Journal production processes

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Crystallography Journals Online

Journal production processes

- Overview
- SGML
- Technical editing
- Typesetting
- Proofreading
- Printing
- Online journals

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Technical Editing

ed·it (ĕd′ĭt)
tr.v. **ed·it·ed**, **ed·it·ing**, **ed·its**

1.
   - **a.** To prepare (written material) for publication or presentation, as by correcting, revising, or adapting.
   - **b.** To prepare an edition of for publication: *edit a collection of short stories.*
   - **c.** To modify or adapt so as to make suitable or acceptable: *edited her remarks for presentation to a younger audience.*

2. To supervise the publication of (a newspaper or magazine, for example).
3. To assemble the components of (a film or soundtrack, for example), as by cutting and splicing.
4. To eliminate; delete: *edited the best scene out.*

n.

An act or instance of editing: *made several last-minute edits for reasons of space.*

Why edit?

Maintain consistent style throughout the journal – house style

Make articles easier to read

Maintain accuracy

Add value through links and other features

Technical editing is done on screen and on paper

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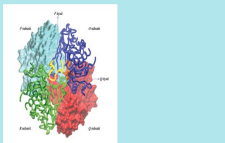
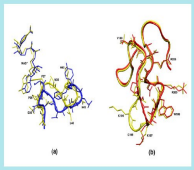
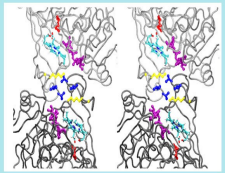
OR

OR



+

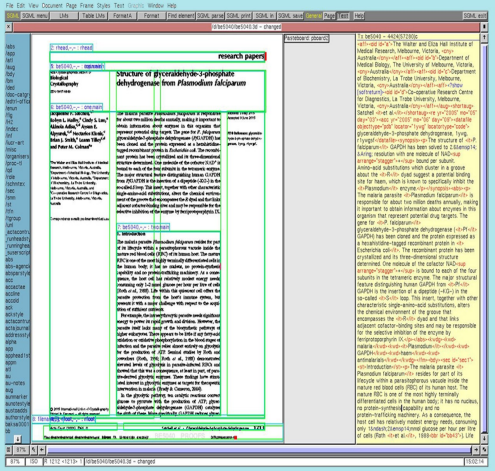




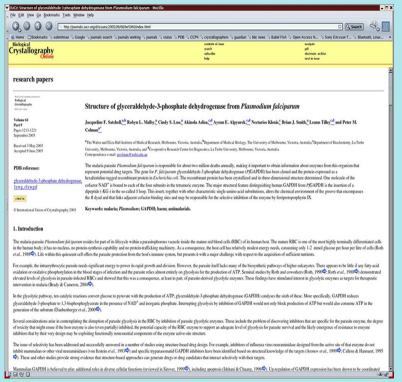
Author's files

SGML editing

Typesetting

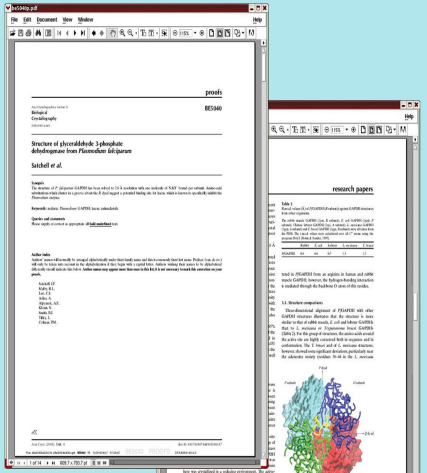


Conversion to HTML



Online version

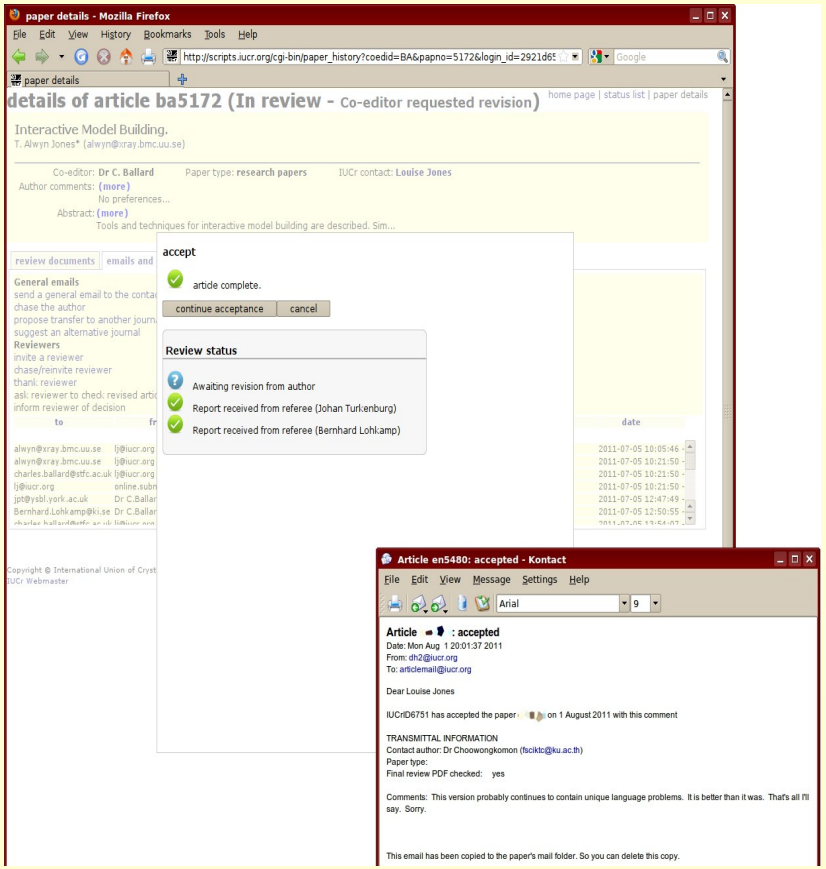
Proofreading



Conversion to PostScript & PDF

Print version

Acceptance



- Author's files transferred across from the submission system to the production system, technical editor e-mailed, production database updated
- Before acceptance make sure final version has all the changes asked for
- After acceptance, website for the submission is closed to the authors, editors get access to e-mails and files depending on status of article *e.g.* proofs, HTML

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What files do we have?

File for text and tables of the article

Processed file for each figure or scheme

Author's original files

Supplementary materials file(s)

Review PDF file

Files giving details about the article, *e.g.* received and accepted dates

All article files follow a naming convention using the co-editor code

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What is SGML and why do we use it?

- SGML = standard generalized markup language
- Structured ASCII document
- Contains tags which may or may not have attributes
- Conforms to our document type definition (DTD)
- Is an archival format
- Used for typesetting, conversion to HTML (online journals)
- Used to create metadata and content for other online platforms
- Future – may change to XML

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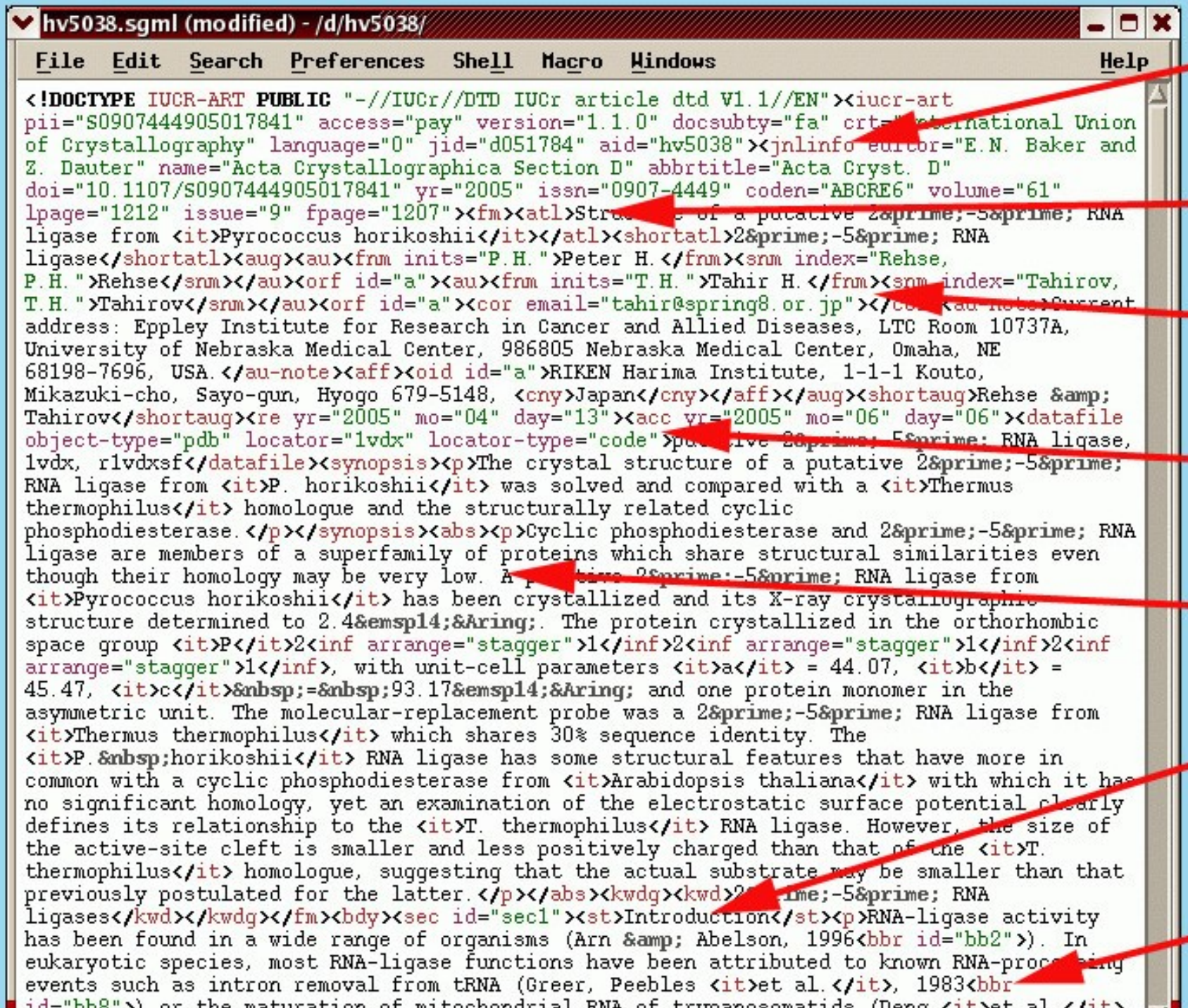
hv5038.sgml (modified) - /d/hv5038/
File Edit Search Preferences Shell Macro Windows Help
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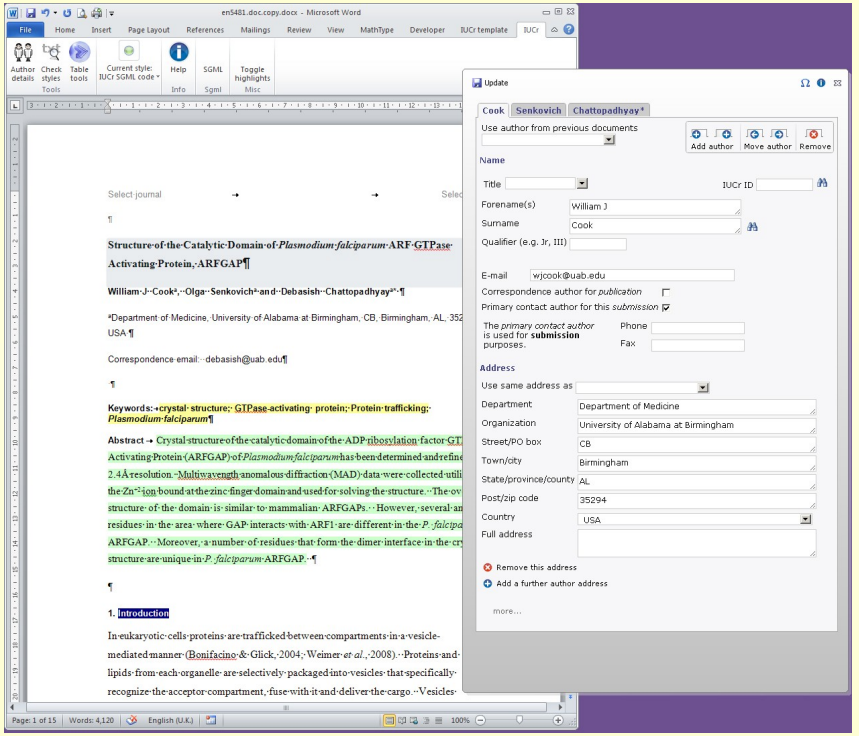
Z. Dauter" name="Acta Crystallographica Section D" abbrtitle="Acta Cryst. D"
doi="10.1107/S0907444905017841" yr="2005" issn="0907-4449" coden="ABCRE6" volume="61"
lpage="1212" issue="9" fpage="1207"><fm><atl>Structure of a putative 2′-5′ RNA
ligase from <it>Pyrococcus horikoshii</it></atl><shortatl>2′-5′ RNA
ligase</shortatl><aug><au><fnm inits="P.H.">Peter H.</fnm><snm index="Rehse,
P.H.">Rehse</snm></au><orf id="a"><au><fnm inits="T.H.">Tahir H.</fnm><snm index="Tahirov,
T.H.">Tahirov</snm></au><orf id="a"><cor email="tahir@spring8.or.jp"></cor><au-note>Current
address: Eppley Institute for Research in Cancer and Allied Diseases, LTC Room 10737A,
University of Nebraska Medical Center, 986805 Nebraska Medical Center, Omaha, NE
68198-7696, USA.</au-note><aff><oid id="a">RIKEN Harima Institute, 1-1-1 Kouto,
Mikazuki-cho, Sayo-gun, Hyogo 679-5148, <cny>Japan</cny></aff></aug><shortaug>Rehse &
Tahirov</shortaug><re yr="2005" mo="04" day="13"><acc yr="2005" mo="06" day="06"><datafile
object-type="pdb" locator="1vdx" locator-type="code">putative 2′-5′ RNA ligase,
1vdx, r1vdxsf</datafile><synopsis> The crystal structure of a putative 2′-5′
RNA ligase from <it>P. horikoshii</it> was solved and compared with a <it>Thermus
thermophilus</it> homologue and the structurally related cyclic
phosphodiesterase. </synopsis><abs> Cyclic phosphodiesterase and 2′-5′ RNA
ligase are members of a superfamily of proteins which share structural similarities even
though their homology may be very low. A putative 2′-5′ RNA ligase from
<it>Pyrococcus horikoshii</it> has been crystallized and its X-ray crystallographic
structure determined to 2.4 Å. The protein crystallized in the orthorhombic
space group <it>P</it>2<inf arrange="stagger">1</inf>2<inf arrange="stagger">1</inf>2<inf
arrange="stagger">1</inf>, with unit-cell parameters <it>a</it> = 44.07, <it>b</it> =
45.47, <it>c</it> = 93.17 Å and one protein monomer in the
asymmetric unit. The molecular-replacement probe was a 2′-5′ RNA ligase from
<it>Thermus thermophilus</it> which shares 30% sequence identity. The
<it>P. horikoshii</it> RNA ligase has some structural features that have more in
common with a cyclic phosphodiesterase from <it>Arabidopsis thaliana</it> with which it has
no significant homology, yet an examination of the electrostatic surface potential clearly
defines its relationship to the <it>T. thermophilus</it> RNA ligase. However, the size of
the active-site cleft is smaller and less positively charged than that of the <it>T.
thermophilus</it> homologue, suggesting that the actual substrate may be smaller than that
previously postulated for the latter. </abs><kwdg><kwd>2′-5′ RNA
ligases</kwd></kwdg></fm><bdy><sec id="sec1"><st>Introduction</st> RNA-ligase activity
has been found in a wide range of organisms (Arn & Abelson, 1996<bbr id="bb2">). In
eukaryotic species, most RNA-ligase functions have been attributed to known RNA-processing
events such as intron removal from tRNA (Greer, Peebles <it>et al.</it>, 1983<bbr
Journal details
Article details
Author details
Database details
Synopsis and Abstract
Start of text
Cross references

IUCr DocX Word template

- If article not supplied in the template Technical Editor can use template to produce SGML
- Journal, volume, issue, paper category, title, authors, affiliations, who is the contact author
- General style of article is checked and IUCr styles are applied to the front matter (abstract, synopsis, keywords), sections, headings, captions, tables
- Different parts highlighted in different colours
- References are checked in IUCr database and in PubMed and reformatted if necessary
- IUCr LaTeX conversion program is also used to convert articles in LaTeX to SGML



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Filtering the SGML

- Carries out repetitive tasks
- Corrects some spellings *e.g.* -ise becomes -ize, -isation becomes -ization
- Computer programs, some foreign words, species names *etc.* made italic
- Adds fixed spaces between possible units and values, double spaces are removed
- Some phrases altered *e.g.* indexation --> indexing, to evidence --> to show
- Unit symbols are altered *e.g.* seconds becomes s
- Table attributes are changed *i.e.* to give rules top, bottom and beneath headings, and entries are aligned left
- Sections, figures, tables are given number attributes
- Checks for uncited reference, figure, scheme, table, footnote tags are run
- Cross references to figures, tables, schemes, equations, references are added
- Adds index terms and running footers for authors
- Puts tags around URLs, PDB codes

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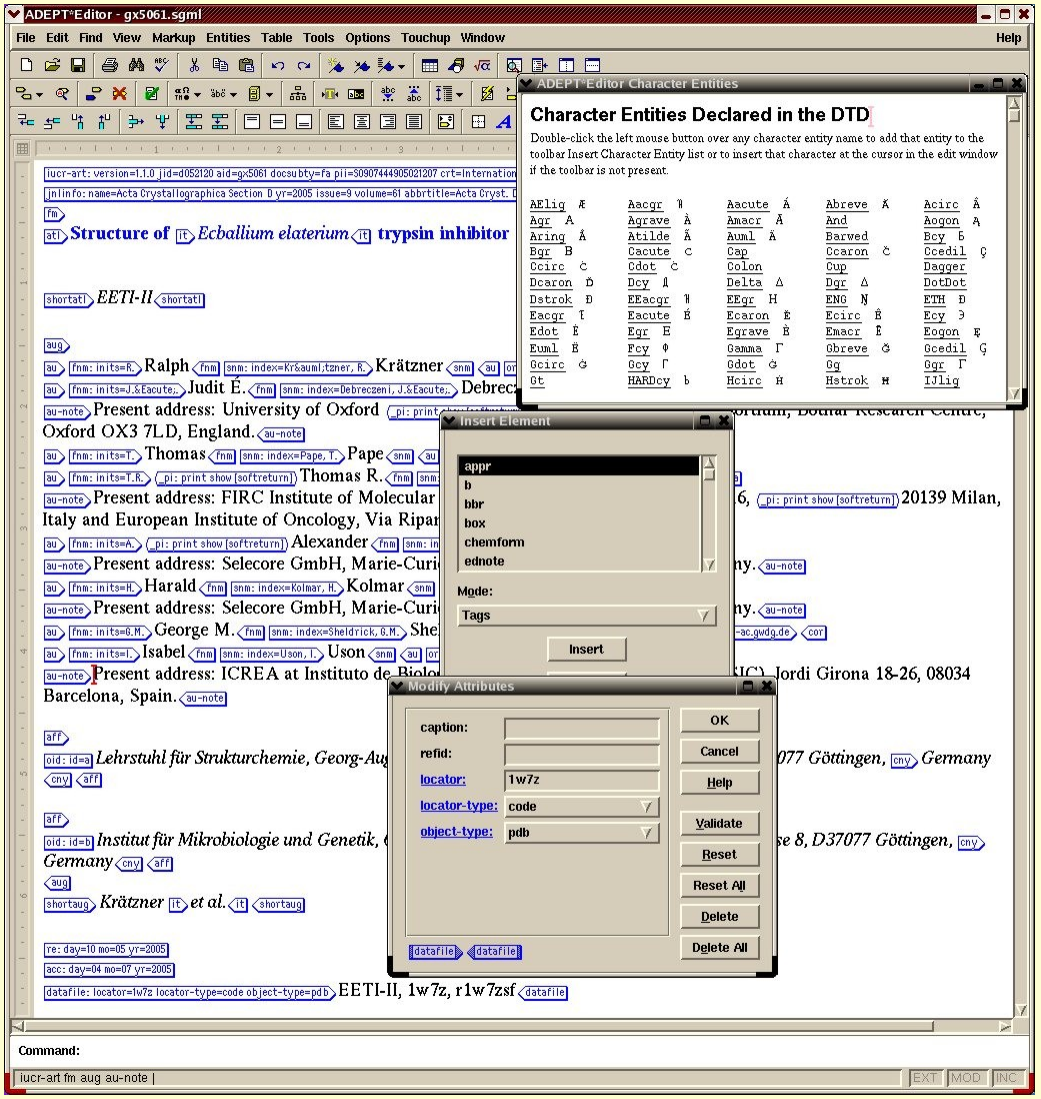
Technical editing on screen



- Using an SGML editor ensures that SGML remains compliant as it will only allow insertion or deletion of elements as allowed by the DTD
- Tags and their attributes can be changed easily

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Checks and changes made in editing

- Authors and affiliations are correct
- Abstract not written in first person
- Spelling
- Grammar
- Clarity/avoidance of ambiguity
- Hyphenation and en rules, *e.g.* adjectival phrases, electron-density plot, en rules used for two distinct elements *e.g.* red–brown crystals
- Consistency between text and tables/figures, especially labels
- Arrangement of data in tables, economic presentation
- Non-standard abbreviations and symbols are defined
- Special symbols such as Greek symbols or mathematical symbols

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Checks and changes made in editing (continued)

- Nomenclature is correct and conforms to IUPAC – use Compendium of Biochemical Nomenclature, IUPAC books
- Units are SI
- Check that tables, figures, schemes are called out in order in the text
- Check that required data have been deposited in databases and any supplementary material is in the correct format for archiving (NB supplementary data is not edited)
- Footnotes are avoided unless absolutely necessary
- Add appropriate links to structural databases *etc*.
- References are checked to conform to our style both in the text and in the reference list
- **Any queries are tagged and appear as bold and underlined in the proofs**

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Spelling

- Follow Oxford English Dictionary
- British English is used unless the authors have used American English
- Historically American delegates wanted American spelling and it was the Technical Editor's job to correct spelling
- In 1962 a professional Technical Editor was appointed, S. A. Bryant, who worked at first from his home in Chester
- Grammar is always British English
- Filter corrects some spellings *e.g.* -ise becomes -ize, -isation becomes -ization

6. 1946–1948: Preparations for the journal

The Journals Subcommittee asked Ewald and Evans (Fig. 5) to find a suitable printer and publisher (Ewald, 1977, 1983). Together, Ewald and Evans prepared a crystallographic text and contacted several printing establishments in France, England, Sweden, Denmark, The Netherlands and Austria, and also the American Institute of Physics. They got prices and specimen settings from seven. The most attractive were from Cambridge University Press (CUP) and the American Institute of Physics. CUP was finally chosen for the printing and distribution of *Acta*, with the American Institute of Physics being responsible for the distribution and collection of subscriptions in North America. Ewald (1977) recalls that when the decision was taken by the Journals Subcommittee to have an international journal, the American delegates insisted that American spelling should be used for American papers. This raised some problems with CUP when they were chosen for the production of the journal! It was finally agreed that the compositors at CUP would not change spellings in the manuscripts and that the responsibility for the spelling would rest with the Technical Editor of the journal. Evans decided on the typeface and specified the design and colour of the cover, which remained the same until 1968. He also assumed the role of Technical Editor. Evans was at the time Lecturer in the Department of Mineralogy and Petrology at Cambridge and attached to the Crystallography Laboratory of the Cavendish Laboratory. His office was across the street from the offices of CUP; it was therefore easy for him to stay in close touch with them. According to Ewald, '*he was a very accurate proof reader and there are hardly any misprints in the first Volumes of Acta*'.

Abbreviations and numerals

Abbreviations

Define abbreviation at first instance

Lower case with full stops or upper case without

Full stops not used when the the last letter of the abbreviation is the last letter of the word

Three-letter amino-acid abbreviations

Standard list of abbreviations needing no explanation, *e.g.* SDS-PAGE, CIF

Numerals

Spell out numbers one to nine if integers, *e.g.* three days but 3 cm

Four digit numbers closed up but longer numbers spaced in threes without commas *e.g.* 1 278 500. If both types adjacent space out, 1 500, 65 000. Not applicable to tables

SUs added in parens not with plus/minus

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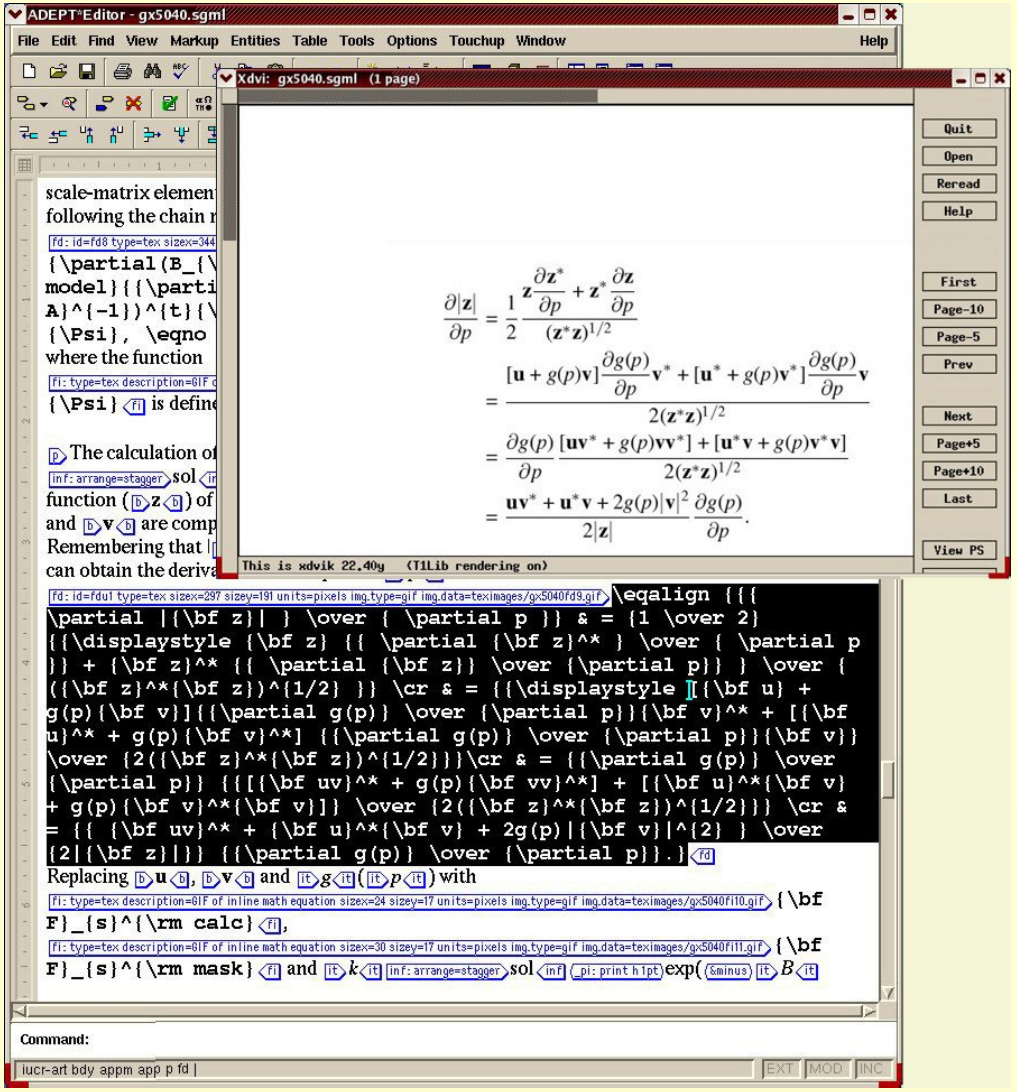
Mathematics



Maths created using Word equation editor is converted to TeX using Mathtype

Mathematical formulae in TeX can be visualized while editing

An external script checks for TeX errors

Future – may use MathML

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Mathematics

Layout and numbering of equations are checked

Displayed equations numbered in one continuous sequence

If sequence is broken then may need to be renumbered

Bold is used for vectors, italic for scalar variables

Nesting of brackets checked

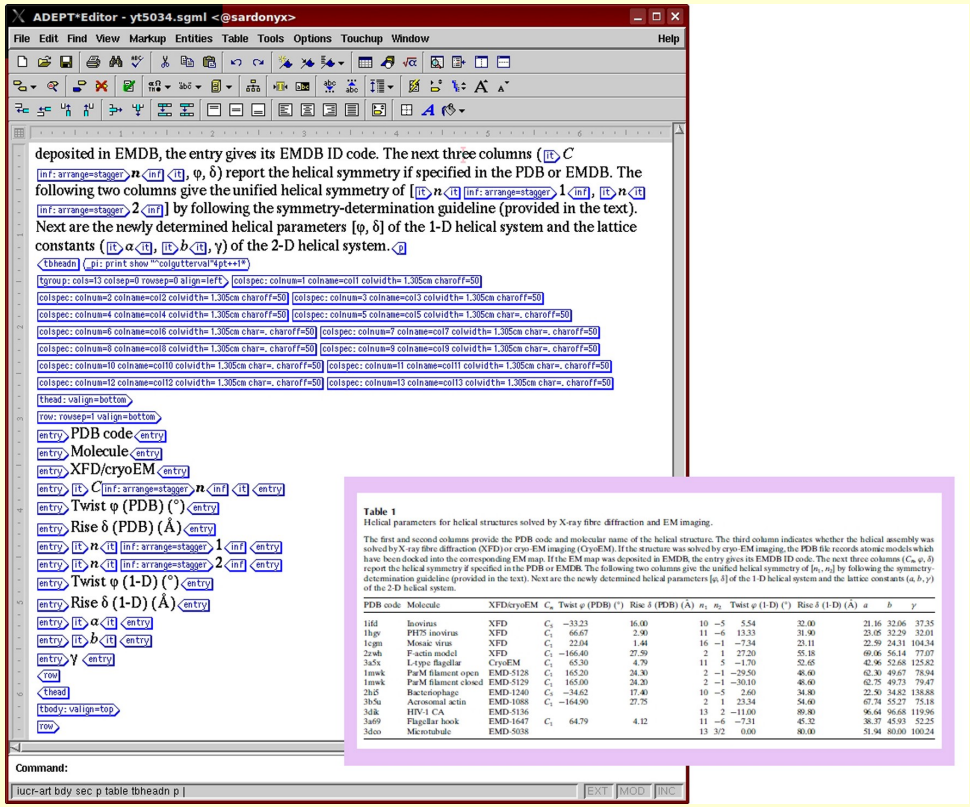
Large fractions broken down

Check that the same symbol does not have for more than one meaning

Non-standard fonts may be substituted

Use power 1/2 not square root sign

Tables



- Arrangement of data in tables, economic presentation
- Check text/figures and tables agree
- Should the table be a figure?
- Landscape tables not possible

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Figures and schemes

System checks on acceptance that figure files are present - does not check if there are meant to be figures but warns if there are no figure files

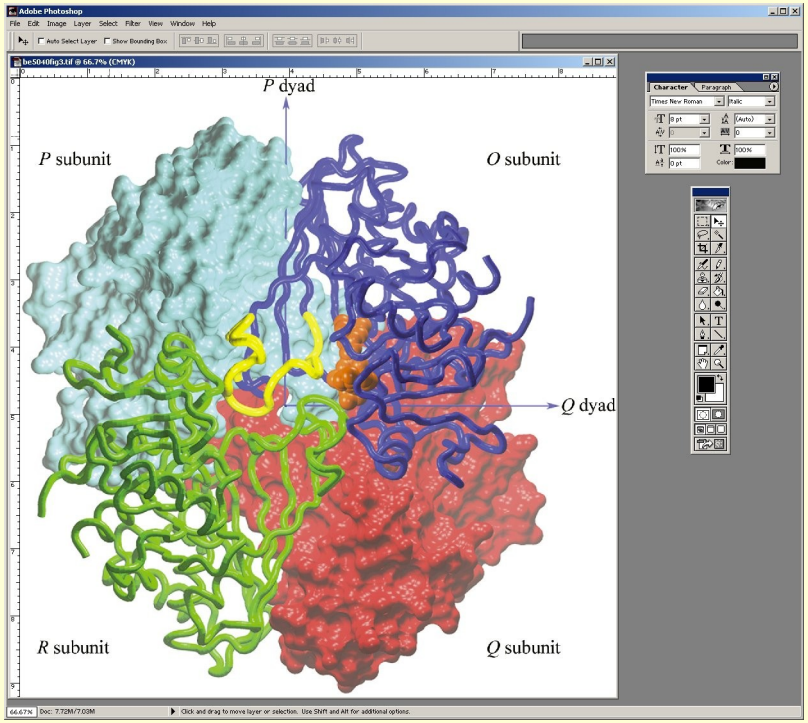
Figure/scheme files are converted to TIFF files of correct size (8.85 cm), resolution (600 d.p.i. for b&w, 400 d.p.i. for colour or halftones/greyscale) and CMYK

For composite figures uploaded as separate parts, lettering (*a*), (*b*) *etc.* is added

Conversion is checked and figures adjusted for size if necessary *e.g.* for stereoviews

Figures may be relabelled or the layout changed for economic use of space

Checks: figures will reproduce well, no red/green problems



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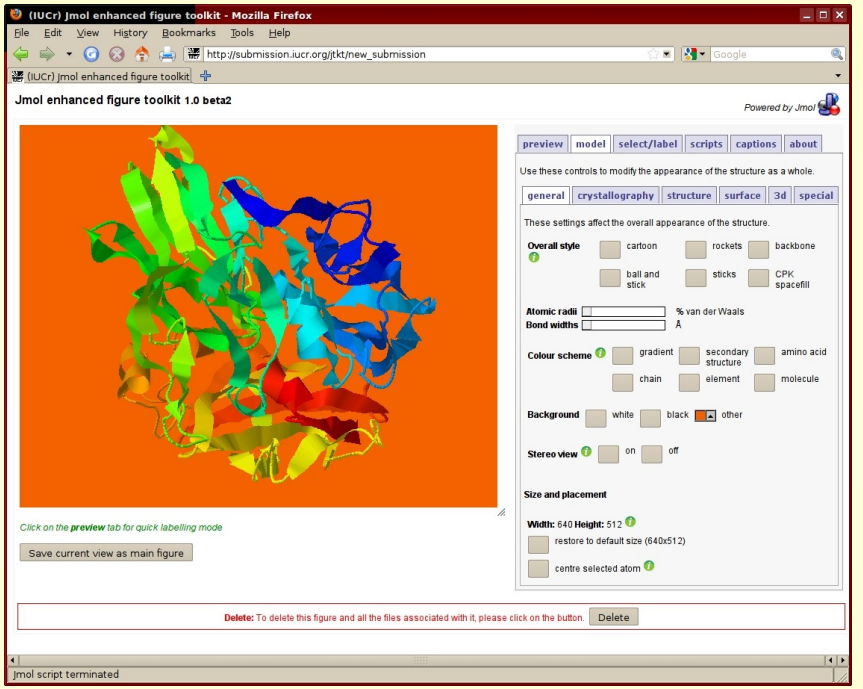
Enhanced figures

- Enhanced figure URL should be included in the submitted paper
- Both a static image and an interactive image created
- When the paper is edited the static image is included in the PDF and the interactive image appears in the online version



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References

Harvard style

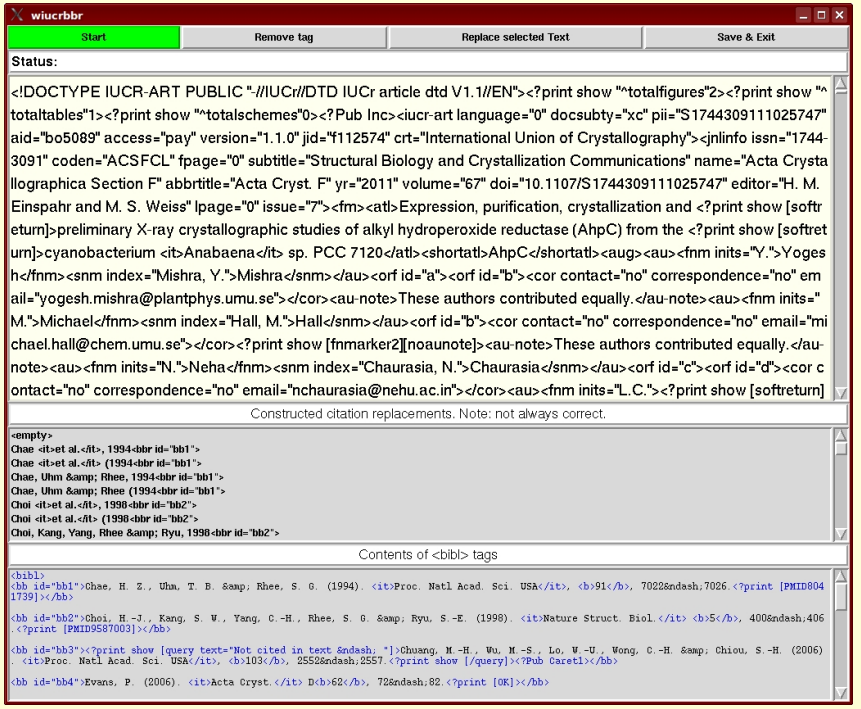
Incorrect format is time consuming to fix so always ask authors for correct format

References are checked to conform to our style both in the text and in the reference list

In text, three or more authors *et al*.

An interactive program makes the conversion and adds cross-referencing tags

In reference list - no titles of articles, too time consuming to correct but may be possible for some in future



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Typesetting

Use the SGML file to typeset the article

Text and figures are imported into the program 3B2

Text edited as little as possible

Figures and tables are placed semi-automatically according to where they are called out in the text

Tables, figures, schemes can be rearranged on the page

Not always possible to place figures or tables exactly where they are called out - there may not be enough text to flow around them or enough space on a page

Footnotes and markers are checked

SGML file updated from within 3B2

May change to a different typesetting method if no longer printing journals

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Given a 3-D unit cell, it is straightforward to generate the entire single crystal with fractional coordinates. The newly generated fractional coordinates are the number of cells (n_a, n_b, n_c) away from the origin (0, 0, 0) along each edge. The Cartesian coordinates of a new cell can be converted from the fractional coordinates by an orthogonal matrix (Evans, 2001) computed from 3-D lattice constants, a, b, c, α, β and γ. However, unlike the 3-D crystal system, a specified helical transformation is needed to generate the helical assembly from a given 1-D or 2-D unit cell. In the following, the equations for the 2-D wrapping and the augmented 1-D helical transformation will be derived and explained in detail.

2.1. 2-D helical system

As stated in §1, a planar sheet of 2-D lattice can be wrapped into a tube. If all sheet units are identical, the two constant integers n_1 and n_2 are sufficient to define all possible distinct tubes obtained by rolling it. Here, n_1 is the number of cells along one edge of the 2-D lattice (a) which are required to make a full round of wrapping and n_2 refers to the number of cells sliding along the other edge of the lattice (b) after wrapping.

If we place edge $\mathbf{a}$ along the x axis of the Cartesian coordinate and a 2-D lattice (a, b, γ) is placed on the xy plane, the wrapping equations for an $[n_1, n_2]$ tube are

$$x_w = -(z_c + r)t_y \sin\alpha + (x_c t_x + y_c t_y)t_x,$$
$$y_w = (z_c + r)t_x \sin\alpha + (x_c t_x + y_c t_y)t_y,$$
$$z_w = (z_c + r)\cos\alpha,$$

where

$$r = [(n_1 a + n_2 b\cos\gamma)^2 + (n_2 b\sin\gamma)^2]^{1/2},$$
$$t_x = n_2 b\sin\gamma/(2\pi r),$$
$$t_y = -(n_1 a + n_2 b\cos\gamma)/(2\pi r),$$
$$\alpha = (-x_c t_y + y_c t_x)/r,$$

(x_w, y_w, z_w) are the wrapped Cartesian coordinates of the tube and (x_c, y_c, z_c) are the Cartesian coordinates of the associated 2-D sheet. In the wrapping equations, the 2-D lattice sheet is at a distance of the tube radius (r) from the tube axis (t_x, t_y, 0). The helical transformation is implicitly specified by the helical twist α and the helical rise $x_c t_x + y_c t_y$. Fig. 1 provides a graphical summary of the 2-D helical transformation. A more detailed description has been given previously (Tsai *et al.*, 2006). Given asymmetric units in a 2-D lattice and a helical symmetry specified by the 2-D helical system in five parameters $[n_1, n_2, a, b, \gamma]$, one can build a complete helical construct based on the 2-D helical transformation equations formulated above.

2.2. Augmented 1-D helical system

Instead of rolling a planar 2-D sheet, a helical structure can also be expressed by a single helix or n helices, with the n helices related by an n-fold screw axis instead of just a rotational axis. Because the helical assembly must consist of identical subunits, the rotational part of the screw axis must display a C_n rotational symmetry and the translational part should be limited by some discrete numbers. In the augmented 1-D helical system, the four parameters $[n_1, n_2, \varphi, \delta]$ indicate that there are n_1 helices in the assembly, with each individual helix characterized by a unit twist (φ) and a unit rise (δ). Because the helices are also related by an n_1-fold screw axis, each helix denoted by $m_1 = 0, 1, 2, \ldots, n_1 - 1$ has an additional twist of $m_1(2\pi/n_1)$ and a rise of $m_1(n_2/n_1)\delta$. Note that the rise, which is specified by n_2 with a quantity of $n_2/n_1\delta$, was not included in the traditional 1-D helical system. Note also that $m_1 = n_1$ refers back to the first helix as specified by (φ, δ), which will give $n_2\delta$ rise after a complete round of n_1 rotations. In the 2-D helical system, this corresponds to the number of cells involved in the helix sliding after a complete wrapping.

A helical structure in the symmetrical construct is identified by the cell coordinates $[m_1, m_2]$. The asymmetric units are given in cell [0, 0] and an $[m_1, m_2]$ cell is located in the m_1 helix m_2 units away from the cell $[m_1, 0]$ along the helix. If the helical axis is parallel to the y axis and passes through the origin (0, 0, 0), the helical transformation equations for an $[m_1, m_2]$ cell in an $[n_1, n_2]$ helical construct are

$$x_w = x_c\cos\alpha + z_c\sin\alpha,$$
$$y_w = y_c + h_y\beta,$$
$$z_w = -x_c\sin\alpha + z_c\cos\alpha,$$

where

$$h_y = m_2 - m_1(n_2/n_1),$$
$$\alpha = h_y\varphi + m_1(2\pi/n_1),$$

(x_w, y_w, z_w) are the transformed Cartesian coordinates for the cell $[m_1, m_2]$ and (x_c, y_c, z_c) are the Cartesian coordinates of asymmetric units in cell [0, 0]. h_y and α specify the overall rise and twist for the $[m_1, m_2]$ cell as specified by an n_1-fold screw axis with n_2 unit shift. In the case of a helical structure with a single helix, in which $n_1 = 1$ and $m_1 = 0$, the helical transformation above reduces to a simple helical operation defined by $[\varphi, \delta]$ only. A graphical summary of the augmented 1-D helical transformation is given in Fig. 2.

2.3. 2-D helical system → augmented 1-D helical system

There are four ways to convert a helical system from 2-D to 1-D: view the continuation of lattice edge $\mathbf{b}$ as a helix, view the continuation of lattice edge $\mathbf{a}$ as a helix or view the continuation along the vector of $\mathbf{a} + \mathbf{b}$ or along the vector of $\mathbf{a} - \mathbf{b}$. The first is the most convenient choice. By selecting the vector $\mathbf{b}$ as an individual helix, the new 1-D helical system retains the same symmetry notation as the 2-D helical system $[n_1, n_2]$. The unit twist φ (in unit of radians) and rise δ of the n_1-start helices are calculated as

$$\varphi = (-x_c t_y + y_c t_x)/r,$$
$$\delta = x_c t_x + y_c t_y,$$

where t_x, t_y are the helical axes of the 2-D helical system and x_c, y_c are the planar Cartesian coordinates at the cell origin

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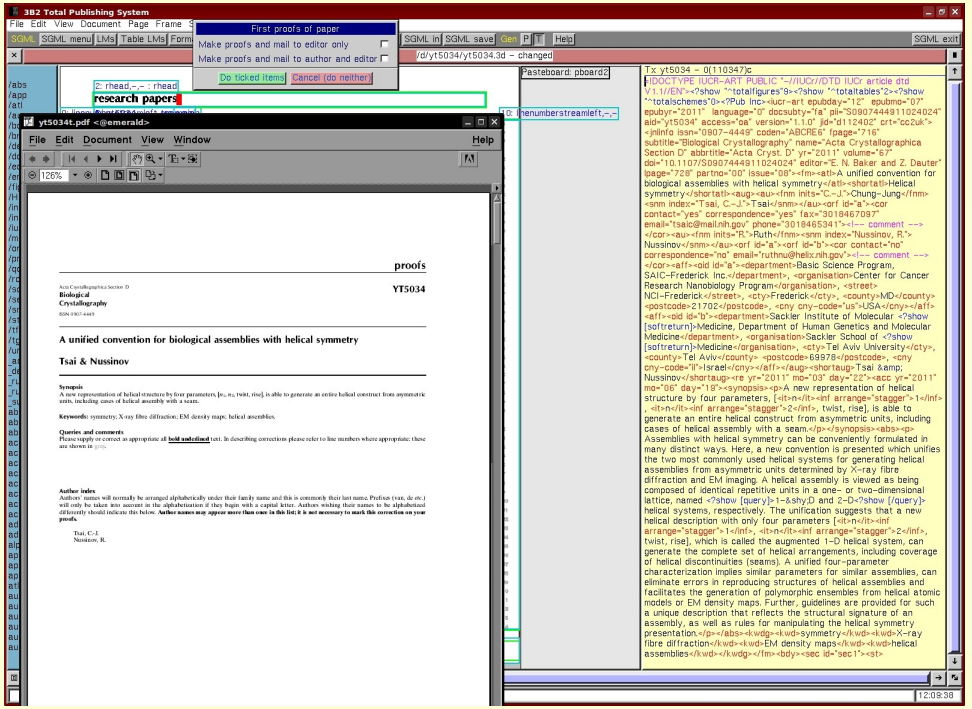

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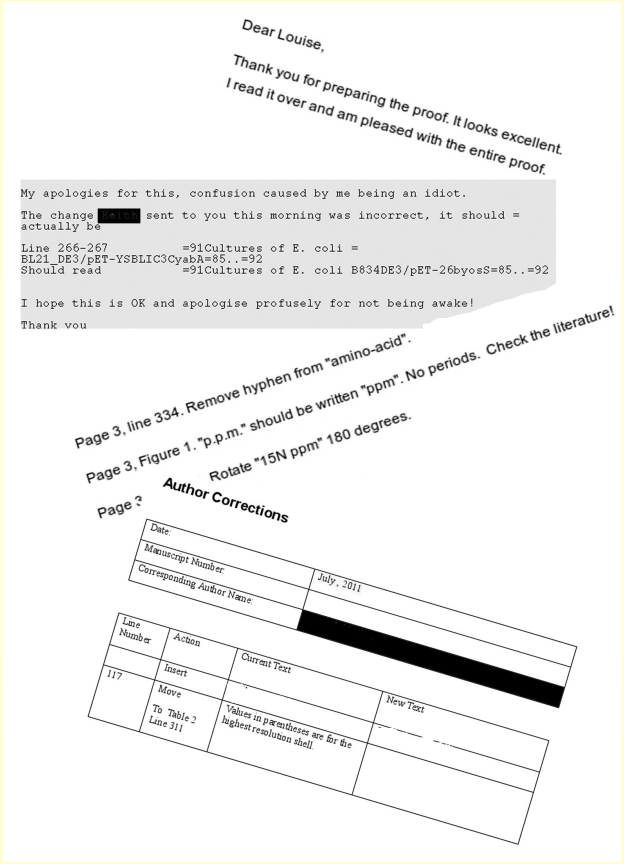

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I read it over and am pleased with the entire proof.

My apologies for this, confusion caused by me being an idiot.

The change [redacted] sent to you this morning was incorrect, it should = actually be

Line 266-267 =91Cultures of E. coli = BL21_DE3/pET-YSBLIC3CyabA=85..=92
Should read =91Cultures of E. coli B834DE3/pET-26byosS=85..=92

I hope this is OK and apologise profusely for not being awake!

Thank you

Page 3, line 334. Remove hyphen from "amino-acid".

Page 3, Figure 1. "p.p.m." should be written "ppm". No periods. Check the literature!

Page ? Rotate "15N ppm" 180 degrees.

Author Corrections

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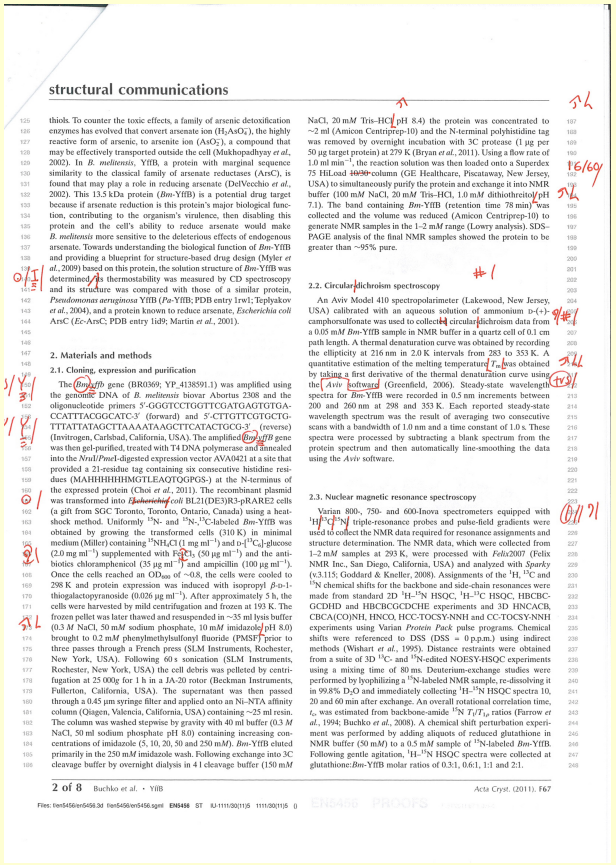

structural communications

thiols. To counter the toxic effects, a family of arsenic detoxification enzymes has evolved that convert arsenate ion ($H_2AsO_4^-$), the highly reactive form of arsenic, to arsenite ion (AsO_3^-), a compound that may be effectively transported outside the cell (Mukhopadhyay *et al.*, 2002). In *B. melitensis*, YfiB, a protein with marginal sequence similarity to the classical family of arsenate reductases (ArsC), is found that may play a role in reducing arsenate (DelVecchio *et al.*, 2002). This 13.5 kDa protein (*Bm*-YfiB) is a potential drug target because if arsenate reduction is this protein's major biological function, contributing to the organism's virulence, then disabling this protein and the cell's ability to reduce arsenate would make *B. melitensis* more sensitive to the deleterious effects of endogenous arsenate. Towards understanding the biological function of *Bm*-YfiB and providing a blueprint for structure-based drug design (Myler *et al.*, 2009) based on this protein, the solution structure of *Bm*-YfiB was determined, its thermostability was measured by CD spectroscopy and its structure was compared with those of a similar protein, *Pseudomonas aeruginosa* YfiB (*Pa*-YfiB; PDB entry 1rw1; Teplyakov *et al.*, 2004), and a protein known to reduce arsenate, *Escherichia coli* ArsC (*Ec*-ArsC; PDB entry 1id9; Martin *et al.*, 2001).

2. Materials and methods

2.1. Cloning, expression and purification

The *BmyfiB* gene (BR0369; YP_4138591.1) was amplified using the genomic DNA of *B. melitensis* biovar Abortus 2308 and the oligonucleotide primers 5′-GGGTCCTGGTTCGATGAGTGTGA-CCATTTACGGCATC-3′ (forward) and 5′-CTTGTTCGTGCTG-TTTATTATAGCTTAAAATAAGCTTCATACTGCG-3′ (reverse) (Invitrogen, Carlsbad, California, USA). The amplified *BmyfiB* gene was then gel-purified, treated with T4 DNA polymerase and annealed into the *Nru*I/*Pme*I-digested expression vector AVA0421 at a site that provided a 21-residue tag containing six consecutive histidine residues (MAHHHHHHMGTLEAQTQGPGS-) at the N-terminus of the expressed protein (Choi *et al.*, 2011). The recombinant plasmid was transformed into *Escherichia coli* BL21(DE3)R3-pRARE2 cells (a gift from SGC Toronto, Toronto, Ontario, Canada) using a heat-shock method. Uniformly ^{15}N- and ^{13}N-,^{13}C-labeled *Bm*-YfiB was obtained by growing the transformed cells (310 K) in minimal medium (Miller) containing $^{15}NH_4Cl$ (1 mg ml^{-1}) and D-[$^{13}C_6$]-glucose (2.0 mg ml^{-1}) supplemented with $FeCl_3$ (50 µg ml^{-1}) and the antibiotics chloramphenicol (35 µg ml^{-1}) and ampicillin (100 µg ml^{-1}). Once the cells reached an OD_{600} of ~0.8, the cells were cooled to 298 K and protein expression was induced with isopropyl β-D-1-thiogalactopyranoside (0.026 µg ml^{-1}). After approximately 5 h, the cells were harvested by mild centrifugation and frozen at 193 K. The frozen pellet was later thawed and resuspended in ~35 ml lysis buffer (0.3 *M* NaCl, 50 m*M* sodium phosphate, 10 m*M* imidazole pH 8.0) brought to 0.2 m*M* phenylmethylsulfonyl fluoride (PMSF) prior to three passes through a French press (SLM Instruments, Rochester, New York, USA). Following 60 s sonication (SLM Instruments, Rochester, New York, USA) the cell debris was pelleted by centrifugation at 25 000*g* for 1 h in a JA-20 rotor (Beckman Instruments, Fullerton, California, USA). The supernatant was then passed through a 0.45 µm syringe filter and applied onto an Ni–NTA affinity column (Qiagen, Valencia, California, USA) containing ~25 ml resin. The column was washed stepwise by gravity with 40 ml buffer (0.3 *M* NaCl, 50 m*M* sodium phosphate pH 8.0) containing increasing concentrations of imidazole (5, 10, 20, 50 and 250 m*M*). *Bm*-YfiB eluted primarily in the 250 m*M* imidazole wash. Following exchange into 3C cleavage buffer by overnight dialysis in 4 l cleavage buffer (150 m*M* NaCl, 20 m*M* Tris–HCl pH 8.4) the protein was concentrated to ~2 ml (Amicon Centriprep-10) and the N-terminal polyhistidine tag was removed by overnight incubation with 3C protease (1 µg per 50 µg target protein) at 279 K (Bryan *et al.*, 2011). Using a flow rate of 1.0 ml min^{-1}, the reaction solution was then loaded onto a Superdex 75 HiLoad 10/30 column (GE Healthcare, Piscataway, New Jersey, USA) to simultaneously purify the protein and exchange it into NMR buffer (100 m*M* NaCl, 20 m*M* Tris–HCl, 1.0 m*M* dithiothreitol pH 7.1). The band containing *Bm*-YfiB (retention time 78 min) was collected and the volume was reduced (Amicon Centriprep-10) to generate NMR samples in the 1–2 m*M* range (Lowery analysis). SDS–PAGE analysis of the final NMR samples showed the protein to be greater than ~95% pure.

2.2. Circular dichroism spectroscopy

An Aviv Model 410 spectropolarimeter (Lakewood, New Jersey, USA) calibrated with an aqueous solution of ammonium D-(+)-10-camphorsulfonate was used to collect circular dichroism data from a 0.05 m*M* *Bm*-YfiB sample in NMR buffer in a quartz cell of 0.1 cm path length. A thermal denaturation curve was obtained by recording the ellipticity at 216 nm in 2.0 K intervals from 283 to 353 K. A quantitative estimation of the melting temperature (T_m) was obtained by taking a first derivative of the thermal denaturation curve using the *Aviv* software (Greenfield, 2006). Steady-state wavelength spectra for *Bm*-YfiB were recorded in 0.5 nm increments between 200 and 260 nm at 298 and 353 K. Each reported steady-state wavelength spectrum was the result of averaging two consecutive scans with a bandwidth of 1.0 nm and a time constant of 1.0 s. These spectra were processed by subtracting a blank spectrum from the protein spectrum and then automatically line-smoothing the data using the *Aviv* software.

2.3. Nuclear magnetic resonance spectroscopy

Varian 800-, 750- and 600-Inova spectrometers equipped with ^{1}H/^{13}C/^{15}N triple-resonance probes and pulse-field gradients were used to collect the NMR data required for resonance assignments and structure determination. The NMR data, which were collected from 1–2 m*M* samples at 293 K, were processed with *Felix*2007 (Felix NMR Inc., San Diego, California, USA) and analyzed with *Sparky* (v.3.115; Goddard & Kneller, 2008). Assignments of the ^{1}H, ^{13}C and ^{15}N chemical shifts for the backbone and side-chain resonances were made from standard 2D ^{1}H–^{15}N HSQC, ^{1}H–^{13}C HSQC, HBCBC-GCDHD and HBCBCGCDCHE experiments and 3D HNCACB, CBCA(CO)NH, HNCO, HCCH-TOCSY-NNH and CC-TOCSY-NNH experiments using Varian *Protein Pack* pulse programs. Chemical shifts were referenced to DSS (DSS = 0 p.p.m.) using indirect methods (Wishart *et al.*, 1995). Distance restraints were obtained from a suite of 3D ^{13}C- and ^{15}N-edited NOESY-HSQC experiments using a mixing time of 80 ms. Deuterium-exchange studies were performed by lyophilizing a ^{15}N-labeled NMR sample, re-dissolving it in 99.8% D_2O and immediately collecting ^{1}H–^{15}N HSQC spectra 10, 20 and 60 min after exchange. An overall rotational correlation time, t_c, was estimated from backbone-amide ^{15}N $T_1/T_{1\rho}$ ratios (Farrow *et al.*, 1994; Buchko *et al.*, 2008). A chemical shift perturbation experiment was performed by adding aliquots of reduced glutathione in NMR buffer (50 m*M*) to a 0.5 m*M* sample of ^{15}N-labeled *Bm*-YfiB. Following gentle agitation, ^{1}H–^{15}N HSQC spectra were collected at glutathione:*Bm*-YfiB molar ratios of 0.3:1, 0.6:1, 1:1 and 2:1.

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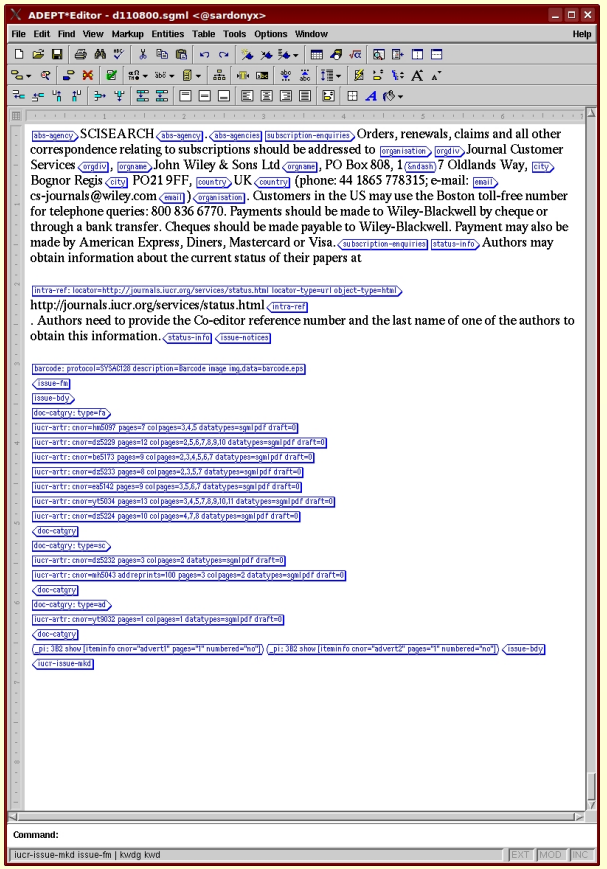

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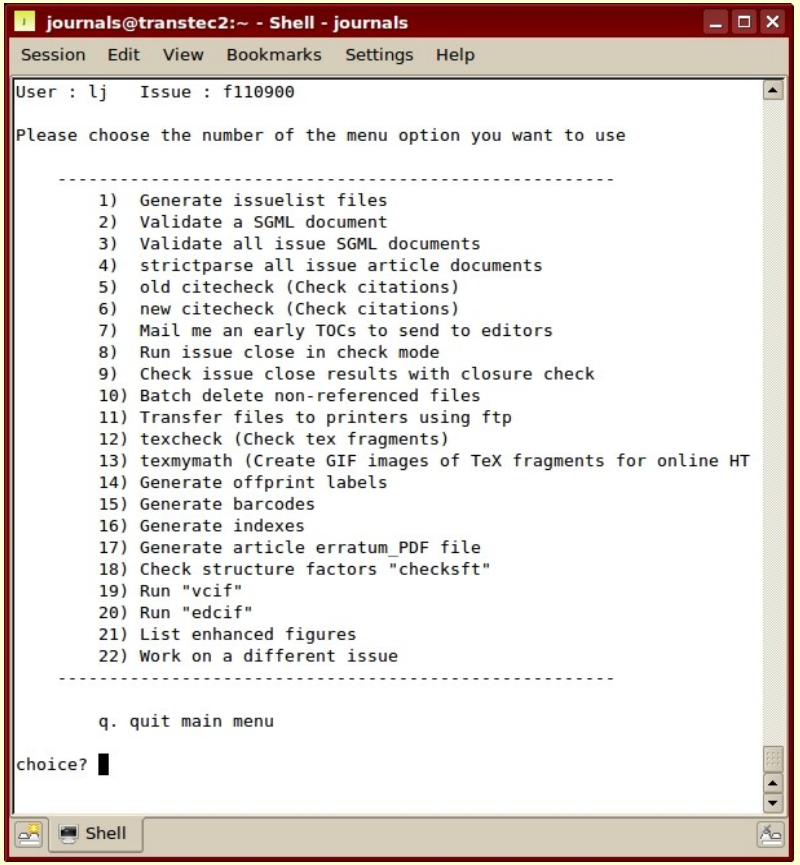

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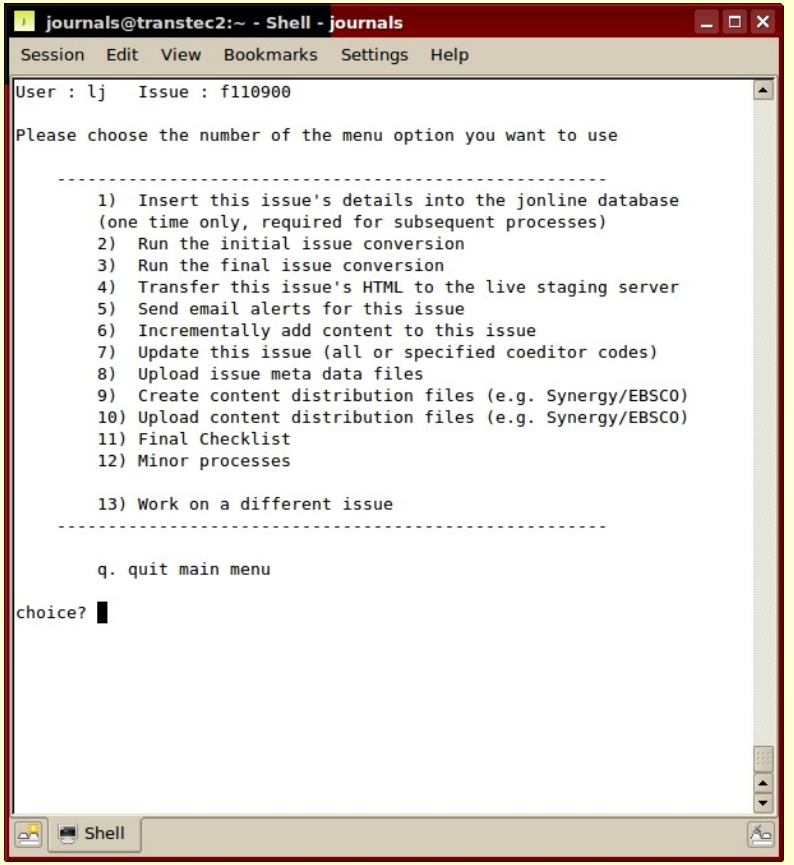

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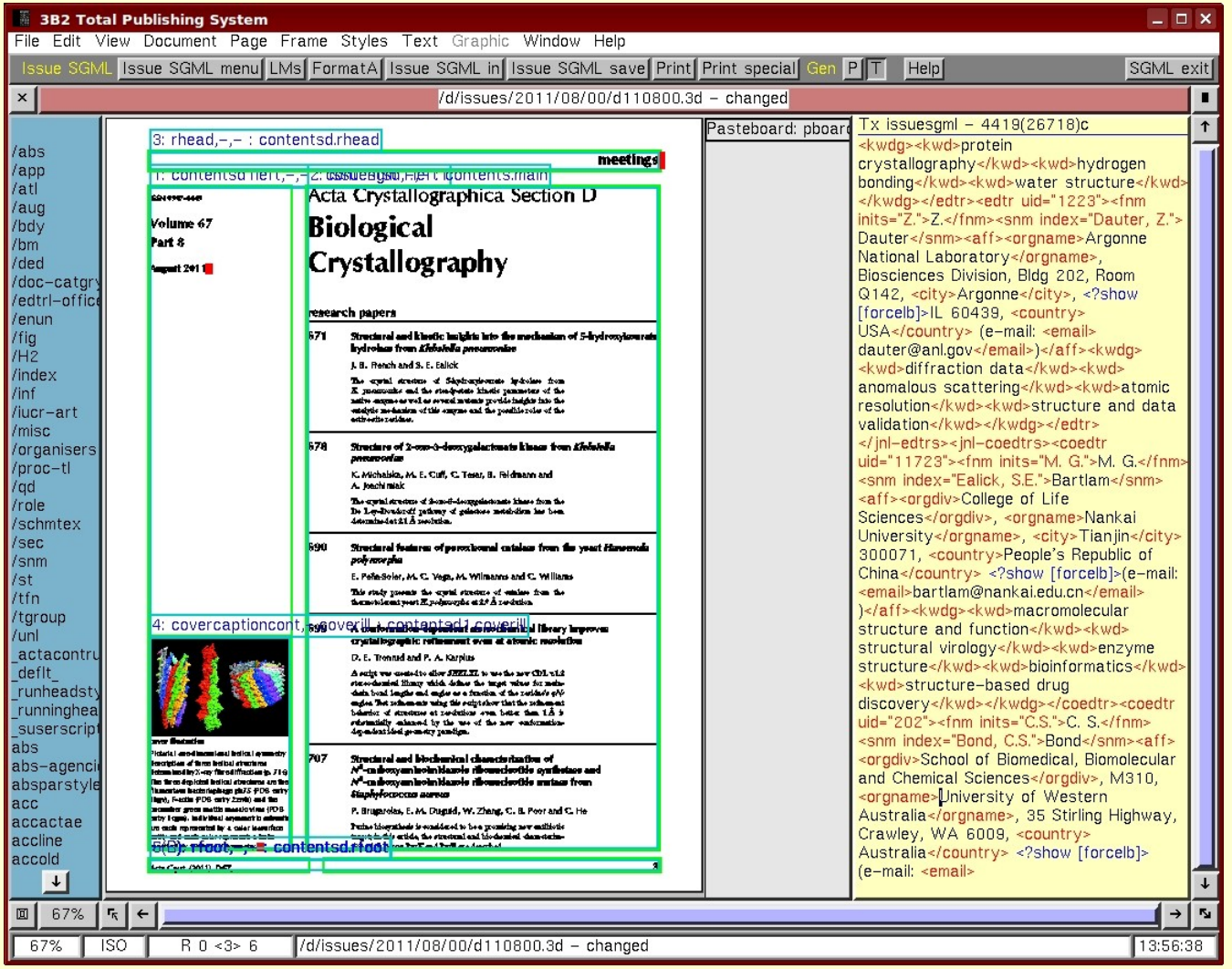

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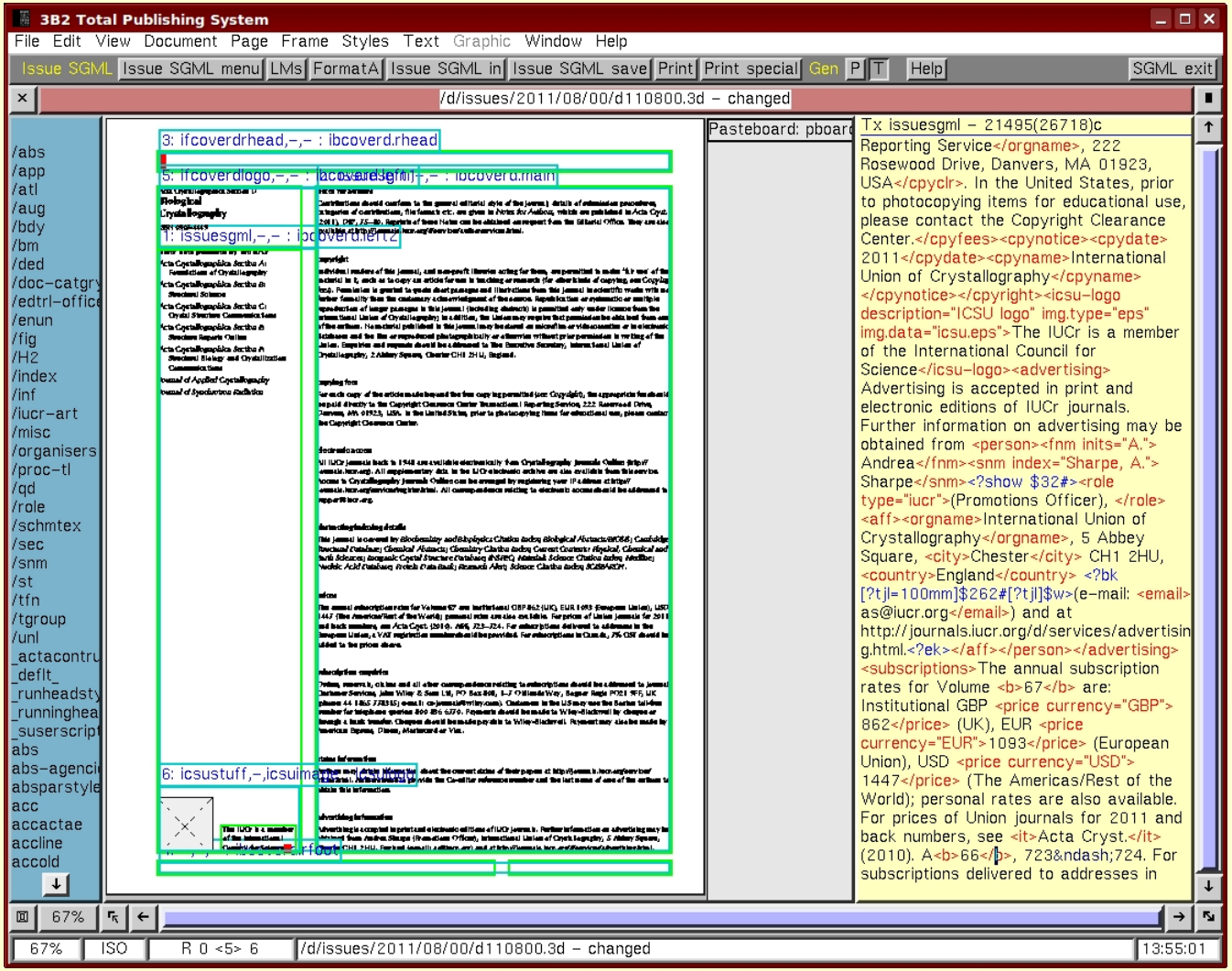

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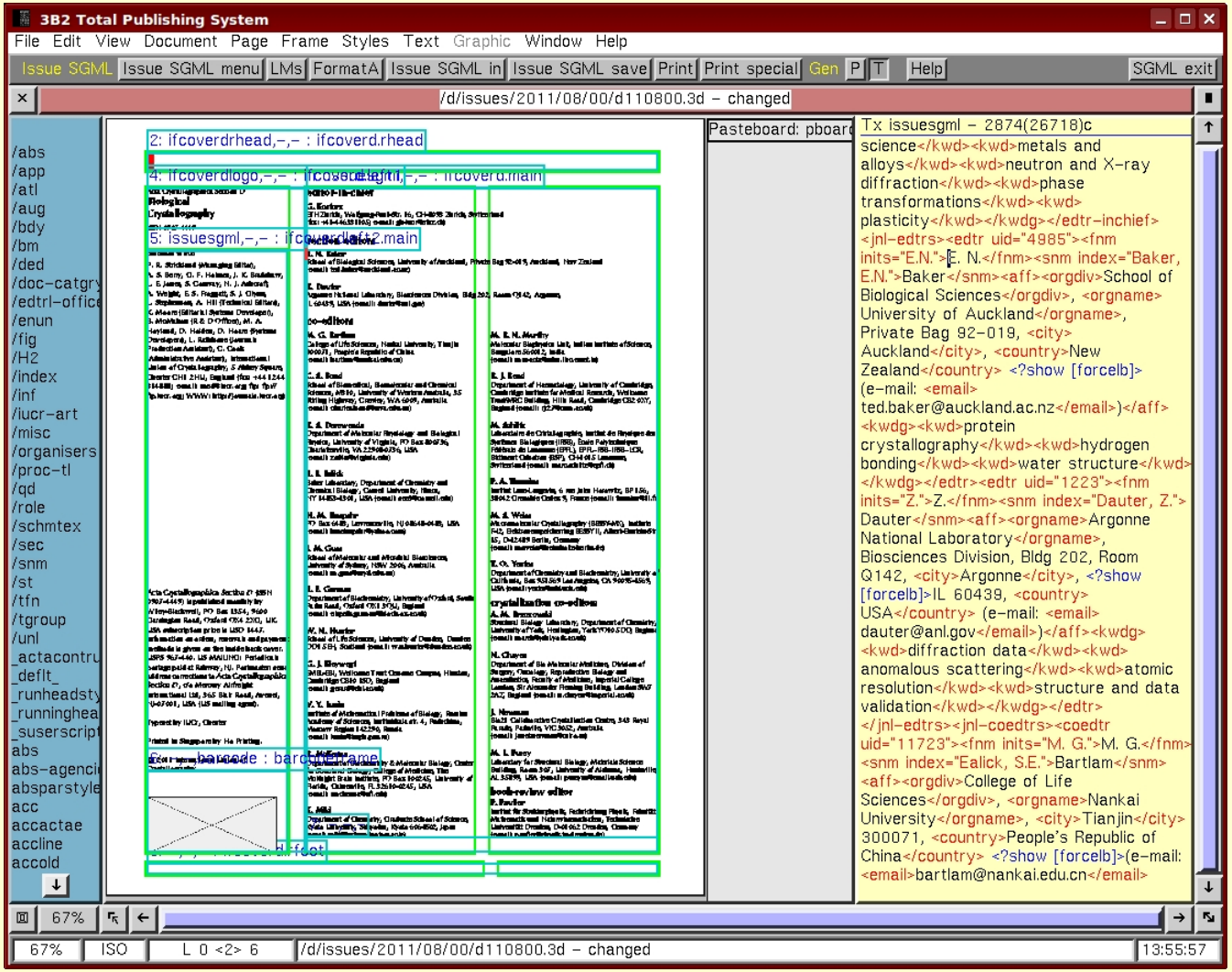

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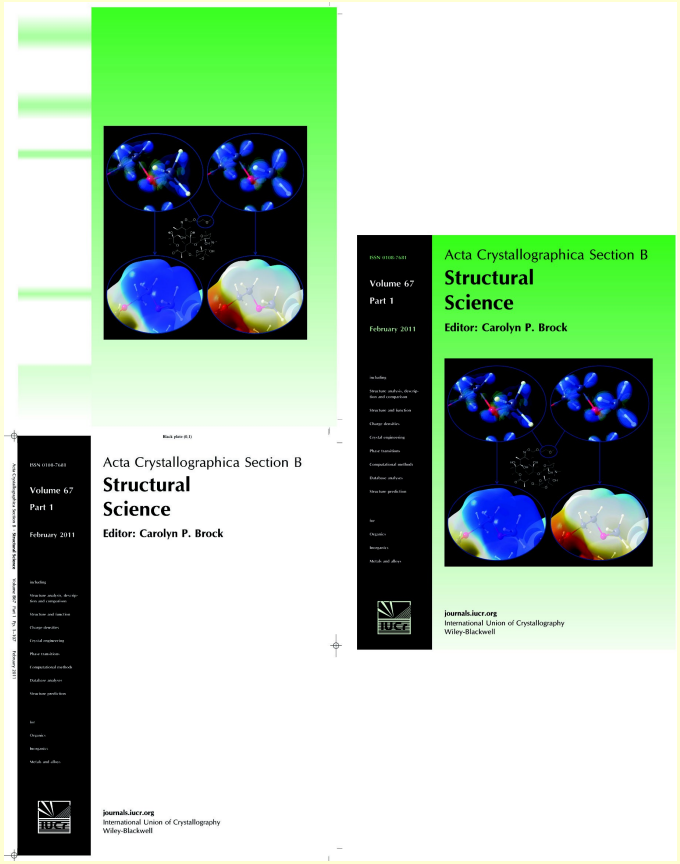

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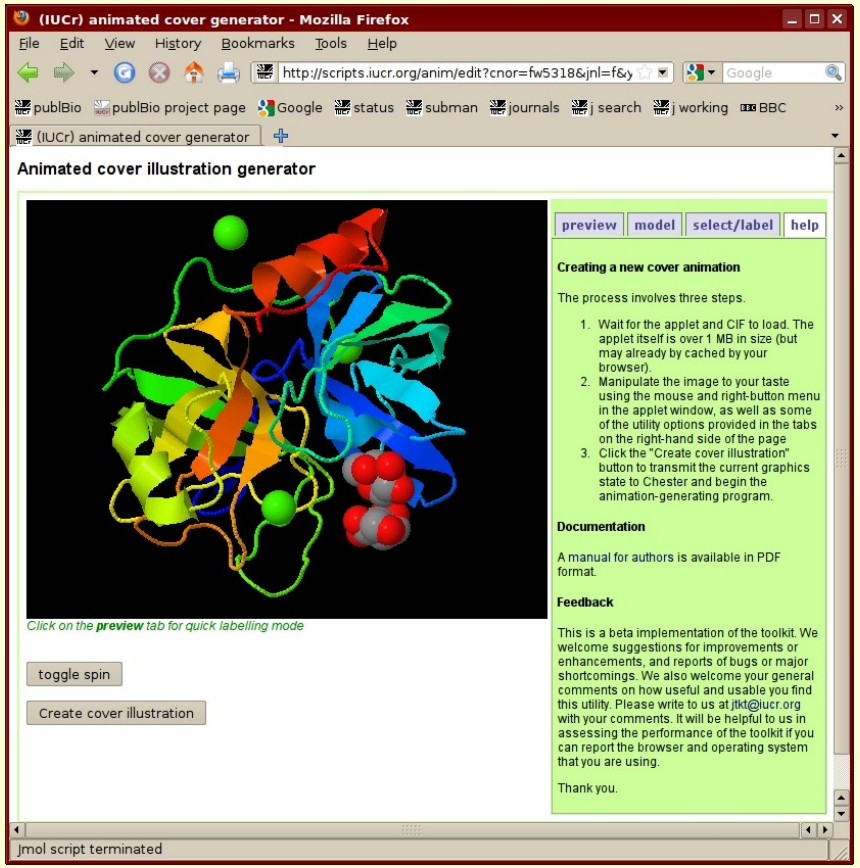

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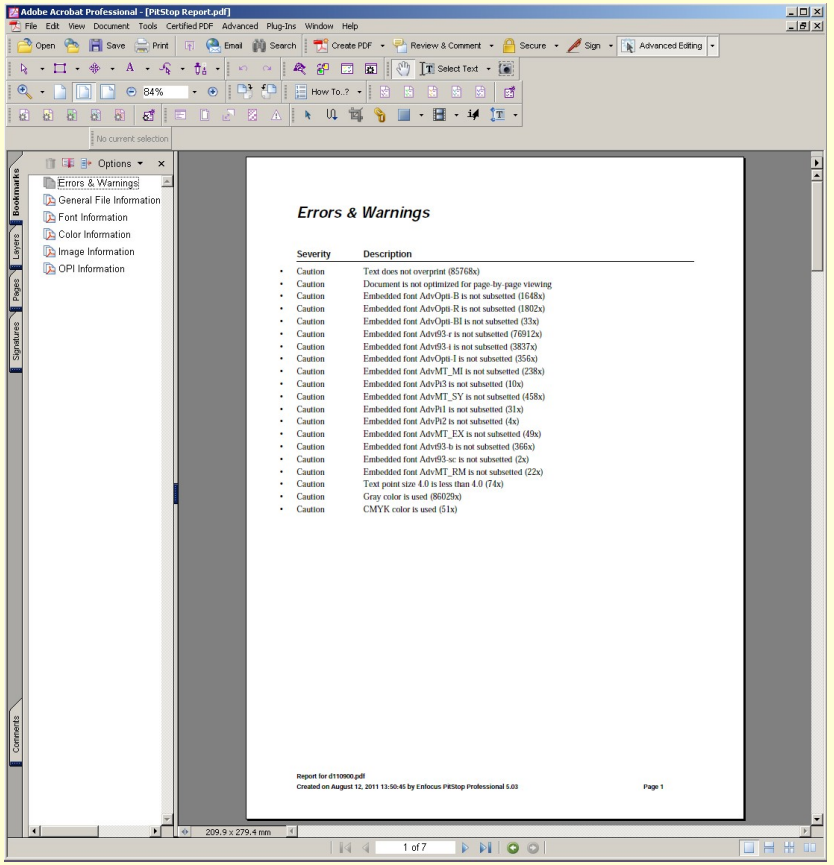

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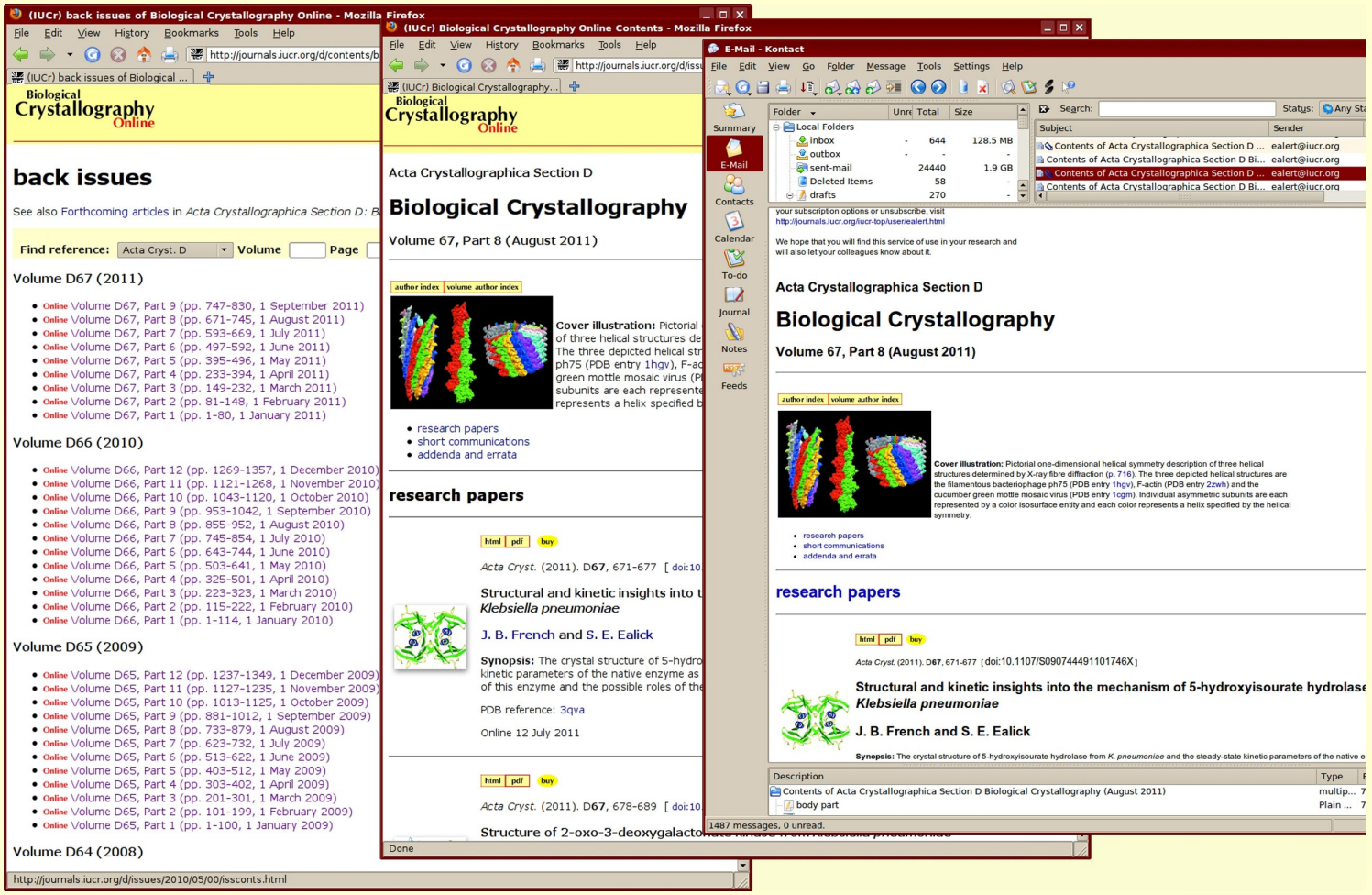

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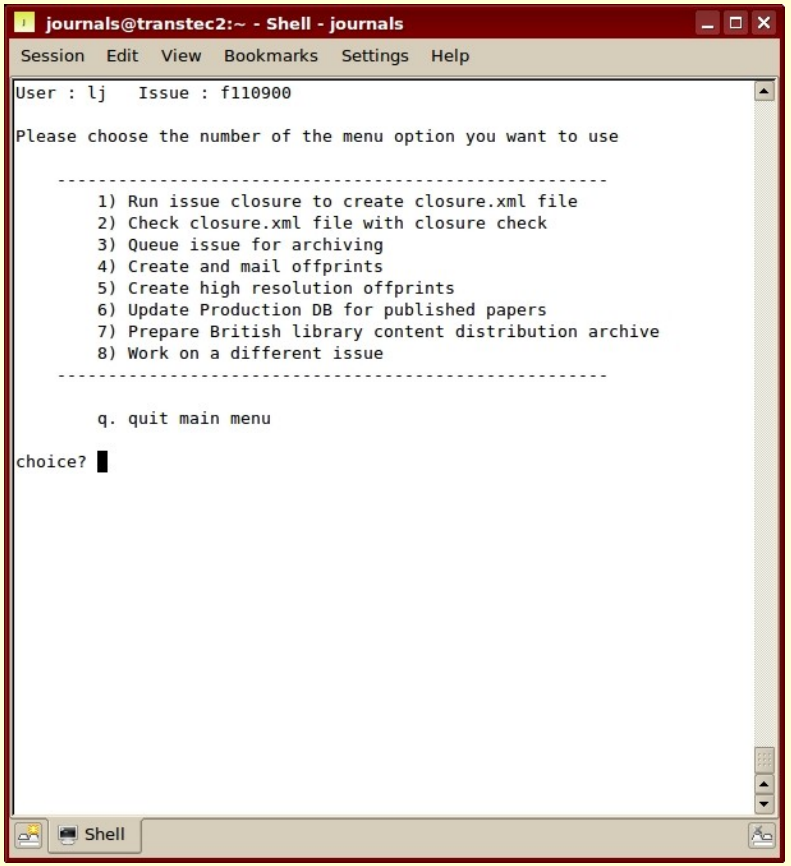

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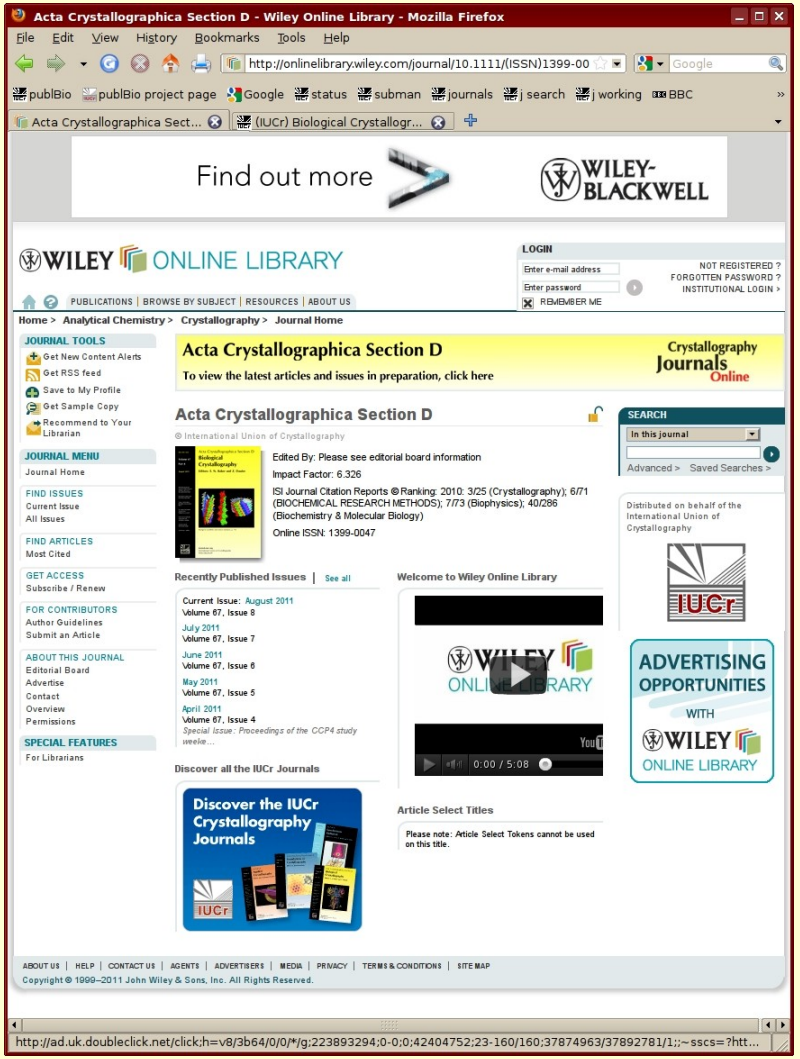

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