Final Report of MX386 at BM16

Several data sets have been collected during the 24h shift at BM16.
Overall the beamline is very user-friendly. In particular, we appreciated the system of automatic centring of the crystal and of the beam-stop. Moreover, the access to the goniometer head is particularly good, making mounting frozen crystals without the arc very easy. The computer set up for data collection, processing and back up is well done and easy to use, although we experienced minor difficulties in mounting our firewire disk on the dedicated linux machine, apparently due to permissions/privileges, which were promptly cured by the beamline scientist, who had in any case to log in as root.
First of all, we performed a SAD experiment on a crystal of Se-Met derivative of the protein WhiE, an aromatase-cyclase from *Streptomyces coelicolor* expressed in *E. coli*. Before starting the data collection we measured the fluorescent spectrum of the crystal to choose the wavelengths for the peak and the remote. Both programs (energy_scan and chooch) are easy to learn and to interpret, as well as the procedure to change wavelength. Given the relatively small cell, we collected 720° with a $\Delta\phi$=2°. Although the initial resolution was 2.6Å, the crystal decayed quite quickly, so we integrated the images at 3.0Å. The remote data collection was performed over only 200°. In the following table there is a summary of the results:

	WhiE (peak)	WhiE (remote)
wavelength	0.9799 Å	0.9184 Å
Space group	P1	
Unit cell dimensions	a= 40.014Å; b= 40.115; c= 49.61; α= 92.49° β= 87.79° γ=109.22°	
Mosaicity	0.57	0.57
Completeness	98.99%	98.99%
Multiplicity	6.85	3.21
Rsym	0.113	0.15
B (Wilson)	30.1	30.5

Table1 summary of data from WhiE

After the SAD experiment we tested several tiny crystals (average size 50μm) of a site-directed mutant of *Schistosoma mansoni* Glutathione S-transferase co-crystallised in the presence of its substrate. Unfortunately none of the crystals tested diffracted better than 3.0Å, so no data collection was performed.
Same fate happened to the crystals of the activation domain of DNR, a DNA transcription protein from *Pseudomonas aeruginosa* expressed in *E. coli*, for which we were aiming to collect a better native data set, but none of the crystals went further 2.2Å, even with 60" exposure. Another series of unfortunate crystals, again impossible to check for diffraction at home given their dimensions, were those of the *Xenopus laevis* endoribonuclease XendoU, co-crystallised with UMP in the presence and in the absence of Mn^{2+}, which did not performed better than 3.1Å; and also those of the cytochrome P450, OleP, from *Streptomyces coelicolor* expressed in *E. coli*, whose diffraction did not reach 8.0Å and which were not even single crystals. In this chain of unfortunate crystals lied also the Xenon derivative of WhiE.

The series finally broke up when exposing crystals of WhiE soaked with Osmium, one of which diffracted to 1.8Å and was collected to completeness at the wavelength of the LI edge of Os (0.9561Å) to get the anomalous signal. 360 frames with $\Delta\phi=2°$ were collected, integrated using the cell refined from the SAD experiment, scaled and checked for the anomalous peaks. The data revealed to be the best and most complete native, with absolutely no sign of heavy metal.
Towards the end of the shift we collected the Xe-derivative of human deoxy hemoglobin crystals at high resolution. A summary is presented below as well as a picture of particular of the electron density map.

HbA-Xe	Data reduction
Space group	$P2_1$
Unit cell dimensions	a=62.64Å, b=82.33Å, c=53.55Å; β=99.79°
Mosaicity	0.43
Completeness (1.45-1.3Å)	99.8% (100%)
Multiplicity (last shell)	5.3 (4.8)
Rsym (last shell)	0. (0.213)
B from Wilson	19.2
	Refinement (50.0-1.3Å)
R	0.18
Rfree	0.23
r.m.s.d. bond length	0.0087
r.m.s.d. bond angle	1.02

Table2. Summary of data from the HbA-Xe

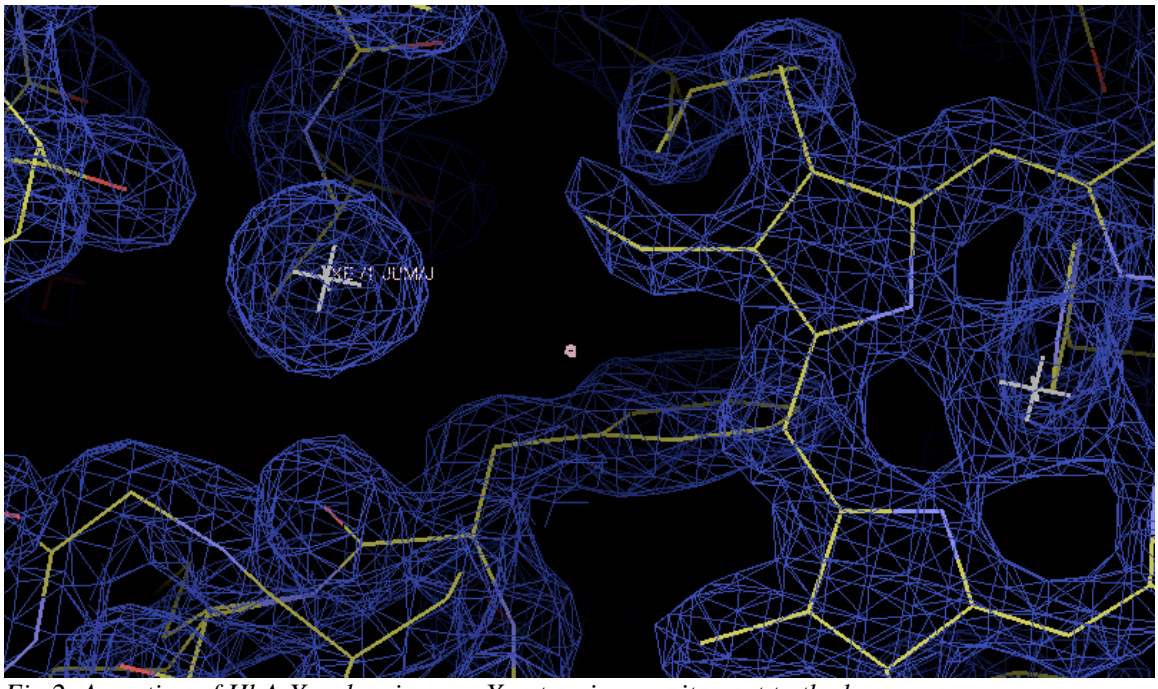

Fig.2. A portion of HbA-Xe, showing one Xe atom in a cavity next to the heme group.