Table 5. Data collection and refinement statistics for UPPS-bisphosphonate crystals

Crystals	BPH-629	BPH-608	BPH-628	BPH-675	BPH-676
			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*	30-1.9 (1.97-1.9)	30-2.0 (2.07-2.0)	30-2.1 (2.18-2.1)	30-2.05 (2.12-2.05)	30-2.5 (2.59-2.5)
Unit cell dimensions					
a, Å	64.02	64.29	63.68	63.54	62.97
b, Å	66.23	68.16	68.16	68.69	68.29
c, Å	111.28	109.91	109.89	110.03	110.23
No. of reflections					
Observed	366,529 (35668)	263,413 (26463)	163,527 (15367)	222,476 (22555)	130,566 (13415)
Unique	39,256 (3877)	33,217 (3267)	28,571 (2794)	30,788 (3048)	16,798 (1639)
Completeness, %	99.8 (100)	99.9 (100)	99.5 (99.1)	99.7 (100)	97.3 (97.1)
R_{merge}, %	5.2 (44.4)	5.8 (46.4)	4.6 (47.0)	4.5 (44.6)	5.8 (41.3)
I/σ(I)	38.2 (5.5)	36.6 (5.0)	34.2 (3.6)	39.9 (4.6)	41.8 (6.3)
			Refinement		
No. of reflections	38,115 (3559)	32,558 (2969)	27,661 (2536)	30,143 (2782)	16,326 (1538)
R_{work}, %	18.7 (20.7)	19.1 (21.3)	20.0 (25.5)	20.9 (26.7)	22.4 (29.7)
R_{free}, %	23.6 (24.4)	23.8 (27.4)	24.2 (30.7)	24.8 (30.5)	28.4 (40.3)
Geometry deviations					
Bond lengths, Å	0.019	0.017	0.015	0.015	0.016
Bond angles, °	1.8	1.6	1.6	1.7	1.7
No. of all protein atoms	3,535	3,545	3,443	3,345	3,470
Mean B-values, Å^2	33.1	36.3	47.1	44.1	53.5
No. of all cofactor atoms	192	145	68	121	90
Mean B-values, Å^2	44.6	51.1	77.1	89.3	85.0
No. of water molecules	458	270	310	301	206
Mean B-values, Å^2	54.1	48.7	59.3	58.1	58.6
Ramachandran plot, %					
Most favored	96.0	94.7	93.0	93.6	92.0
Additionally allowed	4.0	5.3	7.0	6.4	8.0
Generously allowed	0	0	0	0	0

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