



EUROPEAN SYNCHROTRON RADIATION FACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

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: DUNDEE-ST.ANDREWS BAG	Experiment number: LS-2178
Beamline: ID14EH4	Date of experiment: from: 09/05/2002 to: 10/05/2002	Date of report: 25/07/2002
Shifts: 1	Local contact(s): Gordon Leonard	<i>Received at ESRF:</i>
Names and affiliations of applicants (* indicates experimentalists): Charles Bond* School of Life Sciences, University of Dundee		

Report:

* Hje, a second Holliday junction resolvase from *Sulfolobus solfataricus*.

Following up on work from the previous BAG on Hjc, we have obtained crystals of Hje, a second resolvase from *S. solfataricus* which has homology to Hjc. The structure is of interest as Hje and Hjc have quite different DNA cutting patterns. Restriction enzymes in general utilise differing arrangements of monomers in a dimer to vary the cutting pattern, but sequence analysis suggests that Hjc and Hje should have a conserved dimer interface. Time on EH2 on the previous day was used to obtain a good quality native dataset prior to the successful MAD/SAD experiment performed on EH4. Hje contains 2 Met residues per monomer (disregarding the initiating Met) and Matthews coefficient and a K=180 self rotation function peak indicate the presence of a dimer in the AU.

Data: A scan across the selenium edge a strong fluorescence signal with a significant white line, indicating that anomalous data should be collected at energies of 12.661 GeV (peak), 12.6583 GeV (inflection) and 13.2 GeV (remote). Indexing of the initial diffraction pattern confirmed P61/5 spacegroup with typical unit cell of 92.1, 92.1, 72.3, 90, 90, 120 and MOSFLM/STRATEGY suggested collecting wedges of 60 degrees for 4-fold multiplicity of Bijvoet pairs. Scaling and SCALA analysis suggested that a strong anomalous signal was present.

Analysis: While on the beamline still, we ran SOLVE which produced a consistent set of 4 Se sites quickly and very good phasing statistics (FOM > 0.5) in spacegroup P65. The maps both before and after RESOLVE were, however, uninterpretable. At this point we chose to compare the 4 Se sites with an anomalous Patterson calculated using the peak data and decided that they were consistent, so we ran MLPHARE with these sites as SAD phasing using the peak data. The results were excellent. While the MLPHARE FOM was lower than the SOLVE one, at 0.23, DM converged very quickly producing a high quality map which WARP easily interpreted. We have not investigated this further as we are busy analysing the model!

