Tables

Table S1. Statistics of diffraction data and structure refinement

Crystal	MdfA-DXC (Se-peak)	MdfA-Cm	MdfA-LDAO	MdfA-DXC
Data processing				
Beamline	BL1A at KEK	BL1A at KEK	BL17U at SSRF	BL17U at SSRF
Wavelength (Å)	0.9788	1.0000	0.8153	1.0000
Space group	C2	C2	C2	C2
Cell dimensions				
a, b, c (Å)	94.2, 64.4, 101.3	93.9, 63.4, 99.7	94.1, 64.1, 101.3	94.7, 64.2, 101.4
α, β, γ (°)	90, 109.7, 90	90, 106.1, 90	90, 104.2, 90	90, 110.0, 90
Resolution (Å)[a]	50-3.0 (3.1-3.0)	50-2.45 (2.54-2.45)	50-2.2 (2.3-2.2)	50-2.0 (2.1-2.0)
Completeness (%)	99.1 (93.7)	99.6 (97.3)	100.0 (100.0)	98.8 (95.4)
Rmerge (%)	13.0 (65.7)	11.6 (99.6)	12.8 (138.0)	17.2 (65.6)
$CC_{1/2}$	0.994 (0.811)	0.998 (0.623)	0.995 (0.726)	0.986 (0.683)
I /σ(I)	14.6 (2.2)	16.9 (1.7)	15.4 (1.8)	12.1 (1.7)
Unique reflections	11,581 (1,059)	21,233 (2,057)	29,691 (2.960)	38,240 (3.674)
Redundancy	11.7 (7.2)	6.4 (4.8)	8.6 (8.2)	3.4 (2.8)
Refinement				
Resolution (Å)		50-2.45	50-2.2	50-2.0
Number of reflections (test)[b]		21,211 (1,051)	29,641 (1,473)	38,215 (1,891)
Rwork / Rfree (%)		20.4/24.4	20.6/23.2	21.0/23.0
Average B–factor ($Å^2$)				
Protein		56	51	58
Ligand (No. of atoms)		70 (20)	64 (16)	73 (28)
Water (No. of atoms)		51 (14)	46 (16)	53 (18)
R.m.s.d. from ideal geometry				
bond lengths (Å)		0.006	0.005	0.005
bond angles (°)		1.044	1.044	1.039
Ramachandran plot (%)[c]				
favored region		98.0	98.0	98.2
allowed region		2.0	2.0	1.8

[a.] Values in parentheses are for shells with the highest resolution.

[b.] All structures were refined with the same "test" set of R_{free} reference reflections.

[c.] Calculated using *MolProbity*.