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| | **Experiment title: BAG-LEBS-2004-2** | **Experiment number**: MX-350 |
| **Beamline**: ID14 eh1 | **Date of experiment**: from: 25/09/2004 8h to: 27/09/2005 8h | **Date of report**: 22/2/05<br>*Received at ESRF:* |
| **Shifts:** 6 | **Local contact(s)**: Dr S. MACEDO | |

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Report:

The BAG beam time allocation was normally scheduled on ID14- eh3 but because ID14- eh3 was not running on Saturday 25th September 2004, the experiment was transferred at ESRF on ID14-eh1.

**Alpha-glucosyltransferase :**

alpha-Glucosyltransferase (AGT) is a DNA-modifying enzyme encoded by bacteriophage T4 which catalyses the transfer of glucose from UDPG to 5-hydroxymethylcytosine (HMC) in double-stranded DNA. We previously solved the structure of AGT by SAD method. Here, we collected several datasets of AGT in complex with different oligonucleotide:

1- UDP and a 13-mer DNA containing a central HMU:G base pair at 3. Å resolution
2- UDP and a 13-mer DNA containing a central HMU:G base pair at 2.8 Å resolution
3-UDP and a 13-mer DNA containing a central A:G mismatch at 2.6 Å resolution
4- UDP and a 13-mer DNA containing a central A:G mismatch at 2.4 Å resolution
5- UDPG and a 13-mer DNA containing a central HMU:G base pair at 3.2 Å resolution

Datasets 2 and 4 were used for model building and refinement. Two pdbs are deposited and a manuscript is submitted.

**Yeast P-loop protein: YP6:**

We started a systematic structural and functional analysis of yeast P-loop containing proteins of unknown function. The HPr K/P example suggests that some of them could also be protein kinases. We cloned 12 out of them and 5 soluble proteins (called YP4 to YP8) are under crystallization trials. We recently solved the structure of YP6 by SAD method using a mercury derivative. Here, we collected two datasets: a high resolution native dataset at 1.95 Å resolution and a complex with ATP at 1.65 Å resolution. The structures are under-refinement.

**NDP kinase :**

NDP kinase supplies nucleoside triphosphates in the cell. We collected two datasets of NDPK in complex with an analog of nucleotide at 1.65 Å and 2.8 Å resolution. They belong to a different space group. The structures are under-refinement.