Cell, Volume *185*

Supplemental information

Receptor binding and complex structures of human ACE2 to spike RBD from omicron and delta SARS-CoV-2

Pengcheng Han, Linjie Li, Sheng Liu, Qisheng Wang, Di Zhang, Zepeng Xu, Pu Han, Xiaomei Li, Qi Peng, Chao Su, Baihan Huang, Dedong Li, Rong Zhang, Mingxiong Tian, Lutang Fu, Yuanzhu Gao, Xin Zhao, Kefang Liu, Jianxun Qi, George F. Gao, and Peiyi Wang

Supplementary tables:

Table S1. The immobilization and concentrations statistics of SPR assay, Related to Figure 2

Ligand	Sample	Immobilization quantity (units)	Concentrations (nM)
Prototype-RBD	Human ACE2 (PD)	3040.0	200, 100, 50, 25, 12.5
Alpha-RBD	Human ACE2 (PD)	1934.7	200, 100, 50, 25, 12.5
Beta-RBD	Human ACE2 (PD)	3834.4	200, 100, 50, 25, 12.5
Delta-RBD	Human ACE2 (PD)	2896.3	200, 100, 50, 25, 12.5
Gamma-RBD	Human ACE2 (PD)	2885.3	200, 100, 50, 25, 12.5
Omicron-RBD	Human ACE2 (PD)	3632.5	200, 100, 50, 25, 12.5
GD/1/2019-RBD	Human ACE2 (PD)	1415.9	200, 100, 50, 25, 12.5

Table S2. Crystallographic data collection and refinement statistics, Related to Figure 3

	Omicron RBD/hACE2	Delta RBD/hACE2
Data collection		
Space group	$P4_12_12$	$P2_1$
Cell dimensions		
a, *b*, *c* (Å)	104.24, 104.24, 227.18	89.77, 143.65, 106.41
α, β, γ (°)	90.00, 90.00, 90.00	90.00, 95.29, 90.00
Resolution (Å)	50.00-3.00 (3.11-3.00)	50.00-3.35 (3.47-3.35)
Unique reflections	25810 (2509)	38716 (3873)
Completeness (%)	99.9 (100)	100.0 (100.0)
R_{merge}	0.186 (1.067)	0.162 (1.307)
$I/\sigma I$	10.6 (1.8)	9.4 (1.1)
$CC_{1/2}$	0.992（0.692）	0.992 (0.825)
Redundancy	7.8 (7.7)	7.0 (7.2)
Refinement		
Resolution (Å)	46.62-3.00	44.70-3.35
No. reflections	25274	38489
R_{work}/R_{free}	0.2006/0.2324	0.1987/0.2398
No. atoms		
Protein	6532	13024
Ligand/ion	1	2
Water	0	0
B-factors		
Protein	59.2	120.0
Ligand/ion	80.3	108.6
Water		
R.M.S. deviations		

Bond lengths (Å)	0.004	0.012
Bond angles (°)	0.596	1.285
Ramchandran Statistics (%)		
Favored	97.46	94.6
Allowed	2.29	5.34
Disallowed	0.25	0.06

Values in parentheses are for highest-resolution shell.

Table S3. Cryo-EM data processing and refinement statistics, Related to Figure 3

Data Collection & Processing	
Microscope	TFS Titan Krios
Camera	K3
Magnification	74593
Voltage (kV)	300
Total dose (e^{-}/Å^2)	60
Defocus range (μm)	-1.3 to -2.3
Pixel size, Å per pixel	0.67
Symmetry imposed	C1
Final particles images	110,912
Map resolution (Å, FSC=0.143)	3.4
Map sharpening B factor (Å^2)	-200
Map resolution range (Å, FSC=0.143)	2.8-5.0
Refinement	
Initial model used (PDB code)	6LZG
Non-hydrogen atoms	6484
Protein residues	791
Validation	
Clash score	6.79
Poor rotamers (%)	0.72
R.m.s. deviations	
Bond lengths (Å)	0.004
Bond angles (°)	0.589
Ramachandran statistics (%)	
Most favored	96.06
Allowed	3.56
Outliers	0.38