Report of MX497 at the beamline ID23-1 (19/6/2006)

The 3 shifts at ID23-1 were particularly productive for many of our projects and in general we had no problems using the beamline devices.

1) Many crystals of Se-Met derivative of endoglucanase from *Pyrococcus furiosus* were tested, finally we were successful in collecting a MAD experiment at 2.7 Å resolution. A summary of data collection is reported in the following table.

	Se-Met edoglucanase		
Space group	C2		
Unit cell dimensions	a=121.84 Å, b=72.87 Å, c=91.76 Å		
	α=90°, β=100.35°, γ=90°		
	Pk	**Ip**	**Rm**
Resolution (Å)	30.0-2.8		
Wavelength (Å)	0.97925	0.97953	0.97570
Completeness (%)	99.1	98.7	96.4
R_{merge}	0.085	0.139	0.109

2) We tested many crystals of flavodiiron proteins (FDP) from Giardia lamblia; unfortunately most of them did not give good diffraction pattern. Finally we try to collect four different data sets at an initial resolution of ~2.3 Å. Unfortunately collected data were not complete because crystals belonging to the C2 space group with a long unit cell axis (we were forced to collect data with a 0.2/0.5 oscillation range) decade rapidly due to X-ray radiation damage.

3) In order study the role of cavities in neuroglobin (Ngb), we collected data on crystals of murine neuroglobin soaked with Xenon. Moreover we collected data for native crystals. Summary of data collections is reported in the table below.

	Ngb xenon
Space group	R32
Unit cell dimensions	a=89.2 Å, b=89.2 Å, c=111.3 Å
	α=90°, β=90°, γ=120°
Resolution (Å)	30.0-2.8
Wavelength (Å)	1.0
Completeness (%)	88.3
R_{merge}	0.107

	Ngb nativa
Space group	R32
Unit cell dimensions	a=89.7 Å, b=89.7 Å, c=112.4 Å
	α=90°, β=90°, γ=120°
Resolution (Å)[a]	50.0-3.8
Wavelength (Å)	1.0
Completeness (%)	99.5
R_{merge}	0.21

4) The sigma-class glutathione S-transferase from Xenopus laevis (Xlgsts1) is the smallest protein of sigma class GST identified so far as being composed of only 194 amino acid residues. It shows a narrow range of substrate specificity as well as a significantly lower 1-chloro-2,4-dinitrobenzene conjugation capacity than that of other sigma class GSTs. We collected one data set on crystal of Xlgsts1 in complex with glutathione. Data collection summary is reported in the following table.

	Xlgsts1
Space group	$P6_522$
Unit cell dimensions	a=66.67 Å, b=66.67 Å, c=191.12 Å $\alpha=90°, \beta=90°, \gamma=120°$
Resolution (Å)[a]	50.0-2.8
Wavelength (Å)	1.0
Completeness (%)	100%
R_{merge}	0.068