Table S1 Data collection and refinement statistics

Data set	Y194F-Δ270	D159S/Y194F-Δ270
Space group	I222	I222
a (Å)	58.28	56.53
b (Å)	103.37	105.64
c (Å)	119.63	120.08
Resolution Range (Å)	25.77-2.10 (2.21-2.10)	25.72-2.40 (2.53-2.40)
Observed reflections	85,692	56,698
Independent reflections	21,489	14,436
Rmerge (%)[a]	6.8 (29.5)	6.9 (39.7)
I/σ	8.8 (2.6)	8.6 (1.9)
Completeness (%)	99.9 (99.9)	99.9 (100.0)
Refinement		
Reflections in refinement	20,342	13,710
$R_{cryst.}$ (%)[b]	19.62	21.28
R_{free} (%) (test set 5%)[c]	23.94	25.92
r.m.s.d. on bond lengths (Å)[d]	0.009	0.011
r.m.s.d. on bond angles (°)[d]	1.178	1.307

The values in parentheses refer to the highest resolution shells.

[a] Rmerge = $\Sigma h \Sigma i \mid Ih - \langle Ih \rangle \mid / \Sigma h \Sigma i \langle Ih \rangle$ where $\langle Ih \rangle$ is the mean intensity of the *i* observations of reflection *h*.

[b] Rcryst = $\Sigma \mid \mid Fobs \mid - \mid Fcalc \mid \mid / \Sigma \mid Fobs \mid$. where |Fobs| and |Fcalc| are the observed and calculated structure factor amplitudes. respectively. Summation includes all reflections used in the refinement.

[c] Rfree = $\Sigma \mid \mid Fobs \mid - \mid Fcalc \mid \mid / \Sigma \mid Fobs \mid$. evaluated for a randomly chosen subset of 5% of the diffraction data not included in the refinement.

[d] Root mean square deviation from ideal values.