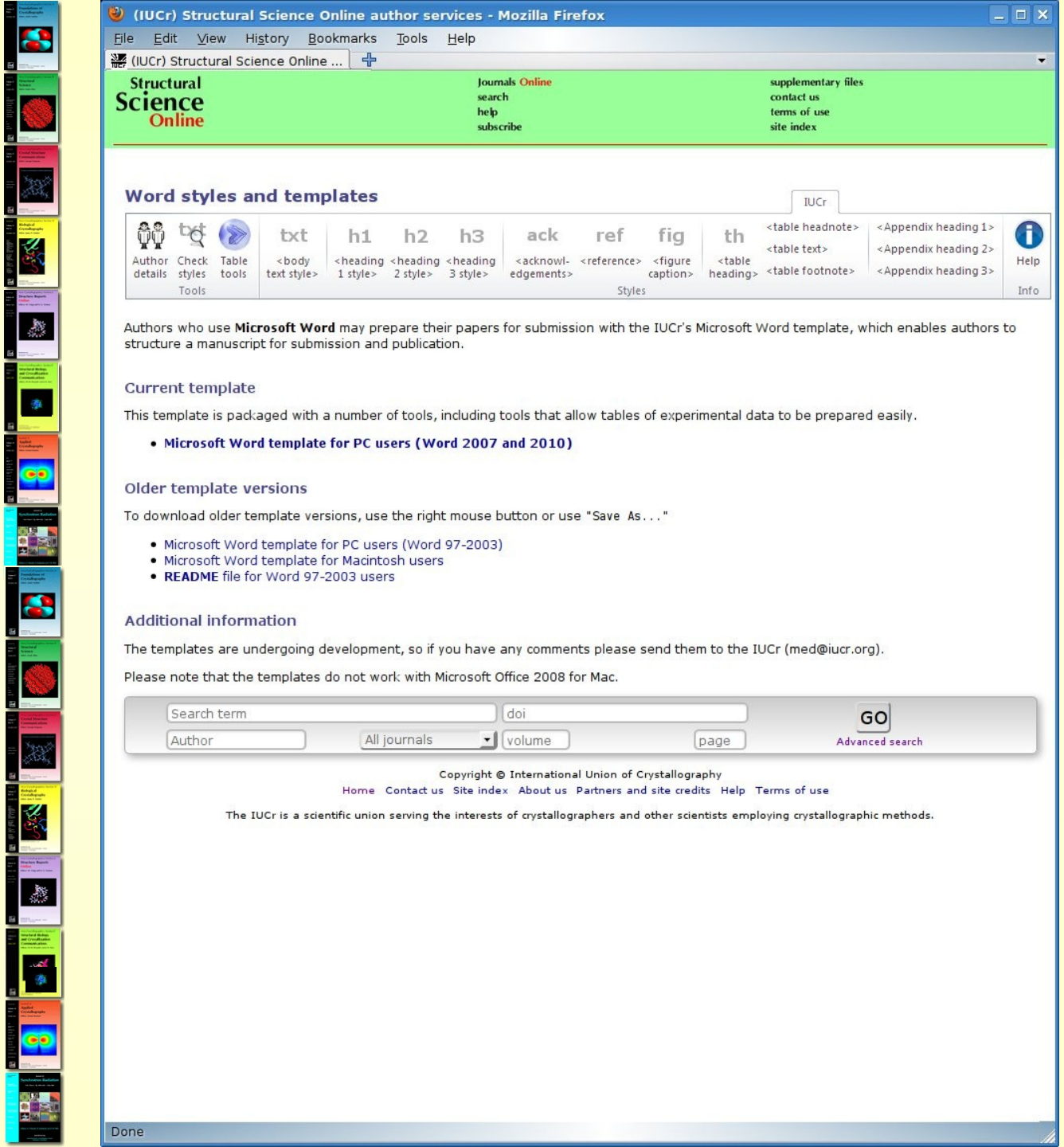
Why templates and author tools

- Provide a structured way of capturing articles
- Save authors' time if integrated with submission procedures
- Avoid rekeyboarding, particularly of data
- Improve efficiency and accuracy of journal production procedures by providing information in a format that can be easily processed
- Allow new features to be introduced to the journals, *e.g.* enhanced figures

Crystallography Journals Online

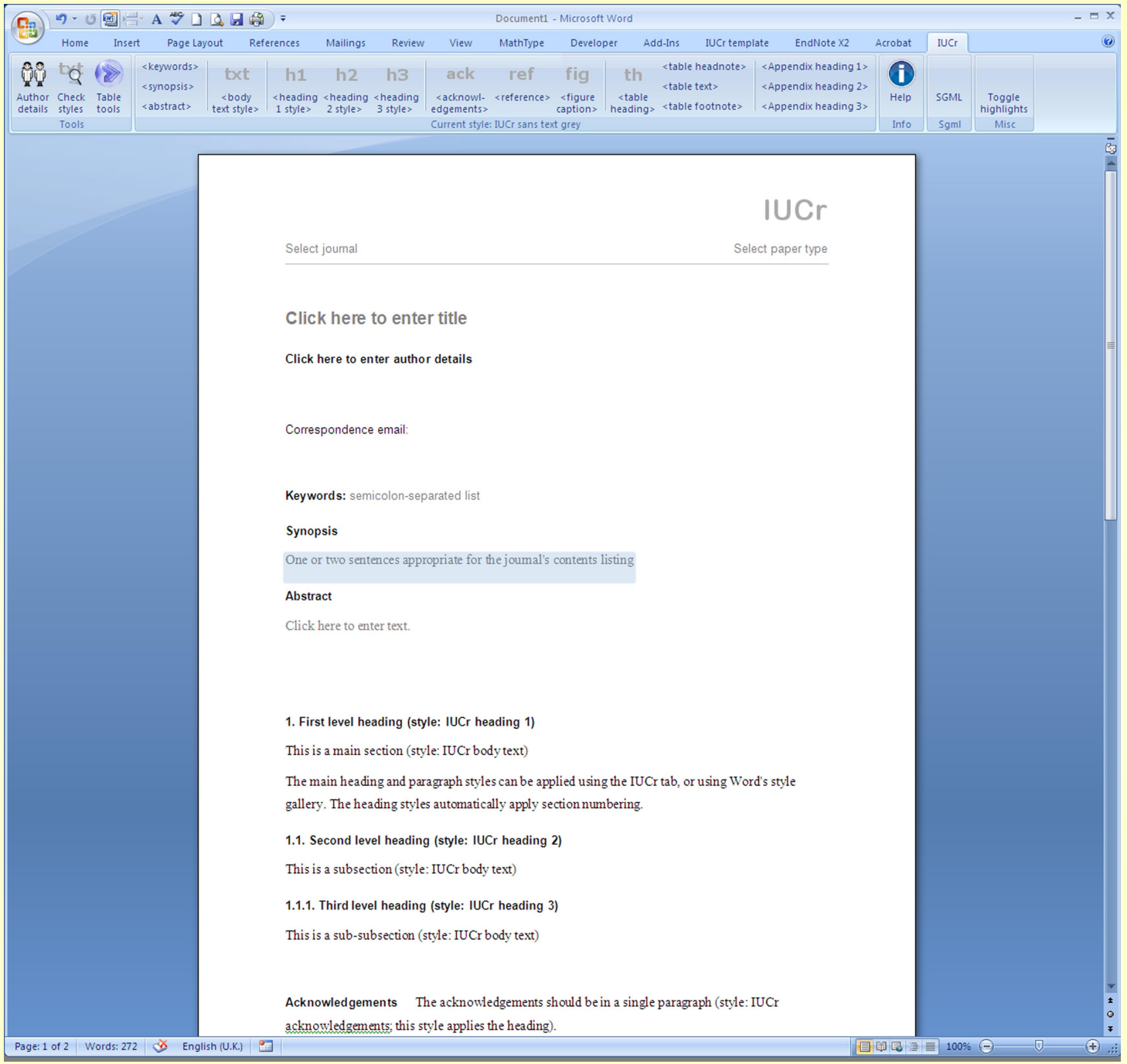
WORD template

Crystallography Journals Online



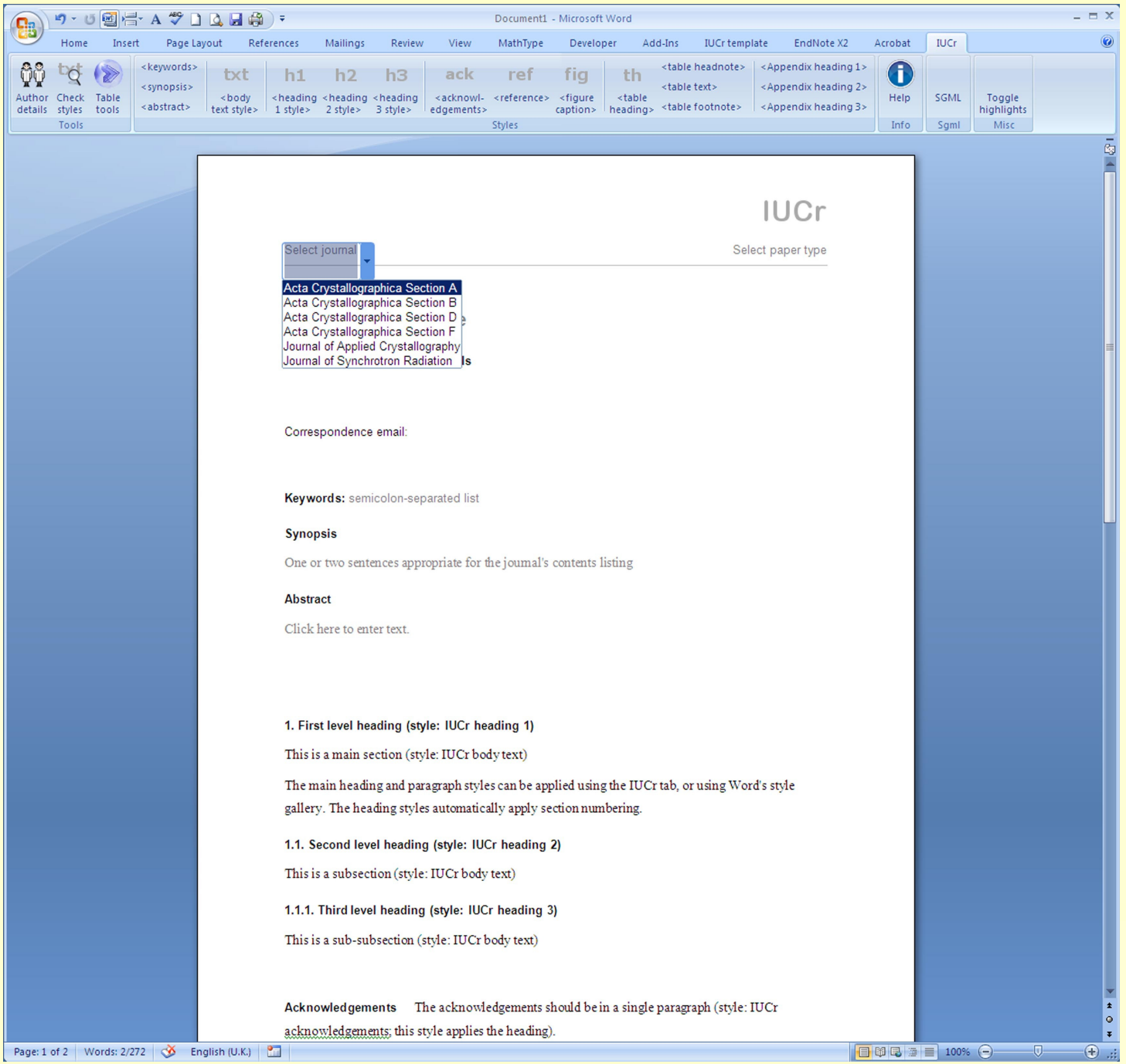
- Template for WORD 2007 and 2010
- Utilizes content management features of WORD
- Older templates also available

Crystallography Journals Online



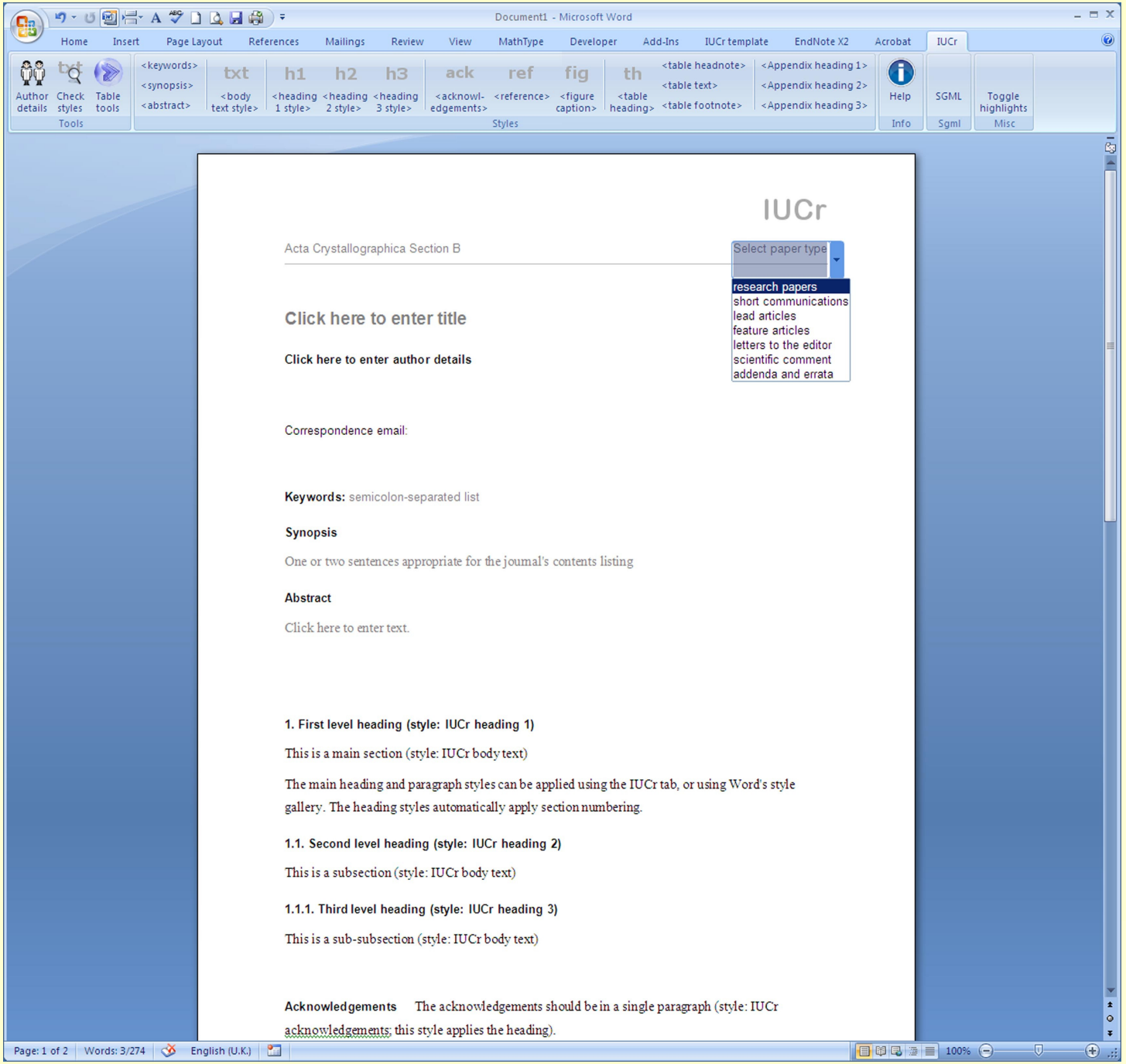
- Template comes packaged with tools
- Interacts with external resources, *e.g.* World Directory
- Allows a personal database of author details to be collected
- Articles can be written in the template or quickly imported and marked up

Crystallography Journals Online



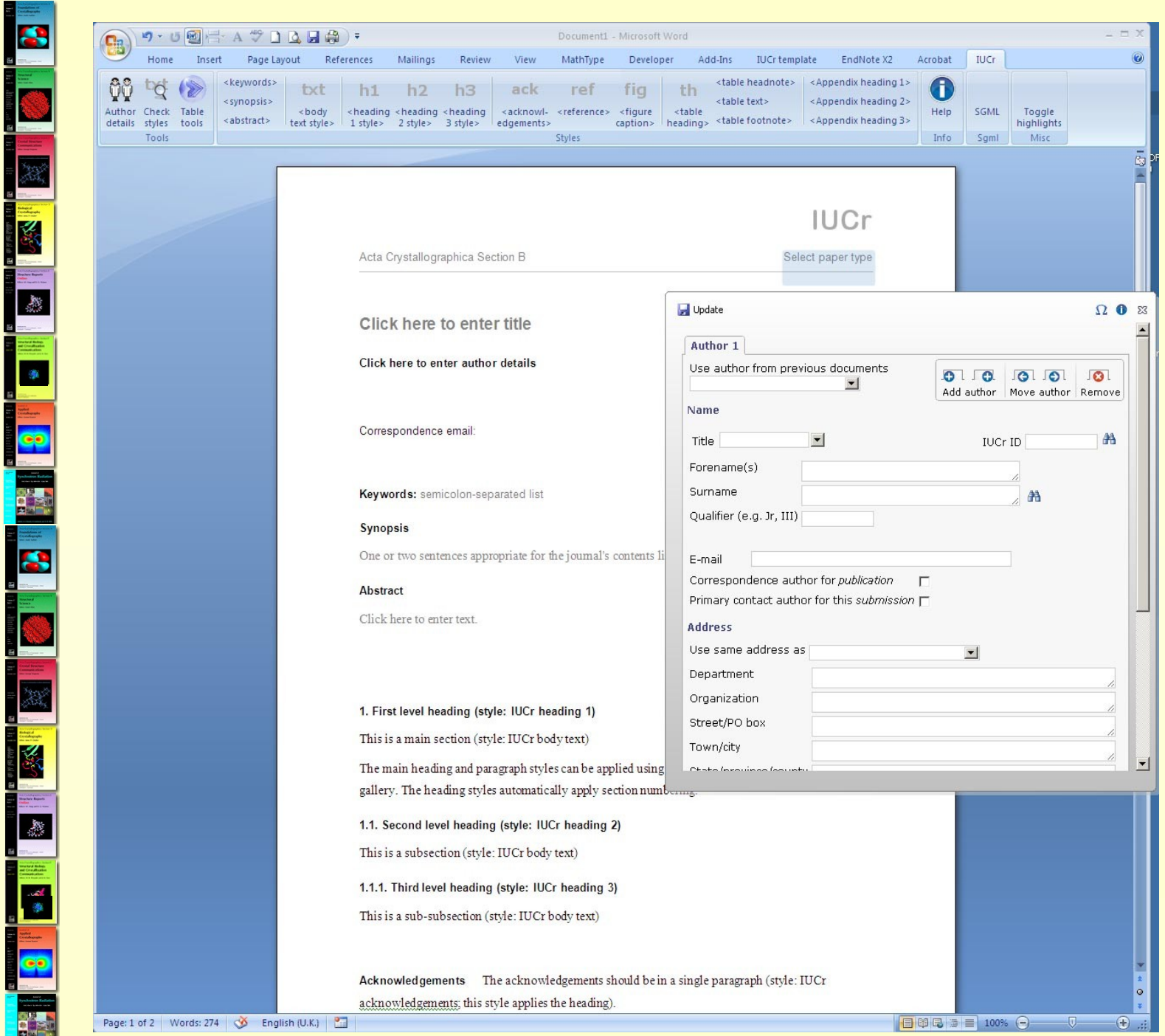
- Use drop-down menu lists to select journal

Crystallography Journals Online



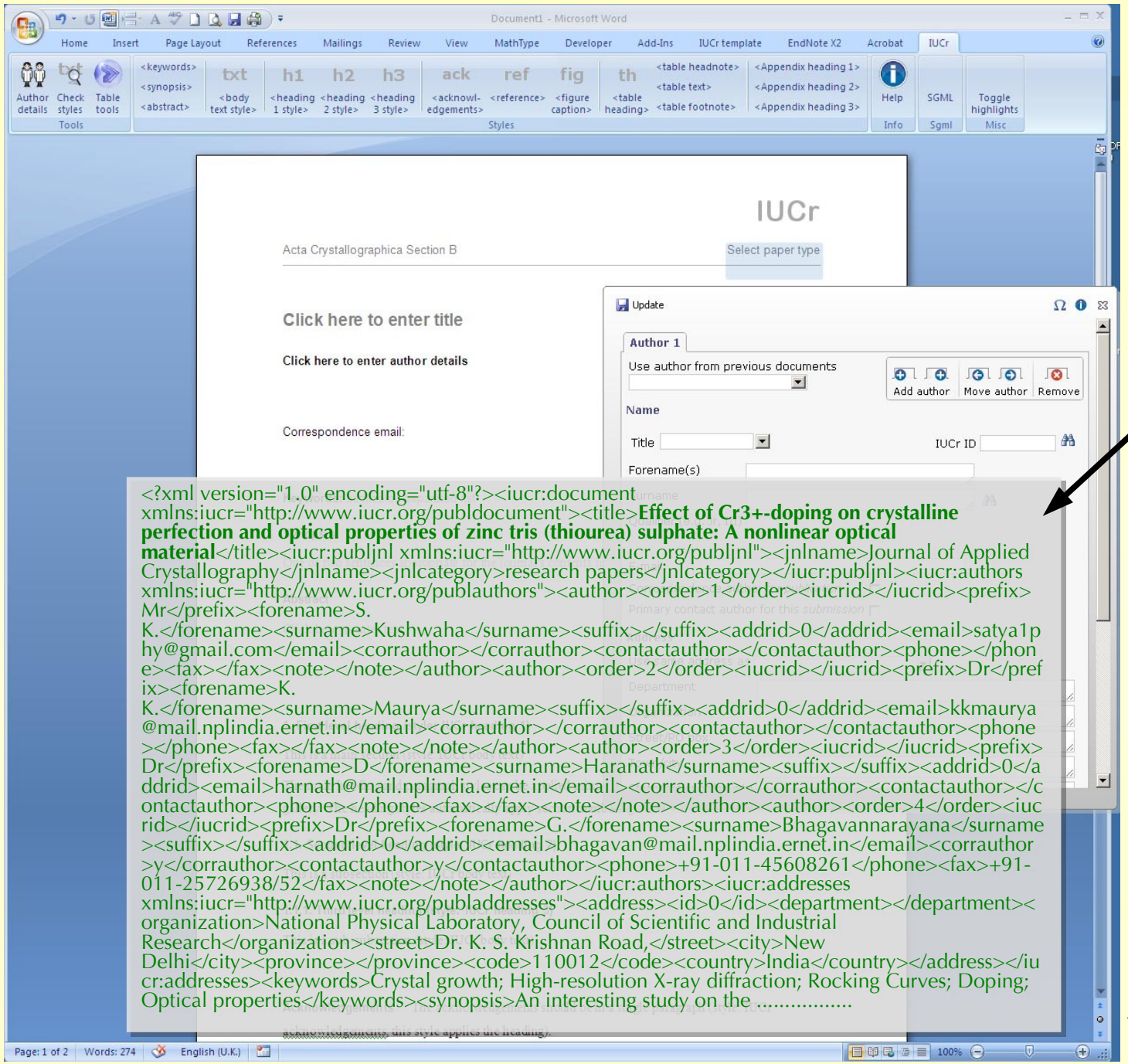
- Select paper type
- Click to add title, keywords, synopsis and abstract

Crystallography Journals Online



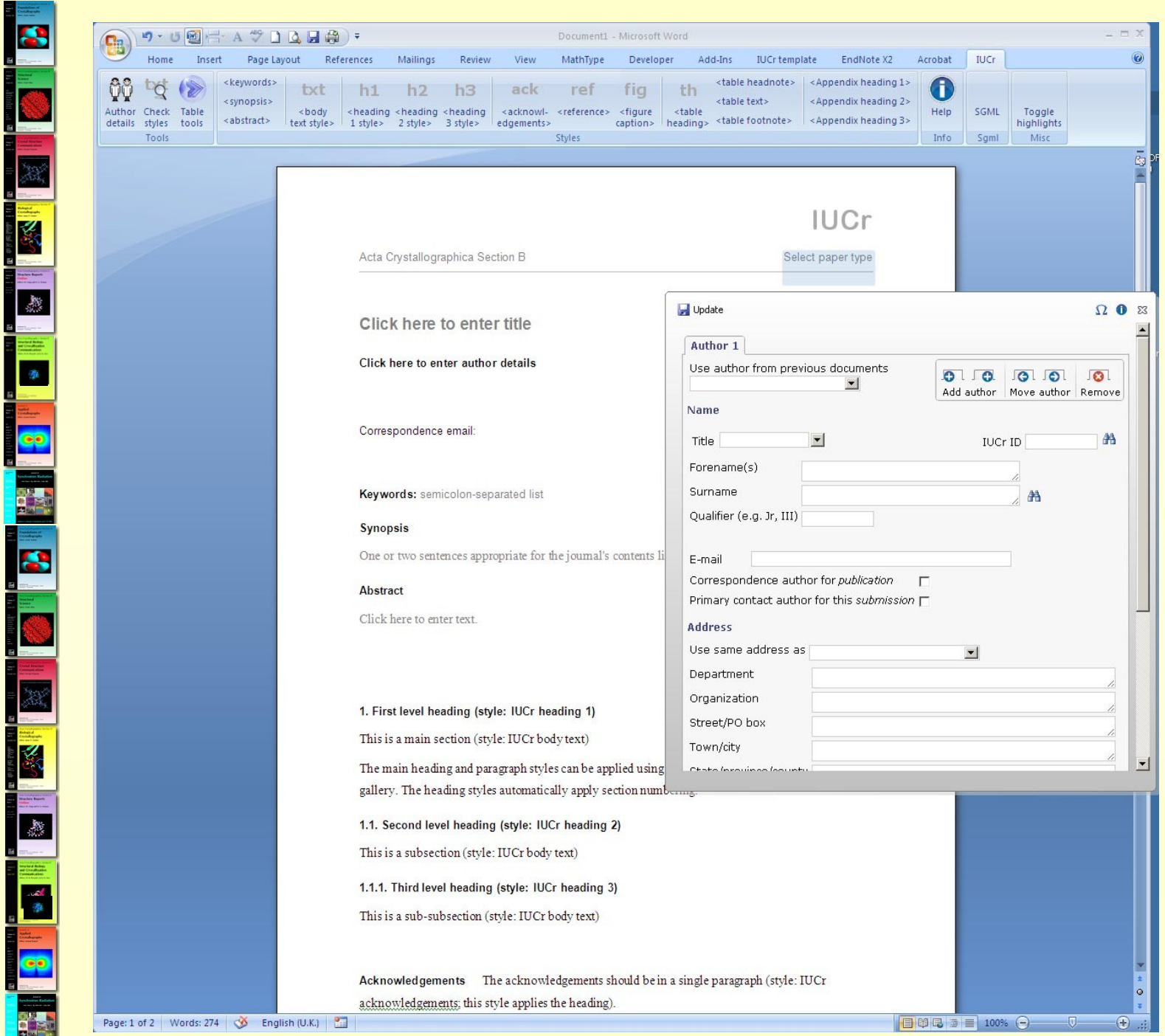
- Author details entered *via* menu
- Details formatted to journal style
- Details stored as XML within document and in local database
- Information can be reused during submission
- Contact and corresponding authors can be distinguished

Crystallography Journals Online



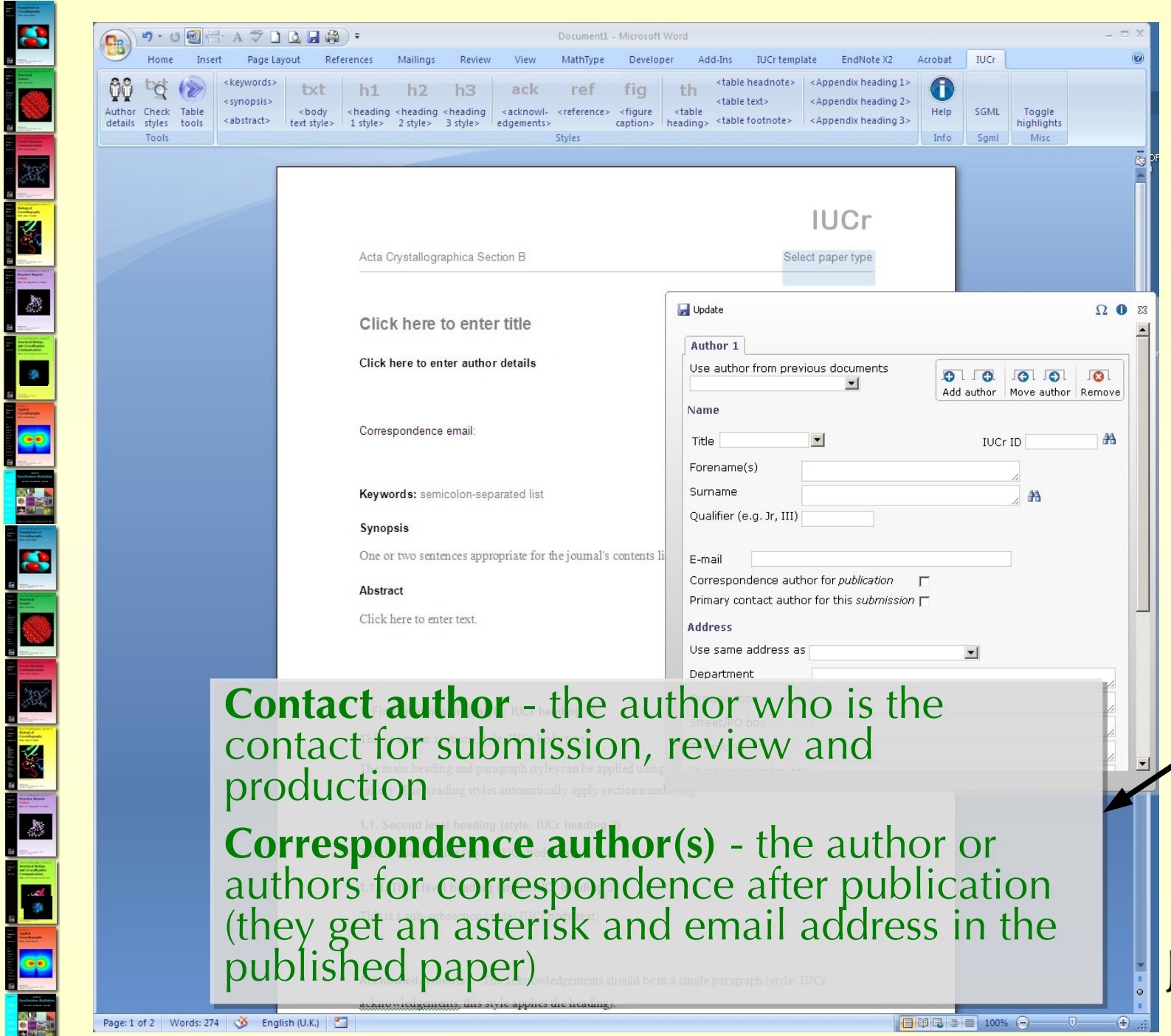
- Author details entered via menu
- Details formatted to journal style
- Details stored as XML within document and in local database
- Information can be reused during submission
- Contact and corresponding authors can be distinguished

Crystallography Journals Online



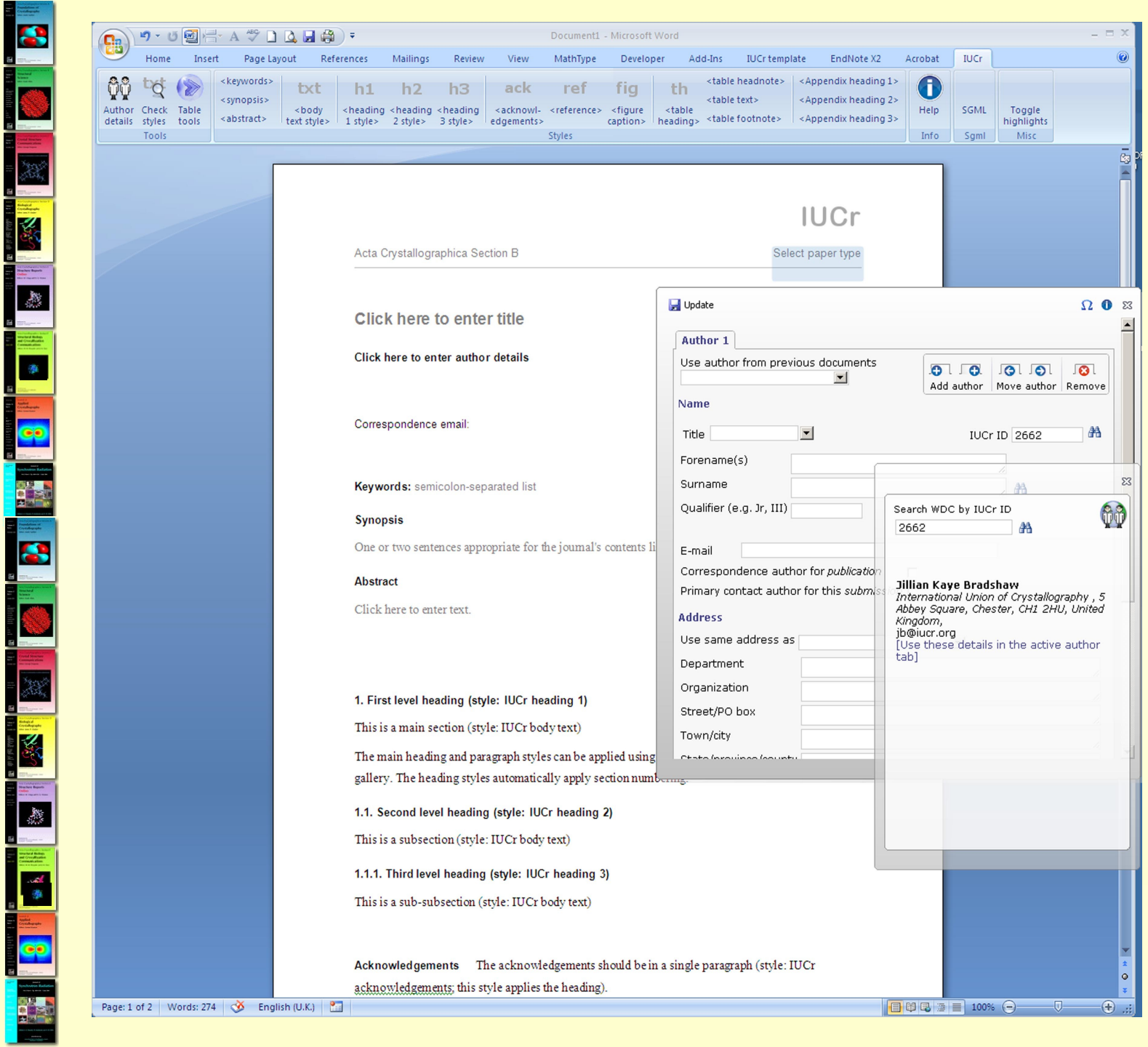
- Author details entered via menu
- Details formatted to journal style
- Details stored as XML within document and in local database
- Information can be reused during submission
- Contact and corresponding authors can be distinguished

Crystallography Journals Online



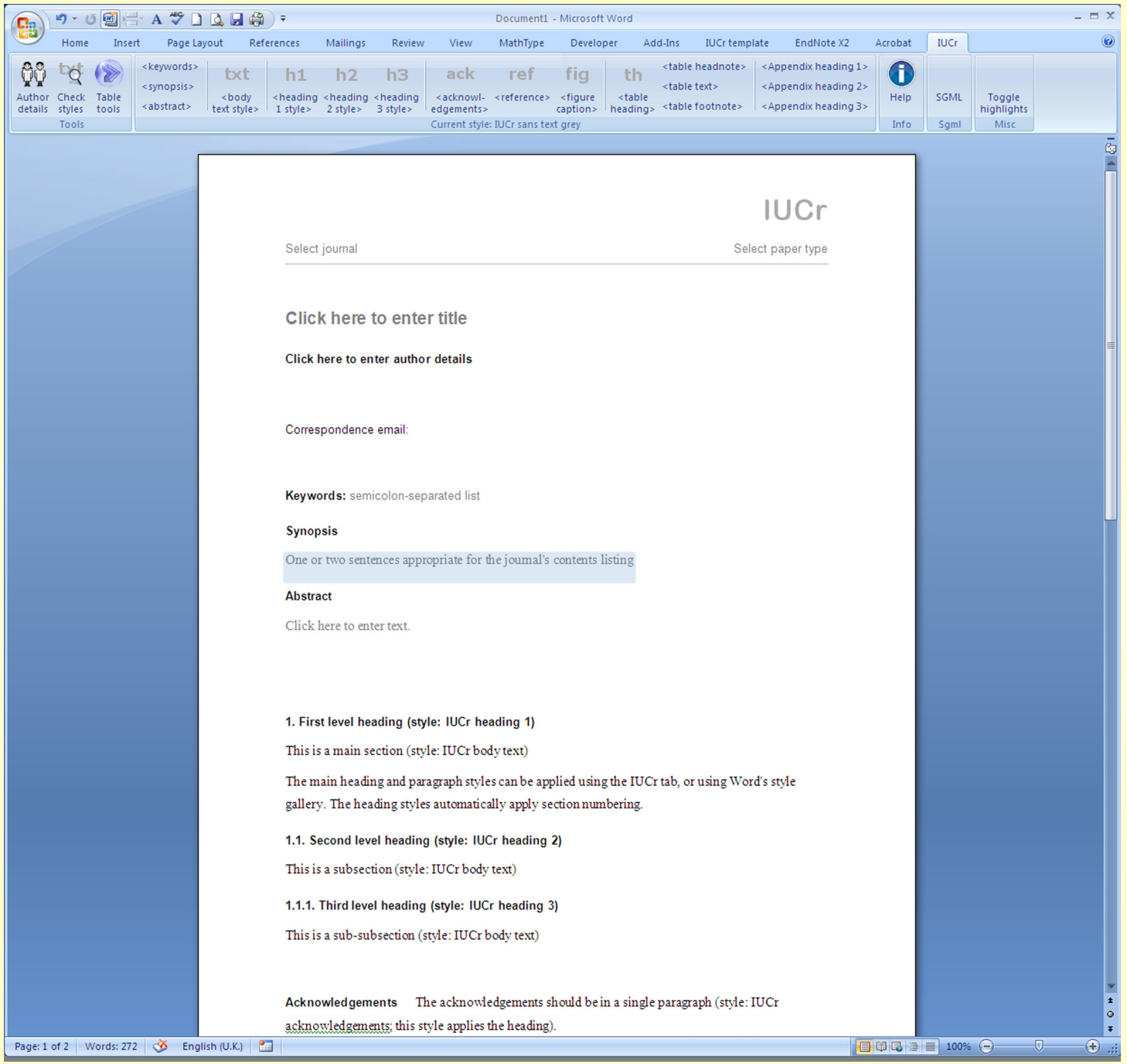
- Author details entered via menu
- Details formatted to journal style
- Details stored as XML within document and in local database
- Information can be reused during submission
- Contact and corresponding authors can be distinguished

Crystallography Journals Online



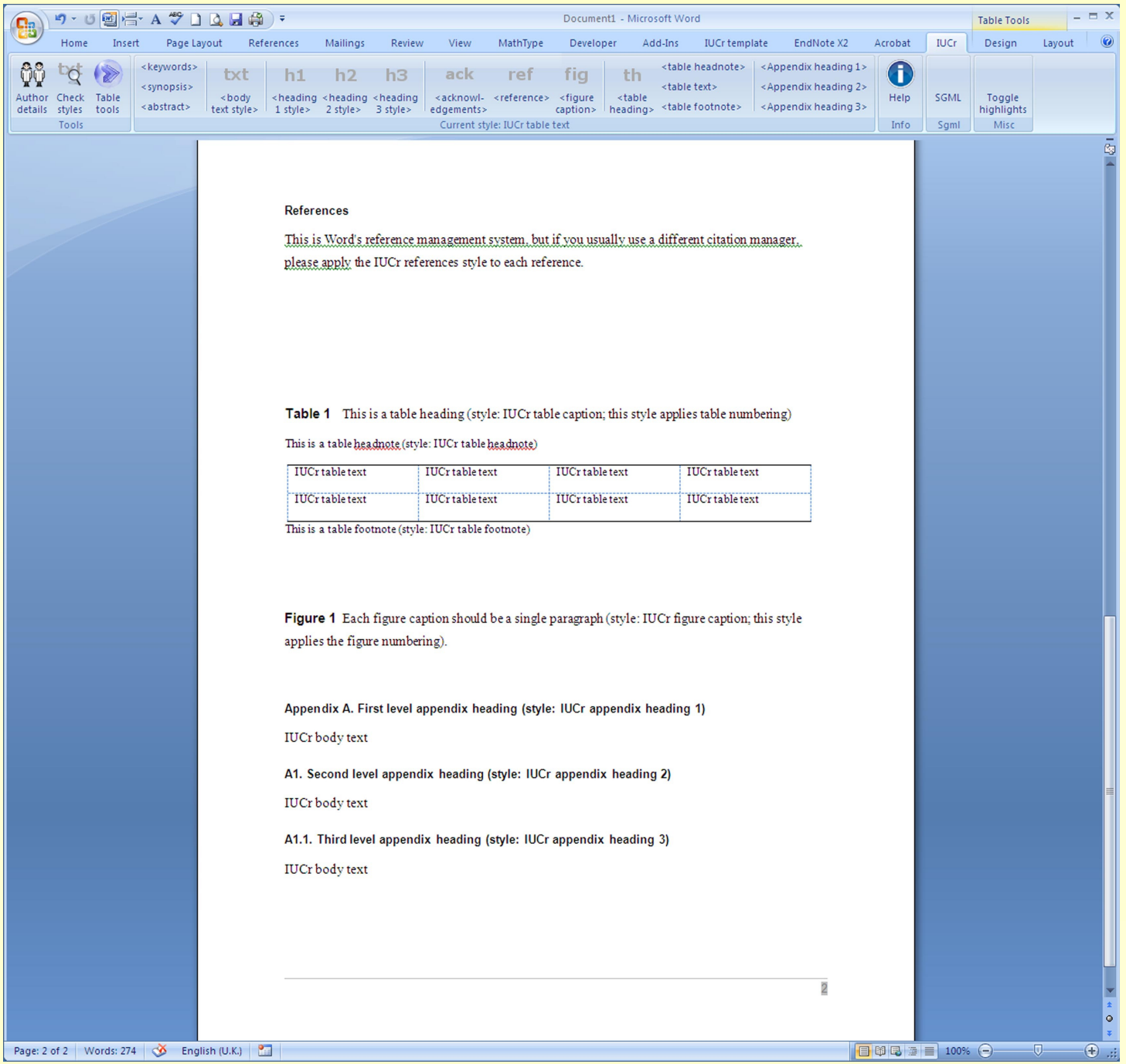
- Details can be retrieved from the World Directory
- In the future, author details could be picked up from services such as ORCID or from previous journal authors

Crystallography Journals Online



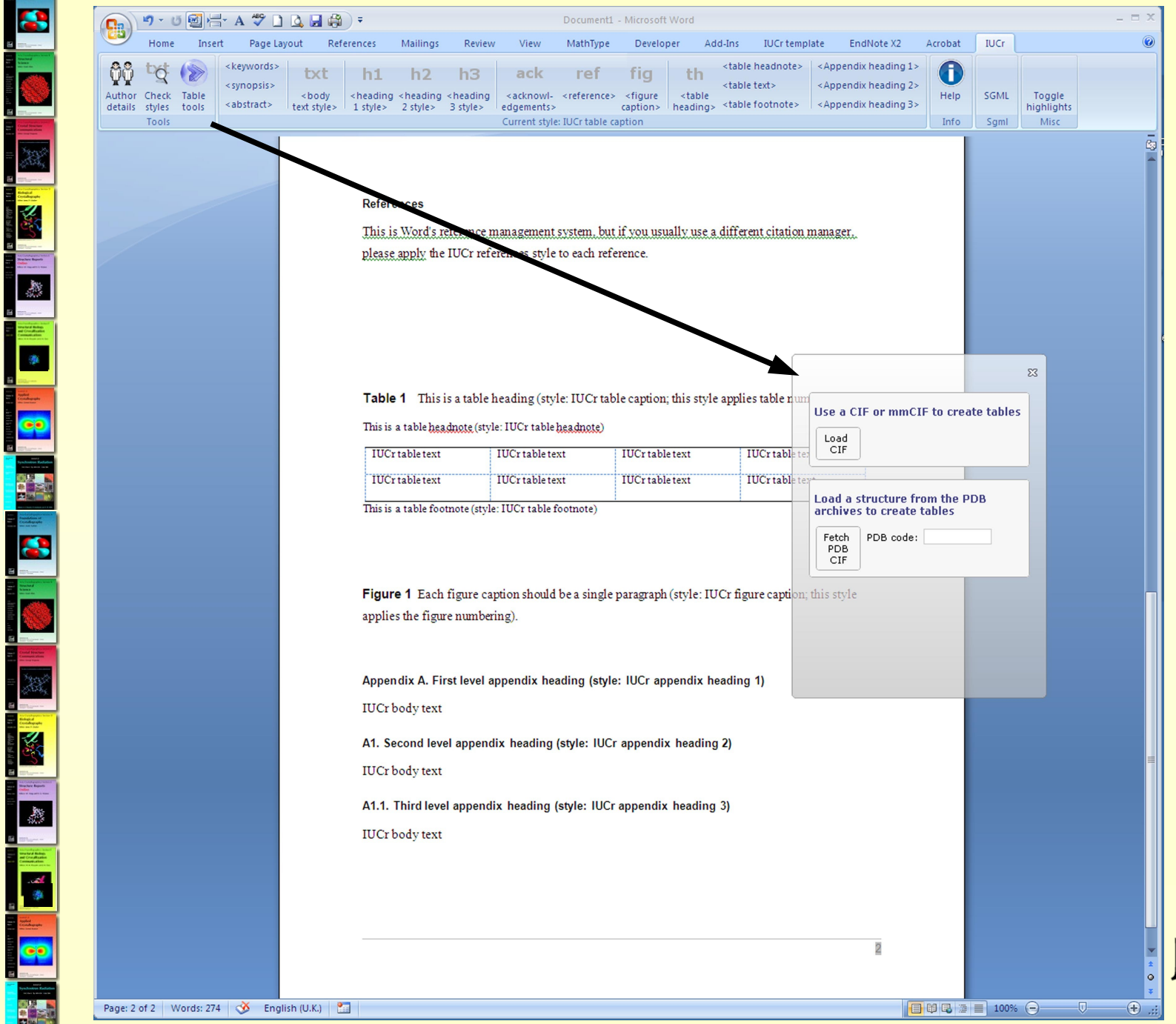
- Mark-up text with styles, *e.g.* for first-, second- or third-level headings
- Styles also available from IUCr ribbon

Crystallography Journals Online



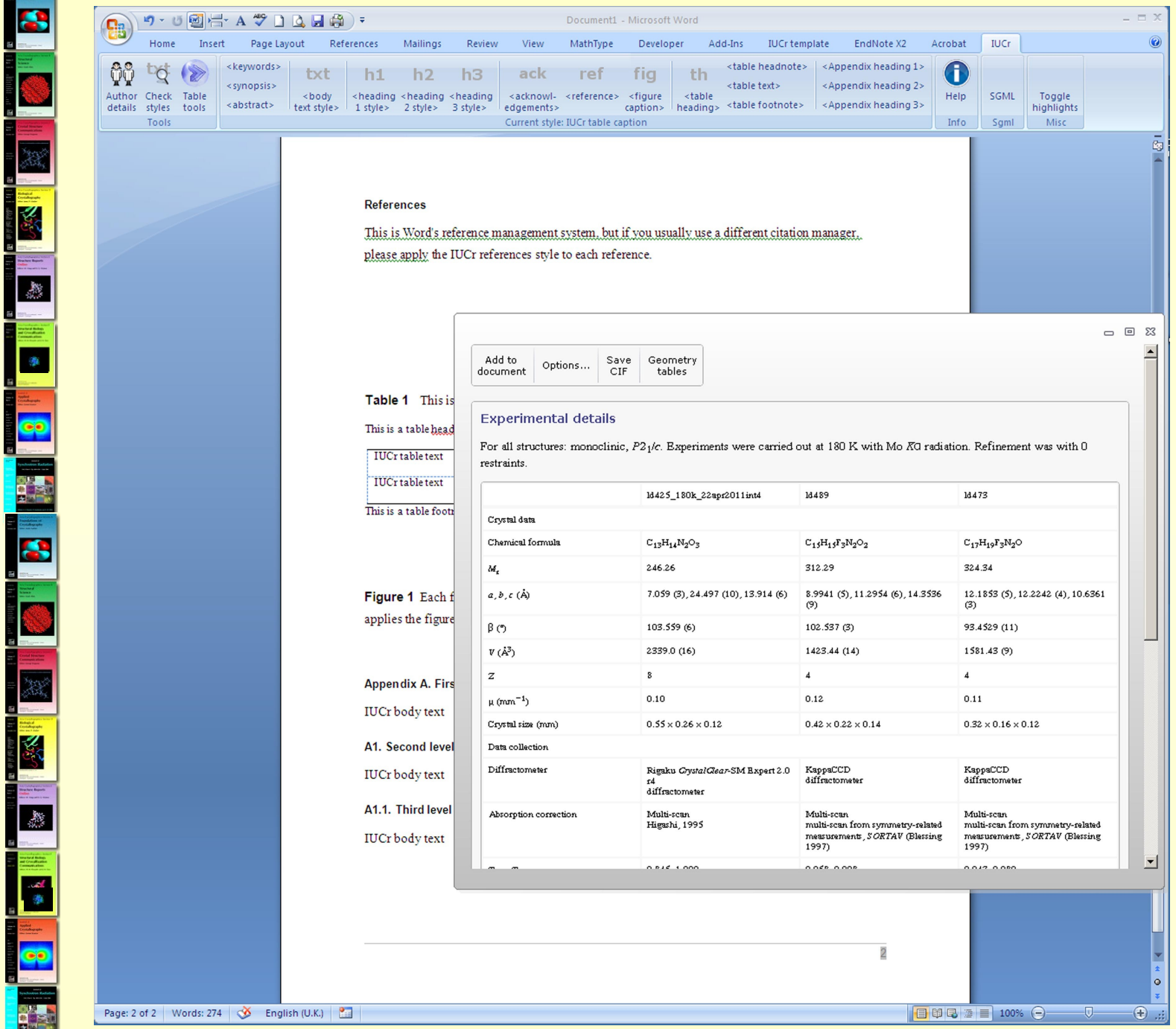
- Tables should be prepared using WORD's table editor with styles applied to caption, headnotes and footnotes
- Experimental tables can be prepared using **Table tools**

Crystallography Journals Online



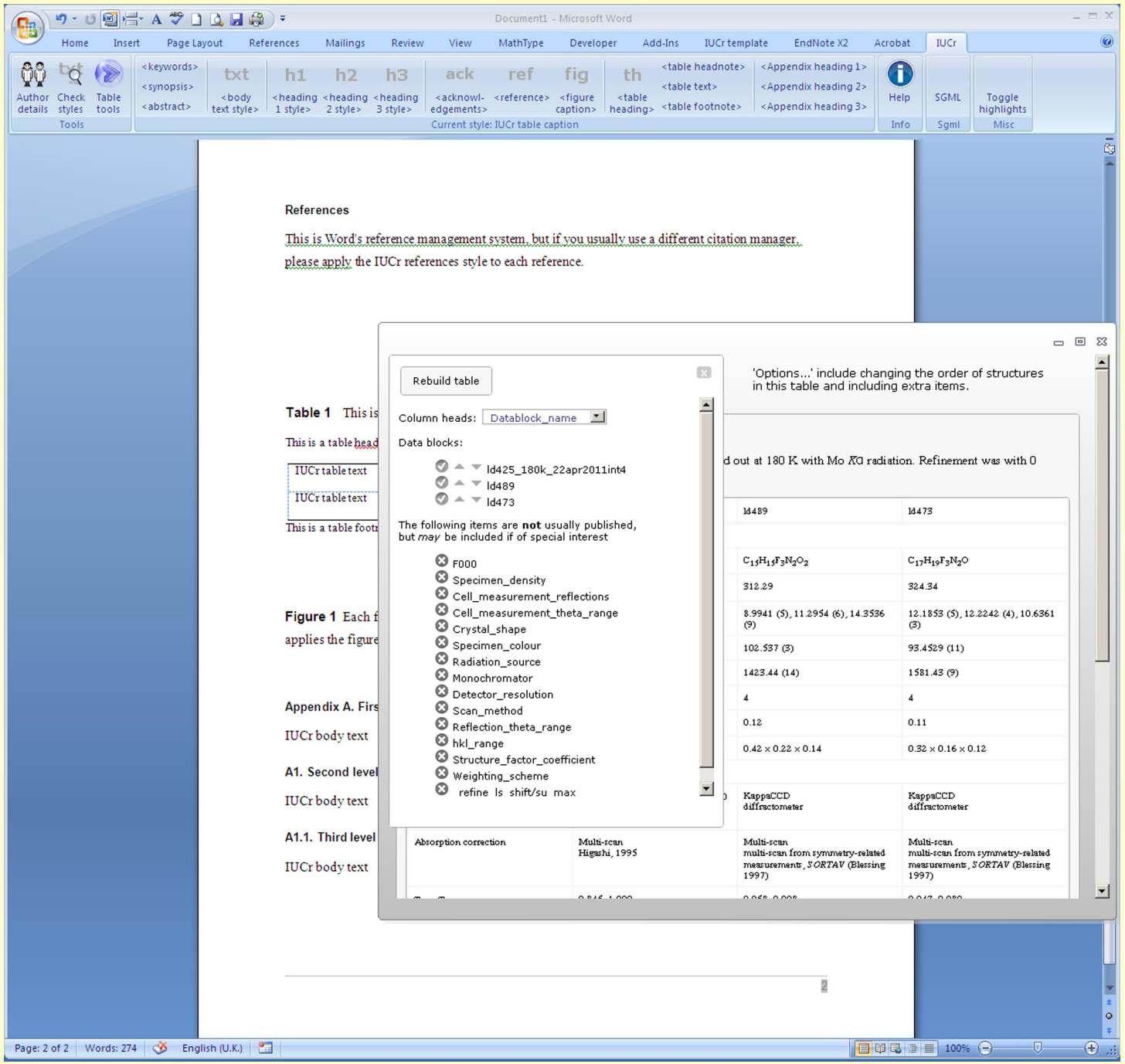
- Use **Table tools** to prepare experimental tables from a CIF for small molecule structures
- For macromolecular structures use PDB code to import mmCIF to create table of experimental details

Crystallography Journals Online



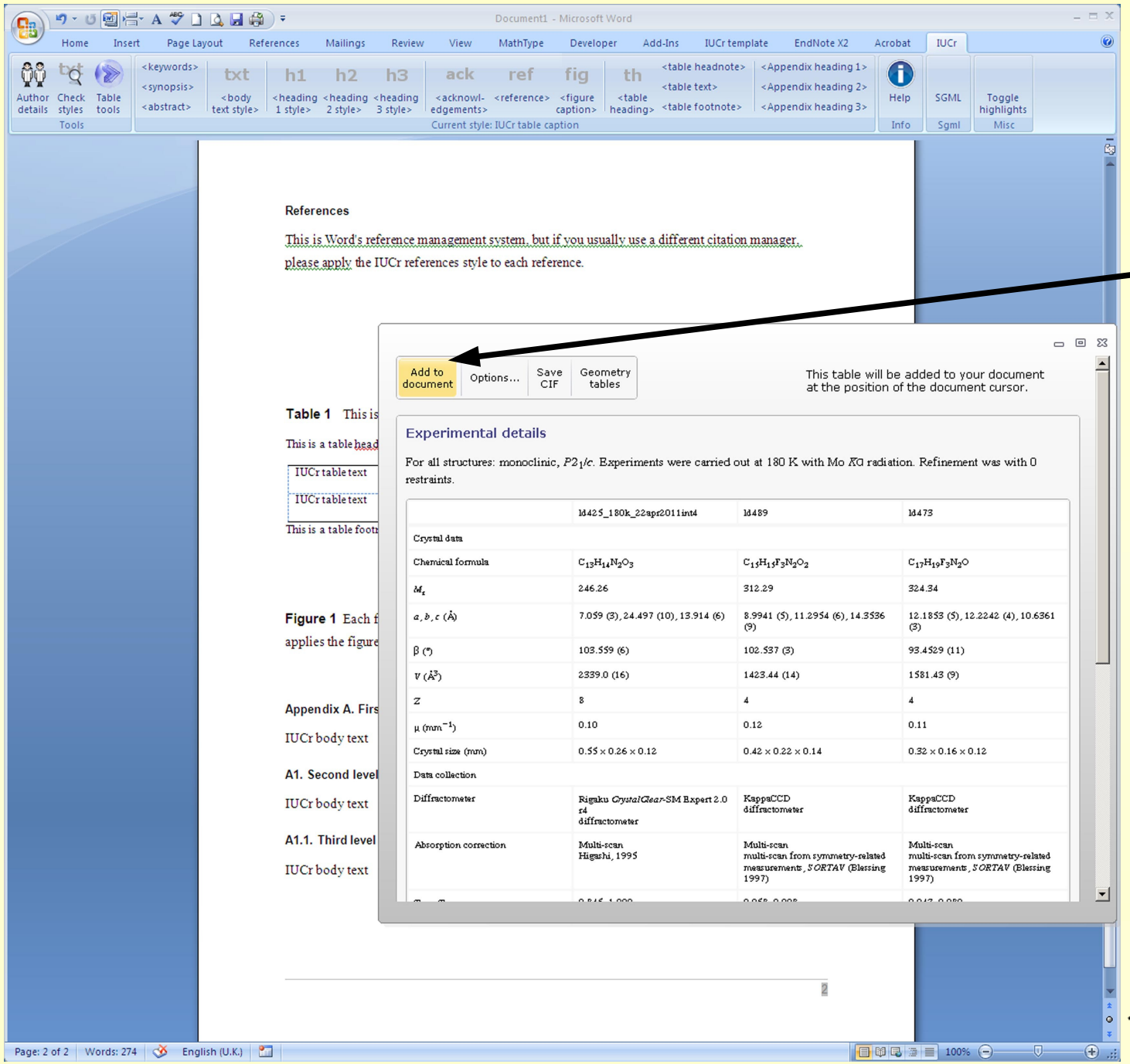
- Each datablock from the CIF appears as column in table

Crystallography Journals Online



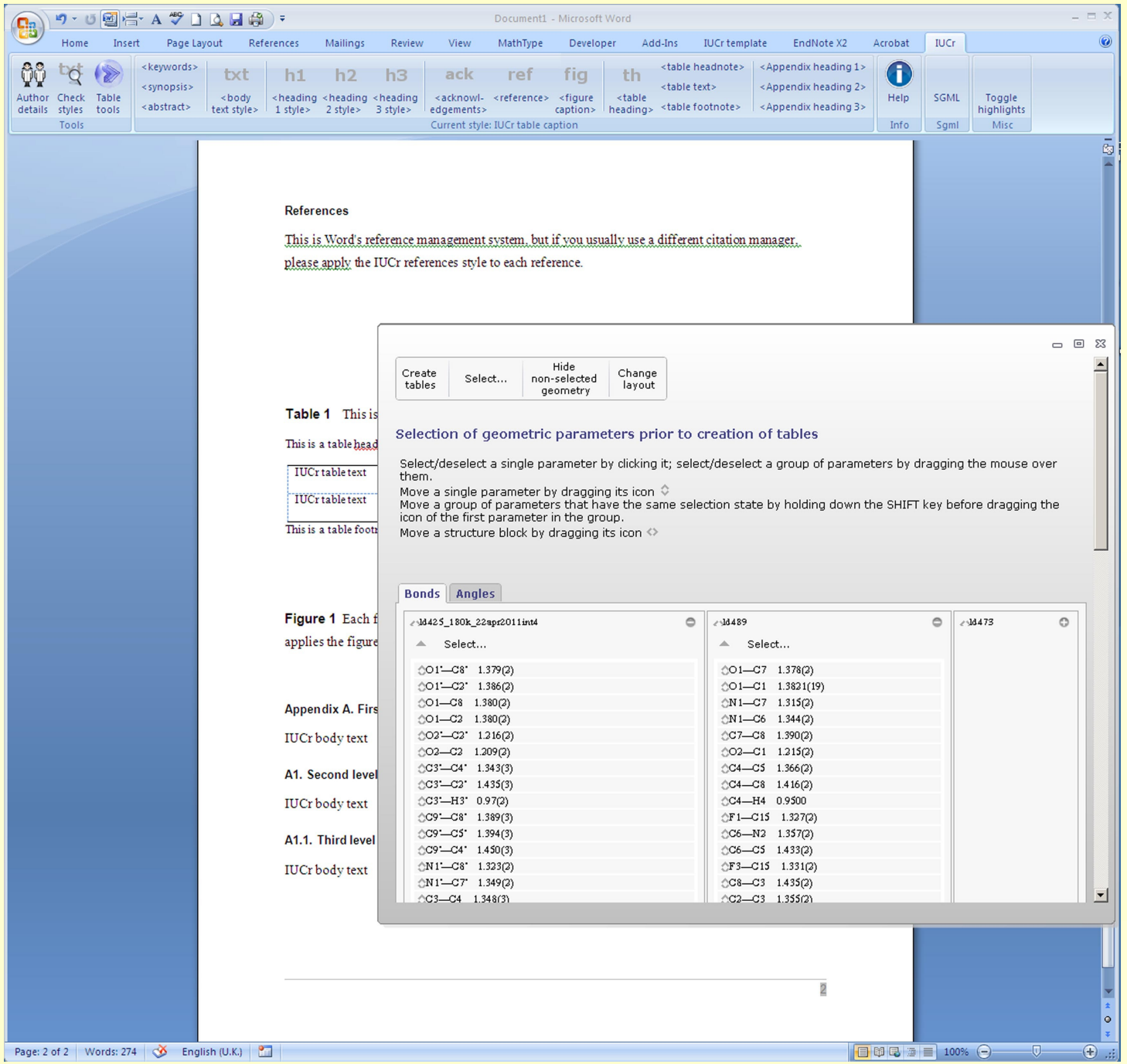
- Extra "non-standard" items present in the CIF can be added to table
- Datablocks can be selected for inclusion or exclusion
- Several types of column headings can be selected
- Small molecule, powder and incommensurate CIFs handled

Crystallography Journals Online



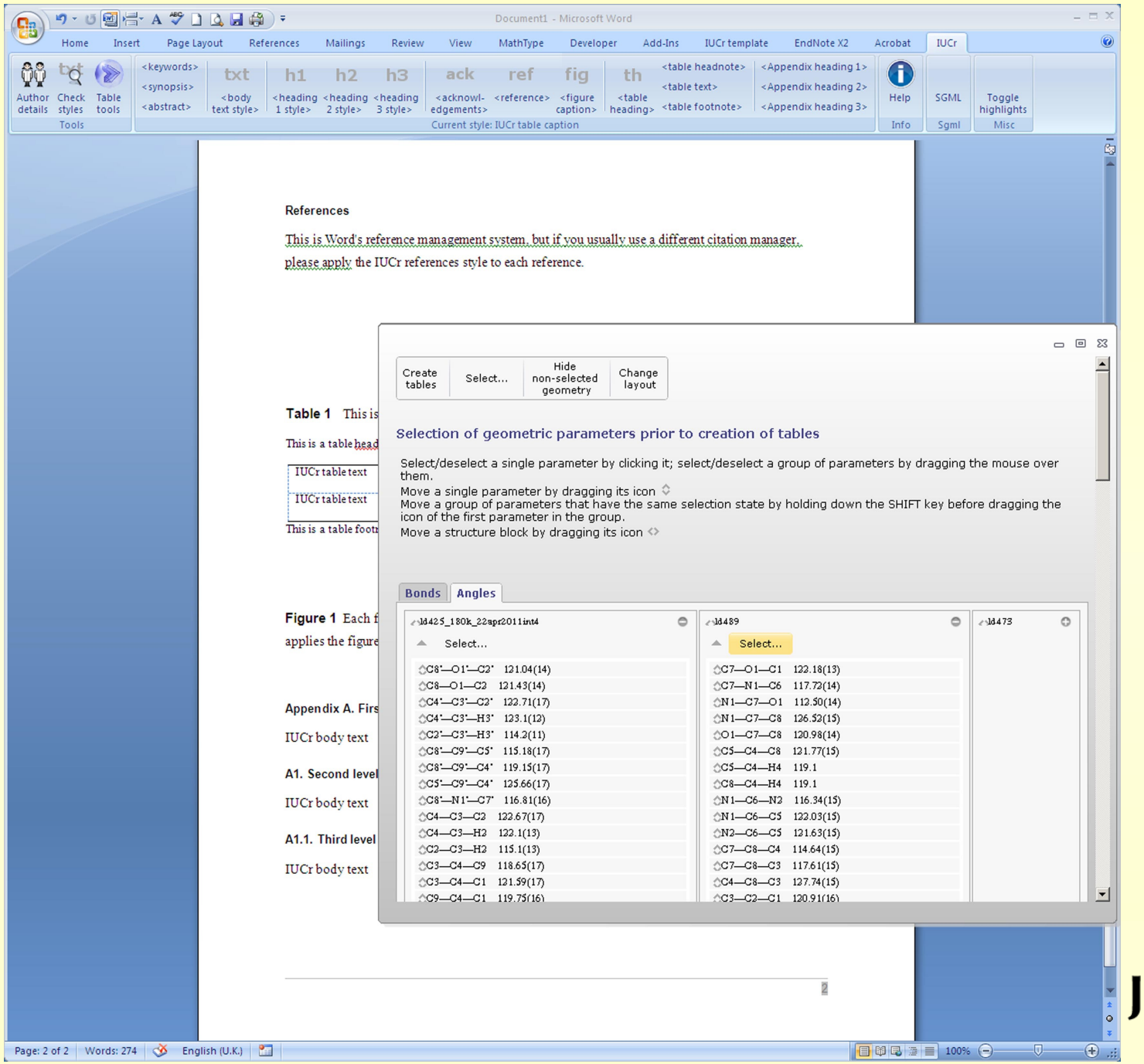
- Once all items have been selected, the experimental table can be added to the document

Crystallography Journals Online



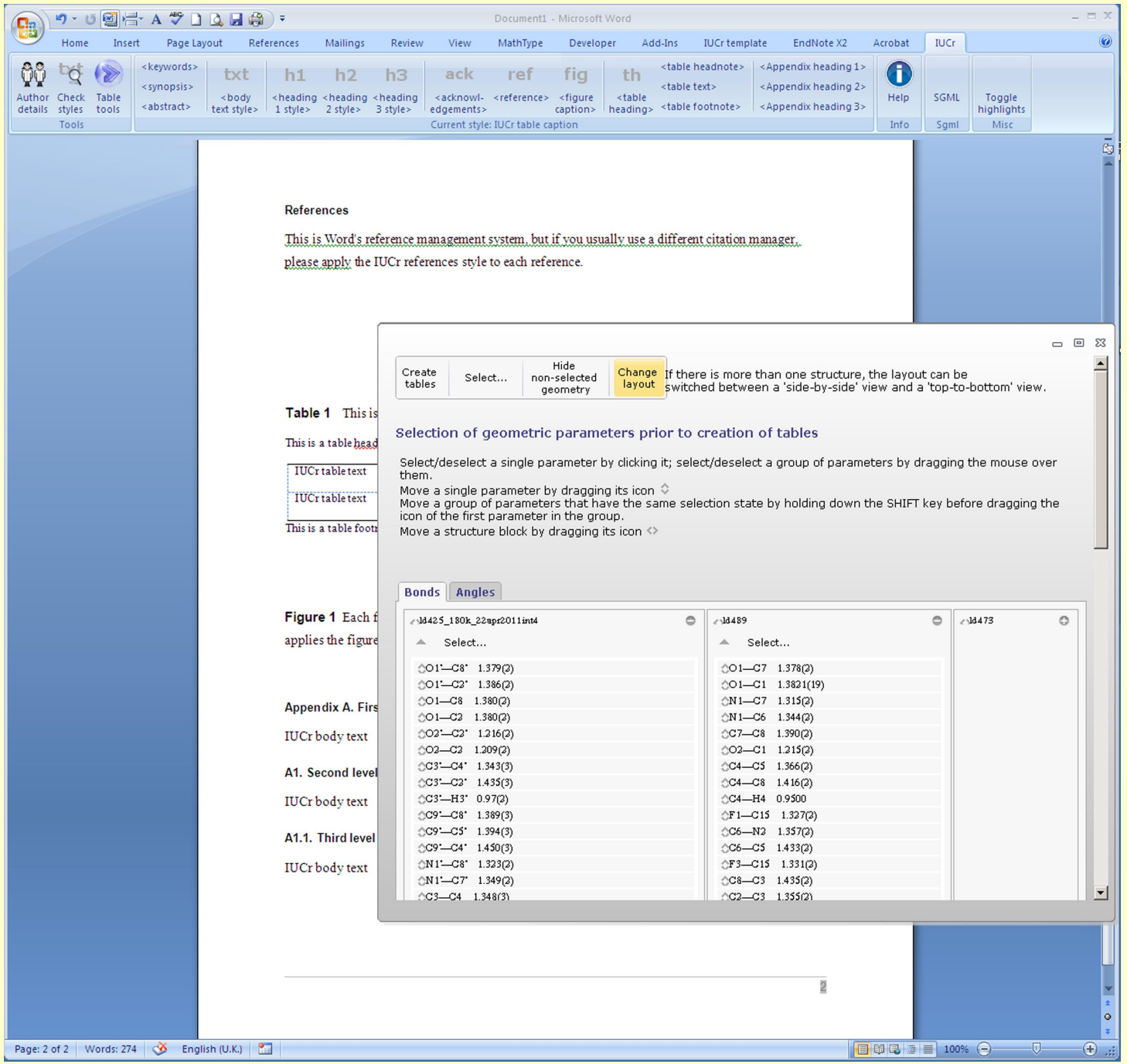
- Can also create geometry tables from CIF

Crystallography Journals Online



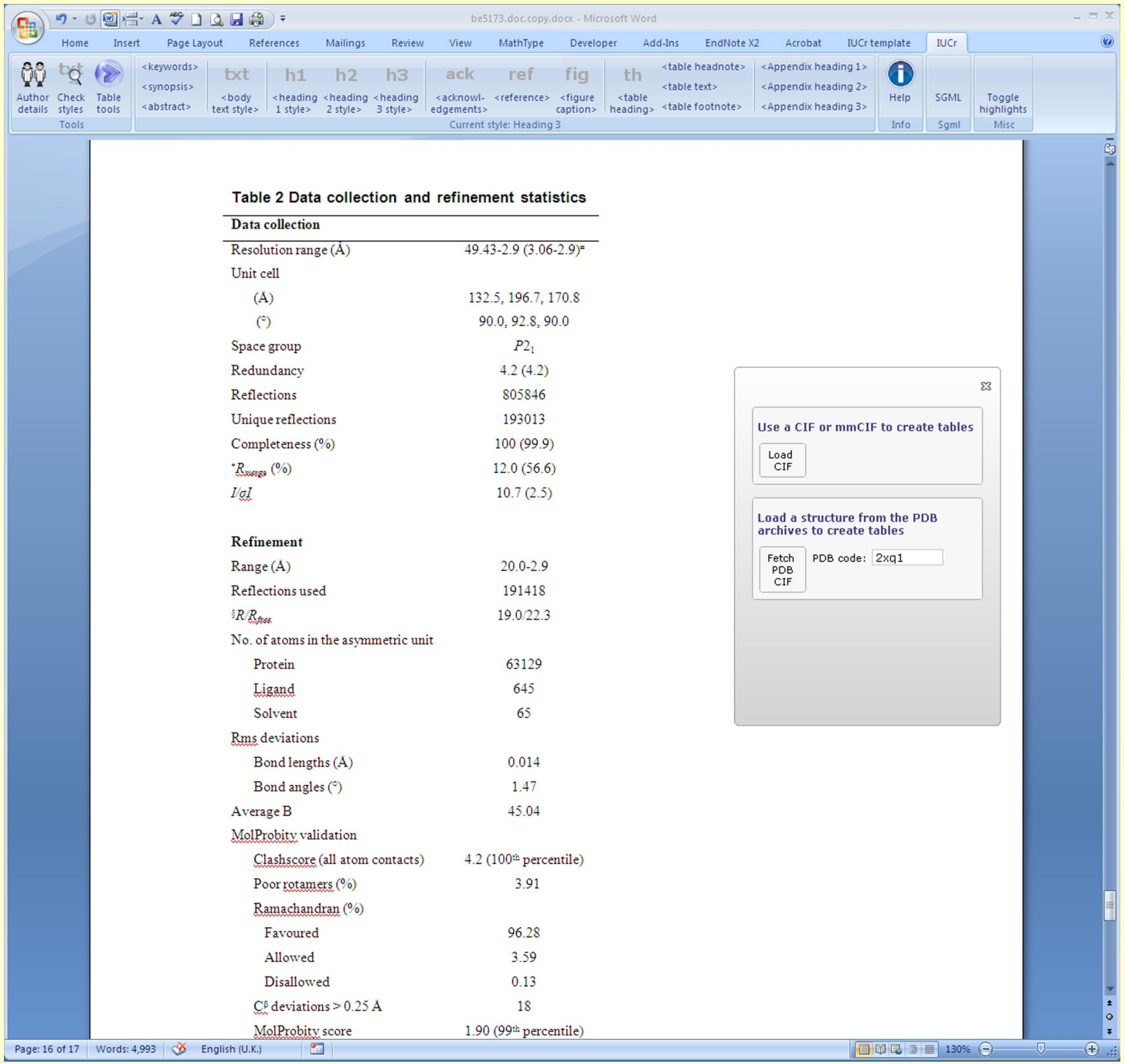
- Can also create geometry tables from CIF
- Can select which bonds and angles to include in table

Crystallography Journals Online



- 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

Crystallography Journals Online



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

Crystallography Journals Online

be5173.doc.copy.docx - Microsoft Word

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

Author details | Check styles | Table tools | Tools

<keywords> <synopsis> <abstract> | txt <body text style> | h1 <heading 1 style> | 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>

Current style: Heading 3

Help | Info | SGML | Sgml | Toggle highlights | Misc

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

Add all tables to document

Add following table to document

Sample information

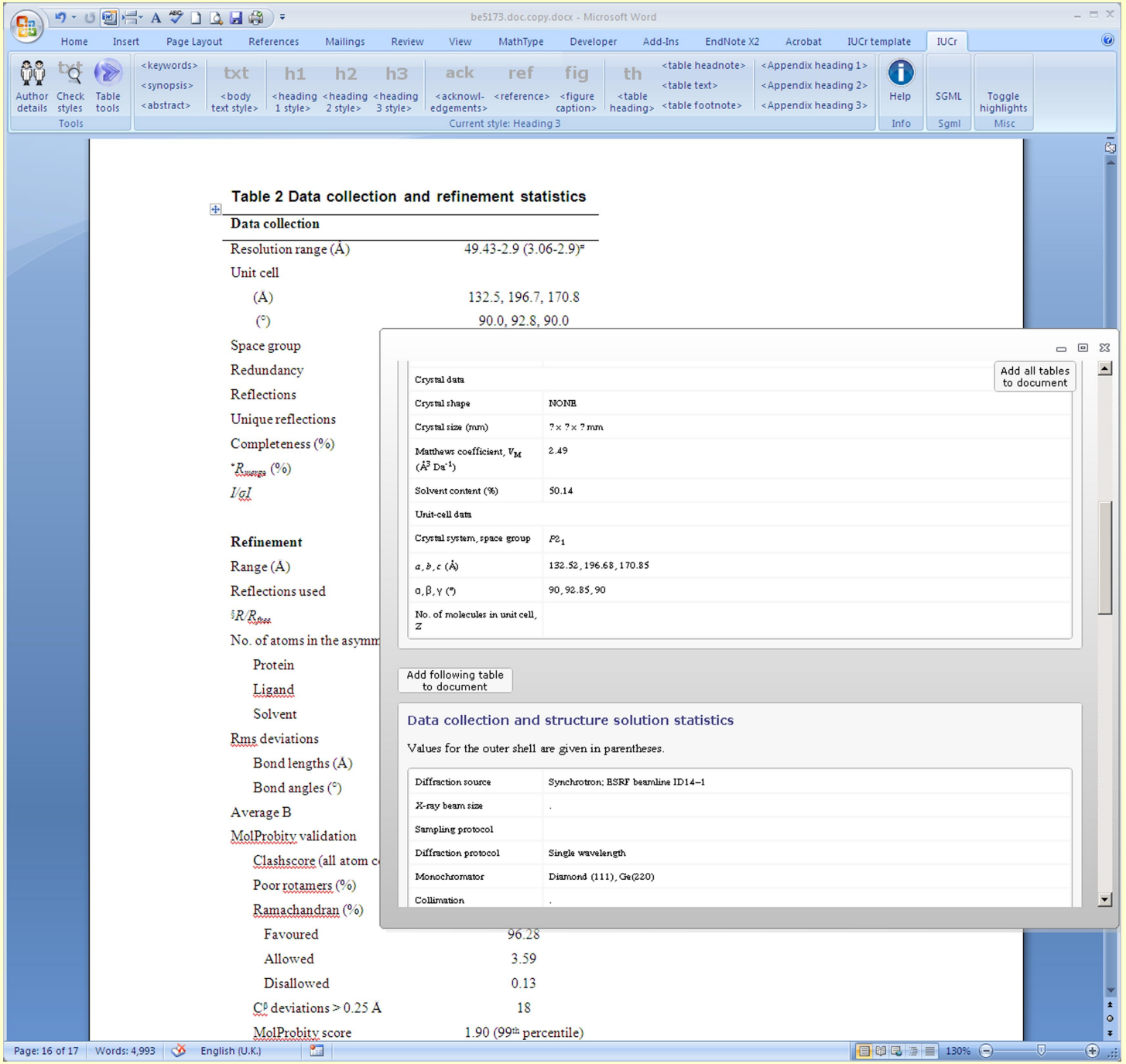
Macromolecule details	
Database code(s)	PDB code: 2XQ1; UNP code: CATA PICAN
Component molecules	Peroxisomal catalase (EC number: 1.11.1.6), protoporphyrin IX containing Fe, water
Macromolecular assembly	
Mass (Da)	
Source organism	PICHIA ANGUSTA
Crystallization and crystal data	
Crystallization method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

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

Tables generated containing

- Sample information

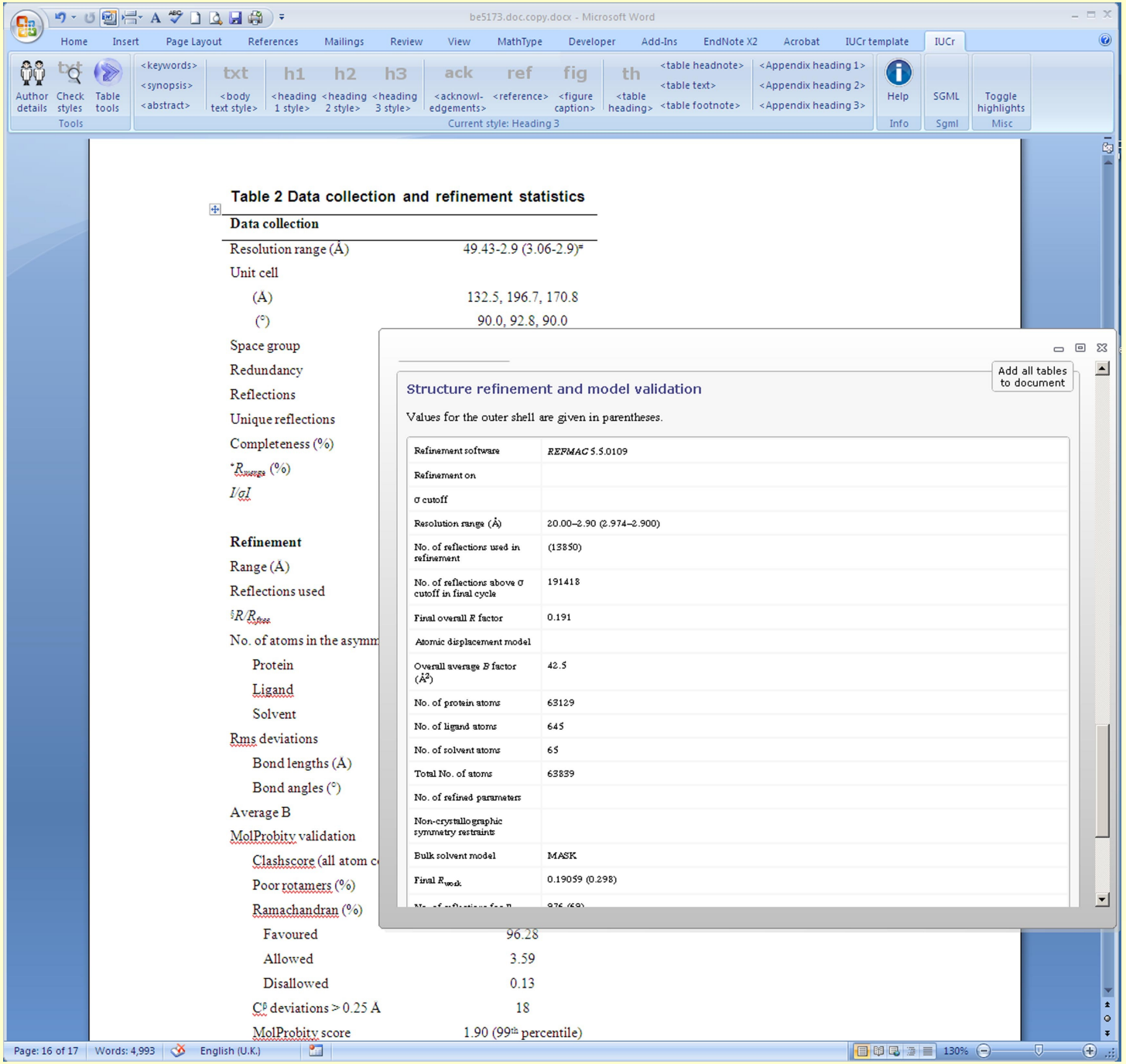
Crystallography Journals Online



Tables generated containing

- Sample information
- Data collection and structure solution statistics

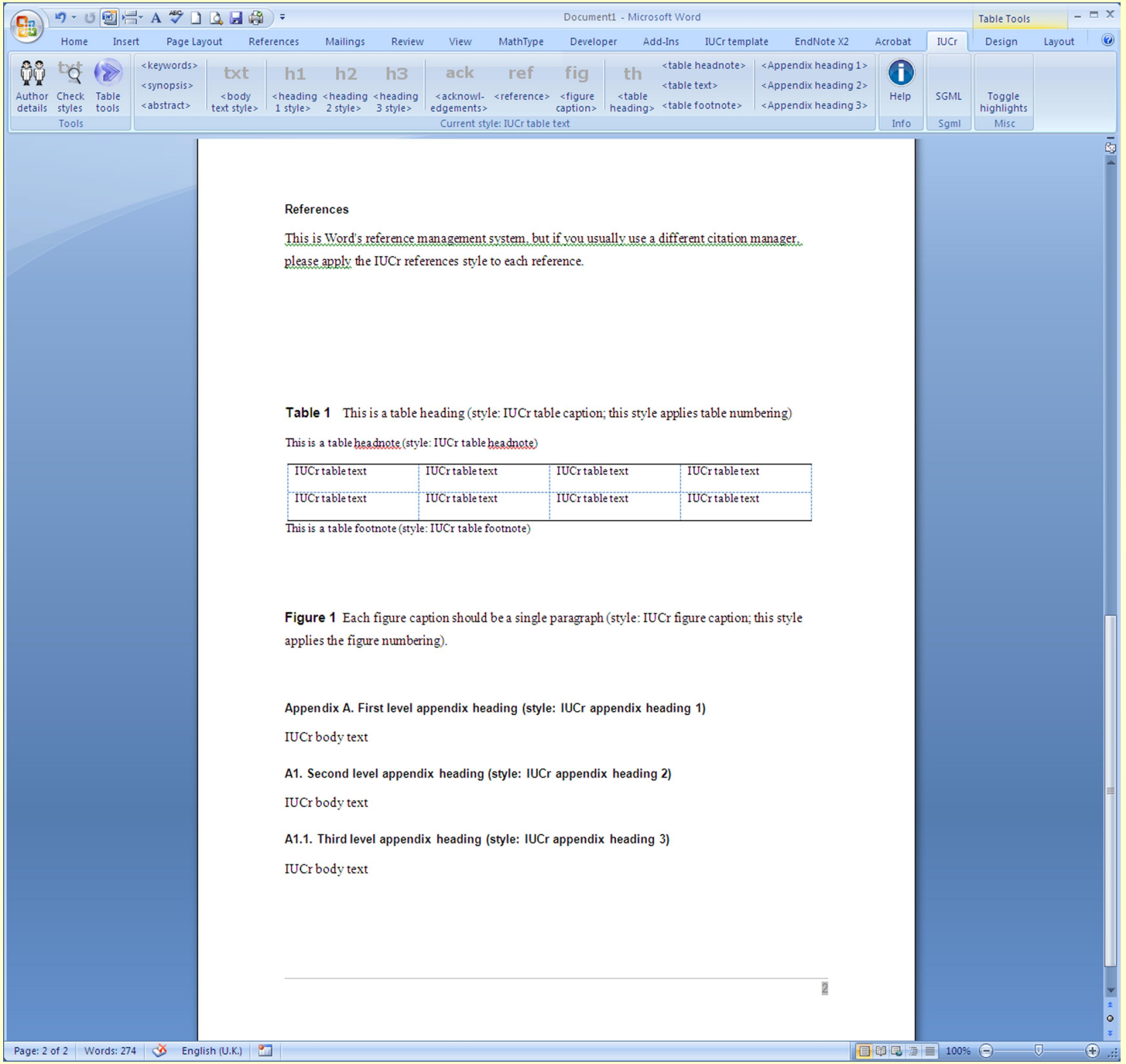
Crystallography Journals Online



Tables generated containing

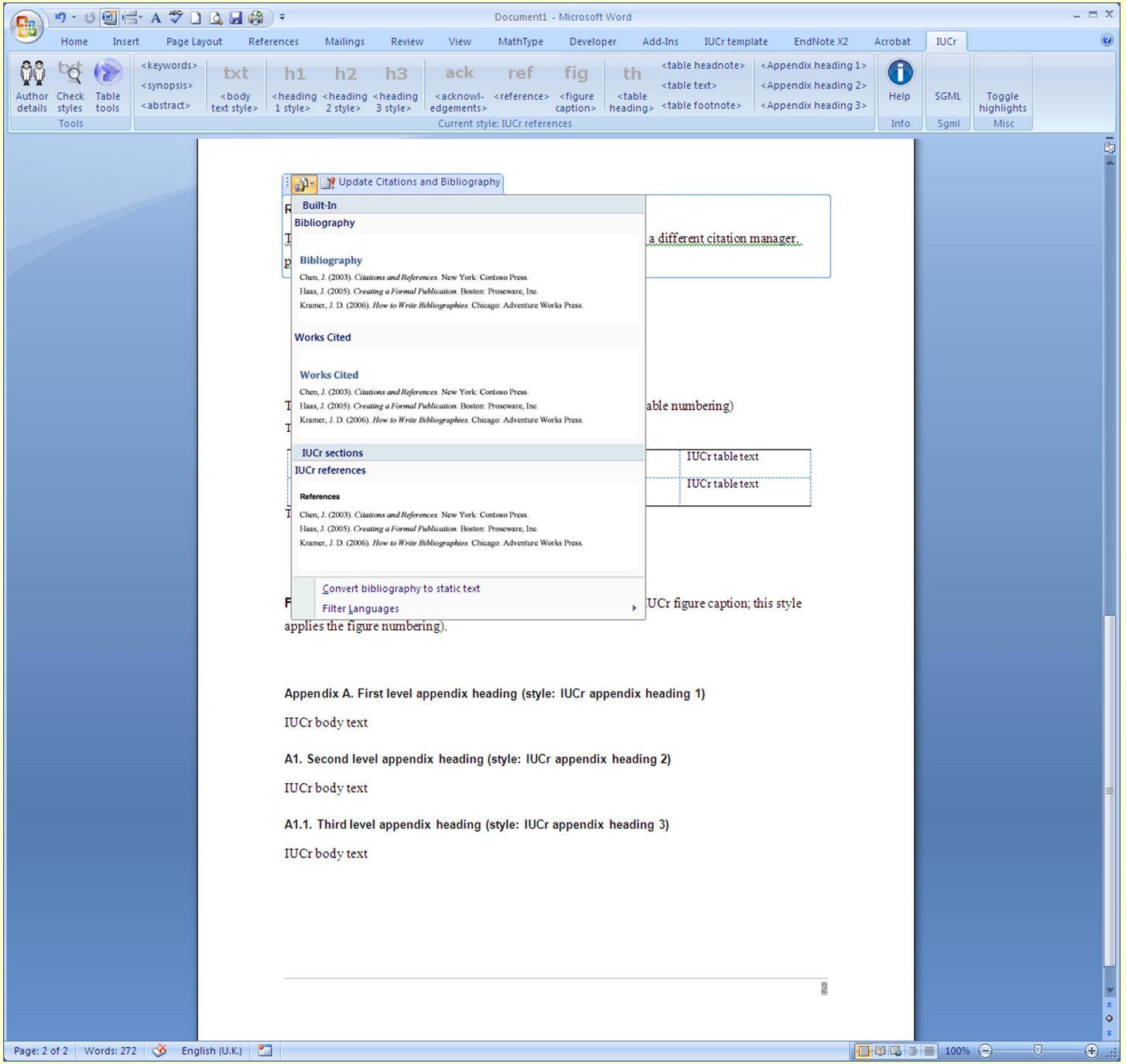
- Sample information
- Data collection and structure solution statistics
- Structure refinement and model validation

Crystallography Journals Online



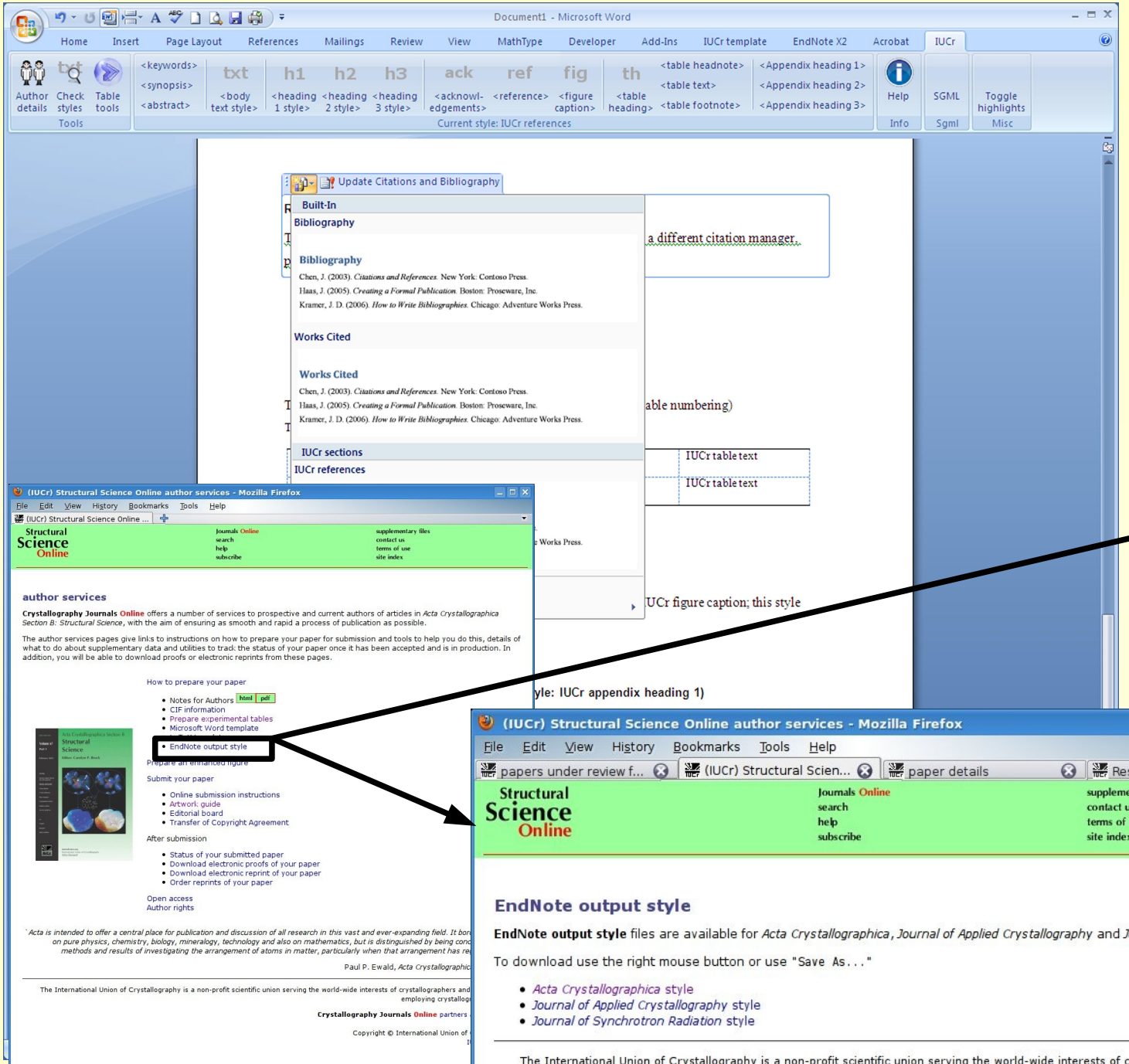
- Figure captions should be listed
- Insert appendices if appropriate
- Headings, tables, figure captions etc. are automatically numbered in journal style

Crystallography Journals Online

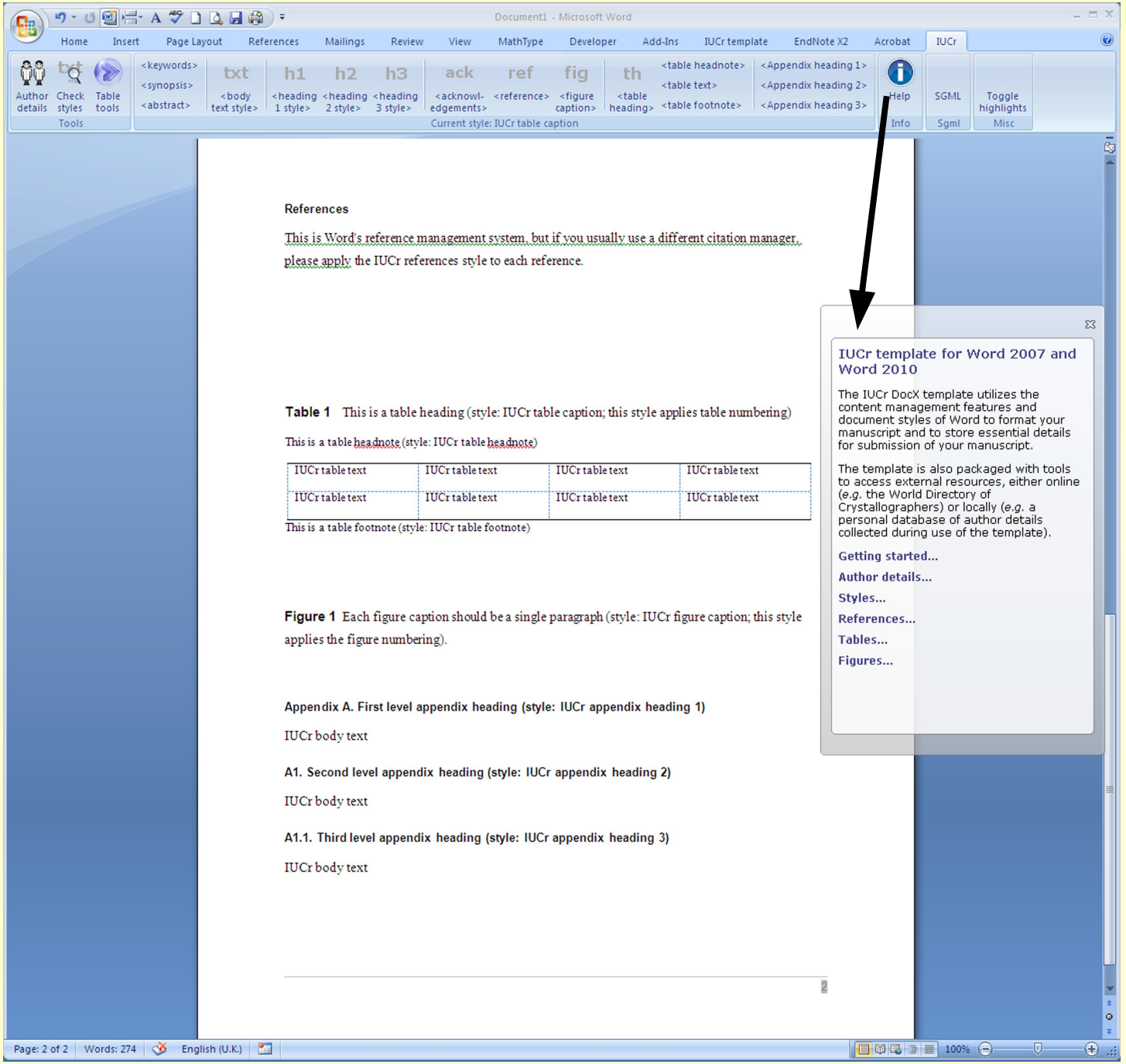


- References added using Microsoft citation manager or EndNote recognised

Crystallography Journals Online



- References added using Microsoft citation manager or EndNote recognised
- EndNote output style files are available



- 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

Crystallography Journals Online

LaTeX template

Crystallography Journals Online

(IUCr) Structural Science Online author services - Mozilla Firefox

File Edit View History Bookmarks Tools Help

(IUCr) Structural Science Online ...

Structural Science Online

Journals Online | search | help | subscribe

supplementary files | contact us | terms of use | site index

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 si
double-spaced version of the paper suitable for review purposes. Use this option for the hard-copy version of the pa
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 trans
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 accordi
style of the journal, including the proper placement of figures and tables. See the specific instructions for preparing c
in such cases

For papers containing long mathematical equations, it is helpful if the author processes the paper without the prepri
initial preparation, 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 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, c
   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. Mar
   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 colu
   They should also send hard-copy versions of the figures, and the CIF file (by email or on diskette). When the p
   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, ther
   to 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 in

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

Done

Mozilla Firefox

File Edit View History Bookmarks Tools Help

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

ftp://ftp.iucr.org/templates/latex/template.ltx

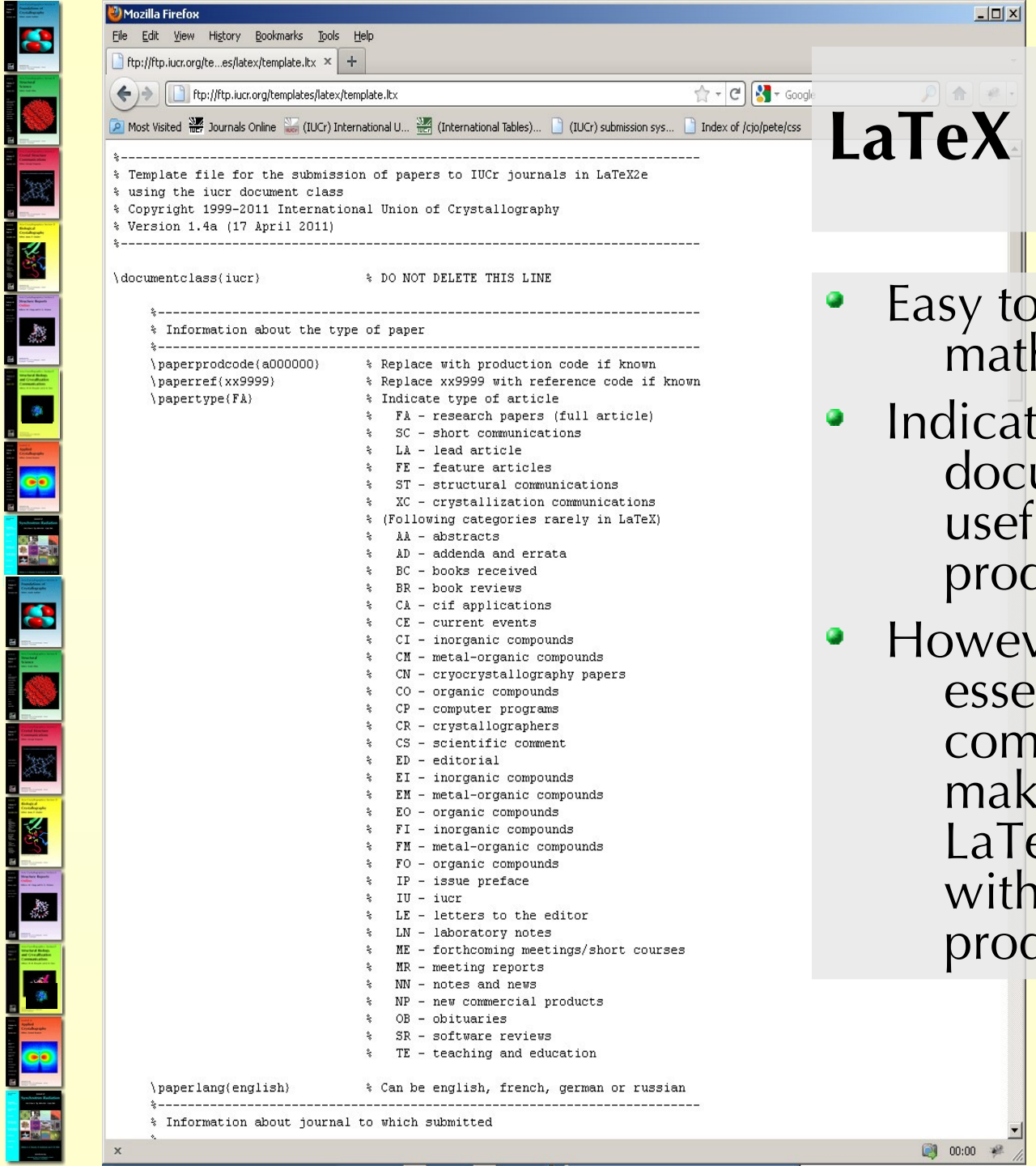
Most Visited | Journals Online | (IUCr) International U... | (International Tables)... | (IUCr) submission sys... | Index of /cjo/pete/css

```
%-------------------------------------------------------------------------------
% 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
```

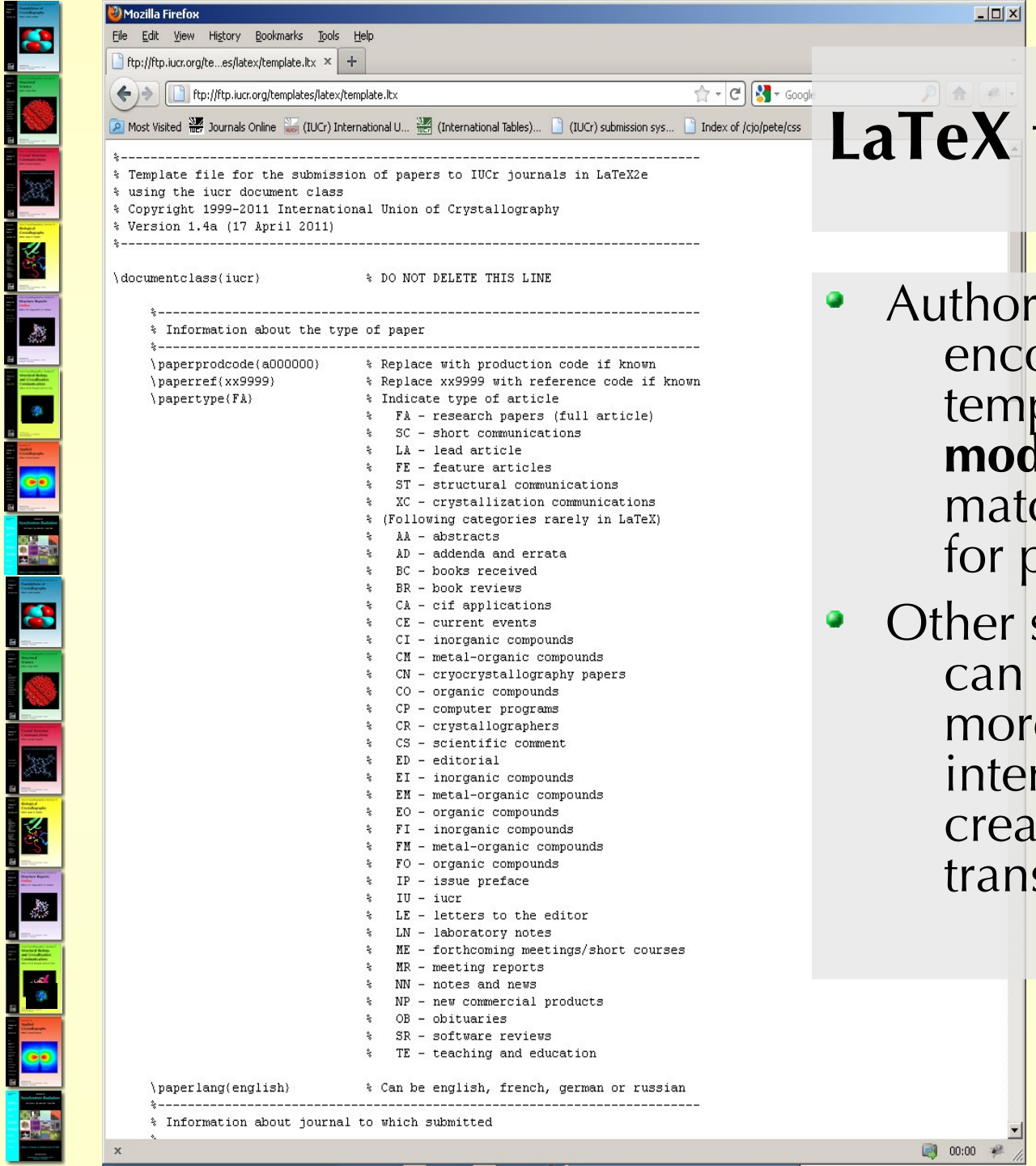
- LaTeX template instructions and files (**template** and **IUCr class file**) from author services page



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

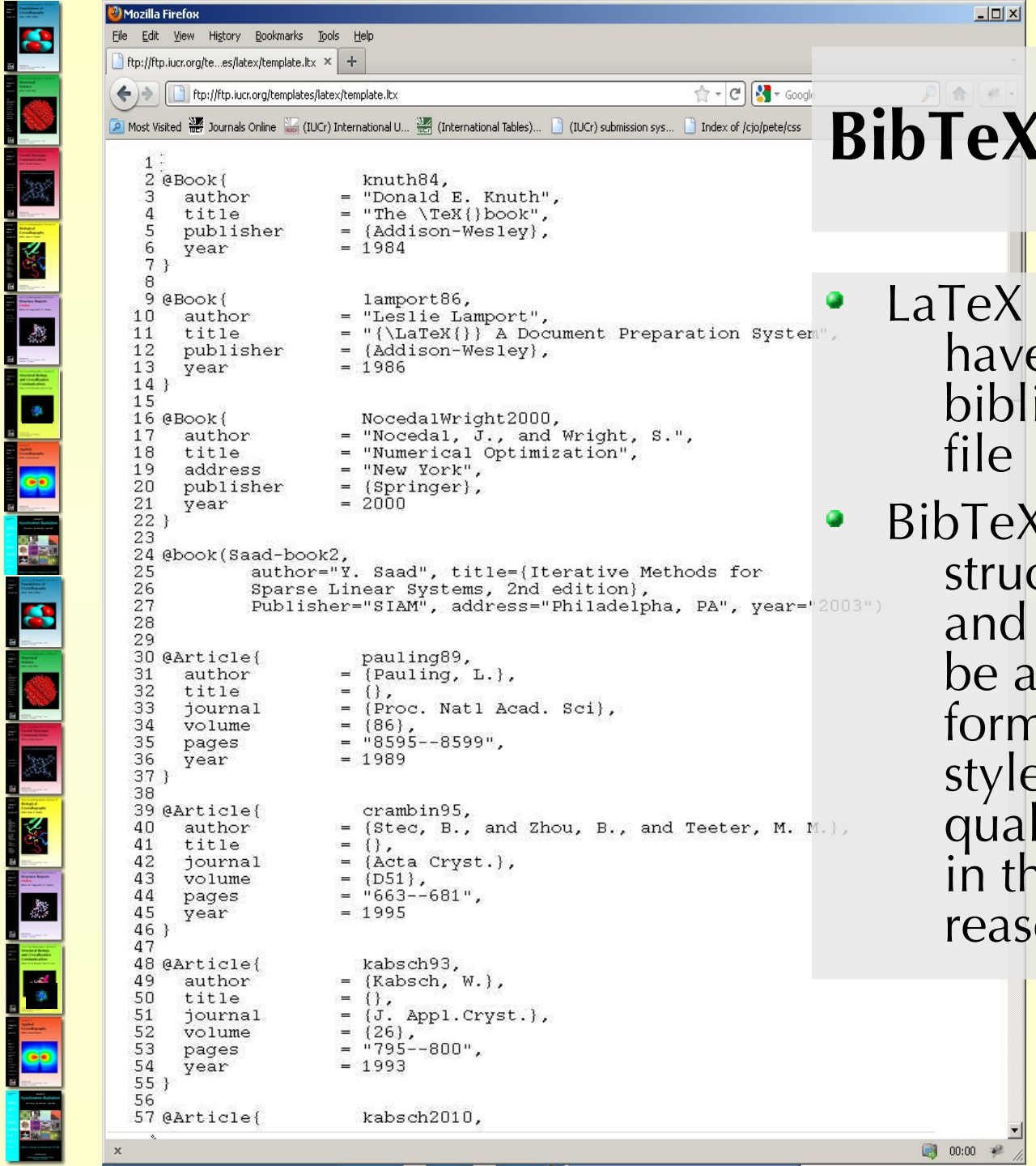
Crystallography Journals Online



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

Crystallography Journals Online



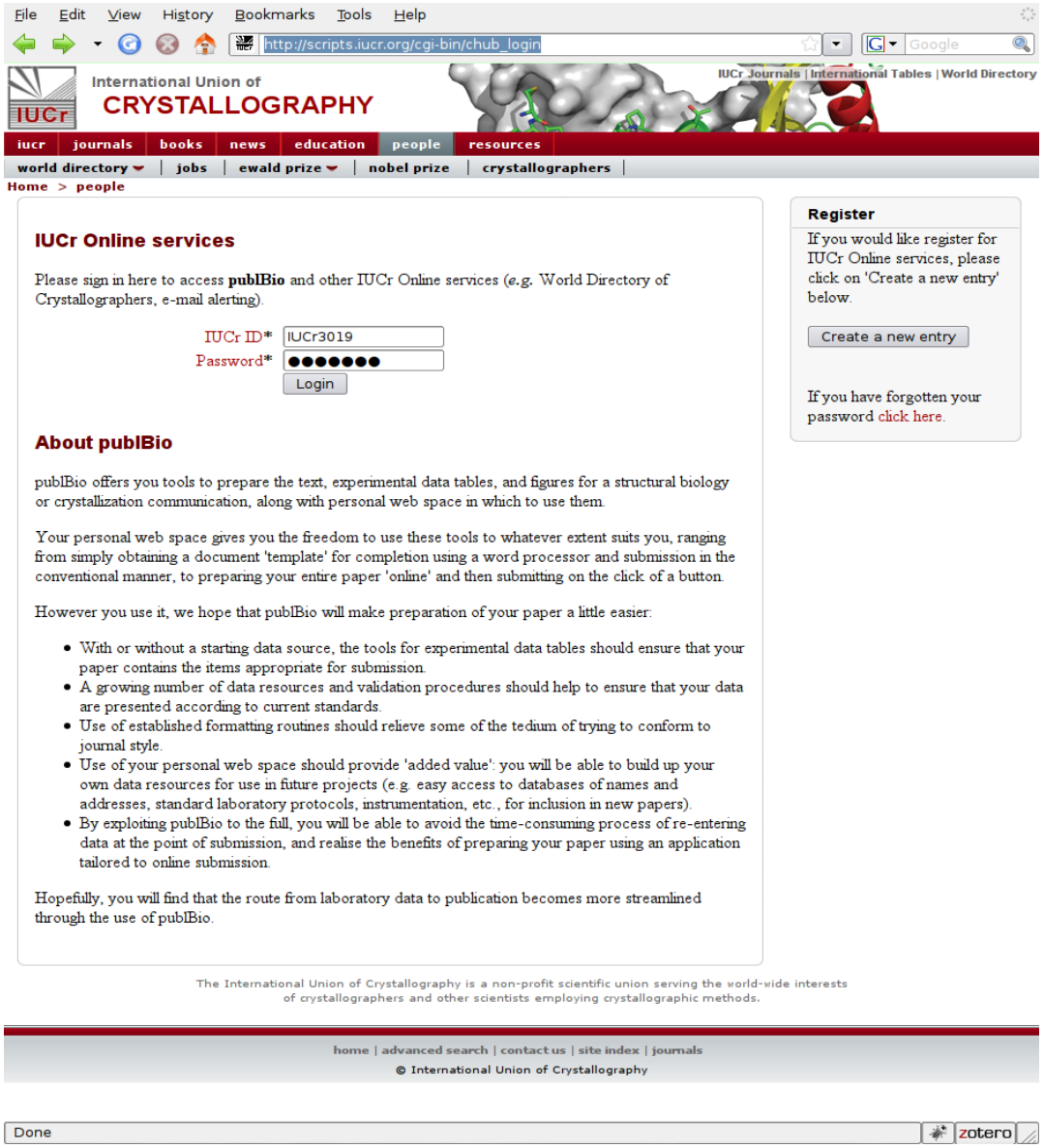
BibTeX

- 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)

Crystallography Journals Online

publBio

Crystallography Journals Online

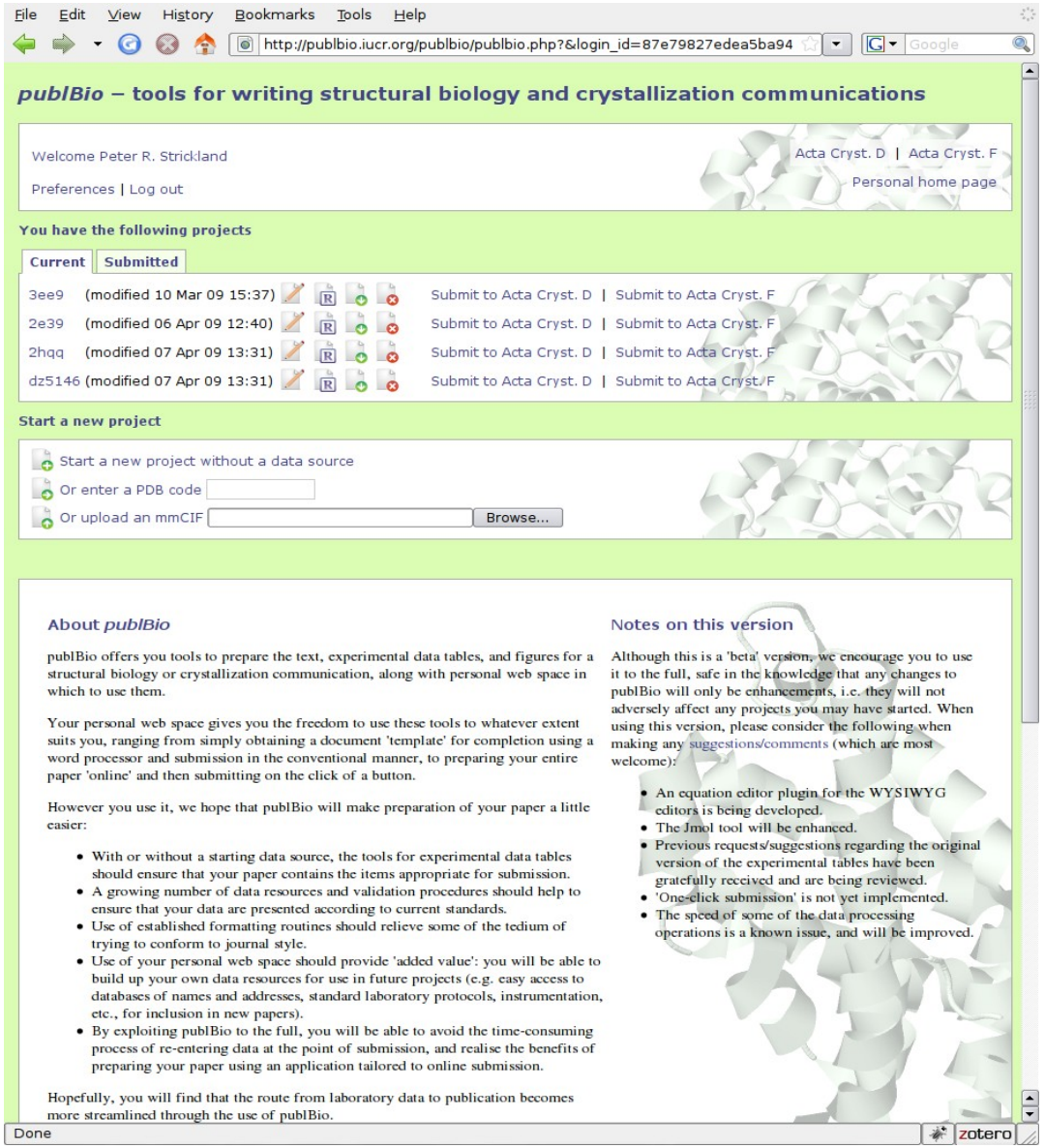


PublBio is a first attempt to provide an online authoring tool for authors in the “cloud”

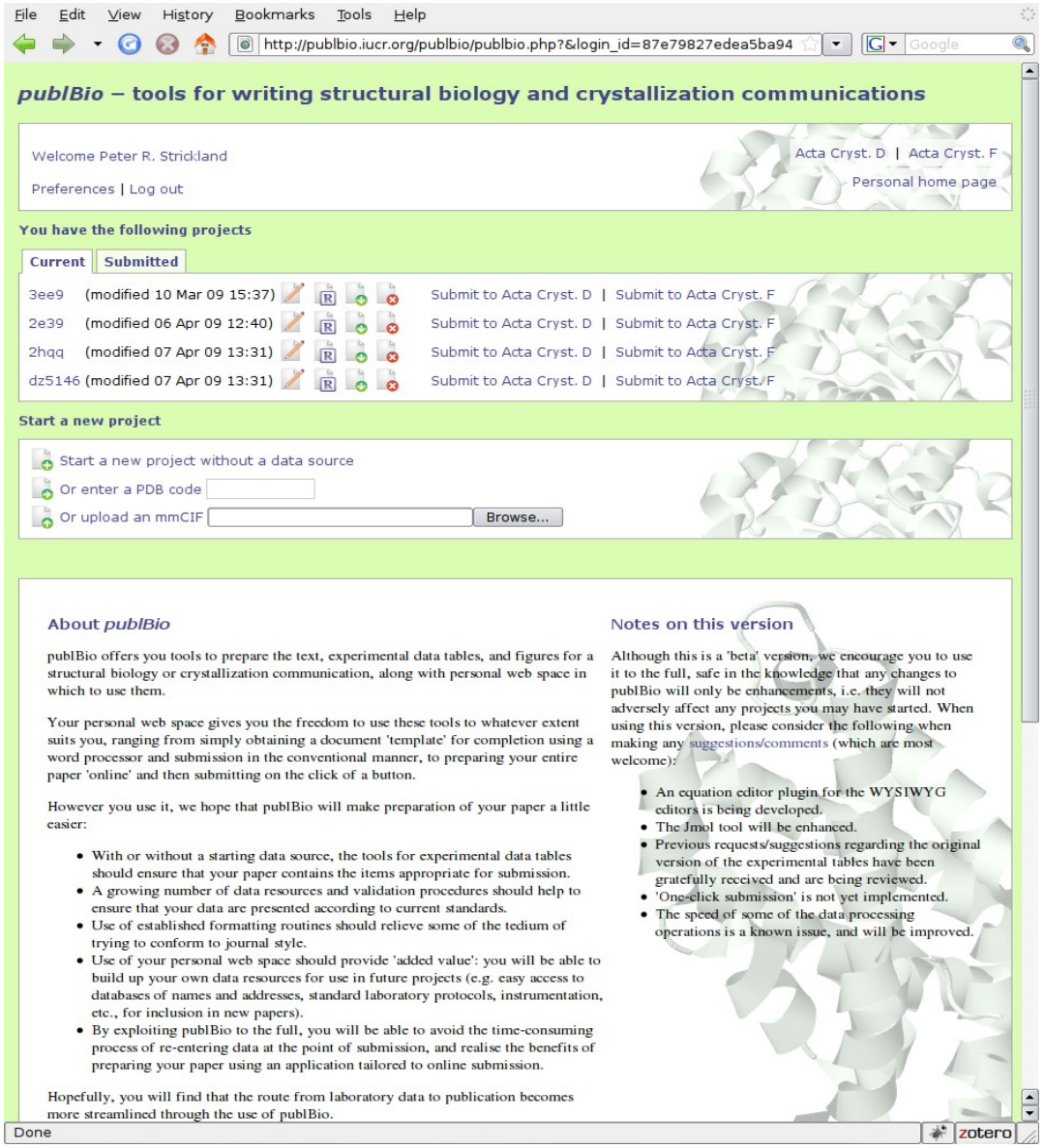
It is currently available to authors of Sections D and F

A quick tour of publBio follows

publBio requires a login and simple registration



your publBio home page shows all your projects



start from scratch

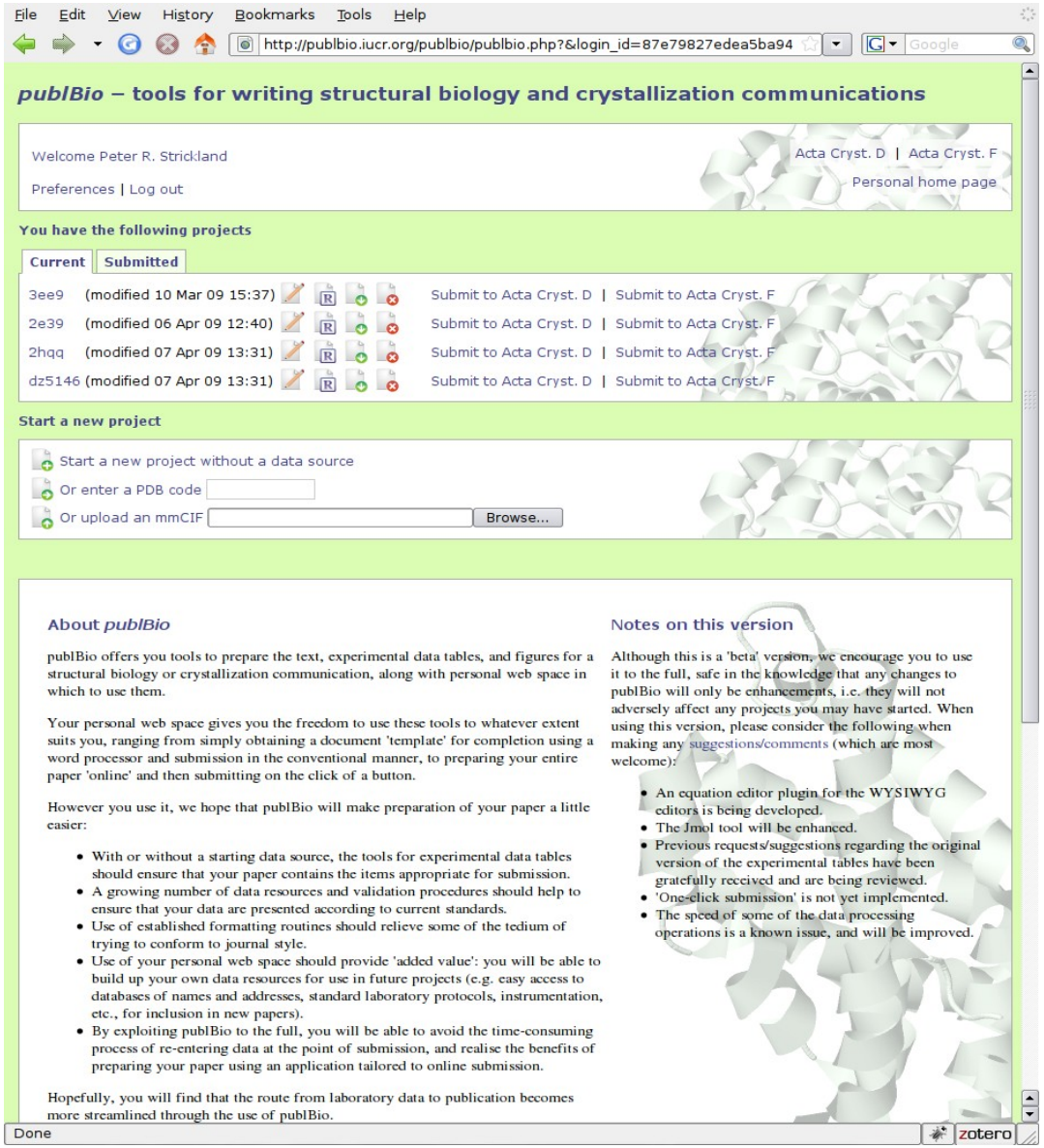
or

enter a PDB code

or

upload an mmCIF

starting a project is simple



rename

edit

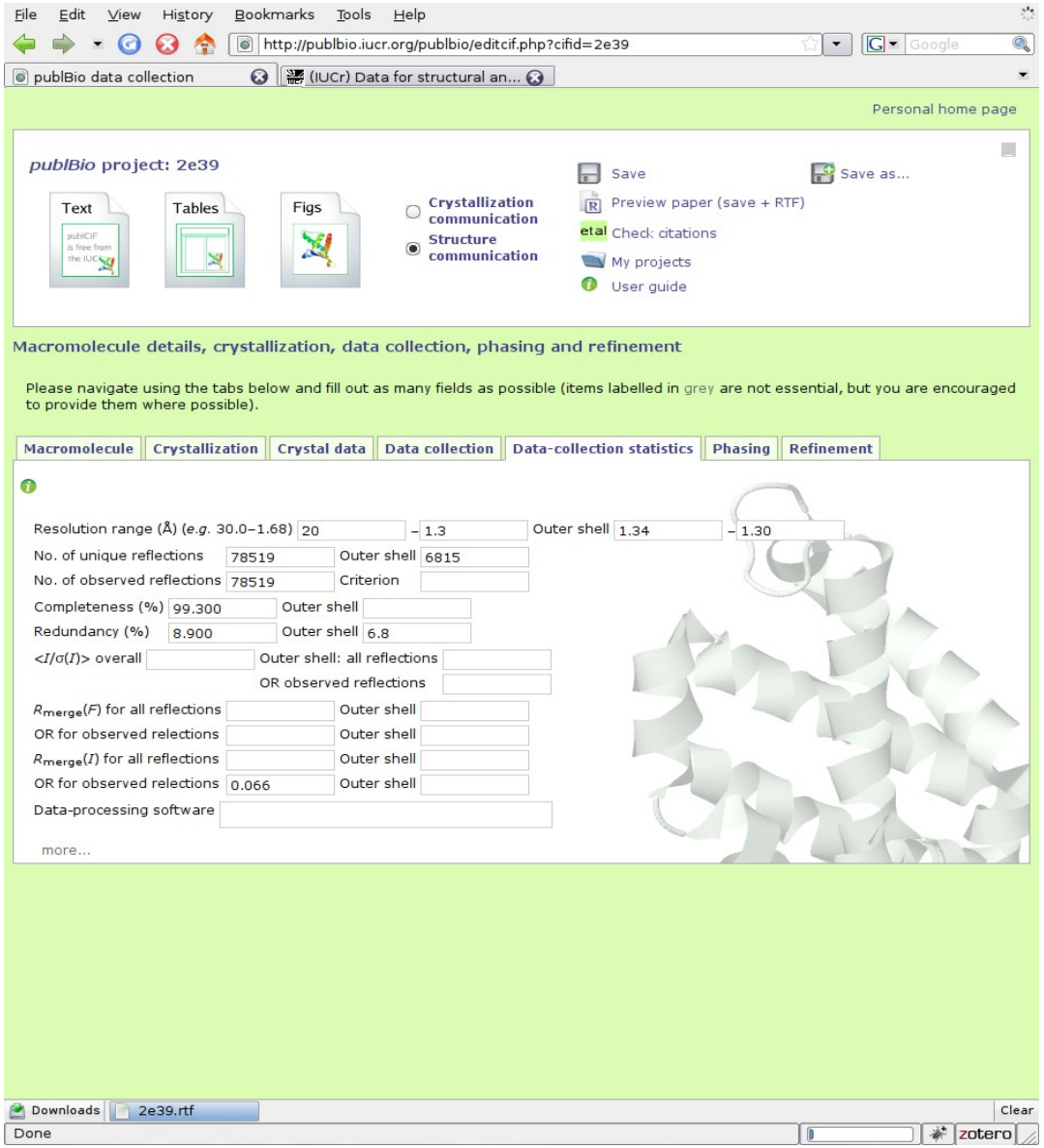
preview

copy

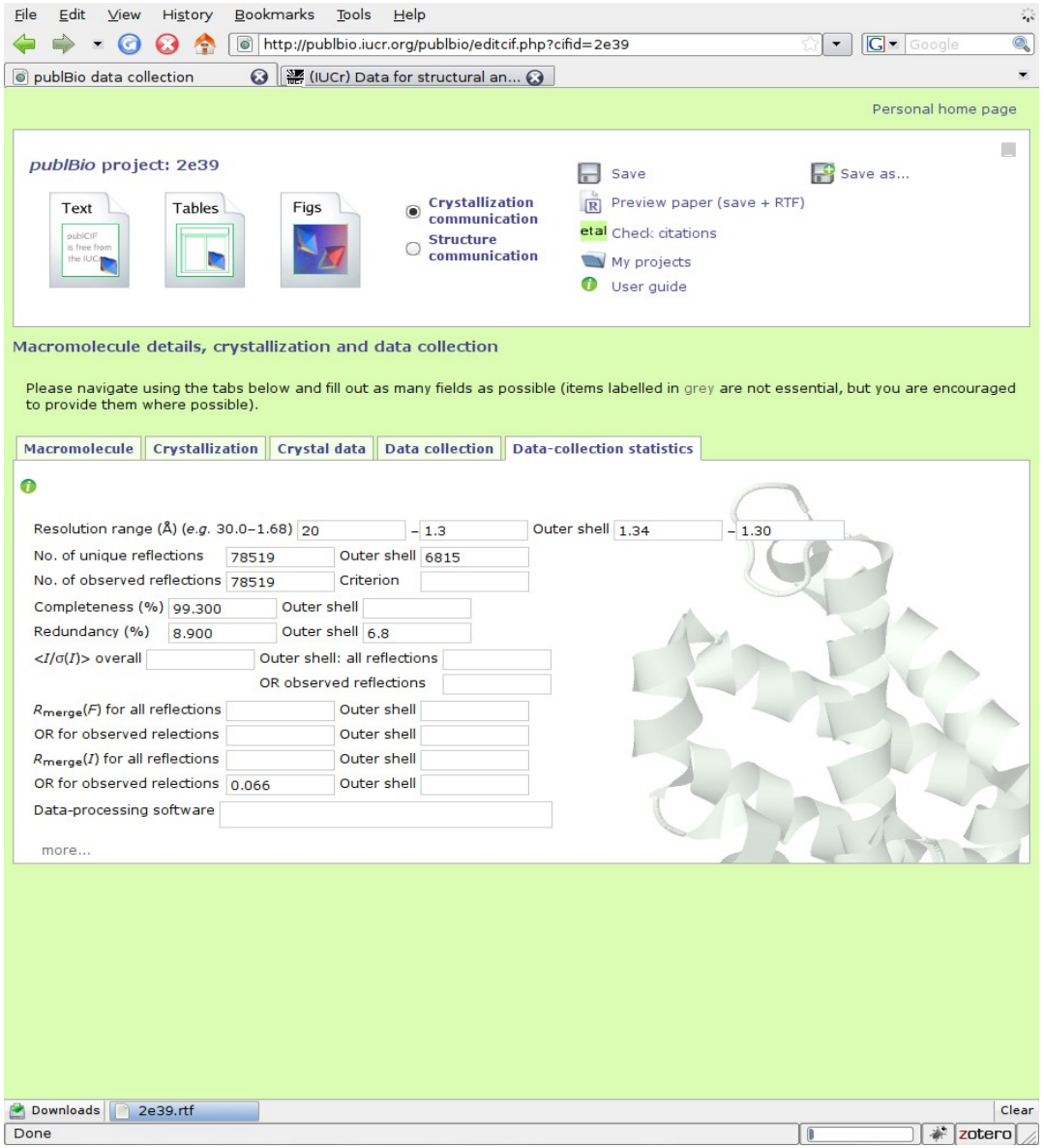
delete

submit

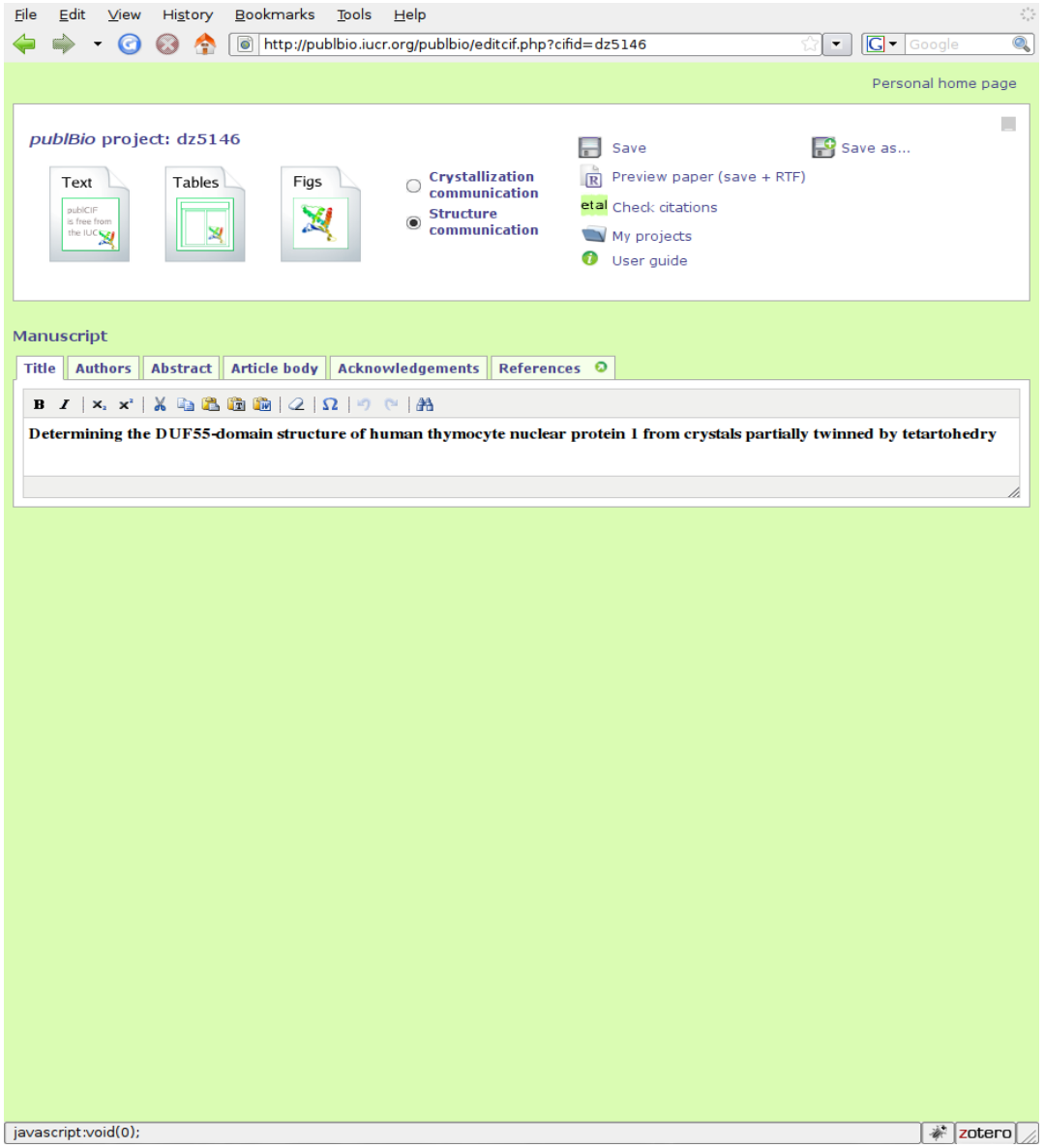
current and submitted projects can be modified



data can be reported for structural studies



or just for crystallization studies



The text tab consists of six tabs

title

authors

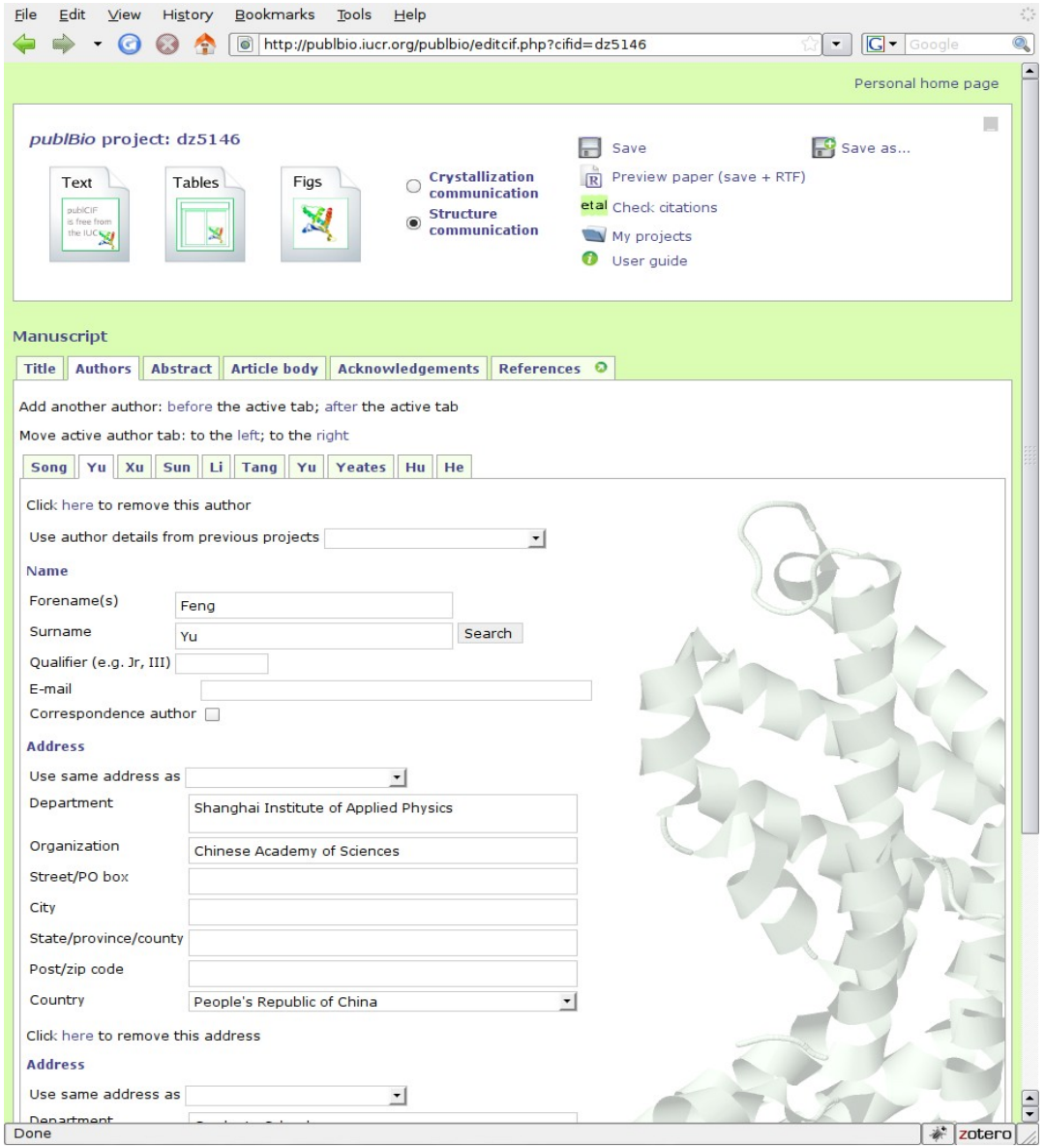
abstract

article body

acknowledgements

references

clicking on a tab opens that part of the article

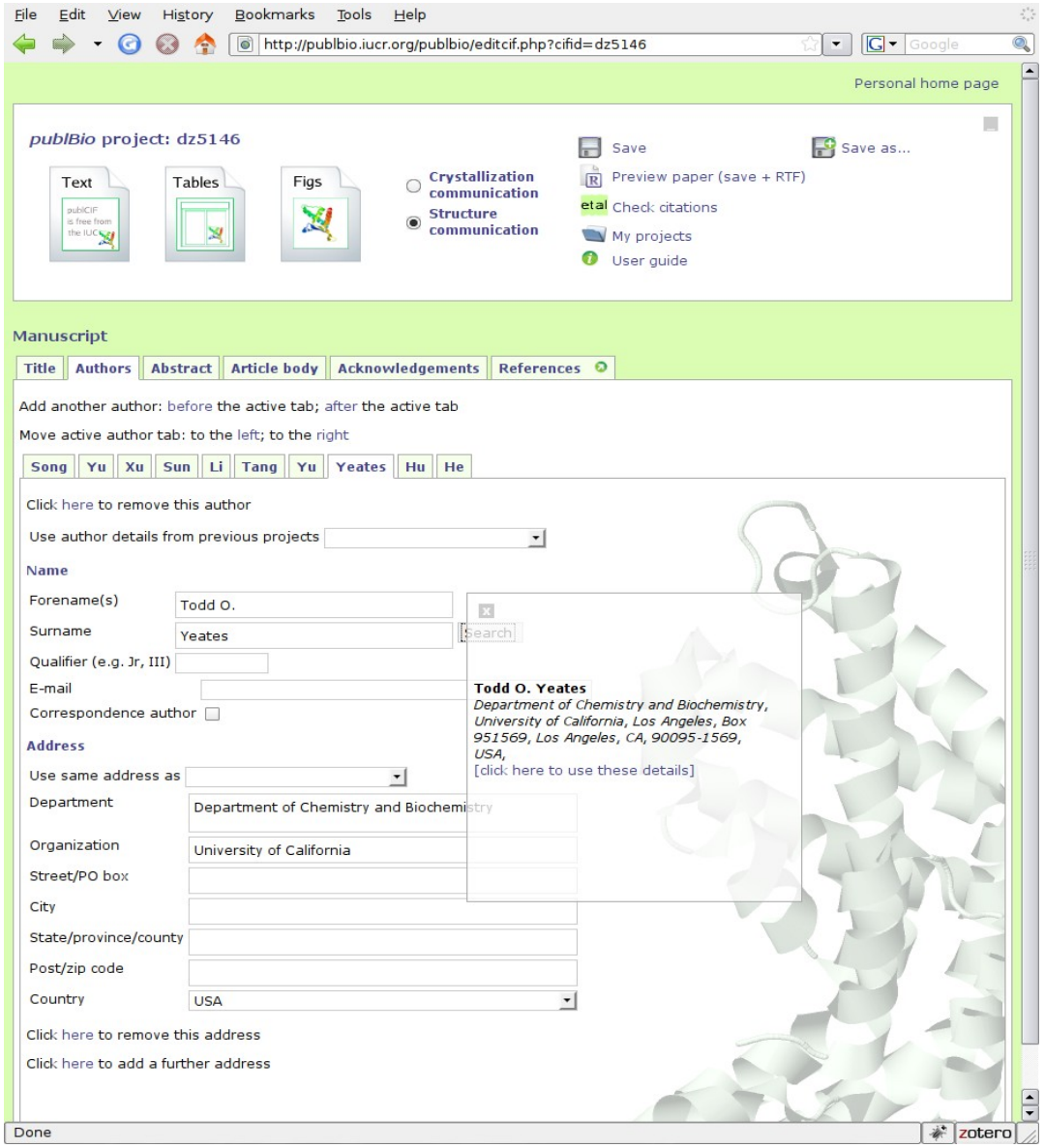


new author tabs may be added

authors may be reordered

authors can have multiple addresses

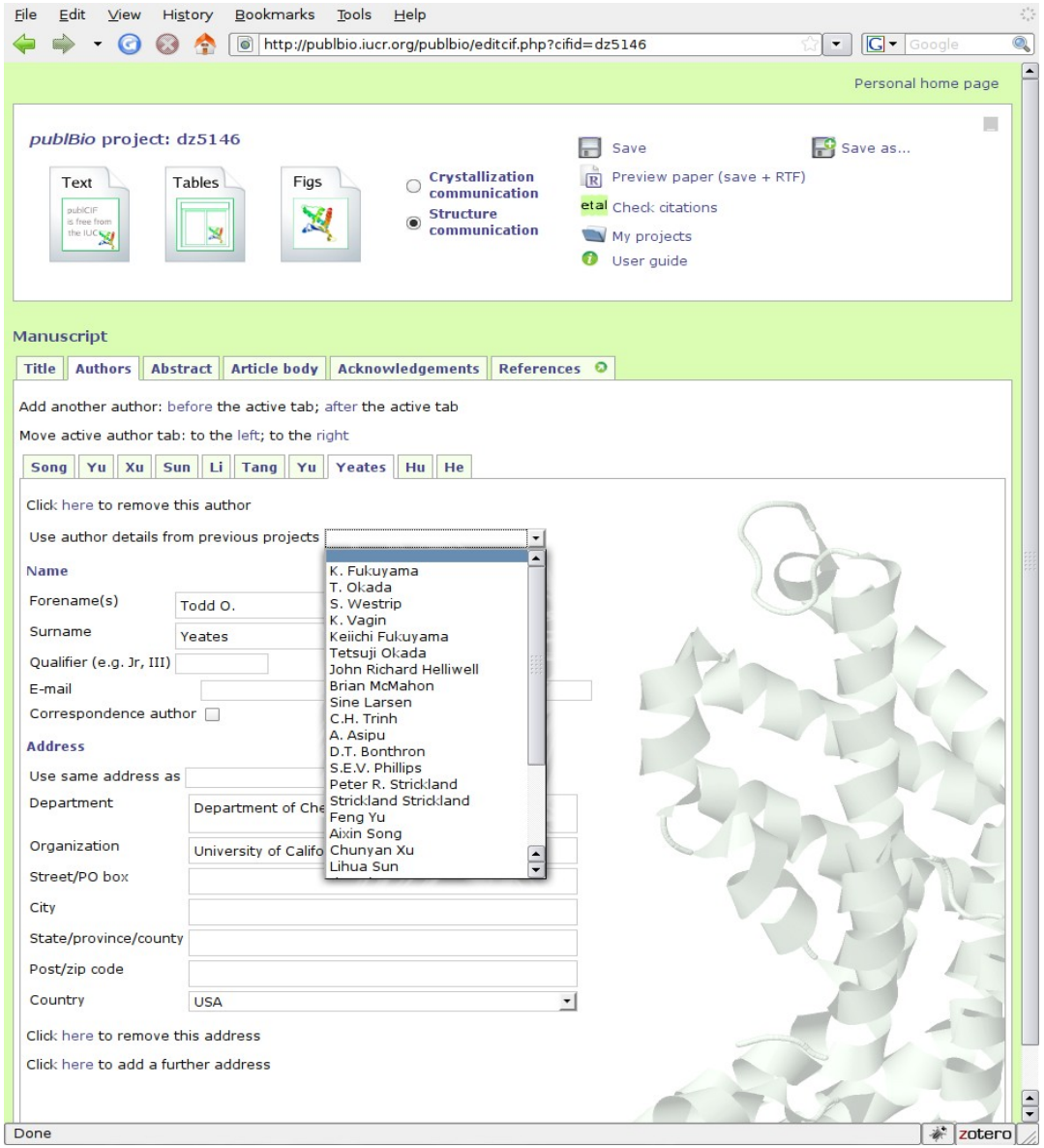
author details may be added manually



click on the search results to add an author

author search is carried out on the World Directory of Crystallographers

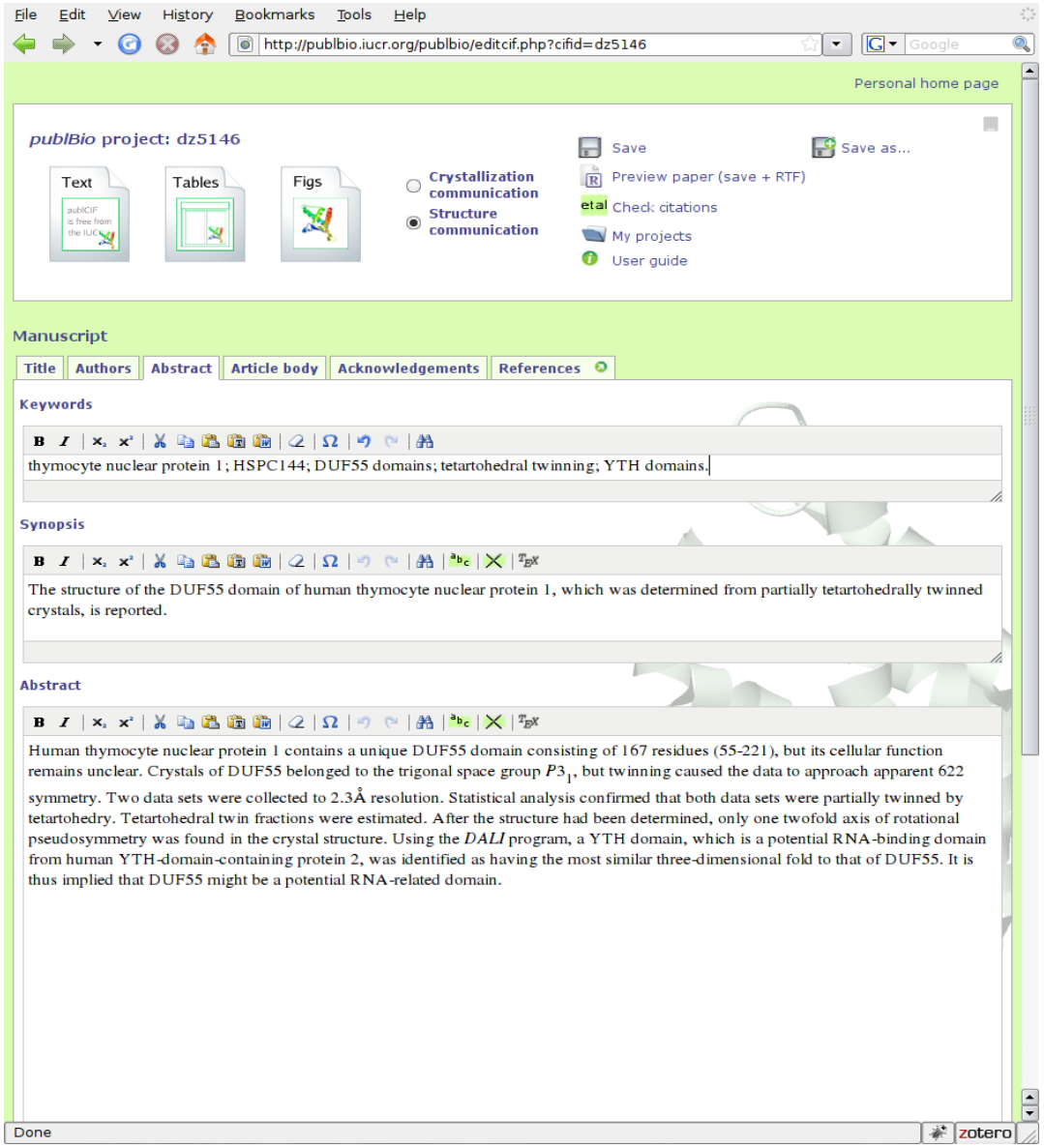
authors may be added by searching



publBio maintains a record of author details used in previous projects

click on a name to add details to the current project

authors may be added from previous projects



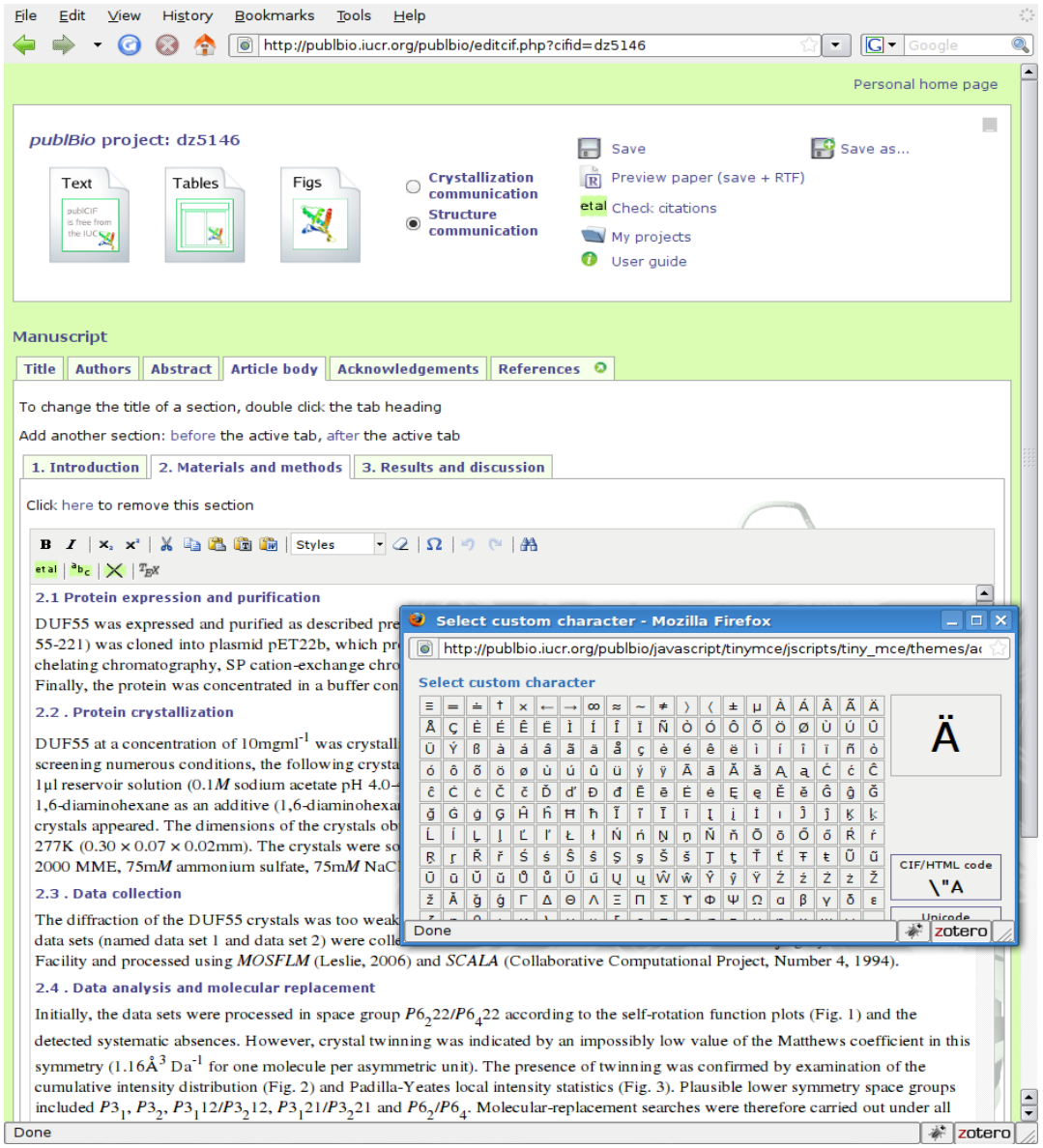
the abstract tab contains the following fields

keywords

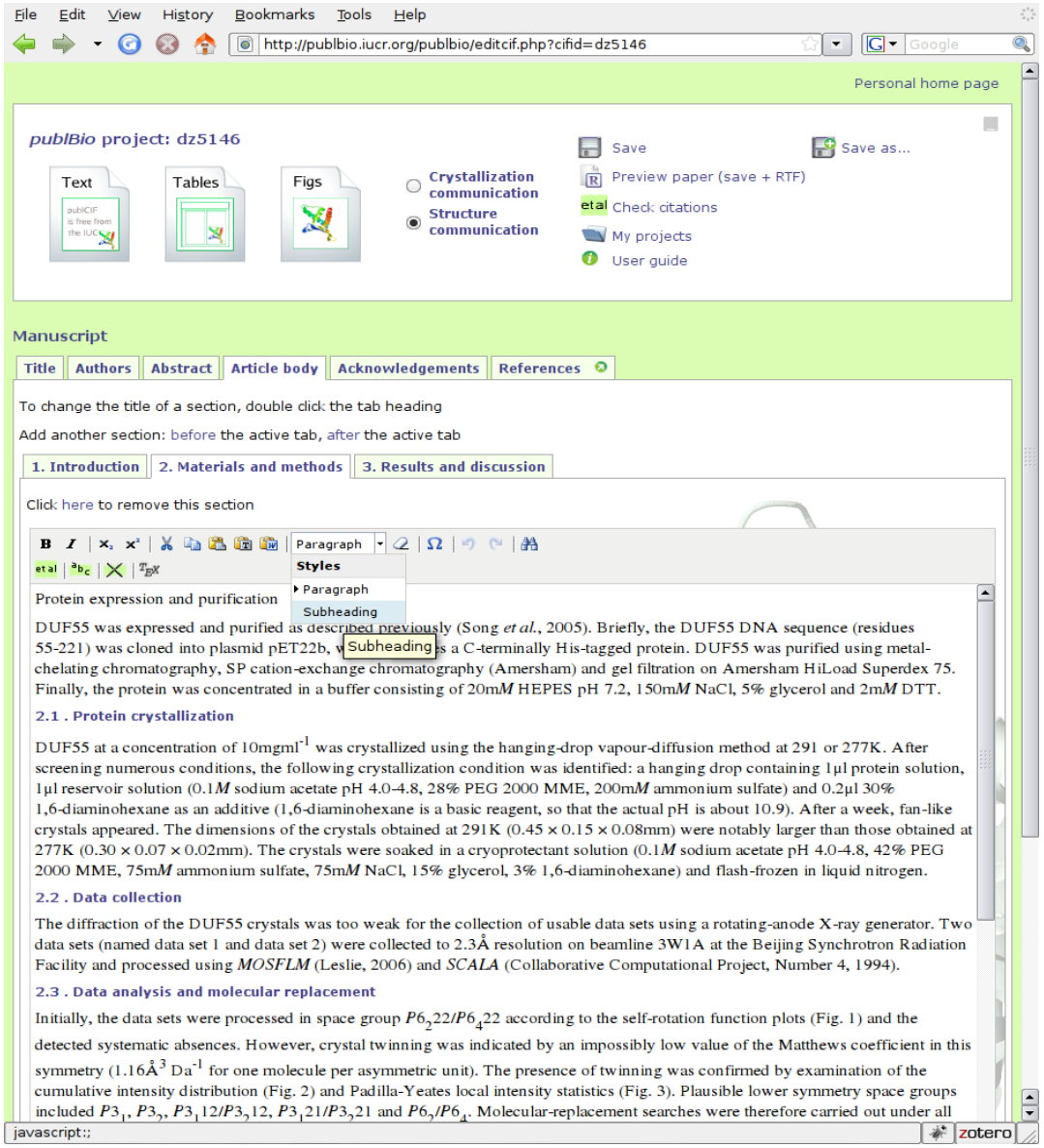
synopsis

abstract

text fields have a WYSIWYG interface



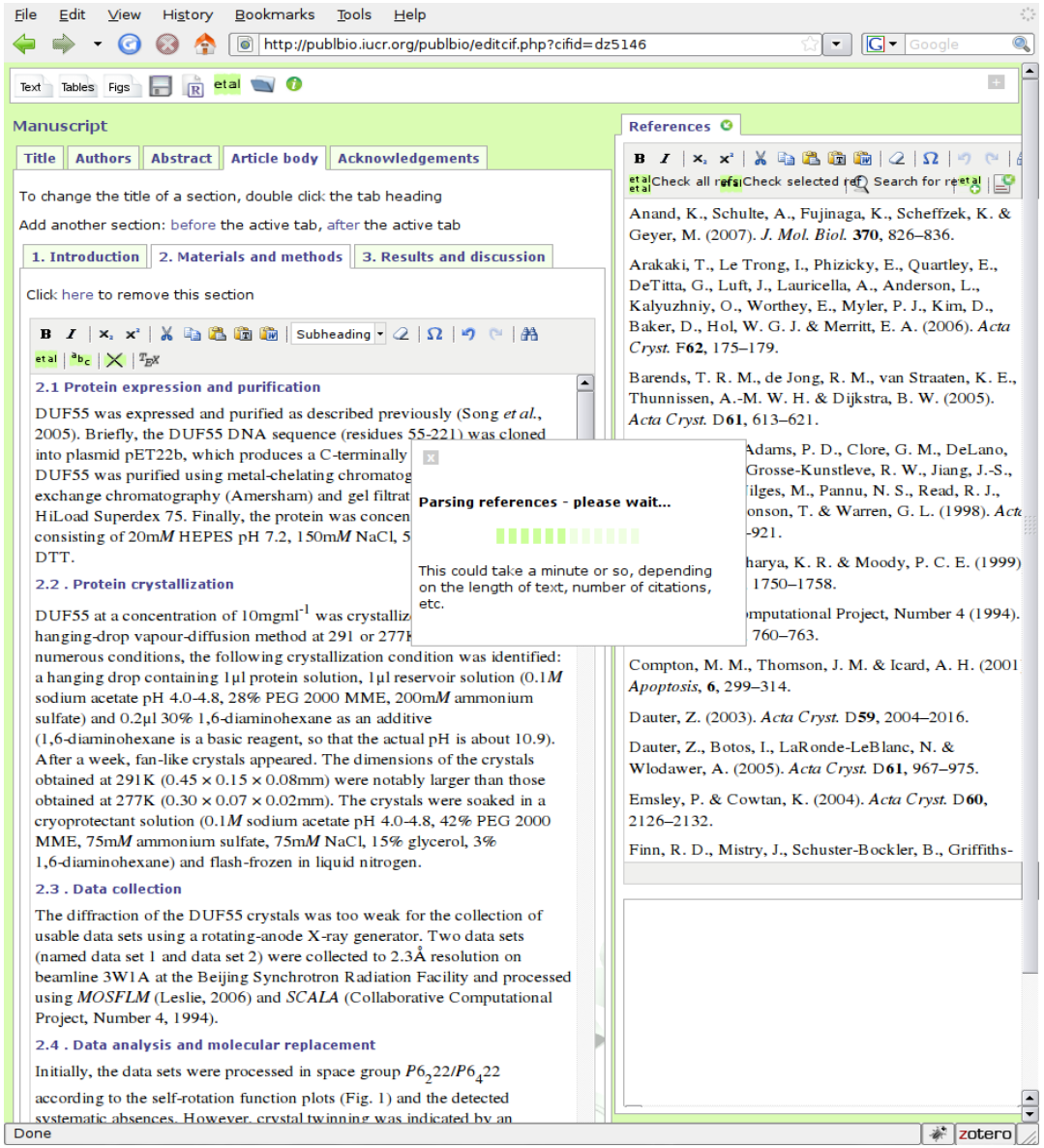
special characters can be inserted



tabs form the main headings

subheadings are inserted by the WYSIWYG editor

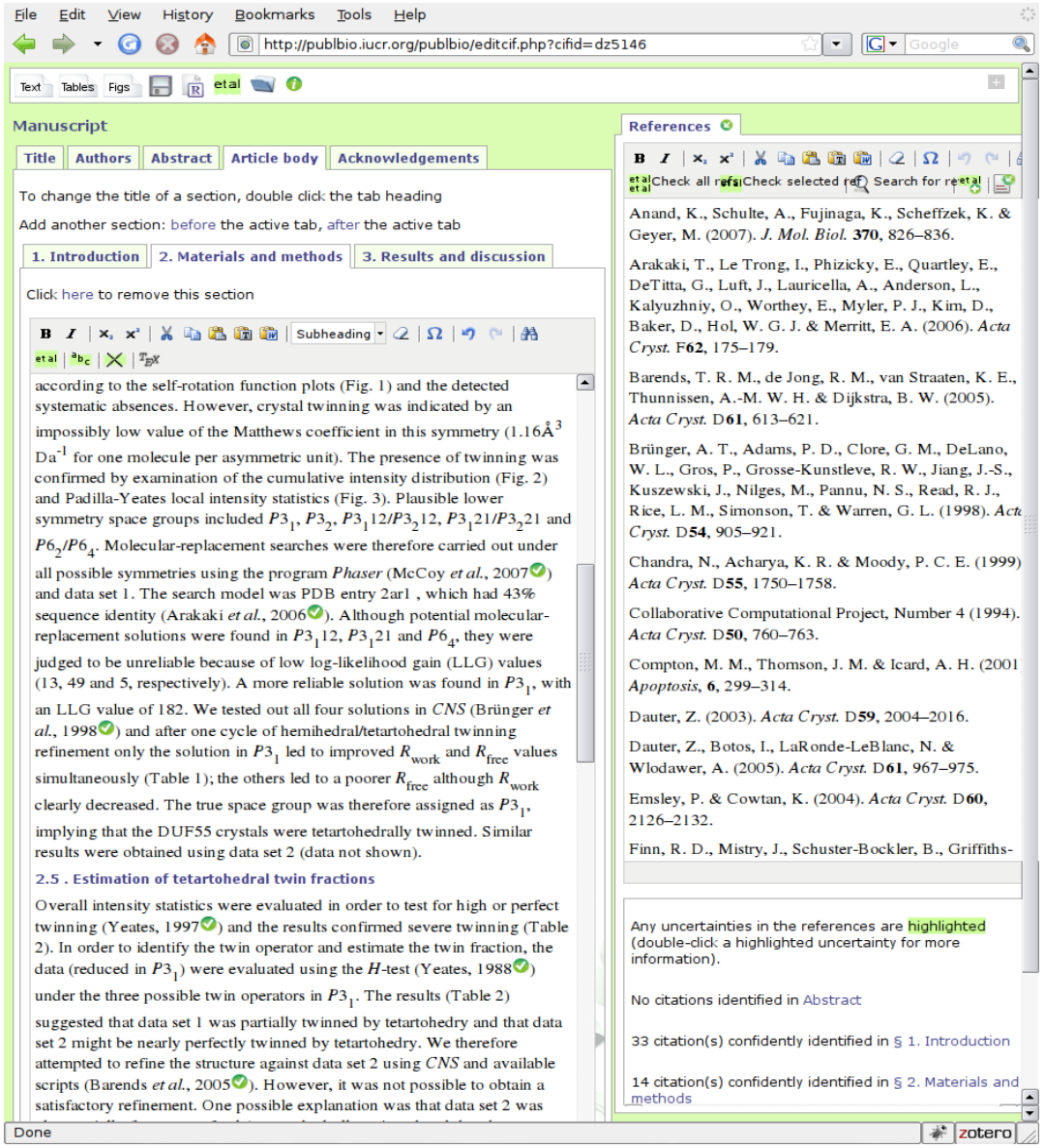
headings and subheadings can be indicated



Check that references in the text are in the reference list

Check that references in the reference list are in the text

references in the text can be checked



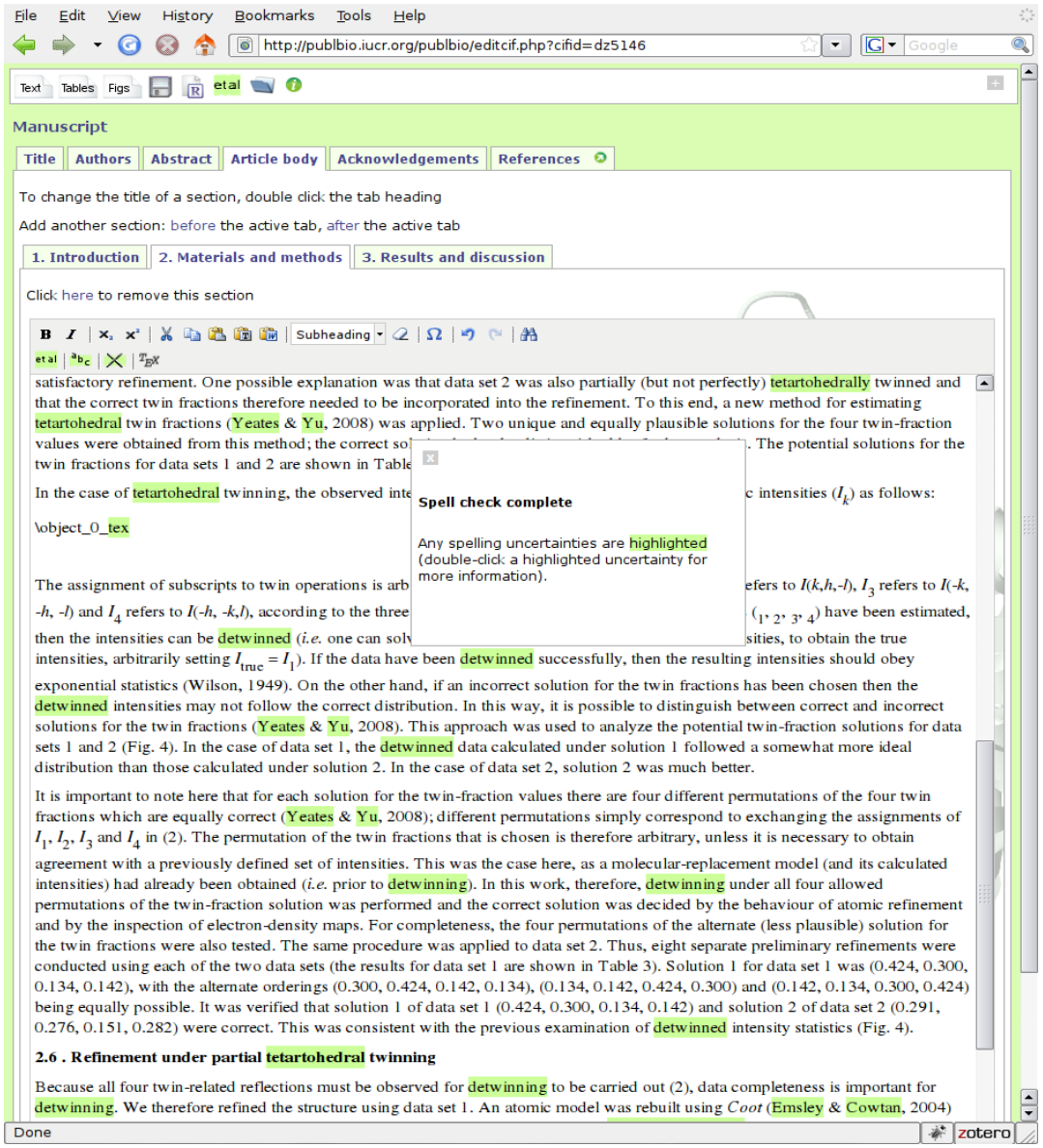
confidently identified references are checked in green

possible citation problems are highlighted

a reference checking report is provided

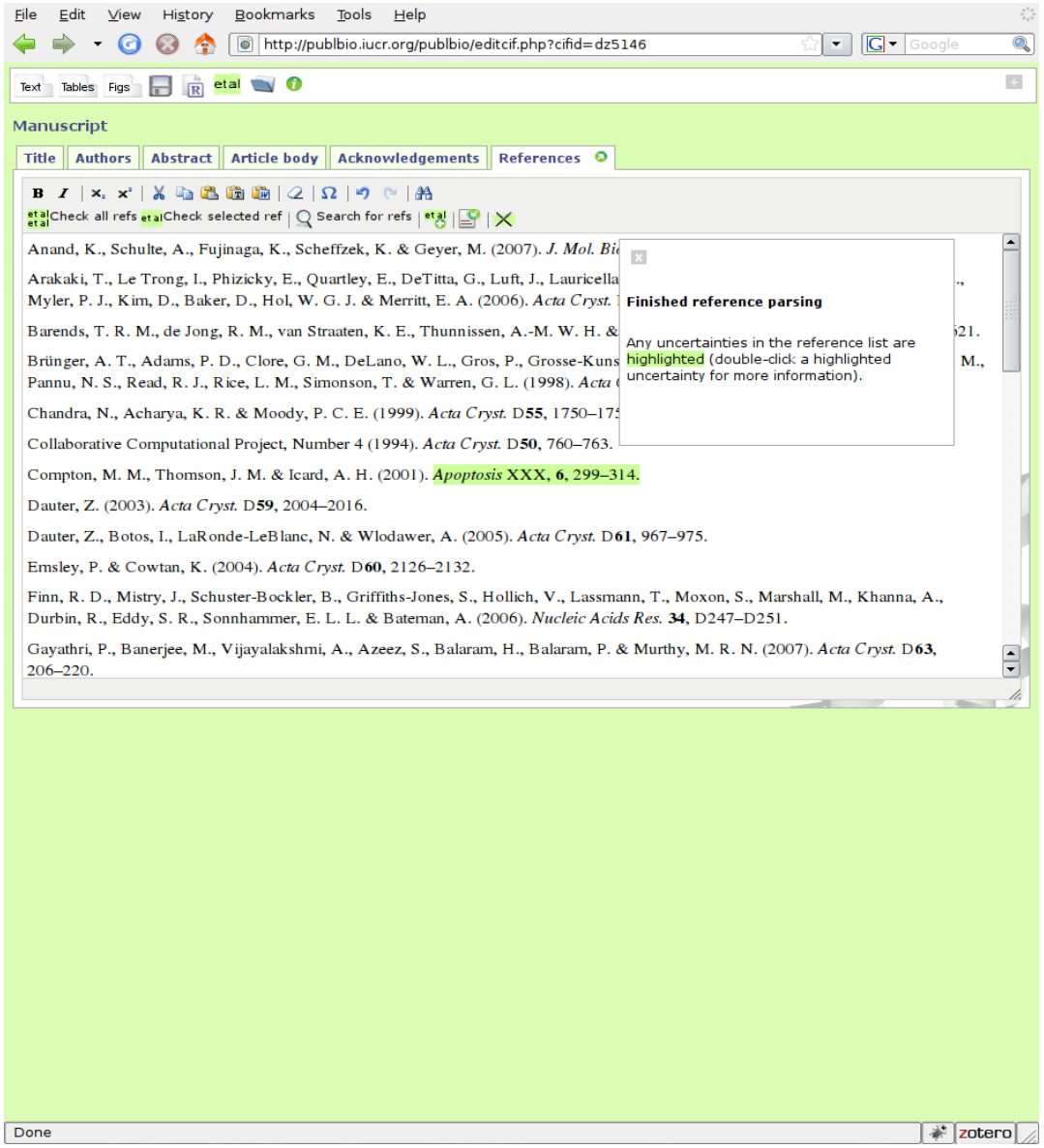
complex mathematics can be handled

mathematics may be input with an equation editor or as TeX



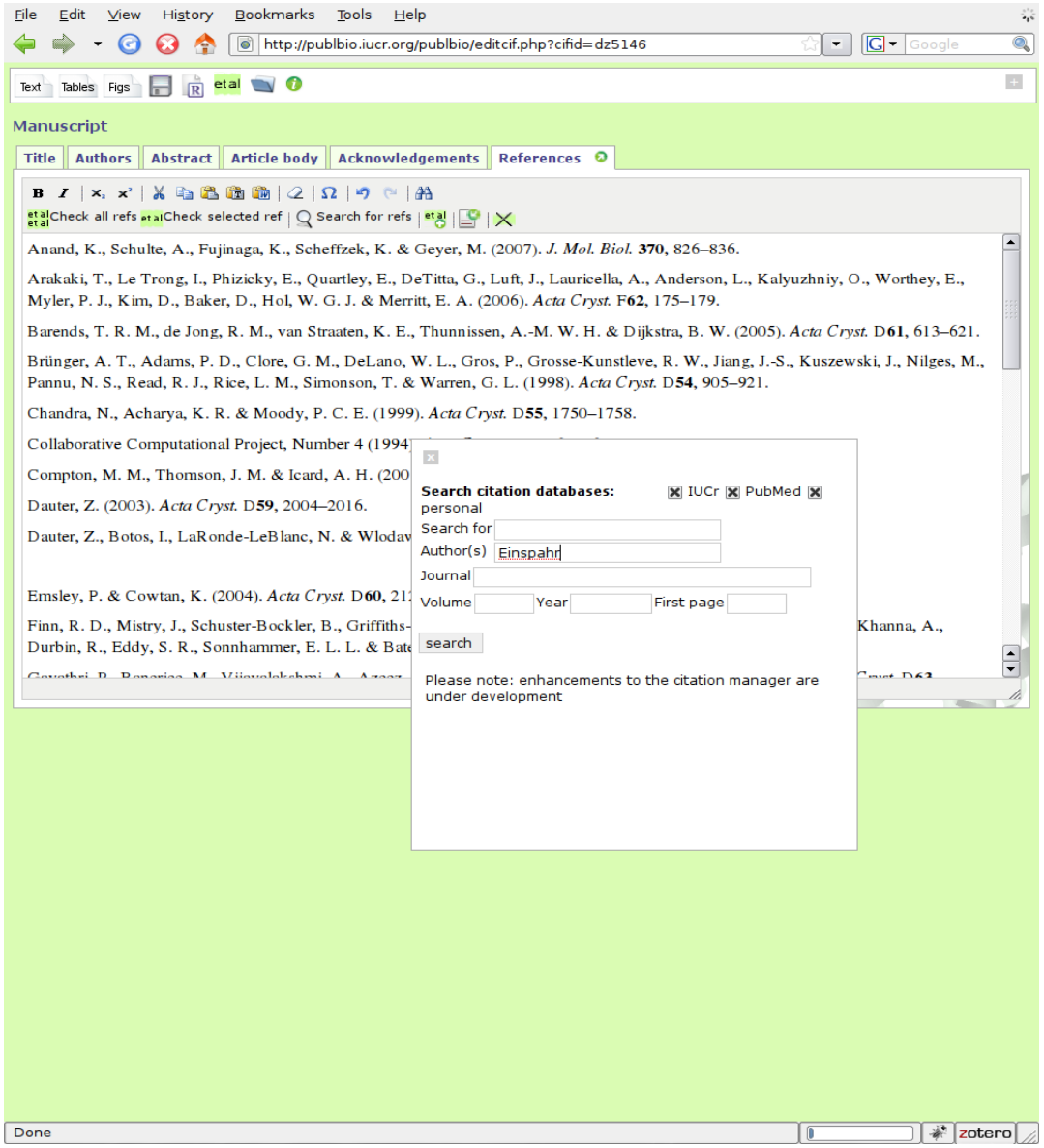
possible spelling problems are highlighted

spell checking is also available



reference list formatting may be checked

possible problems with reference list formatting are highlighted



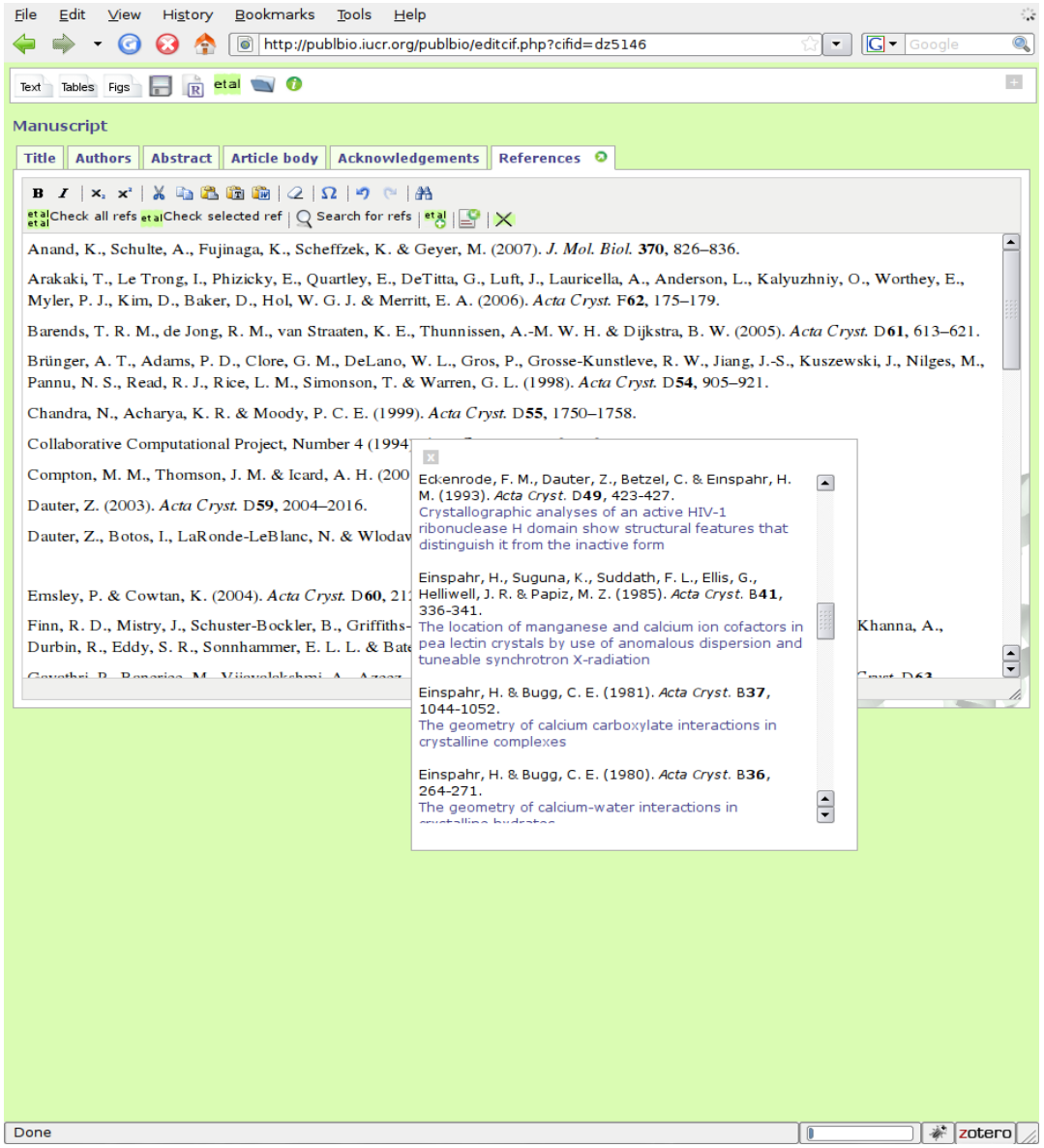
citation databases may be checked

searches can be made on

IUCr Journals

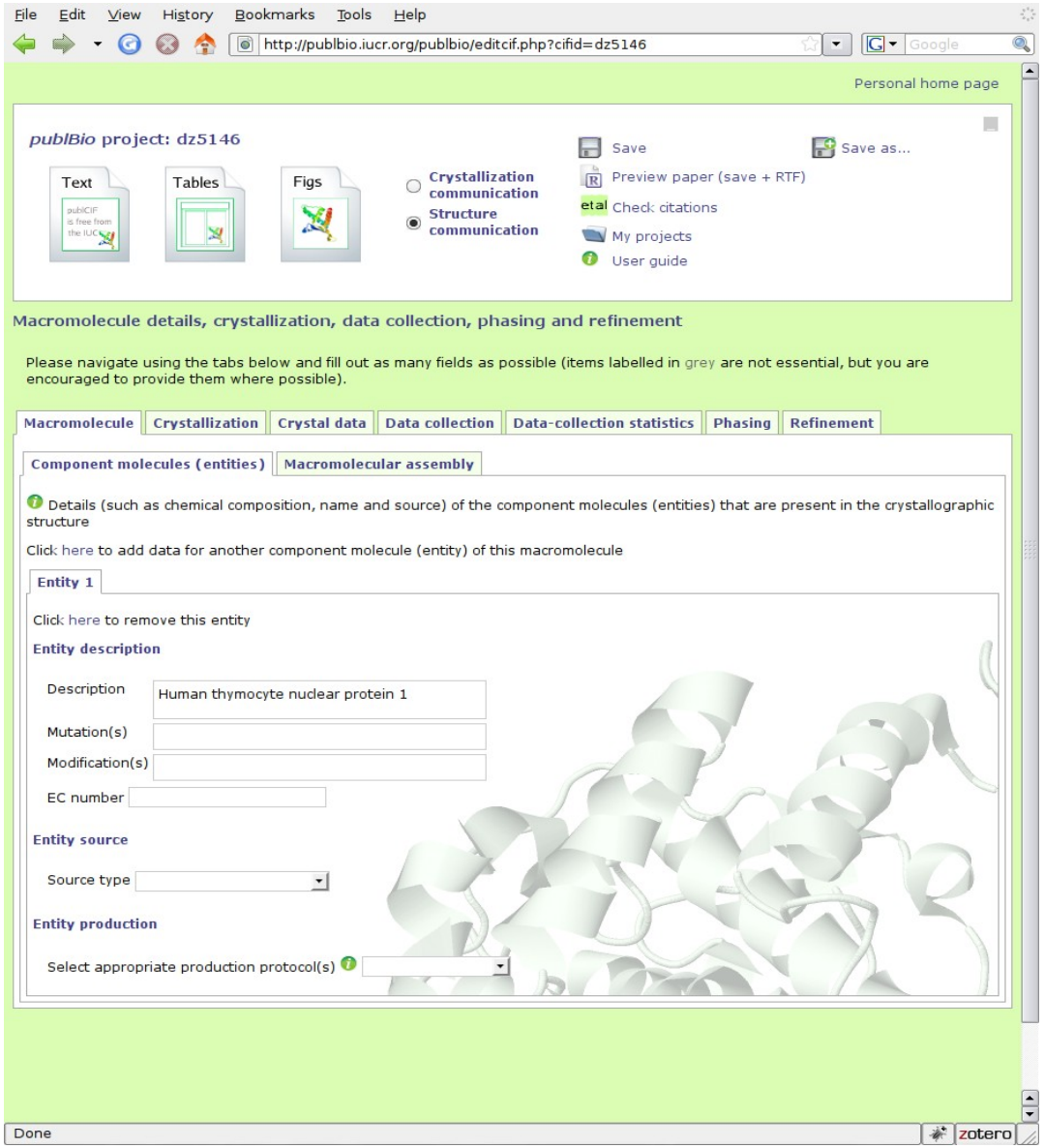
PubMed

personal database



references can be added
from search results
with a single mouse click

results are displayed in a separate window



The tables tab consists of a number of tabs

macromolecule

crystallization

crystal data

data collection

data-collection statistics

phasing

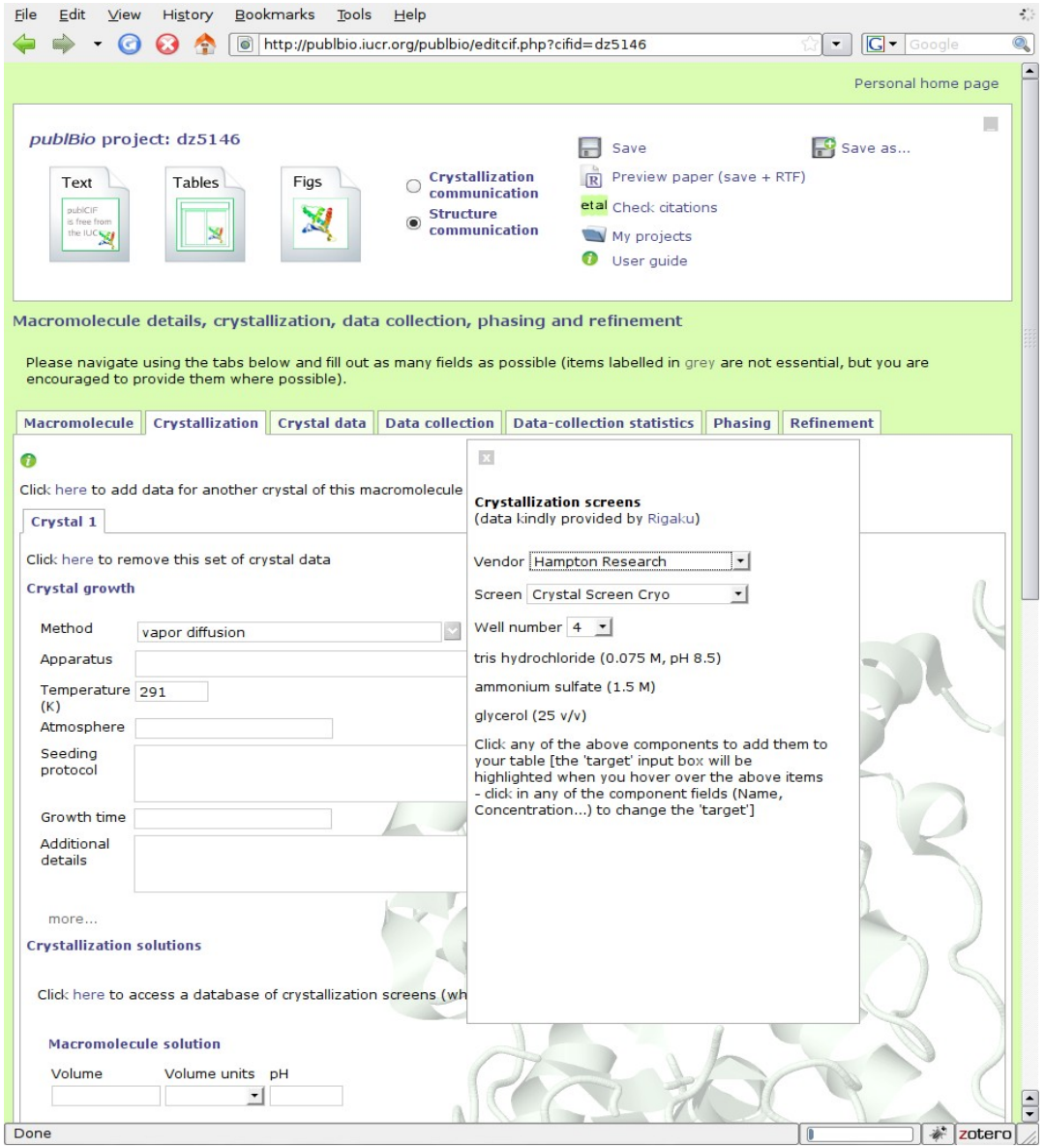
refinement

experimental data can be edited in the tables tabs

data from previous projects are remembered

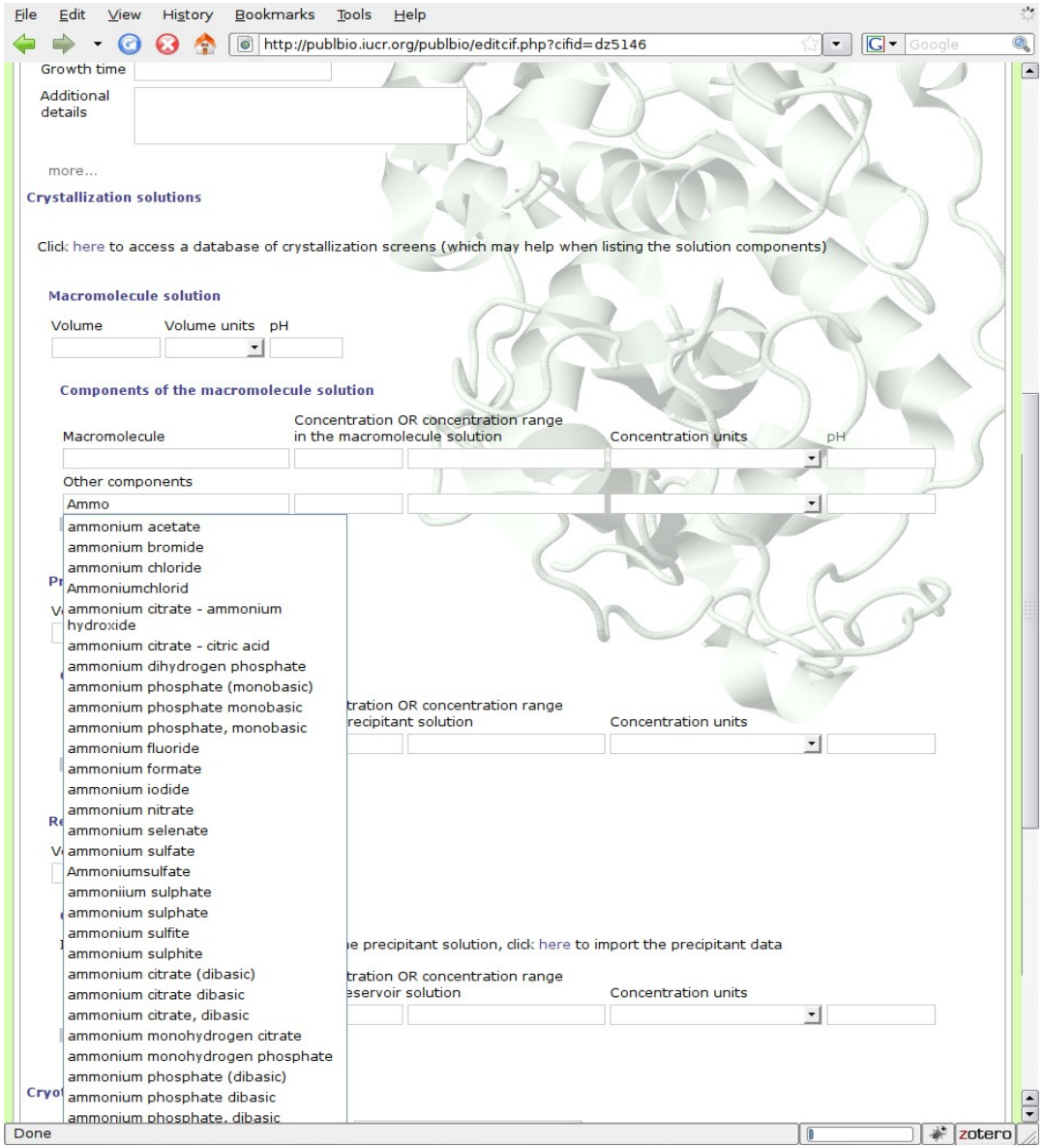
standard descriptions of methods are also offered

input forms suggest possible wording



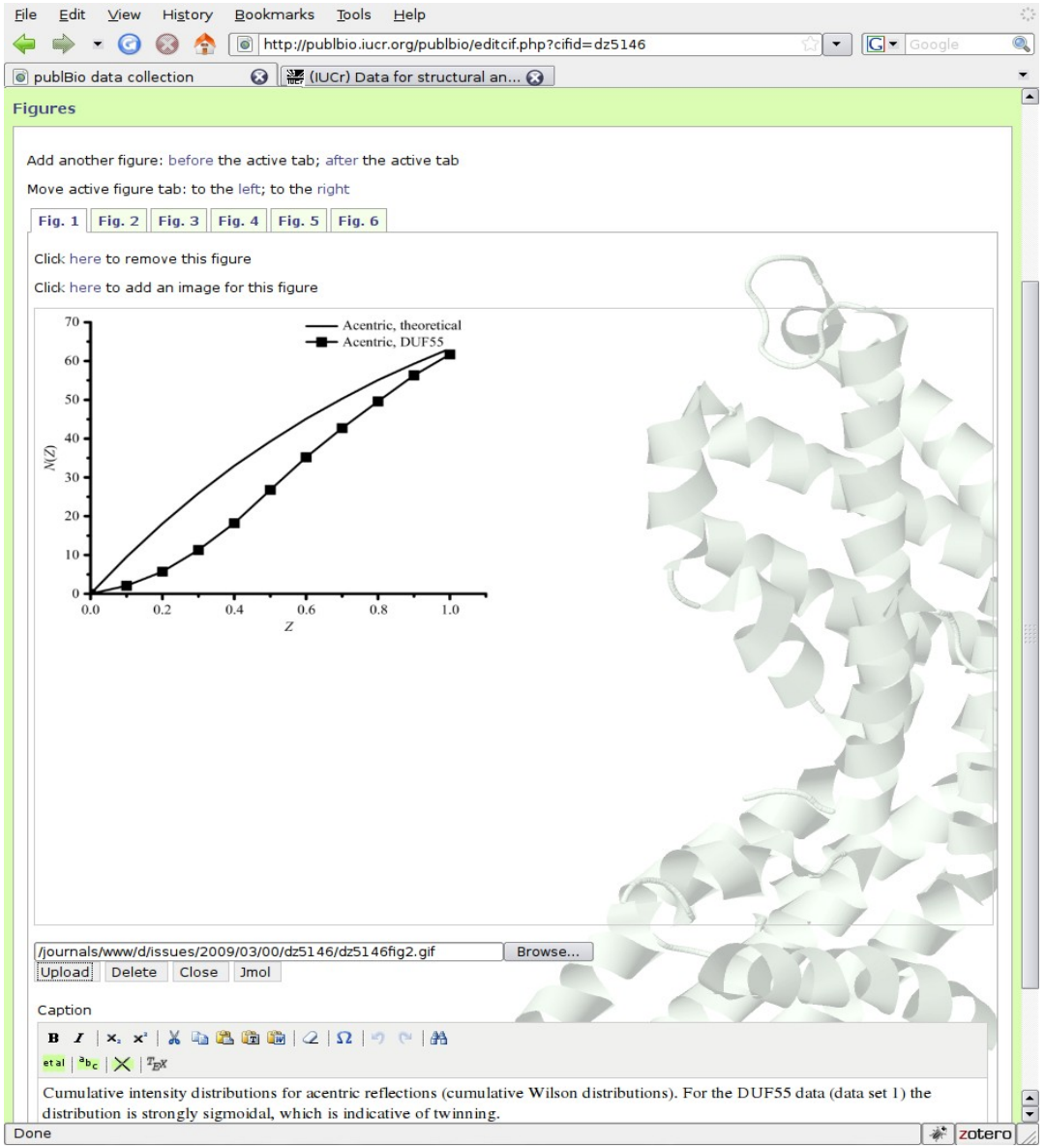
standard commercial crystallization screens can be looked up

crystallization conditions can be added from a database

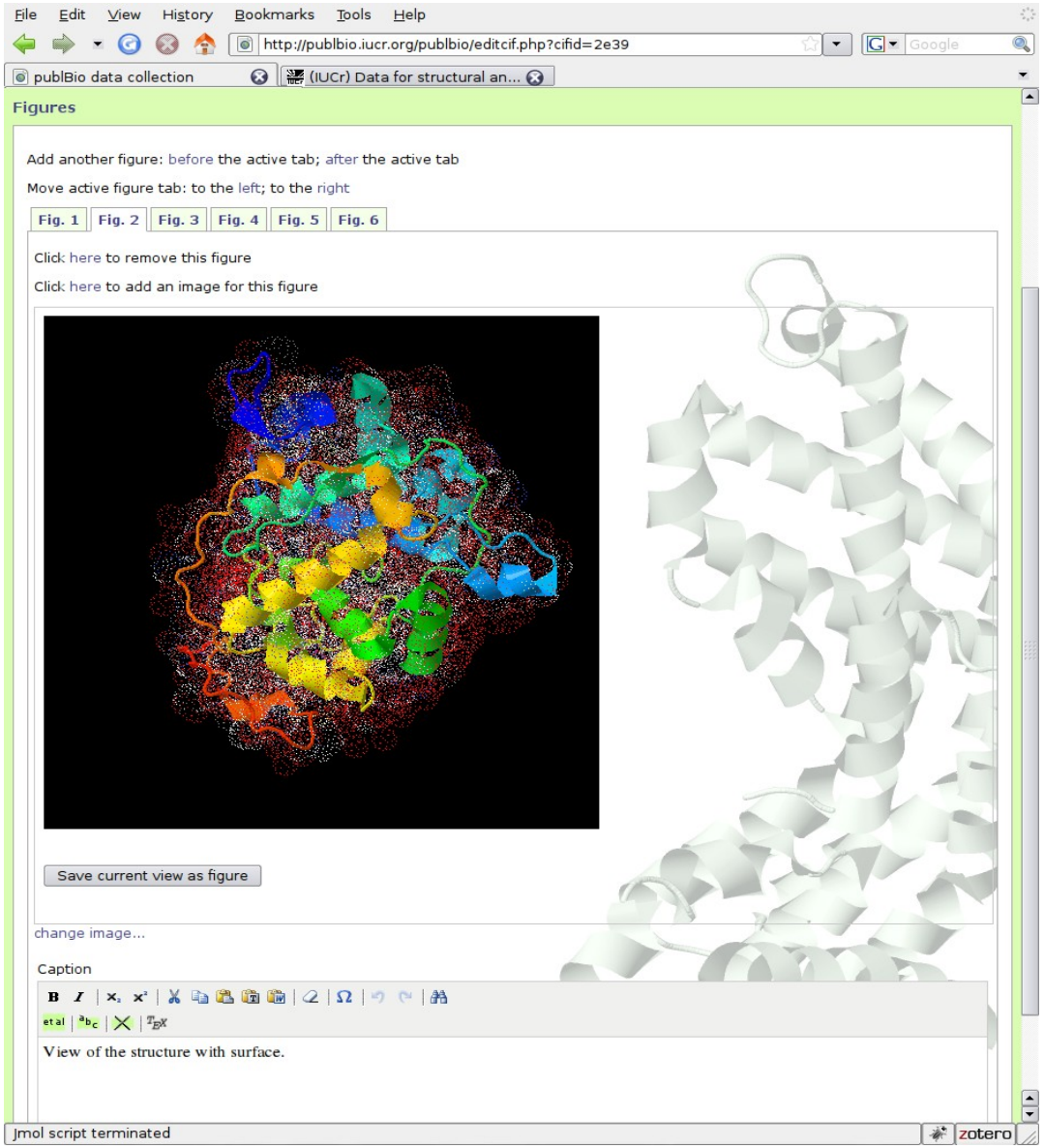


the software predicts the names of standard crystallization components

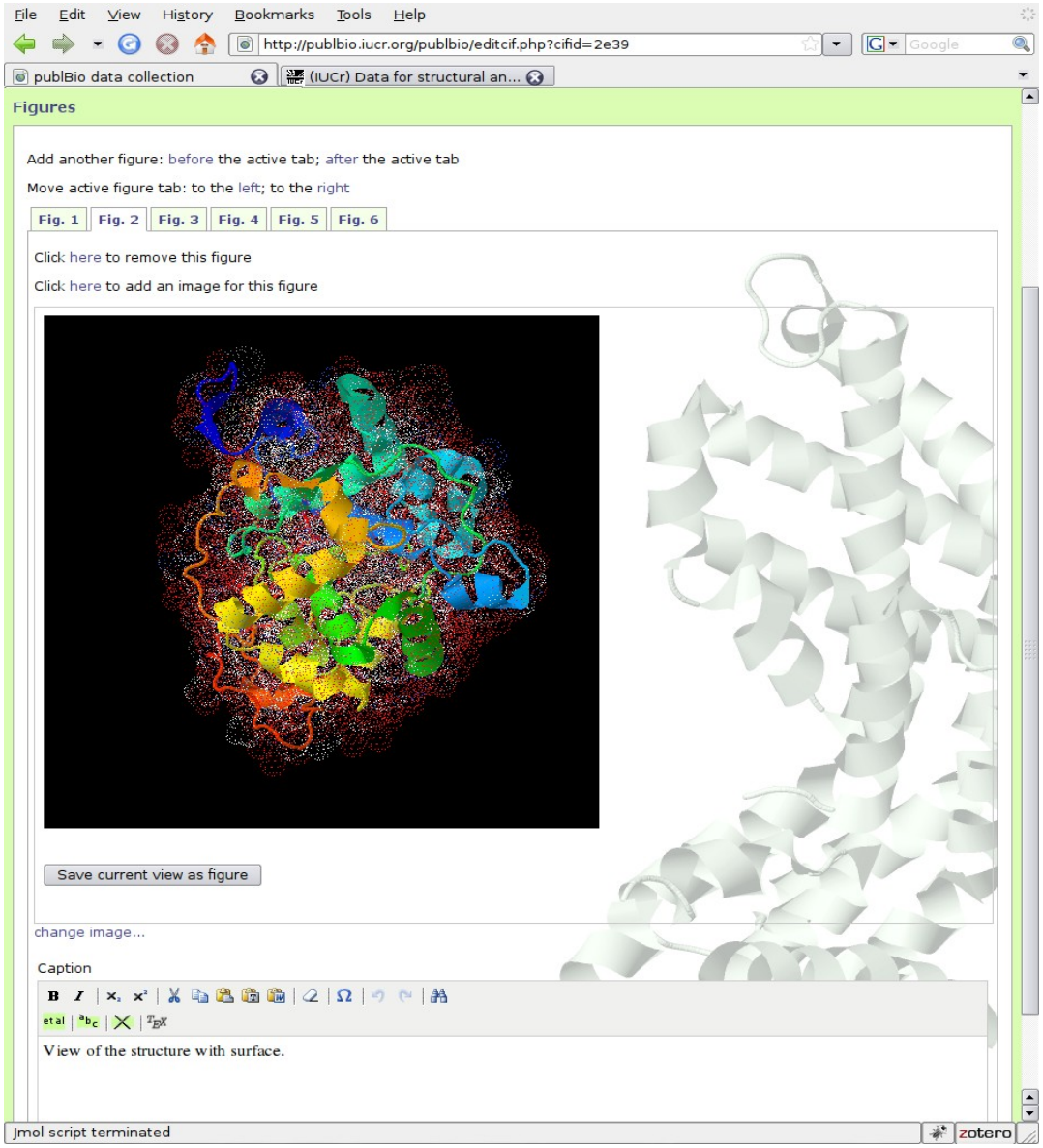
crystallization conditions can be added manually



figures can be added as graphics files



or can be created as interactive JMol figures



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?

Crystallography Journals Online

2013
international year of crystallography

Commission on Journals 2011

Submission to publication

Figure preparation

Crystallography Journals Online

- Online artwork guide available from author services page

Crystallography Journals Online

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

Crystallography Journals Online

Image formats

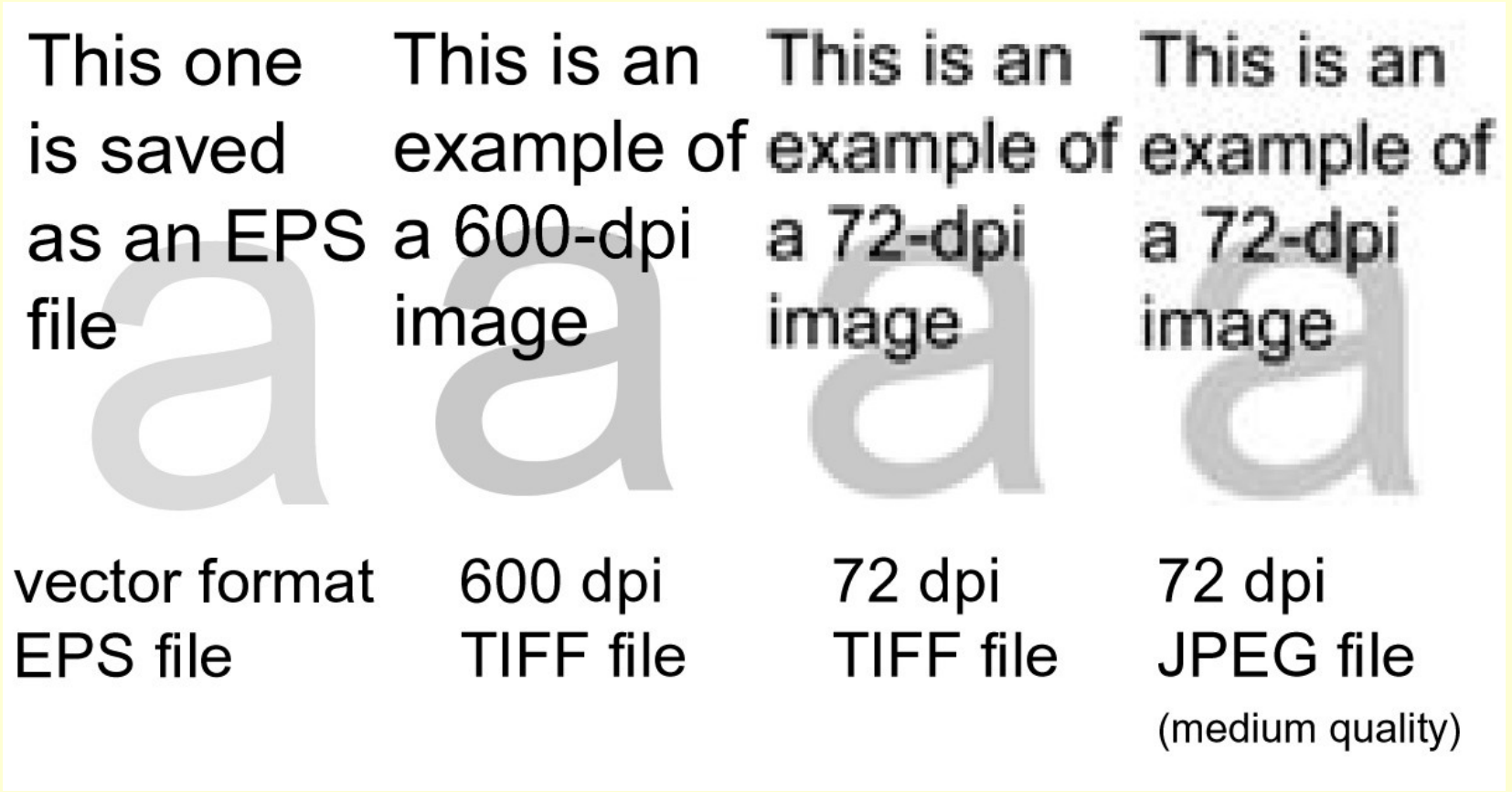
- Recommended formats in Notes for Authors
  - Encapsulated Postscript or PostScript (.eps, .ps) (resolution independent unless there is an embedded bitmap, in which case minimum 600 d.p.i.)
  - Tiff (.tif, minimum resolution 600 d.p.i. final size)
  - HPGL (.hpg) (resolution independent)

  –
- 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

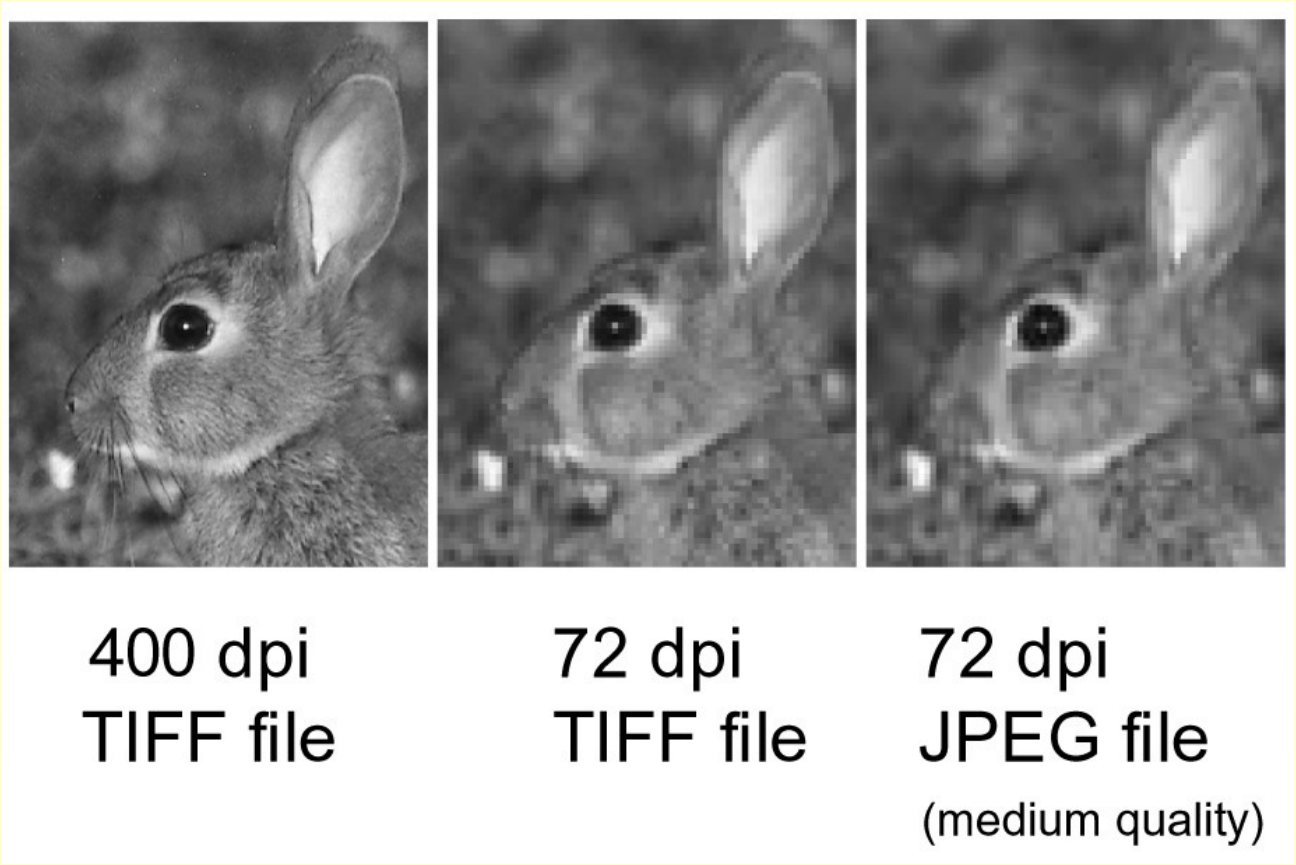
Crystallography Journals Online

Resolution and image formats



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

Resolution and image formats



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

Crystallography Journals Online

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

Table 2. Calculated apatite lattice parameters.

Sample	a(Å)	$\frac{1}{3}c$(Å)
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)

FIGURE OR TABLE?

Crystallography Journals Online

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

Table 2. Calculated apatite lattice parameters.

Sample	*a*(Å)	$\frac{1}{2}c$(Å)
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)

FIGURE OR TABLE

Table 2
Calculated apatite lattice parameters.

Sample	*a* (Å)	*c* (Å)
GI744/1	9.376 (3)	6.888 (4)
GI744/2	9.382 (7)	6.889 (1)
SAR1	9.369 (4)	6.886 (9)
HAI08	9.385 (1)	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 (1)	6.877 (9)
C57	9.438 (8)	6.879 (3)
KH1	9.449 (8)	6.872 (3)

Crystallography Journals Online

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

Table 2. Calculated apatite lattice parameters.

Sample	*a*(Å)	*c*(Å)
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)

FIGURE OR TABLE?

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

Table 2. Calculated apatite lattice parameters.

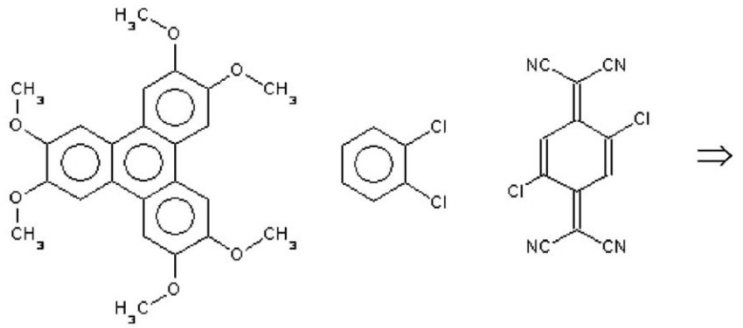
Sample	*a*(Å)	*c*(Å)
GI744/1	9.376(3)	6.888(4)
GI744/2	9.382(7)	6.889(0)
SAR1	9.369(4)	6.886(9)
HAI08	9.385(0)	6.884(3)
988	9.446(7)	6.884(9)
LI95	9.443(9)	6.884(2)
LI95A	9.430(2)	6.883(3)
ELISH	9.449(5)	6.883(6)
ELISH2	9.448(3)	6.884(5)
HAI03	9.404(0)	6.877(9)
C57	9.438(8)	6.879(3)
KH1	9.449(8)	6.872(3)

FIGURE OR TABLE

Sample	*a*(Å)	*c*(Å)
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)

Crystallography Journals Online

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

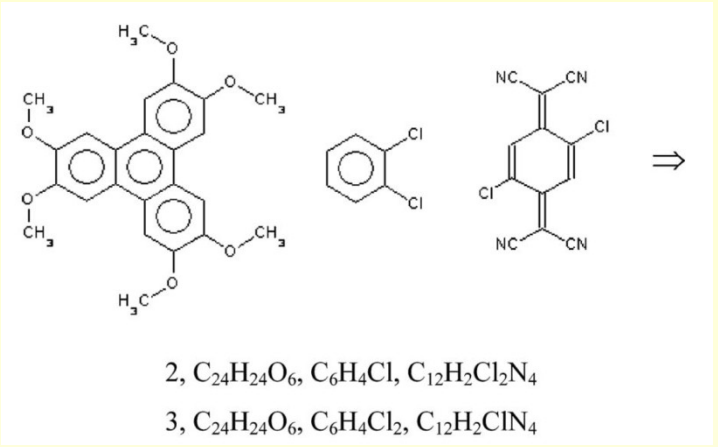


2, $C_{24}H_{24}O_6$, C_6H_4Cl, $C_{12}H_2Cl_2N_4$

3, $C_{24}H_{24}O_6$, $C_6H_4Cl_2$, $C_{12}H_2ClN_4$

Figure 2
Step 1*a* from Fig. 1 in the case of multiple residues: search for the first functional group, –Cl, in the connectivity of every residue. Matches for DAQMUD are shown as examples. For each matching residue, the matching residue number, here 2 and 3, and a representative chemical formula of the entire entry with the functional group removed are stored.

FIGURE



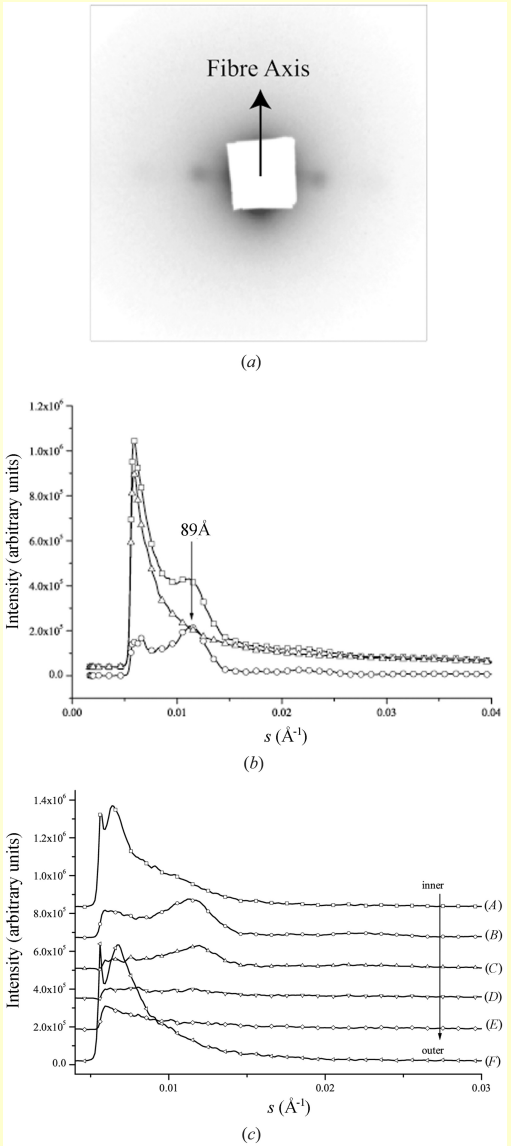
2, $C_{24}H_{24}O_6$, C_6H_4Cl, $C_{12}H_2Cl_2N_4$

3, $C_{24}H_{24}O_6$, $C_6H_4Cl_2$, $C_{12}H_2ClN_4$

SCHEME

Crystallography Journals Online

Composite figures

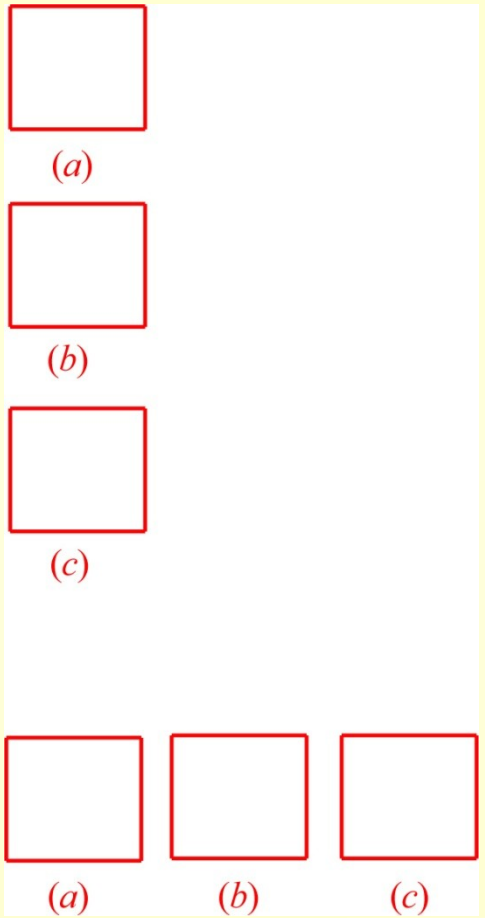


- Parts of figures (*a*), (*b*) etc.; labelling should be in 8pt Times and Times Italic at final size
- Ask authors to revise figures if labelling too small

Crystallography Journals Online

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

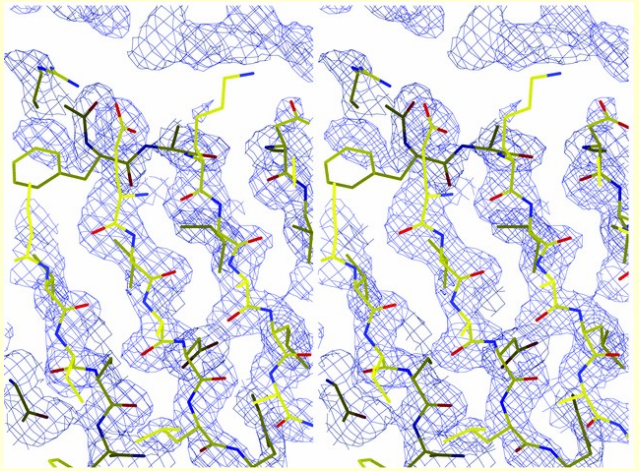


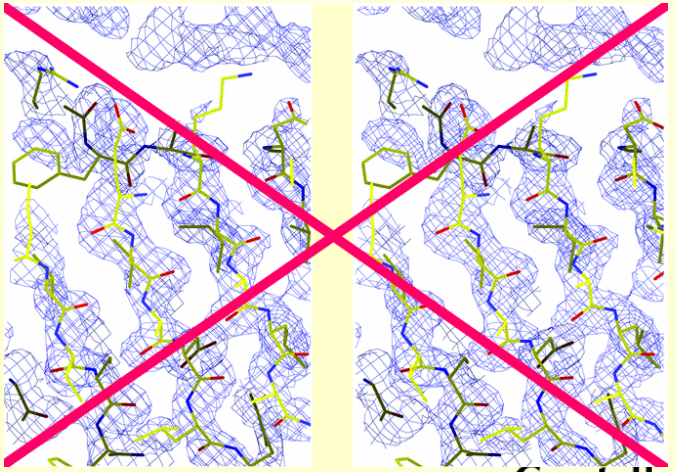
Crystallography Journals Online

Stereoviews

- Left and right views should be within a single figure

- Atom labelling should be on both left and right views in stereo perspective





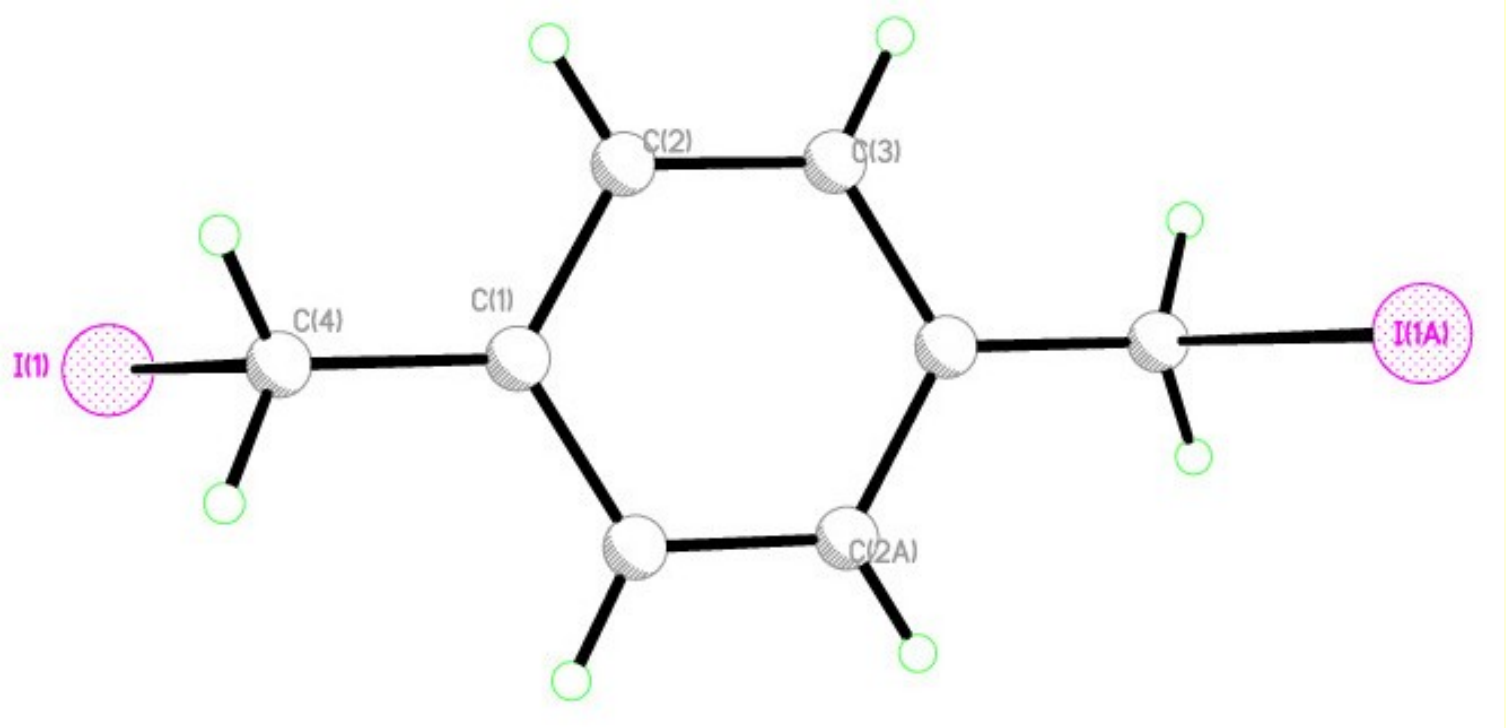
Crystallography Journals Online

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

Crystallography Journals Online

Labelling of structural diagrams



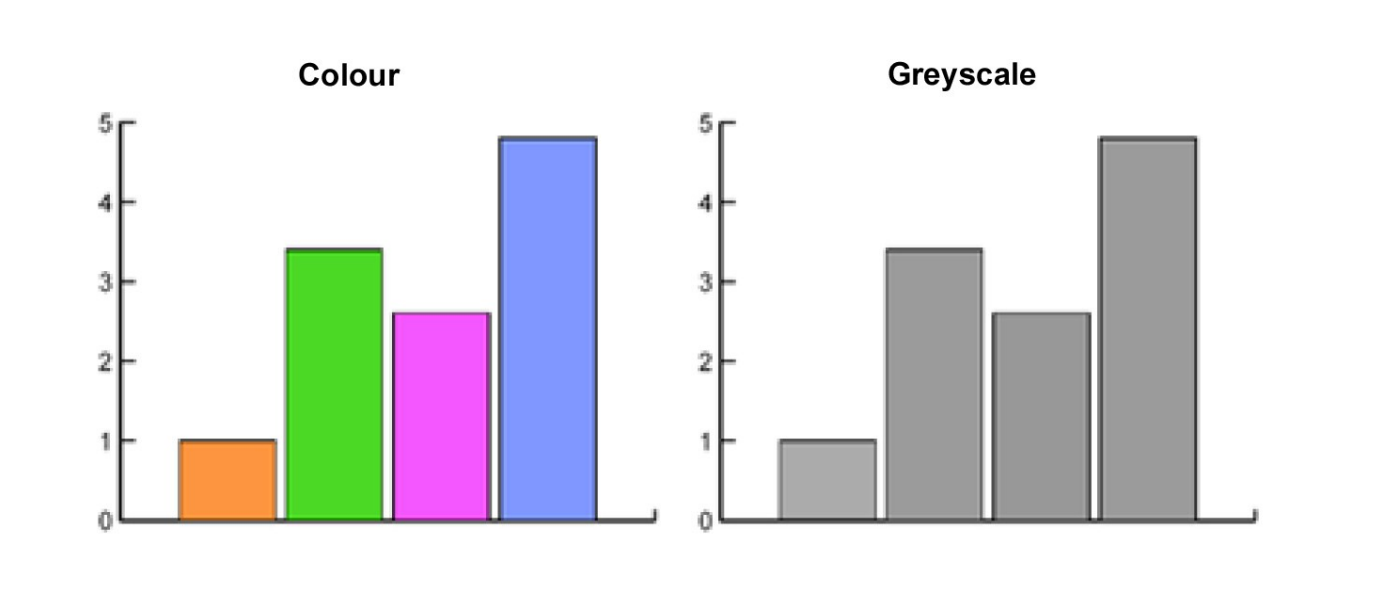
- Atoms should be shown as ellipsoids not spheres
- Atom numbers should usually not be in parentheses
- Atom labels should not intersect with bonds or ellipsoids

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

Crystallography Journals Online

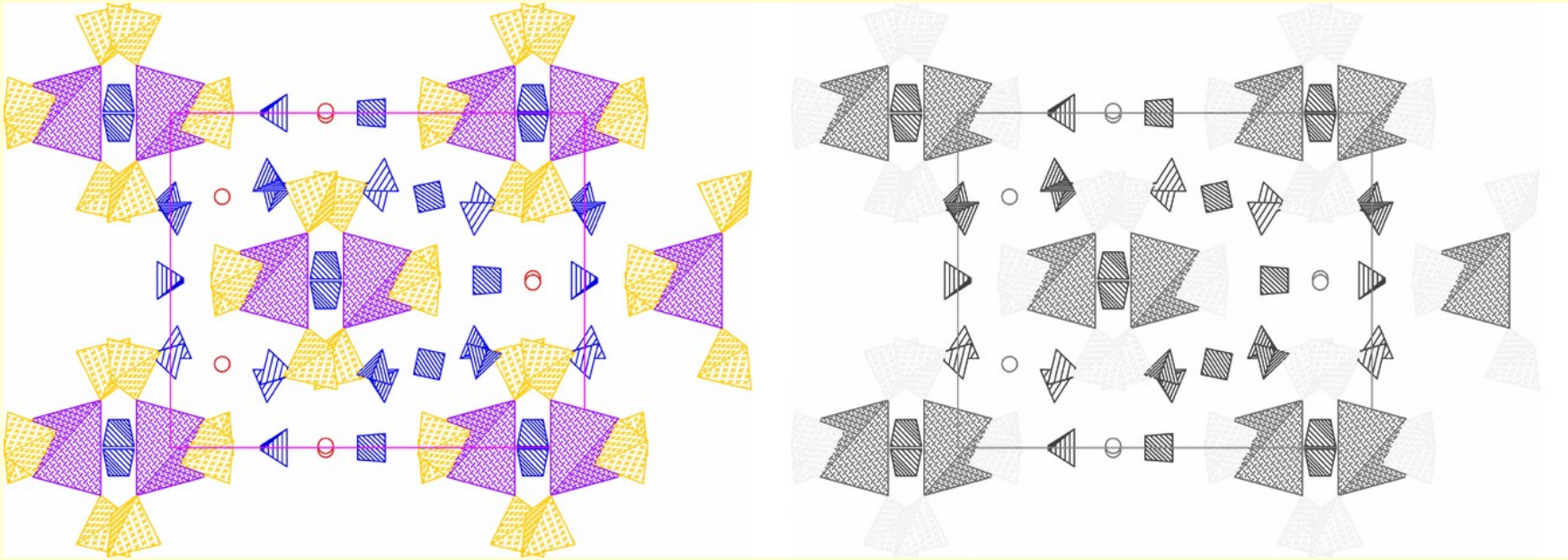
Colour and greyscale



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

Crystallography Journals Online

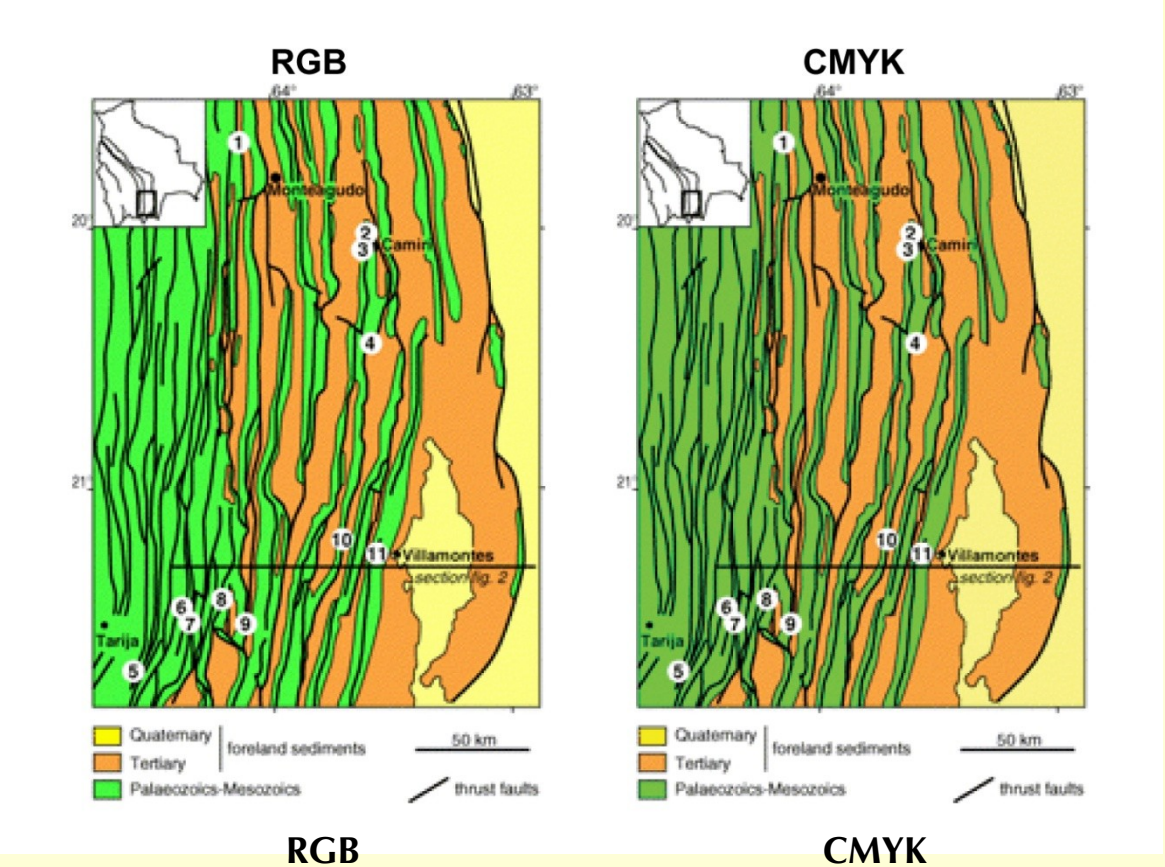
Colour and greyscale



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

Crystallography Journals Online

RGB and CMYK colour



RGB

Red, Green, Blue

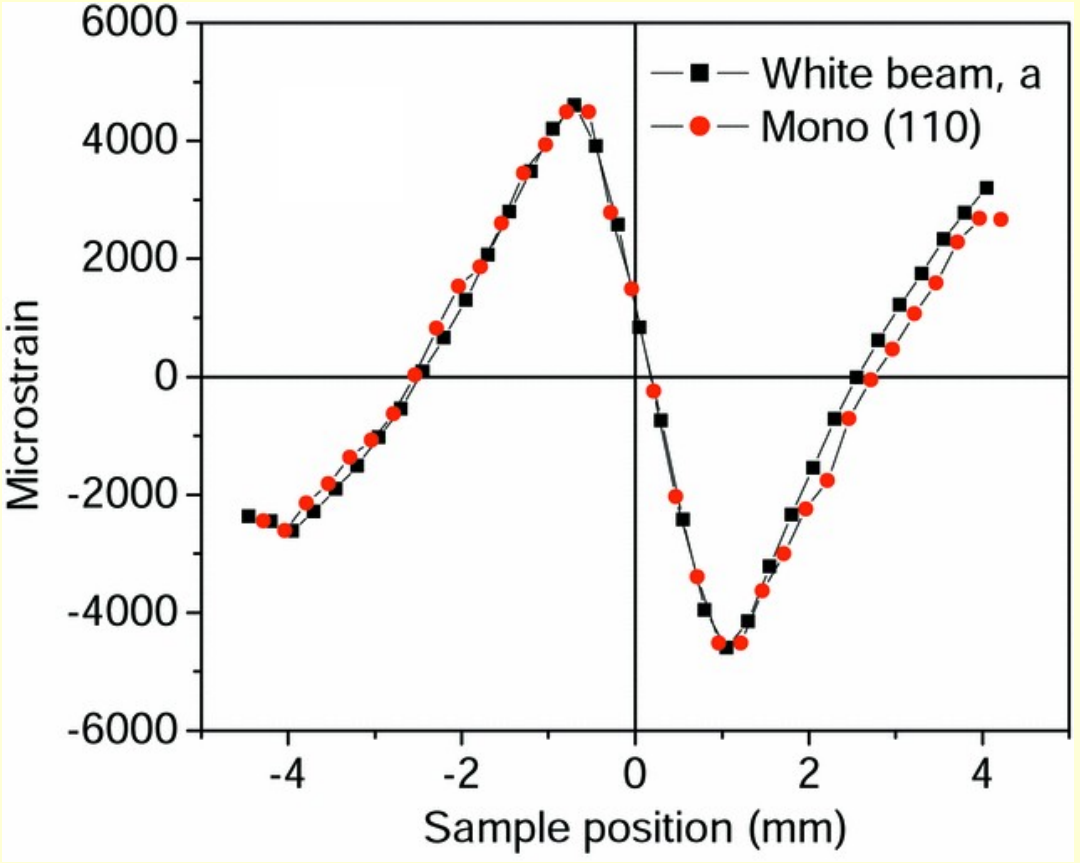
CMYK

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

Crystallography Journals Online

Use of colour



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

Crystallography Journals Online

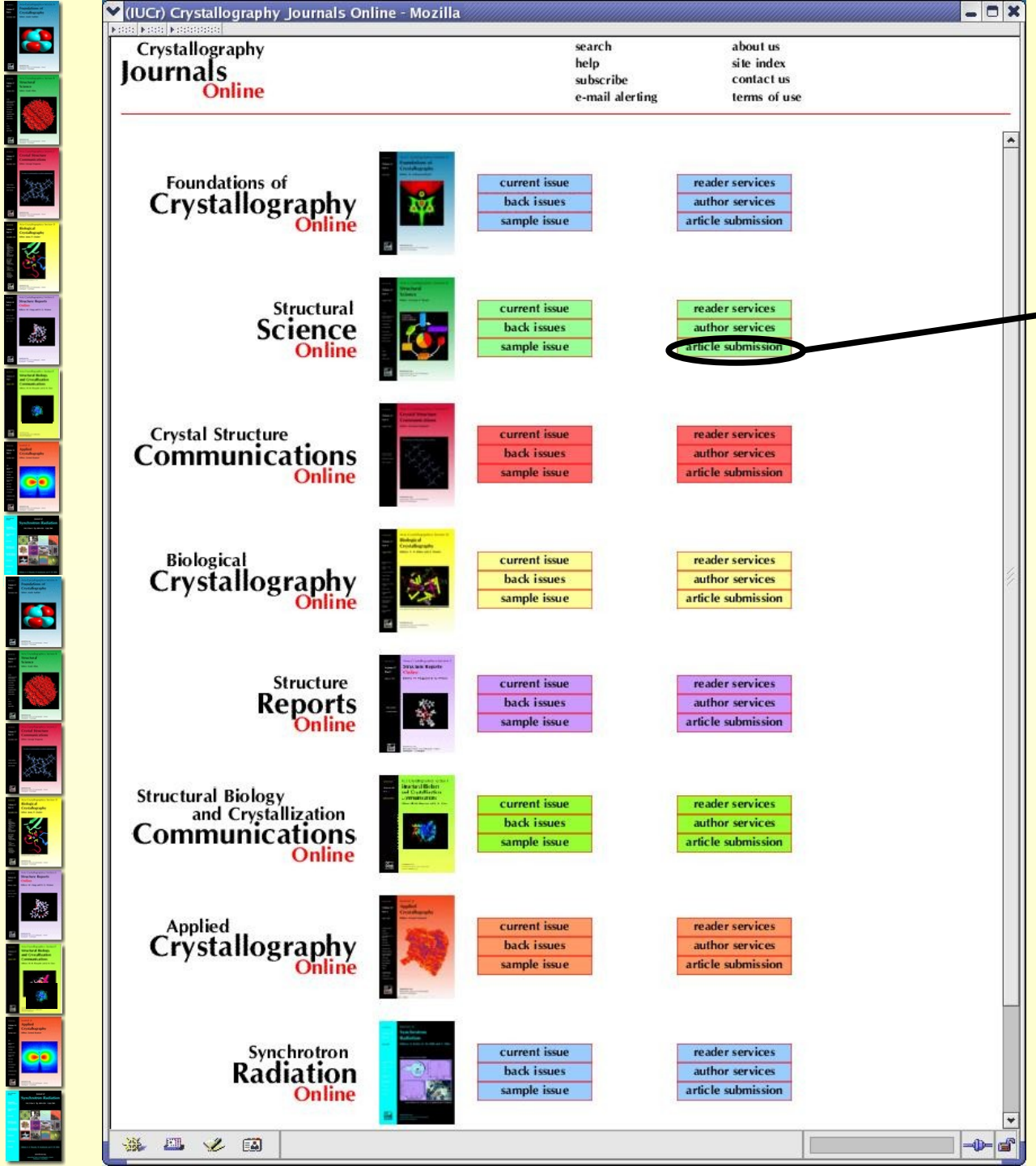
2013 international year of crystallography

Commission on Journals 2011

Submission to publication

Online submission system

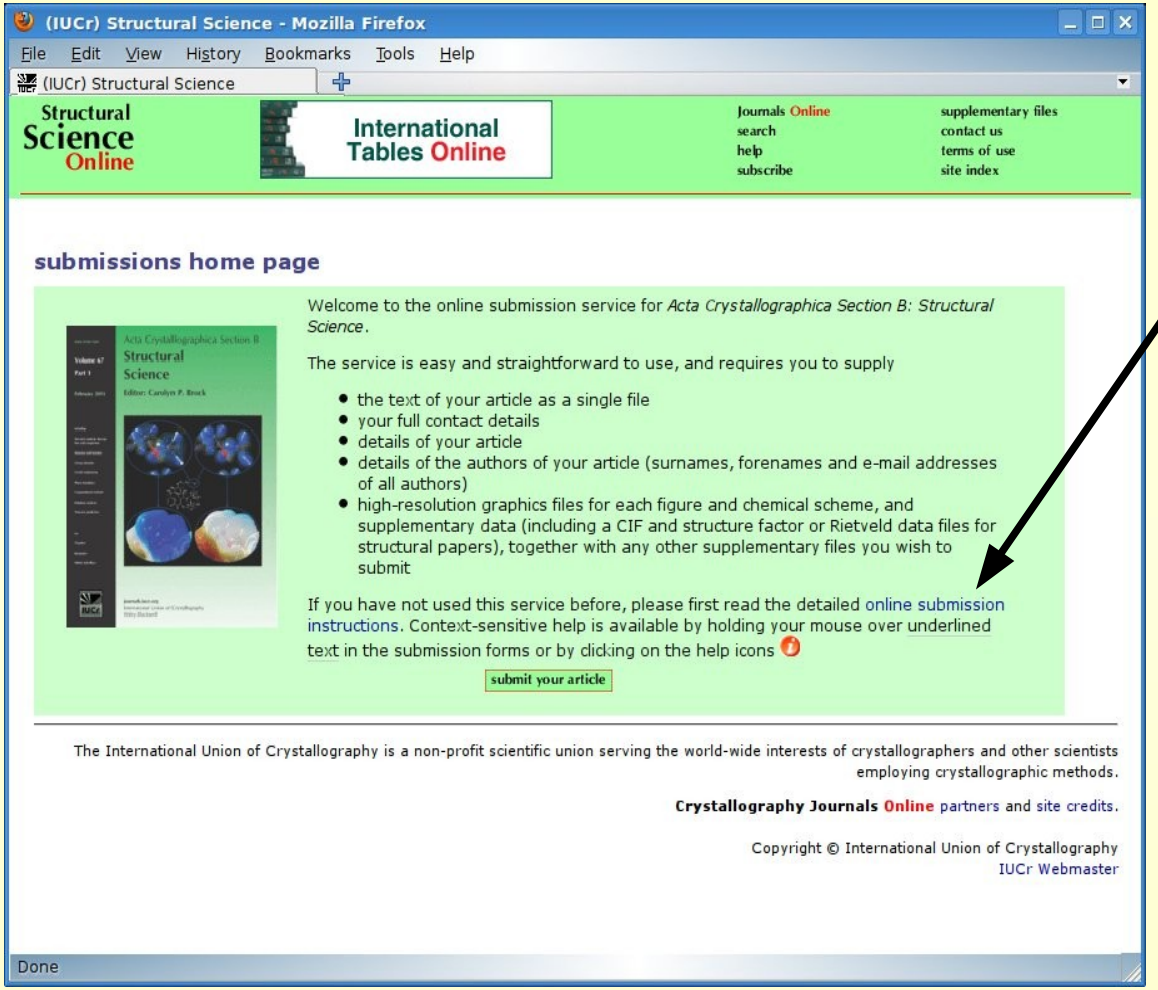
Crystallography Journals Online



- Where to submit?
- journals.iucr.org
- Or from author services on journal home page

Crystallography Journals Online

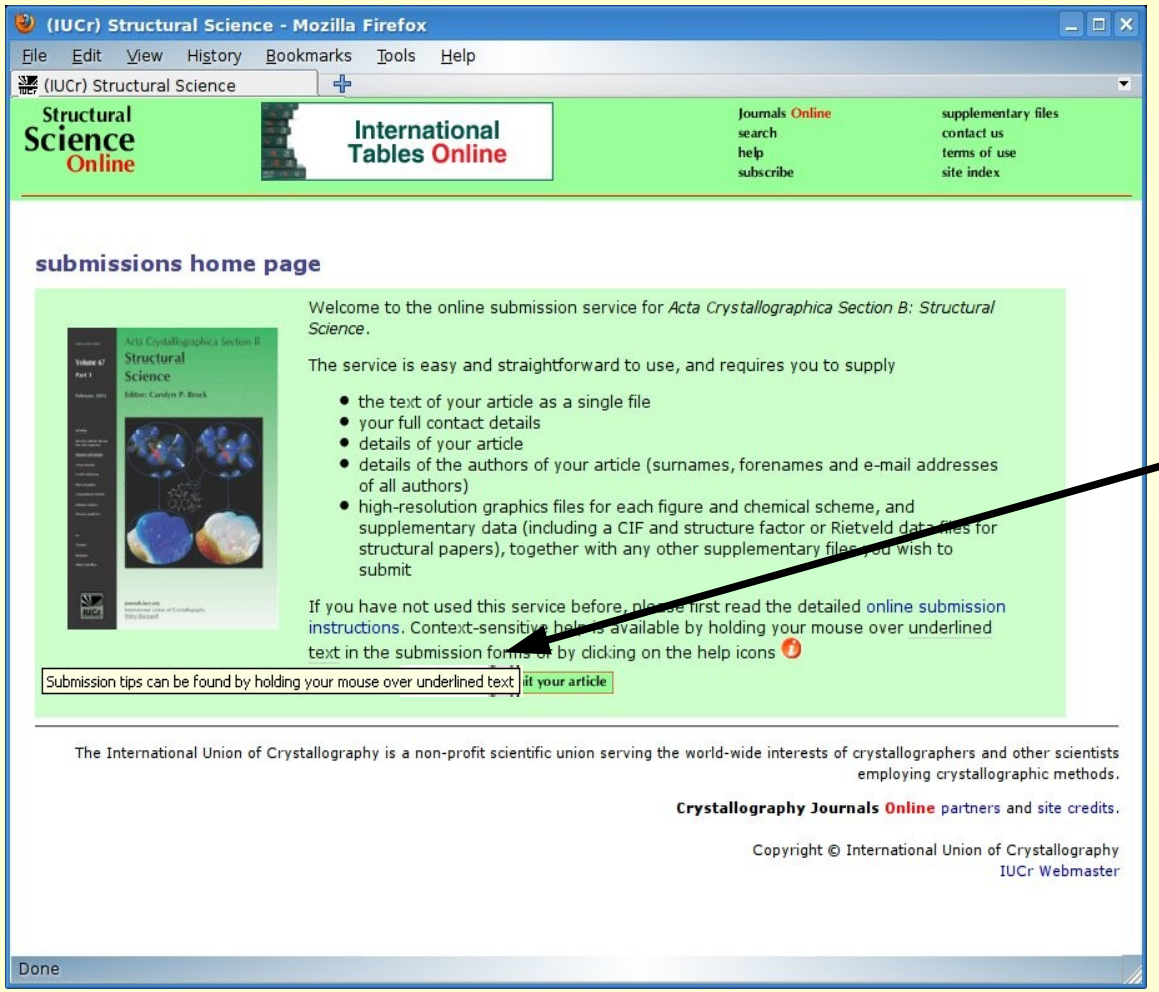
Getting started



- Full submission instructions are available

Crystallography Journals Online

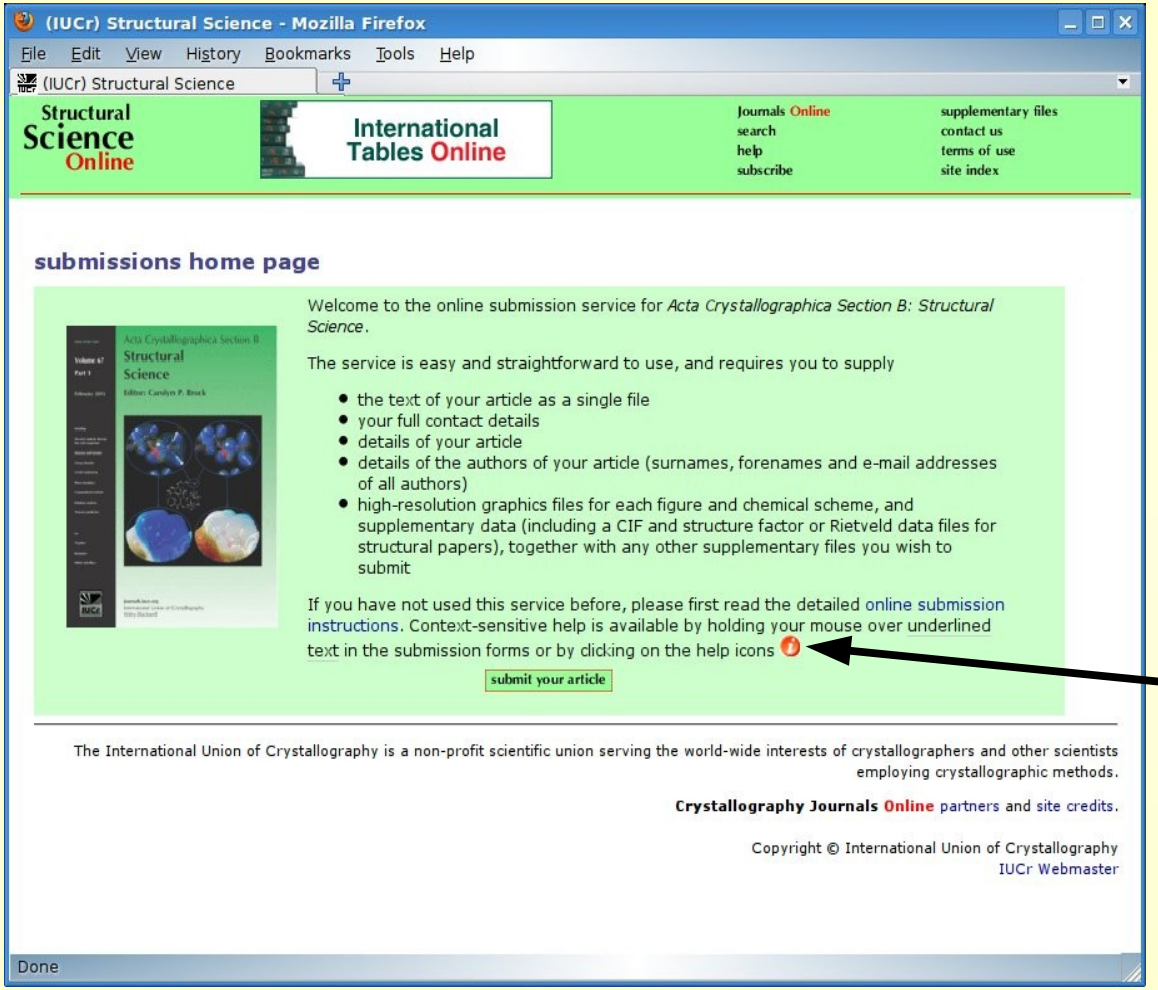
Getting started



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

Crystallography Journals Online

Getting started



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

Crystallography Journals Online

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

Crystallography Journals Online

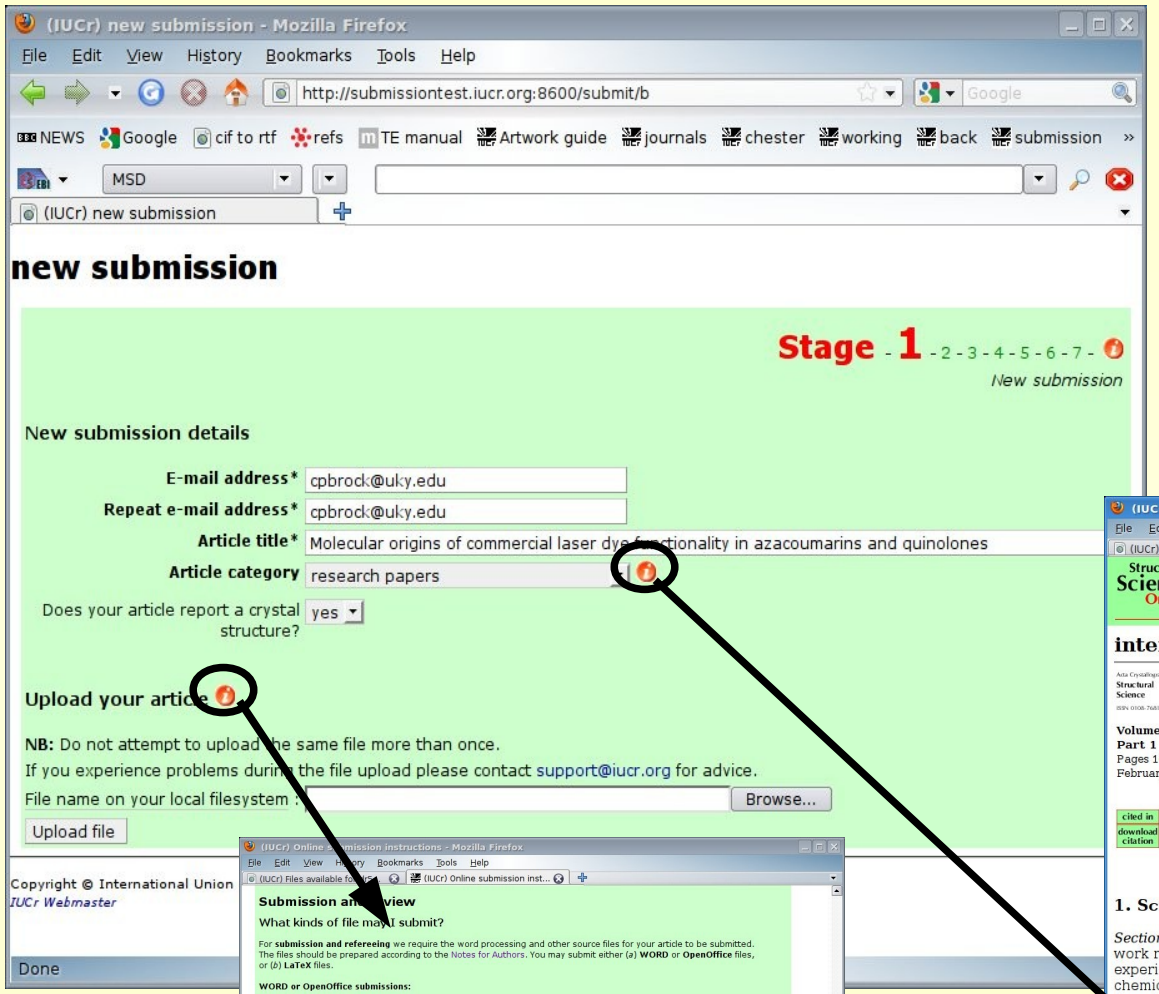
Types of files for submission

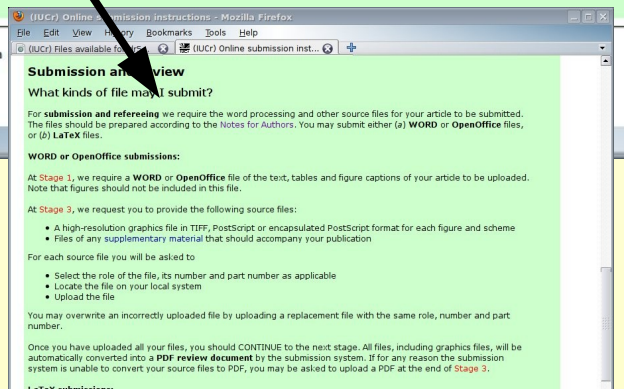
- WORD or OpenOffice file preferably created using **IUCr template**
- LaTeX (using **IUCr template**)
- Figures as PostScript, encapsulated PostScript or TIFF files, but other formats are supported
- Valid CIF/validation report/mmCIF (for structural papers)
- Structure factor/powder data files in CIF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

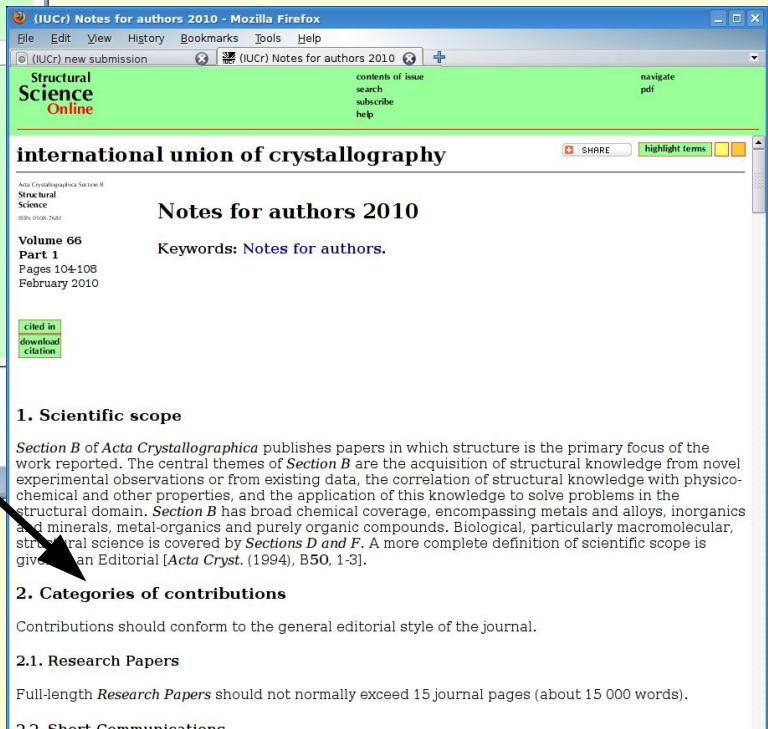
Crystallography Journals Online

Stage 1

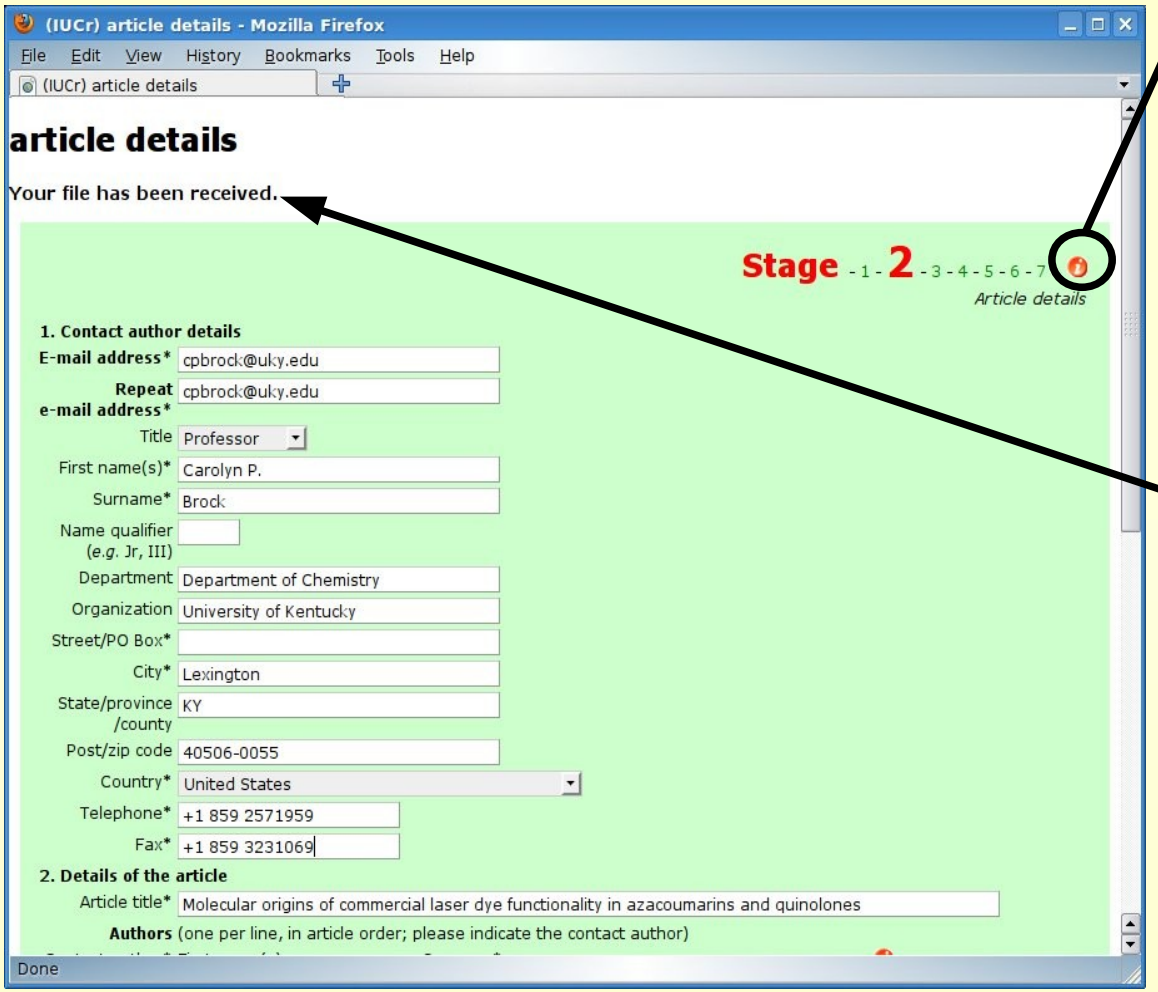
- Contact e-mail address
- Article title
- Category
- **Structural paper?**
- Upload main article text

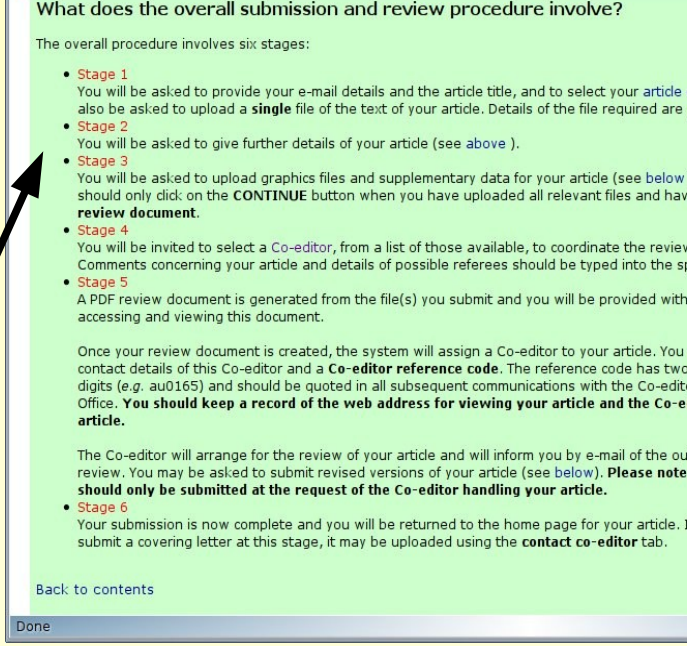






Stage 2

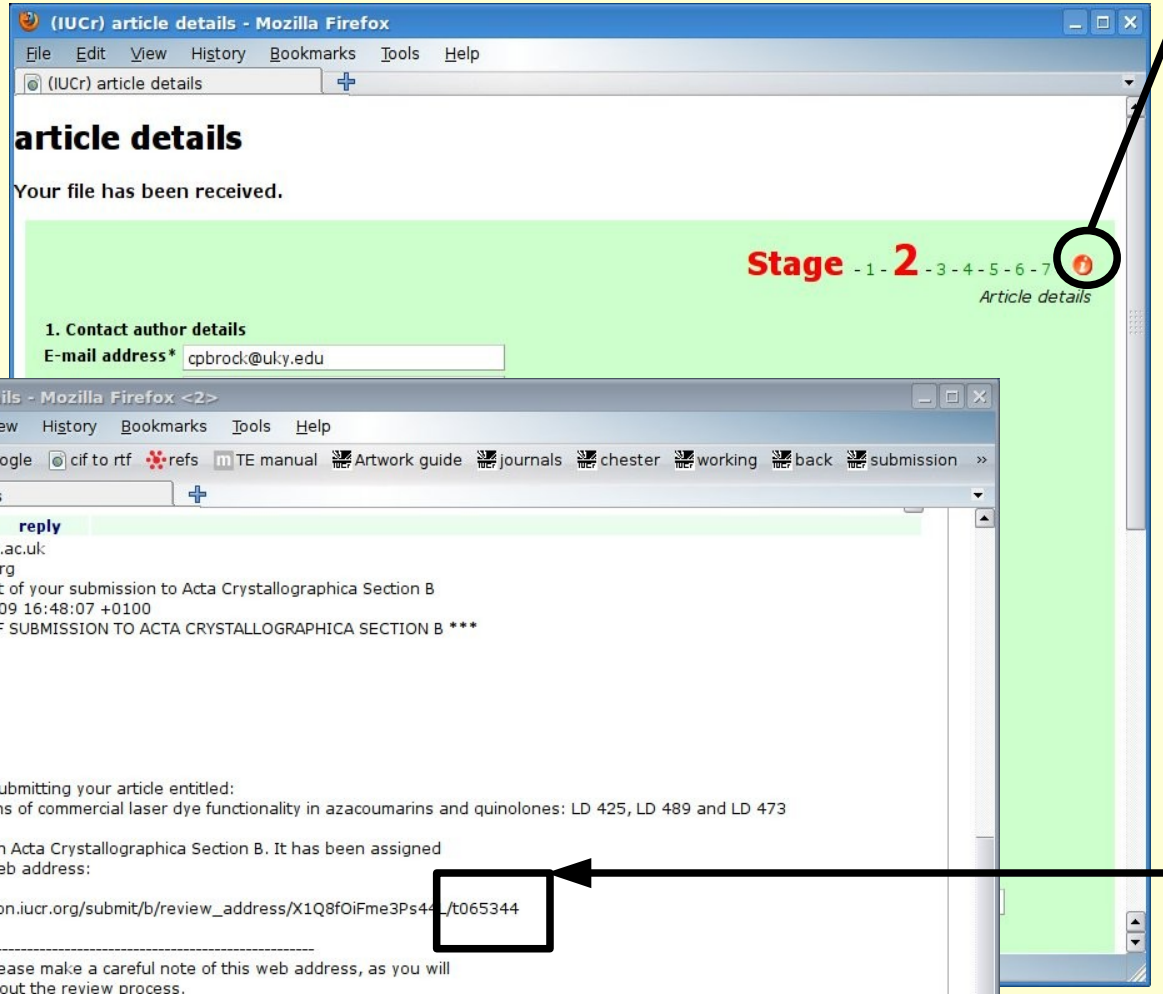


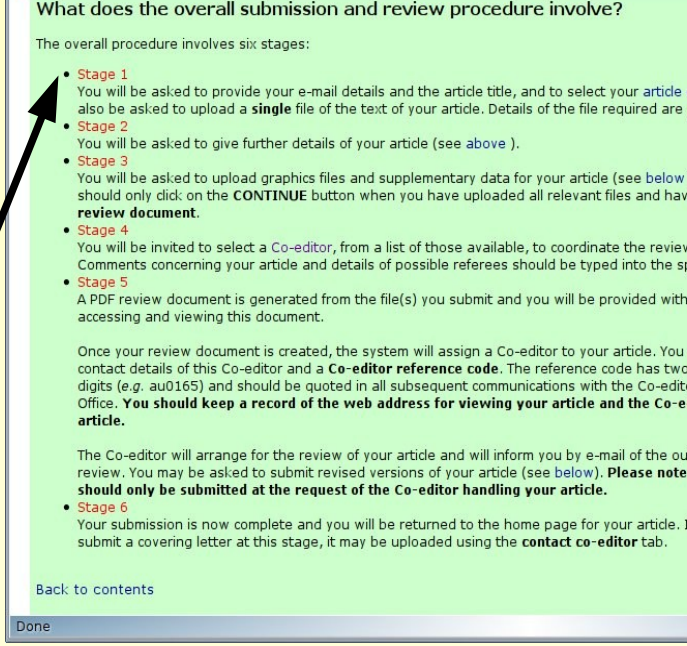


- Confirmation of receipt of file

Crystallography Journals Online

Stage 2





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

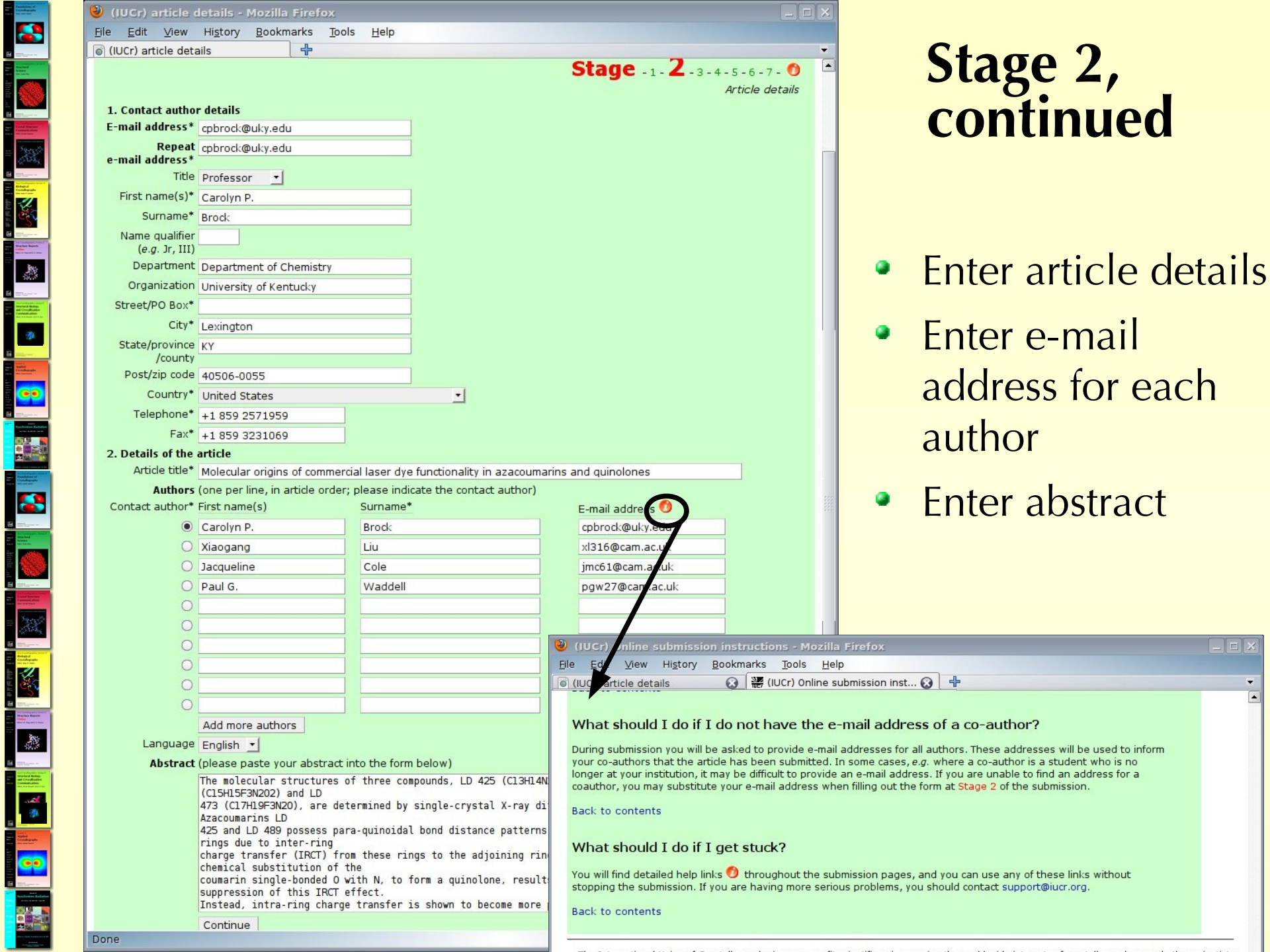
Crystallography Journals Online

Potential problems

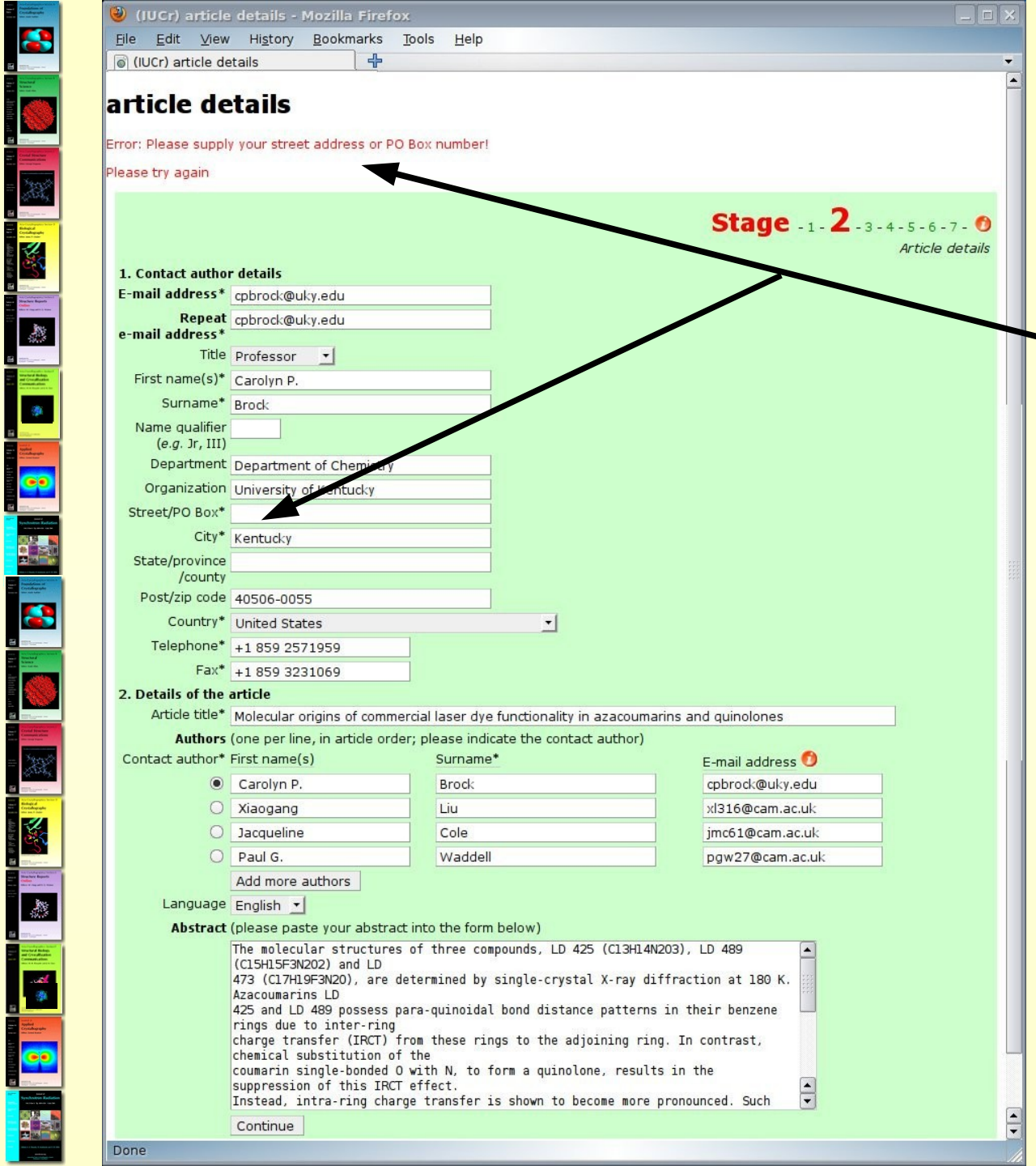
- Title and main article text file are checked against previous submissions in our database
- For journals other than Sections C and E, an **exact duplication** of the title or main article text file with one previously submitted will cause the system to ask the author to contact support rather than 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

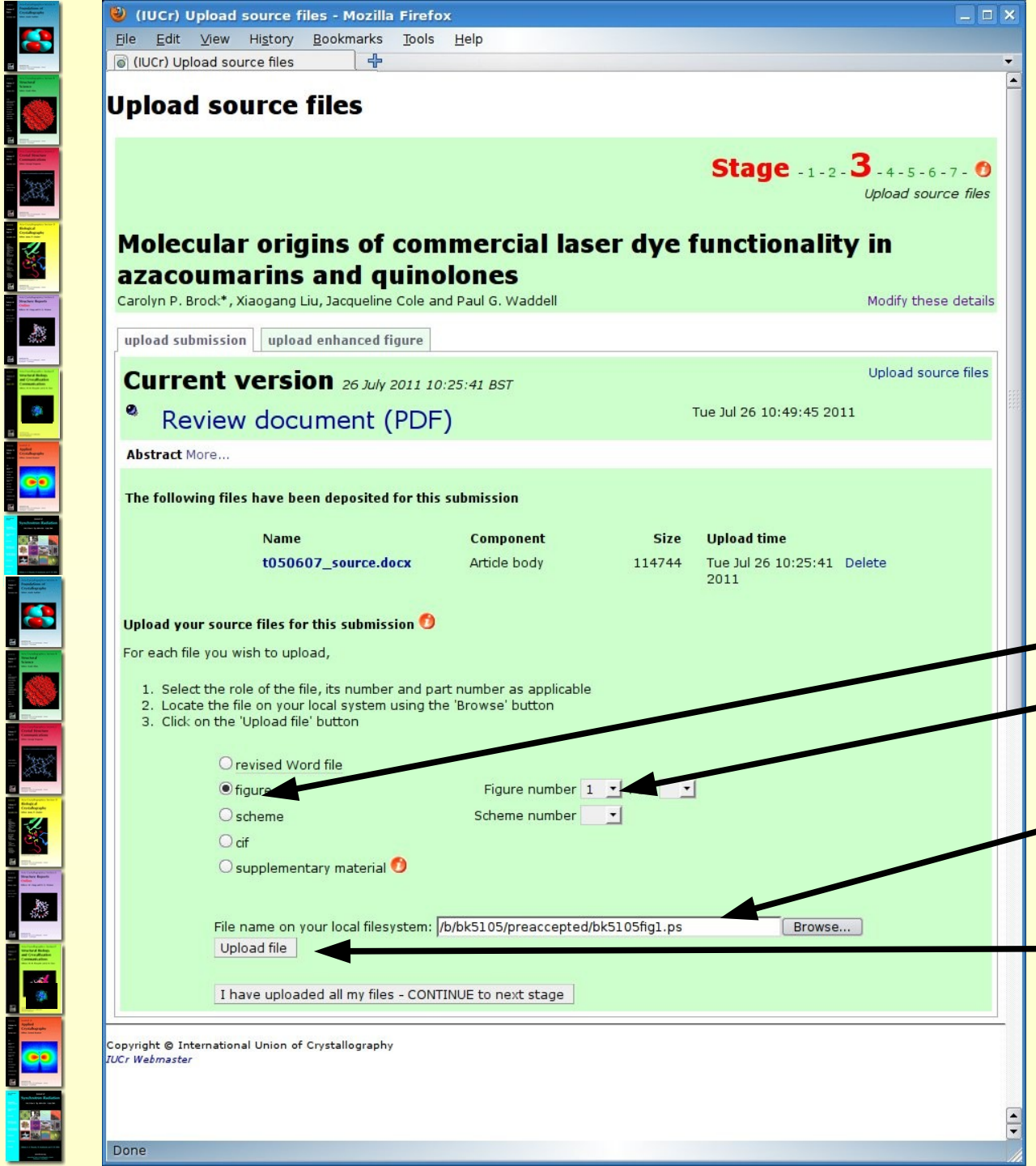


Stage 2, continued



- Must complete fields marked with asterisks

Crystallography Journals Online



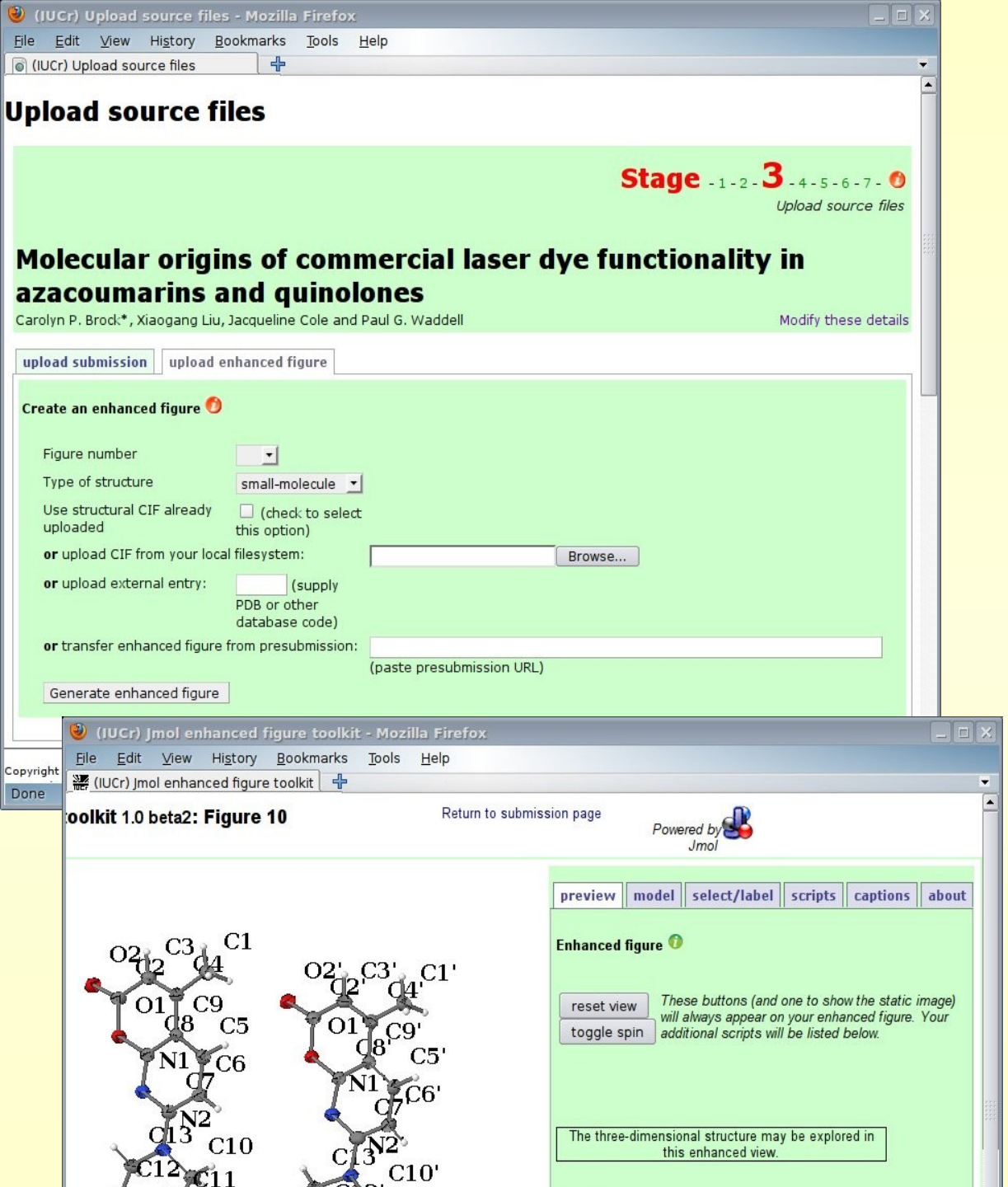
Stage 3

- 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

Crystallography Journals Online

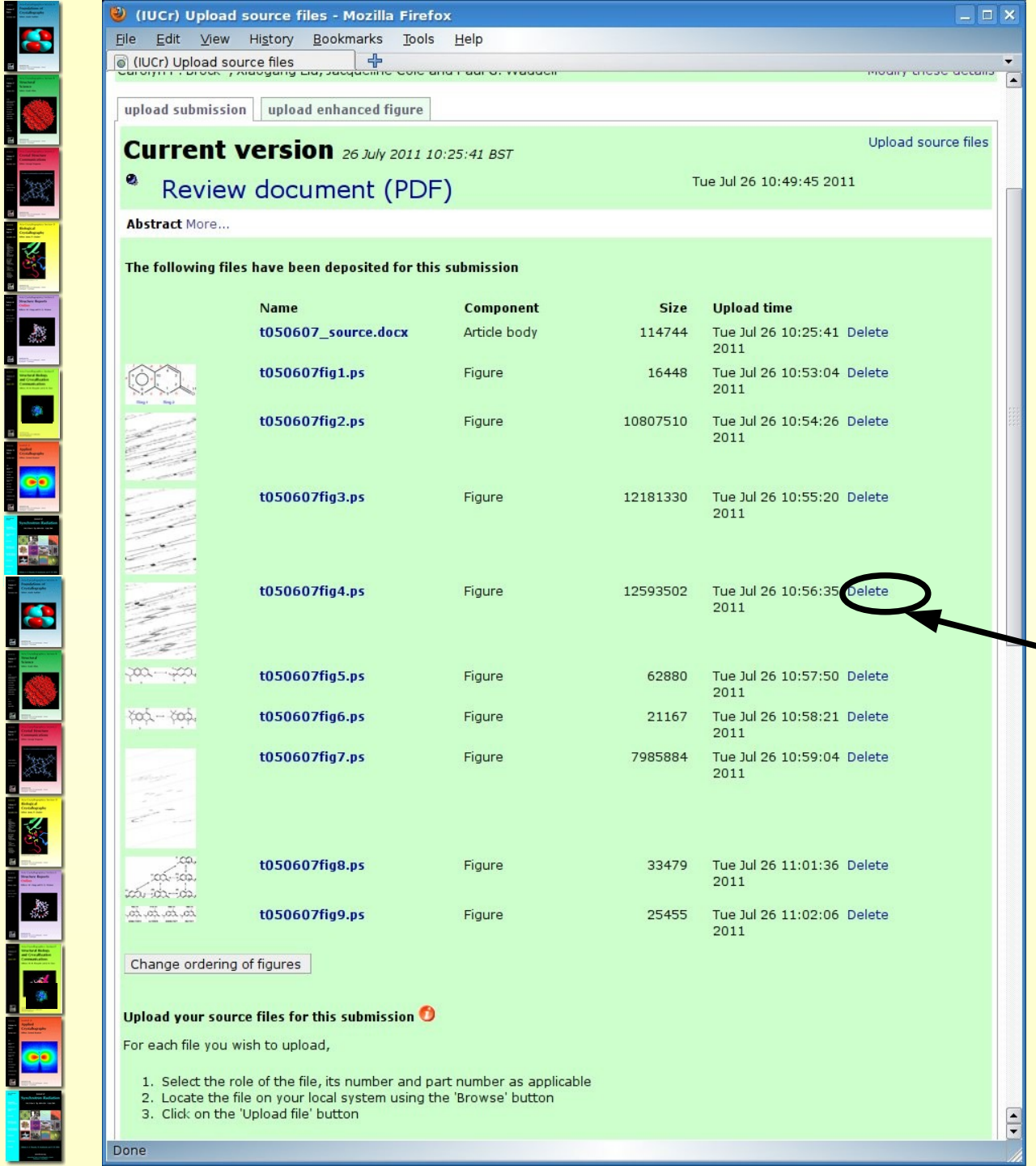


Stage 3, continued

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

Crystallography Journals Online



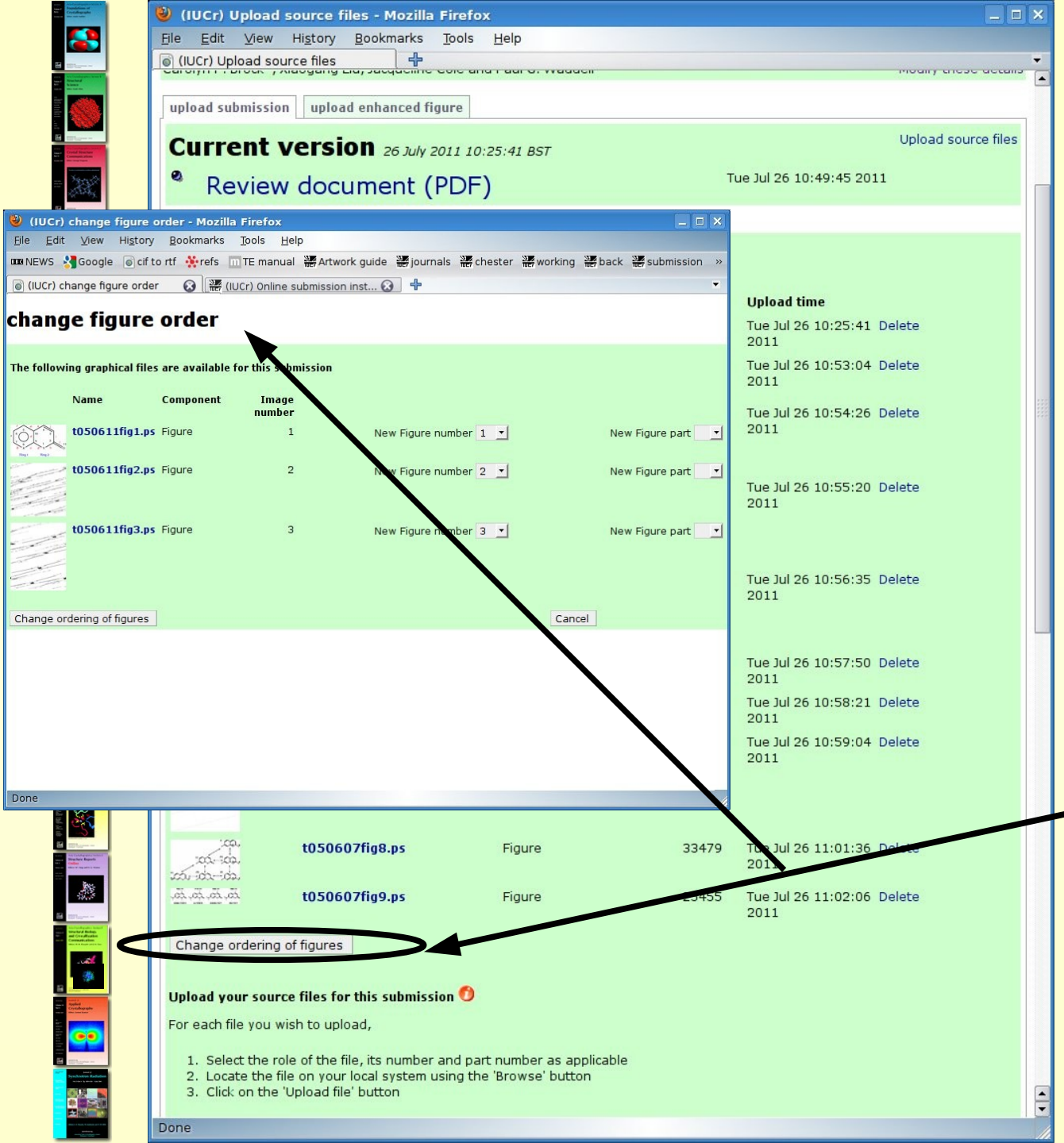
Stage 3, continued

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

Crystallography Journals Online

Stage 3, continued



CORRECTING MISTAKES

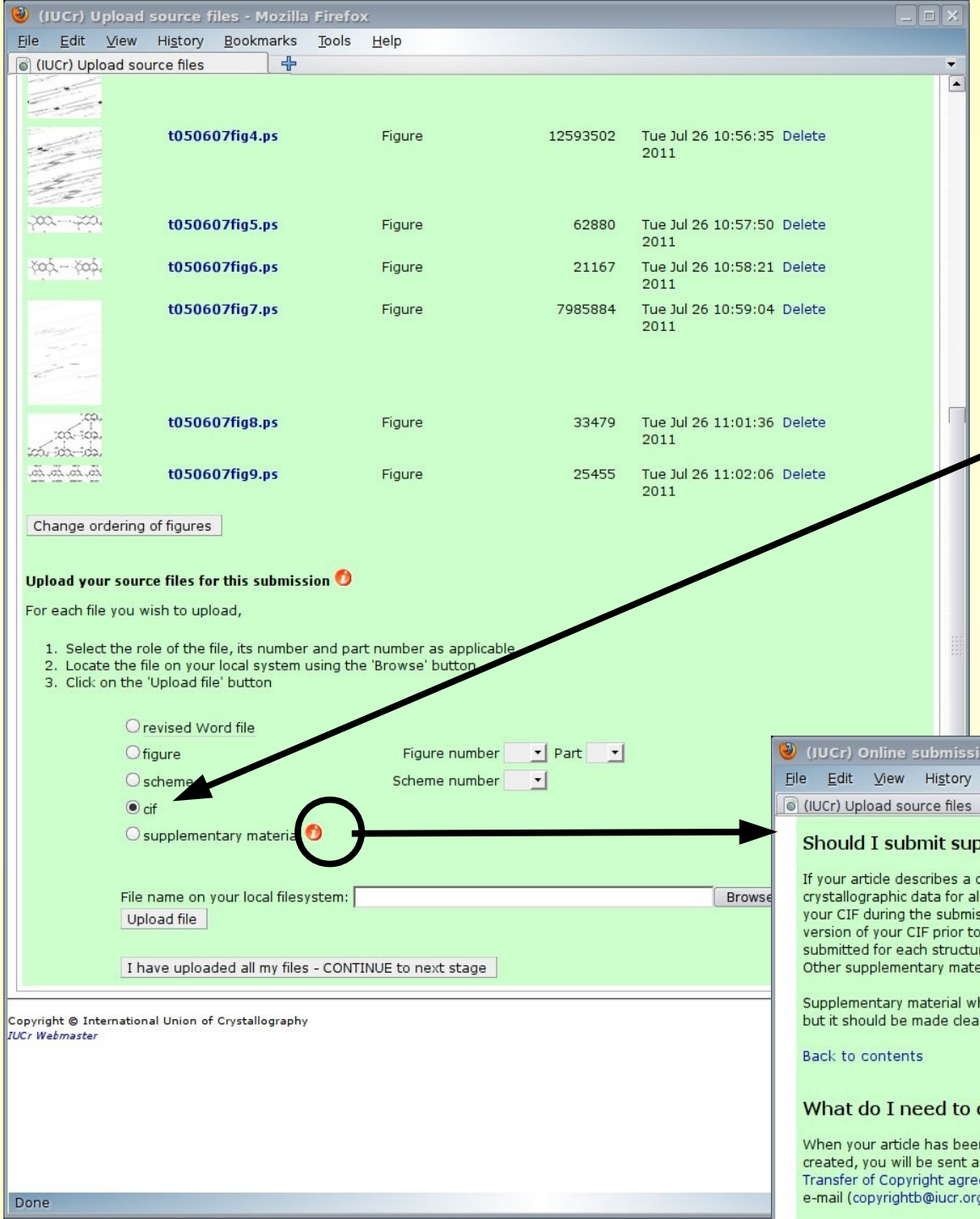
- If wrong file uploaded just reupload and file will be overwritten
- Only use delete to remove no longer required files
- Figure ordering can be corrected

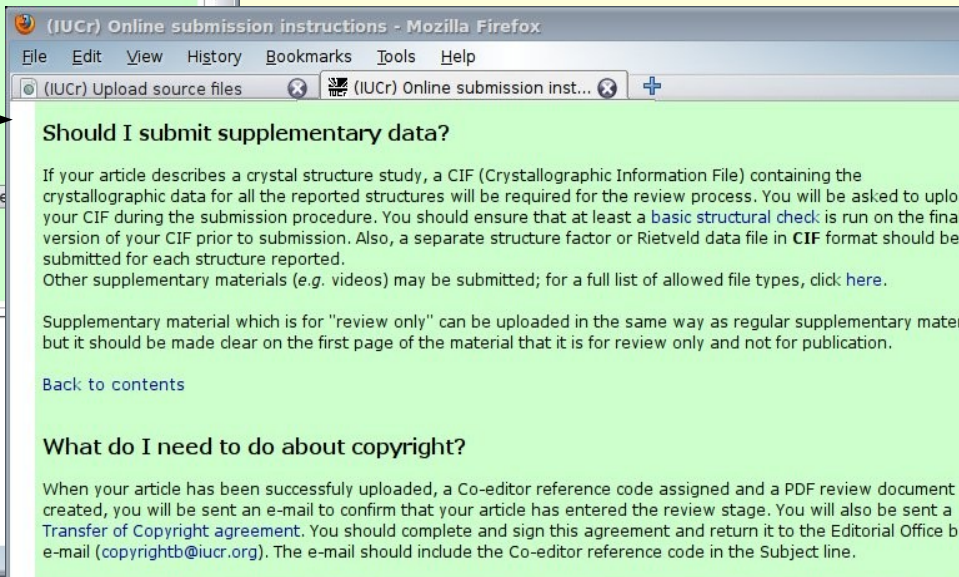
Crystallography Journals Online

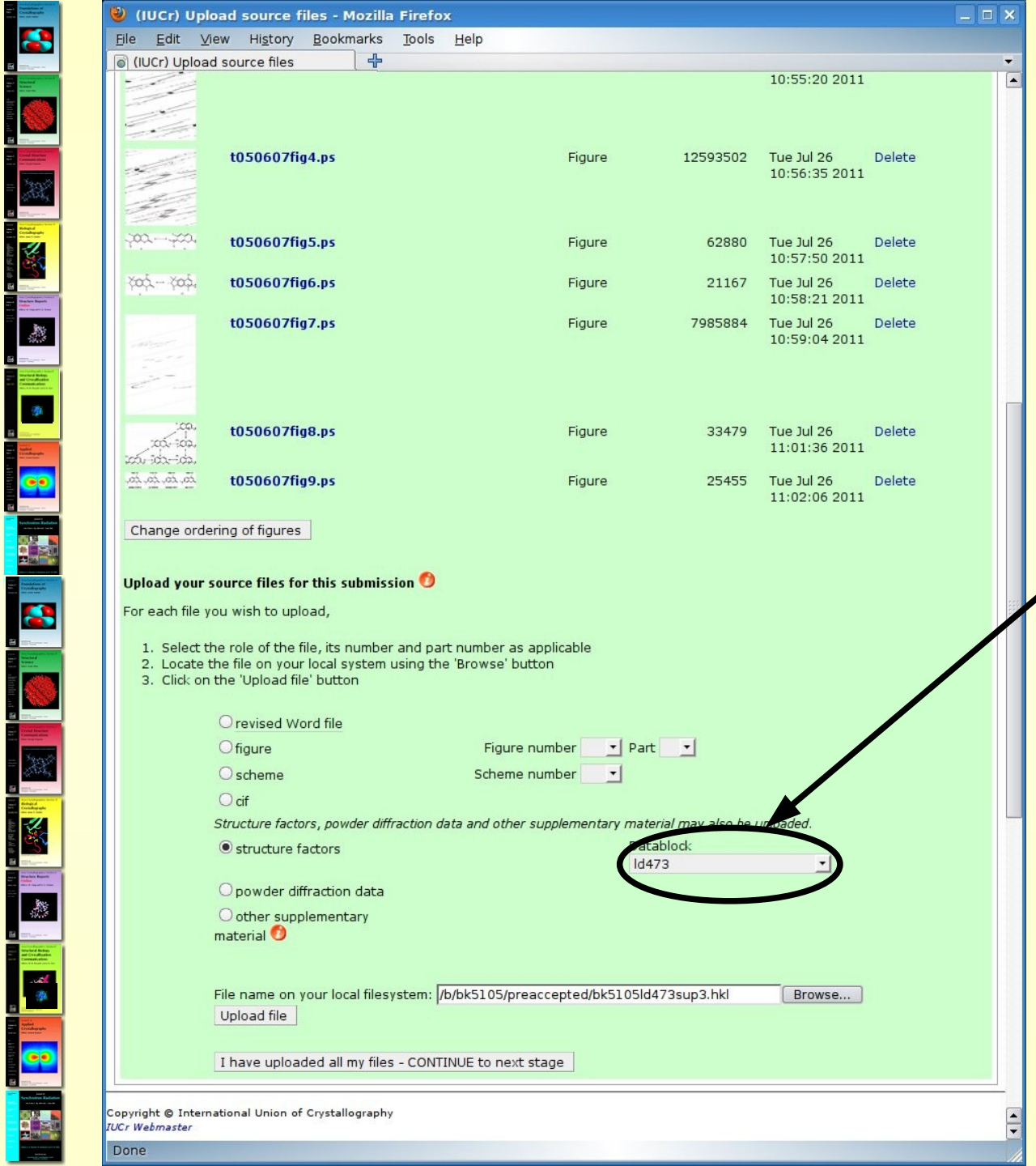
Stage 3, continued

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





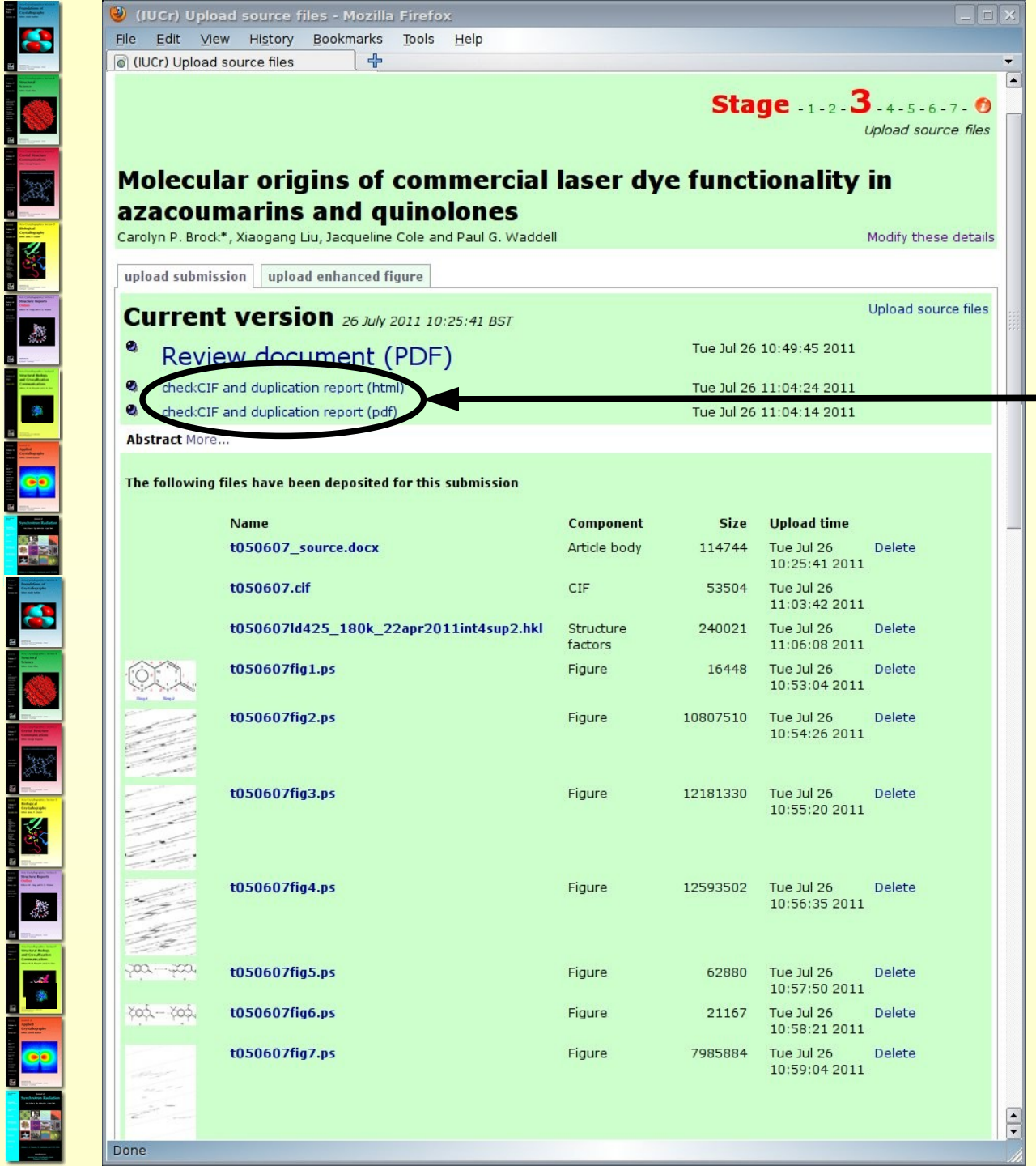


Stage 3, continued

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

Crystallography Journals Online

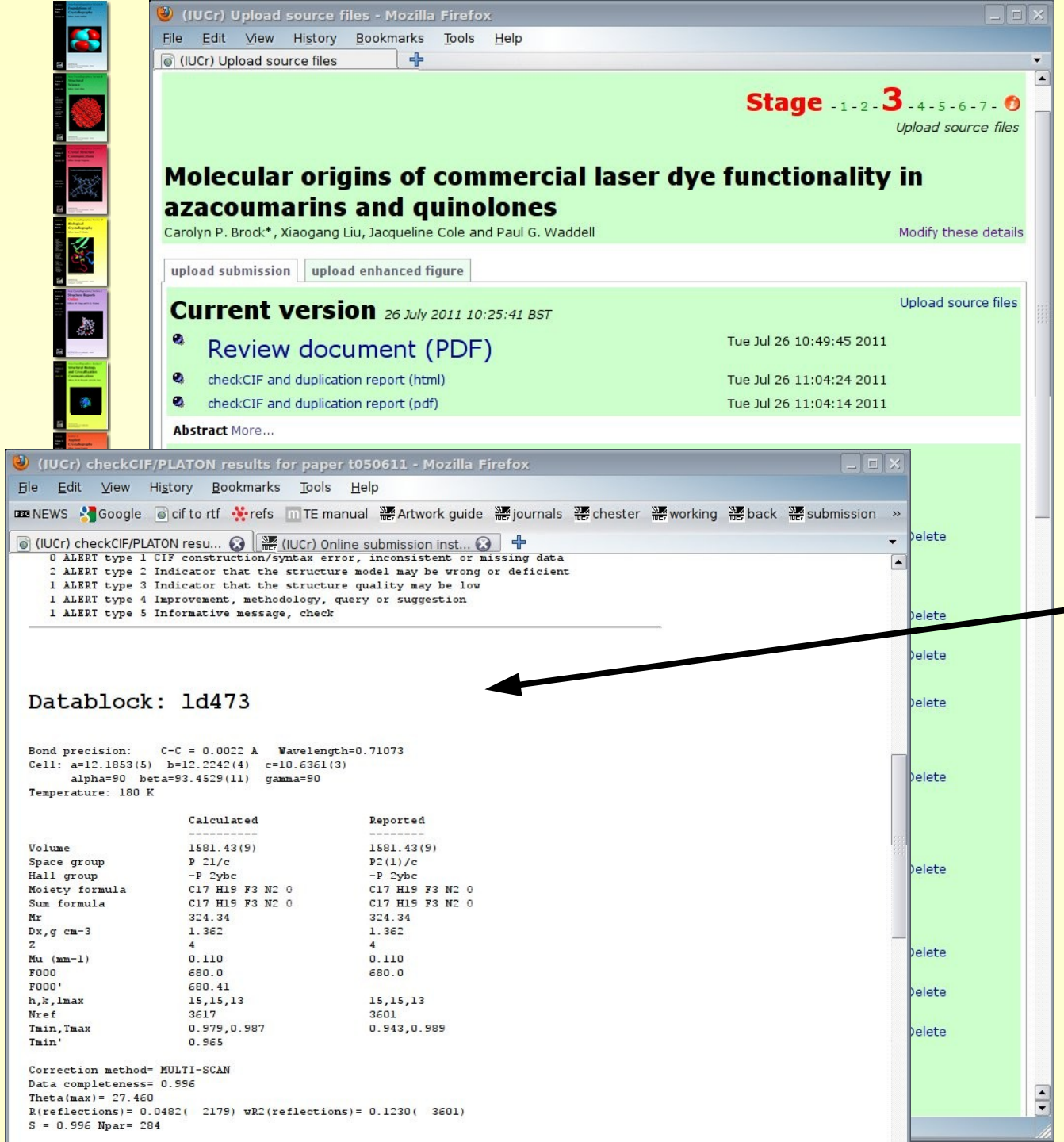


Stage 3, continued

STRUCTURAL PAPER = yes (small molecule structures)

- CheckCIF report appears in html and PDF format

Crystallography Journals Online

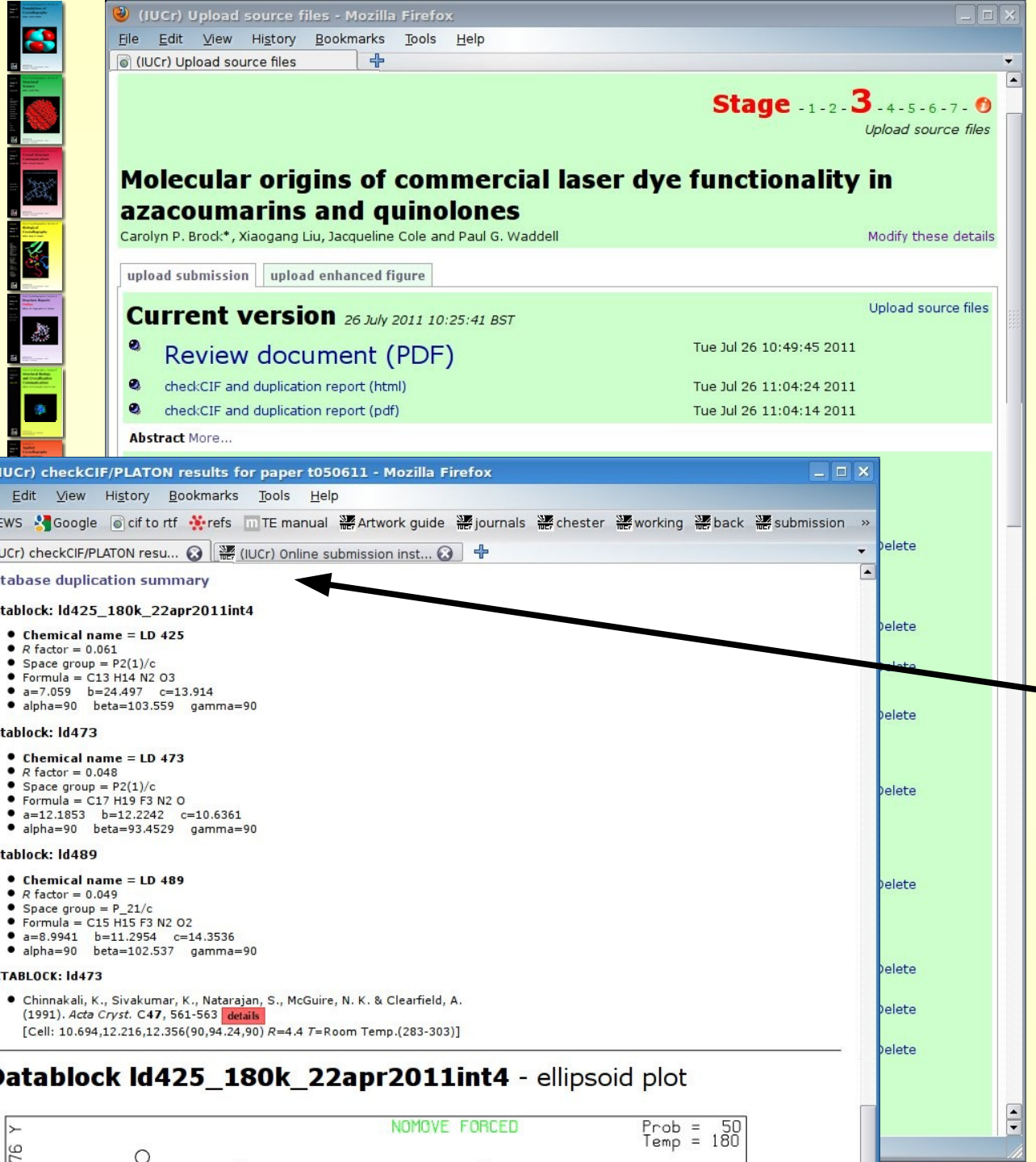


Stage 3, continued

STRUCTURAL PAPER = yes (small molecule structures)

- CheckCIF report appears in html and PDF format
- Report shows
  - checkCIF/PLATON results

Crystallography Journals Online

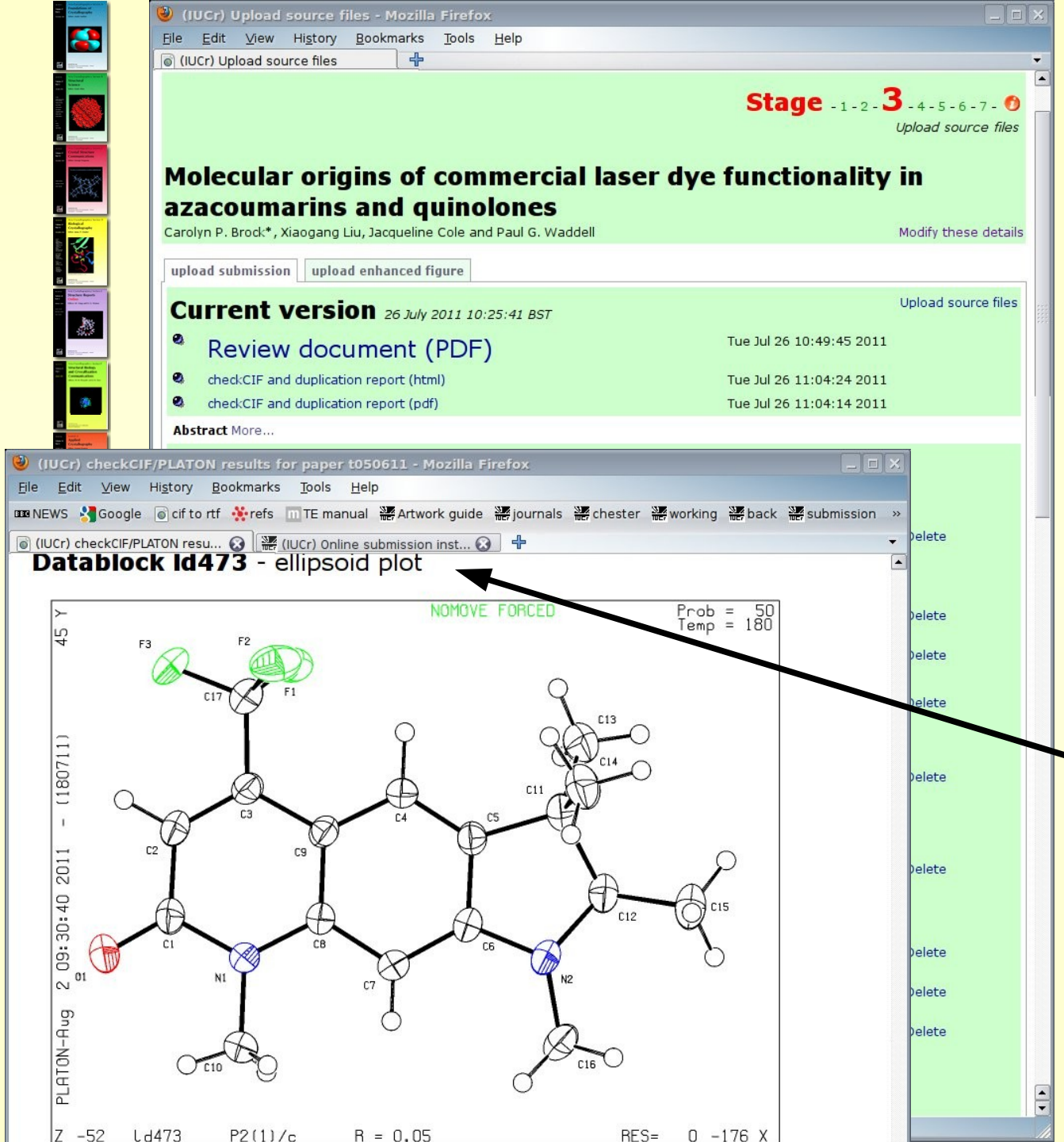


Stage 3, continued

STRUCTURAL PAPER = yes (small molecule structures)

- CheckCIF report appears in html and PDF format
- Report shows
  - checkCIF/PLATON results
  - Database duplication summary

Crystallography Journals Online



Stage 3, continued

STRUCTURAL PAPER = yes (small molecule structures)

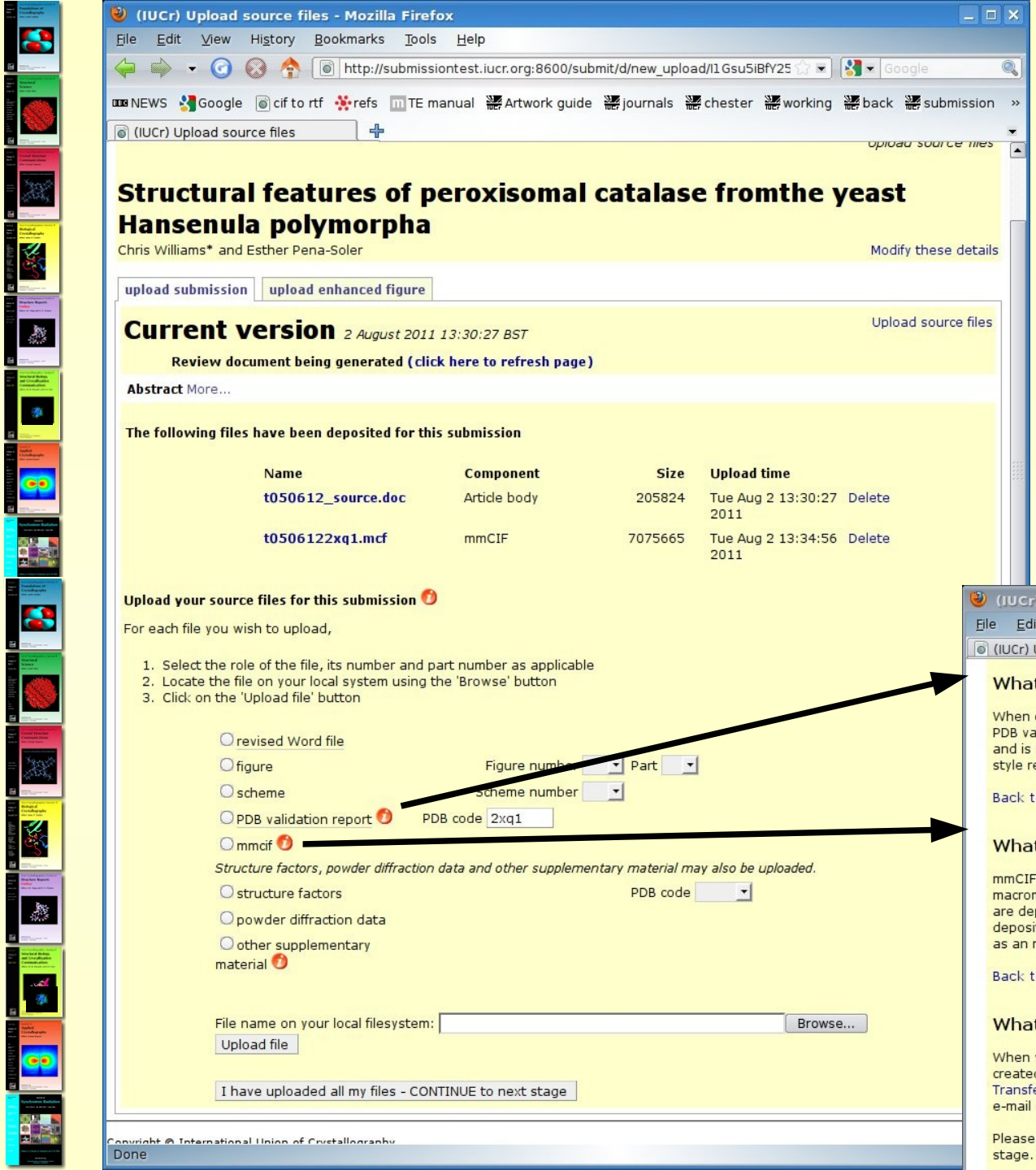
- CheckCIF report appears in html and PDF format
- Report shows
  - checkCIF/PLATON results
  - Database duplication summary
  - Ellipsoid plots

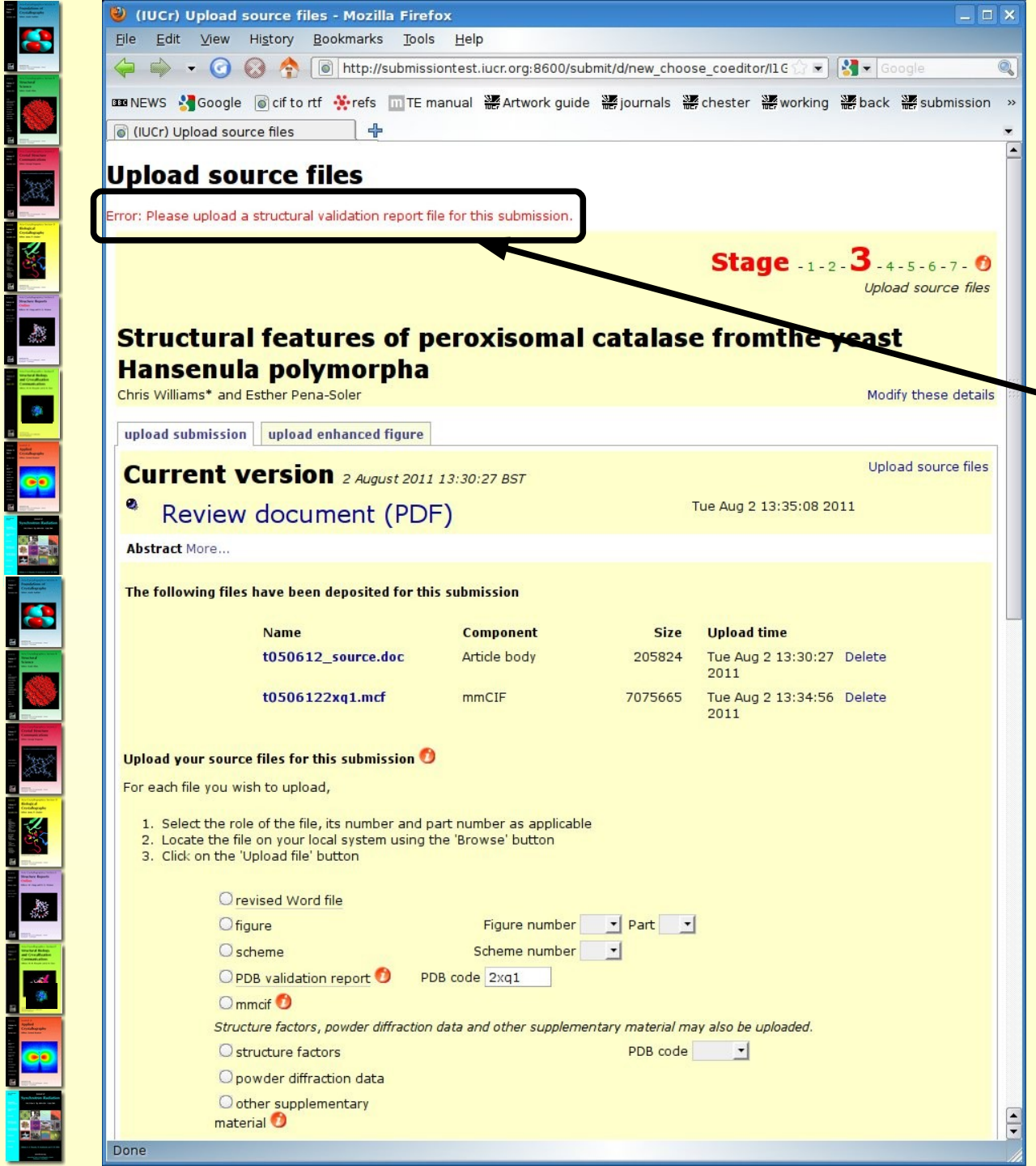
Crystallography Journals Online

Stage 3, continued

STRUCTURAL PAPER = yes (macromolecular structures)

- mmCIF is requested
- PDB validation report required



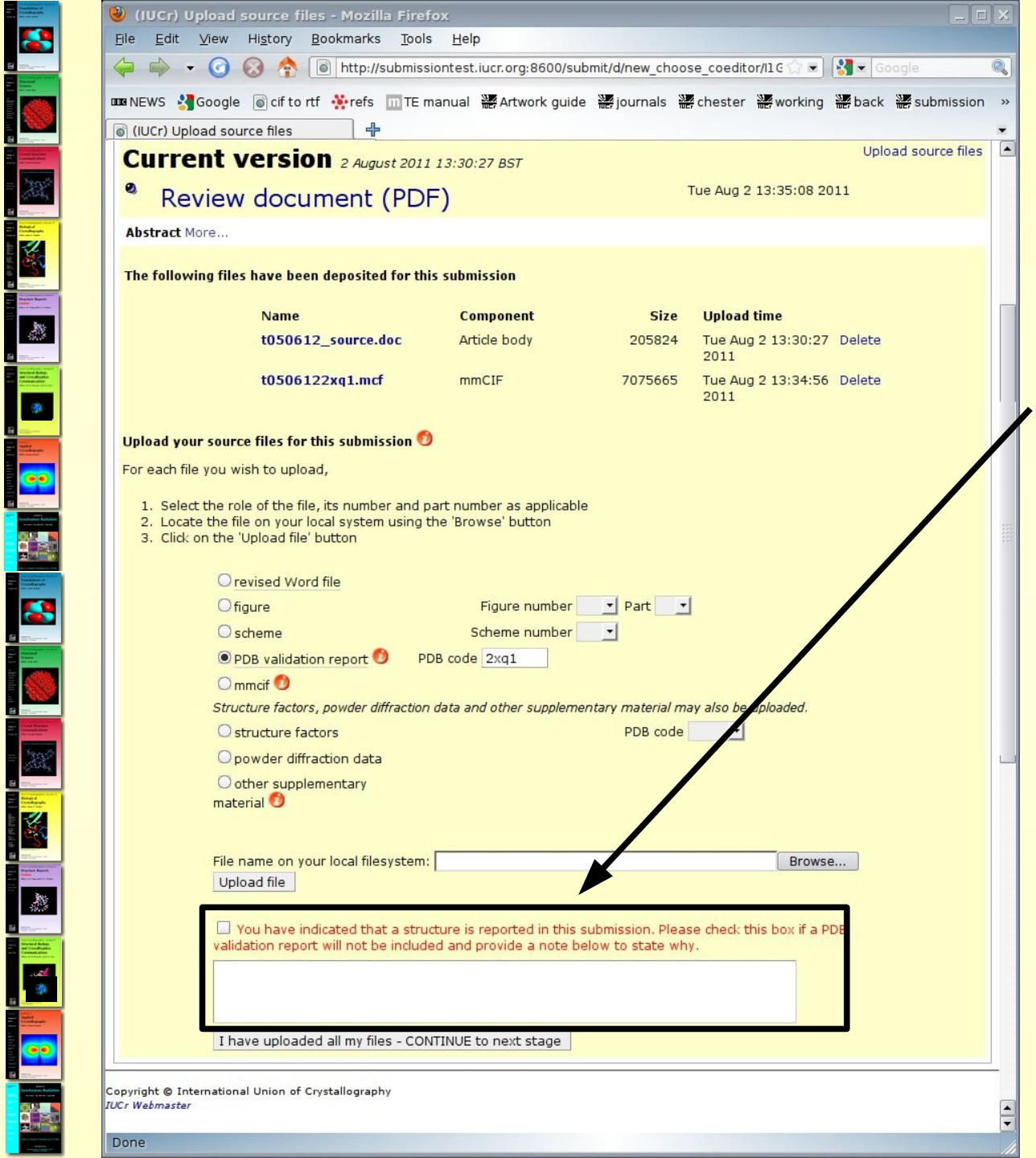


Stage 3, continued

STRUCTURAL PAPER = yes (macromolecular structures)

- Error message appears if authors try to continue without uploading validation report

Crystallography Journals Online

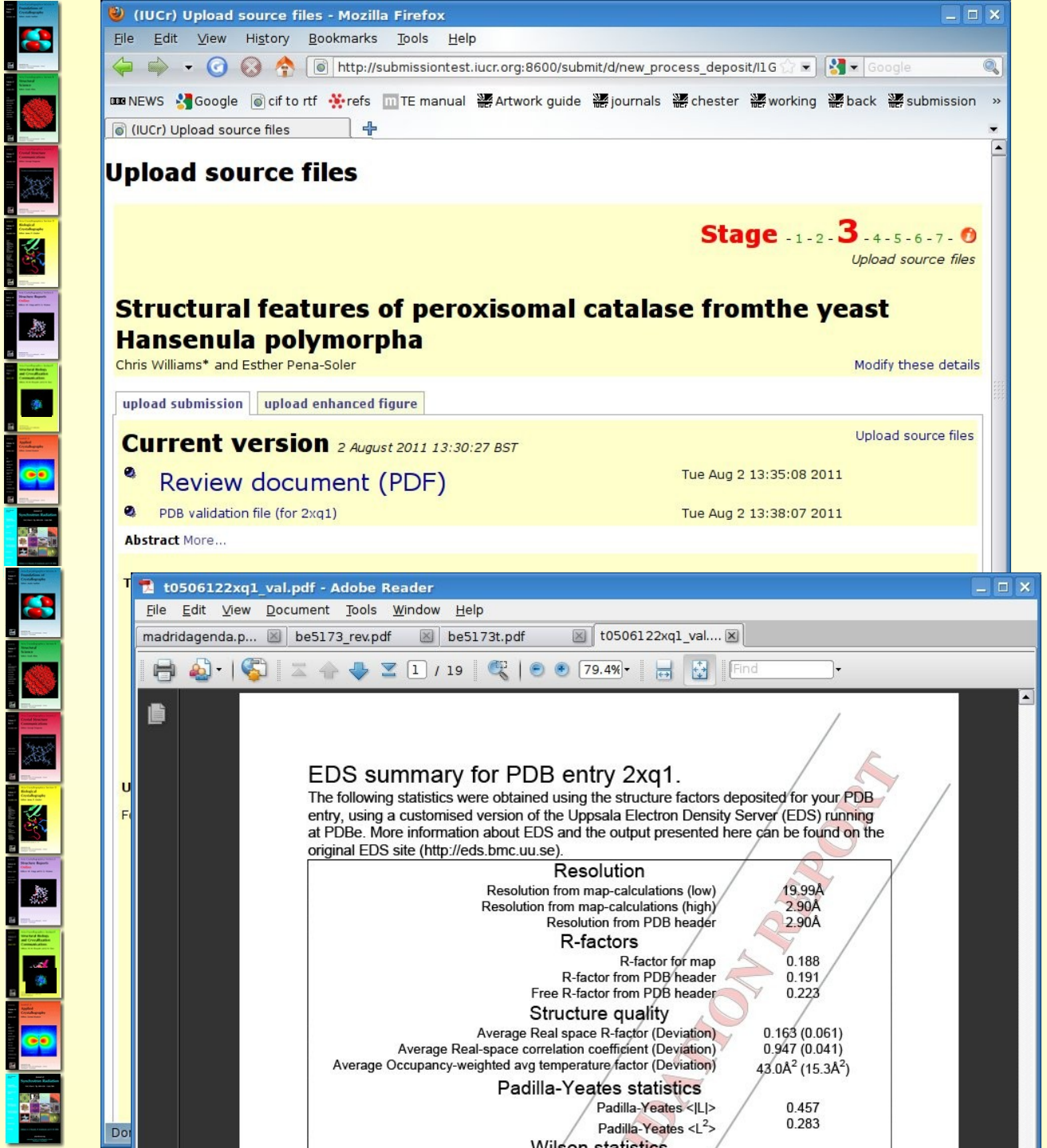


Stage 3, continued

STRUCTURAL PAPER = yes (macromolecular structures)

- If validation report not available can continue if explanation is given

Crystallography Journals Online

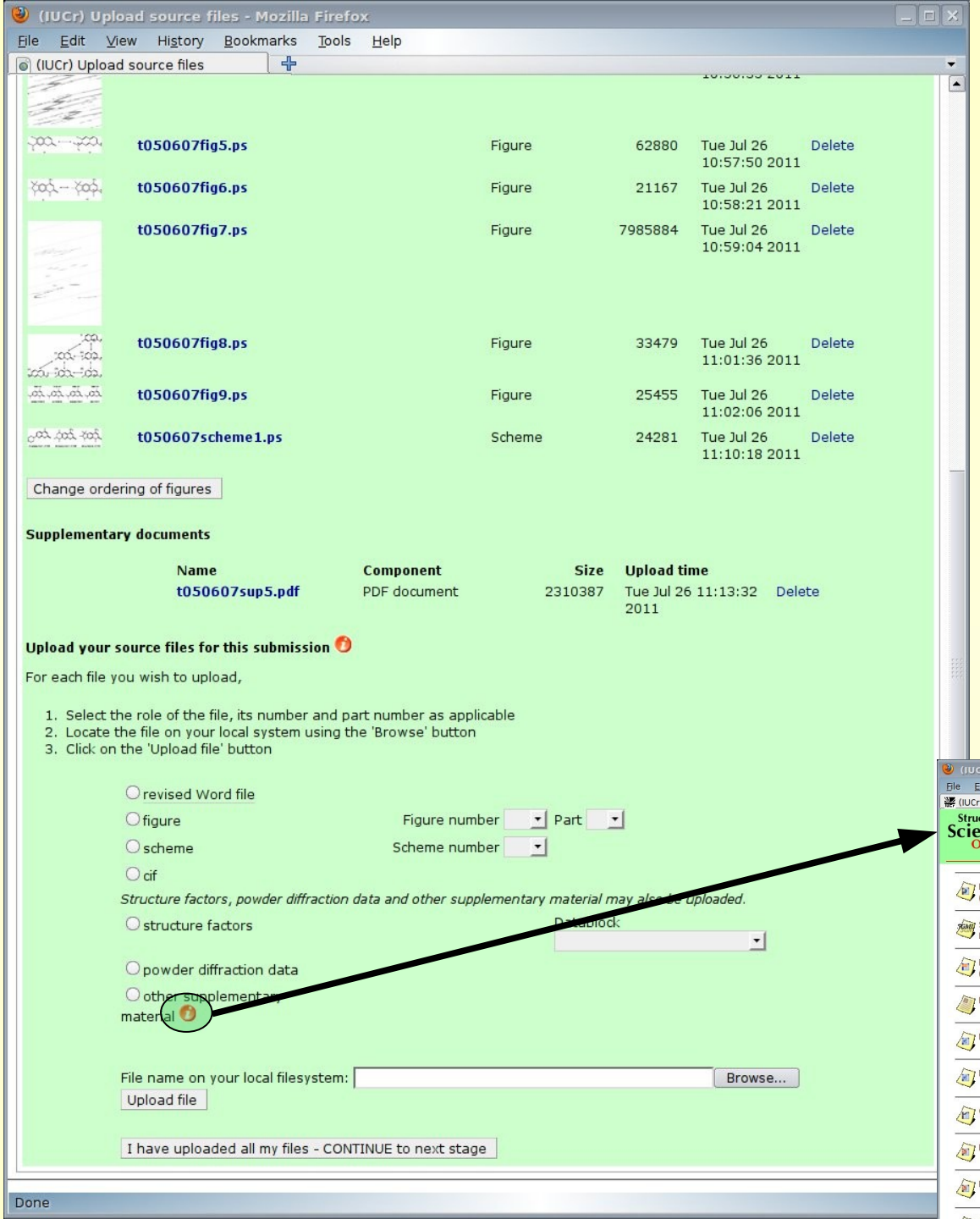


Stage 3, continued

STRUCTURAL PAPER = yes (macromolecular structures)

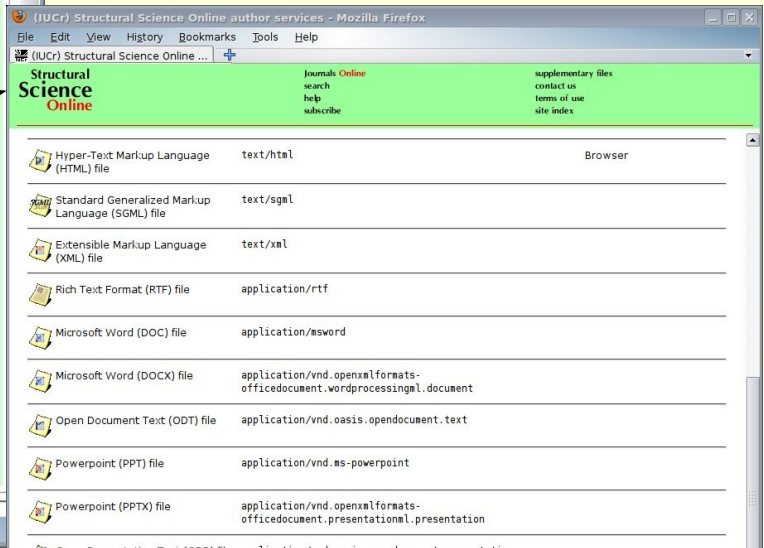
- Validation report usually uploaded as pdf file
- Collecting the report direct from the database is a future option

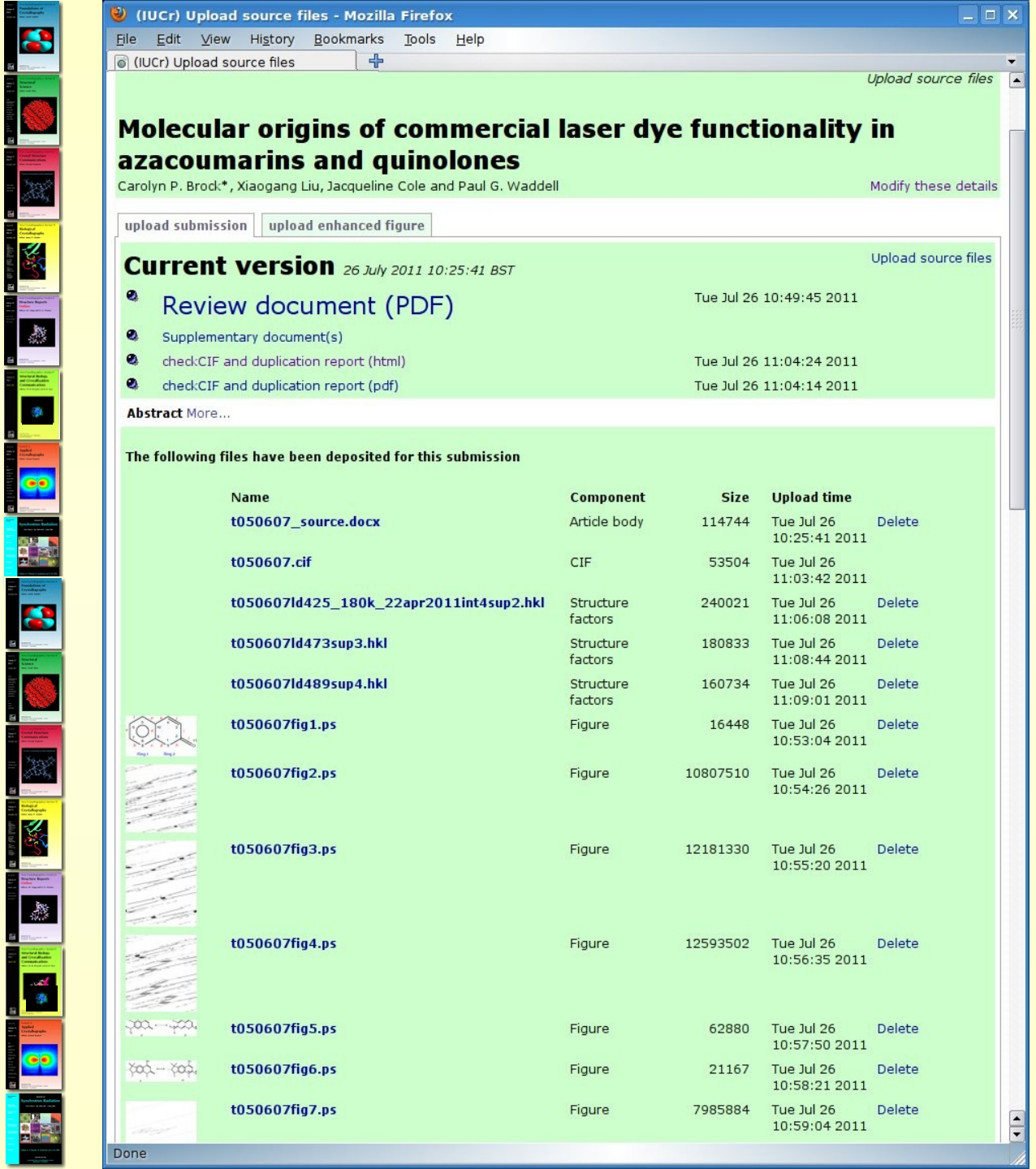
Crystallography Journals Online



Stage 3, continued

- Any other supplementary files can be uploaded
- Full list of file types for supplementary material is available
- 49 different file types supported - chemical connectivity formats added recently

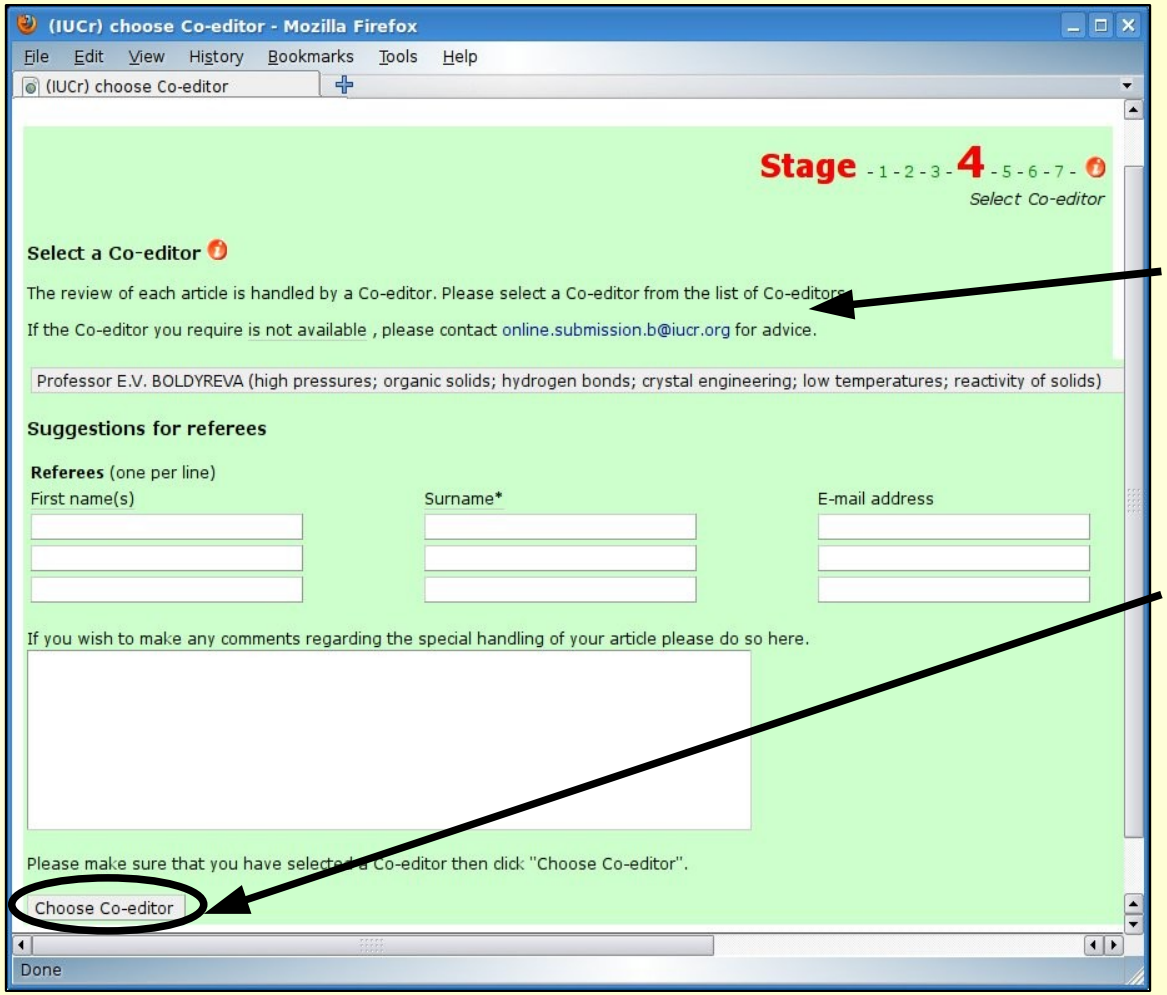




- Final check that all files have been successfully uploaded before moving to Stage 4

Crystallography Journals Online

Stage 4



- Next select a Co-editor from drop-down list
- If Co-editor is not available, author is requested to contact journal support
- Some authors click on `Choose Co-editor' without making a selection – page to be redesigned?

Crystallography Journals Online

Co-editors' availability

What authors see when they submit a paper and get to the Co-editor selection choice, is the COMPLETE list of Coeditors AVAILABLE at that time *i.e.* the ones who are available and whose submission quota for the month has not been exceeded.

The procedure for determining which Co-editors will be available is as follows:

1. Check for conference: if conference select from subset of relevant Co-editors. If no, include all Co-editors.
2. For C/E duplicate structures assign to original Co-editor if Co-editor active (even if quota=0), provided the category is correct.
3. For Addenda/Errata choose relevant Co-editor.
4. Select available Co-editors (*i.e.* active, correct journal, article category and language). Determine the quota, number assigned this week, this month and the number of papers in review for each available Co-editor.

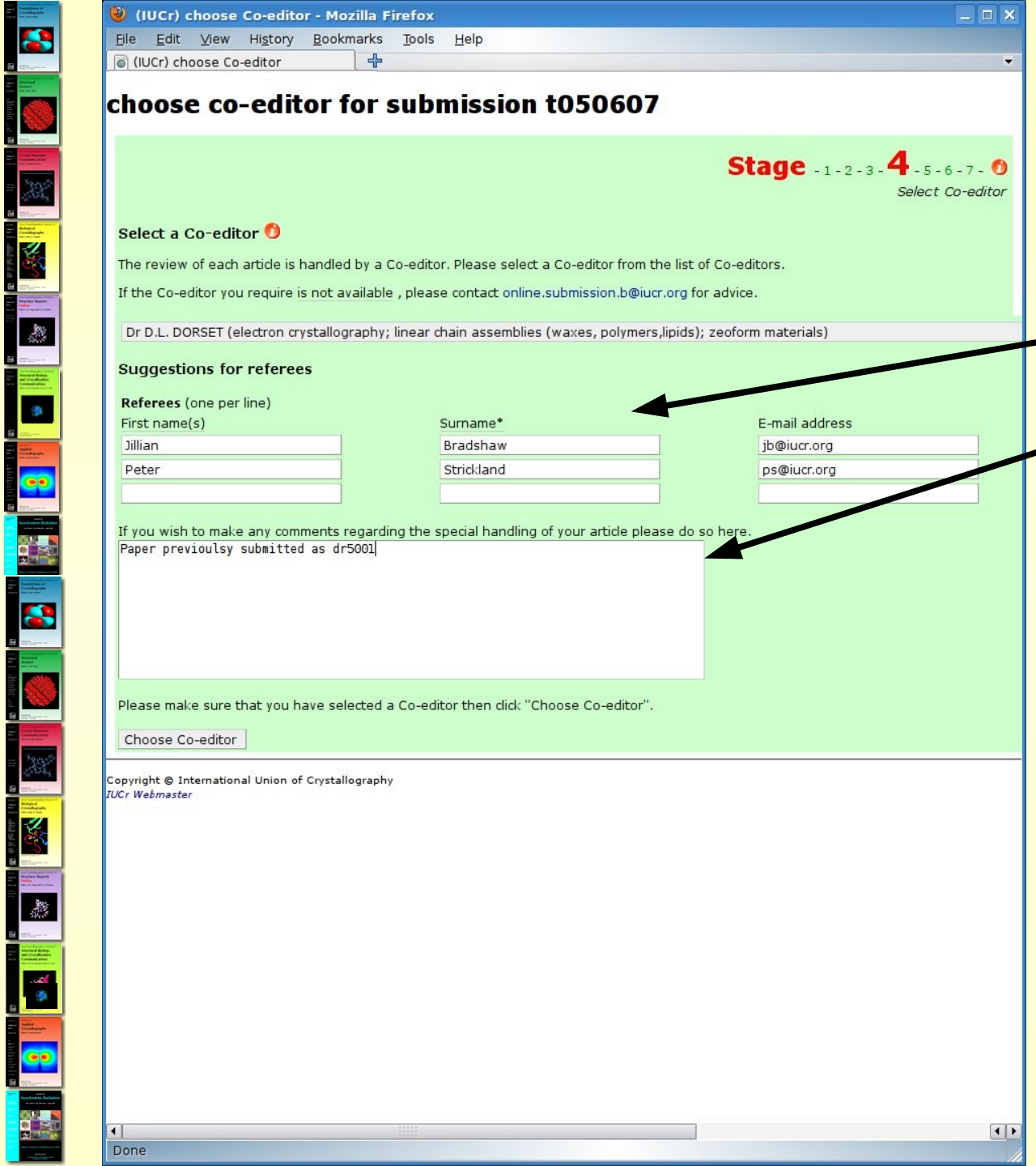
Crystallography Journals Online

Co-editors' availability

5. Select all Coeditors under quota (for C/E monthly and weekly).
6. If none, drop the language test.
7. If still none, factor in the number of articles in review.
8. Total review quota = quota * a journal multiplier
Remove Co-editors with more in review than number determined.
9. If still none repeat with doubling the per month quota.
10. If all else fails, assign to Section Editor.

For some journals, additional tests may be run, *e.g.* has the article "A" validation alerts, is the author on a watchlist, is the word "crystallization" in the title.

Crystallography Journals Online

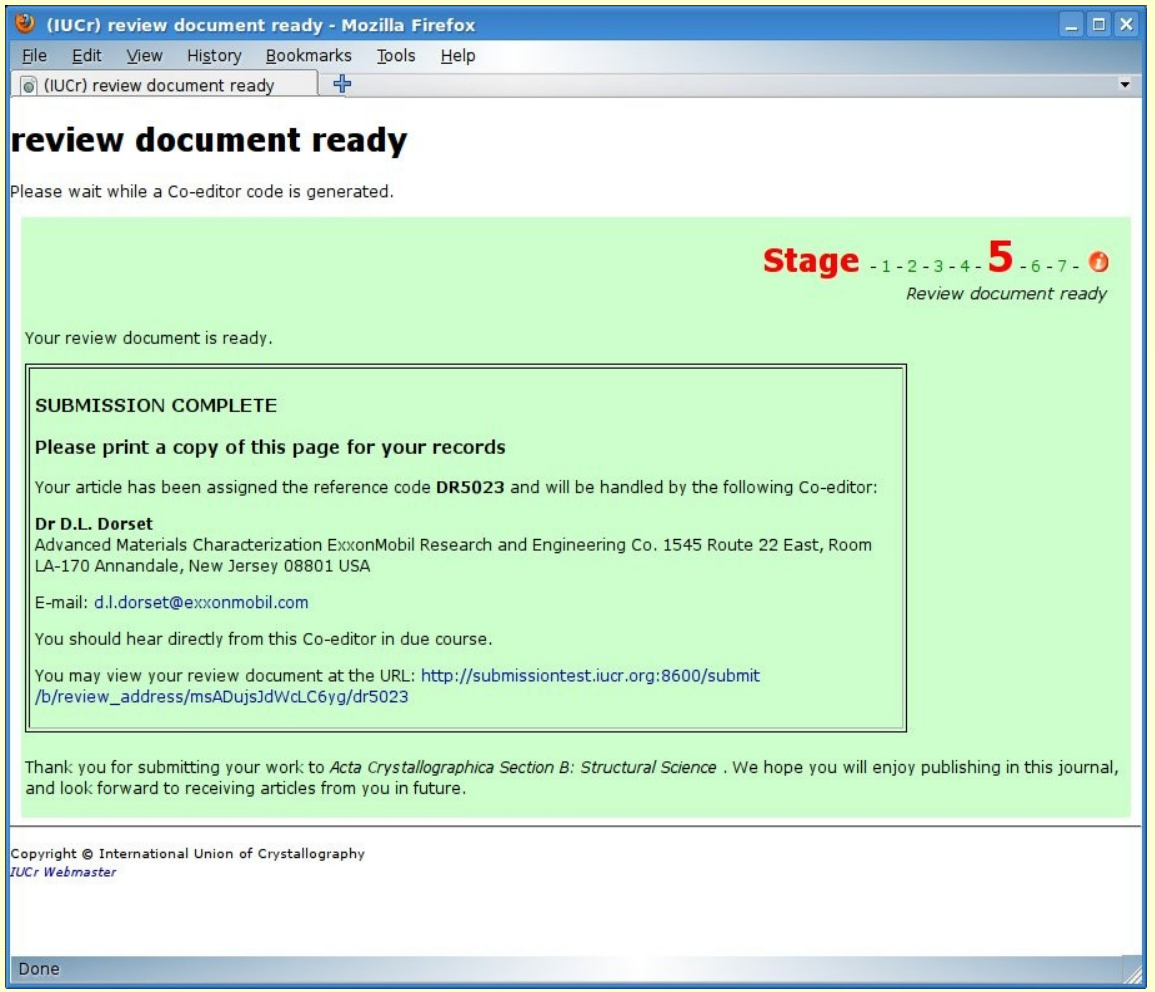


Stage 4

- Can also suggest possible referees
- And make any comments to the Co-editor

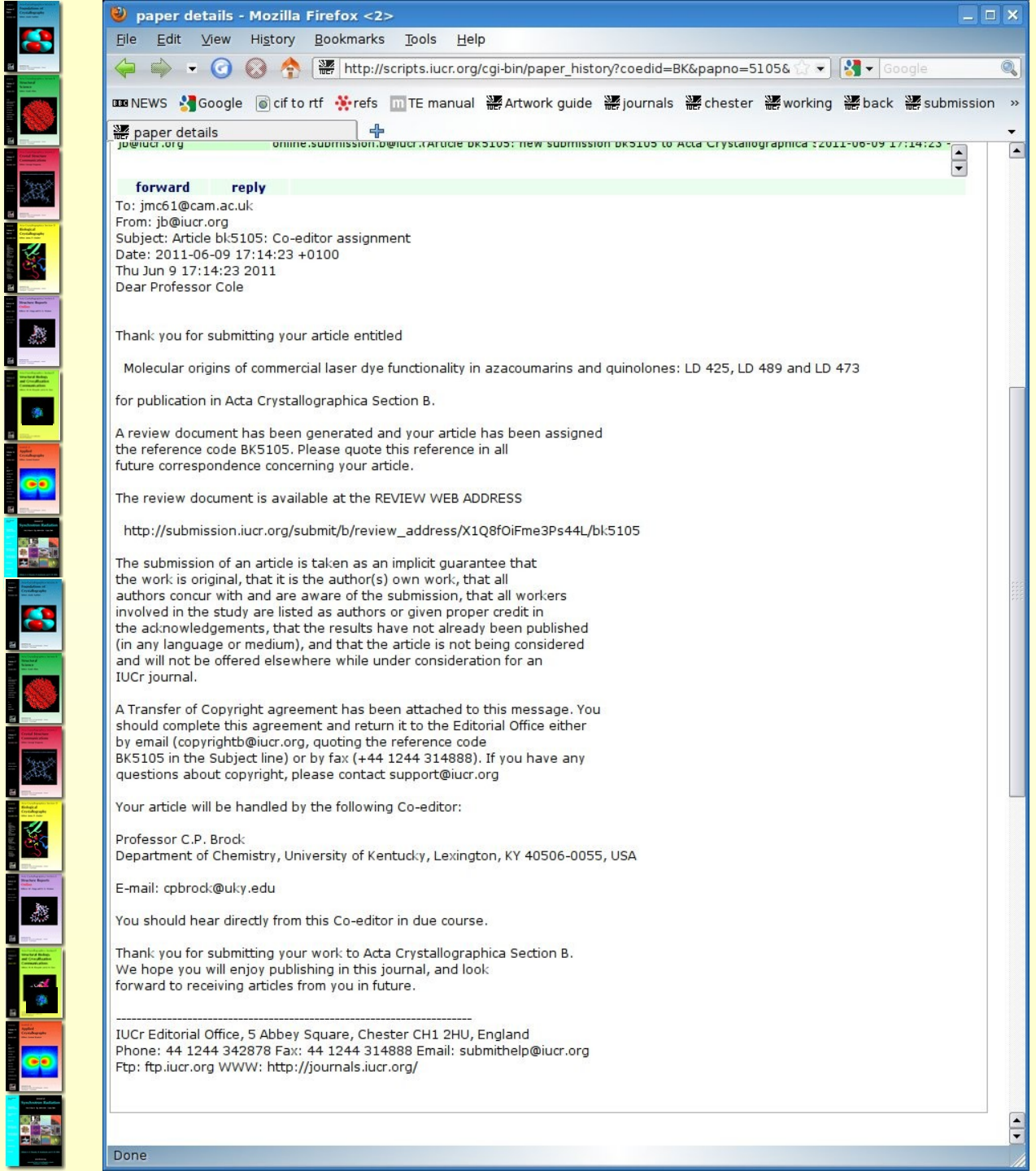
Crystallography Journals Online

Stage 5



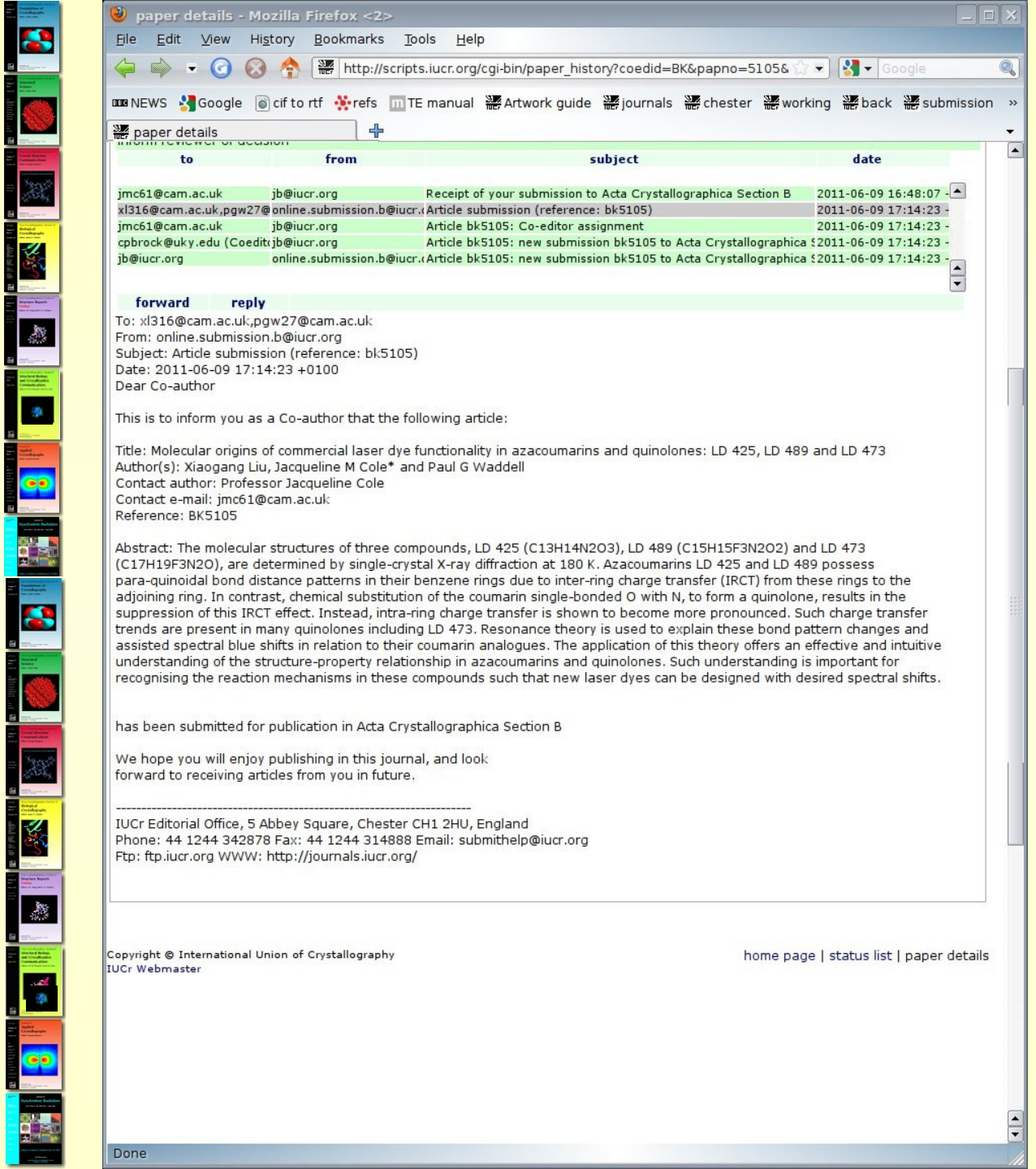
- Submission complete
- E-mails sent
- Chester staff usually check all material present and will query any missing items
- Tracking number replaced by Co-editor code
- Review PDF generated

Crystallography Journals Online



- E-mail sent to author confirming receipt of file
- Co-editor code replaces tracking number

Crystallography Journals Online



- E-mail sent to all co-authors
- Example recently of co-author not being aware of submission of paper – submitted by PhD student

Crystallography Journals Online

paper details - Mozilla Firefox

File Edit View History Bookmarks Tools Help

http://scripts.iucr.org/cgi-bin/paper_history?coedid=BK&papno=5105&

NEWS Google cif to rtf refs TE manual Artwork guide journals chester working back submission

paper details

Electronic review

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 checkCIF report are also available from the web
address below.

The review document is available at the EDITOR WEB PAGE:

http://submission.iucr.org/submit/b/review_address/WCb1Mj4L8OmXQDcO/bk5105

You are recommended to ask your referees to use the ONLINE REVIEW FORM.
To do this, you should either use the 'invite reviewer' facility in the
'e-mails and decisions' tab of the EDITOR WEB PAGE or the status system.

If you prefer your referees not to use the online review form, i.e.
to conduct the review OFFLINE, use the template letter 1A attached
below and the URL given therein.

You may also use the facilities in the 'e-mails and decisions' tab of the
EDITOR WEB PAGE to contact the author, send review comments and request
revisions, and notify the author and the Editorial Office of your decision
(accept, reject, withdraw or transfer). Templates for these actions are also
attached to this message.

Best wishes

Jill Bradshaw
Technical Editor
jb@iucr.org

==========

1A. Template for contacting referees (OFFLINE REVIEW)
---
9 June 2011

Dear

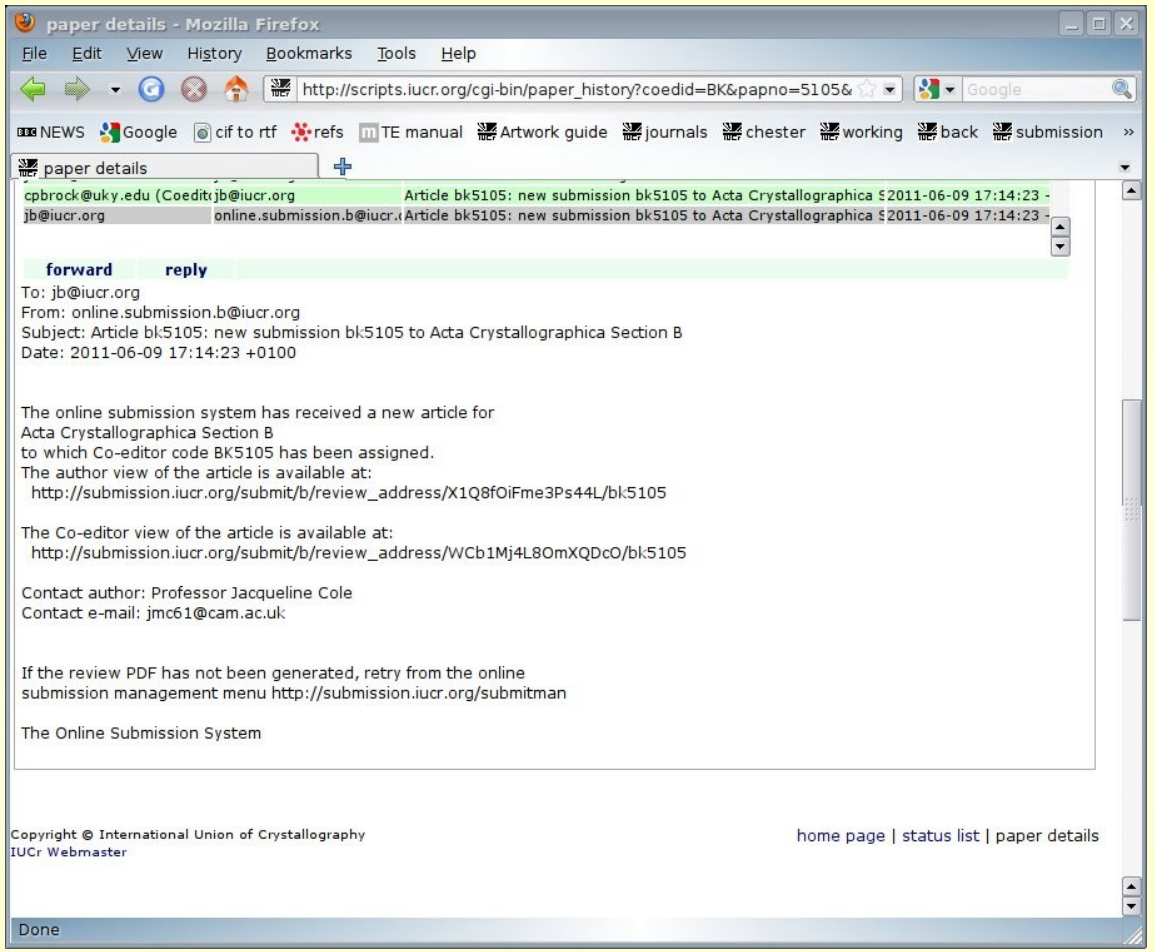
Acta Crystallographica Section B: Structural Science

I would appreciate receiving your comments on the article
(reference: BK5105), which has been submitted for publication in
Acta Crystallographica Section B

Done

- E-mail sent to Co-editor
- E-mail templates for OFFLINE review attached
- Important to only use the urls provided with each submission or *via* the home page

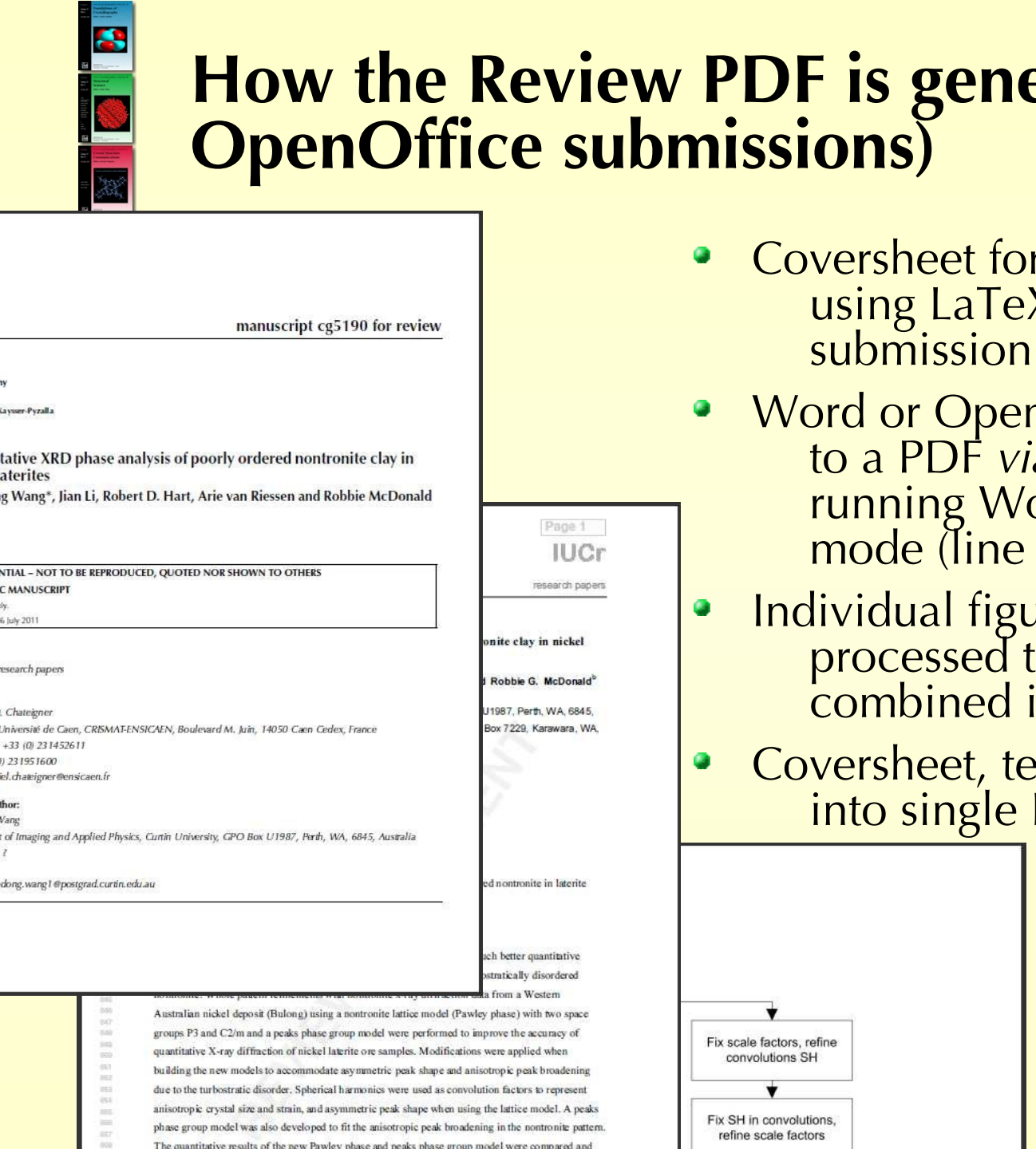
Crystallography Journals Online



- Finally, an e-mail is also sent to Chester

Crystallography Journals Online

How the Review PDF is generated (Word, OpenOffice submissions)



- Coversheet for Review PDF generated using LaTeX from information in submission forms, as .pdf file
- Word or OpenOffice text file converted to a PDF *via* a Windows server running Word 2010 in background mode (line numbering *etc.* added)
- Individual figures automatically processed to .tifs, labelled, and then combined into a figures.pdf file
- Coversheet, text and figures combined into single Review PDF

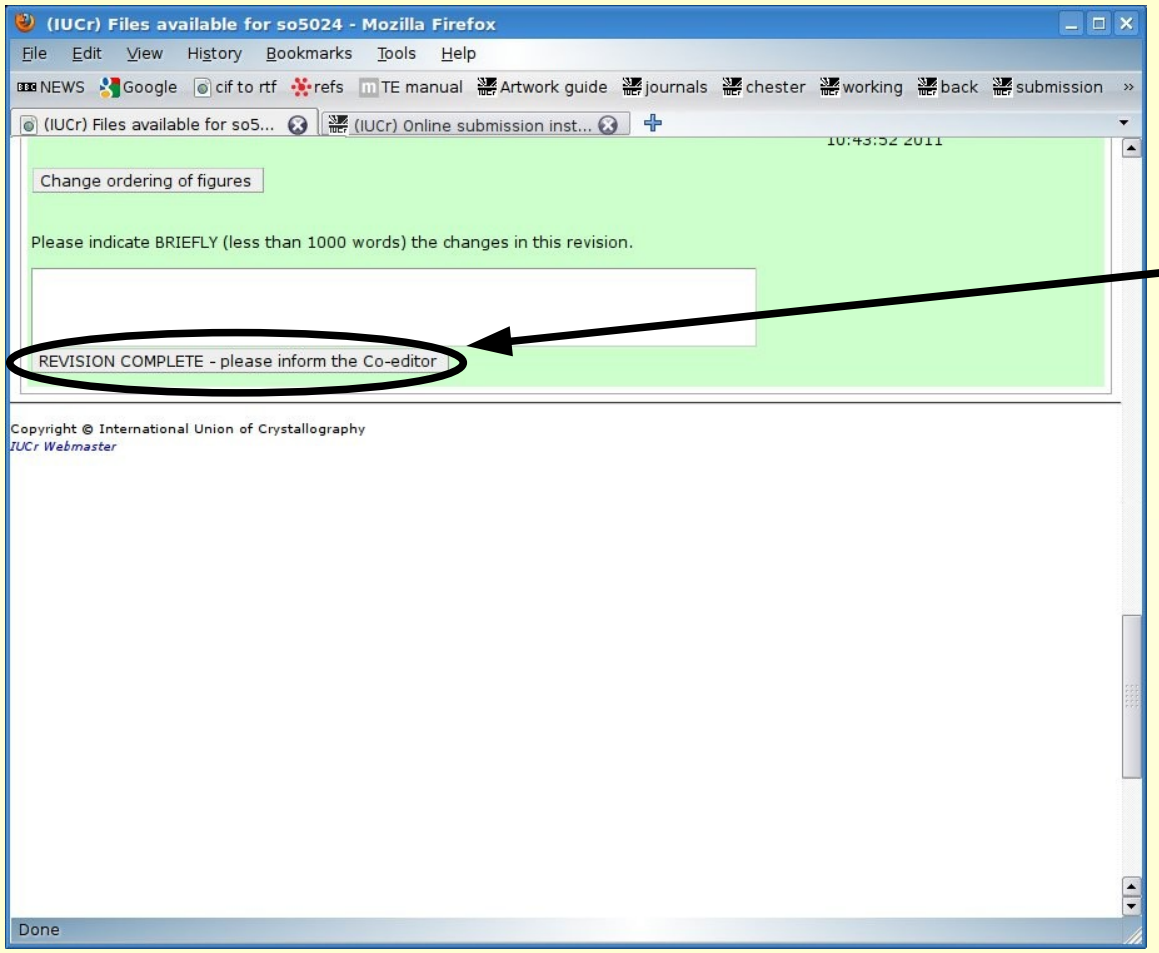
Crystallography Journals Online

How submission system processes LaTeX

- Source file renamed ab1234_source.ltx
- BibTeX renamed ab1234.bib
- Figure files renamed zb1234fig1.ps etc.
- Source file transferred to temporary file ab1234_tmp.ltx – used to create Review PDF file from the transformation:
  - - **authors reference to BibTeX detected and modified** to call in ab1234.bib
  - - **author commands to import figures modified to use new graphics names**, *e.g.* source command \includegraphics{FIGURES\INSTRUMENT.PS} may be changed to \includegraphics{ab1234fig1.ps}
- The system then
  - - runs LaTeX on zb1234_tmp.ltx
  - - if .bib file present BibTeX is run to extract references
  - - LaTeX run again to format citation callouts and bibliography
  - - LaTeX run second time to resolve any remaining cross-references
  - - converts device-dependent output from LaTeX to PDF
  - - if uploaded figures, checks LaTeX file does import these
  - - if not figs are appended to end of review PDF file

Crystallography Journals Online

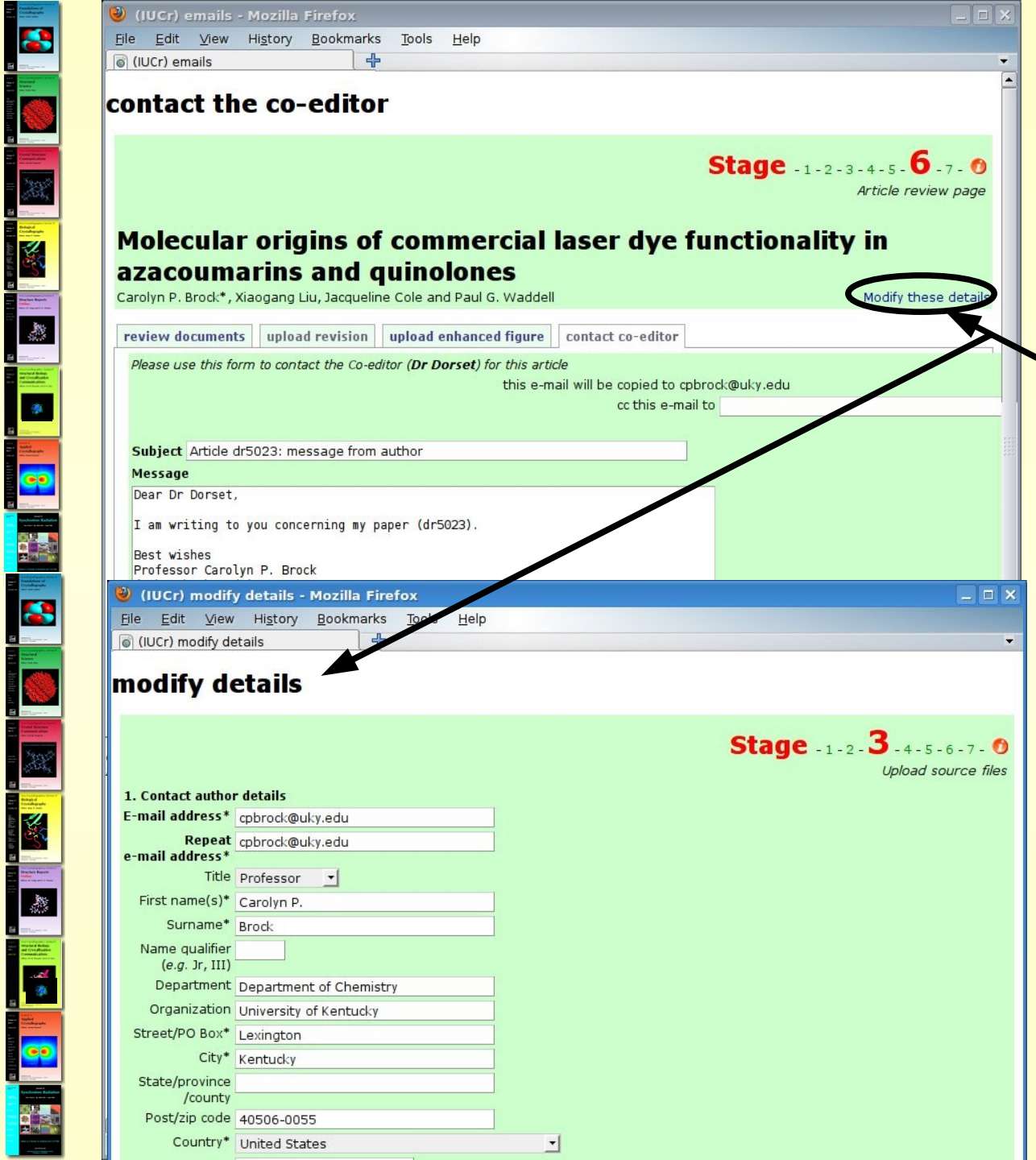
Author revisions



- Co-editor/Chester contacted when revision uploaded
- Author must click on `REVISION COMPLETE – please inform Co-editor' at foot of page
- Document showing **changes** in this revision **available to Co-editors**

Crystallography Journals Online

Author revisions



- Authors can also modify details if any changes to title or authors after submission
- Chester will usually take the information in the manuscript to be correct (**but authors do get proofs**)

Crystallography Journals Online

Some problems

- Review PDF not created
  - files may be password protected
  - file may contain macros
  - file may contain fonts we do not recognise
- Submission not finalized so only tracking number allocated and Co-editor not selected
- Files missing – if author selects `no' at stage 1 in answer to `Does your article report a crystal structure?' then not required to upload CIF
- Missing structure factor/powder data files
- Authors sometimes upload multiple revisions if wrong files uploaded

Crystallography Journals Online

Some problems, continued

- Authors do not complete submission
  - given two months to complete submission but reminder emails sent as authors often lose details of how to proceed
- Multiple submissions using slightly different details and files
- Figures uploaded but do not appear in Review PDF file

Crystallography Journals Online

Some problems - LaTeX

- No BibTex file uploaded or not recognised – no citations will appear in the Review PDF
- Figures in wrong format - LaTeX can handle .ps, .jpg or .png but not .tif
- Names of uploaded figure files differ from those referenced in source LaTeX file
- Author used LaTeX macro libraries that are not standard – the Review PDF will not be created at all (solution: adding non-standard library to collection available to submission system)
- LaTeX file not in preprint mode

Crystallography Journals Online

Future development - submissions

- Feedback very important
- Integration with contributor ID systems such as ORCID
- Plagiarism checking of all articles (using CrossCheck)
- Integration of electronic copyright/licencing transfer into submission procedure
- Improve documentation for authors and make the process clearer
- Transfer of information collected by tools and templates to submission system
- Improved status information for authors
- Home pages to be extended to authors
- Reference checking of submitted articles

Crystallography Journals Online