

Supplemental Information

**Structural Basis for Potent
Neutralization of Betacoronaviruses
by Single-Domain Camelid Antibodies**

Daniel Wrapp, Dorien De Vlieger, Kizzmekia S. Corbett, Gretel M. Torres, Nianshuang Wang, Wander Van Breedam, Kenny Roose, Loes van Schie, VIB-CMB COVID-19 Response Team, Markus Hoffmann, Stefan Pöhlmann, Barney S. Graham, Nico Callewaert, Bert Schepens, Xavier Saelens, and Jason S. McLellan

	Neutralization IC ₅₀ (μg/mL)	
	MERS-CoV England 1	SARS-CoV-1 Urbani
D12 mAb (ctrl)	0.01996	>10
MERS VHH-2	>10	>10
MERS VHH-12	0.13	>10
MERS VHH-15	>10	>10
MERS VHH-20	>10	>10
MERS VHH-34	2.9	>10
MERS VHH-40	0.034	>10
MERS VHH-55	0.014	>10
SARS VHH-1	>10	>10
SARS VHH-6	>10	0.14
SARS VHH-35	>10	>10
SARS VHH-44	>10	5.5
SARS VHH-72	>10	>10

	VHH-72 + SARS-CoV-1 RBD	VHH-55 + MERS-CoV RBD
PDB ID	6WAQ	6WAR
<i>Data collection</i>		
Space group	<i>P</i> 3 ₁ 21	C222 ₁
Cell dimensions		
<i>a, b, c</i> (Å)	88.8, 88.8, 200.8	150.0, 283.3, 173.7
α, β, γ (°)	90, 90, 120	90, 90, 90
Resolution (Å)	43.39-2.20 (2.28-2.20)	66.30-3.40 (3.51-3.40)
Rmerge	0.179 (1.669)	0.999 (3.752)
I/σI	6.2 (1.5)	6.2 (2.1)
CC1/2	0.993 (0.865)	0.485 (0.161)
Completeness (%)	99.8 (99.9)	98.5 (95.7)
Redundancy	8.9 (9.1)	5.8 (5.1)
<i>Refinement</i>		
Rwork/Rfree (%)	20.3/23.6	21.4/26.8
No. atoms		
Protein	4,934	20,270
Glycan (NAG)	42	42
Water	102	0
Average B-factors	78.5	84.3
Protein	78.8	84.3
Ligands	92.5	115.7
R.m.s. deviations		
Bond lengths (Å)	0.01	0.007
Bond angles (°)	0.76	1.05
Ramachandran		
Favored (%)	95.8	97.1
Allowed (%)	4.2	2.5
Outliers (%)	0.0	0.4

Supplementary Table 2: X-ray crystallography data collection and refinement statistics. Related to Figures 2 and 3.