Table 1. Data collection and refinement statistics for substrates and product bound to GGPPS

Names	GGPPs-Mg-IPP	GGPPs-Mg-GPP	GGPPs-Mg-FPP	GGPPs-Mg-FsPP-IPP	GGPPs-GGPP
Ligands	Mg^{2+} and IPP	Mg^{2+} and GPP	Mg^{2+} and FPP	Mg^{2+}, FsPP and IPP	GGPP
Data Collection					
Space group	$P2_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_1$
Resolution, Å*	50-2.08 (2.15-2.08)	30-2.04 (2.11-2.04)	50-2.55 (2.64-2.55)	50-2.13 (2.21-2.13)	30-1.80 (1.86-1.80)
Unit cell dimensions					
a, Å	82.24	47.09	45.77	47.38	82.35
b, Å	47.71	116.60	115.94	116.10	48.82
c, Å	91.83	128.32	126.75	128.25	93.24
β, °	110.71				111.59
No. of reflections					
Observed	201,573 (18579)	264,889 (22131)	114,213 (6232)	178,830 (12671)	278,030 (24278)
Unique	40,504 (3953)	45,635 (4256)	21,952 (1833)	39,101 (3249)	63,682 (6225)
Completeness, %	99.6 (98.4)	99.3 (94.1)	97.3 (82.8)	96.0 (81.3)	98.8 (97.1)
R_{merge}, %	5.1 (25.5)	6.2 (50.3)	6.3 (22.5)	4.1 (18.6)	5.1 (52.2)
I/σ(I)	29.4 (5.9)	28.9 (2.8)	20.3 (3.4)	28.9 (5.1)	28.0 (2.73)
Refinement					
No. of reflections	39,300 (3642)	43,414 (3627)	21,259 (1491)	38,181 (2763)	58,217 (4667)
R_{work}, %	19.8 (25.4)	20.4 (32.5)	18.5 (22.1)	19.6 (24.4)	19.8 (33.2)
R_{free}, %	25.7 (31.7)	24.9 (32.7)	23.9 (29.2)	25.0 (27.9)	24.2 (34.9)
Geometry deviations					
Bond lengths, Å	0.020	0.018	0.011	0.016	0.019
Bond angles, °	1.8	1.7	1.4	1.6	1.7
No. of all protein atoms	4,816	5,014	4,932	4,862	4,730
Mean B-values, $Å^2$	40.2	47.0	37.9	41.6	30.9
No. of all cofactor atoms	60	42	70	80	58
Mean B-values, $Å^2$	44.5	48.6	55.0	63.9	31.3
No. of water molecules	416	350	318	548	980
Mean B-values, $Å^2$	52.1	49.9	42.5	54.3	53.4
Ramachandran plot, %					
Most favored	95.1	95.5	92.5	94.0	96.2
Additionally allowed	4.9	4.3	7.3	6.0	3.8
Generously allowed	0	0.2	0.2	0	0

*Values in the parentheses are for the highest-resolution shells.