EUROPEAN SYNCHROTRON RADIATION FACILITY

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 via the User Portal:

https://wwws.esrf.fr/misapps/SMISWebClient/protected/welcome.do

Reports supporting requests for additional beam time

Reports can 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:** Structural and functional analysis of the chlamydial tail specific protease (Tsp)	**Experiment number**: **MX-1338**
Beamline:	**Date of experiment**: from: 12 Nov 2011 to: 13 Nov 2011	**Date of report**: 28.08.2012
Shifts:	**Local contact(s)**: Christoph Mueller dieckmann (email: christoph.mueller_dieckmann@esrf.fr)	*Received at ESRF:*

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Report:

The major goal of this project was the X-ray structure determination of the Tsp protein CT441 from *C. trachomatis*. For our experiments at the ESRF beamline ID29 we used crystals of TspCt S455A labeled with selenomethionine (SeMet). In total we evaluated diffraction properties of 44 crystals and collected data on four different crystals:

1. On crystal FK1_3 we were able to collect one dataset (894 images) at a standard wavelength and one dataset (3600 images) at 9.69keV (Zn), both to a resolutions of 3.5 Å.
2. Diffraction data (2000 images) of the SeMet containing crystal FK1_7 was collected at 12.7 keV resulting in a resolution of 4.01 Å.
3. On the crystal FK5_4 we collected one full dataset (3600 images) at Se peak-wavelength (12.6613 keV) with a resolution of 3.28 Å and an additional full dataset (3600 images) at Se inflection-wavelength (12.6574 keV) with a final resolution of 3.2 Å.
4. For the crystal FK8_1 we collected one full dataset (3600 images) at Se peak-wavelength (12.6613 keV) with a resolution of 3.26 Å, a full dataset (3600 images) at Se inflection-wavelength (12.6574 keV) with a resolution of 3.18 Å and finally a full dataset (3366 images) at Se remote-wavelength (12.6903 keV) with a resolution of 3.27 Å.

MAD data collected from crystal FK5_4 was indexed (Mosflm, XDS) and scaled (Scala)resulted resulting in final resolution of approx. 3.5-3.8 Å. Unfortunately, we were unable to determine suitable phases for structure solution. This is likely caused by the weak anomalous signal which was detected and the limited resolution of the collected data. Although, it was not possible to detemine the structure of CT441 the results obatined from ESRF enabled us to subsequently improve the crystallization conditions and cryo-protocol to optimize diffration properties of our CT441 crystals. Structure determination is in progress.