Table 1. Interface residues of cRBD and sRBD with ACE2 are shown at 0 ns and 20 ns of simulation. The loss of electrostatic contact can be noted in both states (bold residues).

	RBD-ACE2 interface (0 ns)						RBD-ACE2 interface (0 ns)					
Virus	**RBD**	**ACE2**		**Bond**			**RBD**	**ACE2**		**Bond**		**E** kcal/mol
E kcal/mol	**Dist Å**	**Atom**					**Dist Å**	**Atom**				
SARS-CoV	**Arg426**	**Glu329**	**IH**	**-35.88**	**2.99**	--	Tyr481	Lys353	H	-9.80	2.89	b-
	Gly482	Lys353	H	-7.20	2.80	b-	Tyr436	Asp38	H	-5.80	2.75	--
	Tyr491	Glu37	H	-4.90	2.56	--	Gly488	Gly354	H	-4.00	2.80	bb
	Tyr436	Asp38	H	-3.70	2.53	--	Thr486	Asn330	H	-3.40	2.83	b-
	Asp463	Ser19	I	-1.49	3.61	-b	Asp463	Gln24	H	-2.60	2.78	--
	Asn479	Glu35	H	-1.30	3.18	--	Thr486	Asp355	H	-1.70	2.60	--
	Thr486	Tyr41	H	-1.20	2.99	--	Tyr491	Gly354	A	-0.70	3.86	-b
	Asn473	Gln24	H	-1.00	2.89	--						
SARS-CoV-2	**Lys417**	**Asp30**	**IH**	**-30.83**	**2.71**	--	Gln493	Lys31	H	-11.60	2.85	--
	Tyr505	Glu37	H	-4.60	2.57	--	Tyr449	Asp38	H	-2.80	2.58	--
	Gly502	Lys353	H	-3.60	3.10	bb	Asn501	Lys353	H	-2.80	3.05	b-
	Gln498	Lys353	H	-2.90	3.00	--	Gln474	Gln24	H	-2.70	2.78	--
	Gln506	Gln325	H	-2.60	2.82	--	Asn487	Gln24	H	-2.40	2.85	--
	Asn487	Gln325	H	-1.60	2.80	--	Gln498	Lys353	H	-1.60	3.03	--
	Gln493	His34	H	-0.50	3.07	--	Thr500	Lys353	H	-1.40	2.71	b-
							Tyr489	Phe28	A	-0.60	3.75	b-
							Gln498	Tyr41	A	-0.60	4.52	--

VH, variable heavy chain; VL, variable light chains; H, hydrogen bond; A, aromatic bond; I, ionic (electrostatic) bond; bb, backbone atoms.

Table 2. Iinterface residues of cRBD with anti-SARS mAbs.

mAB Type		cRBD	scFv	Bond	E kcal/mol	Dist Å	Atom
m396	VH	Thr169	Ser31	H	-2.00	2.73	b-
		Gly171	Thr33	H	-2.30	2.94	-b
		Asp74	Asn58	H	-3.10	2.77	--
		Gln175	Val97	H	-4.00	2.92	b-
	VL	Thr45	Ser93	H	-1.70	2.76	--
		Arg77	Ser94	H	-1.10	3.21	b-
		Arg77	Asp95	IH	-19.24	2.89	--
F26G19	VH	Ser44	Thr31	H	-1.50	2.80	-b
		Ser44	Tyr52	H	-1.60	2.93	--
		Asn106	Tyr52	A	-1.20	4.05	--
		Asn106	Asn54	H	-4.20	2.74	-b
		Asn108	Asp56	H	-6.70	2.99	--
		Asn109	Asp56	H	-6.00	2.97	--
		Val172	Gln95	H	-0.80	3.02	-b
	VL	Gly171	Val92	H	-1.00	3.11	bb
		Thr169	Tyr94	H	-5.10	2.88	bb
80R	VH	Gly165	Ser101	H	-1.70	2.81	b-
		Tyr174	Arg100	H	-0.50	3.12	--
	VL	Val114	Trp226	A	-0.50	4.51	--
		Asn119	Arg162	H	-11.70	2.83	--
		Gly154	Thr206	H	-3.20	2.74	b-
		Cys157	Ser197	H	-3.00	2.70	b-
		Gln162	Thr185	H	-2.10	2.77	--
s230	VH	Gln162	Arg54	H	-2.70	2.87	--
		Phe125	Asn55	A	-0.80	4.61	--
		Asn156	Asp60	H	-3.30	2.82	--
		Cys157	Lys63	H	-2.80	3.58	--
		Leu124	Tyr104	H	-3.10	2.62	-b
		Tyr90	Tyr104	A	-0.00	3.91	--

VH, variable heavy chain; VL, variable light chains; H, hydrogen bond; A, aromatic bond; I, ionic (electrostatic) bond; bb, backbone atoms. Residue numbers of the cRBD should be tallied with the top numbers in Figure 1B.

Table 3. Interface residues of cRBD with docked CR3014 and CR3022 mAbs.

mAB Type		cRBD	scFv	Bond	$E^{kcal/mol}$	Dist Å	Atom
CR3014	VL	Asp96	Gln27	H	-2.00	3.21	b-
		Asp96	Tyr92	H	-2.40	2.62	--
		Asp97	Asp1	IH	-13.963	2.80	-b
		Ser128	Tyr32	H	-2.00	3.74	--
		Lys131	Ser91	H	-0.600	3.28	-b
		Pro132	Thr94	H	-1.60	3.01	b-
	VH	Glu134	Arg54	IH	-26.192	2.78	--
		Asp136	Asn58	H	-0.50	3.48	b-
		His188	Arg71	H	-0.60	3.27	b-
CR3022	VL	Arg26	Glu61	IH	-14.70	3.26	--
		Arg135	Tyr56	H	-8.00	2.75	b-
		Arg135	Ser58	H	-3.40	2.96	--
		Phe133	Lys36	H	-2.90	2.87	-b
		Arg24	Tyr56	H	-2.60	3.24	-b
	VH	Glu9	Gly30	H	-6.80	2.80	b-
		Arg26	Ser102	H	-3.80	2.88	--
		Arg26	Tyr34	H	-2.50	2.66	-b
		Leu4	Thr33	H	-2.30	2.78	-b
		Asn29	Trp54	H	-2.90	2.61	-b

VH, variable heavy chain; VL, variable light chains; H, hydrogen bond; A, aromatic bond; I, Ionic (electrostatic) bond; bb, backbone atoms. Residue numbers of the cRBD should be tallied with the top numbers in Figure 1B.