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 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:** Proteins in lipid metabolism	**Experiment number**: LS-1757
Beamline: ID14 4	**Date of experiment**: from: 28-sep-2000 to: 29-sep-2000	**Date of report**:
Shifts: 3	**Local contact(s)**: Sean McSweeney	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

*Henriksen, Anette

*Gotthardt Olsen, Johan

*Blicher, Thomas

Report:

β-Ketoacyl [acyl carrier protein] synthase (KAS I)

A 1.7 Å data has been collected for the *E. coli* K328→A active site mutant. This mutant has ketoacyl transferase activity but no decaboxylation activity. The structure has been refined and structural analysis is in progress.

Data has been collected on the *E. coli* KAS I K328→A active site mutant soaked with malone amide, malonyl-CoA and dodecanoyl-CoA, to 2.1, 2.1 and 2.0 Å resolution, respectively. The malone amide and malonyl–CoA soaked crystals decayed rapidly in the beam and more data need to be collected to obtain complete data sets for these soaks at the high resolution needed for detailed analysis of the decarboxylation process. The strucutre of the KASI K328→A:dodecanoyl complex has not yet been refined, but the data quality is good to 2.0 Å, and the structure solved with molecular replacement shows an interpretable electron density in the lipid binding pocket.

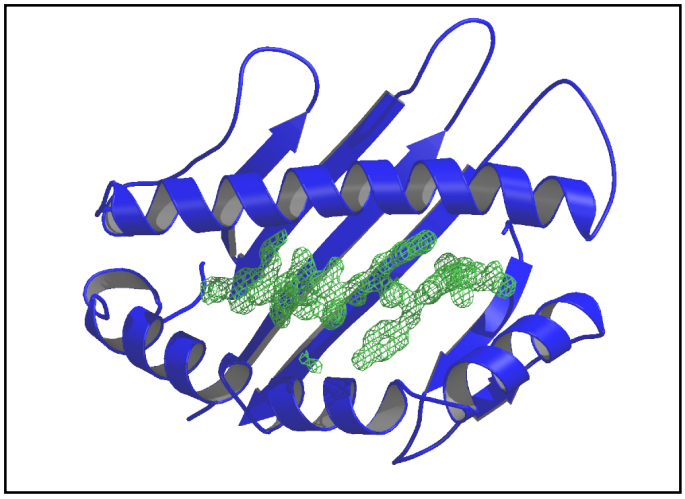
Barley phospolipid transfer protein

1.7 Å data has been collected on the barley lipid transfer protein with a L-α-lysophotadidylcholine, lauroyl molecule in the lipid binding pocket. The structure has been refined and structural analysis is in progress.

HLA-A*1101

Two data sets of the novel MHC class I molecule HLA-A*1101 were collected on two individual crystals diffracting to a resolution of 1.9Å and 1.6Å, respectively. The 1.6Å data set has been processed and the structure of HLA-A*1101 solved by molecular replacement. The structure is currently in the final stages of refinement and provides new insights in the details of peptide binding to MHC molecules.

Figure 1.
Picture showing the important part of HLA-A*1101: The binding cleft with the electron density of the bound peptide.



Beta-2-microglobulin

A native data set to 2.7Å was collected on a crystal of human beta-2-microglobulin, an essential subunit of MHC class I molecules. The data has not yet been analysed.