Writing a Macromolecular Structure Paper with publBio

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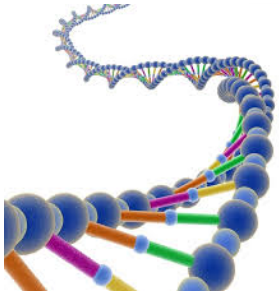
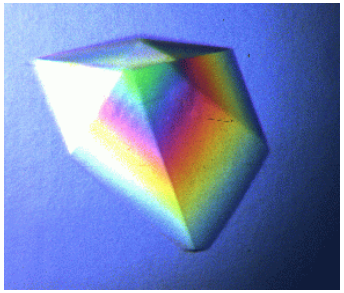
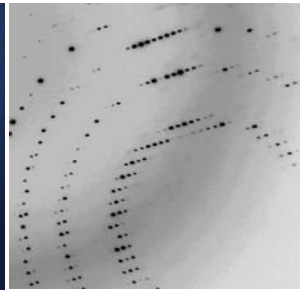
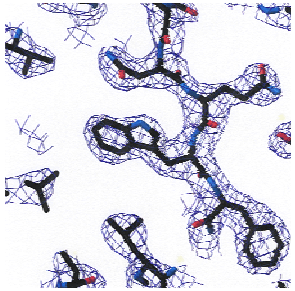
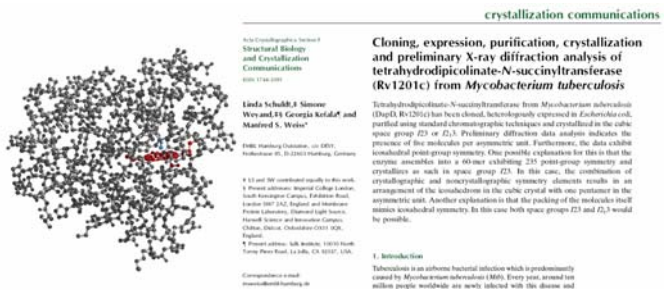
An MX-experiment







crystallization communications

Structural Biology and Crystallization Communications

Cloning, expression, purification, crystallization and preliminary X-ray diffraction analysis of tetrahydrodipicolinate-*N*-succinyltransferase (Rv1201c) from *Mycobacterium tuberculosis*

Linda Schuldt,‡ Simone Weyand,‡‡ Georgia Kefala,* and Manfred S. Weiss*

1. Introduction

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- capture at least some of the unpublished structures in the PDB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

http://publbio.iucr.org

a tool for editing mmcifs

- publBio annotator
- publBio publisher

a tool for writing and submitting articles

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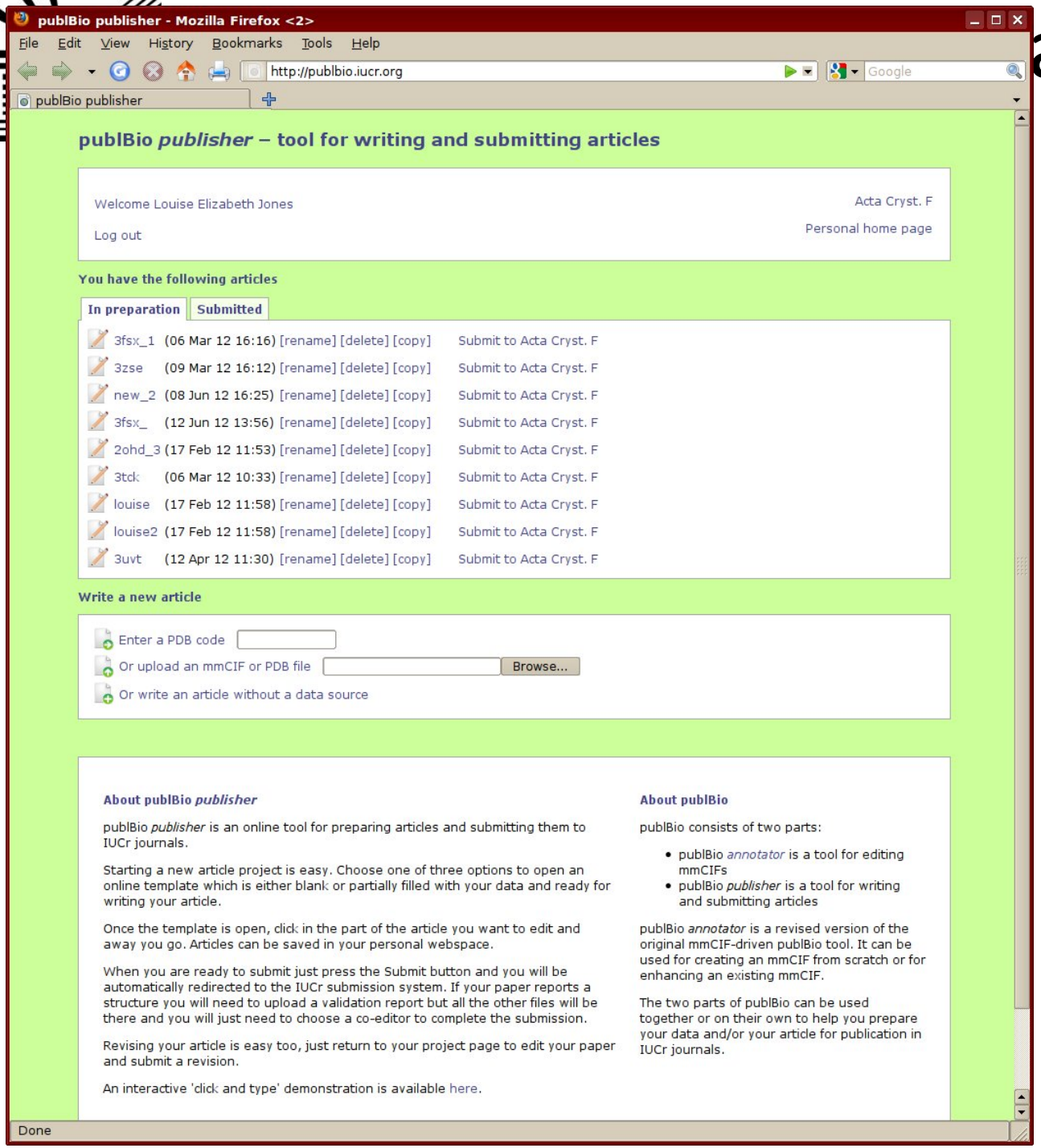
arted



use an annotation project

or

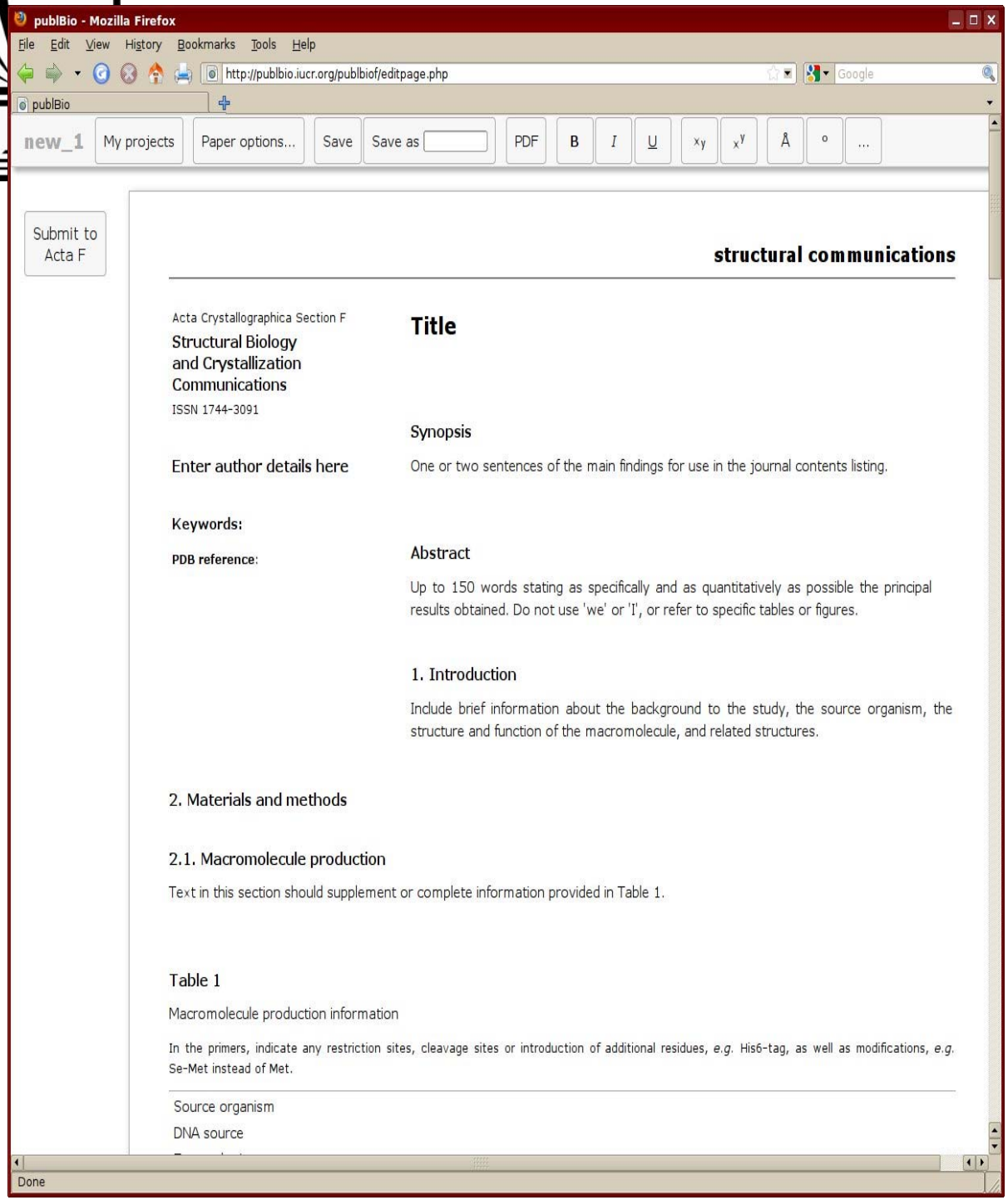
enter a PDB code

or

upload an mmCIF

or

start from scratch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File Edit View History Bookmarks Tools Help
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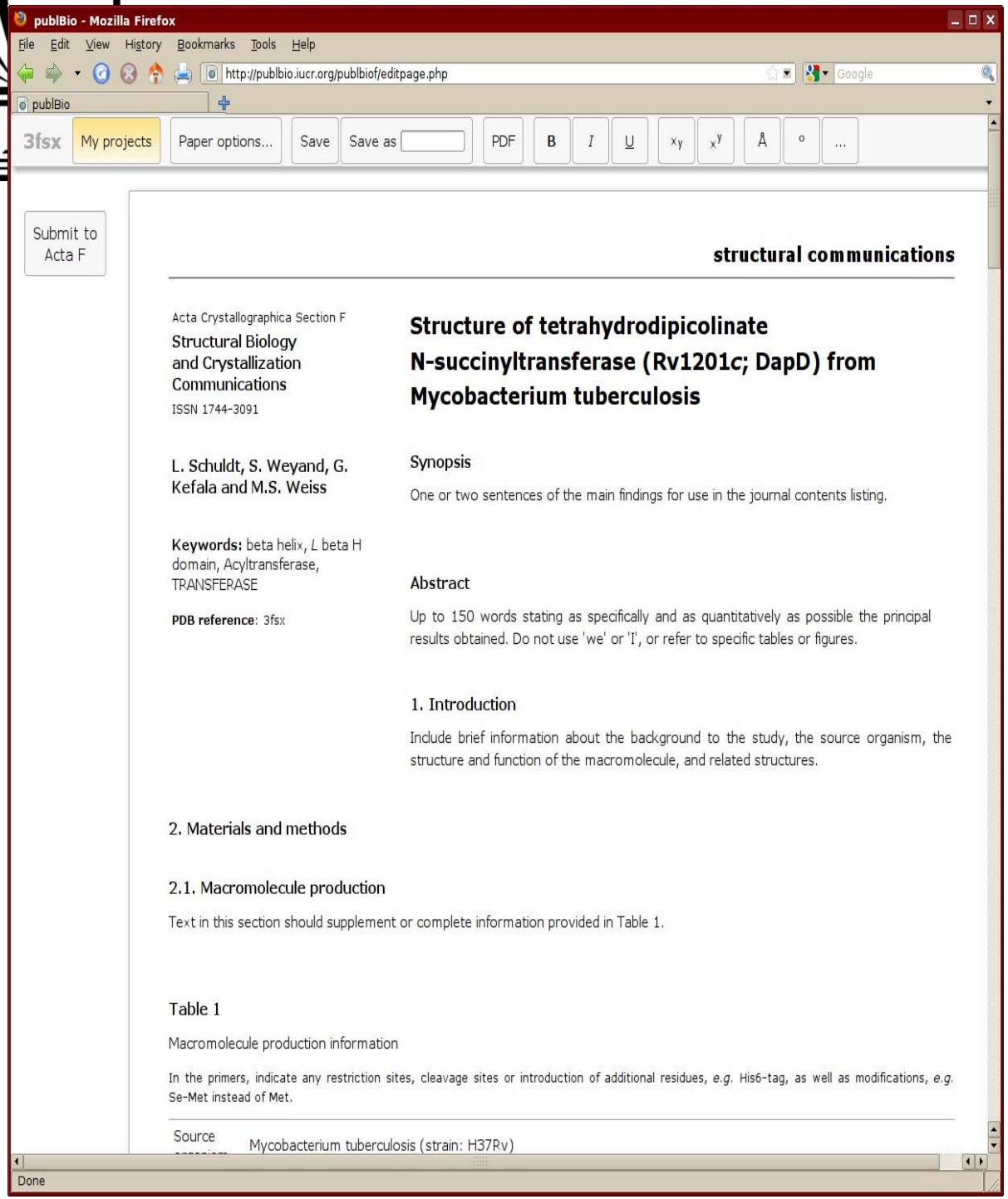
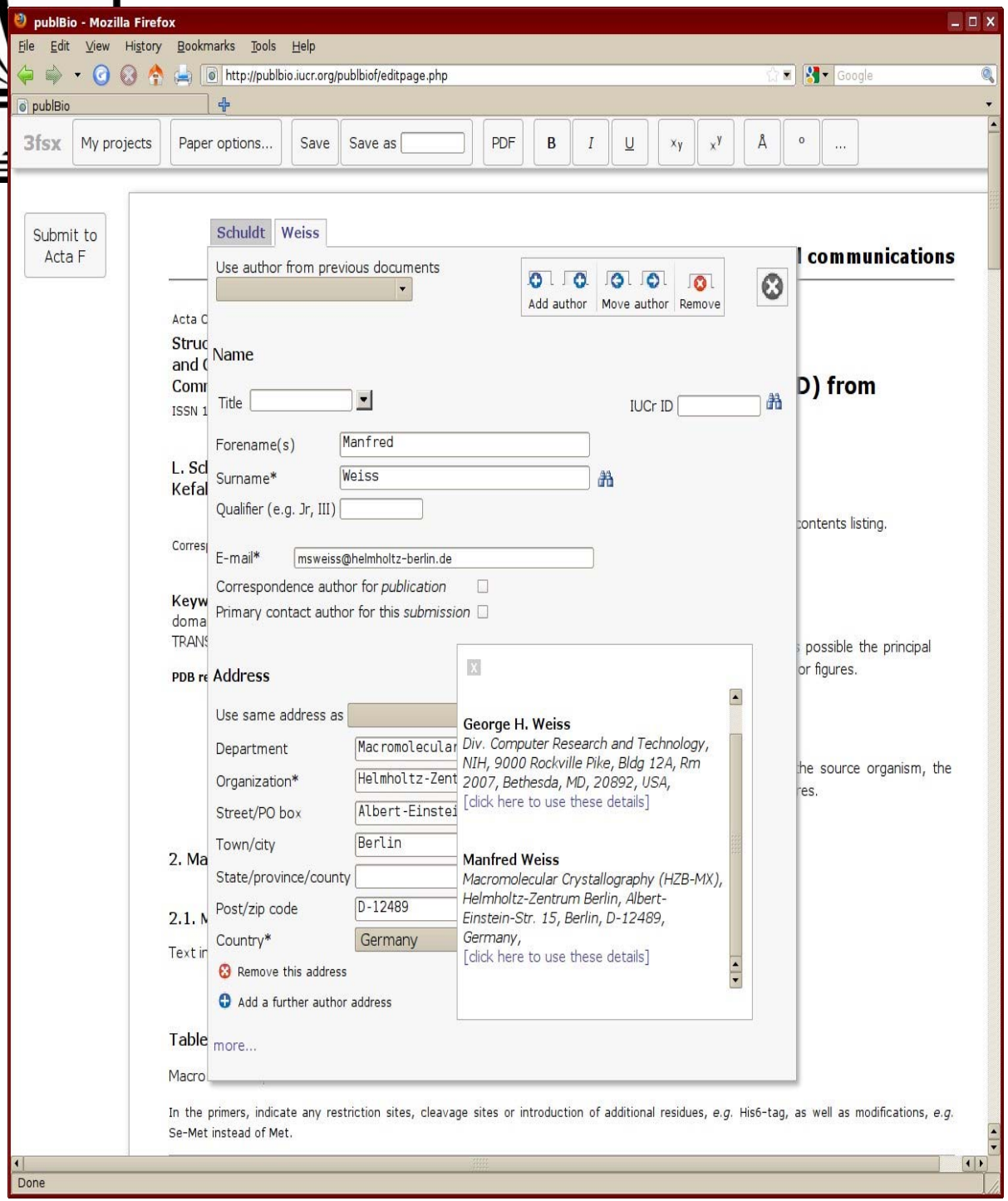
Save as
PDF
Submit to Acta F
structural communications
Acta Crystallographica Section F
Structural Biology and Crystallization Communications
ISSN 1744-3091
Enter author details here
Keywords:
PDB reference:
Title
Synopsis
One or two sentences of the main findings for use in the journal contents listing.
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
Done



details are added from data in the mmCIF or annotation project

click anywhere in the text to start to edit

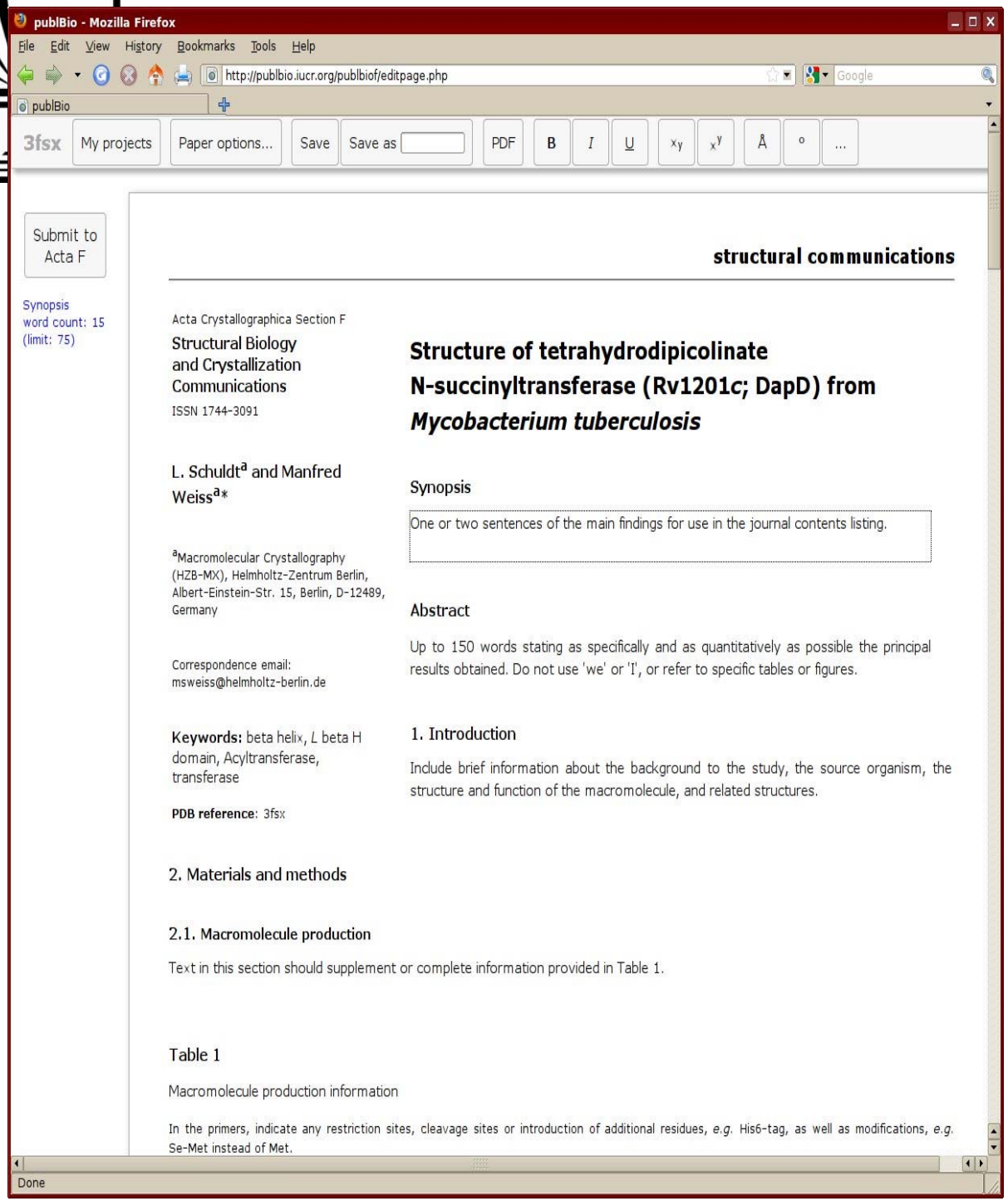


click to edit the author details

search for details using a surname or IUCr-ID

retrieve author details from the WDC

Click on the search results to add an author to the article

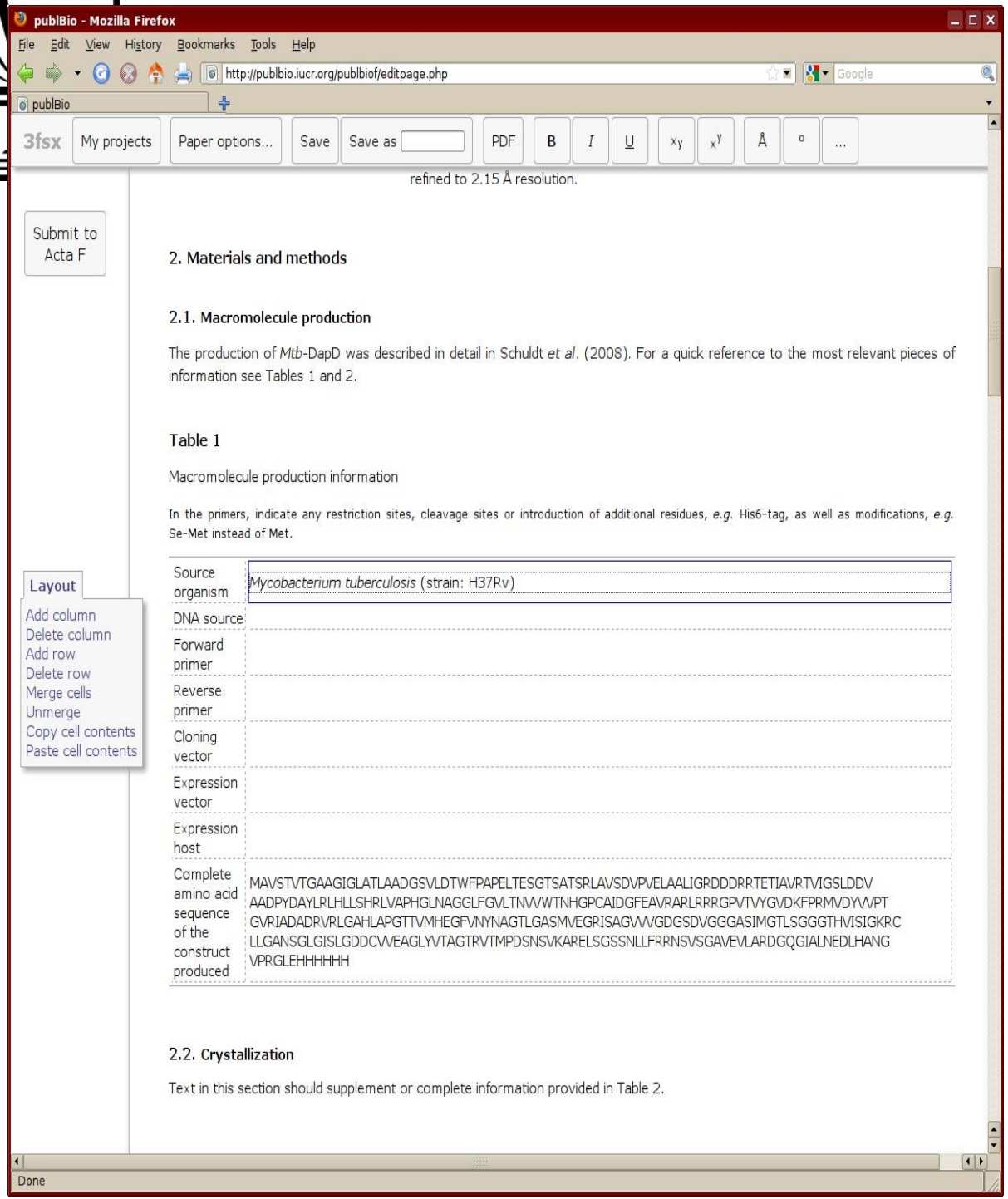


just click to start to edit the text

each section gives a description of what is required

publBio maintains a record of the word count for each section

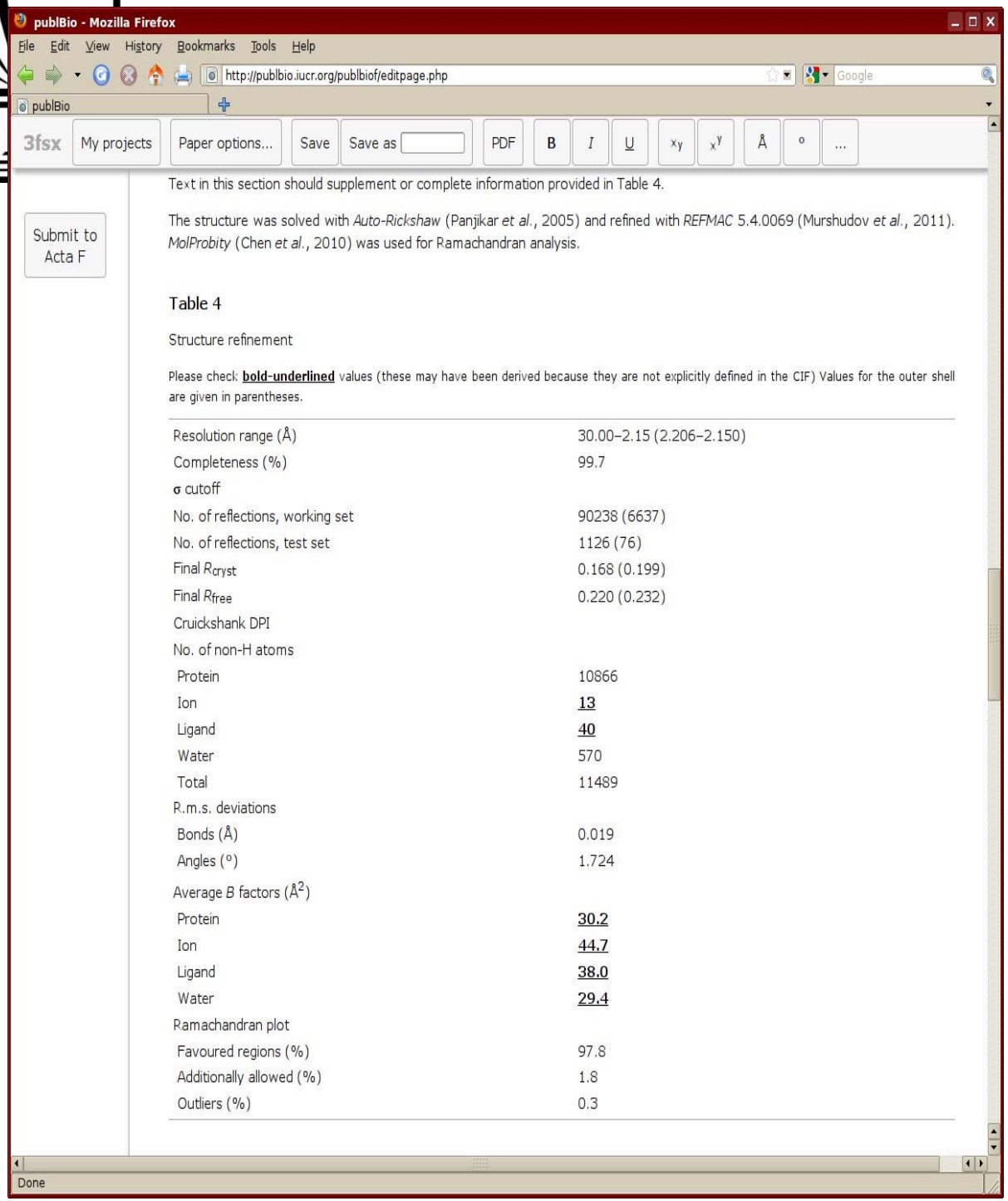
if the word count is ex-ceeded a warning appears



tables are prefilled from data in the mmCIF or annotation project

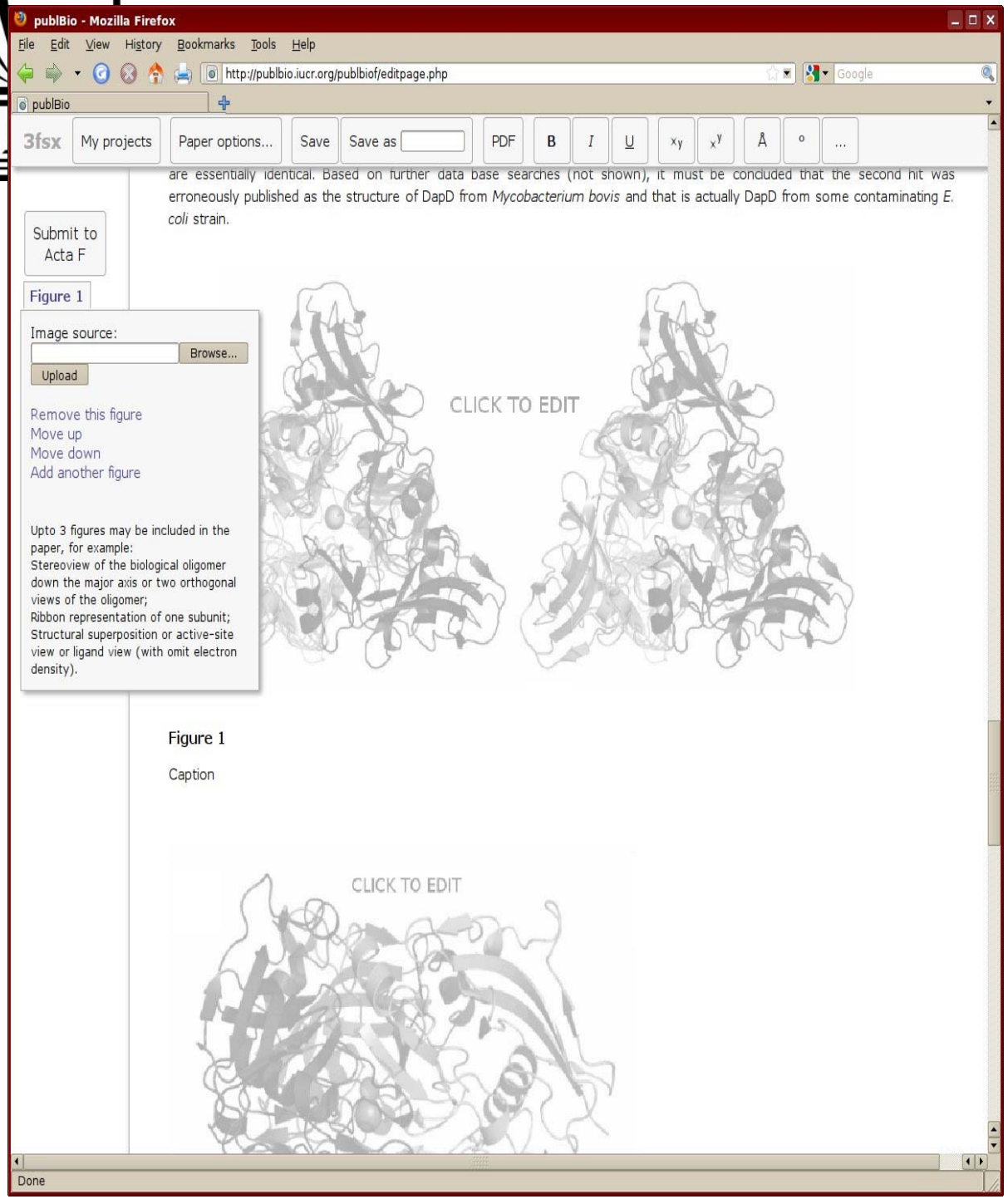
clicking in a table gives a simple table editor

the content and layout of the table can be altered



some values are calculated from data in the mmCIF

bold underlined values should be checked carefully



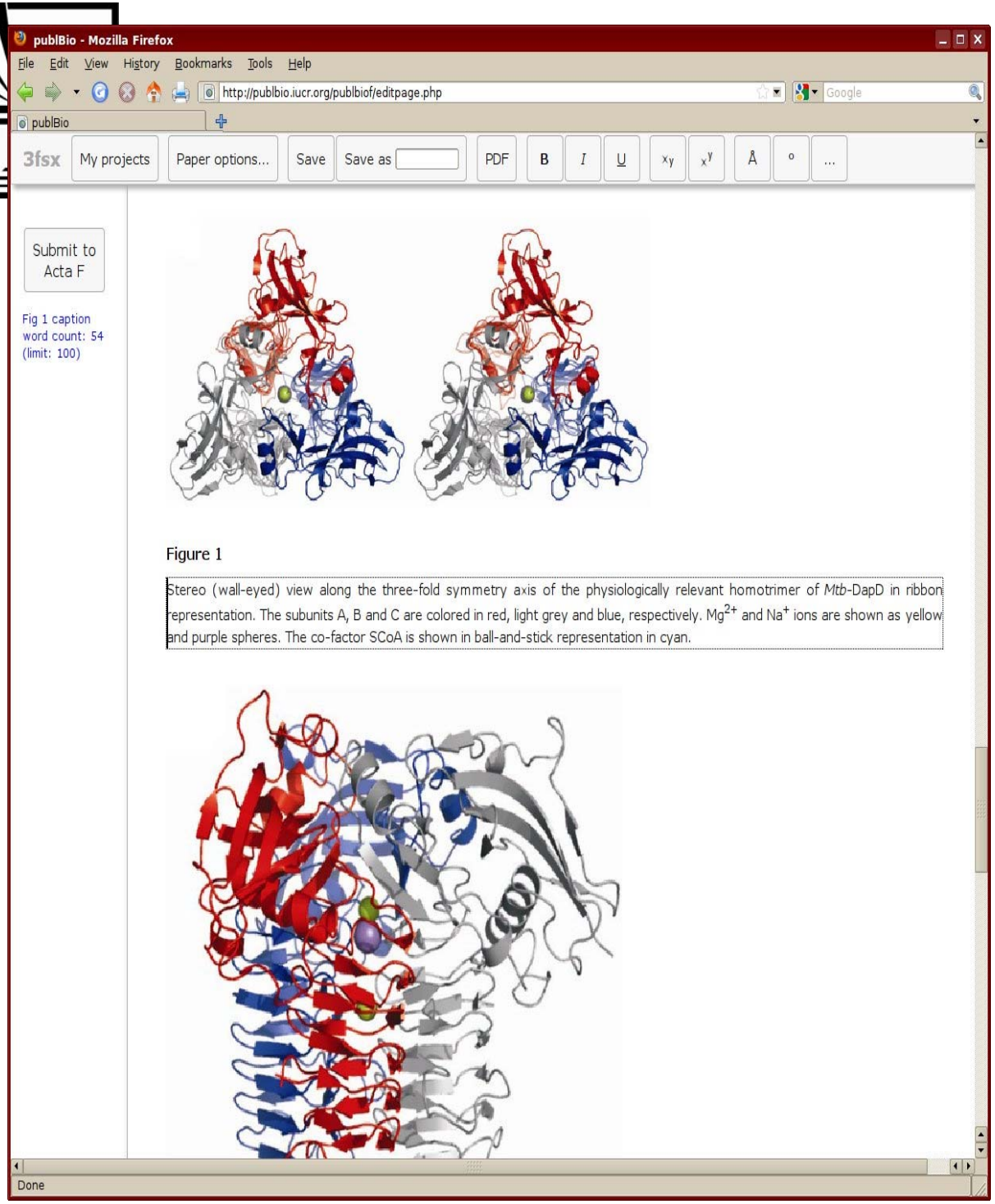
clicking on a figure gives some simple options

upload or remove a figure

change where the figure appears

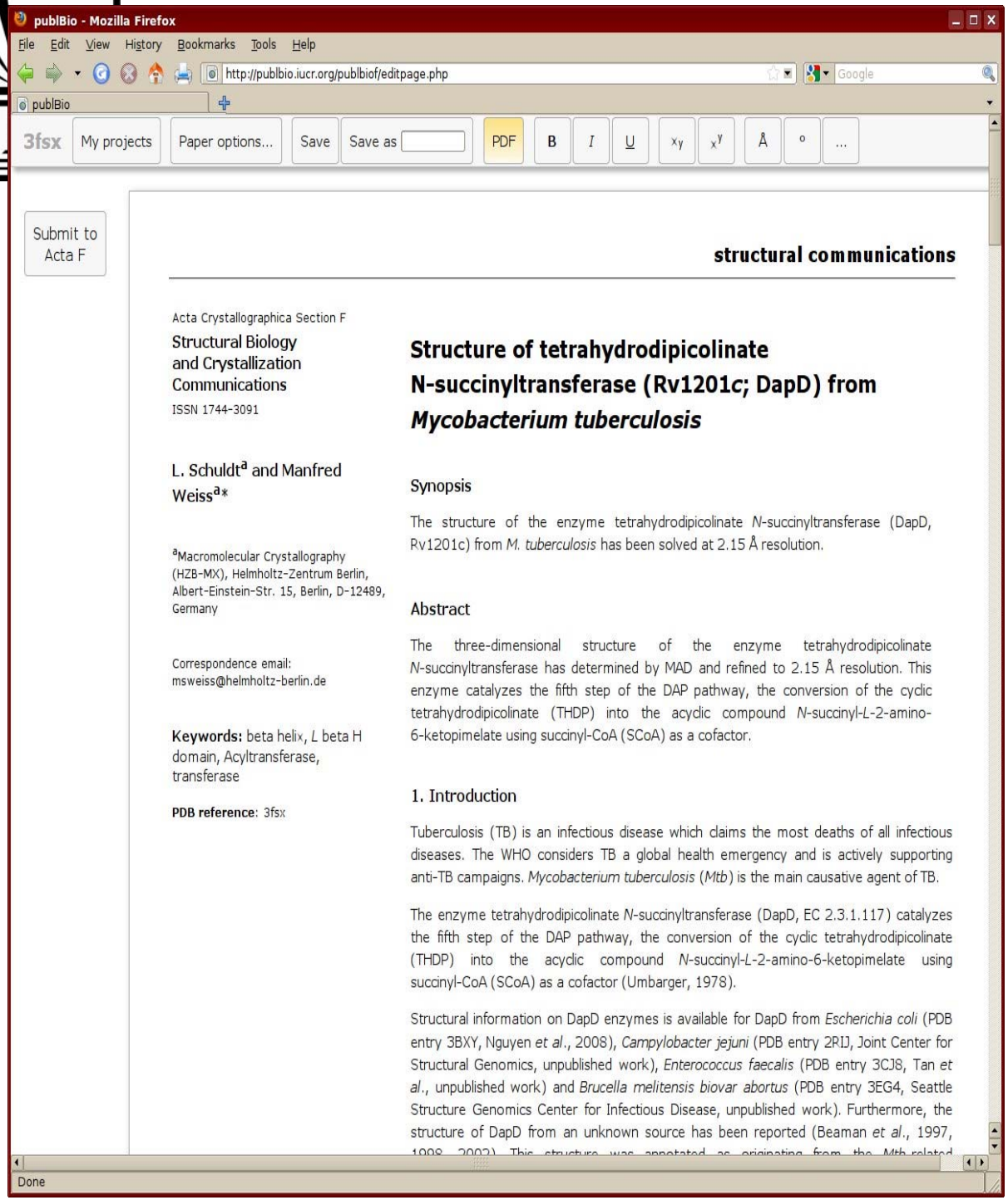
add another figure

suggestions are provided for types of figures

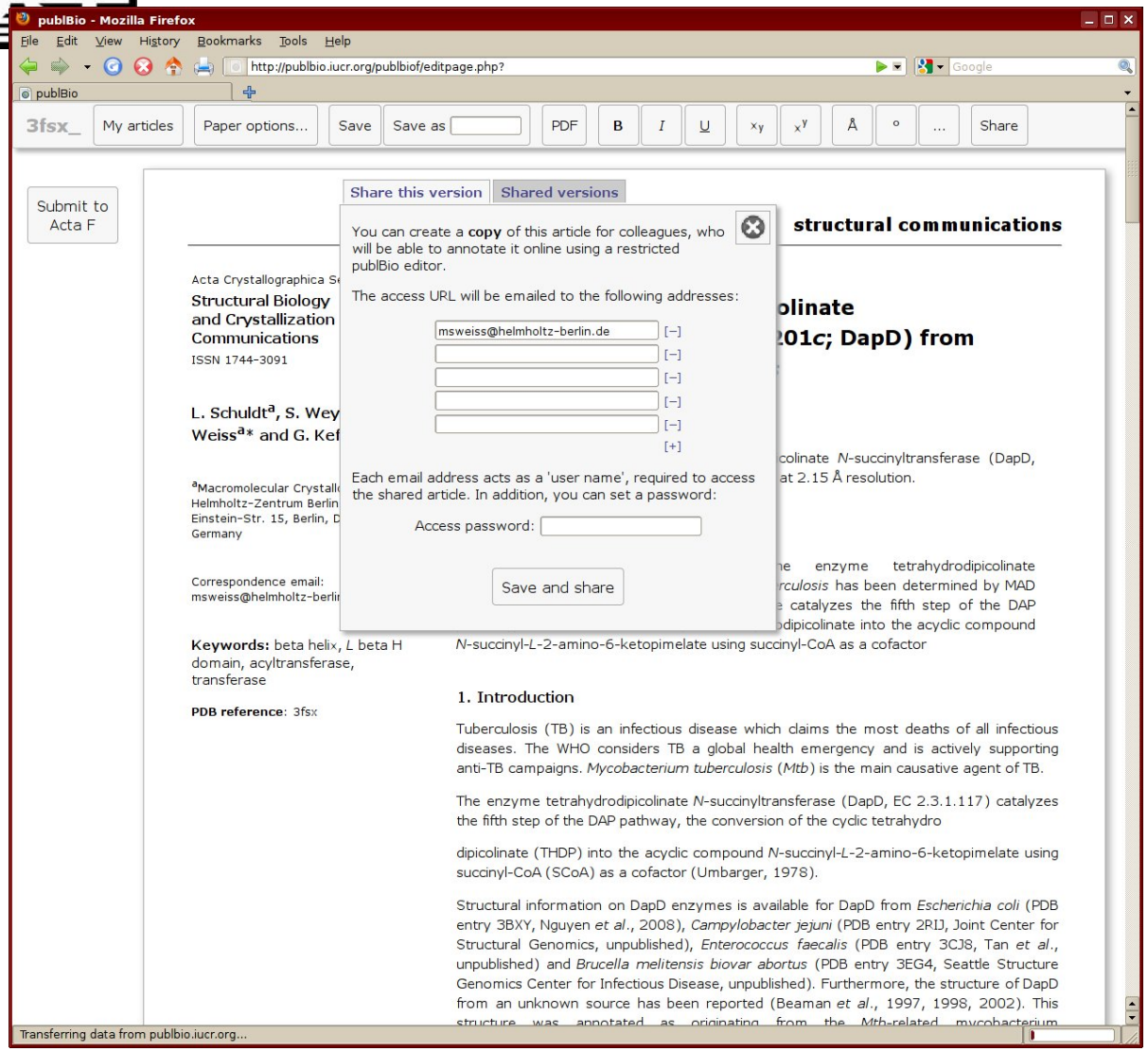


captions can be added to the figures

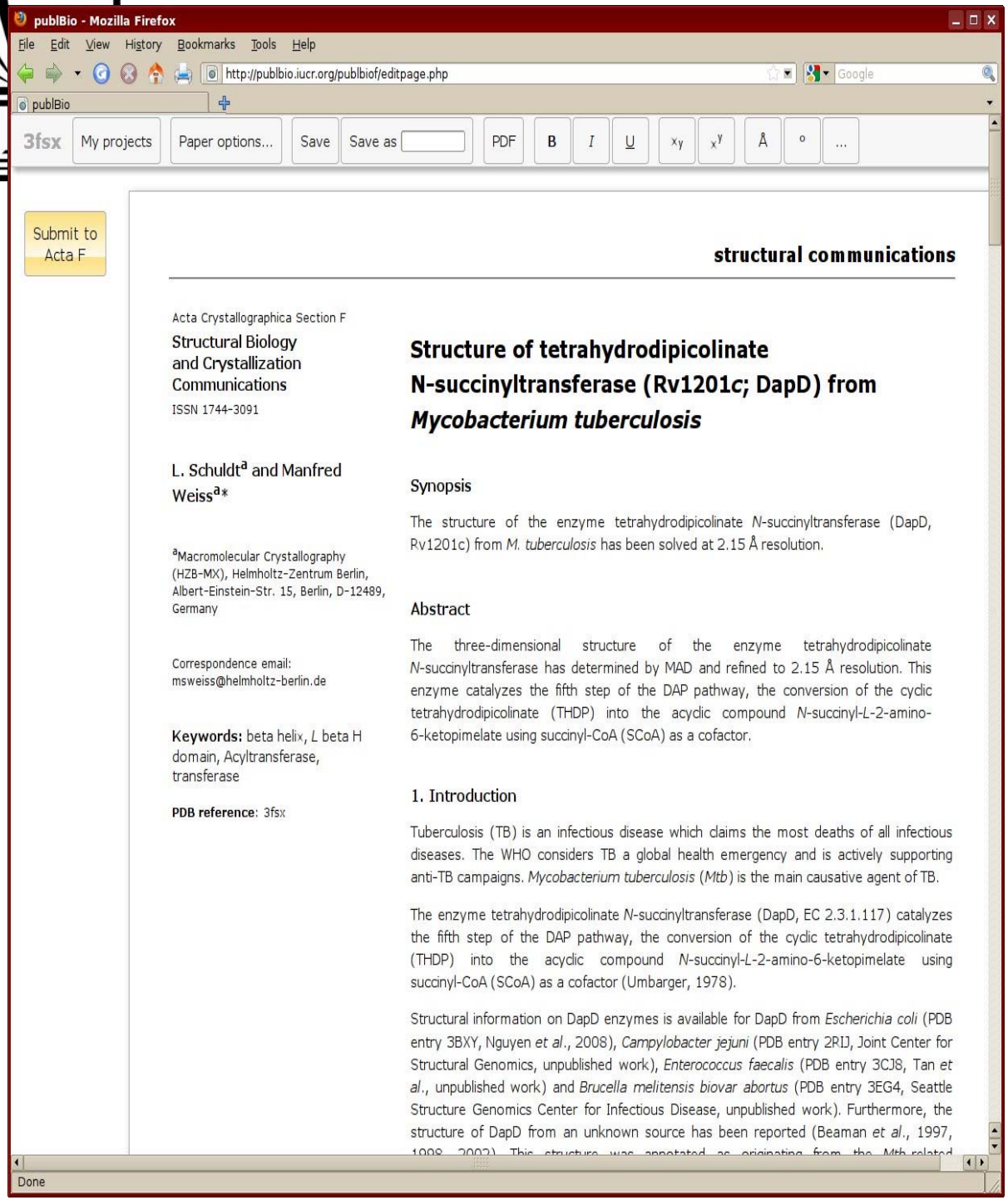
up to three figures are allowed



to view your article a PDF can be created using the PDF button



projects can be shared with colleagues (co-authors)



articles can be submitted to *Acta Cryst. F* directly from within publBio

Summary

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

Try it out …

HZB Helmholtz Zentrum Berlin

http://publbio.iucr.org

People Involved

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

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Thanks for your attention