	Experiment title: Beta glucosyl transferase BAG - CNRS gif sur Yvette	**Experiment number**: LS 1798
Beamline: ID14-H4	**Date of experiment**: from: 3/11/00 to: 3/11/00	**Date of report**: 27/02/01
Shifts: 1	**Local contact(s)**:	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

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Report:

β-glucosyltransferase (BGT) is a DNA-modifying enzyme encoded by bacteriophage T4 which catalyses the transfer of glucose from uridine to 5-hydroxymethylcytosine in double-stranded DNA. We have solved several structures of BGT in complex with UDP and metal ions at high resolution. Six refined structures are described in an article just submitted. Statistic for the data are as follows:

	Free BGT	+UDP	UDP+ Mg^{2+} Form 1	UDP+ Mg^{2+} Form 2	UDP+ Mn^{2+}	UDP+ Ca^{2}
Space group	P 4_1	P 2_1	P $2_12_12_1$	P $2_12_12_1$	P $2_12_12_1$	P 2_1
Resolution (Å)	2.5	1.9	2.5	2.07	1.65	1.65
Measured intensities	74,099	206,775	273,212	381,698	555,036	304,335
Unique reflections	14,640	30,548	12,981	23,440	48,279	49,706
Completeness (%)	100	99.3	90	99.4	99.8	98.8
I/σ	16.5	12.6	15.8	10.7	11.2	10.
Rsym (%)[a]	4.4	6.	7.1	8.8	7.7	4.

Publication :

Solange Moréra, Laurent Larivière, Jürgen Kurzeck, Ursula Aschke-Sonnenborn, Paul S. Freemont, Joël Janin and Wolfgang Rüger (2001).
High resolution crystal structures of T4 phage β-glucosyltransferase: Induced fit and effect of substrate and metal binding. Submitted to *J.Mol.Biol*

Abstract

β-glucosyltransferase (BGT) is a DNA-modifying enzyme encoded by bacteriophage T4 that transfers glucose from uridine diphosphoglucose to 5-hydroxymethyl cytosine bases of T4 DNA. We report six X-ray structures of the substrate-free and the UDP-bound enzyme. Four also contain metal ions which activate the enzyme, including Mg^{2+} in Forms 1 and 2 and Mn^{2+} or Ca^{2}. The substrate-free BGT structure differs by a domain movement from one previously determined in another space group. Further domain movements are seen in the complex with UDP and the four UDP-metal complexes. Mg^{2+}, Mn^{2+} and Ca^{2+} bind near the β-phosphate of the nucleotide, but they occupy slightly different positions and have different ligands depending on the metal and the crystal form. Whilst the metal site observed in these complexes with the product UDP is not compatible with a role in activating glucose transfer, it approximates the position of the positive charge in the oxocarbenium-ion thought to form on the glucose moiety of the substrate during catalysis.