Report for 30-01-816

The C-terminal PASTA domain of the Ser/Thr kinasez Stk1 from *S. aureus* was overexpressed and purified. Crystal hits were obtained for the conditions 65 (0.1 M imidazole, pH 7.5, 1.6 M zinc sulfate) and 66 (0.1 M imidazole, pH 7.5, 0.8 M zinc sulfate) of the "Cations suite" from Nextal (Qiagen). Crystals grew to dimensions of 0.1 × 0.05 × 0.05 mm^3 within 1 week.

Initial X-ray diffraction data sets were collected at 100 K in-house. They belong to the tetragonal space group $P4_122$ with unit-cell parameters a=68.0 Å, b=68.0 Å, c=158.1 Å. The asymmetric unit contains one molecule with a V_M values of 3.5 $Å^3.Da^{-1}$.

Crystal soakings were performed with heavy atom salts (Au, Pt, Hg, Pb) and MAD data were collected at the tunable ESRF MX-beamline FIP-BM30. MAD data were also collected for the zinc K absorption edge. The programs XDS was used for all data processing.

Data phasing was successfully achieved for a MAD data set collected from one of our best diffracting crystal (3.0 Å resolution) at the zinc K absorption edge (Table 1). Crystallization paper is published (1) and structure determination is in progress.

	MAD data collected at the Zn K edge		
	Peak	**Edge**	**Remote**
Wavelength (Å)	1.282535	1.283145	1.275558
Resolution range (Å)	40-3.0 (3.1-3.0)	40-3.0 (3.1-3.0)	40-3.0 (3.1-3.0)
Total oscillation range (°)	180	180	90
No. observations	106557	106374	53867
No. unique reflections	13957	13982	12810
Completeness of data (%)	99.8 (100.0)	99.8 (100.0)	91.9 (94.2)
$\langle I/\sigma(I)\rangle$	18.4 (4.8)	25.1 (9.8)	15.5 (4.1)
Redundancy	7.6	7.6	4.2
R_{merge}† (%)	9.3 (43.7)	6.2 (20.3)	7.1 (37.1)

Values in parentheses are for the highest resolution shell.
†$R_{merge} = \Sigma_{hkl} \Sigma_i |I_i(hkl) - \langle I(hkl)\rangle| / \Sigma_{hkl} \Sigma_i |I_i(hkl)|$where I_i is the i^{th} measurement of reflection $I(hkl)$

1. Paracuellos P, Ballandras A, Robert X, Cozzone AJ, Duclos B, Gouet P. (2009). *Acta Crystallogr Sect F*. 65:1187-9.