

Table 3. Crystallographic summary

Data collection							
Crystal*	Native-pH 6.5	Native-pH 8.0	E201Q-Gln γ but	QC-Acet.	QC-Benz.	QC-Vin.	R54W
Resolution, Å	50-1.66	30-2.35	30-2.22	50-1.56	50-1.64	50-1.68	30-2.22
Cell dimensions, Å, $a = b, c$	119.0, 332.9	119.0, 332.3	119.1, 332.6	119.1, 332.8	119.0, 332.8	118.9, 333.0	119.4, 333.8
Total observations	607669	158563	137268	1224166	405375	475184	166943
Unique reflections	106852	37941	42705	128907	100111	102772	45198
Redundancy	5.7 (5.1) [†]	4.2 (4.0)	3.2 (3.0)	9.5 (7.9)	4.0 (3.4)	4.6 (4.0)	3.7 (3.2)
Completeness, %	99.7 (100.0)	99.2 (99.7)	94.3 (86.3)	99.8 (100.0)	90.1 (93.2)	99.4 (99.1)	98.9 (97.3)
$I/\sigma(I)$	36.9 (3.5)	23.8 (3.6)	16.2 (2.2)	60.1 (4.3)	29.2 (2.6)	32.9 (2.4)	19.3 (3.2)
R_{merge} , %	4.7 (49.0)	7.5 (49.6)	6.4 (47.8)	4.4 (49.8)	4.8 (47.6)	4.7 (49.0)	7.8 (49.0)
Refinement							
Resolution, Å	50-1.66	30-2.35	30-2.22	50-1.56	50-1.64	50-1.68	30-2.22
Reflections, >0 $\sigma(F)$, working/test	96578/5097	33673/1769	37502/1978	117909/6244	91055/4834	92765/4949	39181/2074
$R_{\text{factor}}/R_{\text{free}}$	0.182/0.204	0.185/0.216	0.188/0.226	0.189/0.213	0.177/0.205	0.186/0.212	0.189/0.222
rmsd bond lengths, Å/angles, °	0.013/1.65	0.006/1.30	0.006/1.29	0.015/1.67	0.014/1.87	0.013/1.82	0.009/1.44
Average B factor, Å ² /no. of atoms							
Protein	23.7/5222	36.9/5190	32.3/5190	23.4/5222	20.1/5222	24.3/5222	28.9/5228
Water	34.5/602	44.5/460	40.8/511	34.1/591	30.4/591	34.8/599	32.5/424
Zinc	17.3/2	30.7/2	27.9/2	15.7/2	13.0/2	17.5/2	22.8/2
Sulfate	35.9/10	47.5/10		46.0/10	39.4/10	41.5/10	46.3/10
Substrate			42.8/28				
Inhibitor				25.2/22	19.1/24	28.4/14	
Ramachandran plot, %							
Most favored	89.1	88.5	88.1	88.9	89.6	88.7	88.5
Additionally allowed	10.9	11.0	11.4	10.9	10.0	10.9	11.1
Generously allowed		0.5	0.5	0.2	0.4	0.4	0.4
PDB ID code	2AFM	2AFO	2AFU	2AFW	2AFX	2AFZ	2AFS

Gln γ but, glutamine *t*-butyl ester; Acet., N- ω -acetylhistamine; Benz., 1-benzylimidazole; Vin., 1-vinylimidazole.

*X-ray diffraction experiments were mainly performed at beamline 5, KEK Photon Factory (Tsukuba, Japan). The data for R54W crystals and the crystals grown at pH 8.0 were collected at the Taiwan beamline 12B2, SPring-8 (Hyogo, Japan). Data for the enzyme-substrate complex was collected at Academia Sinica using MSC MicroMax 002. The space group of these crystals is *R*32, containing two QC molecules in an asymmetric unit.

[†]Values in parentheses correspond to highest-resolution shell.