



Writing a Macromolecular Structure Paper with publBio

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Background

- As of Tuesday Aug 20, 2013 at 5 pm PDT, there are **93252** structures in the PDB



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- Acta Crystallographica Section F published **264** crystallization communications in 2012

⇒ Huge backlog in publishing
⇒ Loss of information



Types of Publications

- **CC: crystallization communication**
- **SC: structural communication**



The publBio Idea

- help authors in writing a publication effectively and quickly
- facilitate editing and refereeing
- capture at least some of the unpublished structures in the PDB
- ensure that crystallization information is not lost
- ideally, the information should be minable

⇒ **Publication templates**

⇒ **Most relevant information in tabular form**

⇒ **Tables can be populated from PDB, mmCIF or by hand**

⇒ **Closely linked to the IUCr submission system**



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a tool for editing mmcifs

- **publBio annotator**
- **publBio publisher**

a tool for writing and submitting articles



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new_2 (08 Jun 12 16:25) [rename] [delete] [copy]	Submit to Acta Cryst. F
3fsx_ (12 Jun 12 13:56) [rename] [delete] [copy]	Submit to Acta Cryst. F
2ohd_3 (17 Feb 12 11:53) [rename] [delete] [copy]	Submit to Acta Cryst. F
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louise (17 Feb 12 11:58) [rename] [delete] [copy]	Submit to Acta Cryst. F
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Write a new article

Enter a PDB code

Or upload an mmCIF or PDB file

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About pubBio publisher

pubBio *publisher* is an online tool for preparing articles and submitting them to IUCr journals.

Starting a new article project is easy. Choose one of three options to open an online template which is either blank or partially filled with your data and ready for writing your article.

Once the template is open, click in the part of the article you want to edit and away you go. Articles can be saved in your personal webspace.

When you are ready to submit just press the Submit button and you will be automatically redirected to the IUCr submission system. If your paper reports a structure you will need to upload a validation report but all the other files will be there and you will just need to choose a co-editor to complete the submission.

Revising your article is easy too, just return to your project page to edit your paper and submit a revision.

An interactive 'click and type' demonstration is available [here](#).

About pubBio

pubBio consists of two parts:

- pubBio *annotator* is a tool for editing mmCIFs
- pubBio *publisher* is a tool for writing and submitting articles

pubBio *annotator* is a revised version of the original mmCIF-driven pubBio tool. It can be used for creating an mmCIF from scratch or for enhancing an existing mmCIF.

The two parts of pubBio can be used together or on their own to help you prepare your data and/or your article for publication in IUCr journals.

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structural communications

Acta Crystallographica Section F
**Structural Biology
and Crystallization
Communications**
ISSN 1744-3091

Title

Synopsis
One or two sentences of the main findings for use in the journal contents listing.

Enter author details here

Keywords:

PDB reference:

Abstract
Up to 150 words stating as specifically and as quantitatively as possible the principal results obtained. Do not use 'we' or 'I', or refer to specific tables or figures.

1. Introduction
Include brief information about the background to the study, the source organism, the structure and function of the macromolecule, and related structures.

2. Materials and methods

2.1. Macromolecule production
Text in this section should supplement or complete information provided in Table 1.

Table 1
Macromolecule production information

In the primers, indicate any restriction sites, cleavage sites or introduction of additional residues, e.g. His6-tag, as well as modifications, e.g. Se-Met instead of Met.

Source organism

DNA source

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Acta Crystallographica Section F
Structural Biology
and Crystallization
Communications
ISSN 1744-3091

L. Schultdt, S. Weyand, G.
Kefala and M.S. Weiss

Keywords: beta helix, L beta H
domain, Acyltransferase,
TRANSFERASE

PDB reference: 3fsx

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Source Mycobacterium tuberculosis (strain: H37Rv)

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details are added from
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Schuldt Weiss

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ISSN 1

Name

Title

IUCr ID

Forename(s) Manfred

Surname* Weiss

Qualifier (e.g. Jr, III)

E-mail* msweiss@helmholtz-berlin.de

Correspondence author for publication ☐

Primary contact author for this submission ☐

Keyw
doma
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PDB re

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Organization* Helmholtz-Zent

Street/PO box Albert-Einstei

Town/city Berlin

State/province/county

Post/zip code D-12489

Country* Germany

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George H. Weiss
Div. Computer Research and Technology,
NIH, 9000 Rockville Pike, Bldg 12A, Rm
2007, Bethesda, MD, 20892, USA,
[click here to use these details]

Manfred Weiss
Macromolecular Crystallography (HZB-MX),
Helmholtz-Zentrum Berlin, Albert-
Einstein-Str. 15, Berlin, D-12489,
Germany,
[click here to use these details]

communications

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or figures.

the source organism, the
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2. Ma

2.1. M

Text in

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Macro

In the primers, indicate any restriction sites, cleavage sites or introduction of additional residues, e.g. His6-tag, as well as modifications, e.g. Se-Met instead of Met.

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Synopsis
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structural communications

Acta Crystallographica Section F
Structural Biology
and Crystallization
Communications
ISSN 1744-3091

L. Schultdt^a and Manfred
Weiss^{a*}

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Keywords: beta helix, L beta H
domain, Acyltransferase,
transferase

PDB reference: 3fsx

2. Materials and methods

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Text in this section should supplement or complete information provided in Table 1.

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refined to 2.15 Å resolution.

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2. Materials and methods

2.1. Macromolecule production

The production of *Mtb*-DapD was described in detail in Schuldts *et al.* (2008). For a quick reference to the most relevant pieces of information see Tables 1 and 2.

Table 1

Macromolecule production information

In the primers, indicate any restriction sites, cleavage sites or introduction of additional residues, e.g. His6-tag, as well as modifications, e.g. Se-Met instead of Met.

Source organism	<i>Mycobacterium tuberculosis</i> (strain: H37Rv)
DNA source	
Forward primer	
Reverse primer	
Cloning vector	
Expression vector	
Expression host	
Complete amino acid sequence of the construct produced	MAVSTVTGAAGIGLATLAADGSVLDTWFPAPELTESGTSATSPILAVSDVPVELAALIGRDDRRRTETIAVRTVIGSLDDV AADPYDAYLRHLHSHRLVAPHGLNAGGLFGVLTNNVWTNHGPCAIDGFEAVRARLRGPTVYGVDFKFRMVDYWPT GVRIADADRVRLGAHLAPGTTVMHEGFVNYNAGTLGASMVEGRISAGVW/GDGSVDVGGGASIMGTLSGGGTHVSIQKRC LLGANSGLGISLGDDCWVEAGLYVTAGTRVTMPDSNSVKARELSGSSNLLFRNNSVSGAVEVLAPDGGQIALNEDLHANG VPRGLEHHHHHH

2.2. Crystallization

Text in this section should supplement or complete information provided in Table 2.

Layout

- Add column
- Delete column
- Add row
- Delete row
- Merge cells
- Unmerge
- Copy cell contents
- Paste cell contents

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tables are prefilled from
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simple table editor

*the content and layout of
the table can be altered*

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Text in this section should supplement or complete information provided in Table 4.

The structure was solved with *Auto-Rickshaw* (Panjikar *et al.*, 2005) and refined with *REFMAC* 5.4.0069 (Murshudov *et al.*, 2011). *MolProbity* (Chen *et al.*, 2010) was used for Ramachandran analysis.

Table 4

Structure refinement

Please check **bold-underlined** values (these may have been derived because they are not explicitly defined in the CIF) Values for the outer shell are given in parentheses.

Resolution range (Å)	30.00–2.15 (2.206–2.150)
Completeness (%)	99.7
σ cutoff	
No. of reflections, working set	90238 (6637)
No. of reflections, test set	1126 (76)
Final R_{cryst}	0.168 (0.199)
Final R_{free}	0.220 (0.232)
Cruickshank DPI	
No. of non-H atoms	
Protein	10866
Ion	<u>13</u>
Ligand	<u>40</u>
Water	570
Total	11489
R.m.s. deviations	
Bonds (Å)	0.019
Angles (°)	1.724
Average B factors (Å ²)	
Protein	<u>30.2</u>
Ion	<u>44.7</u>
Ligand	<u>38.0</u>
Water	<u>29.4</u>
Ramachandran plot	
Favoured regions (%)	97.8
Additionally allowed (%)	1.8
Outliers (%)	0.3

Done

some values are
calculated from data
in the mmCIF

bold underlined values
should be checked
carefully

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are essentially identical. Based on further data base searches (not shown), it must be concluded that the second hit was erroneously published as the structure of DapD from *Mycobacterium bovis* and that is actually DapD from some contaminating *E. coli* strain.

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Figure 1

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Upto 3 figures may be included in the paper, for example:
Stereoview of the biological oligomer down the major axis or two orthogonal views of the oligomer;
Ribbon representation of one subunit;
Structural superposition or active-site view or ligand view (with omit electron density).

Figure 1

Caption

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Fig 1 caption
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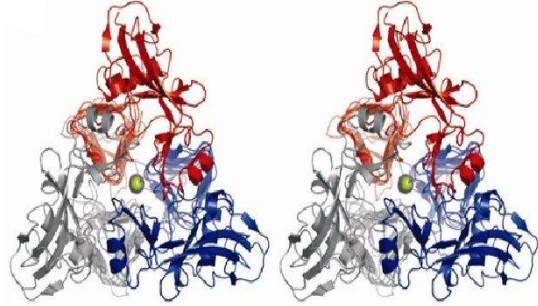
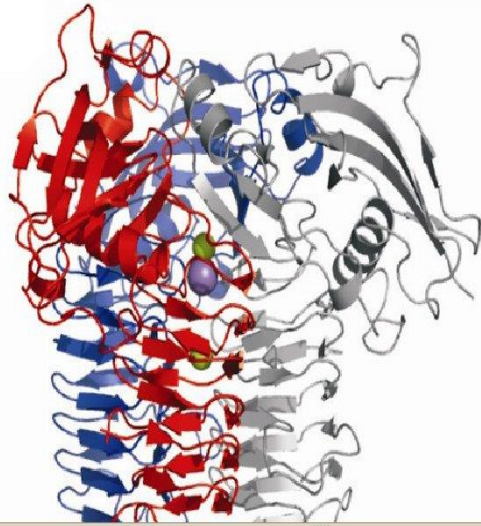


Figure 1

Stereo (wall-eyed) view along the three-fold symmetry axis of the physiologically relevant homotrimer of *Mtb*-DapD in ribbon representation. The subunits A, B and C are colored in red, light grey and blue, respectively. Mg²⁺ and Na⁺ ions are shown as yellow and purple spheres. The co-factor SCoA is shown in ball-and-stick representation in cyan.



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structural communications

Acta Crystallographica Section F
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Keywords: beta helix, L beta H
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transferase

PDB reference: 3fsx

**Structure of tetrahydridipicolinate
N-succinyltransferase (Rv1201c; DapD) from
*Mycobacterium tuberculosis***

Synopsis

The structure of the enzyme tetrahydridipicolinate *N*-succinyltransferase (DapD, Rv1201c) from *M. tuberculosis* has been solved at 2.15 Å resolution.

Abstract

The three-dimensional structure of the enzyme tetrahydridipicolinate *N*-succinyltransferase has determined by MAD and refined to 2.15 Å resolution. This enzyme catalyzes the fifth step of the DAP pathway, the conversion of the cyclic tetrahydridipicolinate (THDP) into the acyclic compound *N*-succinyl-L-2-amino-6-ketopimelate using succinyl-CoA (SCoA) as a cofactor.

1. Introduction

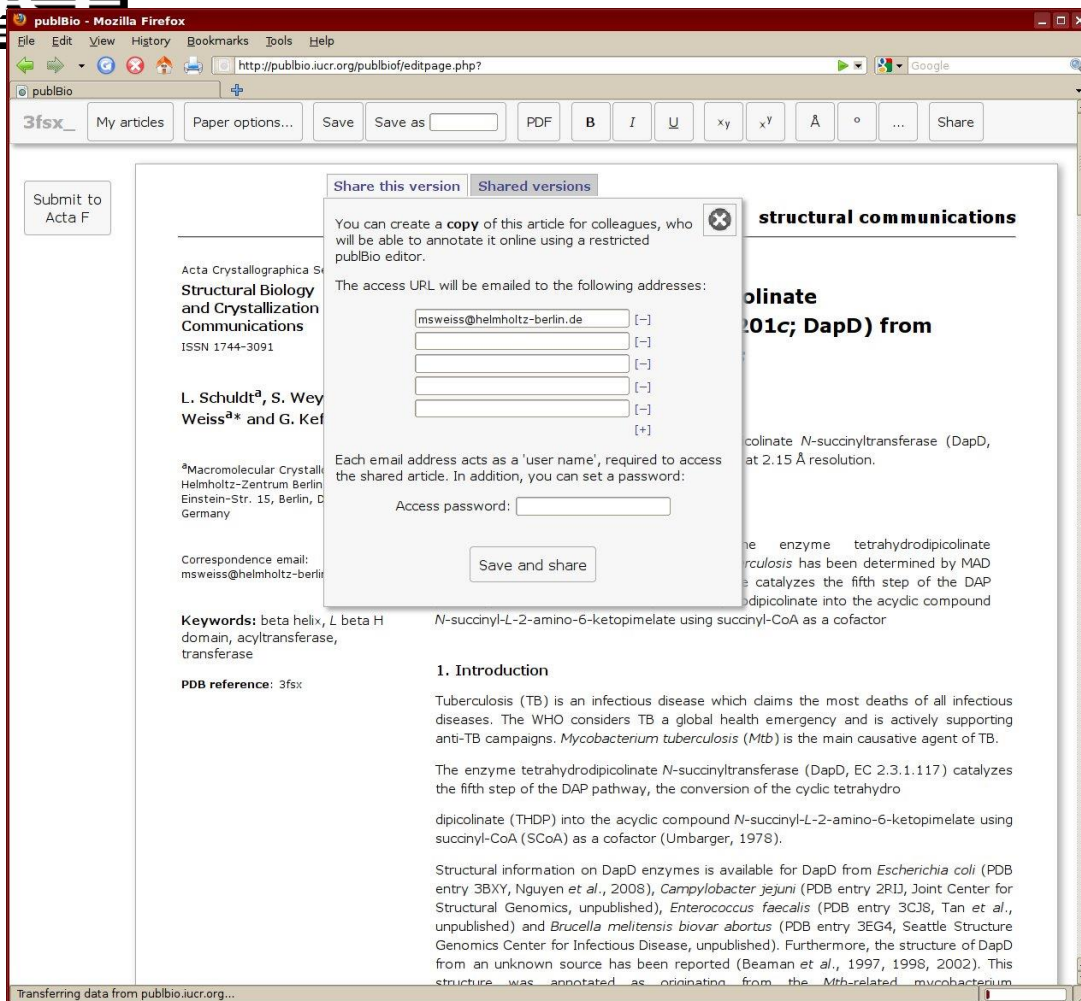
Tuberculosis (TB) is an infectious disease which claims the most deaths of all infectious diseases. The WHO considers TB a global health emergency and is actively supporting anti-TB campaigns. *Mycobacterium tuberculosis* (*Mtb*) is the main causative agent of TB.

The enzyme tetrahydridipicolinate *N*-succinyltransferase (DapD, EC 2.3.1.117) catalyzes the fifth step of the DAP pathway, the conversion of the cyclic tetrahydridipicolinate (THDP) into the acyclic compound *N*-succinyl-L-2-amino-6-ketopimelate using succinyl-CoA (SCoA) as a cofactor (Umbarger, 1978).

Structural information on DapD enzymes is available for DapD from *Escherichia coli* (PDB entry 3BXY, Nguyen *et al.*, 2008), *Campylobacter jejuni* (PDB entry 2RIJ, Joint Center for Structural Genomics, unpublished work), *Enterococcus faecalis* (PDB entry 3CJ8, Tan *et al.*, unpublished work) and *Brucella melitensis biovar abortus* (PDB entry 3EG4, Seattle Structure Genomics Center for Infectious Disease, unpublished work). Furthermore, the structure of DapD from an unknown source has been reported (Beaman *et al.*, 1997, 1998, 2002). This structure was annotated as originating from the *Mtb*-related

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Summary

- **Structured article types (CC, SC)**
- **Standard content**
- **Relevant information in tabular form**
- **Easy to work with**
- **Linked to IUCr submission system**



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People Involved

- Howard Einspahr (Acta F, IUCr)
- Louise Jones (IUCr)
- Janet Newman (CSIRO)
- John Westbrook (PDB)
- Simon Westrip (IUCr)



Thanks for your attention