	Experiment title: Crystal structure of bacterial TMP kinase complexed with different substrates and inhibitors	Experiment number: LS-1685
Beamline: ID14-EH3	**Date of experiment:** from: 08-April-2000 to: 19-June-2000	**Date of report:** 25-Aug-2000
Shifts: 6	**Local contact(s)**: S. Monaco	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Marc DELARUE, C.N.R.S., Unité de Biochimie Structurale, Institut Pasteur, Paris, 75015.

Ines Li De La Sierra-Gallay, Unité de Biochimie Structurale, Institut Pasteur, Paris, 75015.

Report:

During these shifts, data were collected for different complexes between TMP kinase and AZTMP and other dTMP analogues synthesized by P. Herdewijn in Leuven, Belgium, at 1.9 Å resolution. They are currently being refined and analyzed.

Several crystals soaked both with ADP and chemicals intended to form AlF3 in situ were tried, in an attempt to characterize the transition state of the reaction. Preliminary data indicate that at least one of these experiments has been successful, with diffraction extending to 1.8 Å, showing clear electron density for AlF3 and ADP in Fourier difference maps.

A total of **15** useful and full data sets at 2.0 Å resolution or more have been collected and processed during this period. Some of them are still being studied/refined.

Publication

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.