

Table 1. Crystallographic statistics

Data set	WT pH 8.5	WT pH 5.5	T203C pH 8.5	T203C pH 5.5	Y145C	Y145CT203C
Collection statistics						
Source [*]	UTSW	UTSW	X4A	7-1	UTSW	7-1
Resolution, Å	25-1.45	22-1.48	24-1.55	25-1.58	22-1.38	25-1.60
Observed/Multiplicity	36,969/2.8	32,536/3.1	31,021/3.9	30,578/4.7	38,868/3.1	28518/3.0
Completeness, % [†]	93.3 (68.5)	86.2 (72.4)	95.3 (92.4)	99.9 (99.4)	83.5 [‡] (17.9)	95.6 (90.2)
R _{sym} , % [†]	4.1 (30.2)	5.6 (48.1)	5.7 (42.3)	4.6 (43.6)	3.4 (16.8)	7.8 (45.6)
I/σ [†]	22.3 (2.0)	13.0 (2.0)	18.5 (2.5)	24.5 (2.0)	24.2 (2.6)	26.2 (2.0)
Refinement Statistics						
No. of reflections (working/test)	34,744/2224	29,272/3245	28,513/2502	26,510/2938	36,515/2336	25,666/2823
Resolution, Å	25.0-1.45	25.0-1.48	25-1.55	25-1.58	25.0-1.38	25-1.60
R _{work} /R _{free}	18.7/20.1	21.6/23.1	19.4/21.4	20.8/23.3	18.3/20.2	19.3/21.0
Rms deviation:						
Bond lengths, Å	0.01	0.01	0.01	0.01	0.01	0.01
Bond angles, °	1.74	1.69	1.67	1.78	1.74	1.69

^{*} 7-1 at Stanford Synchrotron Radiation Laboratory (Stanford Linear Accelerator Center), X4A at National Synchrotron Light Source (Brookhaven National Laboratory), UTSW home R-axis IV detector Howard Hughes Medical Institute at University of Texas Southwestern Medical Center.

[†] Values for the highest resolution shell are given in parentheses.

[‡] 93.0% completeness from 22 to 1.50 Å; lower completeness to 1.38 Å due to imaging plate size.