

Table 1: Data collection and refinement statistics

Data collection statistics					
	SARS-CoV M^{pro}				TGEV M^{pro}
	I2	N1	N3	N9	N1
Wavelength (Å)	1.5418	1.5418	1.5418	1.5418	1.5418
Space group	P2 ₁	P2 ₁	P2 ₁	P2 ₁	P2 ₁ 2 ₁ 2 ₁
Unit cell (Å, °)	a=50.7 Å b=94.7 Å c=66.2 Å	a=51.7 Å b=95.3 Å c=67.5 Å	a=52.1 Å b=95.7 Å c=67.6 Å	a=52.1 Å b=95.0 Å c=67.6 Å	a=66.6 Å b=90.2 Å c=110.3 Å
	β=103.0°	β=103.6°	β=102.9°	β=103.1°	
Resolution limit (Å)	50.0 – 2.7 (2.8 – 2.70)	50.0 – 2.0 (2.08 – 2.0)	50.0 – 2.3 (2.34 – 2.3)	50.0 – 1.85 (1.93 – 1.85)	50.0 – 2.7 (2.75 – 2.7)
Total reflections	62,720	312,221	217,524	246,270	229,389
Unique reflections	16,799	42,325	28,372	53,796	18,149
Completeness	99.8 (99.6)	99.8 (99.7)	98.0 (96.0)	99.9 (99.5)	96.2 (92.9)
R _{merge} ^a	9.5 (38.0)	7.8 (31.4)	12.0 (52.9)	8.3 (44.7)	12.8 (65.2)
<I/σ(I)>	7.7 (2.5)	13.0 (3.9)	10.0 (3.3)	8.4 (2.1)	12.4 (3.8)
Redundancy	3.7 (3.7)	7.4 (7.0)	7.7 (7.7)	4.6 (4.4)	12.6 (12.8)
Refinement statistics					
	I2	N1	N3	N9	N1
Resolution range (Å)	30.0 – 2.7	30.0 – 2.0	30.0 – 2.3	30.0 – 1.85	30.0 – 2.7
R _{work} ^b (%)	20.9	20.1	19.4	21.5	23.4
R _{free} ^b (%)	28.2	23.9	23.0	24.5	27.1
RMS deviation:					
bonds (Å)	0.010	0.012	0.016	0.006	0.02
angles (°)	1.52	1.89	1.97	1.43	1.94
Ramachandran plot					
favored (%)	79.5	89.8	86.7	89.5	76.2
allowed (%)	18.9	9.0	12.2	9.0	21.3
generously allowed (%)	1.0	0.8	0.8	1.1	2.3
disallowed (%)	0.6	0.4	0.4	0.4	0.2

^aR_{merge} = $\sum_h \sum_l |I_{ih} - \langle I_h \rangle| / \sum_h \sum_l \langle I_h \rangle$, where $\langle I_h \rangle$ is the mean of the observations I_{ih} of reflection h .

^bR_{work} = $\sum (|F_p(\text{obs})| - |F_p(\text{calc})|) / \sum |F_p(\text{obs})|$; R_{free} = R factor for a selected subset (10%) of the reflections that was not included in prior refinement calculation.