Table 2. Crystallographic data statistics

Data collection statistics

Crystal	Space group	Cell dimensions
Native	$P6_522$	a = 185.0 Å, b = 185.0 Å, c = 67.7 Å
SeMet	$P6_522$	a = 185.2 Å, b = 185.2 Å, c = 68.3 Å

Data set	d_{min}, Å	No. of measurements	No. of unique reflections	Completeness, %	I/σ	R_{sym}, %
Native	3.1	128,504	12,651	98.5 (98.1)	13 (2.7)	6.9 (46.9)
SeMet λ1 (peak)	3.2	248,283	11,812	99.5 (98.9)	15 (5.7)	6.4 (48.3)
SeMet λ2 (edge)	3.2	153,292	11,692	98.3 (93.8)	14 (3.9)	6.5 (53.8)
SeMet λ3 (remote)	3.2	155,029	11,703	98.3 (94.2)	14 (3.5)	5.8 (59.7)

MAD phasing statistics

		Peak		Edge		Remote	
		Isomorphous	Anomalous	Isomorphous	Anomalous	Isomorphous	Anomalous
Phasing power	Centric	–	–	0.476	–	0.615	–
	Acentric	–	2.554	0.542	1.179	0.734	1.666
FOM	Centric	0.198					
	Acentric	0.415					
FOM after DM		0.856					

Refinement statistics (native data set)

No. of reflections (working/test)	10,286 / 1,185
No. of nonhydrogen atoms	1,805
Resolution, Å	8.0-3.1
R_{cryst} / R_{free}, %	26.8 / 31.6
Bond length deviation, Å	0.008
Bond angle deviation, º	1.5

Values in parentheses are for the highest-resolution bin.
$R_{sym} = \Sigma_h\Sigma_i|I_i(h) - \langle I(h)\rangle| / \Sigma h\langle I(h)\rangle$, where $I_i(h)$ is the ith measurement and $\langle I(h)\rangle$ is the weighted mean of all measurements of $I(h)$.
Phasing power = $\langle|F_H(\text{calc})|\rangle/\langle E\rangle$, where E is the phase-integrated lack of closure. FOM, figure of merit. FOM after DM, figure of merit after solvent flipping in the program DM.
$R = \Sigma(|F_{obs}| - K|F_{calc}|) / \Sigma|F_{obs}|$. R_{free} is the R value obtained for a test set of reflections that consisted of a randomly selected 8% subset of the diffraction data used during refinement of σ_A value calculations.