

Table S1. Data collection and structure refinement statistics

	PLD α 1-PA	PLD α 1-Apo	Se-Met
Resolution (Å)	34.7-2.30 (2.37-2.30)	37.7-1.80 (1.87-1.80)	38.7-2.00 (2.07-2.00)
Space group	P 2 ₁ 2 ₁ 2 ₁	C 1 2 1	P 2 ₁ 2 ₁ 2 ₁
Until cell			
<i>a</i> , <i>b</i> , <i>c</i> , (Å)	99.04,123.03 138.90	118.89 127.44 55.36	99.23 123.57 140.22
α , β , γ , (°)	90, 90, 90	90 95.472 90	90, 90, 90
Unique reflections	74,502 (6,209) [†]	75,085 (7,370)	117,128 (11,282)
Multiplicity	12.6	13.4	13.2
I/ σ (I)	13.1 (2.3)	27.6 (1.4)	21.6 (1.4)
<i>R</i> _{merge}	0.219 (1.145)	0.096 (0.798)	0.125 (0.872)
Completeness (%)	99.8 (98.3)	99.5 (99.9)	100 (100)
<i>R</i> _{work} / <i>R</i> _{free} [‡] (%)	19.70/24.99	16.64/19.23	
Number of atoms	6,298 ^A /6,298 ^B	6,199	
Ligand			
di8:0PA	28/28		
Ca ²⁺	2	1	
Water	500	595	
Protein residues	1572	771	
r.m.s. deviations			
bonds (Å)	0.010	0.007	
Angles (°)	1.12	0.89	
Average B factor	15.9	21.6	
Protein	15.9	20.8	
Ligand	15.8	13.5	
Water	15.1	30.3	
Ramachandran			
Favored (%)	93.3	95.9	
Allowed (%)	6.7	4.1	

[†] Numbers in parentheses represent the highest-resolution shell.

[‡] $R = \frac{\sum hkl ||F_o| - |F_c||}{\sum hkl |F_o|}$.

^A Chain A; ^B Chain B.