Supplemental Table 1. Data collection and refinement statistics of *apo* SARS-CoV-2 3CL protease and 3CL protease bound to compound 4, GC376, and MAC-5576.

	apo 3CL	3CL with Compound 4	3CL with GC376	3CL with MAC-5576
Data collection				
Space group	*C2*	*C2*	*C2*	*C2*
Cell dimensions				
a, *b*, *c* (Å)	98.7, 82.0, 51.8	97.2, 81.9, 54.2	98.8, 80.2, 52.0	98.3, 82.5, 51.8
α, β, γ (°)	90, 114.9, 90	90, 117.1, 90	90, 114.3, 90	90, 114.83, 90
Resolution (Å)	60.4-1.85 (1.88-1.85)*	59.5-1.80 (1.82-1.80)*	59.9-1.83 (1.86-1.83)*	60.58-1.73 (1.76-1.73)*
R_{merge} (%)	7.2 (65.7)	18.7 (57.6)	14.7 (60.5)	4.1 (68.8)
I/σI	13.4 (2.1)	10.2 (2.4)	12.7 (2.2)	23.5 (2.3)
Completeness (%)	98.9 (97.4)	98.8 (99.0)	98.5 (96.0)	99.2 (88.3)
Redundancy	6.8 (6.5)	6.7 (6.5)	6.9 (6.1)	6.8 (6.6)
CC1/2	99.8 (95.1)	0.99 (0.91)	0.99 (0.93)	100 (0.90)
Refinement				
Resolution (Å)	47.0-1.85 (1.88-1.85)*	48.2-1.80 (1.82-1.80)*	47.38-1.83 (1.86-1.83)	47.0-1.73 (1.75-1.73)
No. reflections	31,710 (3,219)	34,294 (3,497)	31,972 (3,134)	38,879 (3,899)
R_{work} / R_{free} (%)	16.8 (25.2)/19.8 (29.3)	18.7 (25.7)/22.3 (30.7)	17.4 (25.0)/20.6 (28.7)	16.6 (26.8)/19.0 (27.6)
No. atoms				
Protein	2,329	2,370	2,340	2,298
Ligand/ion	5	44	28	16
Water	128	293	163	245
B-factors				
Protein	50.0	35.2	41.4	40.5
Ligand/ion	52.6	36.6	42.4	43.7
Water	53.5	46.7	48.2	50.7
R.m.s deviations				
Bond lengths (Å)	0.006	0.007	0.006	0.006
Bond angles (°)	0.8	0.8	0.8	0.8

*Highest resolution shell is shown in parenthesis.