

Experiment Report Form

The double page inside this form is to be filled in by all users or groups of users who have had access to beam time for measurements at the ESRF.

Once completed, the report should be submitted electronically to the User Office using the **Electronic Report Submission Application:**

<http://193.49.43.2:8080/smis/servlet/UserUtils?start>

Reports supporting requests for additional beam time

Reports can now be submitted independently of new proposals – it is necessary simply to indicate the number of the report(s) supporting a new proposal on the proposal form.

The Review Committees reserve the right to reject new proposals from groups who have not reported on the use of beam time allocated previously.

Reports on experiments relating to long term projects

Proposers awarded beam time for a long term project are required to submit an interim report at the end of each year, irrespective of the number of shifts of beam time they have used.

Published papers

All users must give proper credit to ESRF staff members and proper mention to ESRF facilities which were essential for the results described in any ensuing publication. Further, they are obliged to send to the Joint ESRF/ ILL library the complete reference and the abstract of all papers appearing in print, and resulting from the use of the ESRF.

Should you wish to make more general comments on the experiment, please note them on the User Evaluation Form, and send both the Report and the Evaluation Form to the User Office.

Deadlines for submission of Experimental Reports

- 1st March for experiments carried out up until June of the previous year;
- 1st September for experiments carried out up until January of the same year.

Instructions for preparing your Report

- fill in a separate form for each project or series of measurements.
- type your report, in English.
- include the reference number of the proposal to which the report refers.
- make sure that the text, tables and figures fit into the space available.
- if your work is published or is in press, you may prefer to paste in the abstract, and add full reference details. If the abstract is in a language other than English, please include an English translation.



	Experiment title: St. Andrews Dundee BAG	Experiment number: LS-2087
Beam line: 14.2	Date of experiment: from: 4 th July to: 5 th July	Date of report: 09/08/01
Shifts: 3	Local contact(s):	<i>Received at ESRF:</i>
Names and affiliations of applicants (* indicates experimentalists): Adam Staines* Chiang Jiang Dong* James H. Naismith		

Report:

UDP- Galactopyranose mutase (mutase):

Crystals of mutase from *Mycobacterium Tuberculosis* were taken to Grenoble both as prefrozen samples and in hanging drop plates (stored at 4°C during transit). Fresh protein was also brought with the intention of producing new crystals.

Diffraction of crystals with the in-house source has proven unsuccessful therefore crystals had to be screened for diffraction quality at Grenoble. Despite a large number of crystals (both prefrozen and frozen on site) none diffracted beyond 3.2Å (which corresponds to the best resolution dataset achieved to date). Fresh crystals grown onsite overnight also failed to give improved resolution. Attempts to improve resolution by alteration of freezing conditions also proved unsuccessful.

RT dataset 1: resolution: 3.4 Å space group: P4 cell: 140 140 153 90 90 90
no. of frames collected: 5 mosaicity: 0.9, collection stopped due to radiation damage

RT dataset 2: resolution: 3.2 Å space group: P4 cell: 140 140 151 90 90 90 no. frames collected: 3 mosaicity: 0.8, collection stopped due to radiation damage

frozen dataset 1: resolution: 3.6 Å space group: cell: 140 140 150 90 90 90

no. of frames collected: 10 mosaicity: 0.6, collection stopped as processing revealed poor resolution

frozen dataset 2: resolution: 3.4 Å space group: P4 cell: 140 140 151 90 90 90

no. of frames collected: 15 mosaicity: 1.1, collection stopped as processing revealed poor resolution and high mosaicity

WbID

Bordetella pertussis is the causative agent of whooping cough. Although the vaccine of killed bacteria is effective there are well known severe side effects which can occur in a small number of infants. Parents have always been concerned about having their children vaccinated against whooping cough for this reason. Carbohydrate based vaccines, such as those *H. Influenzae* B (HIB) and *N. meningitis* C (MENEC) have excellent safety and efficacy. A carbohydrate based vaccine for whooping cough has been developed and tested, whilst very safe its efficacy has been called into question. The efficacy could be improved by adding further components, in particular the outer carbohydrate of the LPS molecule. We have shown that the functional assignment of the gene sequence for the outer part of the LPS molecule of *B. pertussis* is wrong. As a result the biosynthetic pathway is incorrect. To determine the biosynthetic pathway we have crystallised the wbID enzyme. Using the MAD structure determination we performed using BM14 UK , we molecular replaced the native data.

Table 1 Preliminary data (refinement in progress)

	Native
Wavelength	0.933
Cell constants	a = 77.73Å b = 89.86Å c = 123.25Å
Space group	P212121
Resolution	62 – 1.6
Total measurements	1907354
Unique reflection	135118
Completeness	96.2
Rmerge	12.4
R-factor	24.6
R-free	26.9
RMSD bond	0.018
RMSD Angle	1.86