Supplementary Table I

Table 1 Data collection, phasing and refinement statistics

	Wild type (crystal 1)				Wild type (crystal 2)	ΔApp mutant	a4 mutant
Data collection							
Space group	$I4_1$				$I4_1$	$I4_1$	$P2_1$
Cell dimensions							
a, *b*, *c* (Å)	126,1, 126.1, 101.3				127.4, 127.4, 99.6	129.1, 129.1, 98.0	44.3, 212.2, 54.3
α, β, γ (º)	90, 90, 90				90, 90, 90	90, 90, 90	90, 97.0, 90
	Inflection	*Peak*	*Remote 1*	*Remote 2*			
Wavelength	0.9794	0.9793	0.9817	0.9734	0.9797	1.0	1.0
Resolution (Å)	50-3.2 (3.31-3.2)	50-3.2 (3.31-3.2)	50-3.25 (3.37-3.25)	50-3.3 (3.42-3.3)	50-3.1 (3.21-3.1)	20-2.9 (3.0-2.9)	50-2.4 (2.49-2.4)
R_{merge}	0.065 (0.451)	0.065 (0.371)	0.063 (0.372)	0.087 (0.394)	0.066 (0.363)	0.074 (0.350)	0.098 (0.323)
$I/\sigma I$	21.3 (3.1)	23.4 (8.5)	21.4 (8.37)	19.3 (7.0)	22.9 (4.5)	20.7 (5.5)	11.0 (3.7)
Completeness (%)	99.8 (100)	99.9 (100)	99.8 (100)	99.9 (100)	99.6 (100)	99.8 (100)	99.6 (93.5)
Redundancy	7.56	7.58	7.55	7.54	7.64	6.47	3.8
Refinement							
Resolution (Å)					20-3.1	20-2.9	50-2.4
No. reflections					14449	16852	38523
$R_{work/}$ R_{free}					0.236 /0.264	0.238 /0.269	0.215 /0.270
No. atoms							
Protein					1698	1622	7204
Ligand/ion					0	0	1 (Ca^{2+})
Water					0	0	197
B-factors							
Protein					84.8	74.8	54.7
Ligand/ion							54.6
Water							36.3
R.m.s deviations							
Bond lengths (Å)					0.0057	0.0072	0.0051
Bond angles (º)					1.03	1.10	0.959

Highest resolution shell is shown in parenthesis.