	Experiment title: Diffraction studies of ancestral thioredoxin (Atrx) and TRYP6 (L Major), and two bacterial proteins from Psedomonas Putida: MCPs	**Experiment number**: MX1106
Beamline: ID14-1/ID23	**Date of experiment**: from: 15/05/2010 to: 16/05/2010	**Date of report**: 27, August 2010
Shifts: 3	**Local contact(s)**: Dr. Elspeth GORDON	*Received at ESRF:*

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Report:

Diffraction studies of ancestral thioredoxin

Crystals of several ancestral thioredoxins, named ATrx250, ATrx325, grown by the counterdiffusion method were subject to data collection at ID14. Among them two data set were of sufficient quality to attempt the structural resolution by MR. Current status is as follow:

	ATrx250	**ATrx325**
Wavelength (Å)		
Space group	$P2_1$	P1
Cell parameters (Å)	55.00 30.19 59.00 90.0 116.0 90.0	32.15 36.29 48.12 90.76 107.97 111.01
Resolution range (Å)	48.45-1.52 (1.6-1.52)	45.32-1.75 (1.84-1.75)
Observed reflections	93980	70312
Independent reflections	26670	18887
Data completeness (%)	97.6 (84.7)	97.6 (88.7)
R_{merge} (%)[†]	5.3 (56.8)	10.5 (39.6)
Average I/σ (I)	16.9 (1.8)	8.5 (2.7)
Multiplicity	3.5 (2.7)	3.7 (2.9)
Mol/Asym	2	2
Matthews coefficient ($Å^3$ Da^{-1})	1.92	2.16
Solvent content (%)	35.82	43.1
Refinement		
R-work	17.4	21.5
R-free	20.5	28.7

NOTE: At this point, and after the initial diffraction-selection-test, the communication between the detector and the beam-line control software fail. After the intervention of the Local Contact the informatics engineer they decided that the problem could not be fix right the way and we move to ID23.

Diffraction studies of TRYP6

We did not have any useful crystal of TRYP6 (L Major) by the time of data collection and this system was substituted by the **B5/D48G mutant of Alpha-spectrin SH3 domain**, designed to improve the hydrophobic core and as a consequence the protein stability. Two data sets were collected to be merged and to solved the structure at 1 Å. The description has already been published (see reference) and a resume of the data collection and refinement statistics is summarized as follow:

Values in parentheses are for the highest resolution bin.

Data collection	
Space group	P212121
Unit-cell parameters (Å)	a=24.79,b=37.23,c=62.95
Resolution range (Å)	20 - 1.08
No. of observations	87782 (11438)
Unique reflections	25256 (3590)
Data completeness (%)	99.2 (98.4)
R_{merge} (%)†	7.1 (33.2)
Average I/σ (I)	11.1 (3.2)
Multiplicity	3.5
Wilson B factor (Å^2)	9.37
Refinement	
Protein residues	56
Solvent molecules	66
Rwork (%)	16.8
Rfree (%)	18.5
PDB. ID	3NGP

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High-resolution structure of an -spectrin SH3-domain mutant with a redesigned hydrophobic core
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Diffraction studies of MCPS (+ Citrate)

Approximately 20 crystals were tested for diffraction. Among them we collected two data sets composed of 150 frames with a maximum resolution limit of 2.7 Å. Crystals belong to the P222 space group with unit cell dimension 63.51 128.03 143.89 Å, for a, b, and c, respectively. Besides MR will be attempt with those data, crystal quality and size improvement is on going.

Diffraction studies of PTXS

Crystal of PTXS grown with and without ADN were tested at both beam lines, ID14 and ID23 (more than 12). The diffraction quality was very poor for PTXS and slightly better for crystals co-crystallize with ADN. PTXS-ADN crystals are of good visual quality when inspected by microscopy and therefore we think that the cryo-protection protocol could have an important influence on it. In situ cryo-protection of capillary counter-diffusion crystal grown crystal will be subject to analysis in future opportunities.