	Experiment title: X-ray analysis on the bacterial chemoreceptor McpS and the transcription regulator PtxS both from P.Putida	**Experiment number**: 16-01-765
Beamline: BM16	**Date of experiment**: from: 20/11/2010 to: 22/11/2010	**Date of report**: 2, March 2012
Shifts: 6	**Local contact(s)**: Mickael Cherrier (email: mickael.cherrier@ibs.fr) Eva Rosenbaum (email: eva.rosenbaum@esrf.fr)	*Received at ESRF:*

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Report:

Diffraction studies of McpS

We had previously collected native datasets on this protein together with one of its natural ligands, malic acid at BM16 (proposal CRG-1610-727). The lack of a model for MR brings us to the production of the Se-methionine to be tested at both BM-16 (proposal MX-1017) and Id14-4. With data collected at both BM16 (MX1017 and CRG-1610-727) and Id14-4 (MX-1016) we have solved the structure of MCPs together with malic acid (PDB ID. 2YFA) and succinate (PDB ID. 2YFB) (Submitted to PNAS and accepted in Acta Crust. F). This beam-time was initially intended to collect full data sets of McpS bound to citrate to complete our analysis since structures of McpS with malate and succinate, already solved. Unfortunately we were not able to produce crystals of sufficient quality and therefore the allocated time was used to diffract crystal of several systems including: a) Ancestral thioredoxines (ATrx365: 6 crystals, ATrx324: 8 crystals, ATrx325: 15 crystals, ATrx212: 15 crystals, ATrx205: 17 crystals); b) HbII from *L. pectinate* at pH 6.0 (31 crystals).

Diffraction studies of ancestral thioredoxin ATrx365

The structure has been refined and it is ready for deposit at the PDB.

	Trx365
Wavelength (Å)	0.98
Resolution range (Å)	20- 2.2 (2.28- 2.2)
Space group	P 21 21 21
Unit cell	37.5 42.8 55.9 90 90 90
Total reflections	51159
Unique reflections	4904
Multiplicity	10.4 (10.7)
Completeness (%)	100.00 (100.00)
I/sigma(I)	23.26 (4.95)
Wilson B-factor	29.19
R-sym	0.103 (0.487)
R-factor	0.1916
R-free	0.2486
Number of atoms	1751
Protein residues	105
Water molecules	41
RMS(bonds)	0.005
RMS(angles)	0.85
Ramachandran favored (%)	99
Ramachandran outliers (%)	0
Clashscore	16.97
Average B-factor	31.30

Diffraction studies of HbII at pH 6.0

These data will allow us to complete previous data set collected in the range of pH 4.0 to 9.0. The structure is still under refinement. Current statistics are shown below.

	HbII
Wavelength (Å)	0.98
Resolution range (Å)	15 - 2.45 (2.54 - 2.45)
Space group	P 42 21 2
Unit cell	75.3 75.3 153 90 90 90
Total reflections	204671
Unique reflections	16611
Multiplicity	12.3 (12.5)
Completeness (%)	98.60 (100.00)
I/sigma(I)	24.53 (3.41)
Wilson B-factor	49.75
R-sym	0.081 (0.763)
R-factor	0.2879
R-free	0.3092
Number of atoms	4912
Protein residues	305
Water molecules	42
RMS(bonds)	0.017
RMS(angles)	1.62
Ramachandran favored (%)	96
Ramachandran outliers (%)	0
Clashscore	57.19
Average B-factor	59.80