



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://www.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.

**Experiment title:**

Structure based drug design to gain more insights into the inhibitor binding for further drug development for Dengue (**DENV-3**) and **FtsZ**

Experiment**number:**

MX1782

Beamline:	Date of experiment: 5 th April 2016 (ID23-2), 13 th July 2016 (ID30A1-Massif Beamline) and 11 th June 2016 (ID30B)	Date of report:
Shifts:	Local contact(s):	<i>Received at ESRF:</i>

Names and affiliations of applicants (* indicates experimentalists):

Dr. Sandeep Kumar Talapatra, UCL School of Pharmacy, 29-39 Brunswick Square, London WC1N 1AX

Report:

DENV-3 is a part of the flavivirus RNA-dependent RNA polymerase (RdRp) located at the C-terminus of nonstructural protein NS5 of the Dengue virus. Collected multiple datasets (around 25) in the range of 1.8 – 3.0 Å. These measurements were completed during the 5th April and 13th July visits.

Currently, the manuscript is in preparation from these visits and respective PDBs will be submitted in the next few weeks.

FtsZ is a protein that assembles into a ring at the future site of the septum of bacterial cell division. It is a prokaryotic homologue to the eukaryotic protein tubulin. We will employ structure based drug design along with other biochemical methods to improve on the already available inhibitors of FtsZ. We have obtained native protein structure with datasets within a range of 1.8 – 2.0 Å during the 11th June visit that will now be used for further structure based drug discovery.

