

**Supplementary information Table S2: Table of Crystallization Statistics**

<b><u>Data Collection</u></b>	<b><u>PDB ID 6WTT</u></b>
Structure	SARS-CoV-2 M <sup>pro</sup> + GC-376
Space Group	P 3 <sub>2</sub> 21
Cell Dimension	
a, b, c (Å)	101.82, 101.82, 160.01
α, β, γ (°)	90, 90, 120
Resolution (Å)	50.00 - 2.15
	(2.19 - 2.15)
R <sub>merge</sub>	0.110 (0.889)
<I>/σ<I>	28.6 (1.9)
Completeness (%)	100.0 (99.7)
Redundancy	9.5 (7.3)
<b><u>Refinement</u></b>	
Resolution (Å)	45.64 - 2.15
	(2.22 - 2.15)
No. reflections/free	52574 / 2714
R <sub>work</sub> /R <sub>free</sub>	0.22 /0.30
No. Atoms	7430
Protein	6963
Ligand/ion	107
Water	340
B-Factors (Å <sup>2</sup> )	
Protein	66.75
Ligand/ion	67.17
Solvent	63.79
RMS Deviations	
Bond Lengths (Å)	0.014
Bond Angles (°)	1.93
Ramachandran Favored (%)	94.78
Ramachandran Allowed (%)	5.22
Ramachandran Outliers (%)	0.00
Rotameric Outliers (%)	2.33

\* Numbers in parentheses represent the highest resolution shell.