

**Table 2. Summary of data collection and structure refinement statistics**

Data collection				
Data set	Native	MnCl <sub>2</sub>	Mn/Zn/AMP	Mn/Zn/UMP
Beam line	DESY X13	BESSY BL1	MAXLAB 911-2	Home source
Soak	–	10mM MnCl <sub>2</sub>	5mM MnCl <sub>2</sub>	5mM MnCl <sub>2</sub>
			0.5mM ZnCl <sub>2</sub>	0.5mM ZnCl <sub>2</sub>
			5mM AMP	5mM UMP
Space group	P3 <sub>1</sub> 21	P3 <sub>1</sub> 21	P3 <sub>1</sub> 21	P3 <sub>1</sub> 21
Unit cell, Å				
a = b	110.34	110.68	110.85	110.57
c	80.26	79.729	79.87	79.33
Wavelength, Å	0.8048	1.50	1.043	1.542
Resolution (outer shell), Å	95–2.1 (2.18–2.10)	36–2.25 (2.33–2.25)	95–2.3 (2.38–2.30)	95–2.7(2.80–2.70)
No. of observations (unique)	334,137 (34,393)	269,714 (27,124)	232,707, (25,665)	244,172 (15,774)
Completeness (outer shell), %	98.5 (91.3)	99.7 (98.8)	99.9 (100.0)	98.4 (92.9)
Data redundancy (outer shell)	4.9 (3.6)	5.6 (4.9)	5.3 (5.1)	4.1 (3.0)
Mean I/σ <sub>1</sub> (outer shell)	25.6 (2.6)	34.6 (4.9)	25.0 (2.3)	18.7 (1.5)
R <sub>sym</sub> (outer shell), %	5.8 (50.3)	4.0 (34.1)	5.3 (72.6)	6.1 (66.6)

Refinement				
Data set	Native	MnCl <sub>2</sub>	Mn/Zn/AMP	Mn/Zn/UMP
Resolution range used (outer shell), Å	95–2.1	36–2.25	95–2.3	95–2.7
No. of reflections used (free set)	30,976 (3,087)	26,390 (2,646)	24,433 (2,459)	14,609 (1,465)
Residual R-factor (outer shell), %	23.3 (33.0)	22.3 (29.9)	23.8 (32.2)	21.9 (33.3)
Residual free R (outer shell), %	29.2 (36.5)	27.9 (37.8)	28.9 (35.4)	28.7 (37.9)
No. of atoms (solvent atoms)	3.441 (201)	3.492 (252)	3.392 (127)	3.398 (135)
Rms deviation on bond lengths, Å	0.008	0.007	0.007	0.007
Rms deviation on bond angles, °	1.34	1.27	1.24	1.32
Luzzati error (cross-validated), Å	0.32 (0.40)	0.31 (0.40)	0.34 (0.41)	0.37 (0.48)
Ramachandran plot statistics, %				
Most favorable regions	84.3	84.4	85.5	84.0
Additionally allowed regions	14.3	13.4	13.4	14.0
Generously allowed regions	1.4	2.2	1.1	2.0
Disallowed regions	0.0	0.0	0.0	0.0