



	Experiment title: Studies of new derivatives for MAD/SAD experiments	Experiment number: LS-1794
Beamline: ID14-4	Date of experiment: from: 9-11-00 to: 10-11-00	Date of report: 2-2-01
Shifts: 3	Local contact(s): E. GORDON	<i>Received at ESRF:</i>

Names and affiliations of applicants (* indicates experimentalists):

Eric Girard

Richard Kahn*

Jean Vicat*

Report:

The protein is a chimera form of OTC_{ase}.

A first experiment, made at the L_{III} gadolinium absorption edge (BM14, 9-Oct-2000), allowed to determine phases to a resolution of 3 Å resolution.

In order to extend the phases at higher resolution, six data sets were collected at a wavelength of 0.98 Å. Due to a rapid decrease in resolution, induced by radiation damage, data sets were collected on three gadolinium derivative crystals on the one hand, and on three native crystals on the other hand. During the data collection, each crystal was translated several times using 50 µm increments. Data have been processed with DENZO and have been scaled and merged with SCALA.

The statistics for the merged gadolinium derivative data are listed in the following table :

Maximum resolution (Å)	2.6
Highest resolution shell (Å)	2.73 – 2.59

Space group	P2 ₁
Cell parameter (Å)	a=111.45, b=220.01, c=125.45, β=111.27°
Number of measurements	652384
Unique reflections	145621
R factor	8.8 (21.9)
R ano	5.3 (23.6)
I/sigma(I)	5.6 (2.2)
Completeness	94.3 % (76.3 %)
Multiplicity	4.4 (2.5)

Values between parenthesis refer to the highest resolution shell

The statistics for the merged native data are listed in the following table :

Maximum resolution (Å)	2.5
Highest resolution shell (Å)	2.64 – 2.50
Space group	P2 ₁
Cell parameter (Å)	a=111.38, b=220.79, c=124.87, β=110.93°
Number of measurements	825558
Unique reflections	172279
R factor	5.8 (25.2)
I/sigma(I)	9.1 (2.0)
Completeness	95.1 % (81.0 %)
Multiplicity	4.5 (2.9)

Values between parenthesis refer to the highest resolution shell