Table S2. X-ray data collection and crystallographic refinement statistics.

	D168A PC	**D168A P_4-1**	**D168A P_4-2**	**WT P_4-3**	**WT P_4-4**	**D168A P_4-4**	**D168A P_4-5**	**D168A P_4-6**	**D168A P_4-7**	**WT P_4P_5-2A**	**D168A P_4P_5-2A**	**WT P_4P_5-2B**	**D168A P_4P_5-4**	**D168A P_4P_5-5**	**D168A P_4P_5-6**
PDB ID	6UE3	6PIZ	6PIY	6DIT	6DIU	6PJ1	6PJ0	6PIW	6PIV	6DIR	6DIV	6DIQ	6PJ2	6PIX	6PIU
Resolution (Å)	1.56	1.89	1.86	1.79	1.87	1.89	2.05	1.90	2.14	1.75	1.83	1.58	2.10	1.87	2.28
Space group	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$
Molecules in AU[a]	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
Cell dimensions:															
a (Å)	55.6	54.9	55.2	55.3	55.1	54.4	55.2	54.1	55.2	55.1	55.5	55.5	54.4	54.2	54.8
b (Å)	58.5	58.6	58.7	58.6	59.6	58.5	58.5	58.6	58.7	59.8	58.7	58.5	59.6	58.6	59.6
c (Å)	59.9	59.9	59.8	59.8	58.5	60.0	59.7	59.9	60.0	58.5	60.0	59.9	58.6	59.7	58.6
β (°)	90	90	90	90	90	90	90	90	90	90	90	90	90	90	90
Completeness (%)	98.3	99.7	99.5	98.1	97.4	98.6	99.1	95.7	99.9	97.0	98.1	91.3	99.1	98.1	99.8
Total reflections	249313	109214	113571	118729	110776	104473	73797	104326	77445	119548	115996	250177	77900	110082	53741
Unique reflections	28103	15981	16808	18610	16126	15695	12209	14973	11259	19508	17556	25037	11513	15984	9233
Average I/σ	25.2	20.0	27.5	14.5	12.7	20..7	18.7	19.5	26.6	8.8	12.8	7.9	16.6	34.2	14.0
Redundancy	8.9	6.8	6.8	6.4	6.9	6.6	6.0	7.0	6.9	6.1	6.6	10	6.7	6.9	5.8
R_{sym} **(%)**[b]	4.7 (14.3)	9.5 (28.2)	7.0 (28.7)	7.1 (28.4)	6.3 (19.6)	8.5 (36.6)	9.1 (34.8)	9.5 (36.7)	7.4 (17.9)	4.3 (18.3)	7.0 (21.6)	5.7 (15.2)	11.9 (40.1)	5.7 (19.3)	11.9 (50.0)
RMSD[c] **in:**															
Bond lengths (Å)	0.015	0.009	0.006	0.004	0.02	0.005	0.01	0.01	0.002	0.009	0.006	0.007	0.002	0.01	0.03
Bond angles (°)	1.6	1.2	1.2	0.8	0.6	1.1	0.7	1.3	0.7	1.3	1.1	1.0	0.76	1.3	0.8
R_{factor} **(%)**[d]	14.4	16.0	15.8	18.2	18.3	16.4	17.7	16.9	17.4	14.6	16.1	15.1	18.2	15.2	19.3
R_{free} **(%)**[e]	17.0	19.8	17.5	22.9	23.3	20.1	21.5	20.9	20.6	19.3	19.4	18.3	21.4	19.1	23.5

[a]AU, asymmetric unit.

[b]$R_{sym} = \Sigma \mid I - \langle I \rangle \mid / \Sigma I$, where I = observed intensity, $\langle I \rangle$ = average intensity over symmetry equivalent; values in parentheses are for the highest resolution shell.

[c]RMSD, root mean square deviation.

[d]$R_{factor} = \Sigma \mid\mid F_o \mid - \mid F_c \mid\mid / \Sigma \mid F_o \mid$.

[e]R_{free} was calculated from 5% of reflections, chosen randomly, which were omitted from the refinement process.