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Supplementary information

SARS-CoV-2 neutralizing antibody structures inform therapeutic strategies

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Supplementary Table 1. X-ray crystallography data collection and refinement statistics

	C102 SARS-CoV-2 RBD	C102 Fab	C002 Fab	C110 Fab	C121 Fab	C135 Fab
PDB ID	**7K8M**	**7K8N**	**7K8O**	**7K8P**	**7K8Q**	**7K8R**
Data collection[a,b]						
Space group	$P2_12_12_1$	$P6_522$	$P3_121$	P2	$P6_122$	$P4_1$
Cell Dimenstions						
a, b, c (Å)	54.6, 89.3, 175.1	88.8, 88.8, 218.93	92.3, 92.3, 130.9	48.5, 62.7, 78.4	71.3, 71.3, 404.8	102.3, 102.3, 53.3
α, β, γ (°)	90, 90, 90	90, 90, 90	90, 90, 120	90, 97.5, 90	90, 90, 120	90, 90, 90
Resolution (Å)	48.85-3.2 (3.31-3.2)	37.93-1.65 (1.71-1.65)	34.1-1.92 (1.99-1.92)	38.7 - 1.80 (1.86-1.80)	39.1-2.0 (2.05-2.0)	45.7-2.0 (2.07 -2.0)
R_{merge} (%)	16.0 (49.2)	9.58 (148)	7.21 (203)	8.7 (107)	58.1 (136)	8.5 (213)
R_{pim} (%)	6.8 (23.2)	2.27 (33.4)	2.38 (71.4)	4.1 (81.9)	11.4 (81)	3.5 (88.9)
$CC_{1/2}$ (%)	98.7 (97.4)	99.8 (80.7)	99.9 (80.7)	99.6 (78.2)	99.5 (24.8)	99.8 (30.5)
<I/σI>	6 (0.86)	15.3 (1.6)	13.02 (0.88)	7.7 (2.0)	8.4 (0.6)	10.5 (0.76)
Completeness (%)	99.7 (99.5)	99.97 (99.95)	76.9 (8.41)	98.8 (99.2)	99.2 (97.7)	99.4 (98.4)
Redundancy	6.5 (6)	19.2 (19.3)	9.9 (8.7)	4.7 (2.0)	26.3 (26.8)	6.8 (6.6)
Wilson *B*-factor	28.5	28.5	32.1	23.8	44.3	52.6
Refinement and Validation						
Resolution (Å)	48.5 - 3.2	37.9 - 1.65	34.1-1.92	38.9 - 1.80	36.4 - 2.0	45.7 - 2.0
Unique Reflections	14,722 (1413)	62,121 (6095)	38260 (413)	42,891 (4,284)	42,233 (2,989)	37,324 (3071)
Number of atoms						
Protein	4,731	3,280	3,337	3,345	3,269	3,315
Ligand	14	58	53	n/a	14	18
Waters	0	78	63	172	12	30
R_{work}/R_{free} (%)	18.7/23.8	19.6/21.2	19.7/22.7	20.9/23.4	20.7/23.9	20.8/23.7
R.m.s. deviations						
Bond lengths (Å)	0.002	0.02	0.007	0.01	0.005	0.004
Bond angles (°)	0.5	1.7	0.9	1.1	0.7	1.02
Poor rotamers (%)	0.9	2.2	2.1	0	0.8	0.27
Ramachandran plot						
Favored (%)	94.7	97.4	97.5	97.9	97.5	97.2
Allowed (%)	5.1	2.6	2.3	2.1	2.5	2.5
Disallowed (%)	0.2	0	0.2	0	0	0
Average *B*-factor (Å)	80.2	42.6	43.2	32.8	53.5	59.8

[a]For each structure reported, data were derived from a single crystal.

[b]Numbers in parentheses correspond to the highest resolution shell

Supplementary Table 2. cryo-EM data collection and refinement statistics.

	C002 SARS-CoV-2 S 2P (state 1)	C002 SARS-CoV-2 S 2P (state 2)	C104 SARS-CoV-2 S 2P (open state)	C110 SARS-CoV-2 S 2P (open state)	C119 SARS-CoV-2 S 2P (open state)	C121 SARS-CoV-2 S 2P (state 1)	C121 SARS-CoV-2 S 2P (state 2)	C135 SARS-CoV-2 S 2P (open state)	C144 SARS-CoV-2 S 6P (closed state)
PDB	**7K8S**	**7K8T**	**7K8U**	**7K8V**	**7K8W**	**7K8X**	**7K8Y**	**7K8Z**	**7K90**
EMD	**22729**	**22730**	**22731**	**22732**	**22733**	**22734**	**22735**	**22736**	**22737**
Data collection conditions									
Microscope	Titan Krios	Titan Krios	Titan Krios	Titan Krios	Titan Krios	Titan Krios	Titan Krios	Titan Krios	Talos Arctica
Camera	Gatan K3 Summit	Gatan K3 Summit	Gatan K3 Summit	Gatan K3 Summit	Gatan K3 Summit	Gatan K3 Summit	Gatan K3 Summit	Gatan K3 Summit	Gatan K3 Summit
Magnification	105,000x	105,000x	105,000x	105,000x	105,000x	105,000x	105,000x	105,000x	45,000x
Voltage (kV)	300	300	300	300	300	300	300	300	200
Recording mode	counting	counting	counting	counting	counting	counting	counting	counting	counting
Dose rate (e$^-$/pixel/s)	22.1	22.1	23.1	22.1	22.1	23.1	22.1	23.5	15.28
Electron dose (e$^-$/Å^2)	60	60	61	60	60	60	60	60	60
Defocus range (μm)	1.0 - 2.5	1.0 - 2.5	1.0 - 2.6	1.0 - 2.5	1.0 - 2.5	1.0 - 2.5	1.0 - 2.5	1.0 - 2.5	0.8 - 2.2
Pixel size (Å)	0.836	0.836	0.836	0.836	0.836	0.836	0.836	0.836	0.869
Micrographs collected	3,471	3,471	3,383	4,995	3,626	5,481	5,481	3,882	2,530
Micrographs used	3,105	3,105	2,668	2,923	3,069	3,671	3,671	3,184	2,184
Total extracted particles	1,691,930	1,691,930	1,181,957	840,293	1,381,582	892,954	892,954	634,621	376,586
Refined particles	51,915	49,238	40,469	43,981	140,378	40,489	14,999	101,114	212,876
Symmetry imposed	C1	C1	C1	C1	C1	C1	C1	C1	C3
Nominal Map Resolution (Å)									
FSC 0.143 (unmasked/masked)	4.4/3.4	4.6/3.4	6.6/3.7	5.3/3.8	4.4/3.6	4.4/3.6	8.4/4.4	7.4/3.5	3.9/3.2
FSC 0.143 local (unmasked/masked)	5.8/3.7	6.5/3.8	7.4/4.3	8.2/4.1	7.2/3.7	7.8/3.9	10.2/5.6	9.2/3.8	7.9/3.7
Refinement and Validation									
Initial model used	6VXX	6VYB	6VYB	6VYB	6VYB	6VYB	6VYB	6VYB	6XKL
Number of atoms									
Protein	28,865	28,871	23,852	25,365	25,662	27,399	25,098	23,436	28,466
Ligand	795	779	671	649	837	357	262	789	627
MapCC (global/local)	0.83/0.82	0.86/0.81	0.86/0.82	0.80/0.72	0.74/0.73	0.78/0.74	0.79/0.78	0.81/0.82	0.8/0.77
Map sharpening B-factor	88	79.1	135.1	98.4	80.7	58.1	42.4	71.4	66.9
R.m.s. deviations									
Bond lengths (Å)	0.01	0.01	0.01	0.01	0.01	0.003	0.002	0.006	0.003
Bond angles (°)	0.81	0.9	0.84	0.81	1	0.6	0.5	0.8	0.6
MolProbity score	2.56	2.14	2.27	2.33	2.46	2.06	2	2.3	2.37
Clashscore (all atom)	16.5	15.2	18.9	19.7	18.1	11.2	20.9	16.3	9.7
Poor rotamers (%)	0	0	0	2.1	2.4	2.4	0	0.2	1.3
Ramachandran plot									
Favored (%)	92.6	92.9	91.7	95.9	93.7	96.7	97.1	87.2	94
Allowed (%)	6.9	6.5	8.3	4.1	6.3	3.2	2.7	12.4	5.6
Disallowed (%)	0.5	0.6	0	0	0	0.1	0.2	0.4	0.4