New Routes to Crystallographic Data Publication

Presentation:

Data Publishing in *Acta Crystallographica* Section F

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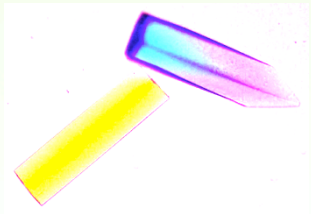

Journals : Databases

Deposition mmCIF to journal:

"streamlining"

Publication mmCIF for database:

crystallization data

Thoughts on further evolution

Crystallography Journals Online

***Acta Crystallographica* Section F**

http://journals.iucr.org/f/

New Routes to Crystallographic Data Publication

Streamlining project: Essentially completed

Collaboration: **RCSB & Acta F**

Objectives: speed publication, enhance database archive

RCSB: Relational transformation (mmCIF)

More data in tables (fewer text entries)

PDB_EXTRACT

ActaF: Streamlining publication *via* deposited data

Deposition mmCIF converted to journal tables

Expand, retool mmCIF dictionary

Identify data required for publication

Enhanced figure preparation

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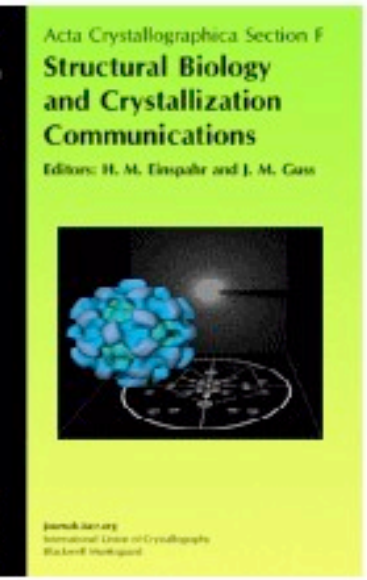

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New Author Services page

experimental tables for *Acta Crystallographica Section F*

This service is provided to enable authors who have deposited their structure with the PDB to prepare experimental tables for publication in *Acta Crystallographica Section F*. To obtain an RTF file for inclusion in your article, indicate the phasing method used, and then either upload an mmCIF or enter the PDB code of your structure.

Indicate the phasing method used:

☐ MAD ☐ MIR ☐ MIRAS ☐ MR
☐ SAD ☐ SIR ☐ SIRAS ☐ not known

mmCIF file name:

Browse...

or

PDB code:

Prepare experimental tables

Done

Click to "experimental details table" page

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Table 3. Structure refinement and model validation
Values for the outer shell are given in parentheses.

Refinement software	X-PLOR
Refinement on	F^2
σ cutoff	$F > 2.0\sigma(F)$
Resolution range (Å)	10.00–2.00 (2.09–2.00)
No. of reflections used in refinement	15067 (1058)
No. of reflections above σ cutoff in final cycle	15067 (?)
Final overall *R* factor	? (?)
Atomic displacement model	iso
Overall average *B* factor (Å^2)	25.2
No. of protein atoms	1990
No. of ligand atoms	21
No. of solvent atoms	106
Total No. of atoms	2117
No. of refined parameters	8362
Non-crystallographic symmetry restraints	0
Bulk solvent model	?; B_{SOL} = ?, K_{SOL} = ?
Final R_{work}	0.242 (0.302)
No. of reflections for R_{free}	743 (52)
Final R_{free}	0.312 (0.367)

RTF File With Three Tables:

1 - Sample
2 - Data Collection
3 - Refinement

PDB code 1i37
AR-LBD
Pre-PDB_EXTRACT

http://journals.iucr.org/f/services/authorservices.html

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publCIF: parallel editing of tables & CIF

publCIF - //Fileserver1/natronscr/av1218.cif (modified)

CIF Edit Preprint Tools Help

```
268 al.</i> (1997). Crystallization in Et~2~O/<i>n</i>-hex
269 crystals of (I) suitable for X-ray diffraction.
270 ;
271
272 #=============================================================
273
274 data_I
275
276 _audit_creation_method            SHELXL97
277 _chemical_name_systematic
278 ;
279 Diethyl [(Z)-1-iodo-2-phenyl-1-hexenyl]phosphonate
280 ;
281 _chemical_name_common             ?
282 _chemical_melting_point           ?
283 _chemical_formula_iupac           'C16 H24 I O3 P'
284 _chemical_formula_moiety          'C16 H24 I O3 P'
285 _chemical_formula_sum             'C16 H24 I O3 P'
286 _chemical_formula_weight          422.22
287
288 _symmetry_cell_setting            monoclinic
289 _symmetry_space_group_name_H-M    'P 21/n'
290 _symmetry_space_group_name_Hall   '-P 2yn'
291
292 loop_
293  _symmetry_equiv_pos_as_xyz
294  'x, y, z'
295  '-x+1/2, y+1/2, -z+1/2'
296
```

Col: 49 View log

Crystallization in Et_2O/*n*-hexane yielded single crystals of (I) suitable for X-ray diffraction.

(I)

Crystal data

$C_{16}H_{24}IO_3P$	D_x = 1.489 Mg m^{-3}
M_r = 422.22	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 1006 reflections
a = 11.7324 (18) Å	θ = 2.4–27.4°
b = 12.3985 (19) Å	μ = 1.79 mm^{-1}
c = 13.228 (2) Å	T = 293 (2) K
β = 101.817 (3)°	Irregular, colourless
V = 1883.4 (5) Å^3	0.48 × 0.42 × 0.26 mm
Z = 4	

Designations for Crystallization Data

Example: Simple list of recommended and required data

1.3. Crystallization

Crystallization specifics

- **Crystallization method**
- **Temperature (K)**
- **Additional details**
- **Volumes and pHs of crystallization solutions**
- **Compositions of crystallization solutions**

Cryo treatments

- **Final cryoprotection solution**
- **Soaking**
- **Cooling**
- **Annealing**

And more …

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Special Standards for Crystallization Data

The complete sequence of the molecule crystallized should be provided.
This may take the form of a database code to indicate the canonical sequence, but it should include **sequences and attachment points of any tags or remnants of tags** and any known covalent modifications. In the case that the preparation and purification steps have been previously published and a paper containing their description is cited, the authors should provide a brief summary of the key aspects of sample preparation that makes the final sequence clear to readers.

Explicit definition of crystallization conditions.
Authors are required to define the compositions and volumes of the protein and precipitant solutions used to produce the optimized crystals used for structure determination as accurately as possible. Also required in the case of vapor diffusion experiments are the volume of reservoir solution and its composition, if different from the precipitant.

http://journals.iucr.org/f/services
/structuralcommunications/mmcifreqditems.html

Crystallization Databases: Impact

"Requirements" standards and expansion of mmCIF dictionary have created a virtual template

This template invoked and visualized by publCIF

Online tools based on publCIF being developed to create mmCIF from tables based on real template

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crystallization data tool

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It will take a few moments to set up the editor - please wait until the whole page has finished loading. . . . . .

Macromolecule details, crystallization and data collection

continue

Please navigate using the tabs below and fill out as many fields as possible (items labelled in grey are not essential, but you are encouraged to provide them where possible). When you have finished, click 'continue' to preview your experimental data tables.

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

Unit-cell data

Crystal system [ ] Space group P 32 2 1

a (Å) 107.516 *b* (Å) 107.516 *c* (Å) 338.487

α (°) 90.00 β (°) 90.00 γ (°) 120.00

No. of molecules in unit cell *Z*

Crystal characteristics

Click here to add data for another crystal of this macromolecule

Crystal 1

Click here to remove this set of crystal data

Dimensions (mm) max: mid: min:

radial:

Matthews coefficient V_M (Å^3 Da^{-1}) 3.23

Solvent content (%) 61.97

more...

Done zotero

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New Tool

Template has been much requested by authors.

To be used by authors to make writing, submitting and editing easier

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

Click here to add data for another crystal of this macromolecule

Crystal 1

Click here to remove this set of crystal data

Crystal growth

Method

Apparatus

Temperature (K)

Atmosphere

pH OR pH range

Seeding protocol

Growth time

Additional details

Crystallization solutions

Macromolecule solution

Volume Volume units pH

Components of the macromolecule solution

Name Concentration OR concentration range Concentration units

+

Precipitant solution

Volume Volume units pH

Components of the precipitant solution

Name Concentration OR concentration range Concentration units

+

Reservoir solution

Volume Volume units pH

Components of the reservoir solution

Name Concentration OR concentration range Concentration units

+

Cryotreatment

Select appropriate cryotreatment protocol(s)

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Pages

Pull down menus

Deposition of Crystallization Data in PDB: addressing concerns

- **Compliance might improve if deposition convenient**
- **Crystallization data not accepted without structure**
- **Crystallization data inconvenient after deposition:**
  revalidation
- **But for crystallization papers preceding structure reports, authors could be encouraged to add mmCIF of crystallization data from Acta Cryst. F to their structure data for simultaneous deposition.**

WORLDWIDE PDB
PROTEIN DATA BANK

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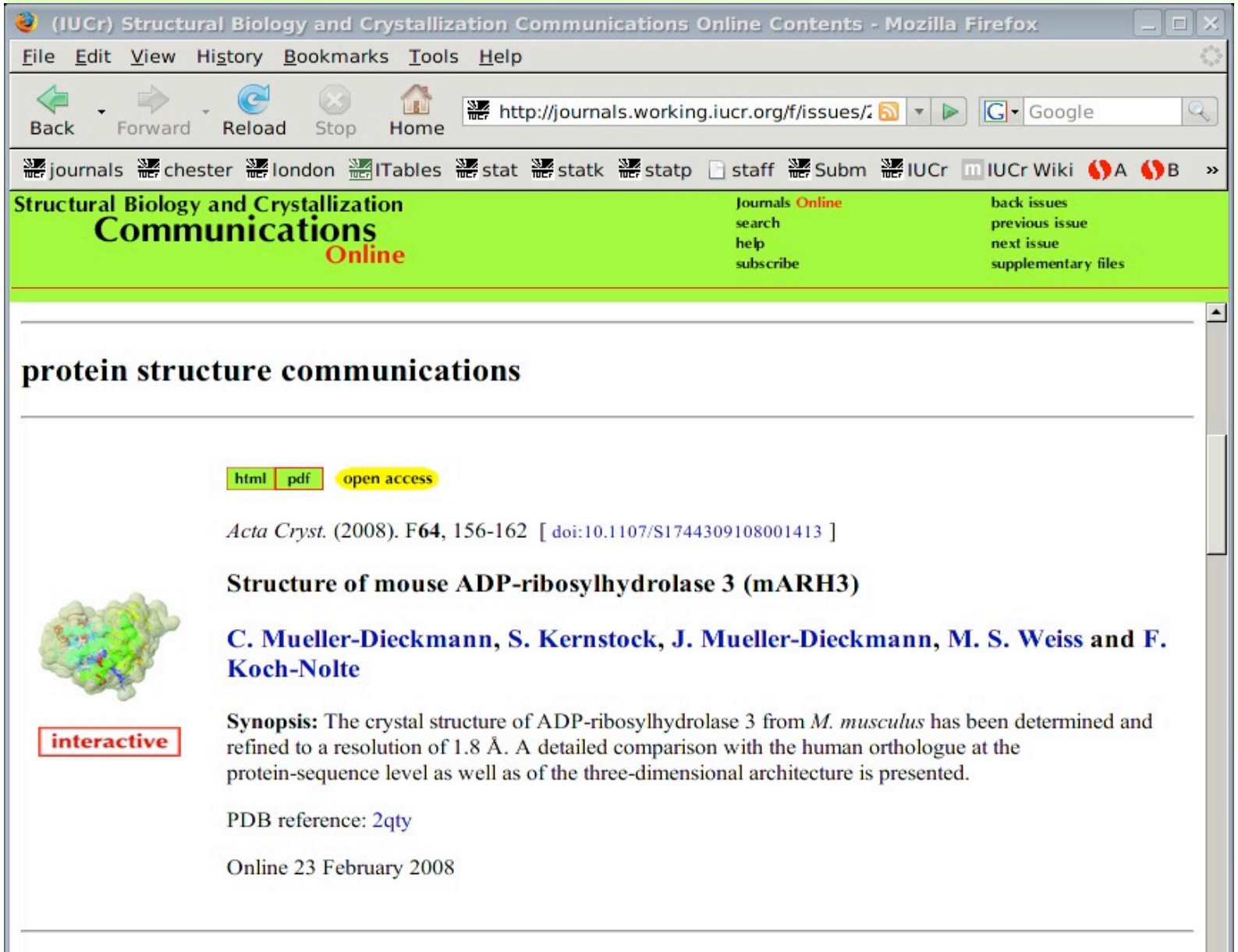
If no structure is produced?
Or crystallization communication too late for deposition?



Acta Cryst. F proposes to make crystallization data of all articles available in perpetuity.

Freely available to all databases, crystallization or otherwise.

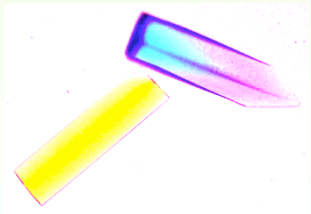
Future Options, Future Issues

Generalization to non-crystallization data

Improved data presentation for extraction

Extension to authors targeting other journals

Generalization of procedures to accommodate deposition in chunks and in any order



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