Table S1. Main characteristics of relevant target proteins.

Protein [1]	Gene [2]	Code [3]	Name [4]	Organism	Length [5]
CD46	CD46	P15529	Membrane cofactor protein	Homo sapiens	392
EP	E	P0DTC4	Envelope small membrane protein	SARS-CoV-2	75
MP	M	P0DTC5	Membrane protein	SARS-CoV-2	222
NP	N	P0DTC9	Nucleoprotein	SARS-CoV-2	419
SP	S	P0DTC2	Spike glycoprotein	SARS-CoV-2	1273

Note.1. Generally accepted protein abbreviation; 2. Gene's nomenclatural designation; 3. Common protein code recommended by UniProt.; 4. Nomenclature name recommended by UniProt.; 5. Length of the primary sequence in amino acid residues.

Table S2. Experimental 3D models of relevant target proteins.

Protein	PDB Code
CD46	1CKL, 2O39, 3INB, 3L89, 3O8E, 5F08
EP	7K3G
MP	—
NP	6M3M, 6VYO, 6WJI, 6WKP, 6WZO, 6WZQ, 6YI3, 6YUN, 6ZCO, 7ACS, 7ACT, 7C22, 7CDZ, 7CE0, 7DE1, 7KGO, 7KGP, 7KGQ, 7KGR, 7KGT, 7RGS
SP	6LVN, 6LXT, 6LZG, 6MO5, 6M17, 6M1V, 6VSB, 6VW1, 6VXX, 6VYB, 6W41, 6WPS, 6WPT, 6X29, 6X2A, 6X2B, 6X2C, 6X6P, 6X79, 6XC2, 6XC3, 6XC4, 6XC7, 6XCM, 6XCN, 6XDG, 6XE1, 6XEY, 6XF5, 6XF6, 6XKL, 6XKP, 6XKQ, 6XLU, 6XMO, 6XM3, 6XM4, 6XM5, 6XR8, 6XRA, 6XS6, 6YLA, 6YM0, 6YOR, 6YZ5, 6YZ7, 6Y2M, 6Z43, 6Z97, 6ZB4, 6ZB5, 6ZBP, 6ZCZ, 6ZDG, 6ZDH, 6ZER, 6ZFO, 6ZGE, 6ZGG, 6ZGI, 6ZH9, 6ZHD, 6ZLR, 6ZOW, 6ZOX, 6ZOY, 6ZOZ, 6ZP0, 6ZP1, 6ZP2, 6ZP5, 6ZP7, 6ZWV, 6ZXN, 7A25, 7A29, 7A4N, 7A5R, 7A5S, 7A91, 7A92, 7A93, 7A94, 7A95, 7A96, 7A97, 7A98, 7AD1, 7B17, 7BEH, 7BEI, 7BEJ, 7BEK, 7BEL, 7BEM, 7BEN, 7BEO, 7BEP, 7BWJ, 7BYR, 7BZS, 7C01, 7C2L, 7C8D, 7C8J, 7C8V, 7C8W, 7CAB, 7CAC, 7CAH, 7CAI, 7CAK, 7CAN, 7CDI, 7CDJ, 7CH4, 7CH5, 7CHB, 7CHC, 7CHE, 7CHF, 7CHH, 7CJF, 7CM4, 7CN9, 7CT5, 7CWL, 7CWM, 7CWN, 7CWO, 7CWS, 7CWU, 7D2Z, 7D30, 7DCC, 7DCX, 7DD2, 7DD8, 7DDD, 7DDN, 7DF3, 7DF4, 7DK3, 7DK4, 7DK5, 7DK6, 7DK7, 7DMU, 7DPM, 7JJC, 7JJI, 7JJJ, 7JMO, 7JMP, 7JMW, 7JV2, 7JV4, 7JV6, 7JVA, 7JVB, 7JVC, 7JW0, 7JWB, 7JWY, 7JX3, 7JZL, 7JZM, 7JZN, 7JZU, 7K43, 7K45, 7K4N, 7K8M, 7K8S, 7K8T, 7K8U, 7K8V, 7K8W, 7K8X, 7K8Y, 7K8Z, 7K90, 7K9Z, 7KDG, 7KDH, 7KDI, 7KDJ, 7KDK, 7KDL, 7KE4, 7KE6, 7KE7, 7KE8, 7KE9, 7KEA, 7KEB, 7KEC, 7KGJ, 7KGK, 7KJ2, 7KJ3, 7KJ4, 7KJ5, 7KKK, 7KKL, 7KL9, 7KLG, 7KLH, 7KLW, 7KMB, 7KMG, 7KMH, 7KMI, 7KMK, 7KML, 7KMS, 7KMZ, 7KN5, 7KN6, 7KN7, 7KNB, 7KNE, 7KNH, 7KHI, 7KS9, 7KSG, 7KSJ, 7KXK, 7KZB, 7L02, 7L06, 7L09, 7L0N, 7L2C, 7L3N, 7L5B, 7L7F, 7L7K, 7LCN, 7LD1, 7LOP, 7ND3, 7ND4, 7ND5, 7ND6, 7ND7, 7ND8, 7ND9, 7NDA, 7NDB, 7NDC, 7NDD, 7NEH

Table S3. Adequate resolved isolated subunits of experimental 3D models of human CD46 membrane cofactor protein.

PDB Code	Chain [1]	Designation [2]	Length [3]	Range [4]
1CKL	A	CD46_1CKL-A	126	35-160
1CKL	B	CD46_1CKL-B	126	35-160
1CKL	C	CD46_1CKL-C	126	35-160
1CKL	D	CD46_1CKL-D	126	35-160
1CKL	E	CD46_1CKL-E	126	35-160
1CKL	F	CD46_1CKL-F	126	35-160
2O39	C	CD46_2O39-C	126	35-160
2O39	D	CD46_2O39-D	126	35-160
3INB	C	CD46_3INB-C	126	35-160
3INB	D	CD46_3INB-D	126	35-160
3L89	M	CD46_3L89-M	126	35-160
3L89	N	CD46_3L89-N	126	35-160
3L89	O	CD46_3L89-O	126	35-160
3L89	P	CD46_3L89-P	126	35-160
3L89	Q	CD46_3L89-Q	125	35-160
3L89	R	CD46_3L89-R	126	35-160
3L89	S	CD46_3L89-S	126	35-160
3L89	T	CD46_3L89-T	124	35-160
3L89	U	CD46_3L89-U	126	35-160
3L89	V	CD46_3L89-V	126	35-160
3L89	W	CD46_3L89-W	125	35-160
3L89	X	CD46_3L89-X	126	35-160
3O8E	B	CD46_3O8E-B	252	35-286
3O8E	D	CD46_3O8E-D	248	35-286
5FO8	C	CD46_5FO8-C	129	158-286

Note. 1. According to their designations in the original 3D model. 2. Designation of the isolated resolved subunit and the name of the pdb file containing this subunit. 3. Length of the isolated resolved subunit in amino acid residues. 4. The starting and ending numbers of the amino acids in the continuous resolved sequence.

Table S4. Adequate resolved isolated subunits of experimental 3D models of SARS-CoV-2[1] envelope protein (EP).

PDB Code	Chain	Designation	Length	Range
7K3G	A	EP_7K3G-A	31	8-38
7K3G	B	EP_7K3G-B	31	8-38
7K3G	C	EP_7K3G-C	31	8-38
7K3G	D	EP_7K3G-D	31	8-38
7K3G	E	EP_7K3G-E	31	8-38

Note. 1. The column designations correspond to Table S3.

Table S5. Adequate resolved isolated subunits of experimental 3D models of SARS-CoV-2 [1] nucleocapsid protein (NP).

PDB Code	Chain	Designation	Length	Range
6M3M	A	NP_6M3M-A_102-174	73	102-174
6M3M	A	NP_6M3M-A_49-96	48	49-96
6M3M	B	NP_6M3M-B_48-97	50	48-97
6M3M	B	NP_6M3M-B_99-174	76	99-174
6M3M	C	NP_6M3M-C_47-96	50	47-96
6M3M	C	NP_6M3M-C_98-173	76	98-173
6M3M	D	NP_6M3M-D_101-174	74	101-174
6M3M	D	NP_6M3M-D_48-99	52	48-99
6VYO	D	NP_6YVO-D	125	49-173
6WJI	A	NP_6WIJ-A	108	257-364
6WJI	B	NP_6WIJ-B	108	257-364
6WJI	C	NP_6WIJ-C	108	257-364
6WJI	D	NP_6WIJ-D	108	257-364
6WJI	E	NP_6WIJ-E	108	257-364
6WJI	F	NP_6WIJ-F	108	257-364
6WZO	A	NP_6WZO-A	108	257-364
6WZO	B	NP_6WZO-B	111	254-364
6WZO	C	NP_6WZO-C	108	257-364
6WZO	D	NP_6WZO-D	110	255-364
6WZQ	A	NP_6WZQ-A	114	251-364
6WZQ	B	NP_6WZQ-B	114	251-364
6WZQ	C	NP_6WZQ-C	116	249-364
6WZQ	D	NP_6WZQ-D	115	250-364
6YI3	A	NP_6YI3-A	137	44-180
6YUN	A	NP_6YUN-A	116	249-364

6YUN	B	NP_6YUN-B	118	247-364
6ZCO	A	NP_6ZCO-A	118	247-364
7ACS	A	NP_7ACS-A	137	44-180
7ACT	A	NP_7ACT-A	137	44-180
7C22	A	NP_7C22-A	109	256-364
7C22	B	NP_7C22-B	113	252-364
7C22	C	NP_7C22-C	112	253-364
7C22	D	NP_7C22-D	108	257-364
7CDZ	A	NP_7CDZ-A	128	4-131
7CDZ	B	NP_7CDZ-B	127	4-130
7CDZ	C	NP_7CDZ-C	126	5-130
7CDZ	D	NP_7CDZ-D	127	5-131
7CE0	A	NP_7CE0-A	110	255-364
7CE0	B	NP_7CE0-B	110	255-364
7CE0	C	NP_7CE0-C	110	255-364
7CE0	D	NP_7CE0-D	110	255-364
7DE1	A	NP_7DE1-A	108	257-364
7DE1	B	NP_7DE1-B	115	250-364

Note. 1. The column designations correspond to Table S3.

Table S6. Adequate resolved isolated subunits of experimental 3D models of SARS-CoV-2 [1] spike protein (SP).

PDB Code	Chain	Designation	Length	Range
6XR8	A	SP_6XR8-A	1107	14-1162
6XR8	B	SP_6XR8-B	1107	14-1162
6XR8	C	SP_6XR8-C	1107	14-1162
6ZWV	A	SP_6ZWV-A	985	27-1151
6ZWV	B	SP_6ZWV-B	985	27-1151
6ZWV	C	SP_6ZWV-C	985	27-1151
7DDD	A	SP_7DDD-A	1088	14-1147
7DDD	B	SP_7DDD-B	1088	14-1147
7DDD	C	SP_7DDD-C	1088	14-1147
7JJI	A	SP_7JJI-A	1109	14-1146
7JJI	B	SP_7JJI-B	1109	14-1146
7JJI	C	SP_7JJI-C	1109	14-1146
7L7K	A	SP_7L7K-A	973	27-1146
7L7K	B	SP_7L7K-B	973	27-1146
7L7K	C	SP_7L7K-C	973	27-1146

Note. 1. Column designations correspond to Table S3.

Table S7. Validity indicators of adequate resolved isolated subunits from experimental 3D models of human CD46 membrane cofactor protein.

Designation [1]	QMEAN4 [2]	Designation [1]	QMEAN4 [2]
CD46_1CKL-A	-4.95	CD46_3L89-P	-0.47
CD46_1CKL-B	-0.66	CD46_3L89-Q	-1.37
CD46_1CKL-C	-3.40	CD46_3L89-R	-0.05
CD46_1CKL-D	-2.09	CD46_3L89-S	-0.44
CD46_1CKL-E	-1.62	CD46_3L89-T	-0.37
CD46_1CKL-F	-0.50	CD46_3L89-U	0.16
CD46_2O39-C	-1.39	CD46_3L89-V	-0.68
CD46_2O39-D	-0.86	CD46_3L89-W	-0.53
CD46_3INB-C	-6.13	CD46_3L89-X	-0.18
CD46_3INB-D	-6.94	CD46_3O8E-B	0.96
CD46_3L89-M	-0.48	CD46_3O8E-D	1.42
CD46_3L89-N	-0.73	CD46_5FO8-C	0.08
CD46_3L89-O	-0.26		

Note. 1. Designation of the pdb file containing the respective isolated subunit. 2. The validity assessment function for the 3D model [Benkert, 2011].

Table S8. Validity Indicators of Adequate Resolved Isolated Subunits from Experimental 3D Models of SARS-CoV-2[1] Envelope Protein (EP).

Designation	QMEAN4	Designation	QMEAN4
EP_7K3G-A	-2.90	EP_7K3G-D	-2.90
EP_7K3G-B	-2.94	EP_7K3G-E	-2.90
EP_7K3G-C	-2.87		

Note. 1. The column designations correspond to Table S7.

Table S9. Validity Indicators of Adequate Resolved Isolated Subunits from Experimental 3D Models of SARS-CoV-2 Nucleocapsid Protein (NP).

Designation	QMEAN4	Designation	QMEAN4	Designation	QMEAN4
NP_6M3M-A_102-174	0.17	NP_6WZO-A	-0.12	NP_7C22-B	0.12
NP_6M3M-A_49-96	-1.40	NP_6WZO-B	0.07	NP_7C22-C	-0.23
NP_6M3M-B_48-97	-0.71	NP_6WZO-C	0.07	NP_7C22-D	-0.15
NP_6M3M-B_99-174	-0.17	NP_6WZO-D	0.01	NP_7CDZ-A	0.94
NP_6M3M-C_47-96	-1.10	NP_6WZQ-A	0.22	NP_7CDZ-B	1.57
NP_6M3M-C_98-173	-0.74	NP_6WZQ-B	0.10	NP_7CDZ-C	0.83
NP_6M3M-D_101-174	-0.34	NP_6WZQ-C	0.37	NP_7CDZ-D	1.27

NP_6M3M-D_48-99	-1.20	NP_6WZQ-D	-0.27	NP_7CE0-A	0.11
NP_6YVO-D	1.19	NP_6YI3-A	not valid [2]	NP_7CE0-B	0.20
NP_6WIJ-A	-0.16	NP_6YUN-A	0.39	NP_7CE0-C	0.37
NP_6WIJ-B	-0.19	NP_6YUN-B	0.13	NP_7CE0-D	0.26
NP_6WIJ-C	-0.14	NP_6ZCO-A	-0.04	NP_7DE1-A	0.00
NP_6WIJ-D	-0.17	NP_7ACS-A	not valid [2]	NP_7DE1-B	0.18
NP_6WIJ-E	0.04	NP_7ACT-A	-3.22		
NP_6WIJ-F	-0.16	NP_7C22-A	-0.25		

Note. 1. The column designations correspond to Table 7. 2. QMEAN values are exceeding the permissible range,

Table S10. Validity Indicators of Adequate Resolved Isolated Subunits from Experimental 3D Models of SARS-CoV-2 [1] Spike Protein (SP).

Designation	QMEAN4	Designation	QMEAN4
SP_6XR8-A	-0.57	SP_7DDD-C	-1.68
SP_6XR8-B	-0.65	SP_7JJI-A	0.87
SP_6XR8-C	-0.72	SP_7JJI-B	0.91
SP_6ZWV-A	-1.28	SP_7JJI-C	0.91
SP_6ZWV-B	-1.26	SP_7L7K-A	-2.16
SP_6ZWV-C	-1.20	SP_7L7K-D	-3.33
SP_7DDD-A	-1.65	SP_7L7K-C	-2.15
SP_7DDD-B	-1.67		

Note. 1. The column designations correspond to Table S7.

Table S11. Valid Subunits Representing the Experimental 3D Structure of Human CD46 Membrane Cofactor Protein.

Designation	Length	Range	QMEAN4
CD46_3L89-R	126	35-160	-0.05
CD46_3O8E-B	252	35-286	0.96
CD46_3O8E-D	248	35-286	1.42
CD46_5FO8-C	129	158-286	0.08

Table S12. Valid Subunits Representing the Experimental 3D Structure of SARS-CoV-2 Nucleocapsid Protein (NP).

Designation	Length	Range	QMEAN
NP_6YVO-D	125	49-173	1.19
NP_6WZQ-C	116	249-364	0.37
NP_6YUN-A	116	249-364	0.39
NP_7CDZ-B	127	4-130	1.57
NP_7CDZ-D	127	5-131	1.27
NP_7CE0-C	110	255-364	0.37

Table S13. Valid Subunits Representing the Experimental 3D Structure of SARS-CoV-2 Spike Protein (SP).

Designation	Length	Range	QMEAN
SP_6XR8-A	1107	14-1162	-0.57
SP_6XR8-B	1107	14-1162	-0.65
SP_6XR8-C	1107	14-1162	-0.72
SP_6ZWV-A	985	27-1151	-1.28
SP_6ZWV-B	985	27-1151	-1.26
SP_6ZWV-C	985	27-1151	-1.20
SP_7DDD-A	1088	14-1147	-1.65
SP_7DDD-B	1088	14-1147	-1.67
SP_7DDD-C	1088	14-1147	-1.68
SP_7JJI-A	1109	14-1146	0.87
SP_7JJI-B	1109	14-1146	0.91
SP_7JJI-C	1109	14-1146	0.91

Table S14. Reliability of Homology-Based Full 3D Models of Human CD46 Protein and SARS-CoV-2 Envelope Protein (EP), Membrane Protein (MP), Nucleocapsid Protein

Protein	C-score for Model No.				
	1	2	3	4	5
Human CD46	-0.84	-3.27	-2.29	-3.39	-3.77
EP SARS-CoV-2	-0.85	-1.66	-1.01	-1.05	-3.90
MP SARS-CoV-2	-3.35	-3.43	-4.81	-5.00	-4.94
NP SARS-CoV-2	-1.58	-1.95	-3.18	-2.73	-3.04
SP SARS-CoV-2	-2.07	-2.12	-2.37	-2.61	-2.69

Table S15. Ranking of Validity Assessment for Homology-Based Full-Size 3D Models of Human CD46 Protein and SARS-CoV-2 Envelope Protein (EP), Membrane Protein (MP), Nucleocapsid Protein (NP), and Spike Protein (SP).

Experimental Subunit	Rank													
	DALI			PDBeFold			TM-score			FATKAT			$Rank_{Mean}$	$Rank_{Model}$
	Z	RSMD	Q	P	Z	RSMD	RSMD	TM	p	Score	$RSMD_{opt}$	$RSMD_{chain}$		
Human CD46 Membrane Protein														
Model1														**8.02**
CD46_3O8E-B	3	1	1	3	5	1	7	4	1	3	1	1	2.58	
CD46_3O8E-D	5	2	4	4	7	4	1	13	1	7	4	4	4.67	
CD46_5FO8-C	10	9	9	9	9	9	18	17	1	11	9	9	10.00	
CD46_3L89-R	16	13	11	13	13	13	19	14	15	18	18	15	14.83	
Model2														9.10
CD46_3O8E-B	4	2	3	1	6	3	9	5	1	2	3	3	3.50	
CD46_3O8E-D	7	2	5	2	8	5	3	18	1	6	5	5	5.58	
CD46_5FO8-C	9	10	18	14	17	18	20	16	10	10	10	10	13.50	
CD46_3L89-R	15	16	13	11	12	14	15	3	16	16	19	16	13.83	
Model3														10.06
CD46_3O8E-B	5	7	7	5	1	7	11	1	1	4	7	7	5.25	
CD46_3O8E-D	8	7	8	6	2	8	5	20	1	8	8	8	7.42	
CD46_5FO8-C	13	12	19	14	19	19	13	19	12	14	12	12	14.83	
CD46_3L89-R	14	13	12	12	11	11	14	6	14	17	16	13	12.75	
Model4														8.56
CD46_3O8E-B	1	2	2	7	3	2	10	2	1	1	2	2	2.92	
CD46_3O8E-D	2	2	5	8	4	6	4	12	1	5	5	5	4.92	
CD46_5FO8-C	10	10	20	14	17	20	17	15	10	12	11	11	13.92	
CD46_3L89-R	12	13	10	10	10	12	16	9	13	15	16	14	12.50	
Model5														15.08
CD46_3O8E-B	17	19	14	14	15	15	6	8	17	9	14	19	13.92	
CD46_3O8E-D	19	17	16	14	20	16	2	7	19	13	20	20	15.25	
CD46_5FO8-C	20	20	17	14	16	17	12	10	18	19	13	18	16.17	
CD46_3L89-R	18	18	15	14	14	10	8	11	20	20	15	17	15.00	

SARS-CoV-2 Envelope Protein (EP)													
						Model1							3.90
EP_7K3G-A	—	—	5	4	6	3	7	5	2	2	2	3	3.90
						Model2							6.80
EP_7K3G-A	—	—	6	6	7	7	5	7	8	7	8	7	6.80
						Model3							4.10
EP_7K3G-A	—	—	4	5	3	4	6	4	5	5	3	2	4.10
						Model4							5.60
EP_7K3G-A	—	—	7	7	5	6	4	6	6	6	5	4	5.60
						Model5							7.80
EP_7K3G-A	—	—	8	8	8	8	8	8	7	8	7	8	7.80
						QHD43418							**2.10**
EP_7K3G-A	—	—	3	3	4	1	3	3	1	1	1	1	2.10
SARS-CoV-2 Nucleocapsid Protein (NP)													
						Model1							21.53
NP_6WZQ-C	—	—	24	16	24	21	34	3	29	27	11	25	21.40
NP_6YUN-A	—	—	32	16	23	23	35	4	26	25	34	29	24.70
NP_6YVO-D	—	—	23	16	25	17	15	1	25	28	20	10	18.00
NP_7CDZ-B	—	—	26	16	26	16	14	5	30	30	21	18	20.20
NP_7CDZ-D	—	—	25	16	27	18	16	2	28	29	30	11	20.20
NP_7CE0-C	—	—	27	16	22	24	28	12	27	26	35	30	24.70
						Model2							24.89
NP_6WZQ-C	—	—	18	16	17	31	31	7	36	33	12	36	23.70
NP_6YUN-A	—	—	17	16	28	19	32	6	32	32	16	34	23.20
NP_6YVO-D	—	—	—	—	—	—	33	15	32	34	31	19	27.33
NP_7CDZ-B	—	—	—	—	—	—	29	8	34	35	26	20	25.33
NP_7CDZ-D	—	—	—	—	—	—	30	14	34	36	23	20	26.17
NP_7CE0-C	—	—	19	16	18	32	36	9	31	31	10	34	23.60
						Model3							15.43
NP_6WZQ-C	—	—	22	16	30	28	23	11	17	16	19	33	21.50
NP_6YUN-A	—	—	21	16	31	30	24	10	18	17	18	32	21.70

NP_6YVO-D	6	9	9	15	12	9	3	34	9	8	9	9	11.00	
NP_7CDZ-B	5	8	7	13	10	7	1	27	7	5	7	7	8.67	
NP_7CDZ-D	4	7	8	14	11	8	2	25	8	4	8	8	8.92	
NP_7CE0-C	—	—	20	16	29	22	13	26	16	18	17	31	20.80	
							Model4							18.41
NP_6WZQ-C	—	—	29	16	19	25	18	19	21	20	36	26	22.90	
NP_6YUN-A	—	—	30	16	20	26	20	24	19	19	32	28	23.40	
NP_6YVO-D	12	14	15	5	7	13	6	23	14	14	23	17	13.58	
NP_7CDZ-B	10	10	13	6	8	11	4	36	10	13	22	12	12.92	
NP_7CDZ-D	11	12	11	8	9	14	5	32	11	11	25	15	13.67	
NP_7CE0-C	—	—	28	16	21	27	17	30	20	21	33	27	24.00	
							Model5							18.79
NP_6WZQ-C	—	—	31	16	33	33	27	17	24	23	14	24	24.20	
NP_6YUN-A	—	—	33	16	32	29	26	20	22	22	13	22	23.50	
NP_6YVO-D	15	14	14	7	13	15	7	21	15	15	26	16	14.83	
NP_7CDZ-B	13	11	12	9	14	10	9	31	13	12	29	13	14.67	
NP_7CDZ-D	14	12	10	10	15	12	8	33	12	10	28	14	14.83	
NP_7CE0-C	—	—	16	16	16	20	25	29	23	24	15	23	20.70	
							QHD43423							**6.36**
NP_6WZQ-C	8	3	4	2	2	3	19	13	1	7	3	3	5.67	
NP_6YUN-A	7	1	2	1	1	1	21	16	1	6	1	1	4.92	
NP_6YVO-D	2	4	1	4	4	4	11	35	1	1	4	5	6.33	
NP_7CDZ-B	3	6	5	11	5	6	12	21	6	3	6	6	7.50	
NP_7CDZ-D	1	5	3	12	6	5	10	18	5	2	5	4	6.33	
NP_7CE0-C	9	2	6	3	3	2	22	28	1	9	2	2	7.42	
							SARS-CoV-2 Spike Protein (SP)							
							Model1							40.45
SP_6XR8-A	47	4	64	59	54	25	66	69	1	27	38	52	42.17	
SP_6XR8-B	25	24	58	59	68	61	15	19	1	10	33	48	35.08	
SP_6XR8-C	22	9	56	59	63	54	15	20	1	9	32	49	32.38	
SP_7DDD-A	30	49	66	59	66	67	69	67	1	34	43	57	50.63	

SP_7DDD-B	31	48	69	59	57	8	46	38	1	60	11	2	35.83	
SP_7DDD-C	31	51	66	59	66	67	65	66	1	32	34	54	49.29	
SP-6ZWV-A	71	46	16	24	23	17	41	49	64	46	70	59	43.83	
SP-6ZWV-B	68	39	17	18	24	15	70	59	72	69	72	72	49.58	
SP-6ZWV-C	59	52	18	17	20	20	33	35	65	55	7	63	37.00	
SP_7JJI-A	13	62	57	42	60	60	25	39	55	51	24	50	44.79	
SP_7JJI-B	37	26	59	59	64	58	12	12	1	5	27	43	33.58	
SP_7JJI-C	9	28	59	59	64	58	11	10	1	6	27	43	31.25	
							Model2							32.16
SP_6XR8-A	53	36	31	19	17	27	67	68	1	28	49	9	33.75	
SP_6XR8-B	31	5	23	25	19	46	24	23	1	11	42	25	22.88	
SP_6XR8-C	31	11	28	29	31	52	23	23	1	12	38	25	25.29	
SP_7DDD-A	52	33	41	37	36	43	58	57	1	40	53	37	40.67	
SP_7DDD-B	49	61	71	59	58	35	47	38	57	65	65	7	50.96	
SP_7DDD-C	49	41	42	36	37	44	51	56	1	36	53	13	38.25	
SP-6ZWV-A	61	45	5	5	6	21	42	44	1	45	3	40	26.46	
SP-6ZWV-B	60	2	4	3	4	19	64	52	67	68	6	67	34.67	
SP-6ZWV-C	56	44	6	4	5	18	32	33	68	59	35	70	35.83	
SP_7JJI-A	25	63	25	21	33	47	29	40	1	49	30	36	33.25	
SP_7JJI-B	44	16	21	30	26	37	5	7	1	8	53	31	23.21	
SP_7JJI-C	22	16	21	30	26	37	2	3	1	7	53	31	20.71	
							Model3							33.40
SP_6XR8-A	53	35	29	23	18	26	59	65	1	31	61	12	34.38	
SP_6XR8-B	37	20	26	26	22	31	18	16	1	21	46	29	24.38	
SP_6XR8-C	31	11	33	27	28	31	18	16	1	22	45	29	24.33	
SP_7DDD-A	46	40	44	47	50	39	60	59	1	42	59	33	43.33	
SP_7DDD-B	43	56	72	59	71	29	48	38	61	64	44	62	53.88	
SP_7DDD-C	49	43	43	45	50	40	54	58	1	37	59	10	40.75	
SP-6ZWV-A	65	50	10	12	10	12	43	43	1	47	16	56	30.42	
SP-6ZWV-B	64	2	11	10	10	13	53	46	70	71	18	70	36.50	
SP-6ZWV-C	58	60	12	10	10	11	35	33	63	58	10	68	35.67	

SP_7JJI-A	7	64	24	20	25	30	30	40	54	54	30	34	34.29	
SP_7JJI-B	44	8	19	35	32	31	5	8	1	23	46	23	22.88	
SP_7JJI-C	14	9	19	34	30	34	3	4	1	24	46	23	20.04	
							Model4							36.53
SP_6XR8-A	27	42	45	44	47	48	68	68	1	33	64	11	41.46	
SP_6XR8-B	1	13	37	55	59	70	21	18	1	16	62	16	30.75	
SP_6XR8-C	4	13	40	58	61	69	22	20	1	15	62	16	31.71	
SP_7DDD-A	21	33	47	50	55	50	57	52	1	41	49	25	40.08	
SP_7DDD-B	19	67	70	59	62	36	39	33	53	66	19	4	43.88	
SP_7DDD-C	19	38	46	48	56	51	50	55	1	39	49	8	38.29	
SP-6ZWV-A	63	47	8	14	14	10	37	39	1	50	8	38	27.42	
SP-6ZWV-B	62	1	9	15	15	16	56	46	58	72	9	61	34.96	
SP-6ZWV-C	67	32	7	15	15	14	31	32	66	62	14	64	34.88	
SP_7JJI-A	10	66	51	46	72	71	27	36	56	52	68	18	47.71	
SP_7JJI-B	40	21	49	59	69	65	8	7	1	17	66	21	35.21	
SP_7JJI-C	10	21	49	59	69	65	4	3	1	17	66	21	32.04	
							Model5							**31.34**
SP_6XR8-A	47	36	36	32	20	28	62	65	1	30	49	5	34.25	
SP_6XR8-B	15	7	27	33	34	49	17	17	1	14	38	14	22.13	
SP_6XR8-C	15	5	32	38	39	62	18	18	1	13	38	15	24.50	
SP_7DDD-A	31	31	39	43	43	42	55	54	1	38	58	35	39.17	
SP_7DDD-B	37	69	68	59	39	9	44	35	1	63	12	1	36.38	
SP_7DDD-C	42	30	38	41	43	41	49	55	1	35	53	6	36.13	
SP-6ZWV-A	69	55	1	9	7	5	38	40	1	48	2	39	26.17	
SP-6ZWV-B	70	68	2	7	7	6	52	45	69	70	14	66	39.67	
SP-6ZWV-C	57	57	3	8	9	7	36	35	62	56	5	65	33.29	
SP_7JJI-A	5	65	30	22	35	45	28	37	52	53	29	25	35.50	
SP_7JJI-B	41	13	34	39	45	56	5	6	1	19	35	19	26.08	
SP_7JJI-C	7	16	34	39	45	56	1	2	1	20	35	19	22.88	
							QHD43416							34.90
SP_6XR8-A	22	59	61	54	38	22	63	67	1	25	24	51	40.58	

SP_6XR8-B	1	23	48	49	48	55	13	16	1	3	22	47	27.17
SP_6XR8-C	1	25	52	57	49	53	14	17	1	4	23	45	28.42
SP_7DDD-A	29	54	62	56	42	24	71	67	1	29	13	58	42.17
SP_7DDD-B	17	71	65	53	29	1	45	37	1	61	4	3	32.25
SP_7DDD-C	17	53	63	51	41	23	60	63	1	26	26	53	39.71
SP-6ZWV-A	72	58	15	6	1	2	40	48	59	44	69	55	39.04
SP-6ZWV-B	66	29	14	2	3	4	72	61	71	67	71	69	44.08
SP-6ZWV-C	55	70	13	1	1	3	34	35	60	57	1	60	32.50
SP_7JJI-A	6	72	53	28	53	64	26	40	51	43	17	46	41.58
SP_7JJI-B	27	16	54	13	13	72	10	11	1	1	20	41	23.21
SP_7JJI-C	10	26	55	52	52	63	9	8	1	1	20	41	28.13

Table S16. Validity Assessment of Homology-Based Full-Size 3D Models of SARS-CoV-2 Membrane Protein (MP).

Model	QMEAN	Model	QMEAN
Model1	-10.78	Model4	-16.07
Model2	-12.58	Model5	-11.80
Mode3	-12.65	**QHD43419**	**-5.79**

Table S17. Energetic Characteristics of Protein-Protein Complexes of Human CD46 and SARS-CoV-2 Envelope Protein (EP), Membrane Protein (MP), Nucleocapsid Protein (NP), and Spike Protein (SP).

Complex	Program	ΔE, kcal/mol	Complex	Program	ΔE, kcal/mol
CD46 receptor — EP, MP, NP, SP ligands			**EP, MP, NP, SP receptors — CD46 ligand**		
CD46—EP	Cluspro2	-1218	EP—CD46	Cluspro2	-1217
CD46—EP	GRAMM1	20558	EP—CD46	GRAMM1	20558
CD46—EP	Hex8	-286.5	EP—CD46	Hex8	-278.8
CD46—EP	SwarmDock	-179.0	EP—CD46	SwarmDock	-247.7
CD46—EP	ZDOCK3	1815	EP—CD46	ZDOCK3	1815
CD46—MP	Cluspro2	-1300	MP—CD46	Cluspro2	-1355
CD46—MP	GRAMM1	21735	MP—CD46	GRAMM1	22061
CD46—MP	Hex8	-397.2	MP—CD46	Hex8	-412.7
CD46—MP	SwarmDock	-252.3	MP—CD46	SwarmDock	-398.7
CD46—MP	ZDOCK3	2186	MP—CD46	ZDOCK3	2186
CD46—NP	Cluspro2	-1354	NP—CD46	Cluspro2	-1473
CD46—NP	GRAMM1	20286	NP—CD46	GRAMM1	21072
CD46—NP	Hex8	-468.3	NP—CD46	Hex8	-467.1
CD46—NP	SwarmDock	-193.5	NP—CD46	SwarmDock	-178.9
CD46—NP	ZDOCK3	1834	NP—CD46	ZDOCK3	1834
CD46—SP	Cluspro2	-1329	SP—CD46	Cluspro2	-1329
CD46—SP	GRAMM1	68467	SP—CD46	GRAMM1	65242
CD46—SP	Hex8	-518.3	SP—CD46	Hex8	-493.6
CD46—SP	SwarmDock	-294.2	SP—CD46	SwarmDock	-294.2
CD46—SP	ZDOCK3	2219	SP—CD46	ZDOCK3	2219

Note: In Table S17, ΔE is expressed in arbitrary units for the ZDOCK3 program.

The primary energy scoring function for the complexes in different programs is defined as follows:

- Cluspro2 - ELowest: Weighted scoring function of the minimum energy for the given valid complex.
- GRAMM1 - ETotal: Scoring function of the minimum total energy for the given valid complex.
- Hex8 - EInteraction: Scoring function of the minimum energy of protein-protein interaction in the given valid complex.
- SwarmDock - EInteraction: Scoring function of the minimum energy of protein-protein interaction in the most representative cluster of the given valid complex.
- ZDOCK3 - ZDOCKScore: Scoring function of the minimum energy of protein-protein interaction in the given valid complex based on the number of amino acid contacts, expressed in arbitrary units.

Table S18. Full Lists of Binding Amino Acids in the Human CD46 and SARS-CoV-2 Envelope Protein (EP) Protein-Protein Complex.

Human CD46			EP SARS-CoV-2		
Amino Acid	**Position**	**Occurrence**	**Amino Acid**	**Position**	**Occurrence**
THR	**188**	**3**	**PHE**	**20**	**6**
TYR	**189**	**3**	**ILE**	**13**	**5**
SER	**190**	**3**	**VAL**	**5**	**4**
CYS	**191**	**3**	**THR**	**9**	**4**
PRO	**193**	**3**	**LEU**	**12**	**4**
PHE	**200**	**3**	**SER**	**16**	**4**
LEU	**202**	**3**	**VAL**	**17**	**4**
GLU	**205**	**3**	**LEU**	**19**	**4**
SER	**206**	**3**	**PHE**	**23**	**4**
THR	**207**	**3**	**LEU**	**27**	**4**
TYR	**247**	**3**	**VAL**	**29**	**4**
PRO	3	2	**LEU**	**34**	**4**
PHE	11	2	**ARG**	**38**	**4**
TRP	14	2	**ASN**	**45**	**4**
PHE	16	2	**ASN**	**66**	**4**
PRO	17	2	MET	1	3
GLY	18	2	SER	3	3
LEU	20	2	VAL	14	3
LEU	21	2	LEU	18	3
MET	24	2	VAL	25	3
LEU	27	2	LEU	28	3
TYR	29	2	THR	30	3
PHE	31	2	ALA	32	3
ASN	83	2	THR	35	3
HIS	84	2	LEU	39	3
THR	85	2	TYR	42	3
PRO	88	2	ASN	48	3
VAL	89	2	VAL	52	3
SER	90	2	VAL	70	3
PRO	166	2	LEU	73	3
ILE	168	2	VAL	75	3
THR	174	2	PHE	4	2
PHE	175	2	LEU	21	2
LEU	184	2	ALA	22	2
ALA	186	2	VAL	24	2
VAL	187	2	ILE	33	2
ALA	194	2	ALA	36	2
PRO	197	2	CYS	40	2
PRO	199	2	ALA	41	2
TYR	209	2	CYS	43	2
TRP	216	2	CYS	44	2
ALA	219	2	ILE	46	2
ALA	220	2	PRO	54	2
GLU	222	2	TYR	59	2
ILE	239	2	ARG	61	2

PHE	242	2
GLY	243	2
LYS	244	2
LYS	245	2
TYR	248	2
SER	341	2
VAL	351	2
ALA	353	2
LYS	169	1
ASP	192	1
ILE	203	1
PRO	221	1
LYS	237	1
GLN	238	1
SER	240	1
GLY	241	1
LYS	249	1
THR	251	1
MET	253	1
GLU	255	1
TYR	261	1
LEU	262	1
ASP	263	1
GLY	264	1
SER	265	1
ASP	266	1
THR	267	1
VAL	269	1
ASP	271	1
ASP	277	1
PRO	278	1
PRO	279	1
PRO	281	1
THR	292	1
LYS	293	1
PRO	295	1
LEU	297	1
HIS	299	1
SER	300	1
THR	307	1
SER	309	1
PRO	310	1
ALA	314	1
GLY	316	1
PRO	317	1
PRO	323	1
SER	326	1
ASN	327	1
GLY	337	1
ILE	338	1
VAL	62	2
TYR	2	1
SER	6	1
GLU	8	1
THR	11	1
ASN	15	1
PHE	26	1
LEU	31	1
LEU	37	1
VAL	47	1
VAL	49	1
SER	55	1
PHE	56	1
SER	67	1
PRO	71	1
ASP	72	1
LEU	74	1

LEU	339	1
LEU	342	1
TRP	345	1
ILE	352	1
ILE	354	1
VAL	355	1
VAL	358	1
ALA	359	1
VAL	360	1
CYS	362	1
THR	383	1
ARG	385	1
VAL	387	1

Note: Binding amino acids with the highest occurrence are highlighted in bold.

Table S19. Full Lists of Binding Amino Acids in the Human CD46 and SARS-CoV-2 Membrane Protein (MP) Protein-Protein Complex.

Human CD46			**MP SARS-CoV-2**		
Amino Acid	**Position**	**Occurrence**	**Amino Acid**	**Position**	**Occurrence**
PHE	**11**	**4**	**VAL**	**60**	**7**
PRO	**12**	**4**	**PRO**	**59**	**6**
TRP	**14**	**4**	**ALA**	**63**	**6**
PHE	**16**	**4**	**VAL**	**66**	**6**
PRO	**17**	**4**	**VAL**	**70**	**6**
LEU	**20**	**4**	**ASP**	**3**	**5**
MET	**24**	**4**	**LEU**	**56**	**5**
VAL	**25**	**4**	**LEU**	**67**	**5**
LEU	**26**	**4**	**PHE**	**96**	**5**
LEU	**27**	**4**	**MET**	**1**	**4**
TYR	**29**	**4**	**LEU**	**13**	**4**
PHE	**31**	**4**	**TRP**	**20**	**4**
GLU	**36**	**4**	**LEU**	**57**	**4**
ASN	**83**	**4**	**LEU**	**62**	**4**
THR	**85**	**4**	**TYR**	**71**	**4**
ILE	**239**	**4**	**ILE**	**82**	**4**
TYR	**247**	**4**	**LEU**	**90**	**4**
THR	**251**	**4**	**TRP**	**92**	**4**
VAL	**269**	**4**	LEU	17	3
SER	30	3	ILE	24	3
HIS	84	3	GLN	36	3
LYS	237	3	TYR	39	3
SER	240	3	PHE	45	3
GLY	241	3	ILE	49	3
PHE	242	3	TRP	55	3
LYS	249	3	CYS	64	3
MET	253	3	ALA	69	3
SER	265	3	ARG	72	3
ASP	266	3	MET	91	3

THR	267	3	SER	94	3
LEU	342	3	TYR	95	3
VAL	351	3	MET	109	3
VAL	355	3	PHE	112	3
PRO	3	2	LEU	134	3
SER	13	2	GLU	135	3
ARG	15	2	ALA	2	2
LEU	21	2	SER	4	2
LEU	28	2	THR	7	2
SER	32	2	ILE	8	2
ASP	33	2	VAL	10	2
ALA	34	2	LEU	16	2
LEU	184	2	TRP	31	2
ALA	186	2	ILE	32	2
THR	188	2	PHE	37	2
SER	190	2	ALA	40	2
LEU	202	2	ASN	43	2
GLU	205	2	ARG	44	2
SER	206	2	ILE	52	2
THR	207	2	PHE	53	2
GLU	255	2	TRP	58	2
ASP	257	2	PHE	65	2
LYS	258	2	TRP	75	2
TYR	261	2	CYS	86	2
GLY	264	2	LEU	93	2
ALA	314	2	ILE	97	2
PRO	323	2	PHE	100	2
LEU	339	2	PHE	103	2
ASP	340	2	ARG	107	2
SER	341	2	GLU	115	2
VAL	344	2	ASN	117	2
TRP	345	2	HIS	125	2
ILE	347	2	ASP	163	2
ALA	348	2	PRO	165	2
ALA	353	2	GLU	167	2
VAL	360	2	ARG	174	2
HIS	384	2	TYR	178	2
PRO	4	1	GLU	12	1
ARG	6	1	LEU	27	1
CYS	9	1	CYS	33	1
PRO	52	1	LEU	35	1
ASP	104	1	ILE	48	1
ASN	107	1	LYS	50	1
ASN	128	1	LEU	54	1
GLU	129	1	THR	61	1
TYR	132	1	ILE	73	1
THR	163	1	ASN	74	1
LYS	172	1	GLY	78	1
PHE	175	1	LEU	87	1
TYR	183	1	ARG	101	1

ASP	185	1	ARG	105	1
TYR	189	1	PRO	123	1
CYS	191	1	GLY	126	1
ASP	192	1	ILE	128	1
PRO	193	1	GLY	141	1
ALA	194	1	VAL	143	1
PRO	199	1	ARG	150	1
ILE	203	1	ILE	151	1
VAL	215	1	ALA	152	1
ALA	219	1	GLY	153	1
ALA	220	1	ARG	158	1
GLU	222	1	LYS	162	1
LYS	224	1	SER	173	1
GLY	243	1	LEU	176	1
LYS	244	1	GLN	185	1
TYR	248	1	PHE	193	1
ALA	250	1	ILE	201	1
LEU	262	1	GLY	202	1
ASP	263	1	ASN	203	1
SER	272	1	TYR	204	1
PRO	278	1	LYS	205	1
HIS	299	1	GLN	222	1
SER	315	1			
GLY	316	1			
PRO	317	1			
THR	320	1			
LYS	322	1			
SER	326	1			
ASP	343	1			
GLY	357	1			

Note: Binding amino acids with the highest occurrence are highlighted in bold.

Table S20. Full Lists of Binding Amino Acids in the Human CD46 and SARS-CoV-2 Nucleocapsid Protein (NP) Protein-Protein Complex.

Human CD46			NP SARS-CoV-2		
Amino Acid	**Position**	**Occurrence**	**Amino Acid**	**Position**	**Occurrence**
ASP	**343**	**5**	**PHE**	**17**	**4**
VAL	**344**	**5**	**SER**	**21**	**4**
TRP	**345**	**5**	**SER**	**79**	**4**
TYR	**247**	**4**	**HIS**	**145**	**4**
SER	**341**	**4**	**GLY**	**212**	**4**
LEU	**342**	**4**	**ASP**	**216**	**4**
VAL	**346**	**4**	**THR**	**334**	**4**
VAL	**351**	**4**	**GLY**	**335**	**4**
TYR	**132**	**3**	**ALA**	**336**	**4**
ALA	**194**	**3**	**ASP**	**81**	**3**
PRO	**199**	**3**	**ASP**	**82**	**3**
GLU	**205**	**3**	**ASN**	**140**	**3**

TRP	**216**	**3**	**THR**	**141**	**3**
ARG	**218**	**3**	**ALA**	**211**	**3**
PHE	**242**	**3**	**ASN**	**213**	**3**
LYS	**245**	**3**	**LEU**	**219**	**3**
ILE	**338**	**3**	**LEU**	**223**	**3**
LEU	**339**	**3**	**ARG**	**259**	**3**
ASP	**340**	**3**	**ARG**	**277**	**3**
ILE	**347**	**3**	**PRO**	**279**	**3**
ALA	**353**	**3**	**GLN**	**281**	**3**
ILE	**354**	**3**	**THR**	**282**	**3**
VAL	**355**	**3**	**GLN**	**283**	**3**
ALA	**359**	**3**	**GLY**	**284**	**3**
VAL	**360**	**3**	**ASN**	**285**	**3**
TYR	**366**	**3**	**PHE**	**286**	**3**
TYR	**368**	**3**	**ILE**	**304**	**3**
TYR	**378**	**3**	**PRO**	**309**	**3**
THR	**380**	**3**	**PHE**	**314**	**3**
THR	**383**	**3**	**TYR**	**333**	**3**
HIS	**384**	**3**	**ILE**	**337**	**3**
MET	1	2	GLN	7	2
GLU	2	2	GLN	9	2
PRO	3	2	ARG	14	2
GLY	5	2	ILE	15	2
ARG	6	2	THR	16	2
ARG	7	2	ASN	77	2
GLU	8	2	SER	78	2
CYS	9	2	ARG	92	2
PHE	11	2	ILE	94	2
TRP	14	2	ARG	95	2
ARG	15	2	LEU	104	2
PHE	16	2	ARG	107	2
PRO	17	2	LEU	139	2
LEU	19	2	VAL	158	2
LEU	20	2	ARG	177	2
LEU	21	2	GLN	181	2
ALA	22	2	ARG	195	2
ALA	23	2	THR	198	2
MET	24	2	SER	201	2
VAL	25	2	PRO	207	2
LEU	27	2	ALA	208	2
TYR	29	2	ARG	226	2
LEU	133	2	LEU	227	2
GLY	135	2	LEU	230	2
GLU	137	2	GLU	231	2
THR	163	2	GLN	239	2
SER	190	2	GLN	241	2
ASP	192	2	GLN	244	2
PRO	193	2	THR	245	2
GLY	196	2	VAL	246	2
PHE	200	2	GLN	260	2

ILE	203	2	ARG	262	2
TYR	209	2	PHE	274	2
ASN	213	2	GLU	280	2
VAL	215	2	THR	296	2
SER	217	2	TRP	301	2
ALA	219	2	ALA	305	2
GLY	243	2	PHE	307	2
TYR	248	2	ALA	308	2
LYS	249	2	MET	317	2
THR	251	2	SER	318	2
ALA	314	2	ARG	319	2
PRO	317	2	GLU	323	2
SER	326	2	SER	327	2
CYS	362	2	TRP	330	2
PRO	365	2	LEU	331	2
ARG	367	2	LEU	339	2
GLN	370	2	LEU	353	2
ARG	372	2	ILE	357	2
LYS	374	2	THR	393	2
LEU	379	2	LEU	394	2
ASP	381	2	LEU	395	2
GLU	382	2	LEU	400	2
ARG	385	2	PHE	403	2
GLU	386	2	SER	404	2
VAL	387	2	LEU	407	2
PRO	4	1	MET	411	2
PRO	10	1	ASN	11	1
PRO	12	1	SER	23	1
GLY	18	1	ASN	29	1
LEU	26	1	GLY	30	1
TYR	101	1	ARG	32	1
GLN	109	1	SER	33	1
ALA	110	1	GLY	34	1
VAL	111	1	ARG	36	1
PRO	112	1	SER	37	1
TYR	117	1	LYS	38	1
HIS	124	1	ARG	40	1
ILE	126	1	ARG	41	1
CYS	127	1	LYS	61	1
ILE	134	1	ASP	63	1
LEU	161	1	LYS	65	1
PRO	166	1	THR	76	1
ILE	168	1	PRO	80	1
THR	174	1	ILE	84	1
PHE	175	1	ARG	93	1
THR	188	1	LYS	100	1
CYS	191	1	GLY	114	1
PRO	197	1	ALA	119	1
SER	201	1	GLY	120	1
LEU	202	1	TYR	123	1

GLY	204	1
GLY	211	1
SER	214	1
ALA	220	1
GLU	222	1
GLN	238	1
SER	240	1
GLY	241	1
PHE	246	1
ALA	250	1
MET	253	1
GLU	255	1
TYR	261	1
ASP	266	1
THR	267	1
ASP	271	1
SER	272	1
ASN	273	1
THR	275	1
TRP	276	1
ASP	277	1
PRO	279	1
PRO	310	1
SER	313	1
SER	315	1
GLY	316	1
TYR	321	1
LYS	322	1
ASN	327	1
TYR	328	1
TYR	331	1
GLY	357	1
VAL	358	1

GLY	124	1
ALA	125	1
ASN	126	1
LYS	127	1
ASP	128	1
ILE	130	1
ILE	131	1
GLU	136	1
GLY	137	1
ALA	138	1
PRO	142	1
LYS	143	1
ASP	144	1
ALA	173	1
ARG	191	1
ASN	192	1
SER	193	1
SER	194	1
ASN	196	1
SER	197	1
SER	206	1
ARG	209	1
MET	210	1
ALA	217	1
ALA	220	1
PRO	258	1
LYS	261	1
THR	263	1
ALA	264	1
VAL	270	1
ALA	273	1
GLY	278	1
LEU	291	1
GLN	306	1
LYS	338	1
ASP	341	1
LYS	342	1
PRO	344	1
ASN	345	1
LYS	347	1
ASN	354	1
ASP	358	1
LYS	361	1
LYS	388	1
GLN	390	1
VAL	392	1
GLN	409	1
SER	410	1
ASP	415	1
SER	416	1

			GLN	418	1
			ALA	419	1

Note: Binding amino acids with the highest occurrence are highlighted in bold.

Table S21. Full Lists of Binding Amino Acids in the Human CD46 and SARS-CoV-2 Spike Protein (SP) Protein-Protein Complex.

Human CD46			SP SARS-CoV-2		
Amino Acid	**Position**	**Occurrence**	**Amino Acid**	**Position**	**Occurrence**
ARG	**218**	**5**	**VAL**	**3**	**5**
GLN	**122**	**4**	**LEU**	**5**	**5**
GLU	**177**	**4**	**MET**	**1**	**4**
ALA	**219**	**4**	**PHE**	**2**	**4**
LYS	**249**	**4**	**PHE**	**4**	**3**
TYR	**131**	**3**	**VAL**	**6**	**3**
VAL	**178**	**3**	**ASP**	**198**	**3**
PRO	**199**	**3**	**GLY**	**199**	**3**
GLU	**205**	**3**	**GLN**	**271**	**3**
VAL	**215**	**3**	**SER**	**375**	**3**
TRP	**216**	**3**	**ASP**	**405**	**3**
SER	**217**	**3**	**ARG**	**408**	**3**
SER	**240**	**3**	**GLY**	**502**	**3**
PHE	**242**	**3**	**VAL**	**503**	**3**
LYS	**244**	**3**	**LEU**	**1145**	**3**
TYR	**248**	**3**	**ASP**	**1146**	**3**
LYS	**293**	**3**	ASN	61	2
PRO	**295**	**3**	PRO	85	2
LEU	**342**	**3**	ASN	87	2
TRP	**345**	**3**	LYS	113	2
ILE	**347**	**3**	THR	114	2
VAL	**351**	**3**	GLN	115	2
ALA	**353**	**3**	GLU	132	2
VAL	**355**	**3**	ASN	165	2
GLY	**357**	**3**	THR	167	2
ALA	**359**	**3**	TYR	200	2
VAL	**360**	**3**	GLN	321	2
PHE	**389**	**3**	GLY	404	2
THR	40	2	THR	415	2
ILE	71	2	GLY	416	2
PRO	72	2	LYS	417	2
PRO	73	2	ASP	420	2
LEU	74	2	LEU	455	2
ALA	75	2	PHE	456	2
PRO	88	2	TYR	473	2
SER	90	2	GLN	474	2
ASP	92	2	ALA	475	2
TYR	95	2	GLY	485	2
LEU	106	2	PHE	486	2
TYR	117	2	ASN	487	2
HIS	124	2	TYR	489	2
ILE	126	2	GLN	493	2

CYS	127	2	THR	500	2
GLU	129	2	ASN	501	2
LEU	133	2	GLY	504	2
GLU	136	2	ARG	634	2
GLU	137	2	TYR	674	2
ILE	138	2	GLU	725	2
THR	163	2	GLN	762	2
PRO	166	2	ARG	765	2
ILE	168	2	PHE	970	2
LYS	169	2	GLY	971	2
THR	174	2	ILE	973	2
PHE	175	2	GLU	988	2
GLU	179	2	GLN	992	2
TYR	183	2	ARG	995	2
ASP	185	2	GLN	1002	2
THR	188	2	GLU	1017	2
TYR	189	2	ALA	1020	2
SER	190	2	LEU	1024	2
LEU	202	2	ASP	1041	2
GLY	204	2	LYS	1149	2
SER	206	2	GLU	1150	2
TYR	209	2	ASP	1153	2
ASP	212	2	PHE	1156	2
ASN	213	2	SER	1161	2
ALA	220	2	ASN	1178	2
GLU	222	2	ILE	1183	2
GLN	238	2	LEU	1186	2
ILE	239	2	TRP	1214	2
TYR	247	2	ILE	1216	2
MET	253	2	TRP	1217	2
ASP	266	2	LEU	1218	2
THR	267	2	PHE	1220	2
SER	290	2	ILE	1225	2
SER	291	2	MET	1233	2
THR	292	2	LEU	1234	2
PRO	294	2	CYS	1236	2
SER	305	2	CYS	1250	2
THR	306	2	VAL	1268	2
THR	307	2	LYS	1269	2
SER	309	2	HIS	1271	2
SER	313	2	LEU	7	1
SER	315	2	LEU	8	1
TYR	321	2	PRO	9	1
ASN	327	2	LEU	10	1
TYR	328	2	SER	12	1
PRO	329	2	GLN	14	1
TYR	331	2	ARG	21	1
LYS	333	2	GLN	23	1
VAL	344	2	LEU	24	1
VAL	358	2	PRO	26	1

CYS	362	2	TYR	28	1
ARG	367	2	ASN	30	1
LYS	375	2	PHE	59	1
THR	383	2	ASP	80	1
LYS	388	2	ASN	81	1
SER	391	2	PRO	82	1
LEU	392	2	VAL	83	1
ARG	6	1	LEU	84	1
ARG	7	1	PHE	86	1
GLU	8	1	ASP	88	1
CYS	9	1	THR	108	1
PHE	11	1	ASN	196	1
TRP	14	1	ILE	197	1
LEU	20	1	ASN	234	1
MET	24	1	VAL	267	1
VAL	25	1	GLY	268	1
LEU	28	1	TYR	269	1
TYR	29	1	PRO	272	1
SER	30	1	GLU	309	1
GLU	36	1	LYS	310	1
GLU	37	1	GLY	311	1
PRO	38	1	ILE	312	1
LYS	66	1	ASN	317	1
THR	85	1	ARG	319	1
TRP	86	1	PRO	322	1
LEU	87	1	THR	323	1
THR	98	1	GLU	324	1
ASN	107	1	LEU	335	1
VAL	111	1	CYS	336	1
ALA	113	1	PRO	337	1
MET	123	1	GLY	339	1
PHE	125	1	GLU	340	1
ASN	128	1	ASN	343	1
TYR	132	1	ASP	364	1
LEU	139	1	VAL	367	1
TYR	140	1	TYR	369	1
GLU	142	1	SER	373	1
SER	151	1	PHE	374	1
CYS	157	1	THR	376	1
GLU	158	1	PHE	377	1
LYS	159	1	GLY	381	1
LEU	161	1	VAL	382	1
LYS	167	1	SER	383	1
ASN	170	1	PRO	384	1
VAL	180	1	THR	385	1
GLU	182	1	VAL	407	1
LEU	184	1	ASN	437	1
ASP	192	1	GLN	506	1
ALA	194	1	PRO	527	1
ASP	198	1	LYS	529	1

PHE	200	1	ASN	556	1
ILE	203	1	LYS	557	1
SER	214	1	ILE	569	1
PRO	221	1	PHE	592	1
CYS	223	1	THR	604	1
VAL	225	1	SER	605	1
LYS	227	1	ASN	606	1
CYS	228	1	ASP	614	1
ARG	229	1	VAL	615	1
PHE	230	1	ASN	616	1
VAL	232	1	THR	618	1
LYS	237	1	HIS	625	1
GLY	243	1	ALA	626	1
LYS	245	1	ASP	627	1
THR	251	1	GLN	628	1
ASP	257	1	THR	632	1
LYS	258	1	VAL	635	1
LEU	262	1	SER	637	1
ASP	263	1	THR	638	1
SER	265	1	GLY	639	1
VAL	269	1	SER	640	1
ASP	271	1	PHE	643	1
SER	272	1	GLN	644	1
ASN	273	1	ARG	646	1
ASP	277	1	HIS	655	1
PRO	278	1	VAL	656	1
PRO	279	1	GLU	661	1
LYS	282	1	CYS	662	1
LEU	297	1	ASP	663	1
HIS	299	1	PRO	665	1
ARG	318	1	GLY	667	1
LEU	339	1	ALA	668	1
SER	341	1	GLY	669	1
ASP	343	1	SER	673	1
ALA	348	1	GLN	675	1
VAL	349	1	GLN	677	1
ILE	350	1	THR	678	1
ILE	352	1	ILE	693	1
ILE	354	1	MET	697	1
VAL	356	1	LEU	699	1
ILE	361	1	GLY	700	1
PRO	365	1	THR	724	1
THR	377	1	ILE	726	1
ARG	385	1	LEU	727	1
GLU	386	1	TYR	756	1
VAL	387	1	PHE	759	1
			LYS	776	1
			ALA	890	1
			GLY	891	1
			LEU	894	1

ASP	936	1
SER	937	1
SER	939	1
SER	940	1
THR	941	1
ALA	942	1
SER	943	1
GLY	946	1
LYS	947	1
ASP	950	1
ASN	969	1
ALA	972	1
VAL	991	1
ASP	994	1
THR	998	1
LEU	1001	1
GLN	1005	1
GLN	1010	1
LEU	1012	1
ILE	1013	1
ALA	1016	1
ARG	1019	1
SER	1021	1
ALA	1025	1
LYS	1028	1
ARG	1039	1
PHE	1042	1
LYS	1045	1
GLU	1144	1
LEU	1152	1
LYS	1157	1
THR	1160	1
VAL	1176	1
ILE	1179	1
GLN	1208	1
TYR	1215	1
GLY	1219	1
LEU	1224	1
ILE	1227	1
VAL	1228	1
MET	1237	1
CYS	1241	1
SER	1242	1
CYS	1243	1
LEU	1270	1

Note: Binding amino acids with the highest occurrence are highlighted in bold.

Table S22. Key Binding Amino Acids in the Human CD46 and SARS-CoV-2 Envelope Protein (EP), Membrane Protein (MP), Nucleocapsid Protein (NP), and Spike Protein (SP) Protein-Protein Complexes.

Amino Acid	Position	Occurrence	Amino Acid	Position	Occurrence
CD46↔EP Complex					
Human CD46 - 11 amino acids			**SARS-CoV-2 Envelope Protein (EP) - 15 amino acids**		
THR	188	3	PHE	20	6
TYR	189	3	ILE	13	5
SER	190	3	VAL	5	4
CYS	191	3	THR	9	4
PRO	193	3	LEU	12	4
PHE	200	3	SER	16	4
LEU	202	3	VAL	17	4
GLU	205	3	LEU	19	4
SER	206	3	PHE	23	4
THR	207	3	LEU	27	4
TYR	247	3	VAL	29	4
			LEU	34	4
			ARG	38	4
			ASN	45	4
			ASN	66	4
CD46↔MP Complex					
Human CD46 - 19 amino acids			**MP SARS-CoV-2 – 18 amino acids**		
PHE	11	4	VAL	60	7
PRO	12	4	PRO	59	6
TRP	14	4	ALA	63	6
PHE	16	4	VAL	66	6
PRO	17	4	VAL	70	6
LEU	20	4	ASP	3	5
MET	24	4	LEU	56	5
VAL	25	4	LEU	67	5
LEU	26	4	PHE	96	5
LEU	27	4	MET	1	4
TYR	29	4	LEU	13	4
PHE	31	4	TRP	20	4
GLU	36	4	LEU	57	4
ASN	83	4	LEU	62	4
THR	85	4	TYR	71	4
ILE	239	4	ILE	82	4
TYR	247	4	LEU	90	4
THR	251	4	TRP	92	4
VAL	269	4			
CD46↔NP Complex					
Human CD46 – 31 amino acids			**NP SARS-CoV-2 – 31 amino acids**		
ASP	343	5	PHE	17	4
VAL	344	5	SER	21	4
TRP	345	5	SER	79	4
TYR	247	4	HIS	145	4
SER	341	4	GLY	212	4
LEU	342	4	ASP	216	4

VAL	346	4	THR	334	4
VAL	351	4	GLY	335	4
TYR	132	3	ALA	336	4
ALA	194	3	ASP	81	3
PRO	199	3	ASP	82	3
GLU	205	3	ASN	140	3
TRP	216	3	THR	141	3
ARG	218	3	ALA	211	3
PHE	242	3	ASN	213	3
LYS	245	3	LEU	219	3
ILE	338	3	LEU	223	3
LEU	339	3	ARG	259	3
ASP	340	3	ARG	277	3
ILE	347	3	PRO	279	3
ALA	353	3	GLN	281	3
ILE	354	3	THR	282	3
VAL	355	3	GLN	283	3
ALA	359	3	GLY	284	3
VAL	360	3	ASN	285	3
TYR	366	3	PHE	286	3
TYR	368	3	ILE	304	3
TYR	378	3	PRO	309	3
THR	380	3	PHE	314	3
THR	383	3	TYR	333	3
HIS	384	3	ILE	337	3

CD46↔SP Complex

Human CD46 - 28 amino acids			**SP SARS-CoV-2 – 16 amino acids**		
ARG	218	5	VAL	3	5
GLN	122	4	LEU	5	5
GLU	177	4	MET	1	4
ALA	219	4	PHE	2	4
LYS	249	4	PHE	4	3
TYR	131	3	VAL	6	3
VAL	178	3	ASP	198	3
PRO	199	3	GLY	199	3
GLU	205	3	GLN	271	3
VAL	215	3	SER	375	3
TRP	216	3	ASP	405	3
SER	217	3	ARG	408	3
SER	240	3	GLY	502	3
PHE	242	3	VAL	503	3
LYS	244	3	LEU	1145	3
TYR	248	3	ASP	1146	3
LYS	293	3			
PRO	295	3			
LEU	342	3			
TRP	345	3			
ILE	347	3			
VAL	351	3			
ALA	353	3			

VAL	355	3
GLY	357	3
ALA	359	3
VAL	360	3
PHE	389	3

Table S23. Quality Assessment of 3D Models of Human CD46 and SARS-CoV-2 Envelope Protein (EP) Protein-Protein Complexes Obtained Using Different Software Tools.

Program	Number of Key Binding Amino Acids				Percentage of Key Binding Amino Acids[3]				
	CD46_EP[1]		EP_CD46[2]						
	CD46	EP	CD46	EP	CD46[4]	EP[5]	CD46_EP[6]	EP_CD46[7]	All[8]
ClusPro2	11	9	0	0	50.0	30.0	76.9	0.0	38.5
GRAMM1	**11**	**4**	**11**	**4**	**100.0**	**26.7**	**57.7**[9]	**57.7**	**57.7**
Hex8	0	1	0	2	0.0	10.0	3.8	7.7	5.8
SwarmDock	0	9	0	10	0.0	63.3	34.6	38.5	36.5
ZDock3	0	12	0	12	0.0	80.0	46.2	46.2	46.2

Note: 1. In separate subunits of the CD46(receptor)–EP(ligand) complex; 2. In separate subunits of the EP(receptor)–CD46(ligand) complex; 3. Out of the total number of key binding amino acids; 4. In the CD46 subunit of both models; 5. In the EP subunit of both models; 6. In the CD46 (receptor)–EP(ligand) complex; 7. In the EP(receptor)–CD46 (ligand) complex; 8. In both dimeric complexes; 9. Best 3D model.

Table S24. Quality Assessment of 3D Models of Human CD46 and SARS-CoV-2 Membrane Protein (MP) Protein-Protein Complexes Obtained Using Different Software Tools.

Program	Number of Key Binding Amino Acids				Percentage of Key Binding Amino Acids[3]				
	CD46_MP[1]		MP_CD46[2]						
	CD46	MP	CD46	MP	CD46[4]	MP[5]	CD46_MP[6]	MP_CD46[7]	All[8]
ClusPro2	15	7	15	8	78.9	41.7	59.5	62.2	60.8
GRAMM1	4	5	4	12	21.1	47.2	24.3	43.2	33.8
Hex8	0	0	0	0	0.0	0.0	0.0	0.0	0.0
SwarmDock	4	14	4	13	21.1	75.0	48.6	45.9	47.3
ZDock3	**15**	**14**	**15**	**14**	**78.9**	**77.8**	**78.4**[9]	**78.4**	**78.4**

Note: 1. In separate subunits of the CD46(receptor)–MP(ligand) complex; 2. In separate subunits of the MP(receptor)–CD46(ligand) complex; 3. Out of the total number of key binding amino acids; 4. In the CD46 subunit of both models; 5. In the MP subunit of both models; 6. In the CD46 (receptor)–MP(ligand) complex; 7. In the MP(receptor)–CD46 (ligand) complex; 8. In both dimeric complexes; 9. Best 3D model.

Table S25. Quality Assessment of 3D Models of Human CD46 and SARS-CoV-2 Nucleocapsid Protein (NP) Protein-Protein Complexes Obtained Using Different Software Tools.

Program	Number of Key Binding Amino Acids				Percentage of Key Binding Amino Acids[3]				
	CD46_NP[1]		NP_CD46[2]						
	CD46	NP	CD46	NP	CD46[4]	NP[5]	CD46_NP[6]	NP_CD46[7]	All[8]
ClusPro2	0	17	0	17	0.0	54.8	27.4	27.4	27.4
GRAMM1	12	6	18	12	48.4	29.0	29.0	48.4	38.7
Hex8	4	2	4	6	12.9	12.9	9.7	16.1	12.9
SwarmDock	21	22	5	4	41.9	41.9	69.4	14.5	41.9
ZDock3	**20**	**8**	**20**	**8**	**64.5**	**25.8**	**45.2**[9]	**45.2**	**45.2**

Note: 1. In separate subunits of the CD46(receptor)–NP(ligand) complex; 2. In separate subunits of the NP(receptor)–CD46(ligand) complex; 3. Out of the total number of key binding amino acids; 4. In the CD46 subunit of both models; 5. In the NP subunit of both models; 6. In the CD46 (receptor)–NP(ligand) complex; 7. In the NP(receptor)–CD46 (ligand) complex; 8. In both dimeric complexes; 9. Best 3D model.

Table S26. Quality Assessment of 3D Models of Human CD46 and SARS-CoV-2 Spike Protein (SP) Protein-Protein Complexes Obtained Using Different Software Tools.

Program	Number of Key Binding Amino Acids				Percentage of Key Binding Amino Acids3				
	CD46_SP[1]		SP_CD46[2]						
	CD46	SP	CD46	SP	CD46[4]	SP[5]	CD46_SP[6]	SP_CD46[7]	All[8]
ClusPro2	12	2	11	2	41.1	12.5	31.8	29.5	30.7
GRAMM1	8	7	2	3	17.9	31.3	34.1	11.4	22.7
Hex8	9	0	6	0	26.8	0.0	20.5	13.6	17.0
SwarmDock	14	9	8	5	39.3	43.8	52.3	29.5	40.9
ZDock3	**10**	**13**	**10**	**13**	**35.7**	**81.3**	**52.3**[9]	**52.3**	**52.3**

Note: 1. In separate subunits of the CD46(receptor)–SP(ligand) complex; 2. In separate subunits of the SP(receptor)–CD46(ligand) complex; 3. Out of the total number of key binding amino acids; 4. In the CD46 subunit of both models; 5. In the SP subunit of both models; 6. In the CD46 (receptor)–SP(ligand) complex; 7. In the SP(receptor)–CD46 (ligand) complex; 8. In both dimeric complexes; 9. Best 3D model.

Table S27. Key Binding Amino Acids in the Interaction Regions of Subunits in the Best Valid 3D Models of Human CD46 and SARS-CoV-2 Envelope Protein (EP), Membrane Protein (MP), Nucleocapsid Protein (NP), and Spike Protein (SP) Protein-Protein Complexes.

Model	Key Binding Amino Acids	
	CD	Second Subunit
CD46_EP_GRAMM1	THR188, TYR189, SER190, CYS191, PRO193, PHE200, LEU202, GLU205, SER206, THR207, TYR247	ILE13, VAL17, PHE20, VAL29
CD46_MP_ZDock3	PHE11, PRO12, TRP14, PHE16, PRO17, LEU20, MET24, VAL25, LEU26, LEU27, TYR29, PHE31, GLU36, ASN83, THR85	MET1, ASP3, LEU56, LEU57, PRO59, VAL60, LEU62, ALA63, VAL66, LEU67, VAL70, TYR71, TRP92, PHE96
CD46_NP_ZDock3	ILE338, SER341, LEU342, ASP343, VAL344, TRP345, VAL346, ILE347, VAL351, ALA353, ILE354, VAL355, ALA359, VAL360, TYR366, TYR368, TYR378, THR380, THR383, HIS384	PHE17, SER21, ALA211, GLY212, ASN213, ASP216, LEU219, LEU223

CD46_SP_ZDock3	GLU177, VAL178, PRO199, GLU205, ARG218, SER240, TYR248, LYS249, LYS293, PRO295	MET1, PHE2, VAL3, PHE4, LEU5, VAL6, ASP198, GLY199, SER375, ASP405, ARG408, GLY502, VAL503