EUROPEAN **S**YNCHROTRON **R**ADIATION **F**ACILITY

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:** EMBL Grenoble Outstation BAG (Virus structure group of Rob Ruigrok)	**Experiment number**: LS 1814/LS 1945
Beamline: various	**Date of experiment**: from: September 2000 to: August 2001	**Date of report**: 31/8/01
Shifts:	**Local contact(s)**: various	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Dr. Rob Ruigrok, EMBL Grenoble Outstation

Dr. Wim Burmeister

Report:

Crystal structure of the Epstein-Barr virus protease inhibited by diisopropyl-fluorophosphate.

Epstein-Barr virus is a γ-Herpesvirus which infects more than 90% of the world poulation with a life-long persistance, which often leads to lymphomas in immunosuppressed individuals.. The protease of this virus is produced as a polyprotein together with the scaffold protein and is essential for capsid formation and the encapsidation of the genome. It is a good target for the development of antiviral drugs. The protease could be produced as recombinant protein in E. coli. After inhibition with diisopropyl-fluorophosphate (DFP) the protein could be cristallised in space group $P6_122$ with cell parameters of a=b=53.8 Å c=348.6 Å. During congelation of the crystals for the data collection unit cell and symmetry change to $P3_121$ with the parameters a=b=52.8, c=330.5 Å. the resolution of the diffraction increases from 3.3 to 2.3 Å but the crystals become twinned by merohedrie with twinning fractions close to 50 %. This twinning could not be overcome. Still, the structure could be solved by molecular replacement using the structure of the related KSHV protease (50 % identity). The structure was refined to an R_{cryst} of 20% and an R_{free} of 27% against twinned data using CNS. The inhibitor is clearly seen bound to the active site serine. The structure gives some hints how a large loop close to the active site may be involved in substrate recognition. Large parts of the long loops of the structure are visible despite very high temperature factors in these areas.
The large unit cell and weak diffraction required data collections on the undulator beamlines ID29, ID14-1, ID14-3, ID14-4 and in a microfocus experiment on ID13.

Manuscript in preparation: W.P. Burmeister, M. Buisson, J.-F. Hernandez, R. W.H. Ruigrok, E. Drouet and J.M. Seigneurin. **Crystal structure of the Epstein-Barr virus protease inhibited by diisopropyl-fluorophosphate**.