Supplementary Materials

EM-*detwin*: A Program for Resolving Indexing Ambiguity in Serial Crystallography Using the Expectation-Maximization Algorithm

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Table S1. Data collection and refinement statistics.

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	IN-CCD			BLAC			BR		
Data collection									
Space group	P 31 2 1			P 32 2 1			P 63		
Cell dimensions									
a, b, c (Å)	73.20	73.20	66.70	41.84	41.84	233.28	62.32	62.32	111.10
α, β, γ (°)	90.00	90.00	120.00	90.00	90.00	120.00	90.00	90.00	120.00
Number of indexed patterns	27311			12474			15847		
Number of merged patterns	26478			12385			15596		
Resolution (Å)	23.96-2.501 (2.59-2.501) *			34.60-1.70 (1.761-1.70) *			19.35-1.504 (1.558-1.504) *		
R_{split} (%)	9.09 (46.65)			28.58 (62.16)			10.23 (159.89)		
I/σ(I)	7.75 (2.48)			3.33 (2.17)			5.71 (1.81)		
Completeness (%)	99.84 (100.00)			99.88 (99.11)			89.45 (16.33)		
Multiplicity	318.94 (88.79)			34.79 (6.57)			114.62 (2.41)		
$CC_{1/2}$ (%)	99.58 (70.52)			87.23 (43.44)			98.53 (28.69)		
Refinement									
Resolution (Å)	23.96-2.501			34.60-1.70			19.35-1.504		
No. reflections	7434			27377			34650		
R_{work}/R_{free}	0.1828/0.2230			0.2324/0.2620			0.1927/0.2120		
R_{work}/R_{free} (PostRefine#)	0.1844/0.2028			0.2242/0.2534			0.1924/0.2147		
Clashscore	10.40			1.79			1.66		
No. atoms									
Protein	1098			1969			1785		
Water	12			N.A.			N.A.		
B-factor (Å^2)									
Wilson B/Overall B	51.22/61.76			11.54/15.02			22.11/31.61		
Root mean square deviations									
Bond lengths	0.010			0.011			0.010		
Bond angles	1.05			1.05			1.04		

* Values in parentheses are for highest-resolution shell. # The merged data with partiality modeled using the xsphere model in the partialator program.