**E**UROPEAN **S**YNCHROTRON **R**ADIATION **F**ACILITY

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# 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:** CNRS Gif sur Yvette BAG (LEBS) | **Experiment number**: LS 2072 |
|---|---|---|
| **Beamline**: ID14-4 | **Date of experiment**: from: 14/09/2001 to: 15/09/2001 | **Date of report**: 22/02/2002 |
| **Shifts:** 3 | **Local contact(s)**: Dr. Stéphanie MONACO | *Received at ESRF:* |

**Names and affiliations of applicants** (* indicates experimentalists):

Sonia FIEULAINE*****, PhD student, Ines LI de la SIERRA-GALLAY*****, Post-Doc, Joel Janin, Professeur Universite Orsay, Laboratoire d'Enzymologie et Biochimie Structurales (LEBS), CNRS, Gif-sur-Yvette

Marie-Helene Le Du*****, CEA, Marc Graille*****, PhD student, Paula Llinas*****, PhD student, Dépt. Ingéniérie et Etude des Protéines-CEA, Saclay

## Report:

### Sonia FIEULAINE, Ines LI de la SIERRA-GALLAY (1.5 shift)

HPr-kinase/phosphorylase is a bacterial Ser/Thr kinase which has no sequence similarities with other known protein kinases. Sugars enter the cell via the PTS system, then glycolysis produces FBP which activates phosphorylation of the small protein HPr on residue Ser-46, catalysed by HPr-kinase. Further interaction of P-Ser-HPr with the transcription regulator CcpA activates the carbon catabolite repression signalisation pathway. The aim of this study is to understand the catalytic mechanism of the enzyme HPr-kinase/phosphorylase.

In 2000, we solved the structure of the enzyme at 2.8 Å resolution by MAD. Here we collected a 2.5 Å native data set, which has allowed us to improve the quality of the structure. In addition, we collected 2 data sets of a new crystal form, but the data were of insufficient quality for structure solution.

### Marie-Helene Le Du, Marc Graille, Paula Llinas, (1.5 shift)

The parasite *Toxoplasma gondii* is responsible for toxoplasmosis, a worldwide infectious disease that can be life-threatening in immunocompromised individuals and in pregnant woman. The protein P30, present at the surface of the invasive form of the parasite plays a major role in parasite attachment to the host cell. Then, the crystal structure of the complex between P30 and the Fab of a neutralising antibody is of biological importance to map the epitope responsible for parasite entry in the host cell. No protein of known structure possesses a sequence identity sufficiently important to be used as a model to solve the structure by molecular replacement method. Previous crystals of the P30-Fab complex had diffracted to 4.3 Å resolution. No data set have been collected. However, heavy atom derivatives were tested but the crystal diffracted poorly (4.5-5

Å). Then, we need to collect native data set to a higher resolution and to obtain phases from MAD or MIR to solve the structure.

The human urokinase receptor, a highly glycosylated protein, plays an important role in cancer and cell invasion. The elucidation of the structure will be of great importance in the diagnosis and therapy in cancer. This receptor in complex with different peptides crystallise in a cubic space group and one of these complexes contains an anomalous scatterer (Hg). We had previously collected a MAD data set (3.9 Å) from this complex at BM 30 and we wanted to improve this resolution in ID 14-4. We tested the complex that contains the anomalous scatterer and some heavy atom derivatives (and anomalous scatterer) but they did not diffract at better resolution than we already had.