Supplemental Table S2
Data collection and refinement statistics

	WT	D175N	D175N–Δ6S
Space group	*C*2	*C*2	*C*2
Unit cell parameters (Å, deg)	a = 104.8, b = 53.2, c = 70.1, β = 96.6	a = 105.1, b = 53.4, c = 70.2, β = 96.5	a = 105.2, b = 53.3, c = 70.1, β = 96.6
Data collection			
Wavelength (Å)	1.0000	1.0000	1.0000
Resolution limit (last shell)[a] (Å)	50-1.95 (2.02-1.95)	30-2.50 (2.59-2.50)	20-2.02 (2.09-2.02)
Measured reflections	103,030	50,235	96,246
Unique reflections	28,120 (2,595)	13,575 (1,323)	25,199 (2,470)
Redundancy	3.7 (3.1)	3.7 (3.8)	3.8 (3.8)
Completeness (%)	99.0 (91.9)	99.0 (98.4)	98.4 (97.7)
I/σ (I)	16.9 (2.62)	21.5 (4.90)	19.3 (4.30)
R_{merge} (%)	0.060 (0.29)	0.064 (0.35)	0.071 (0.38)
Refinement			
Resolution limit (Å)	50-1.95 (2.00-1.95)	50-2.50 (2.56-2.50)	20-2.02 (2.07-2.02)
Used reflections	26,428 (1,733)	12769 (925)	23,909 (1,696)
Completeness (%)	98.8 (89.5)	98.9 (98.1)	98.3 (96.4)
R-factor (%)	18.9 (23.8)	18.7 (21.5)	17.4 (19.4)
R_{free} (%)	21.3 (29.6)	26.0 (31.6)	20.9 (26.7)
Final model			
No. of molecules /asymmetric unit	1	1	1
No. of nonhydrogen atoms			
Protein	3,250	3,218	3,206
Δ6S	0	0	30
H_2O	109	61	160
Average B-factor (Å^2)			
Protein	25.9	35.8	21.9
H_2O	28.7	31.6	33.5
Δ6S			42.6
r.m.s.d. from ideal			
Bond length (Å)	0.007	0.008	0.007
Bond Angle (deg)	0.957	1.002	0.997
Ramachandran plot (%)			
Favored region	91.4	91.2	90.2
Allowed region	8.6	8.8	9.8
Outlier region	0	0	0

[a] Data in highest resolution shells are given in parentheses.