

Supplemental information

An infectivity-enhancing site on the SARS-CoV-2 spike protein targeted by antibodies

Yafei Liu, Wai Tuck Soh, Jun-ichi Kishikawa, Mika Hirose, Emi E. Nakayama, Songling Li, Miwa Sasai, Tatsuya Suzuki, Asa Tada, Akemi Arakawa, Sumiko Matsuoka, Kanako Akamatsu, Makoto Matsuda, Chikako Ono, Shiho Torii, Kazuki Kishida, Hui Jin, Wataru Nakai, Noriko Arase, Atsushi Nakagawa, Maki Matsumoto, Yukoh Nakazaki, Yasuhiro Shindo, Masako Kohyama, Keisuke Tomii, Koichiro Ohmura, Shiro Ohshima, Toru Okamoto, Masahiro Yamamoto, Hironori Nakagami, Yoshiharu Matsuura, Atsushi Nakagawa, Takayuki Kato, Masato Okada, Daron M. Standley, Tatsuo Shioda, and Hisashi Arase

Table S1. Cryo-EM data collection and processing statistics, related to Figure 5.

Sample	Spike protein			Spike protein with 8D2 Fab			Spike protein with COV2-2490 Fab		
Data collection									
Microscope	Titan Krios			Titan Krios			Titan Krios		
Acc. Voltage (kV)	300			300			300		
Total electron dose (e ⁻ /Å)	50			50			50		
Pixel size (Å)	0.88			0.88			0.88		
Defocus range (μm)	-0.8 – -2.0 (0.15)			-0.8 – -2.0 (0.15)			-0.8 – -2.0 (0.15)		
Magnification	81,000			81,000			81,000		
Corrected Cs (mm)	0.0452			0.059			0.0355		
Data processing									
Software	CryoSparc v3.0.1			CryoSparc v3.0.1			CryoSparc v3.0.1		
# of Micrographs	5,075			2,135			5,177		
# of particles	74,756	161,974	161,524	99,745	743,99	137,974	104,069	33,092	
Symmetry				C1					
# of antibody	-	1	1	1	1	1	3	2	
Resolution (Å, GS-FSC=0.143)	3.36	3.46	3.53	3.82	4.16	3.74	3.15	4.06	
EMDB ID	30915	30916	30117	30918	30919	30920	30921	30922	
Model building									
Method	Homology modeling & Rigid body fitting			Homology modeling & Rigid body fitting			Homology modeling & Rigid body fitting		
Template model (spike)	7KEB			7K8W			7K8W		
Template model (Fab)				5K8M*1			5K8M*1		
Fitting software				MODELL ER v9.23			MODELL ER v9.23		
Fitting Criteria				UCSF Chimera v1.14			UCSF Chimera v1.14		
Correlation after fitting				0.829			0.780		
Modeling software (Fab)				Repertoire Builder			Repertoire Builder		
# of Atoms	13,452			15,212			18,708		
Ramachandran Favored (%)	93			95			95		
Allowed (%)	5			4			4		
Outlier (%)	2			1			1		
Clash score	2			3			1		
RMSZ bound length (Å)	0.87			0.93			0.94		
RMSZ bound angle (°)	0.95			0.91			0.91		
PDBID	7DZW			7DZX			7DZY		
Related figure	Figure 5D Figure S4D	Figure S4E	Figure S4F	Figure 5D Figure S4G	Figure S4H	Figure S4I	Figure 5D Figure S4J	Figure S4K	

*1 The variable region of Fab was modelled by Repertoire Builder. See details in Methods.