

31 AUG 2000



BAG Beam time Progress Report

This represents a summary of the BAG progress in the reporting period, and is in addition to the standard ESRF report sheet for each project which will be used for the Review of the BAG.

BAG Title LS-1685: Structural biology of infectious agents (Institut Pasteur, Paris)

Allocation Period 1 January - 31 July 2000

List of publications resulting from ESRF beam time

Crystallization and preliminary X-Ray analysis of thymidylate kinase from *Mycobacterium tuberculosis*.
Acta Cryst. D (2000) D56, 226-228.

I. Li de la Sierra, H. Munier-Lehmann, A.M. Gilles, O. Barzu & M. Delarue.

Crystallization of the catalytic domain of murine Terminal desoxynucleotidyl Transferase.

N. Sukumar, J.B. Boulé, N. Expert-Bezançon, N. Jourdan, J. Lescar, F. Rougeon, C. Papanicolaou & M. Delarue. Acta Cryst. D. Accepted.

Global Summary

(1) Structural studies of oligomeric protein-protein interactions:

3 mutants of dihydrofolate reductase (DHFR) - resolution ranges 0.9 - 2.5 Å. Refinements in progress.

Wild-type Fc immunoglobulin fragment - 2.1 Å resolution. Refinement in progress.

3 mutants of nucleoside diphosphate kinase (NDK) with substrates - resolution ranges 1.15 - 2.2 Å. Refinements in progress.

(2) Cellobiohydrolase CelS from *Clostridium thermocellum* in complex with substrate - 2.5 Å resolution. Manuscript in preparation.

(3) 3 data sets of trypanosomal sialidases (TrSA) and trans-sialidases with substrates - resolutions ranges 1.6 - 3.0 Å. Refinements in progress.

(4) Glyceraldehyde 3-phosphate dehydrogenase - 2.8 Å resolution. Refinement in progress.

(5) Native and 2 heavy atom derivative data sets from Apoptosis Inducing Factor (AIF). Interpretation of structure in progress.

(6) 2 data sets from Terminal desoxynucleotidyl transferase (TdT) with substrates - resolution ranges 2.7 - 2.8 Å. Structure interpretation in progress.

Global Summary (cont.)

- (7) 15 data sets from Thymidylate kinase (TMK) as complex with different substrate analogues - resolution range 1.9 Å. Interpretation and refinement of structures in progress.
- (8) Anti-HIV protease antibody fragment Fv1696 as complex with peptide epitope - 2.7 Å resolution. Refinement in progress.
- (9) Mutant of MalE (MalE31) - resolution 1.85 Å. Manuscript in preparation.
- (10) *Plasmodium* MSP1-block2 GST fusion protein - resolution 1.85 Å. Refinement in progress.

Visits made to the ESRF

Date(s) of visits	Beamline	No. of Shifts	Short Summary of each Visit
(1) 7.4.2000	ID14-3	3	CelS & substrate; DHFR mutants, Fc of Ig; GPDH
(2) 9.4.2000	ID14-3	3	TdT & TMP substrate complexes
(3) 12.5.2000	ID14-1	3	Fv1696-peptide complex; TMP complexes; 4 hours beam down-time
(4) 19.6.2000	ID14-3	3	TMK & tDt substrate complexes; MSP1-block2/GST fusion protein; Male31
(5) 21.6.2000	ID14-3	3	TrSA with substrates; Mutant NDK with substrates
(6) 23.6.2000	ID14-4	3	AIF native & derivatives; TrSA with substrate