

Supplementary Table I

Diffraction data statistics

Crystal	SeMet AMPPCP-Mg	Wild type AMPPCP-Mn	Wild type AMPPCP without Mg	Wild type 2'I-AMPPNP- Mg
Resolution	100.0-2.50	100.0-2.35	100.0-1.90	100-2.7
Range, Å	(2.56-2.50)	(2.42-2.35)	(1.96-1.9)	(2.8-2.7)
Wavelength, Å	0.9792	1.0	0.9	1.2
Space group	<i>P</i> 4 ₃ 22	<i>P</i> 4 ₃ 22	<i>P</i> 4 ₃ 22	<i>P</i> 4 ₃ 22
Cell <i>a=b</i> , Å	90.982	90.939	90.528	90.560
<i>c</i> , Å	191.973	191.257	191.184	190.214
<i>R</i> _{merge} , %	9.5 (57.8)	7.5 (44.5)	12.9 (58.2)	9.0 (46.4)
<i>I</i> / σ (<i>I</i>)	32.5 (5.0)	34.0 (4.6)	22.6 (3.1)	37.6 (7.6)
Completeness, %	100 (100)	99.8 (99.7)	99.8 (99.7)	99.9 (100)
Redundancy	14.3 (13.9)	8.0 (8.1)	7.4 (7.4)	19.1 (19.4)

Parentheses denote statistics in the highest-resolution shells. To obtain crystals of AMPPCP-bound

CopA-PN without Mg²⁺, we soaked the AMPPCP-Mg²⁺-bound crystals with only AMPPCP. Other

crystals were prepared by co-crystallization.