EUROPEAN **S**YNCHROTRON **R**ADIATION **F**ACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

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:** Structure determination of Epsilon toxin of *Clostridium perfringens*	**Experiment number**: LS1941
Beamline: ID14 EH1	**Date of experiment**: from: 21.04.01 to: 24.4.01	**Date of report**: 20.08.01
Shifts: 6 shifts	**Local contact(s)**: Dr. Hassan Belrhali	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Ambrose Cole*, David Moss, Ajit K. Basak*

Depart of Crystallography,

Birkbeck College,

Malet Street,

London WC1E 7HX,

UK

Report:

Heavy Atom soaks on Epsilon Prototoxin

Two datasets were collected of recombinant epsilon prototoxin, of which a previous native dataset has already been collected to a resolution of 2.5Å. The two compounds chosen had previously produced promising but unsuccessful results with the wild type prototoxin. Both datasets went to a resolution of about 4Å and produced satisfactory statistics with SCALA, scaling in P321. Further processing has however indicated complete none-isomprhism with both the native dataset and each other, even when the data sets are reindexed. This problem has occurred with the wild-type prototoxin and so single crystal experiments will be needed to solve the structure.

	K_2PtCl_4	$NaAuCl_4$
Diffraction Limit (Å)	4	3.8
Rmerge (%)	8.3	10.3
I/sd	19	12.5
Comp (%)	98.7	98.8
Mult (%))	4.8	4.5

Se-Met data from prototoxin and toxin crystals:

Single wavelength datasets were taken of the recombinant Semet derivatives both of these diffracted well to 2.5Å. Upon processing these data sets it became clear that they were however perfectly twinned with the an apparent symmetry of $p6_322$. Checking the twinning fraction also indicated that the twinning fraction was 50%.

	Prototox	Tox
Diffraction Limit (Å)	2.5	2.5
Rmerge (%)	8.8	8.6
I/sd	13.9	15.3
Comp (%)	100	99.7
Mult (%))	7.0	6.9