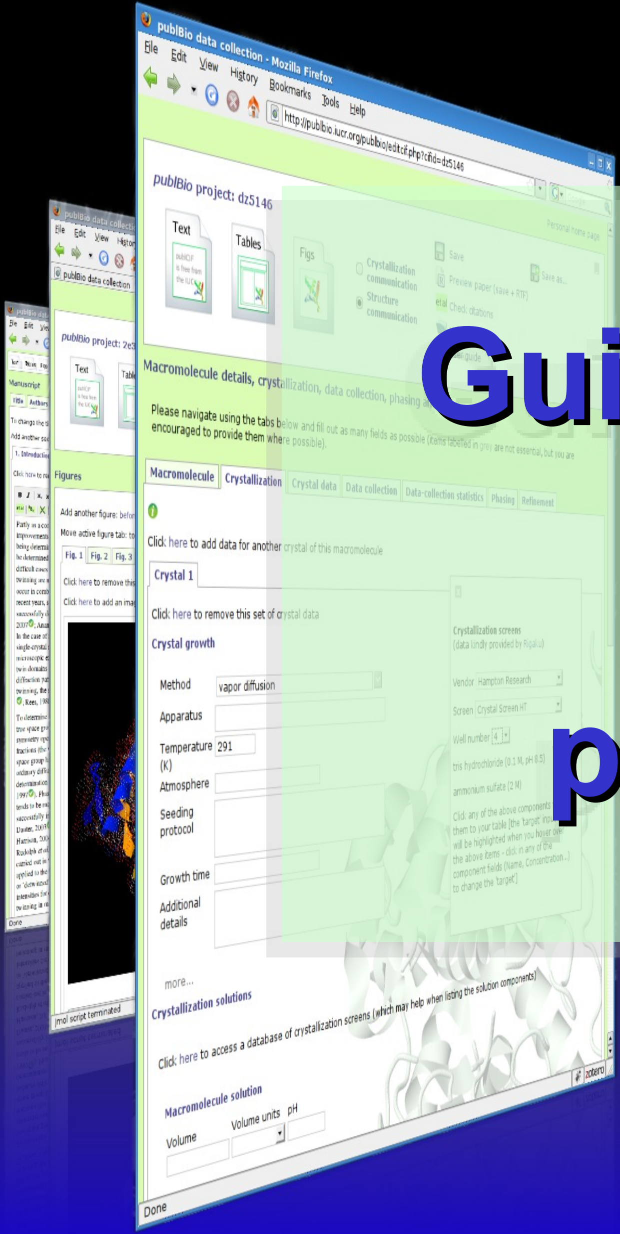

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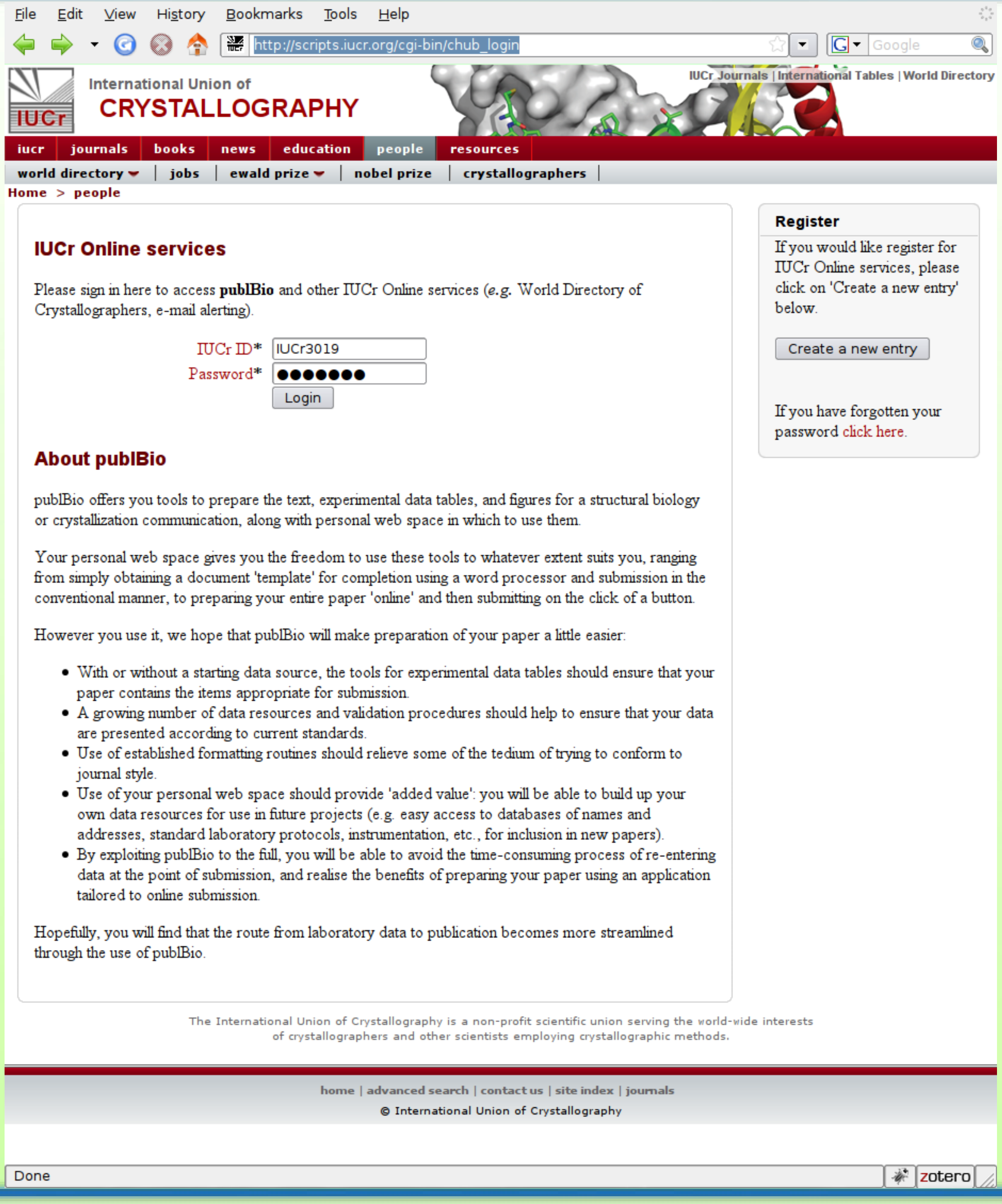

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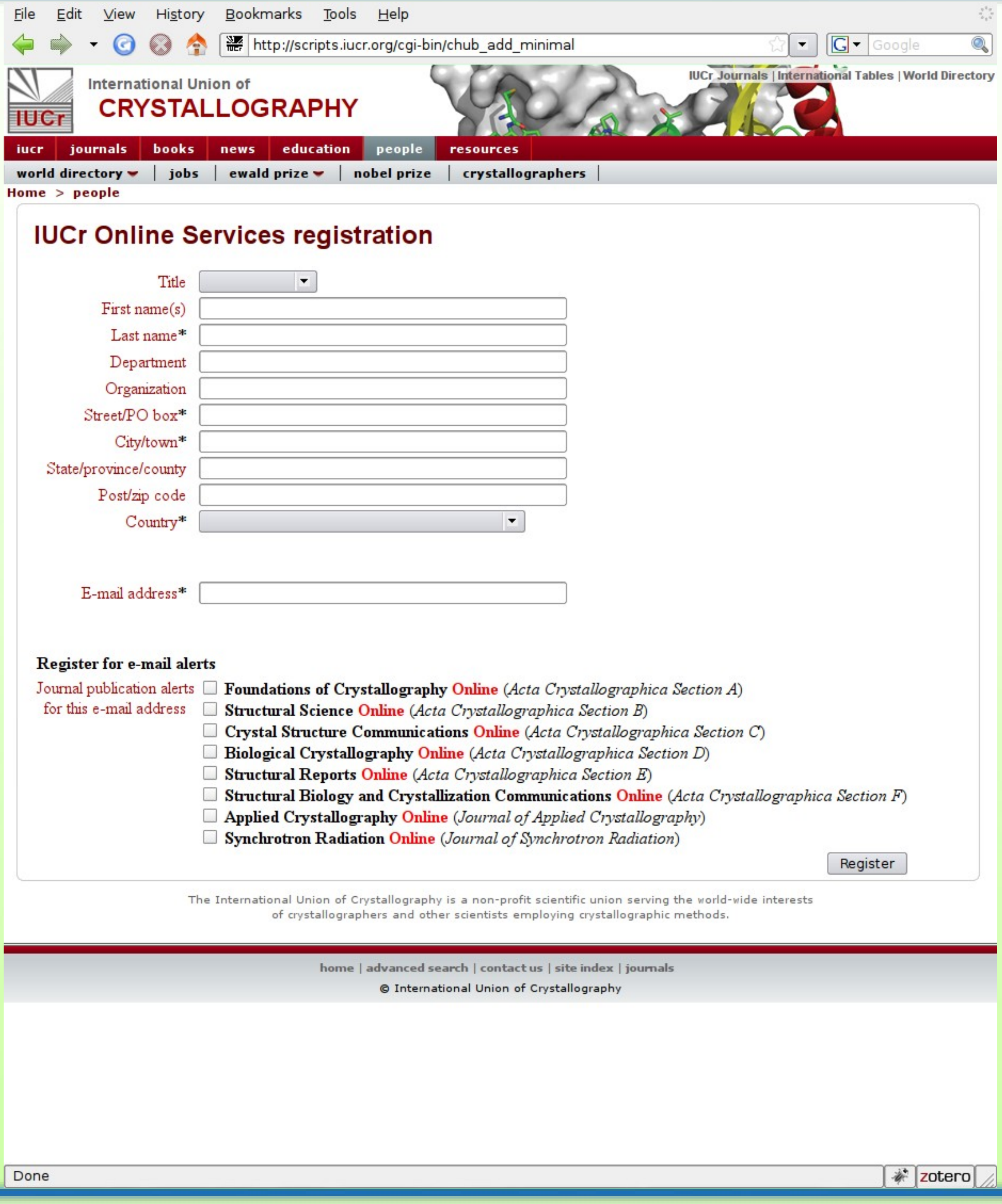

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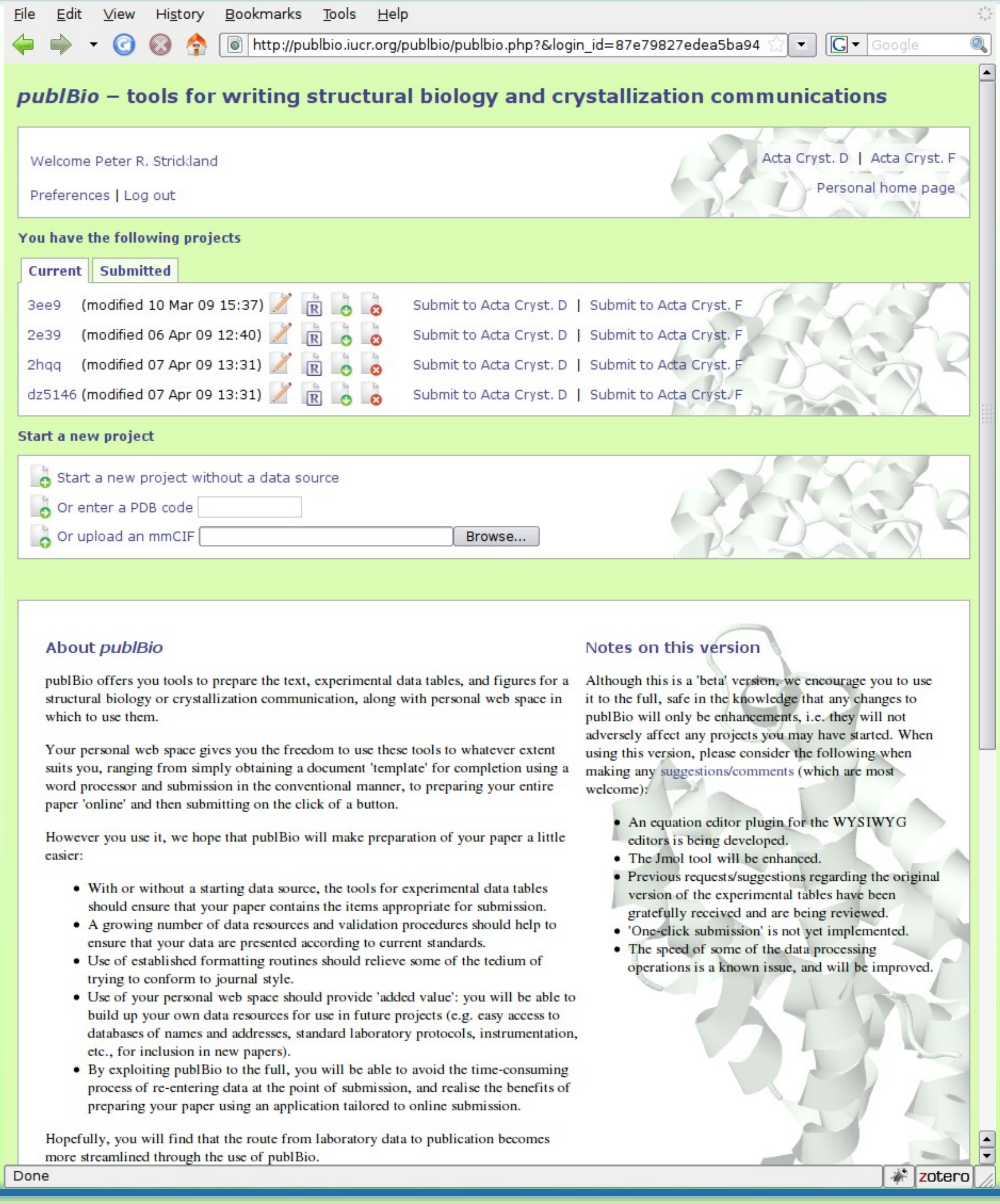

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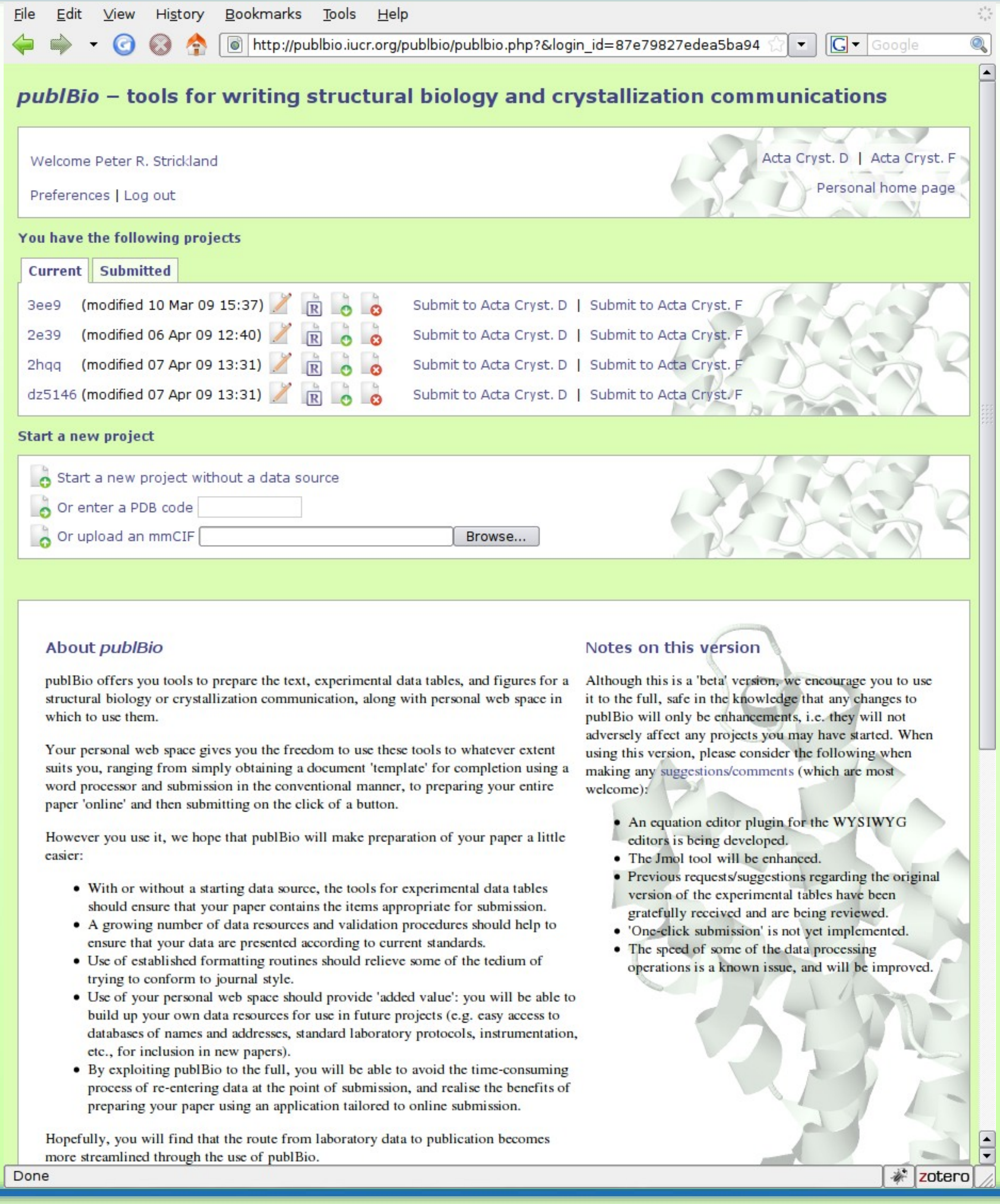

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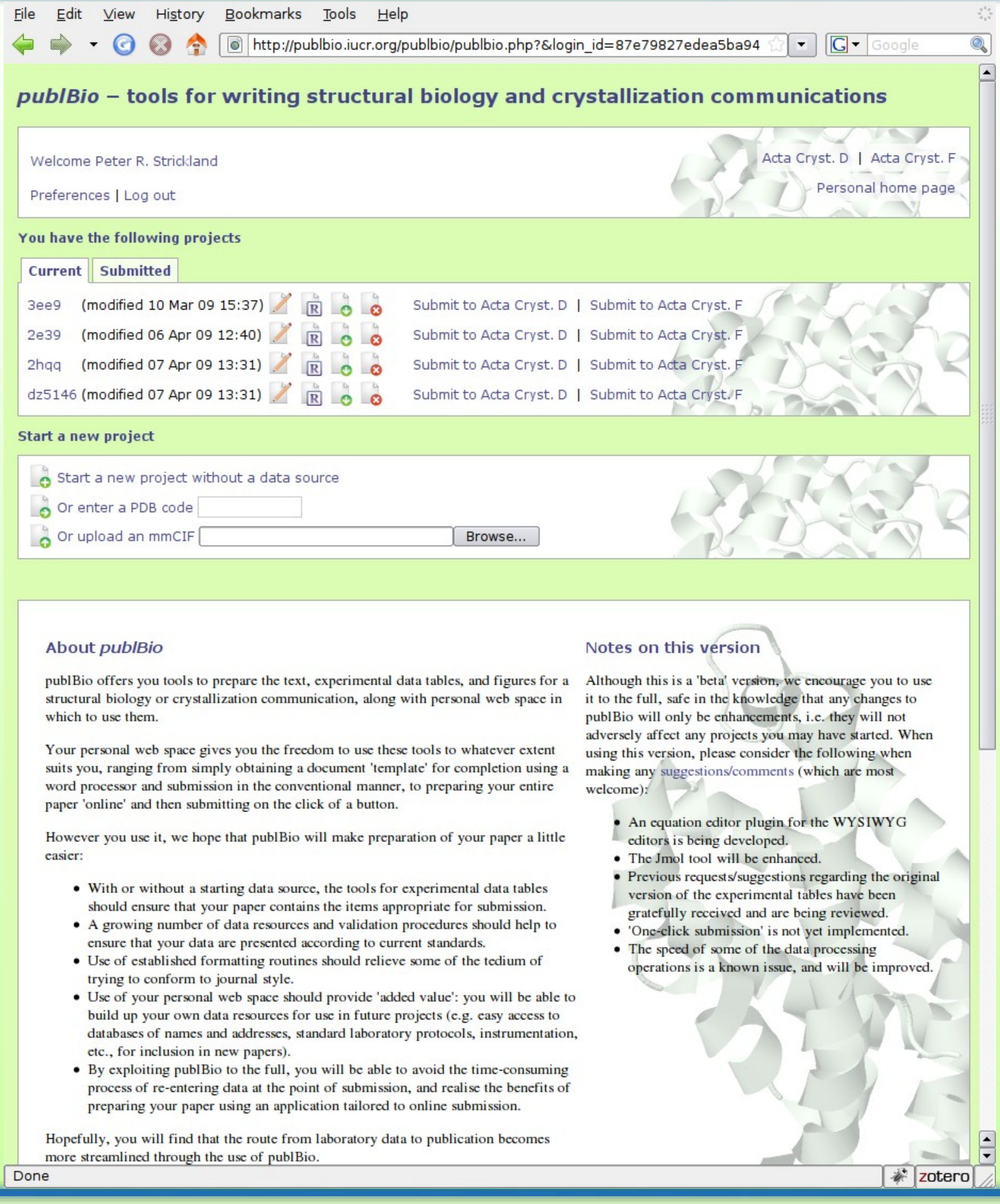

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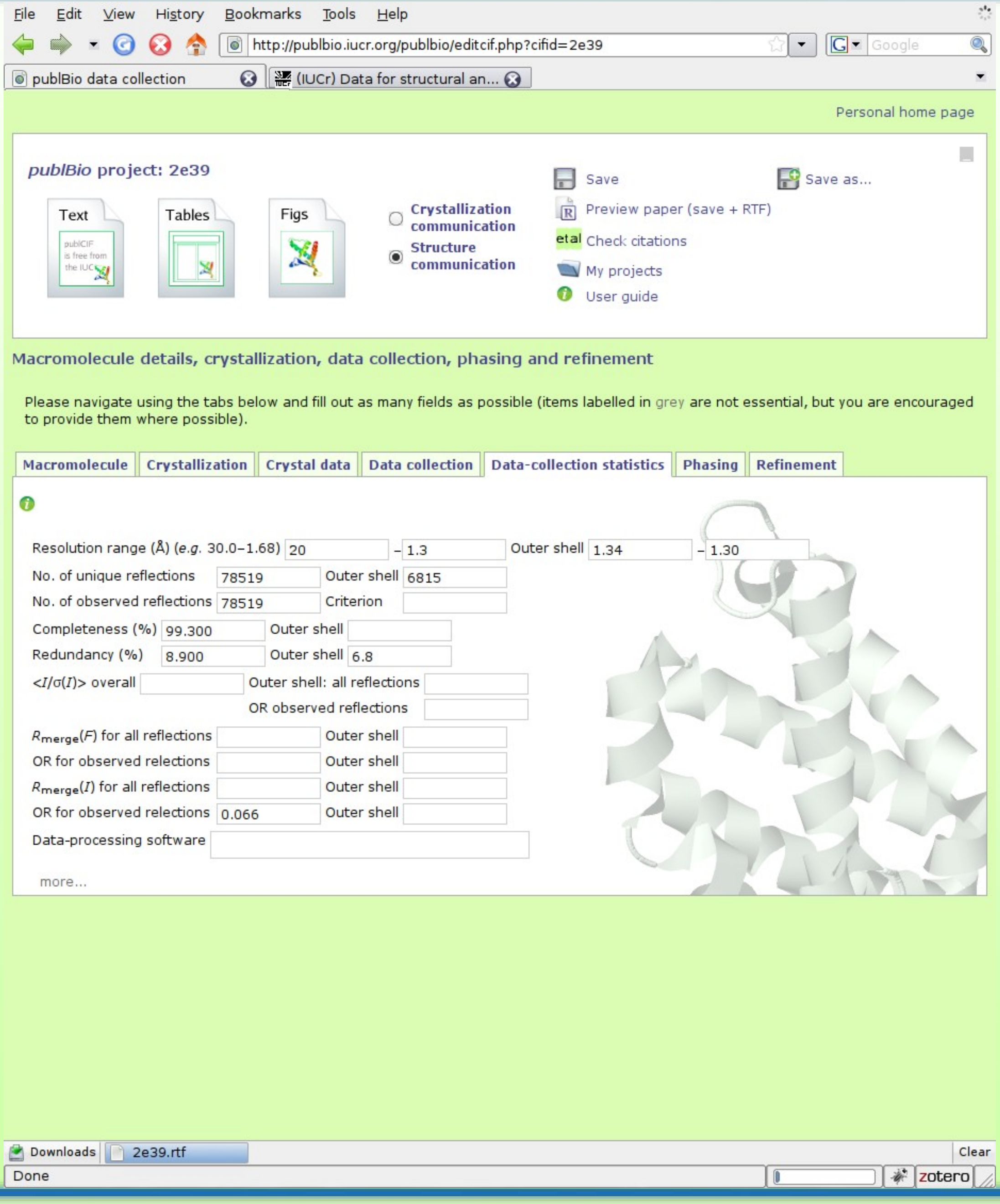

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No. of unique reflections 78519 Outer shell 6815
No. of observed reflections 78519 Criterion
Completeness (%) 99.300 Outer shell
Redundancy (%) 8.900 Outer shell 6.8
$<I/\sigma(I)>$ overall Outer shell: all reflections
OR observed reflections
$R_{merge}(F)$ for all reflections Outer shell
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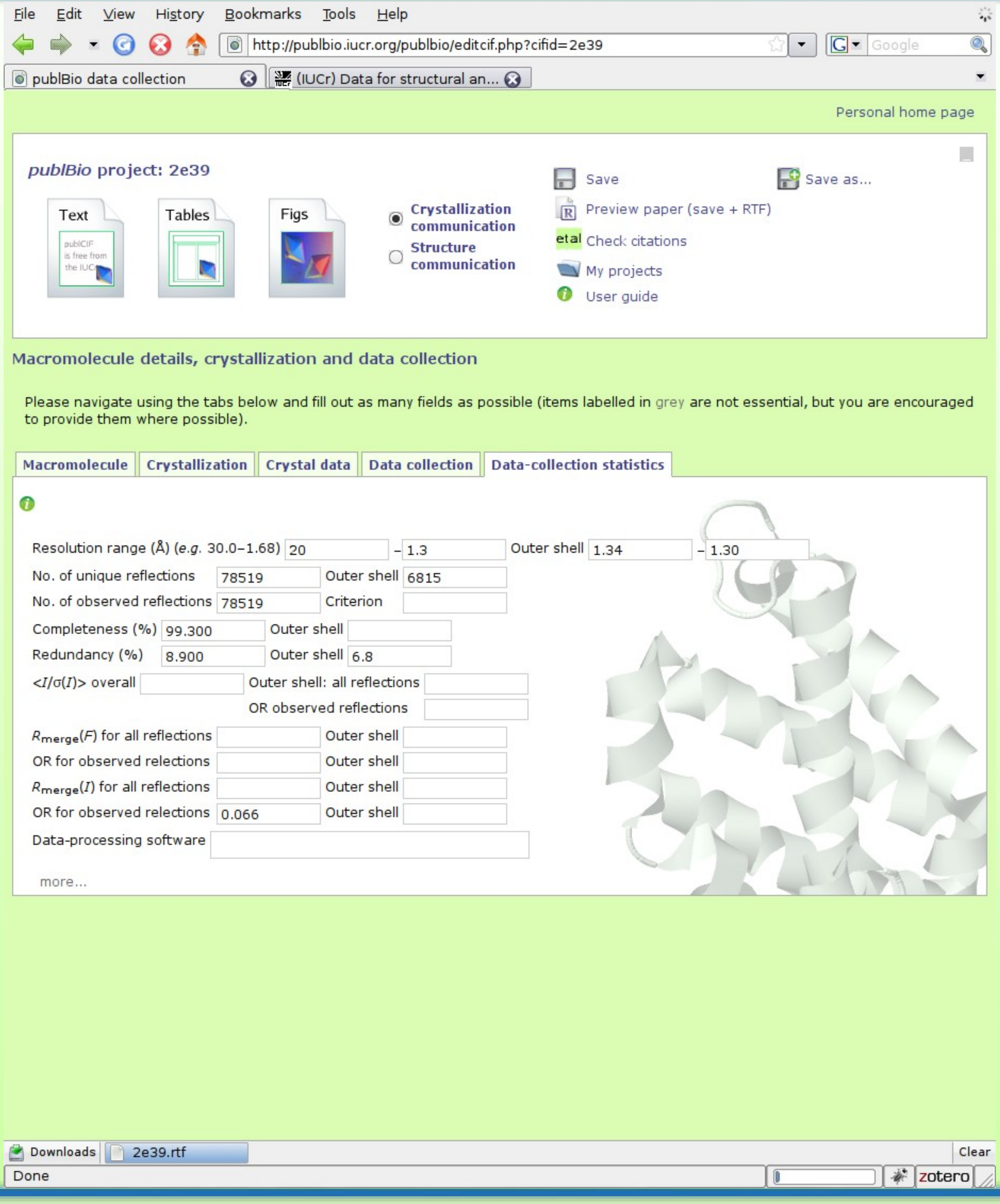

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No. of observed reflections 78519 Criterion

Completeness (%) 99.300 Outer shell

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$<I/\sigma(I)>$ overall Outer shell: all reflections

OR observed reflections

$R_{\rm merge}(F)$ for all reflections Outer shell

OR for observed relections Outer shell

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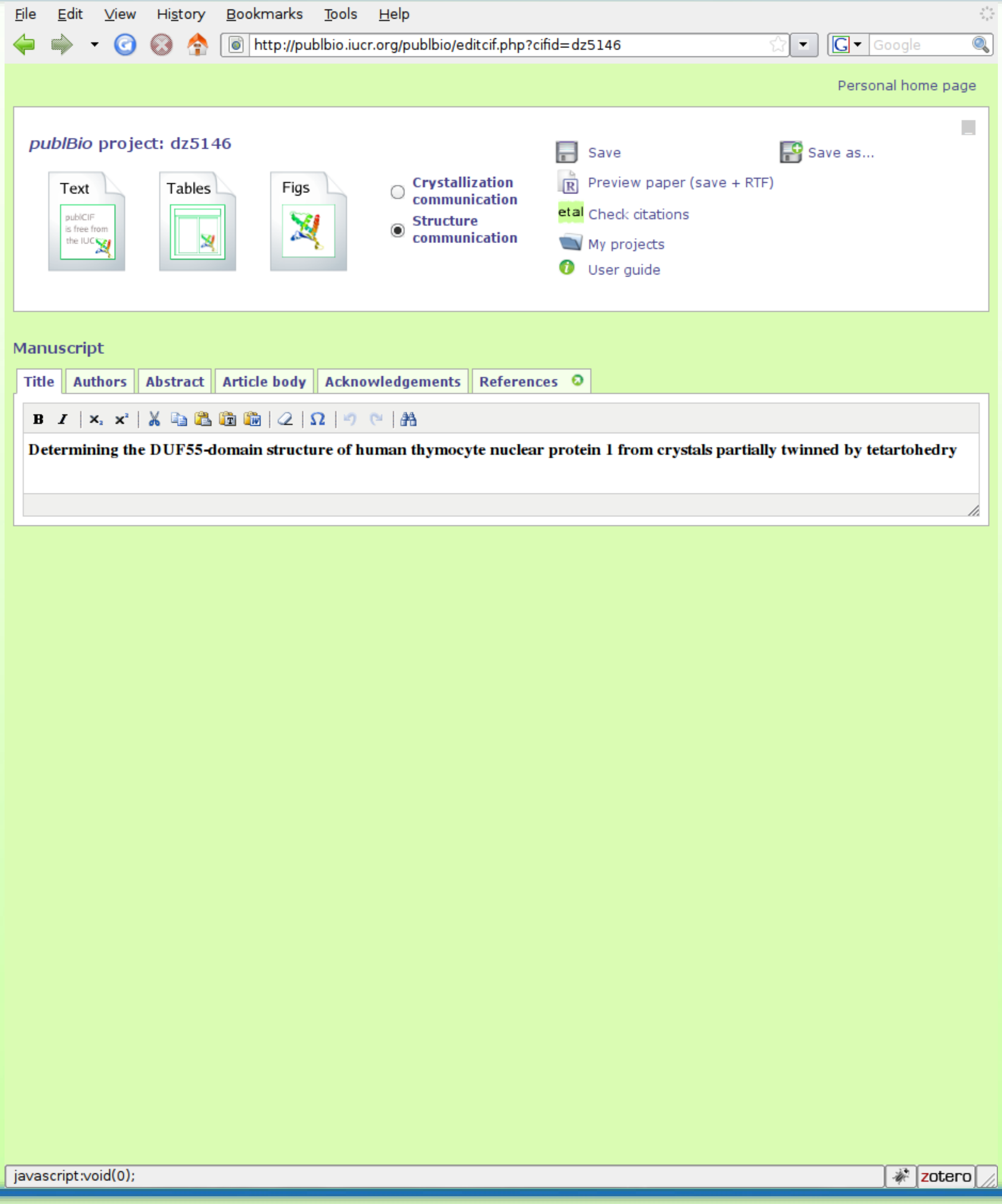

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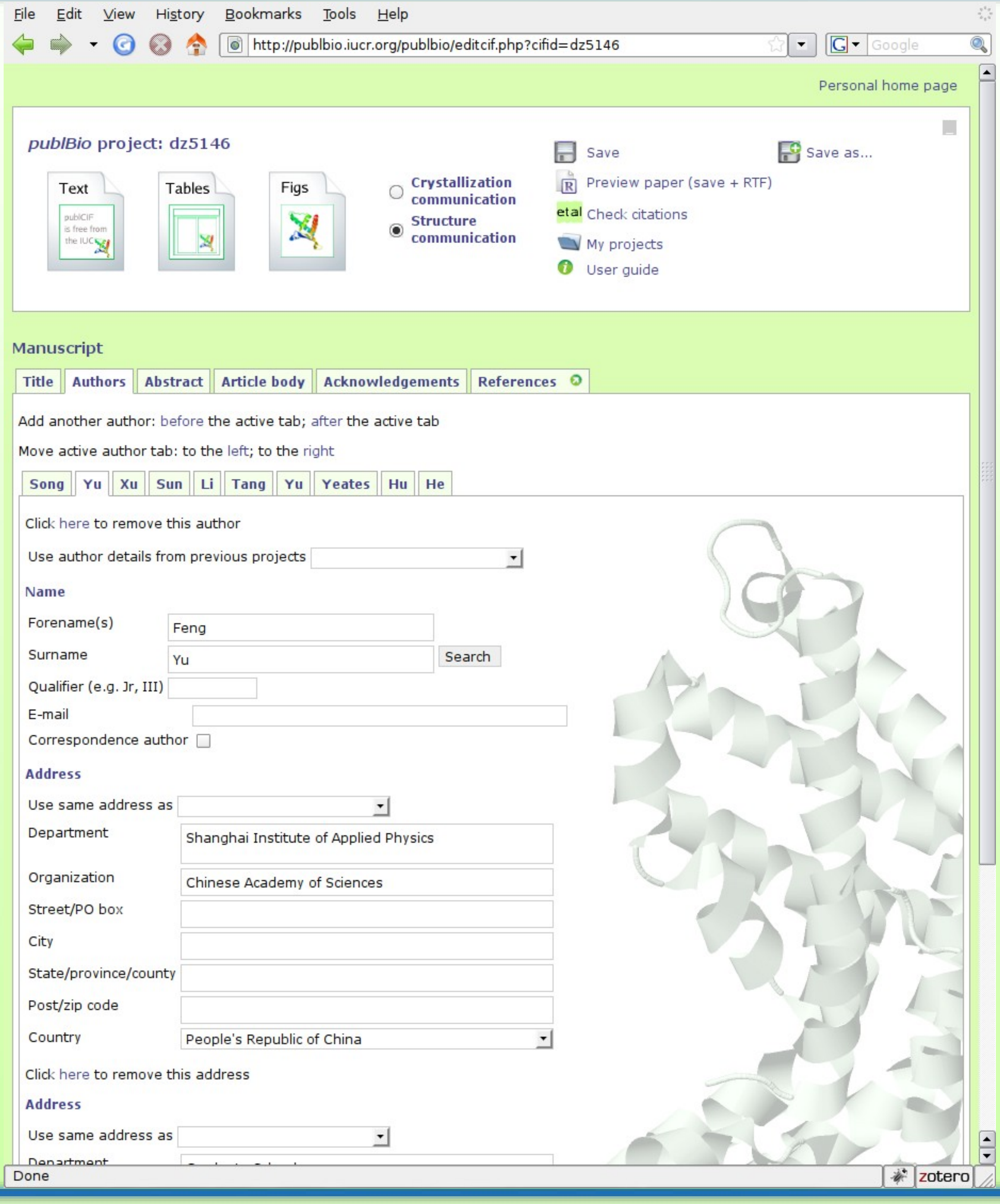

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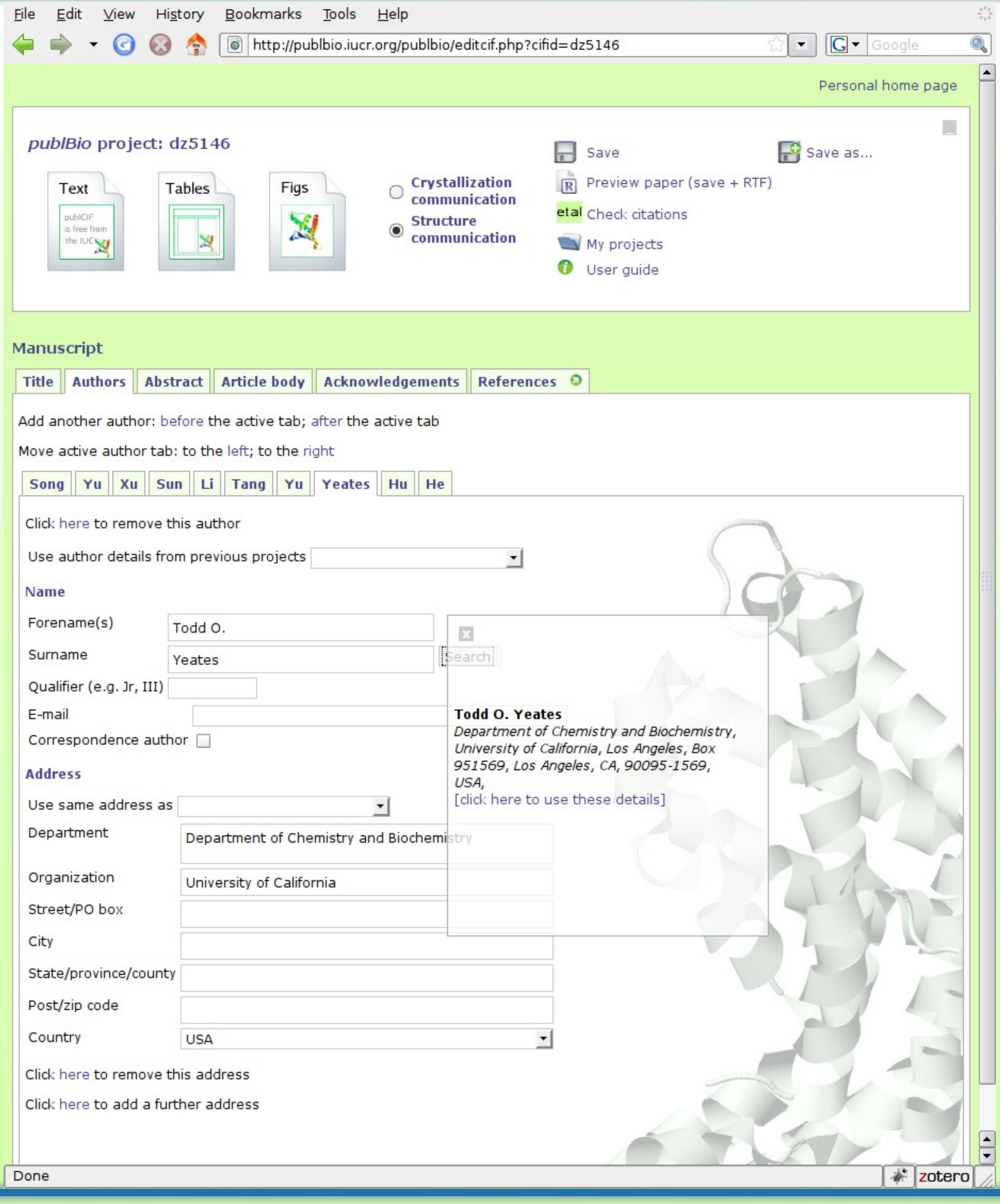

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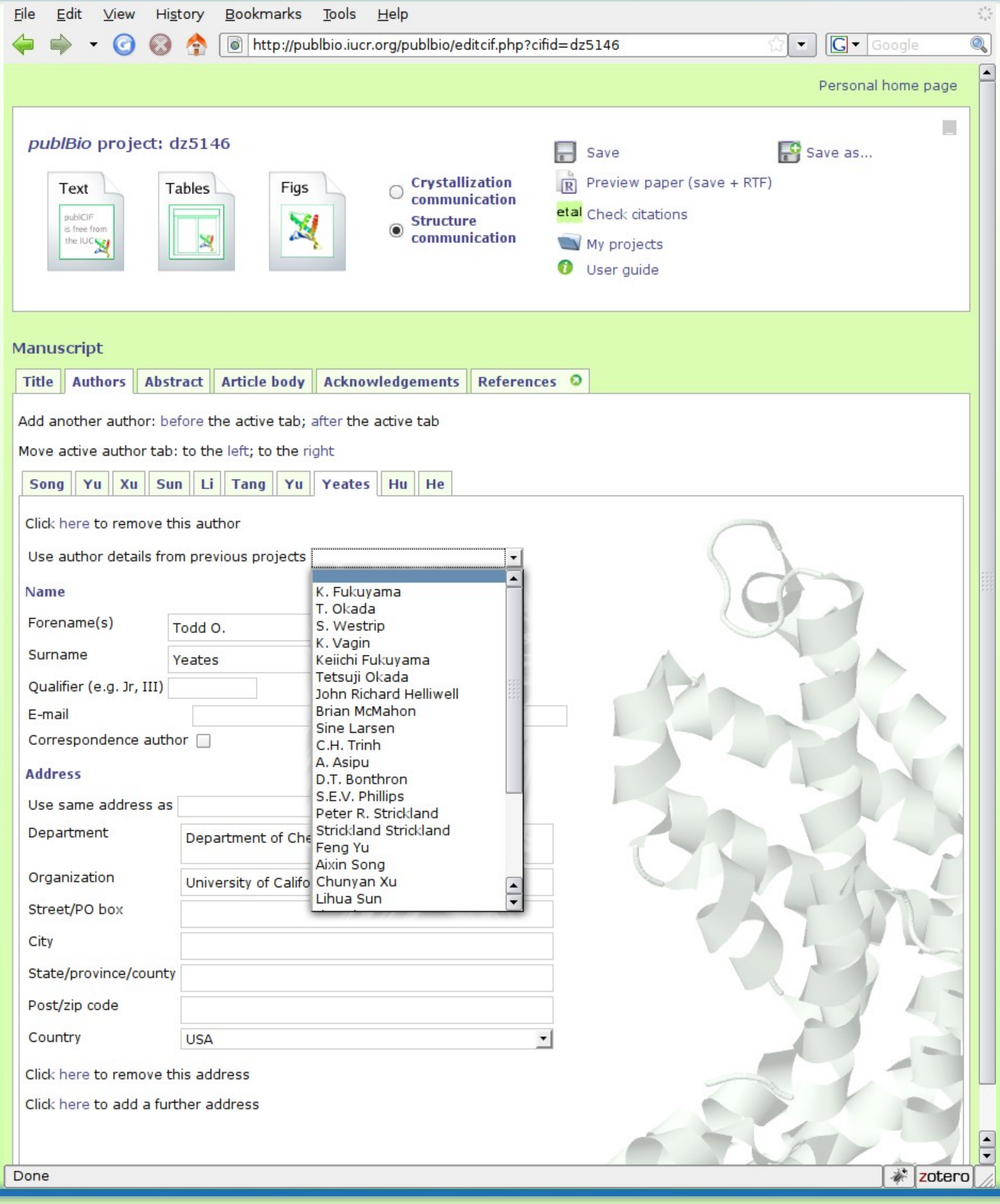

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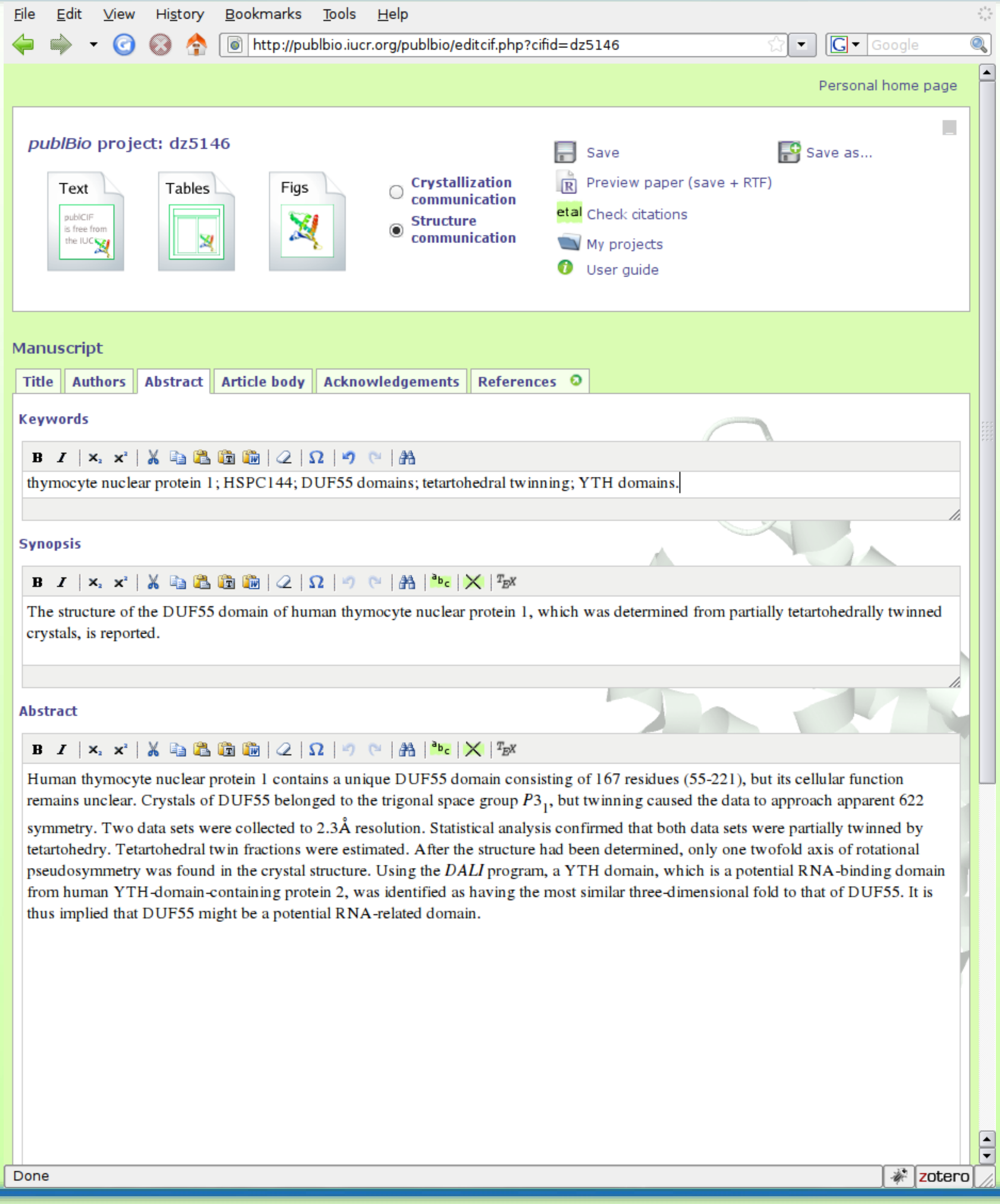

Keywords

thymocyte nuclear protein 1; HSPC144; DUF55 domains; tetartohedral twinning; YTH domains.

Synopsis

The structure of the DUF55 domain of human thymocyte nuclear protein 1, which was determined from partially tetartohedrally twinned crystals, is reported.

Abstract

Human thymocyte nuclear protein 1 contains a unique DUF55 domain consisting of 167 residues (55-221), but its cellular function remains unclear. Crystals of DUF55 belonged to the trigonal space group $P3_1$, but twinning caused the data to approach apparent 622 symmetry. Two data sets were collected to 2.3Å resolution. Statistical analysis confirmed that both data sets were partially twinned by tetartohedry. Tetartohedral twin fractions were estimated. After the structure had been determined, only one twofold axis of rotational pseudosymmetry was found in the crystal structure. Using the *DALI* program, a YTH domain, which is a potential RNA-binding domain from human YTH-domain-containing protein 2, was identified as having the most similar three-dimensional fold to that of DUF55. It is thus implied that DUF55 might be a potential RNA-related domain.

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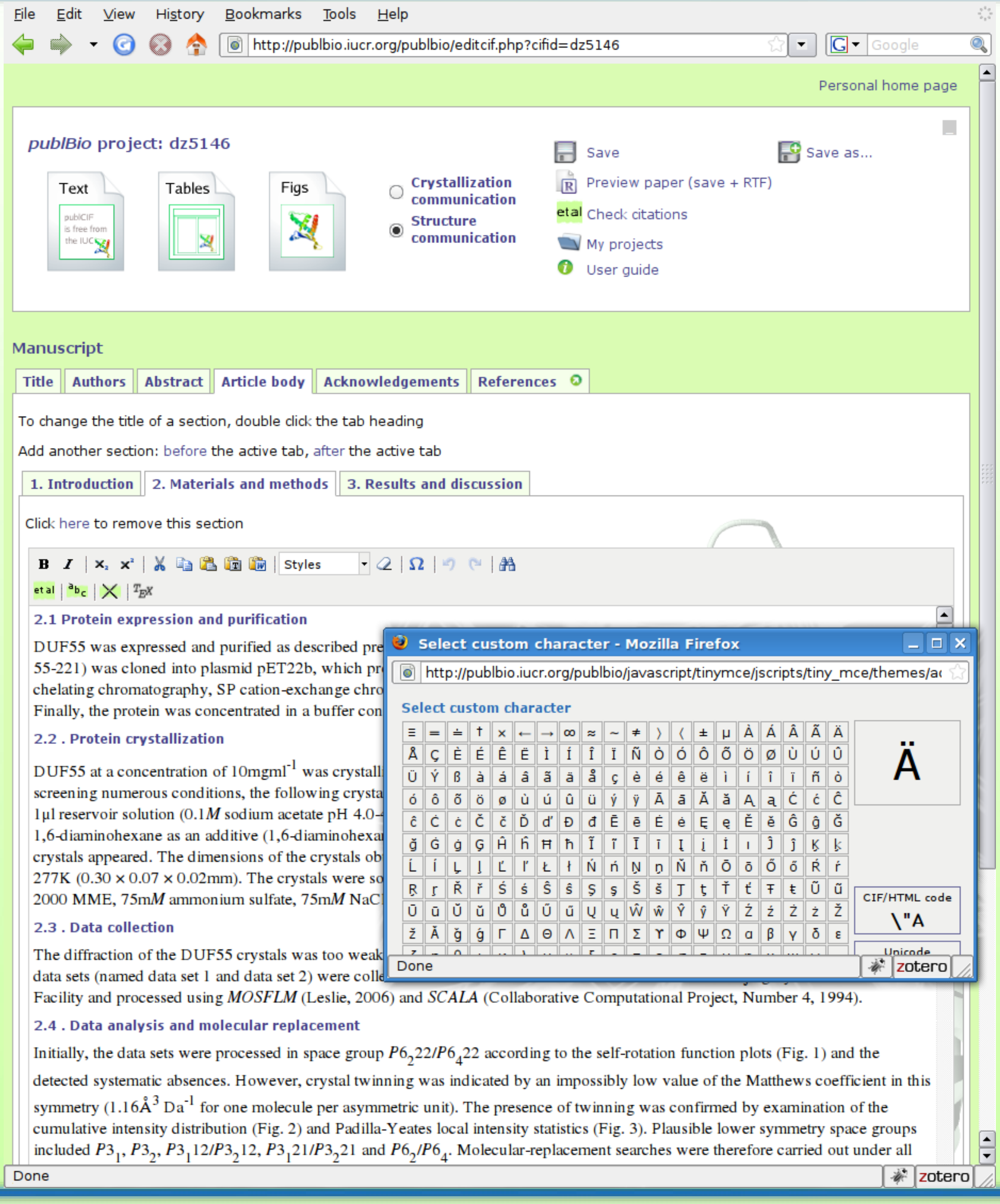

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2.1 Protein expression and purification

DUF55 was expressed and purified as described pre
55-221) was cloned into plasmid pET22b, which pr
chelating chromatography, SP cation-exchange chro
Finally, the protein was concentrated in a buffer con

2.2 . Protein crystallization

DUF55 at a concentration of 10mgml^{-1} was crystalli
screening numerous conditions, the following crysta
1µl reservoir solution (0.1*M* sodium acetate pH 4.0-
1,6-diaminohexane as an additive (1,6-diaminohexa
crystals appeared. The dimensions of the crystals ob
277K (0.30 × 0.07 × 0.02mm). The crystals were so
2000 MME, 75m*M* ammonium sulfate, 75m*M* NaCl

2.3 . Data collection

The diffraction of the DUF55 crystals was too weak
data sets (named data set 1 and data set 2) were colle
Facility and processed using *MOSFLM* (Leslie, 2006) and *SCALA* (Collaborative Computational Project, Number 4, 1994).

2.4 . Data analysis and molecular replacement

Initially, the data sets were processed in space group $P6_222/P6_422$ according to the self-rotation function plots (Fig. 1) and the detected systematic absences. However, crystal twinning was indicated by an impossibly low value of the Matthews coefficient in this symmetry (1.16Å^3 Da^{-1} for one molecule per asymmetric unit). The presence of twinning was confirmed by examination of the cumulative intensity distribution (Fig. 2) and Padilla-Yeates local intensity statistics (Fig. 3). Plausible lower symmetry space groups included $P3_1$, $P3_2$, $P3_112/P3_212$, $P3_121/P3_221$ and $P6_2/P6_4$. Molecular-replacement searches were therefore carried out under all

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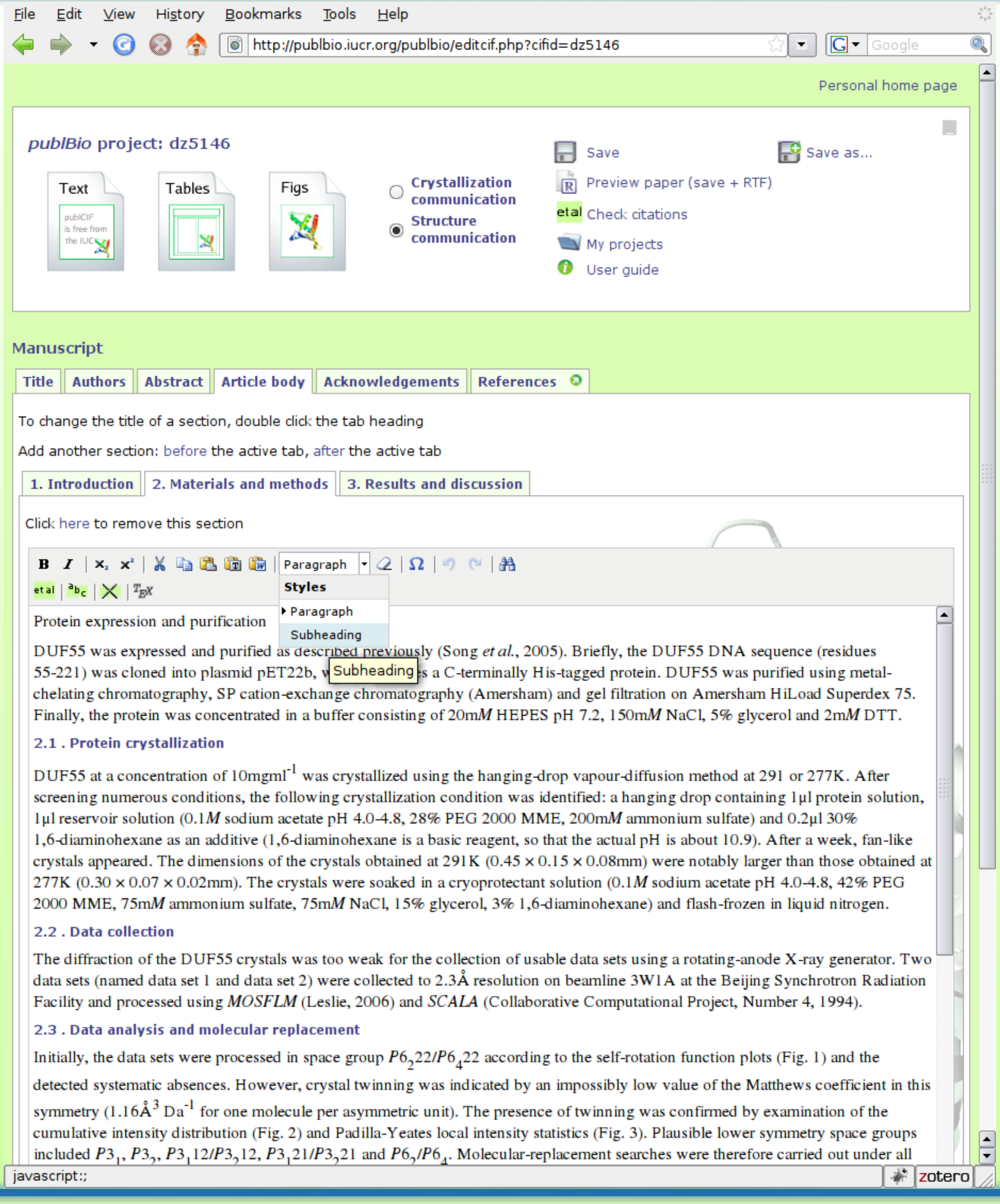

Protein expression and purification

DUF55 was expressed and purified as described previously (Song *et al.*, 2005). Briefly, the DUF55 DNA sequence (residues 55-221) was cloned into plasmid pET22b, w Subheading s a C-terminally His-tagged protein. DUF55 was purified using metal-chelating chromatography, SP cation-exchange chromatography (Amersham) and gel filtration on Amersham HiLoad Superdex 75. Finally, the protein was concentrated in a buffer consisting of 20m*M* HEPES pH 7.2, 150m*M* NaCl, 5% glycerol and 2m*M* DTT.

2.1 . Protein crystallization

DUF55 at a concentration of 10mgml^{-1} was crystallized using the hanging-drop vapour-diffusion method at 291 or 277K. After screening numerous conditions, the following crystallization condition was identified: a hanging drop containing 1µl protein solution, 1µl reservoir solution (0.1*M* sodium acetate pH 4.0-4.8, 28% PEG 2000 MME, 200m*M* ammonium sulfate) and 0.2µl 30% 1,6-diaminohexane as an additive (1,6-diaminohexane is a basic reagent, so that the actual pH is about 10.9). After a week, fan-like crystals appeared. The dimensions of the crystals obtained at 291K (0.45 × 0.15 × 0.08mm) were notably larger than those obtained at 277K (0.30 × 0.07 × 0.02mm). The crystals were soaked in a cryoprotectant solution (0.1*M* sodium acetate pH 4.0-4.8, 42% PEG 2000 MME, 75m*M* ammonium sulfate, 75m*M* NaCl, 15% glycerol, 3% 1,6-diaminohexane) and flash-frozen in liquid nitrogen.

2.2 . Data collection

The diffraction of the DUF55 crystals was too weak for the collection of usable data sets using a rotating-anode X-ray generator. Two data sets (named data set 1 and data set 2) were collected to 2.3Å resolution on beamline 3W1A at the Beijing Synchrotron Radiation Facility and processed using *MOSFLM* (Leslie, 2006) and *SCALA* (Collaborative Computational Project, Number 4, 1994).

2.3 . Data analysis and molecular replacement

Initially, the data sets were processed in space group $P6_222/P6_422$ according to the self-rotation function plots (Fig. 1) and the detected systematic absences. However, crystal twinning was indicated by an impossibly low value of the Matthews coefficient in this symmetry (1.16Å^3 Da^{-1} for one molecule per asymmetric unit). The presence of twinning was confirmed by examination of the cumulative intensity distribution (Fig. 2) and Padilla-Yeates local intensity statistics (Fig. 3). Plausible lower symmetry space groups included $P3_1$, $P3_2$, $P3_112/P3_212$, $P3_121/P3_221$ and $P6_2/P6_4$. Molecular-replacement searches were therefore carried out under all

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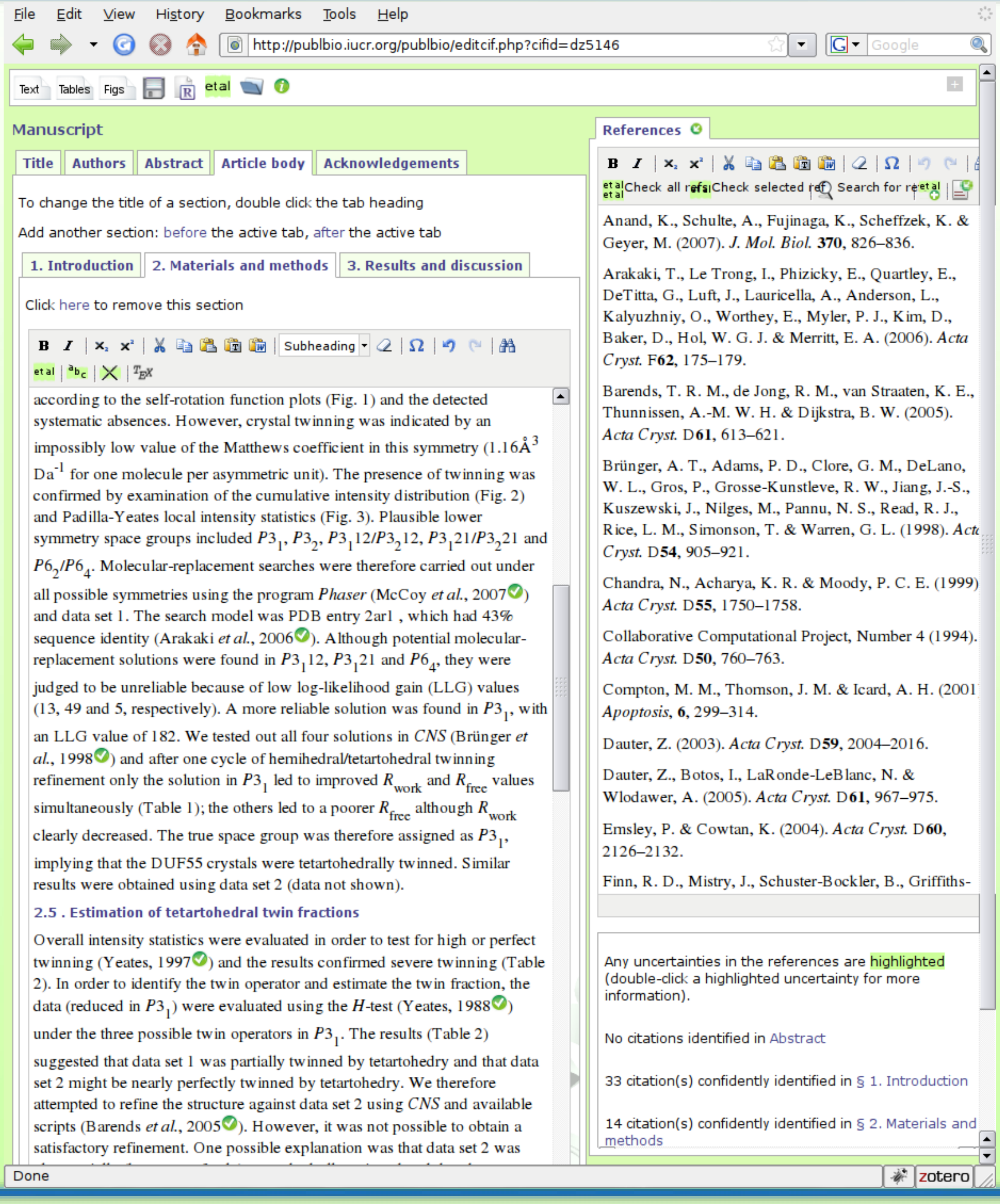

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2.5 . Estimation of tetartohedral twin fractions

Overall intensity statistics were evaluated in order to test for high or perfect twinning (Yeates, 1997✓) and the results confirmed severe twinning (Table 2). In order to identify the twin operator and estimate the twin fraction, the data (reduced in $P3_1$) were evaluated using the *H*-test (Yeates, 1988✓) under the three possible twin operators in $P3_1$. The results (Table 2) suggested that data set 1 was partially twinned by tetartohedry and that data set 2 might be nearly perfectly twinned by tetartohedry. We therefore attempted to refine the structure against data set 2 using *CNS* and available scripts (Barends *et al.*, 2005✓). However, it was not possible to obtain a satisfactory refinement. One possible explanation was that data set 2 was

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It is important to note here that for each solution for the twin-fraction values there are four different permutations of the four twin fractions which are equally correct (Yeates & Yu, 2008✓); different permutations simply correspond to exchanging the assignments of I_1, I_2, I_3 and I_4 in (2). The permutation of the twin fractions that is chosen is therefore arbitrary, unless it is necessary to obtain agreement with a previously defined set of intensities. This was the case here, as a molecular-replacement model (and its calculated intensities) had already been obtained (*i.e.* prior to detwinning). In this work, therefore, detwinning under all four allowed permutations of the twin-fraction solution was performed and the correct solution was decided by the behaviour of atomic refinement and by the inspection of electron-density maps. For completeness, the four permutations of the alternate (less plausible) solution for the twin fractions were also tested. The same procedure was applied to data set 2. Thus, eight separate preliminary refinements were conducted using each of the two data sets (the results for data set 1 are shown in Table 3). Solution 1 for data set 1 was (0.424, 0.300, 0.134, 0.142), with the alternate orderings (0.300, 0.424, 0.142, 0.134), (0.134, 0.142, 0.424, 0.300) and (0.142, 0.134, 0.300, 0.424) being equally possible. It was verified that solution 1 of data set 1 (0.424, 0.300, 0.134, 0.142) and solution 2 of data set 2 (0.291, 0.276, 0.151, 0.282) were correct. This was consistent with the previous examination of detwinned intensity statistics (Fig. 4).

2.6 . Refinement under partial tetartohedral twinning

Because all four twin-related reflections must be observed for detwinning to be carried out (2), data completeness is important for detwinning. We therefore refined the structure using data set 1. An atomic model was rebuilt using *Coot* (Emsley & Cowtan, 2004✓) and simulated annealing and B-factor refinement were then performed employing noncrystallographic symmetry restraints using *CNS*. After about ten cycles of refinement, most of the amino-acid residues could be traced, including four residues which were introduced

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In the case of tetartohedral twinning, the observed intensities (J_k) are related to the true crystallographic intensities (I_k) as follows:

$$\begin{cases} \alpha_1 I_1 + \alpha_2 I_2 + \alpha_3 I_3 + \alpha_4 I_4 = J_1 \\ \alpha_1 I_2 + \alpha_2 I_1 + \alpha_3 I_4 + \alpha_4 I_3 = J_2 \\ \alpha_1 I_3 + \alpha_2 I_4 + \alpha_3 I_1 + \alpha_4 I_2 = J_3 \\ \alpha_1 I_4 + \alpha_2 I_3 + \alpha_3 I_2 + \alpha_4 I_1 = J_4 \end{cases}. \qquad (2)$$

The assignment of subscripts to twin operations is arbitrary, so we can say that I_1 refers to $I(h,k,l)$, I_2 refers to $I(k,h,-l)$, I_3 refers to $I(-k,-h,-l)$ and I_4 refers to $I(-h,-k,l)$, according to the three underlying twin operations. If the twin fractions $({}_1, {}_2, {}_3, {}_4)$ have been estimated, then the intensities can be detwinned (*i.e.* one can solve the equations above, given the observed intensities, to obtain the true intensities, arbitrarily setting $I_{\rm true} = I_1$). If the data have been detwinned successfully, then the resulting intensities should obey exponential statistics (Wilson, 1949✓). On the other hand, if an incorrect solution for the twin fractions has been chosen then the detwinned intensities may not follow the correct distribution. In this way, it is possible to distinguish between correct and incorrect solutions for the twin fractions (Yeates & Yu, 2008✓). This approach was used to analyze the potential twin-fraction solutions for data sets 1 and 2 (Fig. 4). In the case of data set 1, the detwinned data calculated under solution 1 followed a somewhat more ideal distribution than those calculated under solution 2. In the case of data set 2, solution 2 was much better.

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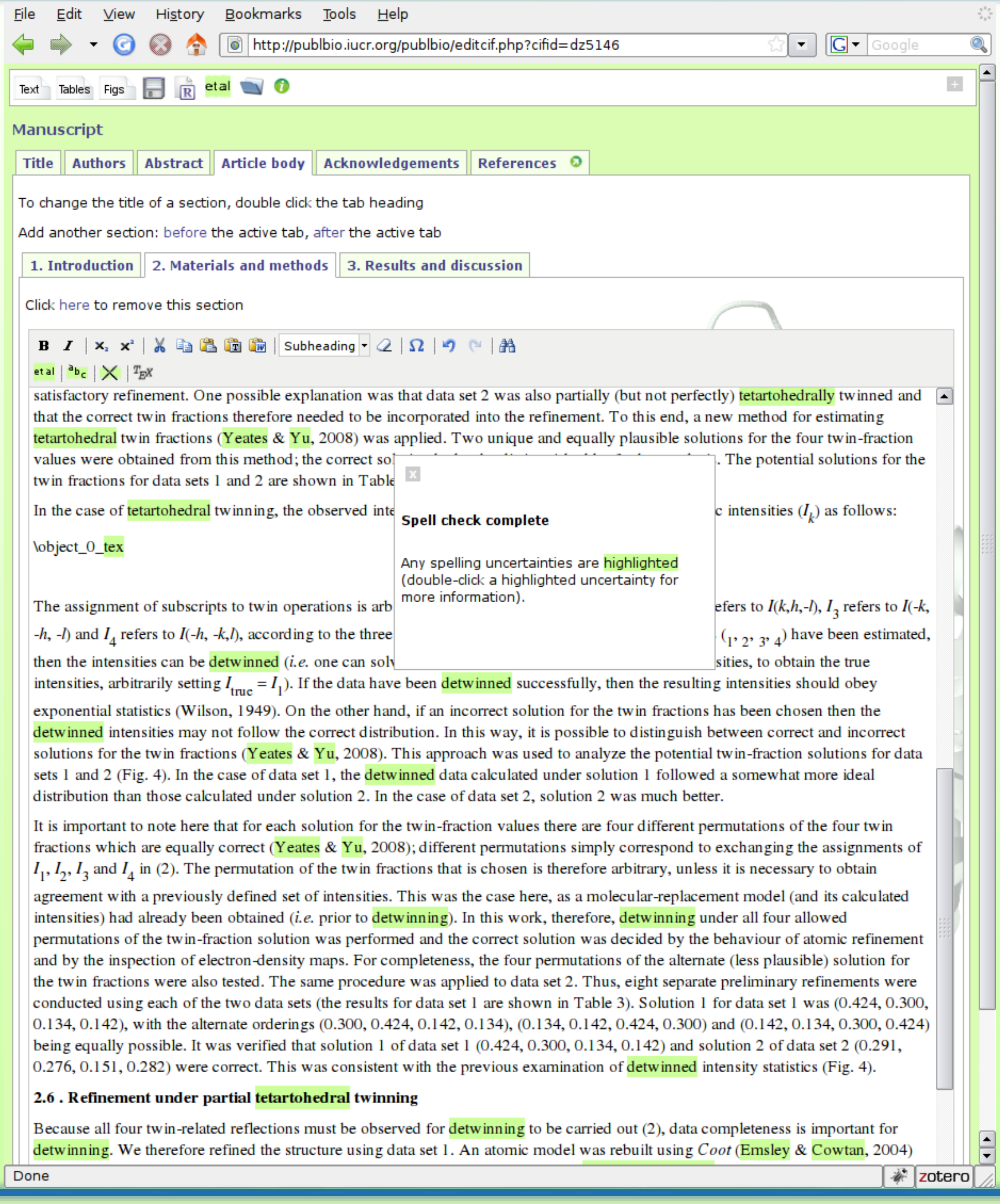

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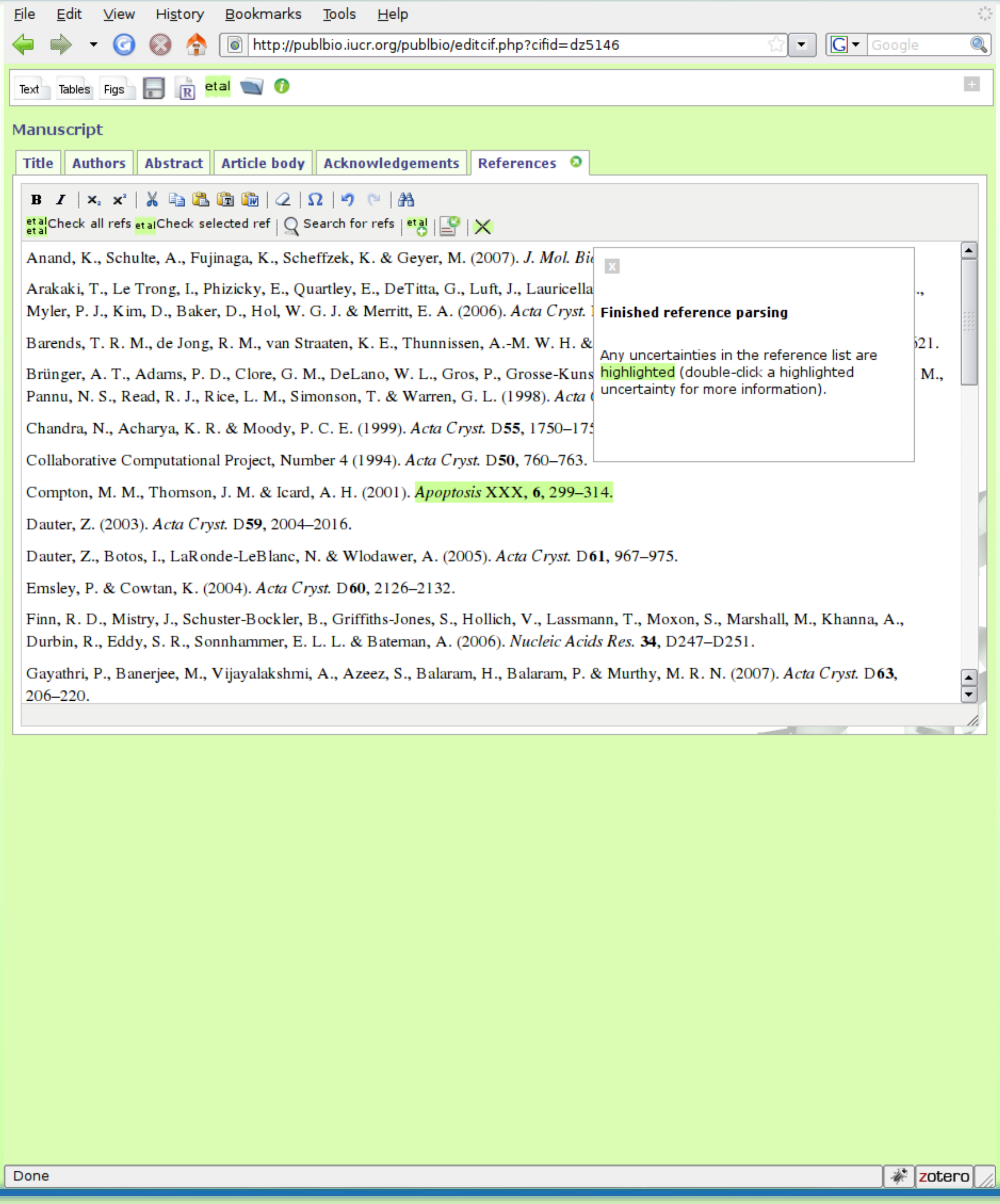

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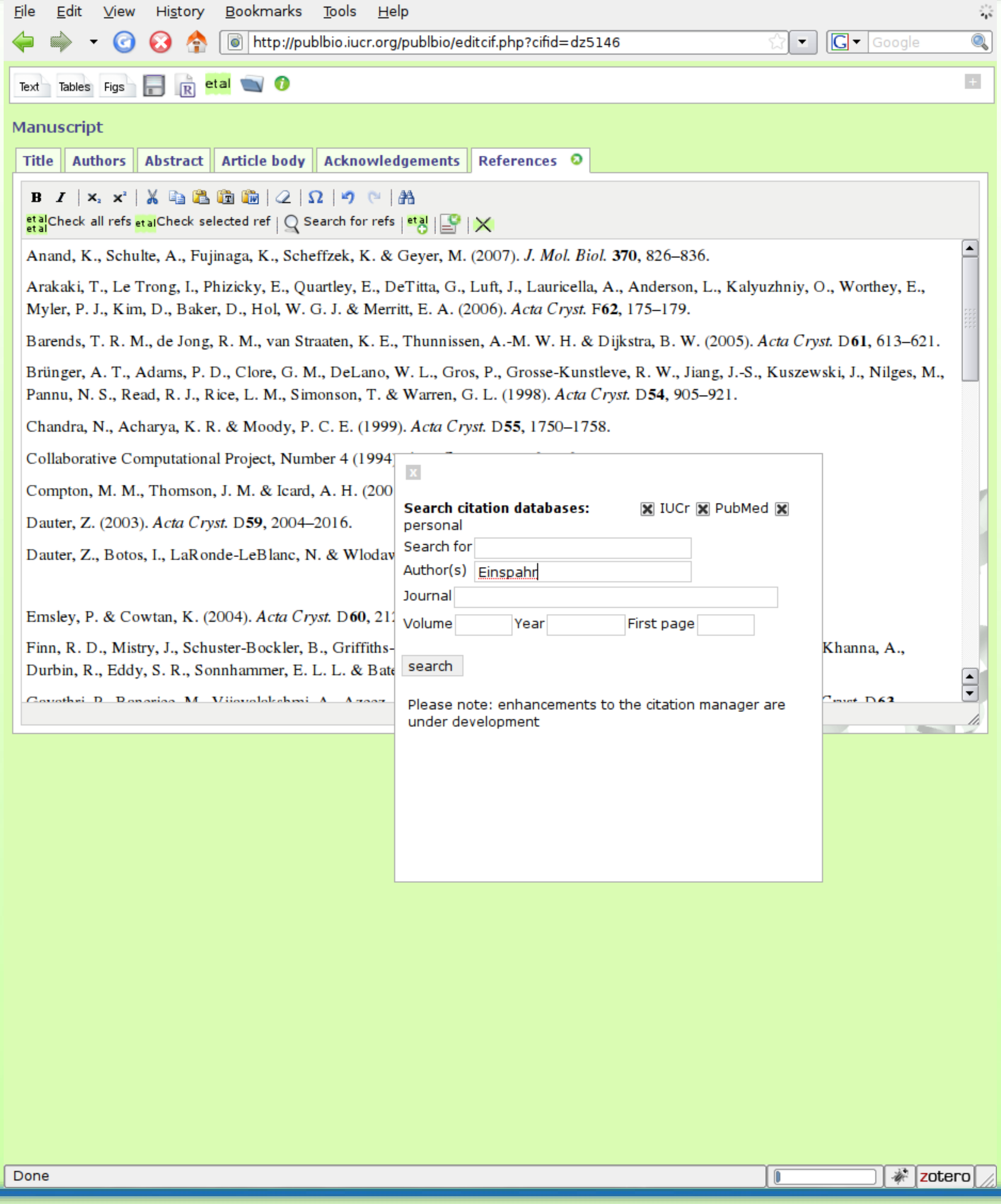

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Finn, R. D., Mistry, J., Schuster-Bockler, B., Griffiths- Khanna, A., Durbin, R., Eddy, S. R., Sonnhammer, E. L. L. & Bate

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searches can be made on

IUCr Journals

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Anand, K., Schulte, A., Fujinaga, K., Scheffzek, K. & Geyer, M. (2007). *J. Mol. Biol.* **370**, 826–836.

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The geometry of calcium carboxylate interactions in crystalline complexes

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The geometry of calcium-water interactions in

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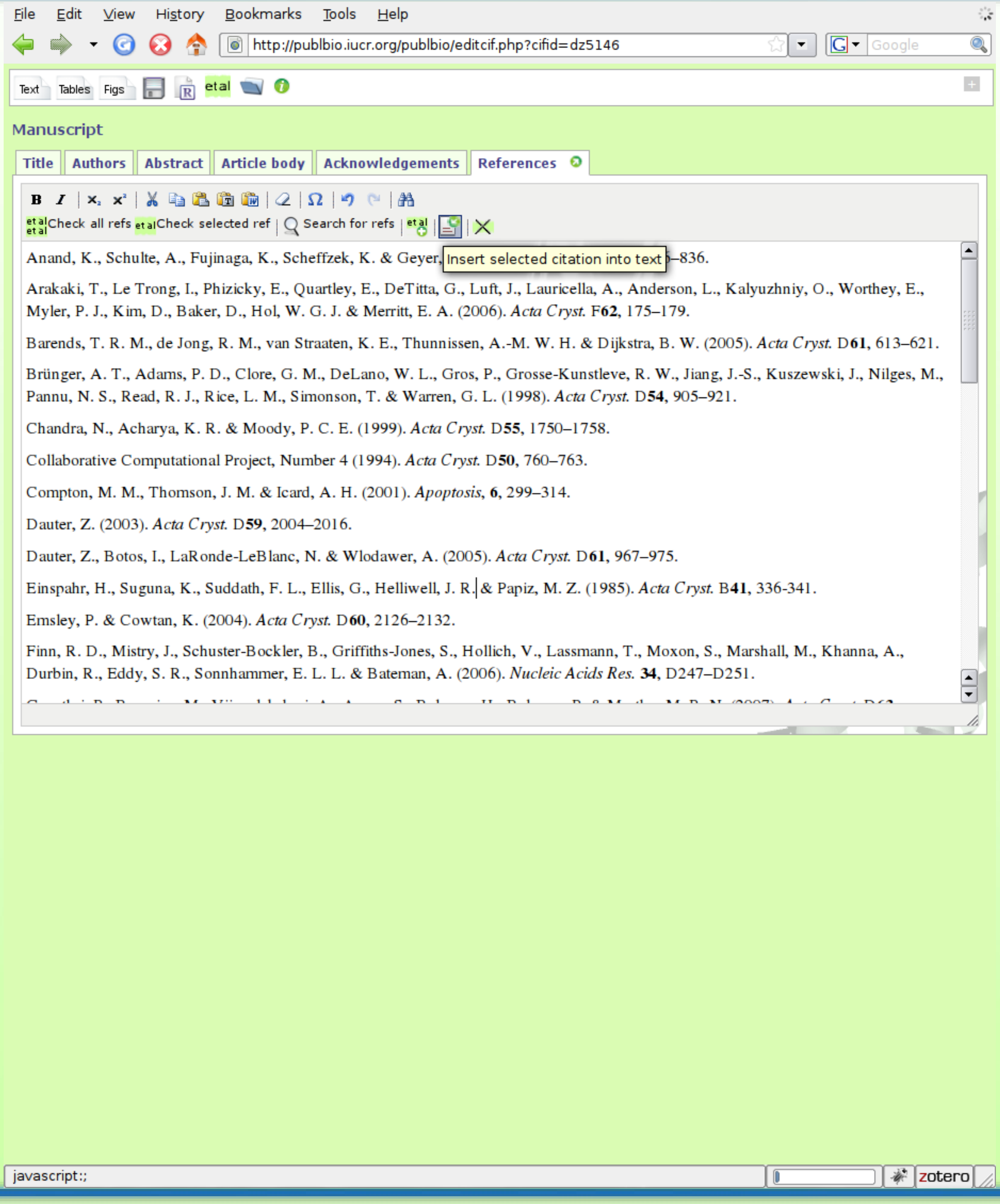

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Arakaki, T., Le Trong, I., Phizicky, E., Quartley, E., DeTitta, G., Luft, J., Lauricella, A., Anderson, L., Kalyuzhniy, O., Worthey, E., Myler, P. J., Kim, D., Baker, D., Hol, W. G. J. & Merritt, E. A. (2006). *Acta Cryst.* F**62**, 175–179.

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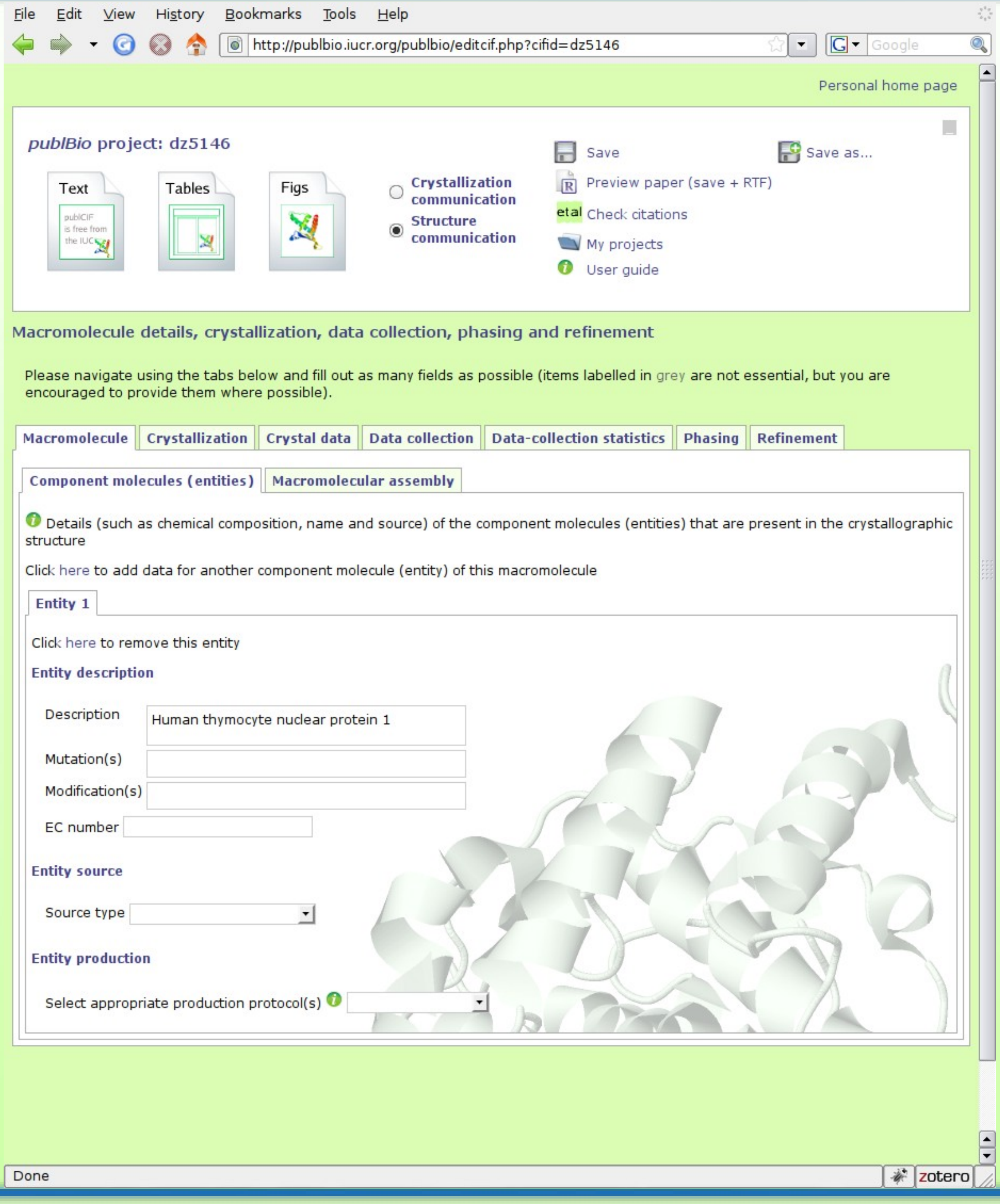

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○ Crystallization communication
● Structure communication

Macromolecule details, crystallization, data collection, phasing and refinement

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).

Details (such as chemical composition, name and source) of the component molecules (entities) that are present in the crystallographic structure

Click here to add data for another component molecule (entity) of this macromolecule

Click here to remove this entity

Entity description

Description: Human thymocyte nuclear protein 1
Mutation(s):
Modification(s):
EC number:

Entity source

Source type:

Entity production

Select appropriate production protocol(s):

The tables tab consists of a number of tabs

macromolecule

crystallization

crystal data

data collection

data-collection statistics

phasing

refinement

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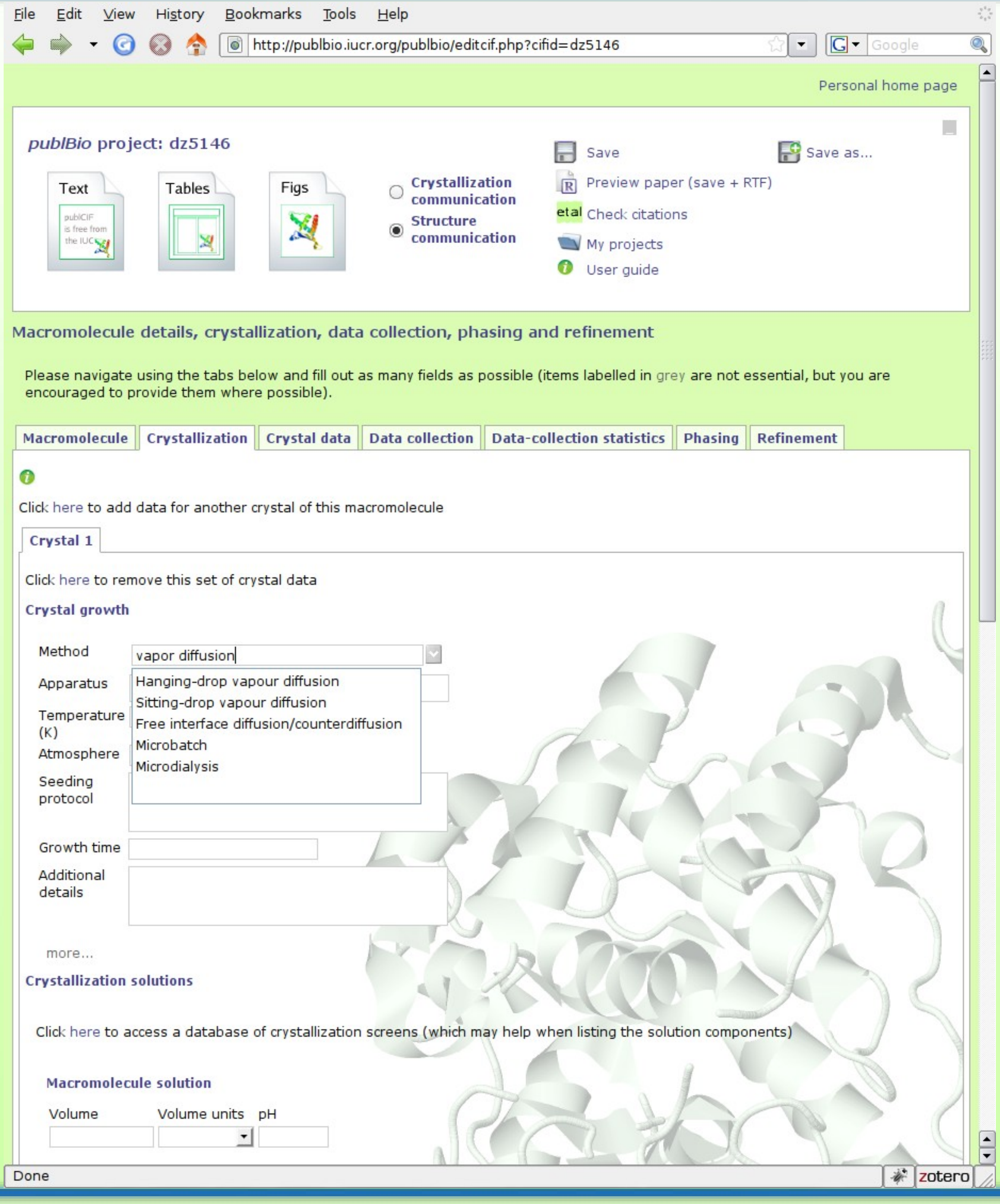
experimental data can be edited in the tables tabs



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○ Crystallization communication
● Structure communication

Macromolecule details, crystallization, data collection, phasing and refinement

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).

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

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: vapor diffusion
- Hanging-drop vapour diffusion
- Sitting-drop vapour diffusion
- Free interface diffusion/counterdiffusion
- Microbatch
- Microdialysis

Apparatus

Temperature (K)

Atmosphere

Seeding protocol

Growth time

Additional details

more...

Crystallization solutions

Click here to access a database of crystallization screens (which may help when listing the solution components)

Macromolecule solution

Volume | Volume units | pH

Done

data from previous projects are remembered

standard descriptions of methods are also offered

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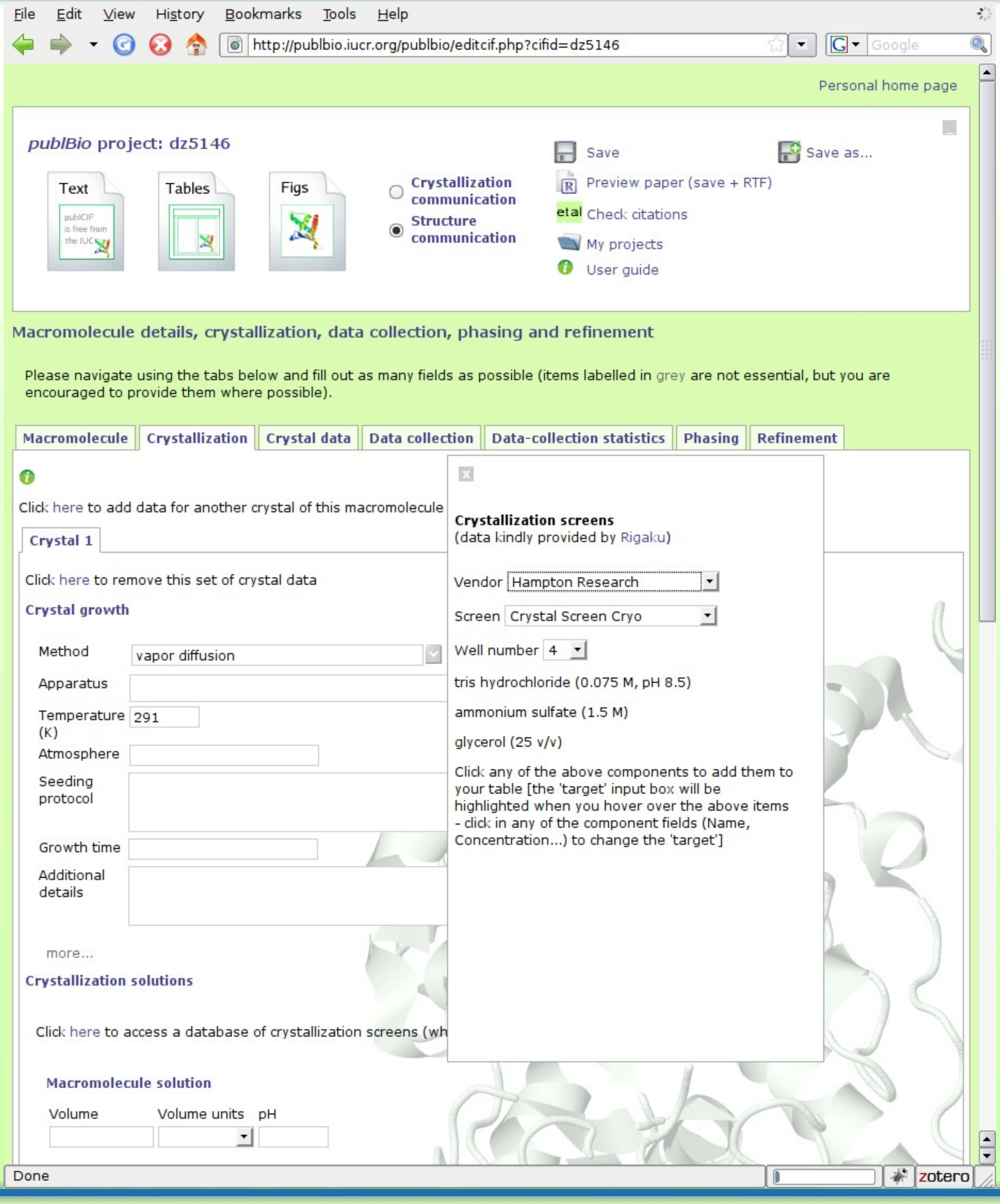
input forms suggest possible wording



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○ Crystallization communication
● Structure communication

Macromolecule details, crystallization, data collection, phasing and refinement

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).

Click here to add data for another crystal of this macromolecule

Click here to remove this set of crystal data

Crystal growth

Method: vapor diffusion
Apparatus:
Temperature (K): 291
Atmosphere:
Seeding protocol:
Growth time:
Additional details:

Crystallization solutions

Click here to access a database of crystallization screens (wh

Macromolecule solution

Volume | Volume units | pH

Crystallization screens
(data kindly provided by Rigaku)

Vendor: Hampton Research
Screen: Crystal Screen Cryo
Well number: 4

tris hydrochloride (0.075 M, pH 8.5)

ammonium sulfate (1.5 M)

glycerol (25 v/v)

Click any of the above components to add them to your table [the 'target' input box will be highlighted when you hover over the above items - click in any of the component fields (Name, Concentration...) to change the 'target']

standard commercial crystallization screens can be looked up

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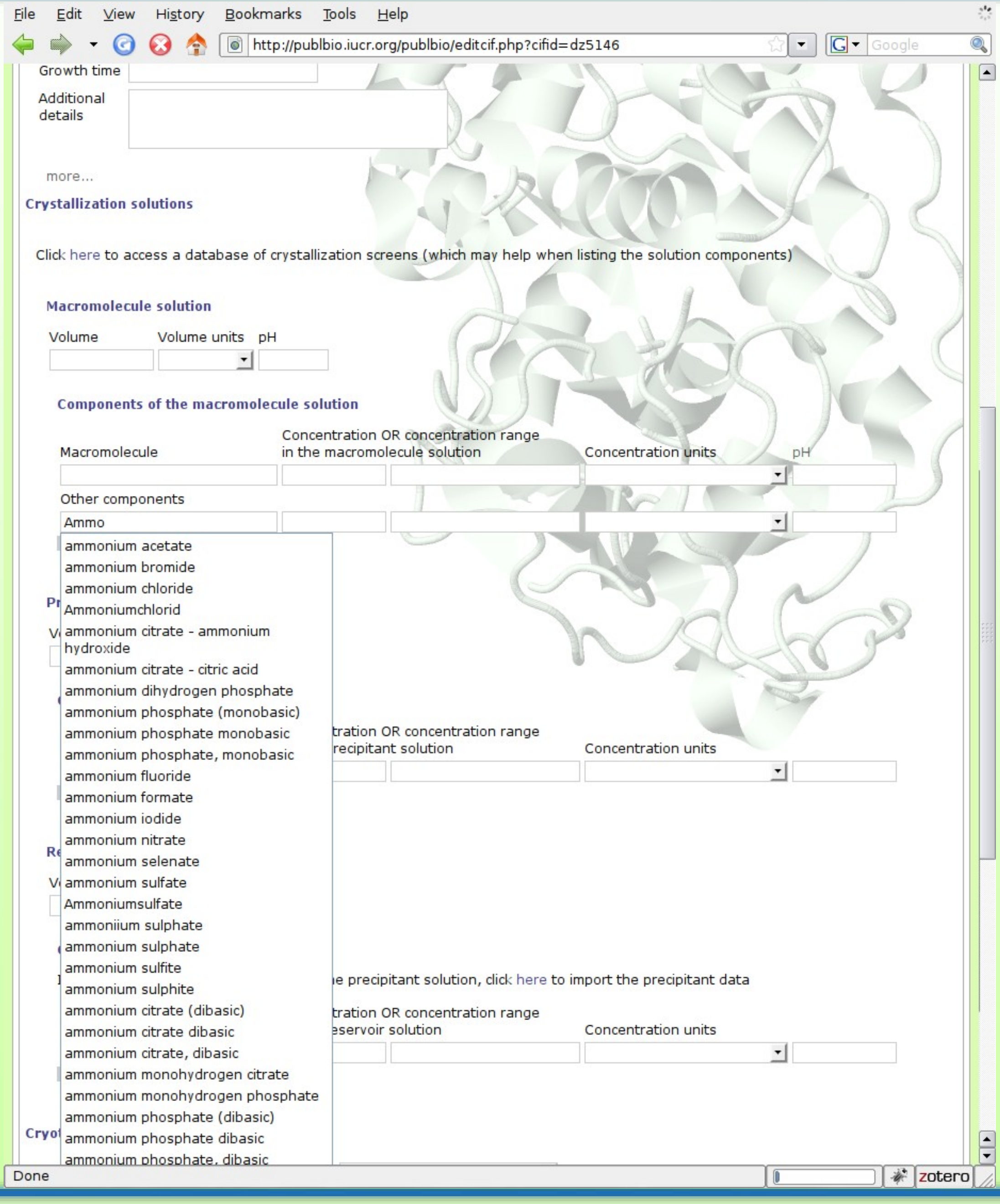
crystallization conditions can be added from a database



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Growth time

Additional details

more...

Crystallization solutions

Click here to access a database of crystallization screens (which may help when listing the solution components)

Macromolecule solution

Volume | Volume units | pH

Components of the macromolecule solution

Macromolecule | Concentration OR concentration range in the macromolecule solution | Concentration units | pH

Other components

Ammo

- ammonium acetate
- ammonium bromide
- ammonium chloride
- Ammoniumchlorid
- ammonium citrate - ammonium hydroxide
- ammonium citrate - citric acid
- ammonium dihydrogen phosphate
- ammonium phosphate (monobasic)
- ammonium phosphate monobasic
- ammonium phosphate, monobasic
- ammonium fluoride
- ammonium formate
- ammonium iodide
- ammonium nitrate
- ammonium selenate
- ammonium sulfate
- Ammoniumsulfate
- ammoniium sulphate
- ammonium sulphate
- ammonium sulfite
- ammonium sulphite
- ammonium citrate (dibasic)
- ammonium citrate dibasic
- ammonium citrate, dibasic
- ammonium monohydrogen citrate
- ammonium monohydrogen phosphate
- ammonium phosphate (dibasic)
- ammonium phosphate dibasic
- ammonium phosphate, dibasic

tration OR concentration range recipitant solution | Concentration units

e precipitant solution, click here to import the precipitant data

tration OR concentration range eservoir solution | Concentration units

the software predicts the names of standard crystallization components

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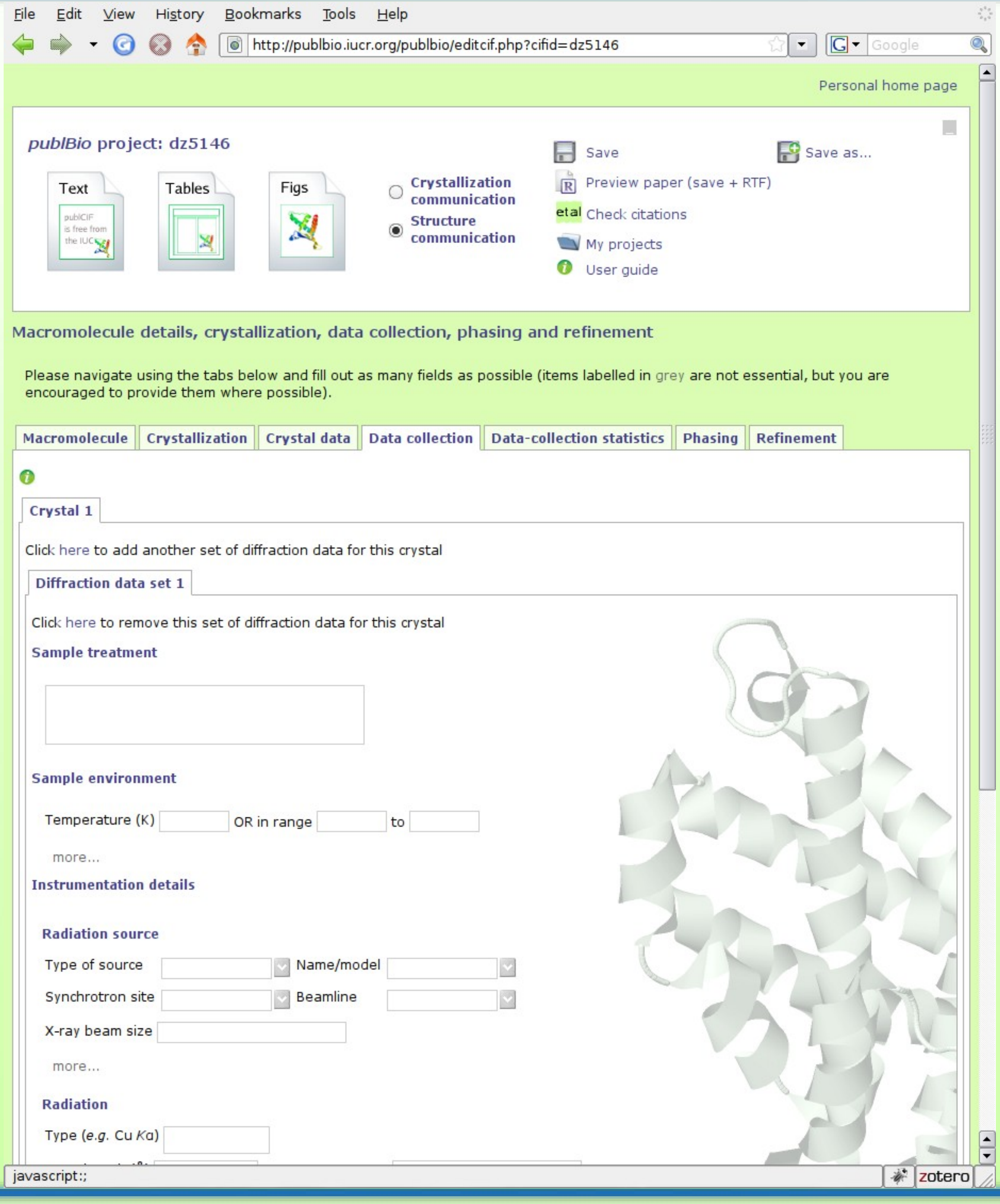
crystallization conditions can be added manually



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○ Crystallization communication
● Structure communication

Macromolecule details, crystallization, data collection, phasing and refinement

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).

Click here to add another set of diffraction data for this crystal

Click here to remove this set of diffraction data for this crystal

Sample treatment

Sample environment

Temperature (K) OR in range to

Instrumentation details

Radiation source

Type of source
Name/model
Synchrotron site
Beamline
X-ray beam size

Radiation

Type (*e.g.* Cu *K*α)

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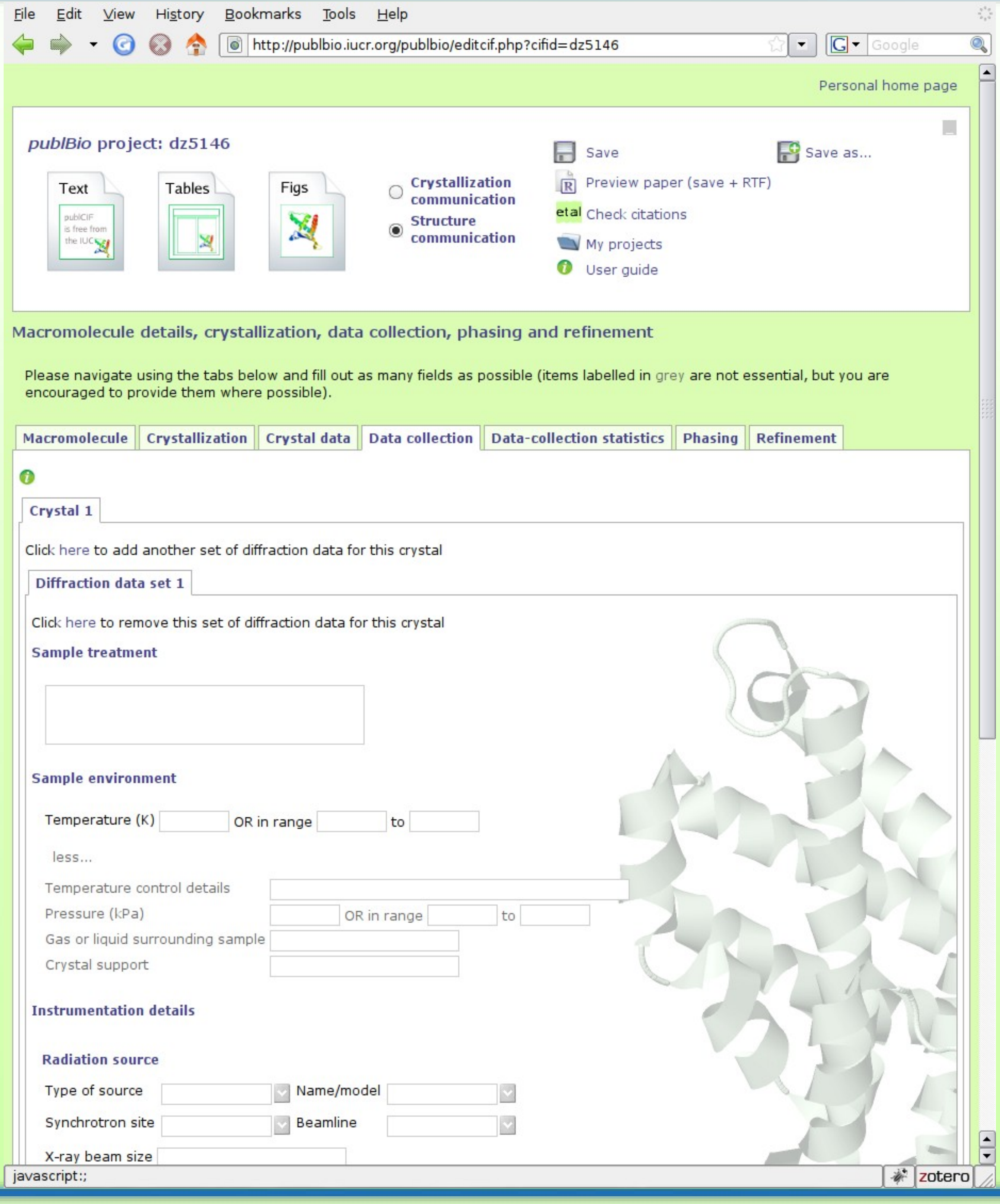
forms request standard information for crystallization studies



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Macromolecule details, crystallization, data collection, phasing and refinement

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).

Click here to add another set of diffraction data for this crystal

Click here to remove this set of diffraction data for this crystal

Sample treatment

Sample environment

Temperature (K) OR in range to

less...

Temperature control details
Pressure (kPa) OR in range to
Gas or liquid surrounding sample
Crystal support

Instrumentation details

Radiation source

Type of source
Name/model
Synchrotron site
Beamline
X-ray beam size

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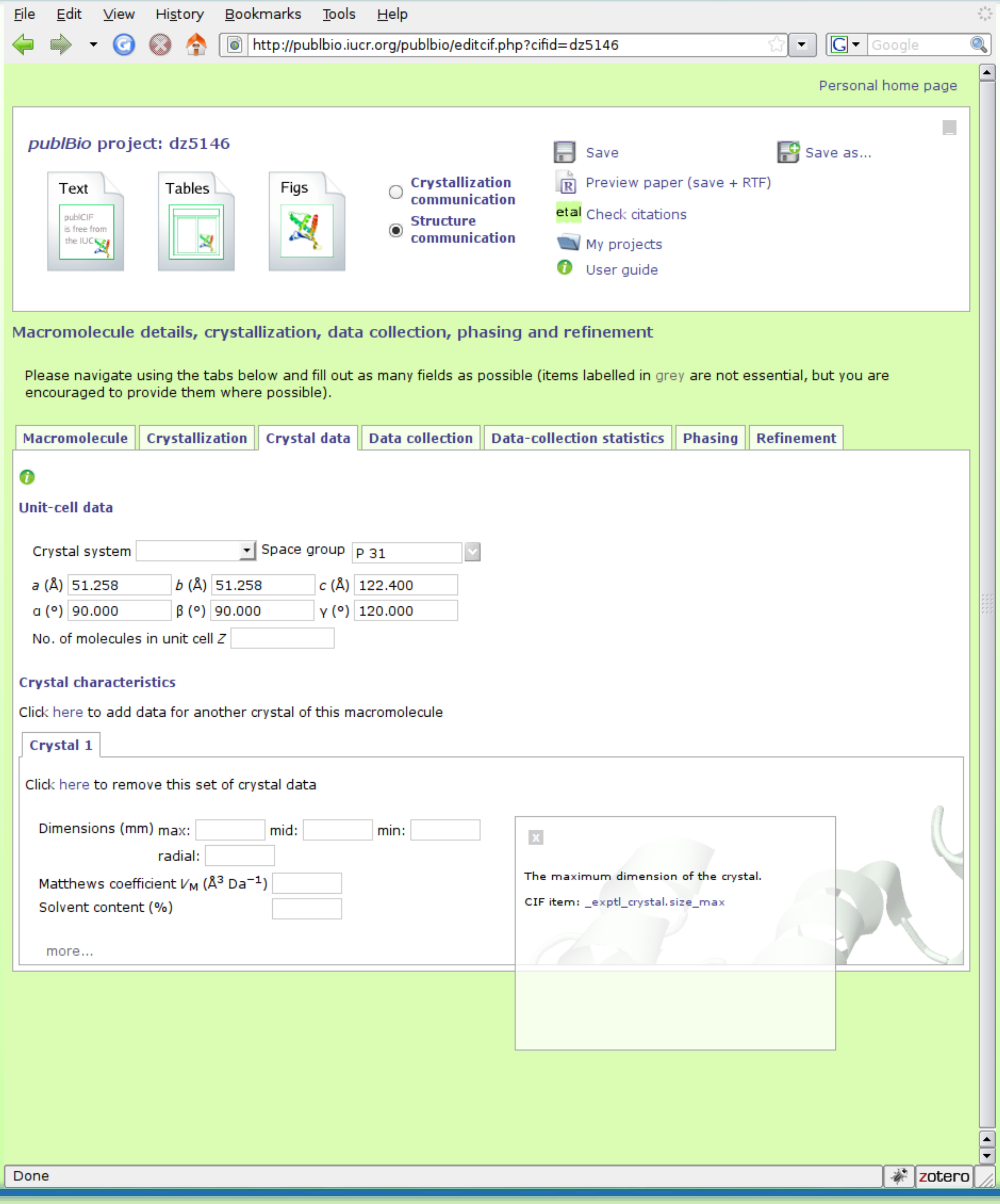
additional information may be added using “more” links



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○ Crystallization communication
● Structure communication

Macromolecule details, crystallization, data collection, phasing and refinement

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).

Unit-cell data

Crystal system Space group P 31

a (Å) 51.258 b (Å) 51.258 c (Å) 122.400

α (°) 90.000 β (°) 90.000 γ (°) 120.000

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})

Solvent content (%)

more...

The maximum dimension of the crystal.

CIF item: _exptl_crystal.size_max

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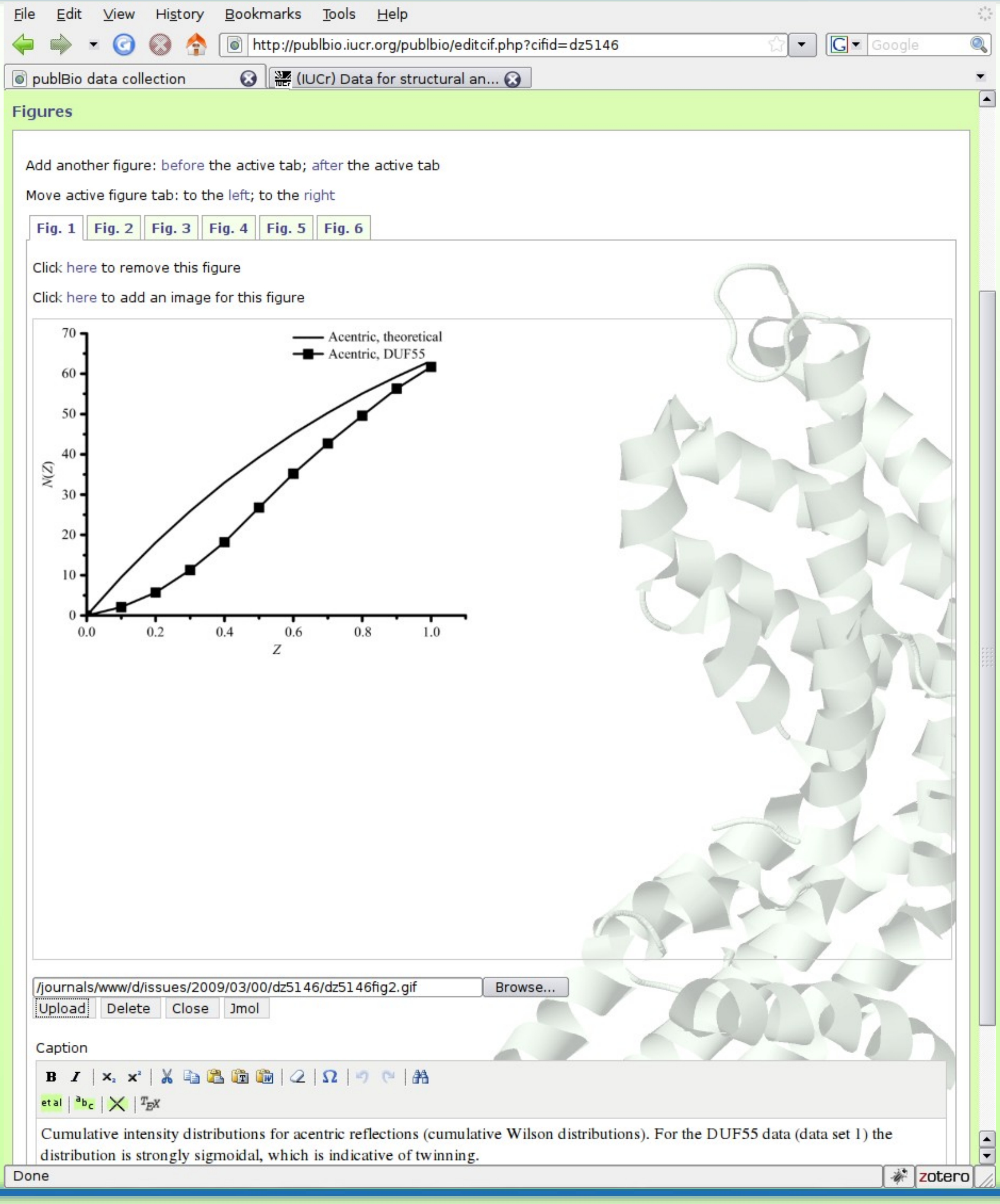
each input box has an associated “help” window



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Caption

Cumulative intensity distributions for acentric reflections (cumulative Wilson distributions). For the DUF55 data (data set 1) the distribution is strongly sigmoidal, which is indicative of twinning.

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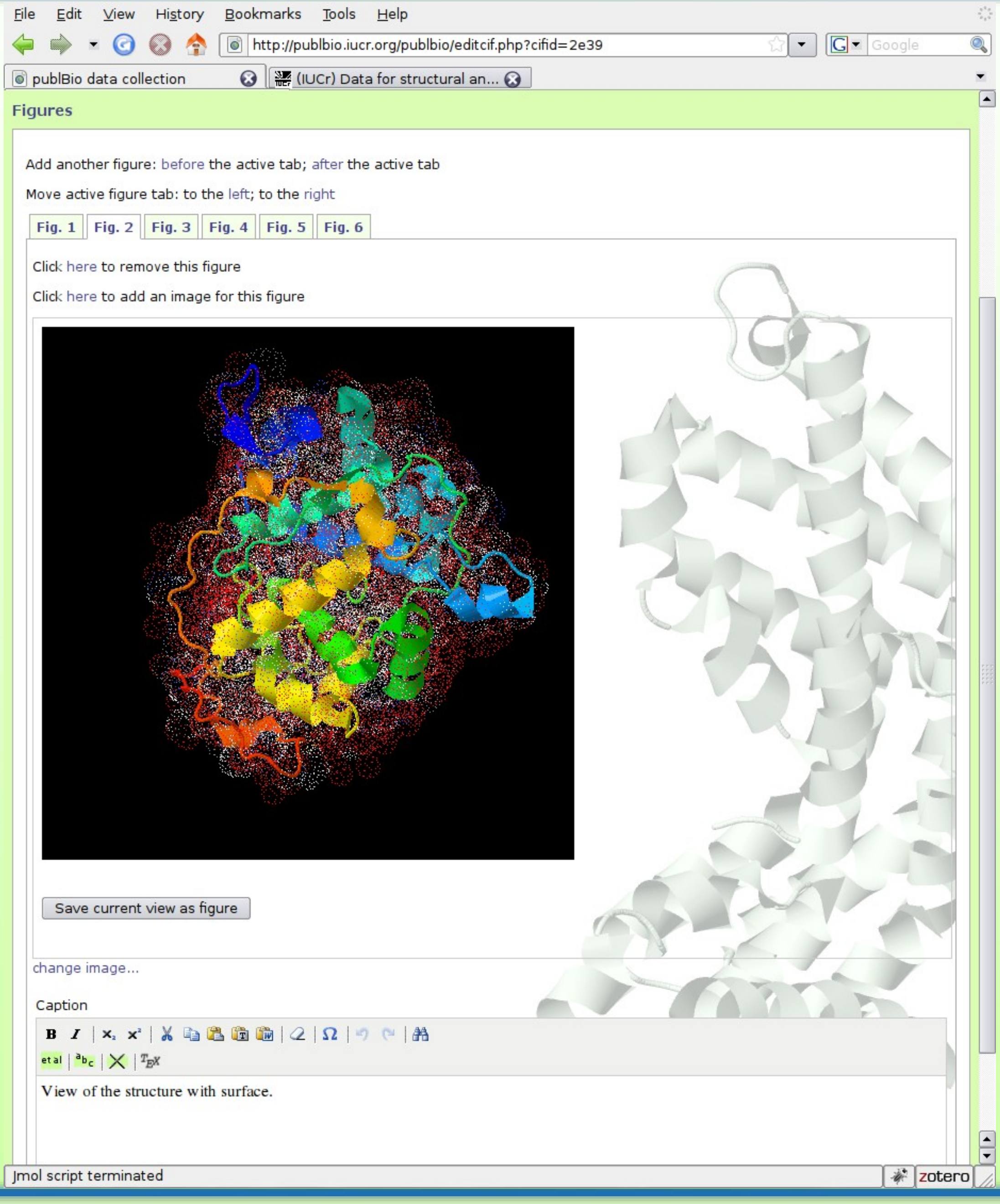

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Caption

View of the structure with surface.

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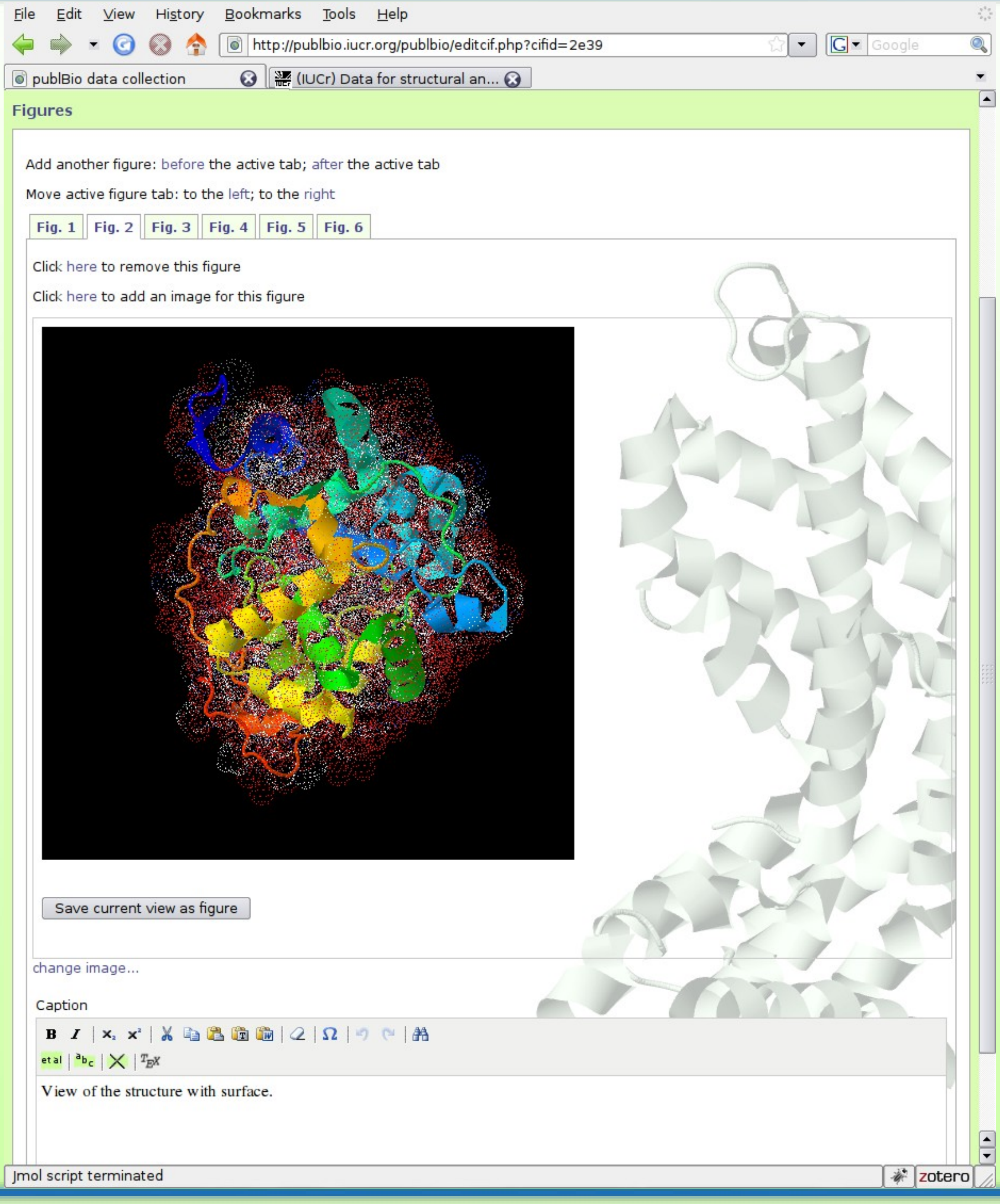

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change image...

Caption

View of the structure with surface.

Jmol script terminated

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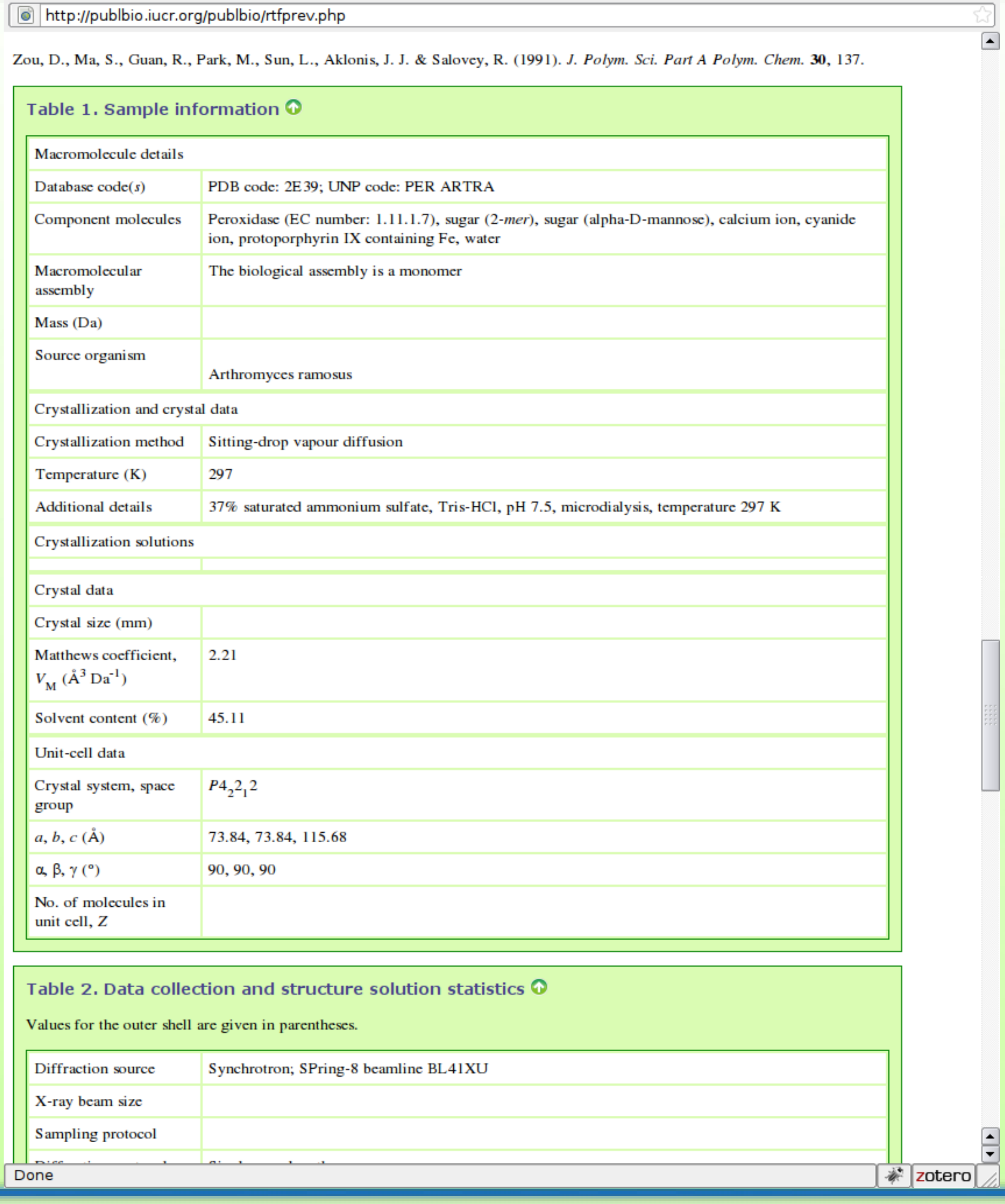

Zou, D., Ma, S., Guan, R., Park, M., Sun, L., Aklonis, J. J. & Salovey, R. (1991). *J. Polym. Sci. Part A Polym. Chem.* **30**, 137.

Table 1. Sample information

Macromolecule details	
Database code(*s*)	PDB code: 2E39; UNP code: PER ARTRA
Component molecules	Peroxidase (EC number: 1.11.1.7), sugar (2-*mer*), sugar (alpha-D-mannose), calcium ion, cyanide ion, protoporphyrin IX containing Fe, water
Macromolecular assembly	The biological assembly is a monomer
Mass (Da)	
Source organism	Arthromyces ramosus
Crystallization and crystal data	
Crystallization method	Sitting-drop vapour diffusion
Temperature (K)	297
Additional details	37% saturated ammonium sulfate, Tris-HCl, pH 7.5, microdialysis, temperature 297 K
Crystallization solutions	
Crystal data	
Crystal size (mm)	
Matthews coefficient, V_M (Å^3 Da^{-1})	2.21
Solvent content (%)	45.11
Unit-cell data	
Crystal system, space group	$P4_22_12$
a, *b*, *c* (Å)	73.84, 73.84, 115.68
α, β, γ (°)	90, 90, 90
No. of molecules in unit cell, *Z*	

Table 2. Data collection and structure solution statistics

Values for the outer shell are given in parentheses.

Diffraction source	Synchrotron; SPring-8 beamline BL41XU
X-ray beam size	
Sampling protocol	

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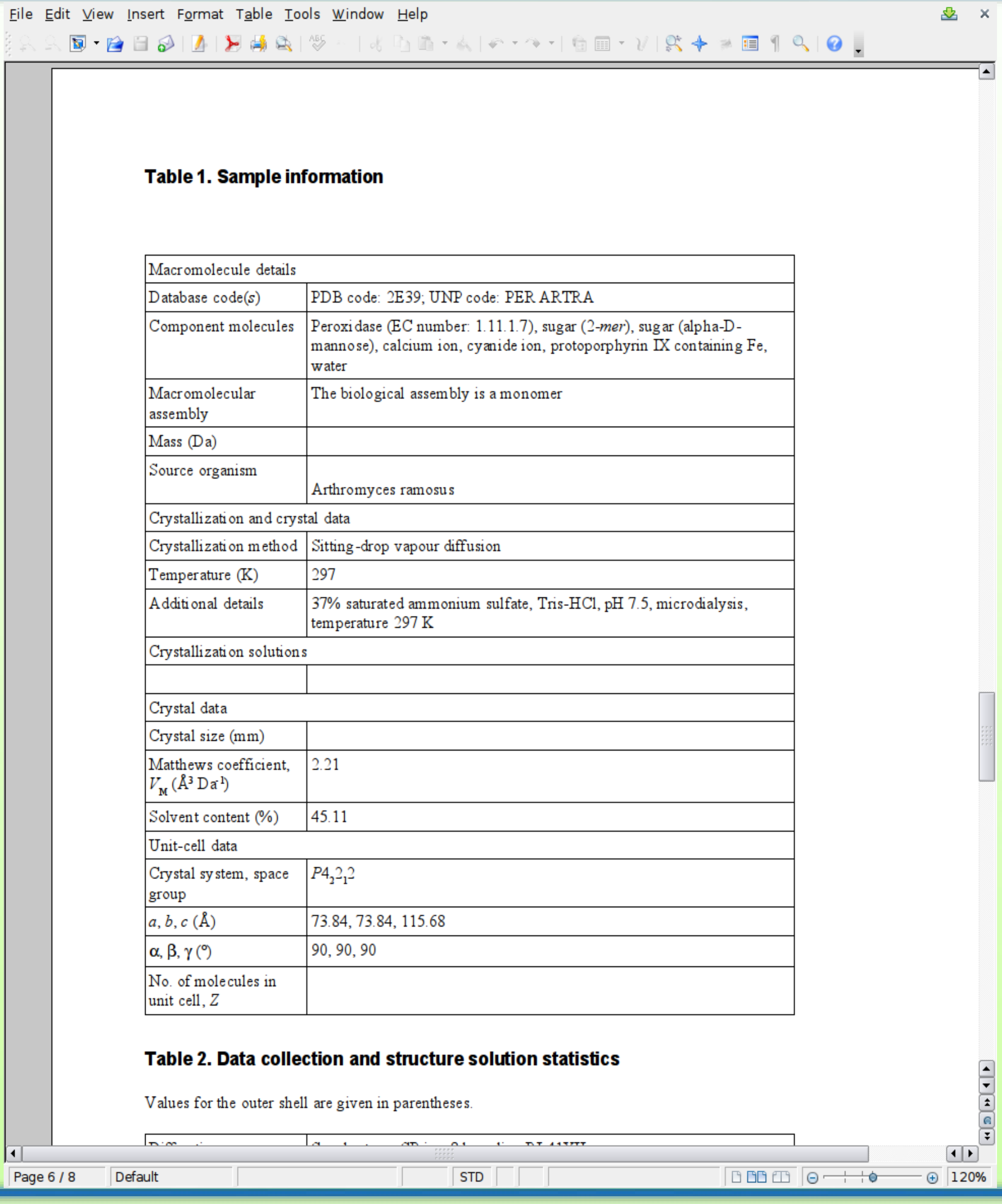

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