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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:** BAG-LEBS-2005-2	**Experiment number**: MX-441
Beamline: BM30A	**Date of experiment**: from: 29/09/05 08:30 to: 29/09/05 8:30	**Date of report**: 24/02/06
Shifts: 3	**Local contact(s)**: Dr. Sonia Fieulaine	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Philip Simister* (post-doctoral researcher), Jean-Christophe Zeeh* (PhD student), Louis RENAULT* (Research Assitant, CR1 CNRS); LEBS, Bât. 34, 1 Avenue de la Terasse, CNRS, 91190, Gif-sur-Yvette, France

Report:

Philip SIMISTER, Jean-Christophe Zeeh (1.5 shifts) : ArnoSec7[E156K]/ΔArf1 small G protein/GDP/inhibitor:

The experiment went well. We tested several crystals and collected one good dataset of this complex with high and low resolution passes. The processing statistics are shown below. The space group and unit cell parameters indicated that the complex had crystallised in the identical space group to the published complex without inhibitor. After refinement, it was clear that there was no density present representing the inhibitor molecule. These data have enabled us to redefine the strategy in order to obtain the desired quaternary complex.

Data collection statistics		
Complex	**Arf1[Δ17] -GDP-ARNO[E156K]-inhibitor**	**Arf1[Δ17] -GDP-ARNO[E156K]***
Space Group	$P3_221$	$P3_221$
Unit Cell a (Å)	104.056	104.018
b (Å)	104.056	104.018
c (Å)	69.378	69.277
Wavelength (Å)	0.934	0.931
Resolution limits (Å)	34.12 - 1.95	30 - 1.46
high resolution shell	2.02 -1.95	1.47-1.46
Reflections: measured	176835	1199546
unique	31441	75051
Completeness (%)	97.0 (93.9)	99.3 (97.0)
R_{symm} (%)	7.3 (28.4)	5.9 (46.2)
I / σ	13.4 (2.01)	26.6 (5.9)

Values in parentheses are for the highest resolution shell.
* Published structure, PDB code: 1R8S

Louis RENAULT (1 shift) : Structural study of innate immunity defense Guanylate binding proteins (GBPs):

Guanylate binding protein (GBP) 1 is a 67kDa multi-domain GTP-binding protein which relays antiviral and anti-angiogenic effects in cells with unknown mechanisms at the molecular level [*Guenzi, E. et al. (2003) The guanylate binding protein-1 GTPase controls the invasive and angiogenic capability of endothelial cells through inhibition of MMP-1 expression. EMBO J. 22, 3772-82*]. GBP1 belongs to the family of dynamin-related GTPases which are multi-domain large GTPases characterized by nucleotide-dependent oligomerizations associated with high-turnover GTPase activities. Their mechanisms of regulation as molecular switch or mechano-chemical enzymes in key cellular pathways remain elusive [*Praefcke, G. J. & McMahon, H. T. (2004) The dynamin superfamily: universal membrane tubulation and fission molecules? Nat Rev Mol Cell Biol 5, 133-47*]. Additionally GBP isoforms have the unique capacity among GTPase to hydrolyze GTP into GDP and GMP. As first model of Guanylate binding proteins we target the molecular mechanism of regulation of GBP1.

We tested on BM30A putative crystals of full length GBP1-GppNHp dimers, GppNHp being a non-hydrolyzable GTP analog. No data set were collected since all crystals showed diffraction patterns heavily splitted.