Table 3. Data collection and refinement statistics for GGPPS-bisphosphonate crystals

Crystals	BPH-91	BPH-261	BPH-629	BPH-364	BPH-675
			Data collection		
Space group	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$
Resolution, Å*	30-2.14 (2.22-2.14)	30-2.31 (2.39-2.31)	50-2.12 (2.20-2.12)	50-2.18 (2.26-2.18)	50-2.2 (2.28-2.2)
Unit cell dimensions					
a, Å	46.66	46.87	45.79	46.57	46.39
b, Å	116.29	116.05	115.82	116.39	116.26
c, Å	126.95	127.73	130.00	128.55	128.70
No. of reflections					
Observed	247,933 (19355)	153,941 (13757)	174,254 (12421)	194,150 (13786)	246,740 (23819)
Unique	39,184 (3795)	30,293 (2866)	38,573 (3357)	36,250 (2997)	36,490 (3555)
Completeness, %	99.5 (98.2)	96.2 (93.1)	96.6 (85.2)	96.8 (81.6)	99.9 (99.9)
R_{merge}, %	10.6 (44.2)	7.3 (45.1)	4.2 (20.9)	4.5 (16.8)	8.5 (42.4)
I/σ(I)	23.1 (4.6)	21.1 (3.3)	28.7 (4.1)	29.6 (4.7)	26.1 (5.5)
			Refinement		
No. of reflections	36,847 (3379)	28,699 (2490)	37,579 (2907)	35,219 (2818)	34,526 (3191)
R_{work}, %	19.7 (24.2)	19.9 (29.4)	16.7 (18.1)	18.0 (21.0)	18.5 (24.0)
R_{free}, %	24.9 (27.5)	25.7 (36.8)	21.7 (24.2)	23.6 (25.5)	24.1 (29.0)
Geometry deviations					
Bond lengths, Å	0.018	0.015	0.020	0.015	0.019
Bond angles, °	1.7	1.6	1.7	1.5	1.7
No. of all protein atoms	4,723	4,749	5,013	4,959	5,128
Mean B-values, Å^2	41.8	48.2	34.7	38.2	40.0
No. of all cofactor atoms	36	44	120	59	51
Mean B-values, Å^2	38.7	51.8	36.5	64.4	61.3
No. of water molecules	470	326	519	657	337
Mean B-values, Å^2	54.9	59.5	48.5	55.6	46.2
Ramachandran plot, %					
Most favored	97.1	94.3	95.3	95.3	94.9
Additionally allowed	2.9	5.7	4.7	4.3	5.1
Generously allowed	0	0	0	0.4	0

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