



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>

Deadlines for submission of Experimental Reports

Experimental reports must be submitted within the period of 3 months after the end of the experiment.

Experiment Report supporting a new proposal (“relevant report”)

If you are submitting a proposal for a new project, or to continue a project for which you have previously been allocated beam time, you must submit a report on each of your previous measurement(s):

- even on those carried out close to the proposal submission deadline (it can be a “*preliminary report*”),
- even for experiments whose scientific area is different from the scientific area of the new proposal,
- carried out on CRG beamlines.

You must then register the report(s) as “relevant report(s)” in the new application form for beam time.

Deadlines for submitting a report supporting a new proposal

- 1st March Proposal Round - **5th March**
- 10th September Proposal Round - **13th September**

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.

Instructions for preparing your Report

- fill in a separate form for each project or series of measurements.
- type your report in English.
- include the experiment number 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: FUNCTIONAL AND STRUCTURAL STUDIES OF REGULATION MECHANISMS OF THE SUMO/UBIQUITIN PATHWAY	Experiment number: MX2348
Beamline: ID30B	Date of experiment: from: 22/4/2021 to: 23/4/2021	Date of report: 12/5/21
Shifts: 2	Local contact(s): Andrew McCarthy	<i>Received at ESRF:</i>
Names and affiliations of applicants (* indicates experimentalists): David Reverter Nathalia Varejao Jara Lascorz Lucia Sanchez Ying Li		

Report:

Crystals measured at the ID30B beamline at the ESRF from April 22th to April 23th in the context of the MX-2348 project. A total of 92 crystals from two projects were checked at the ID30B beamline, for all of them it was the first time diffraction and it was uncertain whether they were crystals of protein or salt, and whether they would diffract. We could finally collect 8 datasets. Next you can find the highlights of the results for the two projects:

1) The structural/function mechanism for the deSUMOylation activity of the **USPL1**, a member of the **USP** de-ubiquitinase family.

Four datasets could be collected for this project. One at high resolution (1.8 Å). Crystals belonged to the monoclinic space group, P2₁, and contained one USPL1-SUMO complex per asymmetric unit. The structure could not be solved by molecular replacement because the sequence identity with the possible models are less than 20 %. We expect in the next future to use heavy atoms soaking to find the phases.

Here you can find a statistic table of the best dataset collection from the program aimless:

	Overall	InnerShell	OuterShell
Low resolution limit	69.93	69.93	1.89
High resolution limit	1.85	9.08	1.85
Rmerge (within I+/I-)	0.079	0.055	0.695
Rmerge (all I+ and I-)	0.088	0.057	0.736
Rmeas (within I+/I-)	0.112	0.078	0.977
Rmeas (all I+ & I-)	0.109	0.071	0.947
Rpim (within I+/I-)	0.079	0.055	0.685
Rpim (all I+ & I-)	0.065	0.043	0.587
Rmerge in top bin	0.060	-	-
Total number observations	75006	613	3412
Total number unique	30339	260	1543

Mean(I)/sd(I)	6.0	14.2	1.2
Mn(I) CC(1/2)	0.991	0.992	0.531
Completeness	94.8	88.2	78.3
Multiplicity	2.5	2.4	2.2
Mean(Chi ²)	0.89	0.83	0.80

2) The structural/function mechanism of the *Nse2* SUMO E3 ligase, which is a subunit of the *Smc5-Smc6* complex.

A few datasets could be collected for this project, the dataset with the highest resolution reached only 4.5 Å. Crystals belonged to the trigonal space group, P3₁21, and contained one complex per asymmetric unit. The structure could be solved by molecular replacement using two components of the complex and the final electron density showed the different chains at this low resolution (4.5 Å). The goal for the next trip to ESRF will be to improve the resolution of the crystals of this complex.

Data set of their best collection:

	Overall	InnerShell	OuterShell
Low resolution limit	98.148	98.148	4.792
High resolution limit	4.511	13.665	4.511
Rmerge (all I+ & I-)	0.161	0.057	1.550
Rmerge (within I+/I-)	0.162	0.055	1.472
Rmeas (all I+ & I-)	0.174	0.063	1.649
Rmeas (within I+/I-)	0.186	0.064	1.673
Rpim (all I+ & I-)	0.063	0.026	0.559
Rpim (within I+/I-)	0.090	0.033	0.788
Total number observations	38767	1412	2140
Total number unique	4978	248	250
Mean(I)/sd(I)	7.7	23.8	1.5
Completeness (spherical)	83.4	98.8	26.0
Completeness (ellipsoidal)	89.8	98.8	43.3
Multiplicity	7.8	5.7	8.6
CC(1/2)	0.997	0.997	0.647

Final low-resolution complex structure of *Nse2*/Smc5-Ubc9-SUMO at 4.5 Å:

