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ESRF

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.

ESRF	**Experiment title:** Crystallographic studies of Staphylococcal exotoxin 1	**Experiment number**: LS-1941
Beamline: ID 14, EH2	**Date of experiment**: from: 21/4/01 to: 23/4/01	**Date of report**: 20/8/01
Shifts: 2	**Local contact(s)**: Hassan Belrhali	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

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Report:

Staphylococcal exotoxin 1 (sET1) is a member of a newly discovered family of superantigen related proteins from *Staphylococcal aureus*. Superantigens in general interact with MHC class II molecules and T-cell receptors in a non-peptide dependent manner, thus eliciting a massive cytokine response from a wide rage of T-lymphocytes, resulting in a range of disease. Experiments with sET1 have failed to elicit this response from T-cells to date, and this protein may thus be able to shed light on the evolution of these toxins, and perhaps on the origin of their function, since utility of a large scale immune response for the bacteria's viability is still unclear.

SET1 is a 24 kDa, 230 residue protein which contains no cysteines and only a single methionine, it has, at best, 24% identity to any known structure. Structure solution is being attempted by standard multiple isomorphous replacement methods. Crystals grow readily using PEG 2k as a precipitant, buffered at pH 8.0 with 0.1M Tricine in the presence of 0.1 M Lithium sulphate. The crystals are in spacegroup $P4_{1/3}2_12$, with cell dimensions a=b=81.7 Å, c=148.0 Å, there are probably 2 molecules in the asymmetric unit. Prevoiusly, crystals formed near-perfect twins (in different crystallisation conditions) which are not detectable from crystal morphology. The new crystallisation conditions (outlined above) gave untwinned crystals, and a native dataset has been obtained to 2.75 Å (molecular replacement has been attempted without success. Two heavy atom derivatives were being screened during this beamtime.

Results:

A Gold Cyanide derivative dataset was collected. This diffracted to 3.6Å, and was processed in MOSFLM/Scala. This gave an R_{sym} = 0.162, with an overall completeness of 100%, and an I/δI of 3.6. Space group was determined as $P4_{1/3}2_12$, with unit cell dimensions of a=b=81 Å, c=147 Å. However, examination of the dataset for heavy atoms was unsucessful, and no phase information could be gained.