ESRF	**Experiment title:** Structure determination of SoxCD	**Experiment number**: MX-1175
Beamline: ID23-1	**Date of experiment**: from: April 2010 to:	**Date of report**: 13-12-2010
Shifts: 1	**Local contact(s)**: Alexander Popov, Daniele de Sanctis	*Received at ESRF:*

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Report:

The sulfur cycle enzyme sulfane dehydrogenase SoxCD is an essential component of the sulfur oxidation (Sox) enzyme system of *Paracoccus pantotrophus*. SoxCD catalyzes a six electron oxidation reaction within the Sox cycle. SoxCD is an $\alpha 2\beta 2$ heterotetrameric complex of the molybdenum cofactor-containing SoxC protein and the diheme c-type cytochrome SoxD with the heme domains D1 and D2. $SoxCD_1$ misses the heme-2 domain D2 and is catalytically as active as SoxCD. The crystal structure of $SoxCD_1$ was solved at 1.33Å. The substrate of SoxCD is the outer (sulfane) sulfur of Cys110-persulfide located at the C-terminal peptide swinging arm of the SoxYZ carrier complex. The $SoxCD_1$ substrate funnel towards the molybdopterin is narrow and partially shielded by side chain residues of SoxD1. For access of the sulfane-sulfur of SoxY-Cys110 persulfide we propose that (I) the blockage by SoxD-Arg98 is opened via interaction with the carboxy terminus of SoxY and (ii) the C-terminal peptide VTIGGCGG of SoxY provides interactions with the entrance path such that the cysteine bound persulfide is optimally positioned near the molybdenum atom. The subsequent oxidation reactions of the sulfane-sulfur are initiated by the nucleophilic attack of the the persulfide anion on the molybdenum atom which is, in turn, reduced. The close proximity of heme-1 to the molybdopterin allows easy acceptance of the electrons. Since SoxYZ, SoxA and SoxB are already structurally characterized, with $SoxCD_1$ the structures of all key enzymes of the Sox cycle are known with atomic resolution.

The publication is accepted for publication in the Journal of Biological Chemistry in a Februar issue 2011: "Structural basis for the oxidation of protein-bound sulfur by the sulfur cycle molybdohemo-enzyme sulfane dehydrogenase SoxCD", Zander, U.; Faust, A.; Klink, B.U.; De Sanctis, D.; Panjikar, S.; Quentmeier, A.; Bardischewski, F.; Friedrich, C.G. & Scheidig, A.J. The structure factors and model coordinates are available from the PDB data base under the PDB-entry 2XTS. The successful structure determination of $SoxCD_1$ was only possible by use of a high-intensity, small X-ray beam by scanning the crystals for parts where the intrinsic inhomogenities were not so great and the diffraction was good. This approach resulted in two data sets with very good data statistics.

Data collection and processing		
Data set	SAD-peak	High resolution
X-Ray source	ID23-1 (ESRF, Grenoble, France)	
Detector	ADSC Quantum Q315r	
Wavelength (Å)	1.74	0.98
Temperature (K)	100 K	
Crystal-to-detector distance (mm)	180	180
Oscillation range (deg.)	1.0	0.5
Total oscillation range (deg.)	360	60
Space group	P3(1)	P3(1)
Cell dimensions (Å)	a=123.19, c=76.42	a=122.97, c=76.39
Resolution limit (Å) [a]	50 - 2.37 (3.0 - 2.37)	50 - 1.33 (1.4 - 1.33)
Completeness (%) [a]	92.4 (88.2)	92 (72.9)
No. observations (overall / unique)	550606 / 48615	507433 / 273185
Average redundancy	11.3 (11.2)	1.8 (1.5)
$\langle I/\sigma(I) \rangle$ [a]	31.4 (19.5)	11.8 (2.6)
$R_{p.i.m.}$ [b]	2.0 (5.9)	4.1 (25.2)
B-factor from Wilson plot (Å^2)	27.0	9.7

Refinement statistics	
Resolution limit (Å) [a]	50 - 1.33
Number of unique reflections [a]	273185
Completeness of data (%) [a]	96.8
R_{cryst} (%) [a, c]	9
R_{free} (%) [a, d]	11
No. of non-H atoms	10432
Protein	9473
Solvent	959
Ramachandran plot (%) [e]	97.1 / 2.8 / 0.1
Coordinate error [f]	0.169
Rms deviations from ideal values	
Bond lengths (Å)	0.028
Bond angles (deg.)	2,368
Mean *B*-factor (Å^2) per protein chain A / B / C / D	10.7 / 13.2 / 10.9 / 12.8