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Supplemental Information

Structurally Resolved SARS-CoV-2 Antibody Shows High Efficacy in Severely Infected Hamsters and Provides a Potent Cocktail Pairing Strategy

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Table S1. Cryo-EM data collection, processing and validation statistics, Related to Figure 1

	S-6P in complex with three BD-368-2 Fabs (PDB ID: 7CHH; EMDB ID: EMD-30374)
Data collection and processing	
Voltage (kV)	300
Microscope	FEI Titan Krios G3
Camera	K2 Summit (Gatan)
Magnification (calibrated)	130,000X
Electron exposure (e^{-}/Å^2)	59.80
Exposure rate (e^{-}/Å^2/s)	7.1875
Number of frames collected per micrograph	32
Energy filter slit width	20 eV
Automation software	SerialEM
Defocus range (μm)	–0.7 to –1.2
Pixel size (Å)	1.055
Micrographs used	5,273
Symmetry imposed	C1
Initial particle images	586,005
Final particle images	85,053
Resolution at 0.5 FSC of masked reconstruction (Å)	3.98
Resolution at 0.143 FSC of masked reconstruction (Å)	3.49
Map sharpening B factor (Å^2)	–52.34
Refinement	
Initial model used (PDB code)	6VSB
Refinement package	Phenix v1.18 (Real-space refinement at 3.49 Å)
Map-model CC	
CC_mask	0.77
CC_box	0.76
CC_peaks	0.64
CC_volume	0.75
Model composition	
Non-hydrogen atoms	29,029
Protein residues	3,704
Ligands	41
R.m.s. deviations	
Bond lengths (Å)	0.007
Bond angles (°)	1.086
B factors (Å^2)	
Protein	84.97
Ligands	80.33
Validation	
MolProbity score	2.04
Clashscore	4.86
Poor rotamers (%)	3.56
Ramachandran plot	
Favored (%)	94.70
Allowed (%)	5.24
Disallowed (%)	0.06
Cβ outliers (%)	0.00
CaBLAM outliers (%)	3.61

Table S3. Crystal data collection and refinement statistics, Related to Figure 6

	BD-236/RBD (PDB ID: 7CHB)	BD-604/RBD (PDB ID: 7CH4)	BD-629/RBD (PDB ID: 7CH5)	BD-236/RBD/BD-368-2 (PDB ID: 7CHE)	BD-604/RBD/BD-368-2 (PDB ID: 7CHF)	BD-629/RBD/BD-368-2 (PDB ID: 7CHC)
Data collection						
Resolution (Å)	2.40	3.15	2.70	3.42	2.67	2.71
Space group	C 2	C 2	P 2_1 2_1 2_1	P 2_1 2_1 2_1	P 2_1 2_1 2_1	P 2_1 2_1 2_1
Unit cell	195.6 Å, 86.8 Å, 56.4 Å, β=100.1 º	197.9 Å, 85.5 Å, 57.1 Å, β=99.8 º	56.0 Å, 102.3 Å, 164.8 Å	100.0 Å, 114.3 Å, 117.0 Å	99.9 Å, 116.2 Å, 115.8 Å	101.9 Å, 105.7 Å, 110.5 Å
Multiplicity	6.8 (6.9)	6.8 (6.8)	12.2 (11.1)	12.7 (11.7)	11.3 (6.2)	13.0 (11.9)
Completeness (%)	99.6 (99.2)	99.7 (99.6)	99.5 (96.4)	94.4 (56.8)	96.0 (70.8)	99.8 (98.9)
Mean I/sigma (I)	15.2 (2.2)	7.8 (2.0)	13.8 (2.5)	11.6 (2.1)	16.2 (2.1)	12.5 (2.0)
Wilson B-factor	43.8	57.3	38.2	64.1	42.3	38.4
R_{merge}	0.17 (0.93)	0.20 (0.68)	0.25 (1.03)	0.28 (1.57)	0.36 (4.21)	0.28 (1.75)
R_{meas}	0.18 (1.01)	0.21 (0.74)	0.26 (1.07)	0.29 (1.64)	0.28 (4.56)	0.29 (1.83)
R_{pim}	0.07 (0.38)	0.08 (0.28)	0.07 (0.31)	0.08 (0.47)	0.11 (1.73)	0.08 (0.52)
$CC_{1/2}$	0.98 (0.80)	0.96 (0.82)	0.99 (0.91)	0.98 (0.69)	0.99 (0.14)	0.99 (0.69)
Refinement						
Reflections used in refinement	36334 (3590)	16331 (1611)	26713 (2557)	17722 (1036)	37204 (2714)	32997 (3192)
Reflections used for R-free	1815 (178)	816 (81)	1337 (128)	1771 (101)	1866 (140)	1649 (139)
R_{work}/R_{free}	0.192/0.227	0.227/0.273	0.226/0.260	0.221/0.234	0.220/0.270	0.212/0.285
Number of non-hydrogen atoms	4893	4729	4687	7955	8008	7985
macromolecules	4676	4729	4687	7955	8008	7985
ligands	28	0	0	0	0	0
solvent	189	0	0	0	0	0
Protein residues	616	619	607	1047	1052	1042
RMS(bonds)	0.003	0.004	0.006	0.027	0.012	0.005
RMS(angles)	0.67	0.79	0.98	2.92	1.45	0.94
Ramachandran favored (%)	95.86	93.29	95.33	93.02	93.74	95.62
Ramachandran allowed (%)	3.97	6.38	4.17	6.69	5.97	4.09
Ramachandran outliers (%)	0.17	0.33	0.50	0.29	0.29	0.29
Average B-factor	50.7	48.4	44.8	54.8	41.2	31.8

Each dataset was collected from a single crystal. Statistics for the highest-resolution shell are shown in parentheses.