Report BM-30, Proposal 30.01.734.

The native and MAD data sets used to solve the NsPCS (Alr0975) structure where collected at beamline BM-30 (see table next page).

Abstract of the submitted paper :

Phytochelatin synthase (PCS) is a key enzyme for the heavy metal detoxification in plants. PCS catalyzes the production of glutathione (GSH)-derived peptides (phytochelatins) that binds heavy metal ions prior to vacuolar sequestration. The enzyme can also hydrolyze GSH and glutathione-S-conjugable xenobiotics. In the cyanobacteria *Nostoc*, the enzyme (NsPCS) contains only the catalytic domain of the eucaryotic synthase, and can act as a GSH hydrolase and weakly as a peptide ligase. The crystal structure of NsPCS in its native form solved at 2.0-Å resolution shows that NsPCS is a dimer which belongs to the papain superfamily of cysteine proteases with a conserved catalytic machinery. Moreover, the structure of the protein solved in complex with GSH at 1.4 Å resolution reveals a γ-glutamyl cysteine acyl-enzyme intermediate stabilized in a cavity of the protein adjacent to a second putative GSH binding site. Dual activities of PCS together with metal requirement are discussed in the light of both structures.

Data collection statistics:

Table I : Summary of crystal parameters, data collection and refinement statistics.

Data Collection		Native			Acyl-enzyme
Beamline		BM-30	BM-30	BM-30	ID-29
Wavelength, Å		0.97950	0.97935	0.974	0.976
Resolution range, Å		19-1.96	18-2.05	19-1.96	29-1.4
Cell parameters:	a	47.86 Å			56.25 Å
	b	62.47 Å			58.26 Å
	c	76.55 Å			72.56 Å
	β	101.38 °			108.87 °
No. of measured reflections		202,889	187,938	206,770	640,767
No. of unique reflections		30,626	27,903	31,117	87418
$R_{sym}{}^{a}$ (last shell)		6.1 (20.1)	6.5 (15.0)	6.5 (22.5)	8.5 (30.5)
I/σI		7.9 (2.7)	7.1 (2.4)	7.6 (3.0)	6.0 (2.1)
Completeness, % (last shell, %)		97 (86.8)	98.8 (98.8)	97.0 (97.0)	99.6 (99.6)
Sites (n)			10		
Figure of Merit[b]			0.44 (0.67)		
Refinement					
Resolution range, Å			18-2.0		29-1.4
R_{cryst} / R_{free}			20.0 / 25.7		17.4 / 18.7
No. of non hydrogen atoms:					
Total			3599		3636
Protein			3339		3212
γ-EC			-		30
Water			259		391
Ion			2		4
Average B-factors, Å² :					
Main-chain			14.8		7.4
Side-chain			17.0		9.4
γ-EC			-		9.0
Water			27.5		24.5
Ion			30.7		13.3
RMSD bonds, Å			0.019		0.008
RMSD angles, °			1.72		1.159

[a] $R_{sym}=\Sigma_h\Sigma_i|I_i(\mathbf{h}) - <I(\mathbf{h})>/ \Sigma_h\Sigma_i I_i(\mathbf{h})$

[b] Value in parenthesis is after solvent flattening