

Report of experiment MX497 on beamline ID14.4

The beamline is very well setup and maintained, and there is also enough space for mounting the crystals in the non-automated way.

We had only one problem: we would have liked to use DENZO to process our data, and for this purpose, we had the correct "cr_info" to run the program, but the program did not work. However we tested many crystals and we collected 10 datasets.

1) We have collected three different datasets on Cyclophilin A from *Schistosoma mansoni*, the crystals we measured have been soaked with two different molecules and displayed the native space group (P_{212121} , with the following cell dimensions $a=41.424$ $b=60.393$ $c=61.533$)

a) CsA (cyclosporinA). The crystal diffracted at 1.6Å resolution. The data set have been processed and unfortunately, the crystals did not contain the molecule.

b) LLPA (peptide). Two crystals have been measured at 1.8 Å and 2.0 Å resolution respectively. The data sets have been processed and unfortunately, the crystals did not contain the molecules.

2) We collected two data sets on two crystals of glutathione S-transferase from *Xenopus laevis*. The best crystal diffracted at 2.5 Å resolution. The crystals are orthorhombic P_{212121} , with the following cell dimension: $a=$

66.6200, $b=115.6080$, $c=191.0810$. We are trying to solve the structure by Molecular Replacement.

3) We collected two data sets on two crystals of flavodiiron proteins (FDP) from *Giardia lamblia*. Two crystals have been measured at 2.8 Å and 2.6 Å resolution respectively.

a) The first data set was 95 % complete; the measured crystal is monoclinic (P_{21}) with the following unit cell dimensions: $a=75.41$; $b=176.44$; $c=128.98$; $\beta=96.24$.

b) The second data set was 85 % complete; the measured crystal is centered monoclinic (C_2) with the following unit cell dimensions: $a=87.55$; $b=149.66$; $c=64.67$; $\beta=114.5$.

4) We collected three data sets on crystals of N-Methyltryptophan oxidase (MTOX), a flavoenzyme from *Escherichia coli*, soaked with the substrate (L-tryptophan).

The best crystal diffracted at 3.0 Å resolution: it is monoclinic (P_2) with the following unit cell dimensions: $a=88.1$; $b=89.7$; $c=91.8$; $\beta=104.73$. We already solved the structure of the native MTOX by Molecular Replacement. Unfortunately in the measured crystals L-tryptophan was not present.