



Journal production processes

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Crystallography
Journals
Online

Journal production processes

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

Technical Editing

ed·it (ēd'it)
tr.v. **ed·it·ed, ed·it·ing, ed·its**

- To prepare (written material) for publication or presentation, as by correcting, revising, or adapting.
 - To prepare an edition of for publication: *edit a collection of short stories*.
 - To modify or adapt so as to make suitable or acceptable: *edited her remarks for presentation to a younger audience*.
- To supervise the publication of (a newspaper or magazine, for example).
- To assemble the components of (a film or soundtrack, for example), as by cutting and splicing.
- 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

SGML editing

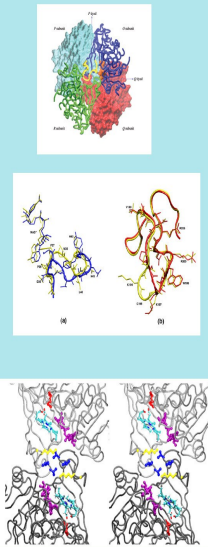
The SGML Editor interface displays a document with a hierarchical structure of tags. A list of authors is visible at the bottom, including names like 'Department of Medical Biology, The University of Melbourne, Victoria, Australia' and 'Department of Biochemistry, La Trobe University, Melbourne, Victoria, Australia'.

OR

A 3D ribbon diagram of a protein structure, colored in shades of blue and green, showing its complex folded shape.

OR

A different view of the protein structure, showing a different orientation and highlighting specific regions in various colors.



Online version

A screenshot of a web browser showing the online version of a scientific paper. The title is 'Structure of glyceraldehyde-3-phosphate dehydrogenase from Plasmodium falciparum'. The page includes an abstract, introduction, and author information.

Conversion to HTML

Proofreading

A proofreading interface showing a document with a search bar and a list of matches. The matches are highlighted in the document, and the search results are displayed in a separate window.

Author's files

A screenshot of a file manager showing a list of files and folders. The files are organized into a tree structure, and the selected file is highlighted.

Conversion to PostScript & PDF

Print version

Typesetting

Acceptance

The screenshot shows a Mozilla Firefox browser window displaying the 'paper details' page for article ba5172. The page is titled 'details of article ba5172 (In review - Co-editor requested revision)'. The author is T. Alwyn Jones. The page includes a sidebar with navigation options like 'review documents' and 'emails and general emails'. A 'Review status' pop-up window is visible, showing 'Awaiting revision from author' and 'Report received from referee'. An email window titled 'Article en5480: accepted - Kontakt' is also open, displaying the acceptance message from the IUCr.

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

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

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

```
<!DOCTYPE IUCR-ART PUBLIC "-//IUCr//DTD IUCr article dtd V1.1//EN"><iucr-art
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of Crystallography" language="0" jid="d051784" aid="hv5038"><jnlinfo editor="E.N. Baker and
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 Pyrococcus horikoshii</atl><shortatl>2'-5' RNA
ligase</shortatl><aug><au><frm inits="P.H.">Peter H.</frm><srn index="Rehse,
P.H.">Rehse</srn></au><orf id="a"><au><frm inits="T.H.">Tahir H.</frm><srn index="Tahirov,
T.H.">Tahirov</srn></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="lvdx" locator-type="code">putative 2'-5' RNA ligase,
lvdx, rlvdxsf</datafile><synopsis><p>The crystal structure of a putative 2'-5'
RNA ligase from P. horikoshii was solved and compared with a Thermus
thermophilus homologue and the structurally related cyclic
phosphodiesterase.</p></synopsis><abs><p>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
Pyrococcus horikoshii has been crystallized and its X-ray crystallographic
structure determined to 2.4 Å. The protein crystallized in the orthorhombic
space group P212121, with unit-cell parameters a = 44.07, b =
45.47, c = 93.17 Å; and one protein monomer in the
asymmetric unit. The molecular-replacement probe was a 2'-5' RNA ligase from
Thermus thermophilus which shares 30% sequence identity. The
P. horikoshii RNA ligase has some structural features that have more in
common with a cyclic phosphodiesterase from Arabidopsis thaliana with which it has
no significant homology, yet an examination of the electrostatic surface potential clearly
defines its relationship to the T. thermophilus RNA ligase. However, the size of
the active-site cleft is smaller and less positively charged than that of the T.
thermophilus homologue, suggesting that the actual substrate may be smaller than that
previously postulated for the latter.</p></abs><kwdg>2'-5' RNA
ligases</kwdg></fm><bdy><sec id="secl"><st>Introduction</st><p>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 <et al.>, 1983<bbr
id="bb8">) or the maturation of mitochondrial RNA of trypanosomatids (Deng <et al.>
```

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

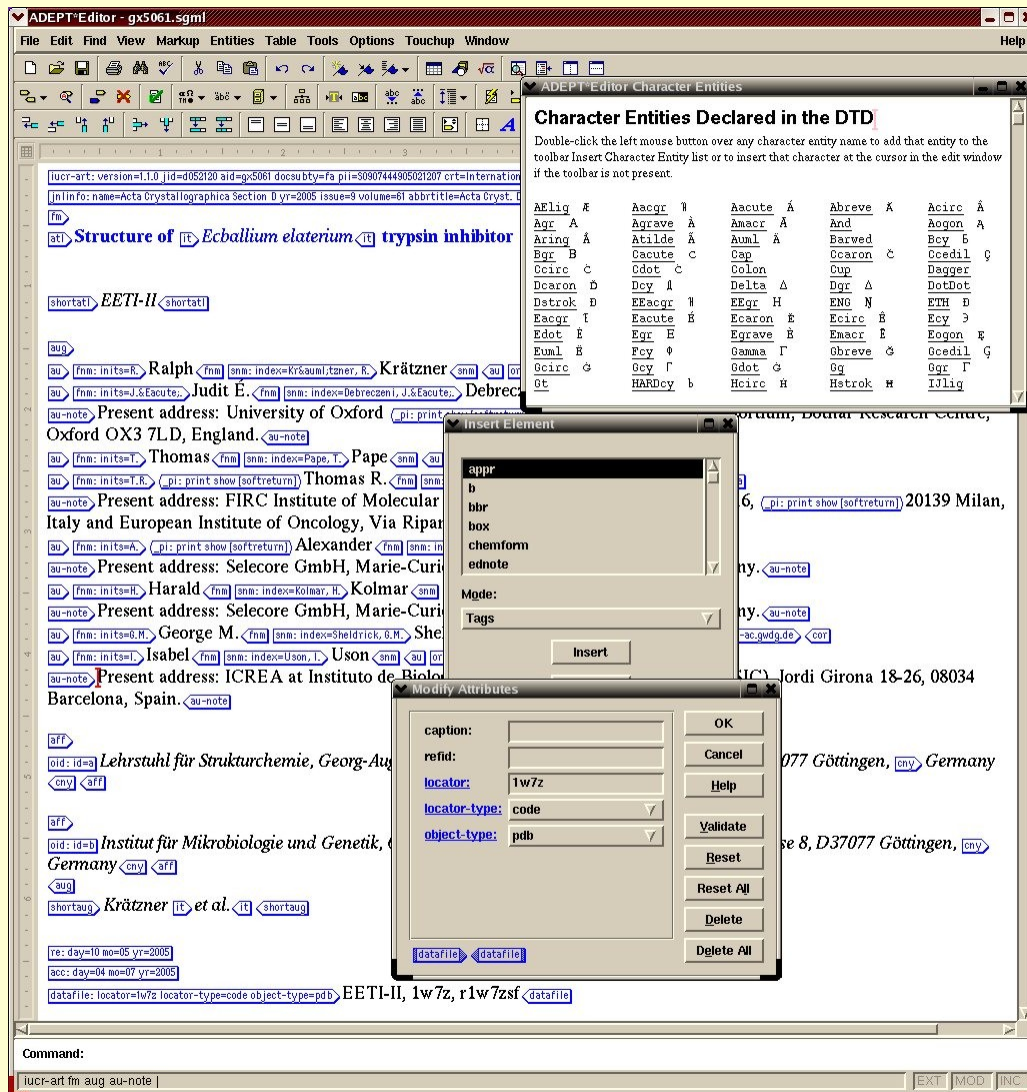
IUCr LaTeX conversion program is also
used to convert articles in LaTeX to
SGML

The screenshot shows a Microsoft Word window with the IUCr DocX template. The main document area displays a title, authors, and affiliation. The abstract and introduction sections are visible, with the abstract text highlighted in yellow. A 'Update' dialog box is open on the right, showing author details for 'Cook, Senkovich, Chattopadhyay' and a form for entering contact information.

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

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.

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

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**

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

Mathematics

The screenshot shows the ADEPT Editor interface. The main window displays a TeX document with the following content:

scale-matrix elemen
following the chain r

$$\frac{\partial |z|}{\partial p} = \frac{1}{2} \frac{z^* \frac{\partial z^*}{\partial p} + z \frac{\partial z}{\partial p}}{(z^* z)^{1/2}}$$

$$= \frac{[u + g(p)v] \frac{\partial g(p)}{\partial p} v^* + [u^* + g(p)v^*] \frac{\partial g(p)}{\partial p} v}{2(z^* z)^{1/2}}$$

$$= \frac{\frac{\partial g(p)}{\partial p} [uv^* + g(p)vv^*] + [u^*v + g(p)v^*v]}{2|z|} \frac{\partial g(p)}{\partial p}$$

The calculation of
function (z) of
and v are comp
Remembering that
can obtain the deriva

```

\eqalignn {{{
\partial |z| \over \partial p} &= {1 \over 2}
{{\displaystyle |z|} {\partial |z|^2 \over \partial p}} \over {\partial p}
+ |z|^2 {\partial |z|^2 \over \partial p} \over {\partial p}
}} \cr &= {{{\displaystyle [|u +
g(p)v] {\partial g(p) \over \partial p} v^* +
[u^* + g(p)v^*] {\partial g(p) \over \partial p} v}
\over {2(|z|^2)^{1/2}}} \cr &= {{{\displaystyle [u v^* +
g(p) v v^*] \over {2(|z|^2)^{1/2}}} \cr &=
{{ |u v^* + g(p) v v^*} \over {2|z|}}
{\partial g(p) \over \partial p}
}} \cr

```

Replacing u , v and p with
 F_s^{calc} ,
 F_s^{mask} and k $\exp(-i k \cdot r)$

Command:
luccr-art bdy appm app p fd |

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

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

The screenshot shows the ADEPT-Editor interface with a table of helical parameters. The table includes columns for PDB code, Molecule, XFD/cryoEM, Rise δ (PDB) (\AA), Twist φ (PDB) ($^\circ$), Rise δ (1-D) (\AA), Twist φ (1-D) ($^\circ$), and lattice constants a , b , γ .

PDB code	Molecule	XFD/cryoEM	C_1	Rise δ (PDB) (\AA)	n_1	n_2	Twist φ (1-D) ($^\circ$)	Rise δ (1-D) (\AA)	a	b	γ
1lfd	Ibotinin	XFD	C_1	-33.23	16.00	10	-5	5.54	21.16	32.06	37.35
1hgs	PHPS Inovirus	XFD	C_1	66.67	2.90	11	-6	13.33	31.90	23.05	32.29
1egm	Mosaic virus	XFD	C_1	22.94	1.44	16	-1	-7.34	23.11	22.59	24.31
2zab	Fusion model	XFD	C_1	-166.40	27.59	2	1	27.20	55.18	60.06	56.14
3a5x	L-type flagellar	CryoEM	C_1	65.30	4.79	11	5	-1.70	52.65	42.96	52.68
1mwk	ParM filament open	EMD-5128	C_1	165.20	24.30	2	-1	-29.50	46.00	62.30	49.67
1mwx	ParM filament closed	EMD-5129	C_1	165.00	24.20	2	-1	-30.10	46.00	62.75	49.73
2h5	Bacteriophage	EMD-1240	C_1	-34.62	17.40	10	-5	2.60	34.80	22.50	34.82
2h5a	Actinonuclear actin	EMD-1088	C_1	-164.00	27.75	2	1	23.84	54.00	67.74	55.27
3dk	HIV-1 CA	EMD-5136	C_1	-34.62	17.40	13	2	-11.00	89.80	96.64	96.68
3a69	Flagellar hook	EMD-1647	C_1	64.79	4.12	11	-6	-7.31	45.32	38.37	45.93
3dco	Microrhabd	EMD-5038	C_1	64.79	4.12	13	32	0.00	80.00	51.94	80.00

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

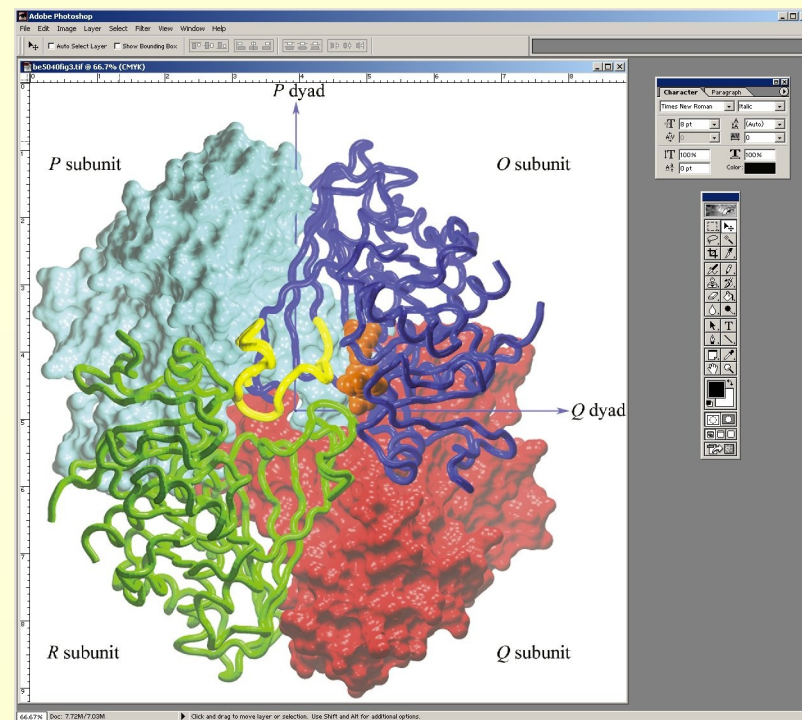
Figure/scheme files are converted to TIFF files of correct size (8.85 cm), resolution (600 d.p.i. for b&w, 400 d.p.i. for colour or halftones/greyscale) and CMYK

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

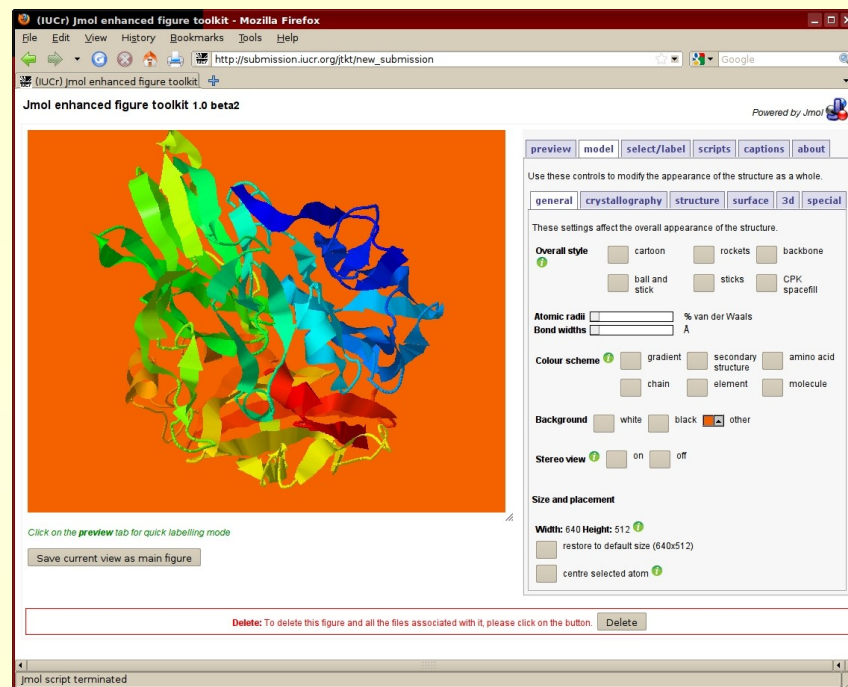


Enhanced figures

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



References

Harvard style

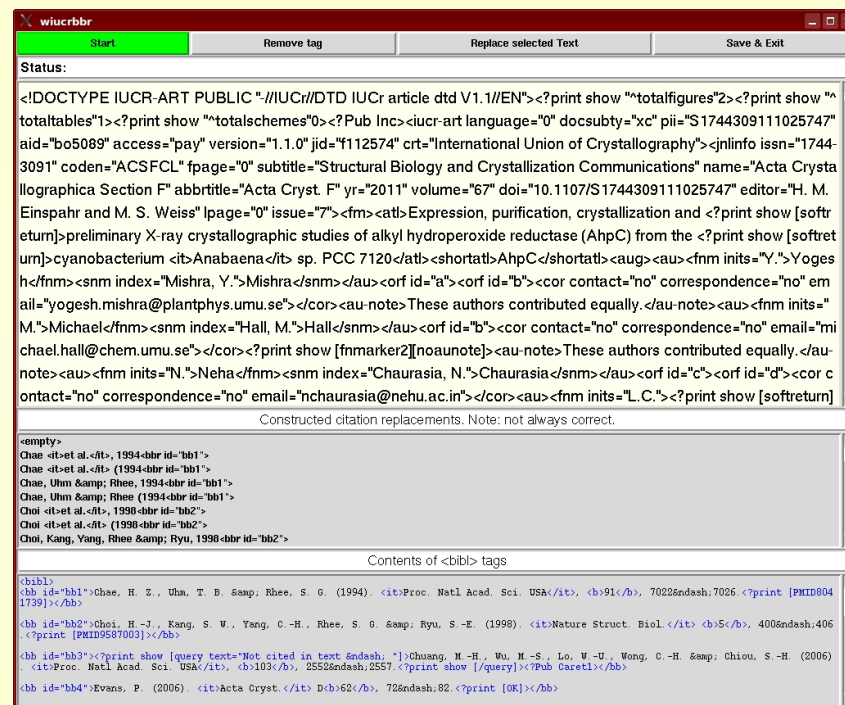
Incorrect format is time consuming to fix
so always ask authors for correct
format

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



```
wiuicrbrb
Start Remove tag Replace selected Text Save & Exit
Status:
<!DOCTYPE IUCR-ART PUBLIC "-//IUCr//DTD IUCr article dtd V1.1/EN"><?print show ""totalfigures"2><?print show ""
totaltables"1><?print show ""totalschemes"0><?Pub Inc<iucr-art language="0" docsbty="xc" pii="S1744309111025747"
aid="bo5089" access="pay" version="1.1.0" jid="f112574" crt="International Union of Crystallography"><jnlinfo issn="1744-
3091" coden="ACSFCL" fpage="0" subtitle="Structural Biology and Crystallization Communications" name="Acta Crysta
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Einspahr and M. S. Weiss" lpage="0" issue="7"><fm><atl>Expression, purification, crystallization and <?print show [softre
tum]>preliminary X-ray crystallographic studies of alkyl hydroperoxide reductase (AhpC) from the <?print show [softret
um]>cyanobacterium <it>Anabaena</it> sp. PCC 7120</at><shortat>AhpC</shortat><aug><au><fnm inits="Y.">Yoges
h</fnm><snm index="Mishra, Y.">Mishra</snm></au><orf id="a"><orf id="b"><cor contact="no" correspondence="no" em
ail="yogesh.mishra@plantphys.umu.se"></cor><au-note>These authors contributed equally.</au-note><au><fnm inits="
M.">Michael</fnm><snm index="Hall, M.">Hall</snm></au><orf id="a"><orf id="b"><cor contact="no" correspondence="no" email="mi
chael.hall@chem.umu.se"></cor><?print show [fnmarker2][noanote]><au-note>These authors contributed equally.</au-
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ontact="no" correspondence="no" email="nchaurasia@nehu.ac.in"></cor><au><fnm inits="L.C."><?print show [softretum]
Constructed citation replacements. Note: not always correct.
<empty>
Chae <it>et al.</it>, 1994<abbr id="bb1">
Chae <it>et al.</it> (1994<abbr id="bb1">
Chae, Uhm &amp; Rhee, 1994<abbr id="bb1">
Chae, Uhm &amp; Rhee (1994<abbr id="bb1">
Choi <it>et al.</it>, 1998<abbr id="bb2">
Choi <it>et al.</it> (1998<abbr id="bb2">
Choi, Kang, Yang, Rhee &amp; Ryu, 1998<abbr id="bb2">
Contents of <abbr> tags
<bb1>
<bb id="bb1">Chae, H. Z., Uha, T. B. &amp; Rhee, S. G. (1994). <it>Proc. Natl. Acad. Sci. USA</it>, <b>91</b>, 7022&dash;7026.<?print [PMID804
1739]</bb>
<bb id="bb2">Choi, H.-J., Kang, S. W., Yang, C.-H., Rhee, S. G. &amp; Ryu, S.-E. (1998). <it>Nature Struct. Biol.</it> <b>5</b>, 4008&dash;406
.<?print [PMID9587003]</bb>
<bb id="bb3"><?print show [query text="Not cited in text &dash;">Chuang, M.-H., Wu, M.-S., Lo, W.-U., Wong, C.-H. &amp; Chiou, S.-H. (2006)
.<it>Proc. Natl. Acad. Sci. USA</it>, <b>103</b>, 2552&dash;2557.<?print show [/query]<?Pub Caret1</bb>
<bb id="bb4">Evans, P. (2006). <it>Acta Cryst.</it> D<b>62</b>, 72&dash;82.<?print [OK]</bb>
```

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

3B2 Total Publishing System
File Edit View Document Page Frame Styles Text Graphic Window Help
SGML SGML menu LMS Table LMS FormatA Format Find elem SGML_parse SGML print SGML in SGML save Gen P T Help
/d/yt5034/yt5034.3d - changed

2: rhead, - : rhead
research papers
6: linenumberleft, 50 @ main, main

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_x, n_y, n_z) 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 (Byrns, 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 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

$$\begin{aligned}x_m &= -(z_m + r)\gamma_2 \sin \alpha + (x_m z_m + \gamma_2 z_m) \\y_m &= (z_m + r)\gamma_2 \sin \alpha + (x_m z_m + \gamma_2 z_m) \\z_m &= (z_m + r) \cos \alpha,\end{aligned}$$

where

$$\begin{aligned}r &= [(n_1 a + n_2 b \cos \gamma)^2 + (n_2 b \cos \gamma)^2]^{1/2}, \\t_2 &= n_2 b \sin \gamma / (2a r), \\t_3 &= -(n_1 a + n_2 b \cos \gamma) / (2a r), \\ \alpha &= (-x_m z_m + \gamma_2 z_m) / r.\end{aligned}$$

(x_m, y_m, z_m) are the wrapped Cartesian coordinates of the tube and (x_m, y_m, z_m) 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 ($z_m, t_2, 0$). The helical transformation is implicitly specified by the helical twist α and the helical rise $x_m z_m + \gamma_2 z_m$. 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 $m_1 = 0, 1, 2, \dots, n_1 - 1$ 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 specified 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

$$\begin{aligned}x_m &= x_m \cos \alpha + z_m \sin \alpha, \\y_m &= y_m + h_m \beta, \\z_m &= -x_m \sin \alpha + z_m \cos \alpha,\end{aligned}$$

where

$$\begin{aligned}h_m &= m_2 - m_1(n_2/n_1), \\ \alpha &= h_m \varphi + m_1(2\pi/n_1).\end{aligned}$$

(x_m, y_m, z_m) are the transformed Cartesian coordinates for the cell $[m_1, m_2]$ and (x_m, y_m, z_m) are the Cartesian coordinates of asymmetric units in cell $[0, 0]$. h_m 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 \rightarrow 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 b as a helix, view the continuation of lattice edge a as a helix or view the continuation along the vector of $a + b$ or along the vector of $a - b$. The first is the most convenient choice. By selecting the vector 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

$$\begin{aligned}\varphi &= (-x_m z_m + \gamma_2 z_m) / r, \\ \delta &= x_m z_m + \gamma_2 z_m,\end{aligned}$$

where t_2, t_3 are the helical axes of the 2-D helical system and x_m, y_m are the planar Cartesian coordinates of the cell origin

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from the 1-D helical system to screwward to generate the and (0, 1) of the new 2-D helical cyl coordinates. The newly we reverse the two wrapped coordare the number of cells planar Cartesian coordinates (x_{2D}, 0, 0) along each edge. The With the new calculated planar coordinates, it is straightfor- ward to calculate the 2-D lattice constants as follows

$$a = (x_a^2 + y_a^2)^{1/2},$$

$$b = (x_b^2 + y_b^2)^{1/2},$$

$$\gamma = (x_a x_b + y_a y_b) / (ab).$$

Fourthly, given the newly determined r , a , b , γ and n_1 , n_2 , the new 2-D helical tube can be determined by solving the quadratic equation $b^2 x^2 + 2rxy \cos \gamma + (ra)^2 - (2rx)^2 = 0$.

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identical subunit, 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 [n₁, n₂, ρ, δ] indicate

We have shown that both the 1-D and 2-D helical systems can be represented by two integers, [n₁, n₂], and that the helical assembly can be built through the helical transformation with the associated parameters. However, the helical symmetry specified by these two integers can also be interpreted in a way different from the helical systems' definitions. In the traditional helical description, an assembly with [n₁, n₂] symmetry can be viewed as two sets of n-start helices in which either the arrangement of the n₁-start helices is specified by n₂ or, vice versa, that of the n₂-start helices is specified by n₁. The best way to illustrate [n₁, n₂] helical symmetry is by using a helical net: an unwrapped flattened 2-D net bound by the circumference in one direction and extended to infinity parallel to the helical axis. Figs 3(a) and 3(b) illustrate an example of wrapping and unwrapping of the helical net with the BM structure of a microtubule with [11, 5] symmetry (Sti & Downing, 2010). The colored circular dots in the helical net represent asymmetric units and a line passing through a set of dots is a helix. The number of intersections (n) between the set of parallel lines with the circumference is exactly the number n of helices that are required to fill the helical assembly. This is the origin of the n-start helices definition. In terms of a helical net description, the helical symmetry can be specified by picking a particular set of two intersecting lines (helices) corresponding to n₁-start and n₂-start lines. The intersections define the locations of repeating asymmetric units in the

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Figure 3
 Illustrations of [n₁, n₂] helical symmetry with respect to helical net. In (a) an BM segment of the microtubule structure is shown in a wrapped helical net with [11, 5] symmetry. The corresponding flattened unwrapped helical net is demonstrated in (b). A section of the corresponding [11, 5] helical net is shown in (c), with the x axis covering the helical circumference, a twist range of 2π and the y axis parallel to the helical axis, corresponding to the helical net. The colored circular dots in the net are the asymmetric subunits and a solid line that passes through a set of dots is a helix. A helical net can be defined by any two sets of lines with their intersections covering all dots. With n₁ lines at 5, there are ten additional sets of helices which can be specific define the same helical structure. See text for an explanation of why only limited sets of helices are feasible with n₁ lines at 5. In (c), feasible sets of helices are marked beside the dots with the value of n₁, colored red. Two of the new helical nets with helical symmetry [8, 5] and [14, 5] are superimposed in (d). The individual helices drawn inside the helical nets is to help in the visualization of individual helical net.

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Author's corrections

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Thank you for preparing the proof, it looks excellent.
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-YSBLIC3Cyab8=85..=92
Should read =91Cultures of E. coli B834DE3/pET-26byoS=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

Date: July, 2011

Manuscript Number: [redacted]

Corresponding Author Name: [redacted]

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120 thiol. To counter the toxic effects, a family of arsenic detoxification
121 enzymes has evolved that convert arsenite ion (AsO₂⁻), the highly
122 reactive form of arsenic, to arsenite ion (AsO₃⁻), a compound that
123 may be effectively transported outside the cell (Mukhopadhyay *et al.*,
124 2002). In *B. melionensis*, YIBB, a protein with marginal sequence
125 similarity to the classical family of arsenite reductases (ArsC),
126 is found that may play a role in reducing arsenite (DeIcco *et al.*,
127 2002). This 13.5 kDa protein (*Bm*-YIBB) is a potential drug target
128 because if arsenite reduction is this protein's major biological func-
129 tion, contributing to the organism's virulence, then disabling this
130 protein and the cell's ability to reduce arsenite would make
131 *B. melionensis* more sensitive to the deleterious effects of endogenous
132 arsenite. Towards understanding the biological function of *Bm*-YIBB
133 and providing a blueprint for structure-based drug design (Meyer *et*
134 *al.*, 2009) based on this protein, the solution structure of *Bm*-YIBB was
135 determined. Its thermostability was measured by CD spectroscopy
136 and its structure was compared with those of a similar protein,
137 *Pseudomonas aeruginosa* YIBB (*Pa*-YIBB; PDB entry 1rwl; Teplovkov
138 *et al.*, 2004), and a protein known to reduce arsenite, *Escherichia coli*
139 ArsC (Ec-ArsC; PDB entry 1dhr; Martin *et al.*, 2003).

2. Materials and methods

2.1. Cloning, expression and purification

The *Bm*-YIBB gene (BR0369; YP_413891.1) was amplified using
the genomic DNA of *B. melionensis* biovar Abortus 2308 and the
oligonucleotide primers 5'-GGGTCTGGTTCCTAATGACGTGGA-
CCATTATAGCCACAGC-3' (forward) and 5'-CTTCTGCTGCTG-
TTTATTATAGCTTAAATAAGCTTCATCACTACCGC-3' (reverse)
(Invitrogen, Carlsbad, California, USA). The amplified *Bm*-YIBB gene
was then gel-purified, treated with T4 DNA polymerase and inserted
into the *Nva*I/*Pme*I-digested expression vector AVA823 at a site that
provided a 21-residue tag containing six consecutive histidine resi-
dues (MAHHHHHHMGLLEAQTGGSS). At the N-terminus of the
expressed protein (Chou *et al.*, 2011). The recombinant plasmid
was transformed into *Escherichia coli* BL21(DE3)R3-*SHARE2* cells
(a gift from SGC Toronto, Toronto, Ontario, Canada) using a heat-
shock method. Uniformly ¹⁵N- and ¹³C-labeled *Bm*-YIBB was
obtained by growing the transformed cells (510 K) in minimal
medium (M9) containing ¹⁵NH₄Cl (1 mg ml⁻¹) and 0-¹³C₆-glucose
(2.0 mg ml⁻¹) supplemented with FeCl₃ (50 µg ml⁻¹) and the anti-
biotics chloramphenicol (35 µg ml⁻¹) and ampicillin (100 µg ml⁻¹).
Once the cells reached an OD₆₀₀ of ~0.8, the cells were cooled to
298 K and protein expression was induced with isopropyl β-D-1-
thiogalactopyranoside (0.025 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 mM sodium phosphate, 10 mM imidazole, 10 mM
brought to 0.2 M phenylmethylsulfonyl fluoride (PMSF) prior to
three passes through a French press (SLM Instruments, Rochester,
New York, USA). Following cell sonication (SLM Instruments,
Rochester, New York, USA) the cell debris was pelleted by centri-
fugation 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 extensively by gravity with 40 ml 0.3 M
NaCl, 50 mM sodium phosphate pH 8.0) containing increasing concen-
trations of imidazole (5, 10, 20, 30 and 250 mM). *Bm*-YIBB eluted
primarily in the 20 mM imidazole wash. Following exchange into 3C
cleavage buffer by overnight dialysis in 41 cleavage buffer (150 mM

NaCl, 20 mM Tris-HCl pH 8.4) the protein was concentrated to
~2 ml (Amicon Centrifuge-10) and the N-terminal polyhistamine tag
was removed by overnight incubation with 3C protease (1 µg per
50 µg target protein) at 270 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 HPLC 4000-column (GE Healthcare, Piscataway, New Jersey,
USA) to simultaneously purify the protein and exchange it into NMR
buffer (100 mM NaCl, 20 mM Tris-HCl, 1.0 mM dithiothreitol/pH
7.1). The band containing *Bm*-YIBB (retention time 78 min) was
collected and the volume was reduced (Amicon Centrifuge-10) to
generate NMR samples in the 1–2 mM range (Lewy 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-(+)-
camphorsulfonate was used to collect circular dichroism data from
a 0.05 mM *Bm*-YIBB 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 20 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, 2000). Steady-state wavelegth
spectra for *Bm*-YIBB were recorded in 0.5 nm increments between
200 and 260 nm at 298 and 353 K. Each reported steady-state
wavelegth 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
¹H/¹³C/¹⁵N 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 mM samples at 293 K, were processed with Felix2007 (Felix
NMR Inc., San Diego, California, USA) and analysed with Jquery
(c.v.115; Goddard & Kneller, 2006). Assignments of the ¹H, ¹³C and
¹⁵N chemical shifts for the backbone and side-chain resonances were
made from standard 2D ¹H-¹⁵N HSQC, ¹³C-¹⁵N HSCQ, HBCBC-
GCHD3 and HBCBCGCCDCHC experiments and 3D HNCACB,
CBCACONH, HNCOC, HEC-TOCSY-NH and CC-TOCSY-NH
experiments using Varian Protein Peak lists programs. Chemical
shifts were referenced to DSS (DSS = 0 p.p.m.) using indirect
methods (Wüthrich *et al.*, 1995). Distance restraints were obtained
from a suite of 2D ¹³C- and ¹⁵N-chemical NOESY-HSQC experi-
ments using a mixing time of 80 ms. Deuterium-exchange studies
were performed by lyophilizing a ¹⁵N-labeled NMR sample, re-dissolving it
in 99.9% D₂O and immediately collecting ¹³C-¹⁵N HSQC spectra for
20 and 60 min after exchange. An overall rotational correlation time,
*t*_r, was estimated from backbone-amide ¹⁵N *T*_ρ ratios (Farrow *et al.*,
1998; Bushkov *et al.*, 2008). A chemical shift perturbation experi-
ment was performed by adding aliquots of reduced glutathione in
NMR buffer (50 mM) to a 0.2 mM sample of ¹⁵N-labeled *Bm*-YIBB.
Following gentle agitation, ¹³C-¹⁵N HSQC spectra were collected at
glutathione:*Bm*-YIBB molar ratios of 0.33, 0.61, 1:1 and 2:1.

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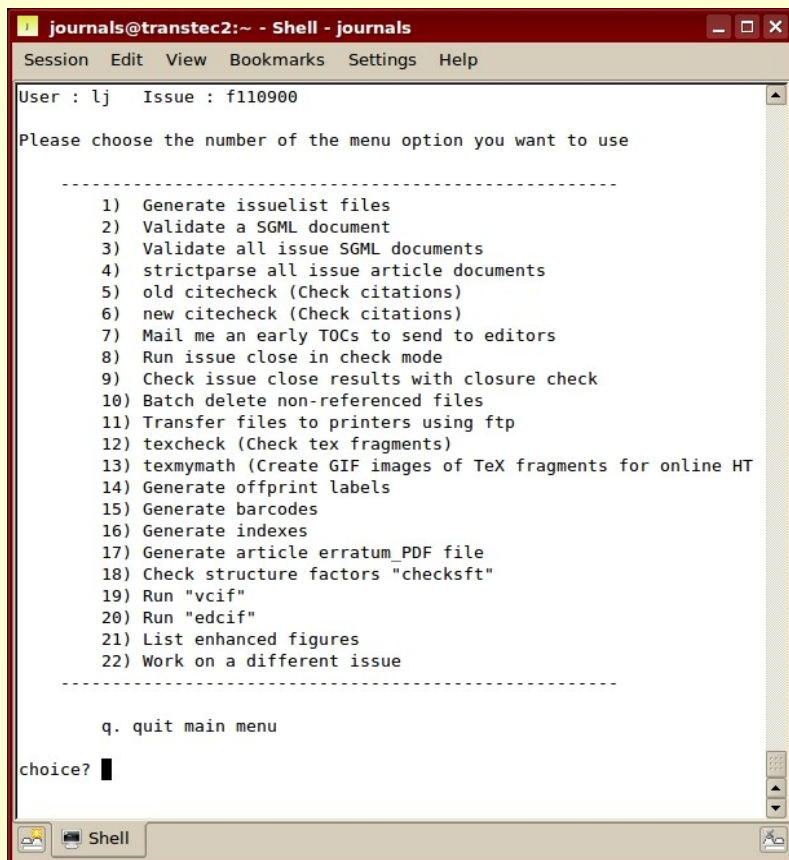
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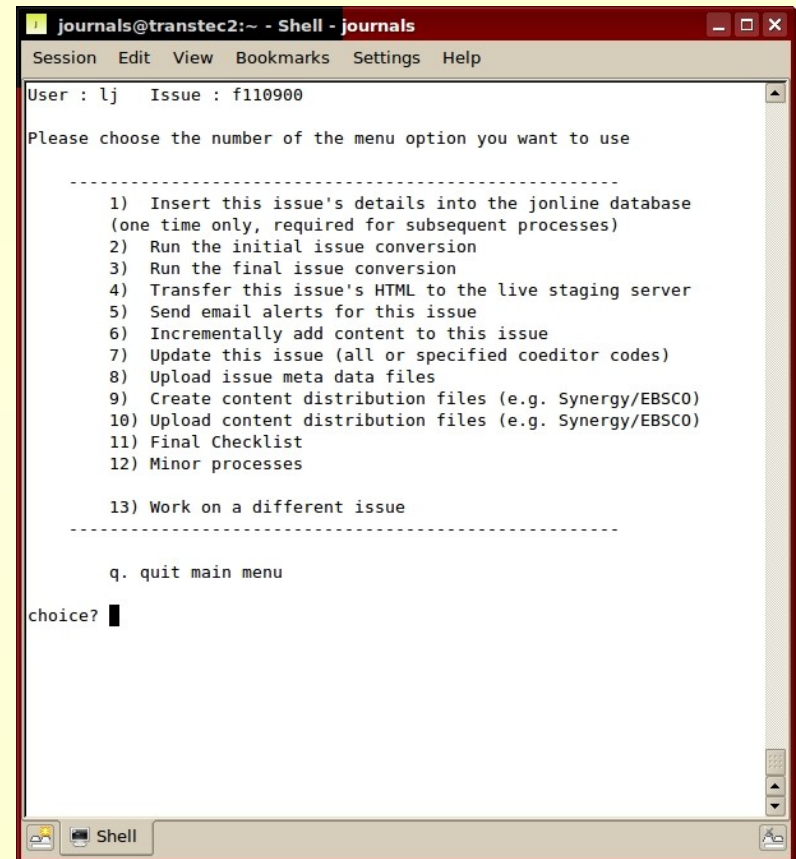
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761 C	762 C	763 GX5184 C	764 C	765 C	766 C	767 C	768 C	769 C	770 C	771 C	772 C	773 C	774 GX5185 C	775 C	776 C
777 C	778 C	779 C	780 C	781 C	782 C	783 C	784 BE5176 C	785 C	786 C	787 C	788 C	789 C	790 C	791 C	792 DZ5228 C
793 C	794 C	795 C	796 C	797 C	798 C	799 C	800 C	801 C	802 C	803 C	804 W- D5155 C	805 C	806 C	807 C	808 C
809 C	810 C	811 C	812 C	813 W- D5158 C	814 C	815 C	816 C	817 C	818 C	819 C	820 C	821 C	822 MH5042 C	823 C	824 C
825 C	826 GX5187 C	827 C	828 C	829 C	830 C	advert1 C	advert2 C								

Contents pages in 3B2

The screenshot displays the 3B2 Total Publishing System interface. The main window shows the contents page for *Acta Crystallographica Section D: Biological Crystallography*, Volume 67, Part 8, August 2011. The page lists several research papers, including:

- 671 Structural and kinetic insights into the mechanism of 5-hydroxymethyl hydroxylase from *Akkalkoala pneumoniae* (J. B. Ranch and S. E. Ealick)
- 678 Structure of 2-oxo-3-deoxyglucosylase kinase from *Akkalkoala pneumoniae* (K. Michalska, M. E. Cliff, C. Tsao, B. Feldman and A. Jochims)
- 690 Structural features of peroxisomal catalase from the yeast *Hansenula polymorpha* (E. Pohlmeier, M. C. Vega, M. Williams and C. Williams)
- 696 Structural features of a novel proteinase from the bacterium *Halobacterium salinarum* (D. E. Tronsted and P. A. Kuppus)
- 707 Structural and biochemical characterization of *N⁶-carboxymethyllysine ribonucleotide synthase* and *N⁶-carboxymethyllysine ribonucleotide surtase* from *Staphylococcus aureus* (P. Bragadoles, E. M. Dugas, W. Zhang, C. B. Poor and C. He)

The interface also shows a left-hand menu with various file paths, a top navigation bar with options like 'File Edit View Document Page Frame Styles Text Graphic Window Help', and a status bar at the bottom indicating the current page and time.

SGML files for articles used to create contents pages

Acta B outside covers



Cover illustration chosen by Editor

Same picture for whole year

Cover is typeset in 3B2

Colour separations produced

Stock covers printed with colour tint and image

Black overlay changes each issue

Acta D outside covers

Editors asked to choose cover illustration from a list on the web for each issue

Acta D cover figure can be from an article in the issue or suggestion from authors

Cover is typeset in 3B2

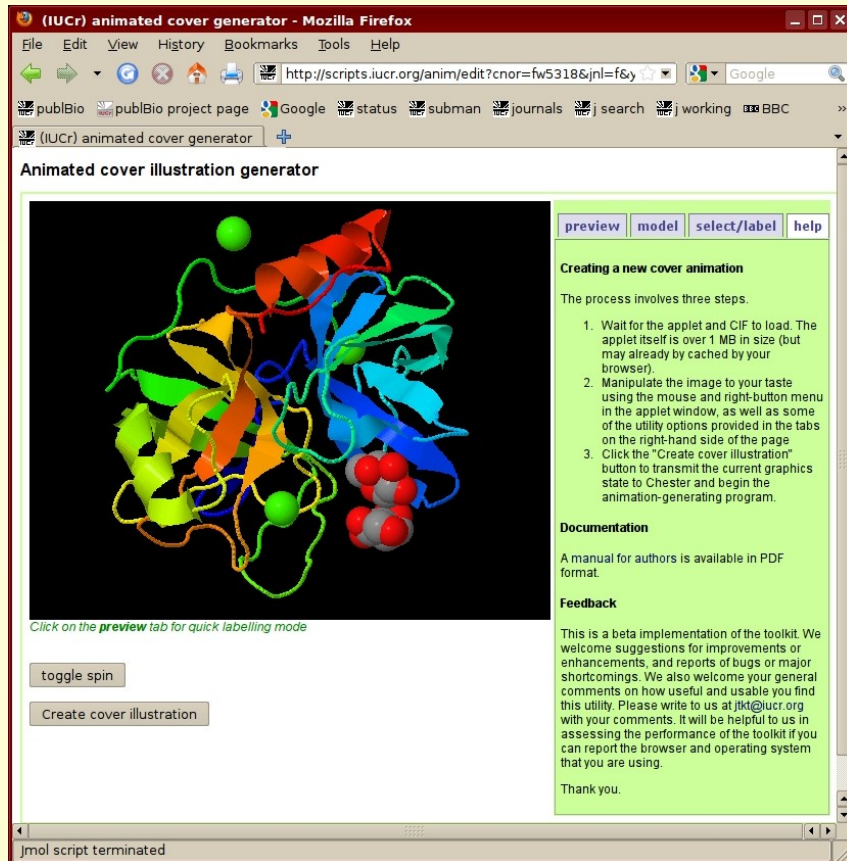
Spine width adjusted depending on number of pages

Adverts added to back cover in 3B2 or Acrobat

Inside covers use information in the issue instance and barcode produced in-house



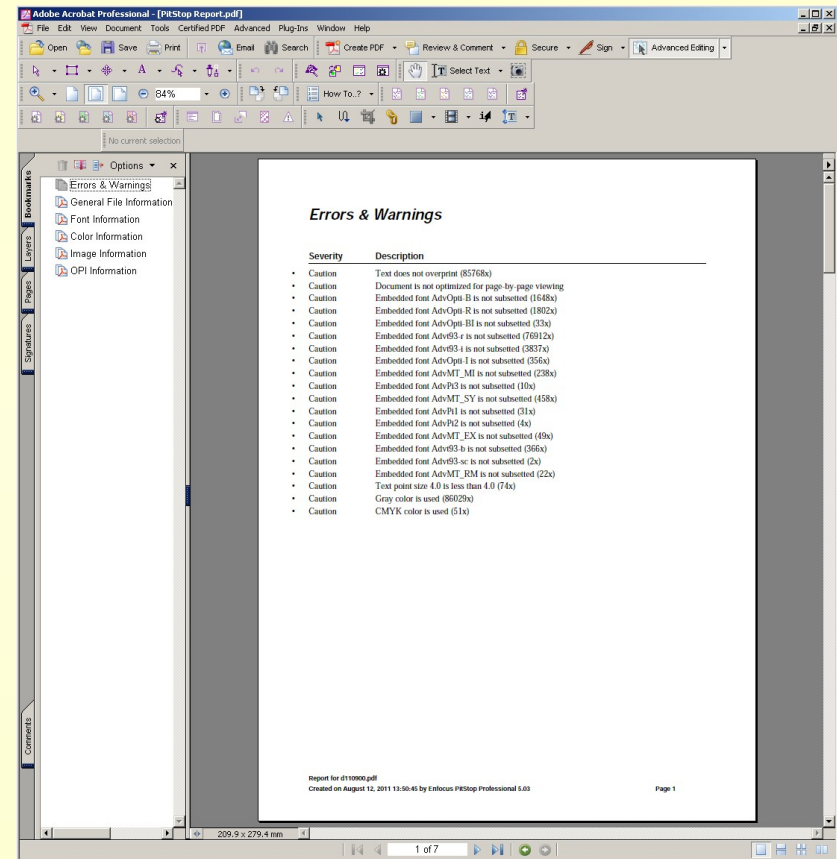
Acta F covers



- Acta F rotating cover created from mmCIF
- Interactive tool for Editors to edit cover illustration
- Automatic script creates rotating cover for web pages

Printing

- High-resolution PDF file of the complete issue created from individual PostScript files
- Corrections checked
- Preflight checks using PitStop Professional
- Checks include: correct fonts embedded, figures correct resolution, CMYK not RGB
- Files for text, covers, issueplan and offprint labels are zipped up and sent by ftp to the printers in Singapore
- Printed by a direct-to-plate method
- Offprints are printed and sent by the printers
- Electronic only journals - digital reprints are produced in-house
- Running sheets (unbound copies of the issue) sent for checking before issue is bound
- Advance bound copies are received approx. two weeks after sending files



Finishing an online issue

Once page numbers have been assigned to articles the online journal is updated
In addition to individual articles, check contents page, back issues page, journal home page, reader services, author services pages

Metadata is created, checked sent by ftp to abstracting and indexing services

Issue content is created for other online platforms such as PubMed Central, Wiley Online Library, checked and sent by ftp

Electronic reprint notifications are sent out to authors

E-mail alerts are sent out

Online pages and e-alerts

The screenshot displays a desktop environment with three main windows:

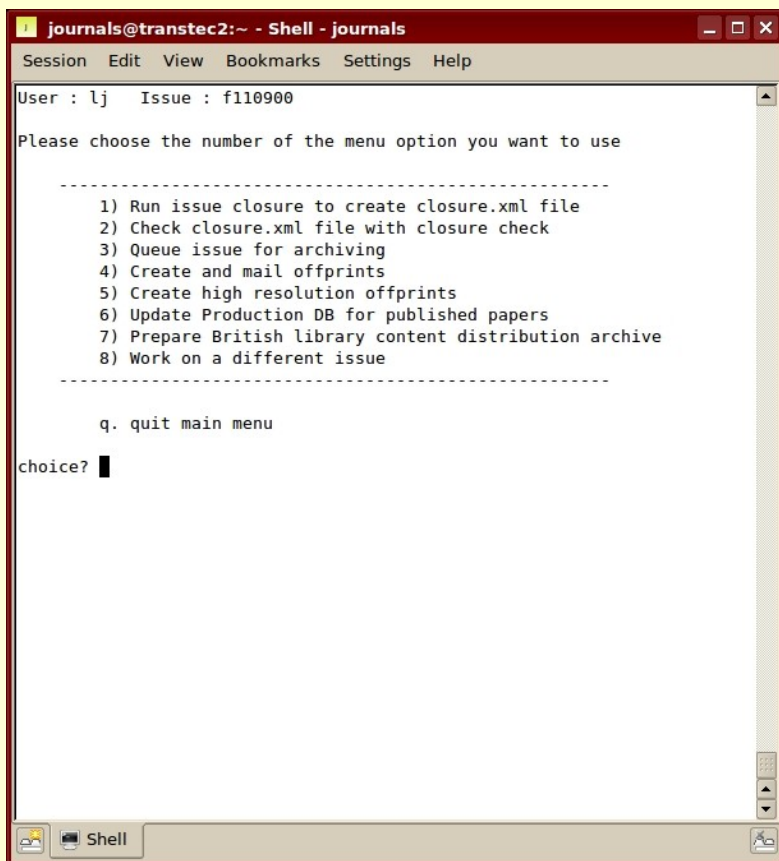
- Left Window:** Mozilla Firefox browser showing the "back issues" page of the IUCr Biological Crystallography Online. It lists back issues from Volume D67 (2011) to Volume D64 (2008). The "back issues" section includes a search bar and a list of articles with their respective page numbers and dates.
- Middle Window:** Mozilla Firefox browser showing the "Acta Crystallographica Section D" page for Volume 67, Part 8 (August 2011). It features a cover illustration of three helical structures and a "research papers" section with a link to a paper on *Klebsiella pneumoniae*.
- Right Window:** E-Mail - Kontact email client showing an inbox with several messages from "ealert@iucr.org" regarding the contents of Acta Crystallographica Section D. Below the inbox, there is a preview of an email with a cover illustration and a "research papers" section.

A vertical sidebar on the far left of the image contains a stack of journal covers from various issues of Acta Crystallographica.

Where content is sent

OhioLINK - The Ohio Library and Information Network, Gale CENGAGE Learning, GNM Healthcare, CILEA Interuniversity Consortium, EBSCO, Minerva, CSA Proquest, Thomsonreuters ISI, National Science Digital Library, Dutch National Library, EBSCO Linking, Consorzio interuniversitario per le Applicazioni di Supercalcolo Per Universita e Ricerca a CASPUR, OCLC Online Computer Library Center, University of Toronto, CNPIEC, Commonwealth Scientific and Industrial Research Organisation (CSIRO), Wiley, QSensei, SCOPUS, PUBMED, British Library (Acta F only), PUBMED crystalopen, CAS, GetInfo, Infotrieve, SWETS, NCBI, CrossRef, DOAJ - Directory of Open Access Journals, AIP, JGATE

Tidying up



```
journals@transtec2:~ - Shell - journals
Session Edit View Bookmarks Settings Help
User : lj Issue : f110900
Please choose the number of the menu option you want to use

-----
1) Run issue closure to create closure.xml file
2) Check closure.xml file with closure check
3) Queue issue for archiving
4) Create and mail offprints
5) Create high resolution offprints
6) Update Production DB for published papers
7) Prepare British library content distribution archive
8) Work on a different issue
-----

q. quit main menu
choice? █
```

Check that all necessary files are in place

Unwanted files from processing are batch deleted

Issue files are archived in Chester

Connecting readers to content

- Browsing
- E-mail alerts
- RSS
- Metadata and content delivery to third parties
 - Wiley Online Library
 - PubMed Central
 - Abstracting and Indexing Databases
 - Search Engines (Google, Scirus, CrossRef, ...)

Browsing

- Tables of Contents
- Crystallography 'What's New'
- Forthcoming articles
- Editor-in-chief's selection
- Highlighted articles in *IUCr Newsletter*

E-mail alerting

- Registered service through World Directory of Crystallographers
- Individual journal contents
- Plain or HTML format

RSS

- Really simple syndication, rich site summary, ...
- Polling model
- Multi-platform; browser plugins
- Tables of contents, forthcoming articles, open-access articles

Metadata

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CrossRef

- Aggregator of bibliographic metadata
- Identifiers based on DOI (www.doi.org)
 - e.g. doi:10.1107/S0021889805016262
- XML schemas for:
 - Deposited articles
 - Books
 - Conference proceedings
 - Article components
- Database interrogation via XML

Wiley Online Library

The screenshot shows the Wiley Online Library interface for Acta Crystallographica Section D. The browser window title is "Acta Crystallographica Section D - Wiley Online Library - Mozilla Firefox". The address bar shows the URL "http://onlinelibrary.wiley.com/journal/10.1111/ISSN1399-00...". The page features a navigation menu with "PUBLICATIONS", "BROWSE BY SUBJECT", "RESOURCES", and "ABOUT US". The main content area includes a "JOURNAL TOOLS" section with options like "Get New Content Alerts", "Get RSS feed", "Save to My Profile", "Get Sample Copy", and "Recommend to Your Librarian". A "JOURNAL MENU" section lists "Journal Home", "Current Issue", "All Issues", "FIND ARTICLES", "GET ACCESS", "FOR CONTRIBUTORS", "ABOUT THIS JOURNAL", and "SPECIAL FEATURES". The central content area displays "Acta Crystallographica Section D" with a "Crystallography Journals Online" logo. It includes a "SEARCH" box, a "Recently Published Issues" list (August 2011, July 2011, June 2011, May 2011, April 2011), and a "Discover all the IUCr Journals" section. The footer contains "ABOUT US", "HELP", "CONTACT US", "AGENTS", "ADVERTISERS", "MEDIA", "PRIVACY", "TERMS & CONDITIONS", and "SITE MAP".

Crystallography
Journals
Online

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IUCr arranges deposition in PubMed Central for articles supported by NIH funding

Authors should not deposit articles themselves

Authors are still advised to make article open access



PubMedCentral

Conservation of a crystallographic interface suggests a role for β -sheet augmentation in influenza virus NS1 multifunctionality - Mozilla

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Journal List > Acta Crystallogr Sect F Struct Biol Cryst Commun > v.67(Pt 8); Aug 1, 2011

Acta Crystallogr Sect F Struct Biol Cryst Commun. 2011 August 1; 67(Pt 8): 858-861. PMID: PMC3151114
Published online 2011 July 13. doi: 10.1107/S17443009111019312

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Conservation of a crystallographic interface suggests a role for β -sheet augmentation in influenza virus NS1 multifunctionality

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Abstract Other Sections

The effector domain (ED) of the influenza virus virulence factor NS1 is capable of interaction with a variety of cellular and viral targets, although regulation of these events is poorly understood. Introduction of a W187A mutation into the ED abolishes dimer formation; however, strand-strand interactions between mutant NS1 ED monomers have been observed in two previous crystal forms. A new condition for crystallization of this protein [0.1 M Bis-Tris pH 6.0, 0.2 M NaCl, 22% (w/v) PEG 3350, 20 mM xylitol] was discovered using the hanging-drop vapour-diffusion method. Diffraction data extending to 1.8 Å resolution were collected from a crystal grown in the presence of 40 mM thieno[2,3-b]pyridin-2-ylmethanol. It was observed that there is conservation of the strand-strand interface in crystals of this monomeric NS1 ED in three different space groups. This observation, coupled with conformational changes in the interface region, suggests a potential role for β -sheet augmentation in NS1 function.

Keywords: effector domains, influenza virus, virulence factors, NS1, β -sheet augmentation

1. Introduction Other Sections

The NS1 protein of influenza virus is an important virulence factor and has been demonstrated to interact with a wide variety of viral and cellular biomolecules (Hale, Randall *et al.*, 2008). In particular, crystallographic structures have been obtained of the N-terminal RNA-binding domain (RBD) in complex with dsRNA (Cheng *et al.*, 2009) and of the C-terminal effector domain (ED) in complex with the F2F3 portion of the cellular processing and specificity factor CPSF30 (Das *et al.*, 2008) and with the iSH2 domain of the PI 3-kinase regulatory subunit p858 (Hale, Kerry *et al.*, 2010). Furthermore, both domains form homodimers *in vitro* (Bornholdt & Prasad, 2006; Chien *et al.*, 1997; Hale, Barclay *et al.*, 2008; Xia *et al.*, 2009). While the conformation of the RBD dimer appears to be conserved, two forms of the ED dimer have been proposed: the strand-strand dimer and the helix-helix dimer (Hale, Barclay *et al.*, 2008; Xia *et al.*, 2009; Bornholdt & Prasad, 2006). The helix-helix dimer is present in all wild-type NS1 ED structures (Kerry *et al.*, 2011) and in the structure of full-length NS1 (Bornholdt & Prasad, 2006). In contrast, the canonical strand-strand dimer has only been observed in crystallographic contacts in a few NS1 ED structures obtained using NS1 from the A/Puerto Rico/8/1999 strain. The structure of the full-length NS1 protein from an HCMV-positive

PubMed articles by these authors

- ▶ Kerry, P.
- ▶ Long, E.
- ▶ Taylor, M.
- ▶ Russell, R.

PubMed related articles

- ▶ A transient homotypic interaction model for the influenza A virus NS1 protein effector domain. [PLoS One. 2011]
- ▶ The RNA-binding and effector domains of the viral NS1 protein are conserved to different extents among influenza A and [Virology. 1996]
- ▶ Structure of an avian influenza A virus NS1 protein effector domain. [Virology. 2008]
- ▶ Review The influenza virus NS1 protein: inhibitor of innate and adaptive immunity. [Infect Disord Drug Targets. 2007]
- ▶ Review The multifunctional NS1 protein of influenza A viruses. [J Gen Virol. 2008]

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- ▶ Taxonomy Tree

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- Search Engines
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- Infotrieve, TIB Info
- Wiley Online Library

Archiving

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- German National Science Library (TIB, Hannover)
- British Library
- Cambridge Crystallographic Data Centre
- PubMed Central
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Redesigning the online journals

Front page to be redesigned completely: more emphasis on journal names

Will include lists of e.g. top downloaded articles, highlighted articles, highly cited articles, newly published articles to encourage downloading and increased citations, search tool to be prominent

Best features that we find on other journal websites

Articles: Tabbed design, closer integration of supplementary materials

More interactive. Graphical, video abstracts, author interviews, ability to comment (e.g. for WDC members)

Citation metrics

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Improve **author and reader service pages** and documentation

Thanks

To everyone who helped in the making of this production

