



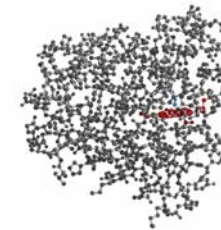
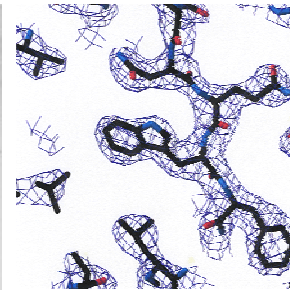
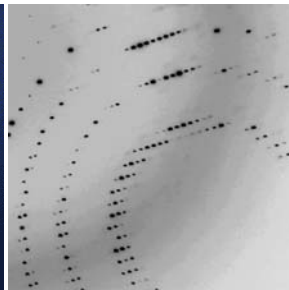
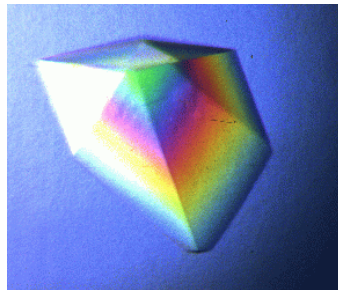
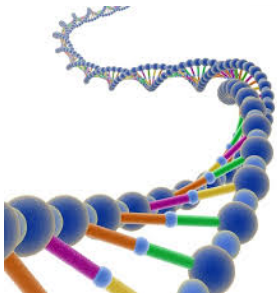
# Writing a Macromolecular Structure Paper with pubBio

**Manfred S. Weiss**

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# An MX-experiment



crystallization communications

Acta Crystallographica Section E  
Structural Biology  
and Crystallization  
Communications  
2010, 17(4), 2001

**Linda Schell, J. Simon  
Wey and D. Georgia Kotla<sup>a</sup> and  
Manfred S. Weiss<sup>b</sup>**

<sup>a</sup>1996 Max-Planck-Gesellschaft, 60528 Frankfurt, Germany  
<sup>b</sup>1996 Max-Planck-Gesellschaft, 60528 Frankfurt, Germany

**Tetrahydrodipicolinate-N-succinyltransferase from *Mycobacterium tuberculosis* (DapD, Rv1291c) has been cloned, heterologously expressed in *Escherichia coli*, purified using standard chromatographic techniques and crystallized in the cubic space group  $I23$  or  $I2_13$ . Preliminary diffraction data analysis indicates the presence of the molecule per asymmetric unit. Furthermore, the data exhibit noncrystallographic point-group symmetry. One possible explanation for this is that the enzyme assembles into a 60-mer exhibiting 232 point-group symmetry and crystallizes as such in space group  $I23$ . In this case, the combination of crystallographic and noncrystallographic symmetry elements results in an arrangement of the monomers in the cubic crystal with one partner in the asymmetric unit. Another explanation is that the packing of the molecules itself mimics icosahedral symmetry. In this case both space groups  $I23$  and  $I2_13$  would be possible.**

<sup>a</sup> 13 and 167 combined results for this work.  
<sup>b</sup> Present address: Max-Planck-Gesellschaft, South Kensington Campus, Fulham Road, London SW7 2AZ, England and Institute of Protein Sciences, University of Bonn, Heinrich Heine University Campus, China, Doherty, Schindlerstr. 0311, 53115, England.  
<sup>c</sup> Present address: NIH, Bethesda, 10815, South Camp Drive, Bethesda, MD, 20892, USA.

Correspondence should be addressed to: [manfred@helmholtz-berlin.de](mailto:manfred@helmholtz-berlin.de)

**1. Introduction**  
Tuberculosis is an airborne bacterial infection which is predominantly caused by *Mycobacterium tuberculosis* (Mtb). Every year, around ten million people worldwide are newly infected with this disease and



# 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
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  - ⇒ **Most relevant information in tabular form**
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**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

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DNA source

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

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

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

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

**PDB reference:** 3fsx

**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.

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Source Mycobacterium tuberculosis (strain: H37Rv)

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data in the mmCIF or  
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Structure and Crystallography

ISSN 1520-4851

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Primary contact author for this submission

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Germany,  
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the source organism, the res.

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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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 Schuldt *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	MAVSTVTGAAGIGLATLAADGSVLDTWFPAPELTESGTSATSRLAVSDVPVELAALIGRDDDRRTETIAVRTVIGSLDDV AADPYDAYLRLLHLLSHRLVAPHGLNAGGLFGLTNVWWTNHGPCAIDGFEAVRARLRRRGPVTVYGVDFPRMVDYVPT GVRADADRVRLLGAHLAPGTTVMHEGFVNYNAGTLGASMVEGRISAGVAVGDSVGGASIMGTLGGGTHMISIGKPC LLGANSGLGISLGDCCVVEAGLYVTAGTRVTMPDSNSVKARELSGSSNLLFRNNSVSGAVEVLARDGGQIALNEDLHANG VPRGLEHHHHHH

### 2.2. Crystallization

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

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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.

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**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 <i>R</i> <sub>cryst</sub>	0.168 (0.199)
Final <i>R</i> <sub>free</sub>	0.220 (0.232)
Cruickshank DPI	
No. of non-H atoms	
Protein	10866
Ion	<b><u>13</u></b>
Ligand	<b><u>40</u></b>
Water	570
Total	11489
R.m.s. deviations	
Bonds (Å)	0.019
Angles (°)	1.724
Average <i>B</i> factors (Å <sup>2</sup> )	
Protein	<b><u>30.2</u></b>
Ion	<b><u>44.7</u></b>
Ligand	<b><u>38.0</u></b>
Water	<b><u>29.4</u></b>
Ramachandran plot	
Favoured regions (%)	97.8
Additionally allowed (%)	1.8
Outliers (%)	0.3

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calculated from data  
in the mmCIF

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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

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. Mg<sup>2+</sup> and Na<sup>+</sup> 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  
Structural Biology and Crystallization Communications  
ISSN 1744-3091

L. Schultd<sup>a</sup> and Manfred Weiss<sup>a\*</sup>

<sup>a</sup>Macromolecular Crystallography (HZB-MX), Helmholtz-Zentrum Berlin, Albert-Einstein-Str. 15, Berlin, D-12489, Germany

Correspondence email: msweiss@helmholtz-berlin.de

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

**PDB reference:** 3fsx

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

**Synopsis**

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

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

L. Schuldt<sup>a</sup>, S. Wey  
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Correspondence email:  
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**Keywords:** beta helix, L beta H domain, acyltransferase, transferase

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**structural communications**

Acta Crystallographica Section F  
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ISSN 1744-3091

L. Schultd<sup>a</sup> and Manfred Weiss<sup>a\*</sup>

<sup>a</sup>Macromolecular Crystallography (HZB-MX), Helmholtz-Zentrum Berlin, Albert-Einstein-Str. 15, Berlin, D-12489, Germany

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- **Louise Jones (IUCr)**
- **Janet Newman (CSIRO)**
- **John Westbrook (PDB)**
- **Simon Westrip (IUCr)**



**Thanks for your attention**