

## Supporting Information

### Elucidation of Teicoplanin Interactions with Drug Targets Related to COVID-19

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**Table S1.** Intermolecular interactions observed in MM/GBSA optimized complexes of teicoplanin and 25 potential COVID-19 targets (AutoDock Vina 1.1.2 was used for molecular docking).

Targets	Hydrogen bonds			Hydrophobic/Electrostatic/Other		
	Compound	Amino acid	Distance (Å)	Type	Amino acid	Distance (Å)
Main protease	H	Pro168	2.05	Alkyl	Leu141	4.97
	H	Ser46	2.21	Alkyl	Pro168	4.85
	H	Gln189	2.67	Alkyl	Leu50	4.26
	O	Met165	2.63			
	O	Gly170	3.04			
	H	Glu166	2.92			
	H	Ser46	2.96			
	H	Glu166	2.37			
	O	Lys157	3.04	$\pi$ -Lone Pair	Tyr264	2.89
	O	Arg166	2.88	Alkyl	Pro247	4.52
	O	Gln269	2.56			
	O	Tyr273	2.17			
	H	Tyr268	2.84			
	H	Leu162	2.26			
	H	Thr301	1.78			
	H	Glu161	1.90			
	H	Thr301	2.56			
Papain-like protease	O	Gly163	2.60			
	O	Arg166	2.70			
	O	Tyr268	2.32			
	H	Tyr268	3.04			
	H	Gln269	2.45			
	H	Asp164	2.22			
	H	Asp164	2.46			
	H	Tyr268	2.79			
	H	Thr301	2.42			
	H	Ala246	2.78			
	H	Tyr264	2.91			
	H	Tyr268	2.69			

RdRp (RTP site)	O	Hie439	2.82	Alkyl	Ala547	4.18
	O	Ile548	2.47	Alkyl	Arg555	4.94
	O	Lys551	2.51	Alkyl	Val557	4.89
	O	Lys551	3.02	Alkyl	Lys551	3.92
	O	Lys551	2.07	Alkyl	Arg555	3.68
	O	Arg553	2.84	Alkyl	Val557	5.48
	O	Asn691	2.08			
	H	Glu811	2.71			
	H	U20	2.09			
	HO	Asp845	2.89			
	H	U20	1.78			
	H	Asp760	2.12			
	H	A19	2.12			
	H	His816	2.93			
	H	A19	2.57			
	H	Ser814	1.76			
	O	Hie439	2.21			
	O	Ala547	2.43			
	O	Lys551	2.58			
	O	Lys798	2.86			
	O	U20	2.53			
	O	A11	2.80			
	H	Asp760	2.91			
	H	A19	2.61			
	H	A19	2.86			
	H	Asp618	2.21			
	H	Asp833	2.30			
	H	U20	2.74			
	H	A19	2.76			
	H	U18	2.56			
	H	Tyr619	2.29			
	H	Ser814	2.36			
	H	Tyr619	2.37			
RdRp (RNA site)	O	Asn496	2.08	Alkyl	Lys500	4.09
	O	Lys500	2.90	Alkyl	Lys593	4.07
	O	Lys545	2.59	$\pi$ -Alkyl	Phe594	5.23
	O	Lys545	2.75			
	O	Thr565	2.65			
	O	Arg569	2.39			
	O	Ser592	2.10			
	H	Asp865	2.80			
	HO	Gly683	1.88			
	H	Asp684	1.89			
	H	Tyr546	1.70			
	H	Ser501	1.87			
	H	Tyr689	1.89			
	O	Lys545	3.05			
	O	Lys545	2.71			
	O	Ala547	2.90			
	O	Ser592	2.64			
	O	Gly683	2.96			

Spike protein (RBD)	H	Ala685	2.80			
	H	Tyr546	3.00			
	O	Tyr453	1.94	-	-	-
	O	Gln493	2.11			
	O	Gln493	2.37			
	HO	Glu484	2.10			
	H	Gly485	1.84			
	H	Gln493	2.23			
	H	Ser494	2.85			
	H	Gly496	1.81			
	O	Arg403	2.49			
	H	Gln493	2.85			
	O	Tyr453	1.72	$\pi$ -Alkyl	Tyr489	4.30
	O	Gly496	1.69	$\pi$ -Alkyl	Tyr505	4.70
Spike monomer	O	Gln498	2.07			
	O	Tyr505	2.14			
	H	Asn501	1.73			
	H	Thr500	1.85			
	O	Tyr495	2.66			
	H	Asp405	2.57			
	H	Tyr505	2.81			
	O	Tyr170	2.01	Alkyl	Pro330	5.26
	H	Arg357	1.93	Alkyl	Ile332	5.27
	H	Glu340	2.11	$\pi$ -Alkyl	Phe168	4.54
	H	Leu335	1.68			
	H	Glu169	2.68			
	H	Glu340	2.19			
	O	Pro337	3.01			
Spike trimer	H	Leu335	2.99			
	H	Asn360	2.95			
	H	Glu340	2.43			
	H	Leu335	2.72			
	H	Leu335	2.65			
	H	Asp979	2.56	Alkyl	Ala972	4.79
	H	Ser968	1.95			
	H	Asp1163	2.81			
	H	Asp1165	1.91			
	H	Asn978	2.22			
	H	Ser975	2.55			
	H	Ser968	2.72			
	O	Gln35	2.12	-	-	-
	O	Lys115	2.05			
S2 protein (post fusion state)	O	Gln35	2.16			
	O	Gln35	2.37			
	O	Arg73	2.16			
	O	Arg73	2.83			
	O	Val78	2.94			
	H	Glu77	1.71			
	H	Met76	1.83			
	O	Gly75	2.81			
	H	Pro33	3.00			
	O	Leu5	2.13	Alkyl	Met3	5.17
N-protein (C domain)						
N-protein (N domain)						

Nsp3 (AMP site)	O	Ser11	2.49	Alkyl	Pro111	5.22
	O	Arg48	2.89			
	O	Tyr69	2.39			
	O	Arg109	1.88			
	H	Asn8	1.66			
	H	Asn114	2.72			
	H	Pro111	2.76			
	H	Asn7	1.94			
	O	Ala10	3.08			
	H	Tyr71	2.38			
	H	Pro111	2.82			
	H	Leu5	2.64			
	H	Leu5	2.52			
	H	Asn7	2.56			
	O	Gly48	2.93	Alkyl	Ala38	3.76
	O	Lys163	2.73	Alkyl	Val49	4.21
	O	Lys163	2.76	Alkyl	Pro125	5.02
	H	Asp22	1.79			
	H	Asn101	1.77			
	H	Gly48	2.48			
	H	Asp22	2.10			
	H	Asp157	1.90			
	O	Gly47	2.45			
	O	Gly47	2.64			
	O	Gly48	2.63			
	O	Val49	2.27			
	O	Gly133	2.76			
	H	Gly130	2.73			
	H	Asp157	2.56			
	H	Gly46	2.52			
	H	Asp157	3.06			
	H	Asp22	2.68			
	H	Asp22	2.86			
Nsp3 (MES site)	O	Asn40	2.94	Alkyl	Val155	4.41
	O	Gly48	2.81	Alkyl	Ile131	4.05
	HO	Gly46	1.71			
	H	Ala129	1.86			
	H	Hie45	3.05			
	H	Gly51	1.90			
	O	Gly46	2.71			
	O	Gly47	2.56			
	O	Lys102	2.82			
	O	Pro136	2.79			
Nsp7	H	Ala129	2.63			
	H	Gly46	2.49			
	H	Gly46	2.60			
	O	Gln31	1.79	-	-	-
	O	Ser57	2.15			
	H	Glu50	2.97			
	H	Ser54	2.38			
	H	Gln31	2.01			

Nsp8	H	Val53	2.11			
	H	Glu50	1.74			
	H	Gln31	1.80			
	O	Lys51	2.55			
	O	Lys51	2.87			
	H	Ser54	3.00			
	H	Glu50	2.87			
	H	Ser54	3.07			
	HO	Met94	2.08	Alkyl	Pro121	3.99
	H	Met129	1.62	Alkyl	Leu117	4.31
	H	Met129	2.92	Alkyl	Pro121	4.12
	H	Thr124	1.96	Alkyl	Val131	5.02
	O	Met90	2.64	Alkyl	Pro121	4.73
	O	Lys97	2.57			
	H	Ser164	2.75			
	H	Met129	2.47			
Nsp9	O	Leu9	2.98	Alkyl	Val110	4.88
	O	Ser13	1.96			
	O	Arg39	1.92			
	HO	Thr109	2.75			
	H	Leu9	1.72			
	H	Asp78	1.84			
	H	Ser105	1.81			
	O	Met12	2.77			
	O	Asn27	2.74			
	H	Leu9	2.90			
	O	Lys4348	2.83	Alkyl	Val4369	4.61
	O	Lys4348	2.80	Alkyl	Val4369	4.75
	H	Asn4338	2.00	$\pi$ -Alkyl	Phe4342	5.46
	H	Pro4337	1.70			
	H	Ile4308	1.95			
Nsp10	O	Pro4339	2.39			
	O	Pro4339	2.57			
	O	Lys4348	2.57			
	H	Pro4337	2.87			
	H	Asn4338	2.59			
	H	Pro4339	2.57			
	H	Cyt4370	2.58			
	H	Phe4342	3.02			
	O	Hie439	1.96	Alkyl	Ala688	4.05
	O	Ala550	1.85	Alkyl	Cys813	5.42
	O	Lys551	2.29	Alkyl	Leu758	4.88
	O	Arg555	2.68	Alkyl	Cys813	3.93
	O	Lys593	2.86			
Nsp12	O	Lys621	2.14			
	O	Asp623	3.00			
	O	Ala688	2.37			
	O	Asn691	2.43			
	O	Gln815	2.52			
	HO	Asp684	2.33			
	H	Asp865	2.14			

Nsp13 (helicase ADP site)	H	Ser814	1.95			
	H	Asp760	1.92			
	O	Ser549	2.72			
	O	Lys551	2.79			
	H	Asp623	2.53			
	H	Tyr619	3.09			
	H	Tyr619	2.40			
	H	Cys813	2.71			
	H	Ser814	2.61			
	H	Asp760	2.54			
	H	Ser549	2.69			
	O	Ser289	2.79	Alkyl	Ala312	3.46
	O	Lys320	2.41	Alkyl	Ala316	3.60
	O	Lys320	2.80			
	O	Lys323	2.18			
	O	Arg442	1.96			
	H	Ser539	1.67			
	H	Ala316	1.82			
	H	Tyr324	1.89			
	H	Arg442	2.16			
	H	Glu319	2.29			
	O	Ser289	2.47			
	H	Arg442	2.91			
	H	Ser289	3.02			
	H	His290	2.93			
	O	Arg178	1.95	Alkyl	Ala312	4.47
	O	Gln531	3.04	Alkyl	Val340	4.04
	H	Asp534	2.53			
Nsp13 (helicase NCB site)	HO	Glu201	1.97			
	H	Asp534	1.95			
	H	Thr530	1.79			
	H	Gln537	2.51			
	H	Ser539	3.08			
	H	Glu375	2.89			
	O	Pro529	2.74			
	O	Ser535	2.53			
	O	Ser535	2.25			
	O	Gly538	2.51			
	H	Asp534	2.38			
	H	Glu201	2.45			
	H	Gln537	2.43			
	H	Thr530	2.46			
	H	Gln537	2.95			
	O	Lys9	2.19	Alkyl	Ala187	4.09
	O	Ser56	2.15	Alkyl	Ala187	5.03
	O	Gly59	2.64			
Nsp14 (ExoN)	O	Phe60	2.84			
	O	Lys61	2.51			
	O	Leu253	2.79			
	H	Gly6	1.88			
	H	Gln245	2.44			
	H	Thr250	3.07			

Nsp14 (N7mtase)	H	Gly251	1.90			
	O	Gly59	2.61			
	O	Gly59	2.69			
	O	Gly59	3.03			
	O	Gly102	2.85			
	O	Gly102	2.98			
	O	Asn252	2.36			
	H	Gly102	2.29			
	H	Gly251	2.82			
	H	Gln245	2.76			
	O	Arg310	2.15	-	-	-
	O	Gln354	2.44			
	O	Ser357	2.04			
	HO	Arg289	1.84			
	H	Asp291	2.75			
	H	Pro355	2.99			
	H	Hie424	2.35			
	O	Lys336	2.47			
	O	Hie235	2.24	Alkyl	Cys291	3.97
	O	Hie235	2.67	$\pi$ -Alkyl	Trp333	5.20
	O	His243	1.99	$\pi$ -Alkyl	Trp333	4.83
	O	Ser244	1.95	$\pi$ -Alkyl	Trp333	4.19
	O	Gln245	2.55	$\pi$ -Alkyl	Trp333	4.61
	O	Cys291	2.19	$\pi$ -Alkyl	Tyr343	3.81
Nsp15 (Exoribonuclease)	H	Gln245	1.78			
	H	His243	1.95			
	H	Ser244	1.74			
	H	Glu340	2.35			
	H	Tyr343	1.79			
	O	Hie235	2.98			
	O	Ser244	3.07			
	O	Gly247	2.96			
	H	Gln245	2.28			
	H	Glu340	2.48			
	O	Lys6935	2.29	Alkyl	Lys6935	4.79
	O	Ser6999	2.03	Alkyl	Lys6935	4.95
	H	Asp6873	2.59	$\pi$ -Alkyl	Tyr6930	5.39
	H	Tyr6930	1.77			
	H	Asn6899	2.66			
	H	Tyr6828	1.92			
	H	Asp6830	2.04			
Nsp16 (GTA site)	H	Asp6928	1.90			
	O	Ser6872	2.62			
	O	Met6929	2.85			
	O	Lys6935	2.61			
	H	Asn6996	2.68			
	H	Gly6869	2.90			
	H	Asp6928	2.62			
	H	Asn6996	2.55			
Nsp16 (MGP site)	O	Ala6808	2.77	$\pi$ -Alkyl	Trp6987	4.56
	H	Ser6800	1.93	$\pi$ -Alkyl	Trp6987	5.00

Nsp16 (SAM site)	H	Gln6804	1.70	$\pi$ -Alkyl	Trp6987	4.67
	H	Ser7074	2.29	$\pi$ -Alkyl	Trp6987	4.20
	H	Ala6808	1.77			
	H	Asn7008	2.83			
	H	Ser7074	2.87			
	O	Thr6854	2.78			
	O	Thr6854	2.74			
	H	Ala6808	2.74			
	H	Thr6856	2.82			
	H	Thr6856	3.00			
	O	Tyr6930	2.78	-	-	-
	O	Lys6935	2.32			
	O	Lys6935	2.97			
	O	Lys6935	2.63			
	O	Ser6999	2.40			
	H	Asp6928	1.82			
	H	Gly6871	1.98			
	H	Asp6897	2.58			
	H	Asp6928	1.92			
	H	Asn6996	1.84			
	O	Gly6829	2.86			
	O	Gly6829	2.50			
	H	Asp6897	2.86			
	H	Asn6996	2.50			

**Table S2.** Computation of MM/GBSA energies of top ten docked poses of teicoplanin in complex with 25 potential COVID-19 targets.

SN	Targets	Docking Models	AutoDock	MM/GBSA						
			Vina $\Delta G_{\text{Bind}}$	$\Delta G_{\text{Bind}}$	$\Delta G_{\text{Coul}}$	$\Delta G_{\text{HBond}}$	$\Delta G_{\text{Lipo}}$	SolvGB	$\Delta G_{\text{vdw}}$	Lig SE
1	Main protease	1M1	-5.7	-64.91	-25.07	-2.64	-49.96	41.57	-53.29	40.50
		1M2	-5.7	-46.33	-27.67	-0.73	-45.85	49.04	-51.94	44.16
		1M3	-5.4	-61.45	-10.99	-1.09	-48.02	44.53	-66.48	42.41
		1M4	-5.4	-97.55	-19.11	-0.68	-59.81	44.25	-68.46	3.87
		1M5	-5.3	-42.53	-5.12	-1.62	-29.12	34.28	-50.01	54.54
		1M6	-5.2	-32.51	-7.36	-3.87	-47.17	46.82	-52.82	71.58
		1M7	-5.2	-58.97	14.97	-1.49	-49.93	38.00	-65.00	36.50
		1M8	-5.2	-67.90	-18.75	-0.65	-53.78	47.89	-58.45	19.15
		1M9	-5.1	-46.37	-14.41	-3.08	-36.69	41.28	-48.26	53.40
		1M10	-5.1	-56.25	-30.91	-1.93	-59.75	54.17	-46.81	42.45
2	Papain-like protease	2M1	-5.4	-78.75	-39.06	-3.33	-58.73	54.34	-42.74	39.85
		2M2	-5.2	-74.17	-25.87	-2.61	-53.59	58.52	-52.61	18.25
		2M3	-5.1	-70.66	-53.54	-4.33	-43.54	56.28	-34.50	38.76
		2M4	-5.1	-47.95	-37.96	-1.05	-34.11	46.03	-41.05	40.92
		2M5	-5.1	-52.18	-10.37	-1.55	-47.00	48.32	-45.61	16.46
		2M6	-4.7	-46.55	-28.60	-0.87	-28.98	37.45	-41.19	21.59
		2M7	-4.7	-25.48	-16.71	-1.45	-35.50	45.65	-57.59	58.92
		2M8	-4.6	-59.04	-33.59	-1.33	-50.31	43.26	-59.09	62.35
		2M9	-4.6	-53.41	-31.57	-2.99	-22.03	48.41	-43.28	9.55
		2M10	-4.6	-51.19	-30.35	-2.22	-56.59	50.69	-43.79	63.80
3		3M1	-9.8	75.76	-124.58	-4.94	-91.90	209.45	-17.65	184.45



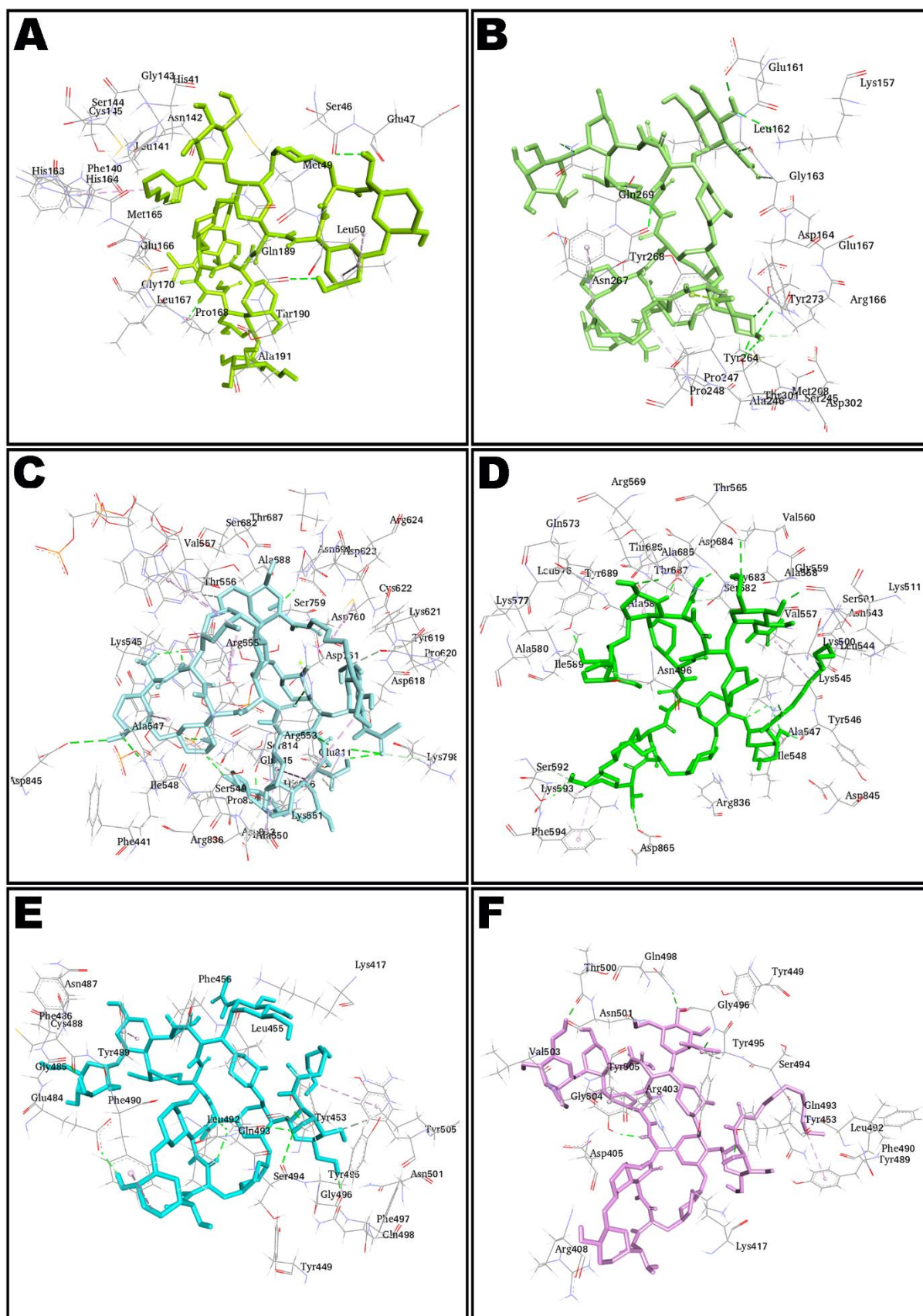
	RdRp (RTP site)	3M2	-9.5	213.43	-48.00	-6.35	-39.95	223.55	-29.34	184.68
		3M3	-9.5	253.29	-114.47	-7.47	-35.74	239.96	-15.42	272.34
		3M4	-9.4	117.68	-117.20	-6.77	-37.75	250.73	-64.96	133.94
		3M5	-9.3	203.79	-41.73	-7.24	-24.03	243.74	-62.70	164.86
		3M6	-9.2	237.92	-60.39	-6.64	-43.14	205.47	20.84	201.55
		3M7	-9.1	217.46	-63.92	-7.47	-37.20	198.79	-1.13	192.32
		3M8	-9.1	223.38	-92.89	-6.56	-39.18	208.35	-0.71	221.88
		3M9	-9	122.55	-133.38	-8.90	-42.75	293.51	-46.87	111.36
		3M10	-8.9	139.53	-135.56	-6.38	-40.16	262.03	-33.97	154.17
		4	RdRp (RNA site)	4M1	-8	-80.86	-31.92	-3.56	-49.26	76.38
4M2	-7.9			-67.31	-64.86	-7.71	-11.69	81.61	-70.62	48.70
4M3	-7.8			-54.12	-40.83	-4.58	-17.85	71.17	-76.88	28.45
4M4	-7.7			-31.16	-27.12	-6.97	-18.03	68.16	-84.02	44.52
4M5	-7.7			-65.71	-42.03	-3.42	-21.59	90.58	-103.70	16.33
4M6	-7.7			-38.91	-32.71	-5.02	-21.65	71.14	-78.36	40.00
4M7	-7.7			-86.33	-68.97	-6.24	-13.97	78.93	-83.45	10.54
4M8	-7.6			-71.88	-35.76	-4.90	-25.19	57.49	-74.53	30.50
4M9	-7.6			-63.35	-3.24	-4.95	-22.01	53.50	-88.85	7.60
4M10	-7.5			-46.32	-29.49	-5.00	-15.19	75.62	-86.77	17.43
5	Spike protein (RBD)	5M1	-6.5	-74.61	-31.09	-4.78	-46.45	32.98	-53.94	30.35
		5M2	-6.3	-91.99	-40.79	-1.98	-46.65	45.40	-51.99	21.37
		5M3	-6.3	-42.47	-32.73	-1.28	-26.75	43.82	-56.38	47.64
		5M4	-6.3	-59.41	-35.06	-2.61	-26.04	50.50	-54.06	31.24
		5M5	-6.2	-61.83	-31.56	-2.27	-44.14	49.98	-54.09	58.67
		5M6	-6.2	-82.43	-40.93	-2.43	-46.19	48.65	-52.83	33.67
		5M7	-6.2	-73.19	-62.56	-4.00	-38.54	52.55	-45.98	21.05
		5M8	-6.1	-95.76	-32.67	-2.13	-54.25	48.60	-66.71	18.19
		5M9	-6	-48.85	-28.39	-1.24	-17.57	43.40	-58.68	38.99
		5M10	-5.9	-37.69	-21.65	-4.11	-29.59	36.16	-51.90	68.18
6	Spike monomer	6M1	-5.9	-66.37	-28.83	-2.87	-33.02	41.91	-53.45	23.41
		6M2	-5.7	-60.41	-20.71	-3.46	-21.67	49.85	-72.35	10.47
		6M3	-5.5	-42.80	-28.25	-4.88	-15.01	46.75	-53.37	29.61
		6M4	-5.4	-68.38	-61.51	-4.39	-13.35	55.98	-50.51	12.74
		6M5	-5.3	-60.45	-35.63	-4.99	-16.62	52.30	-61.41	32.42
		6M6	-5.1	-39.04	-37.69	-5.51	-14.41	43.93	-41.89	40.92
		6M7	-5.1	-32.77	-6.19	-5.53	-15.28	40.33	-61.59	37.39
		6M8	-4.9	-33.54	-33.91	-4.65	-14.65	49.13	-57.05	35.52
		6M9	-4.9	-52.97	-39.13	-5.16	-14.41	30.19	-35.12	18.00
		6M10	-4.9	-21.68	-26.69	-2.91	-12.79	44.51	-39.90	19.71
7	Spike trimer	7M1	-7	-45.17	-31.10	-3.69	-26.16	52.35	-51.26	50.09
		7M2	-7	-40.62	-24.38	-2.45	-27.74	52.50	-64.60	30.83
		7M3	-6.9	-66.87	-27.37	-4.11	-21.53	53.95	-65.20	11.90
		7M4	-6.8	-58.88	-25.84	-4.74	-23.74	43.18	-60.36	36.34
		7M5	-6.8	-30.88	-7.72	-3.99	-22.06	45.59	-65.77	51.27
		7M6	-6.7	-36.28	-20.40	-3.06	-19.38	44.04	-70.13	38.92
		7M7	-6.7	-39.74	-30.06	-2.55	-15.91	55.91	-58.96	19.47
		7M8	-6.7	-14.41	-16.83	-4.29	-23.21	64.93	-70.51	61.70
		7M9	-6.6	-46.41	-1.90	-2.85	-27.63	57.14	-81.01	23.31
		7M10	-6.6	-43.74	-28.36	-2.84	-17.77	48.76	-58.50	20.65
8	S2 protein (post fusion state)	8M1	-5.7	-25.01	-22.12	-3.50	-11.40	61.44	-70.72	30.74
		8M2	-5.6	-16.94	-19.57	-3.37	-10.79	49.75	-59.71	29.01
		8M3	-5.5	-34.28	-20.12	-3.33	-14.41	56.83	-63.82	16.74

9	N-protein (C domain)	8M4	-5.3	-36.93	-23.22	-2.74	-14.11	55.19	-61.27	24.45
		8M5	-5.2	-13.34	-2.29	-0.45	-12.66	44.62	-57.77	31.85
		8M6	-5.2	-8.02	-45.43	-2.78	-13.00	96.04	-60.31	27.81
		8M7	-5.1	-21.95	-21.01	-2.64	-14.25	57.36	-66.30	41.41
		8M8	-5	-8.93	-43.83	-3.07	-12.01	99.61	-56.45	27.36
		8M9	-4.9	-29.72	-45.05	-3.26	-14.98	83.85	-61.54	12.77
		8M10	-4.9	-14.18	-20.44	-2.53	-15.49	79.39	-70.49	29.54
		9M1	-6.1	-34.14	-17.41	-3.14	-18.18	62.01	-63.42	17.77
		9M2	-6.1	-22.10	-38.33	-3.49	-9.96	64.64	-50.20	36.01
		9M3	-5.7	-35.76	-33.37	-4.27	-18.96	69.74	-68.03	29.21
10	N-protein (N domain)	9M4	-5.7	-30.45	-9.78	-4.67	-19.99	48.32	-67.16	38.30
		9M5	-5.6	-42.31	-30.82	-5.06	-16.05	64.88	-62.43	26.93
		9M6	-5.6	-28.79	1.21	-2.26	-18.55	38.59	-55.07	19.45
		9M7	-5.5	-13.17	-4.55	-2.66	-25.30	66.29	-69.88	37.08
		9M8	-5.5	-20.37	-9.70	-1.67	-21.23	41.66	-51.36	34.39
		9M9	-5.4	-40.57	-33.98	-3.22	-17.73	62.10	-58.74	26.57
		9M10	-5.3	-20.59	-13.97	-2.84	-16.50	37.59	-50.91	46.02
		10M1	-8.8	-88.69	-38.01	-5.70	-19.15	47.39	-74.01	14.84
		10M2	-8.7	-64.99	-14.73	-4.54	-19.23	44.95	-73.27	29.76
		10M3	-8.5	-51.02	-20.97	-4.87	-24.51	48.77	-73.49	50.30
11	Nsp3 (AMP site)	10M4	-8.4	-43.37	-31.79	-4.45	-23.05	53.94	-67.14	39.75
		10M5	-8.2	-39.70	-25.53	-4.80	-30.34	58.62	-78.82	59.51
		10M6	-7.9	-45.23	-26.57	-5.48	-25.33	52.24	-66.46	43.61
		10M7	-7.9	-43.37	-39.45	-5.68	-9.95	61.56	-61.00	52.34
		10M8	-7.8	-53.25	-23.28	-4.22	-16.99	44.70	-70.46	47.13
		10M9	-7.7	-13.19	-20.61	-5.13	-10.61	61.16	-68.57	80.32
		10M10	-7.4	-102.13	-40.95	-6.98	-24.95	61.07	-78.69	-0.90
		11M1	-7.3	-37.74	1.62	-2.22	-28.83	39.04	-67.60	36.07
		11M2	-7.3	-58.33	-42.82	-4.38	-25.86	64.42	-71.09	32.93
		11M3	-7.3	-34.25	-2.31	-2.27	-25.57	31.96	-65.18	30.90
12	Nsp3 (MES site)	11M4	-7.1	-44.98	-17.89	-2.56	-25.49	52.30	-70.59	35.64
		11M5	-6.6	-26.80	9.51	-0.47	-21.45	25.16	-60.25	28.75
		11M6	-6.6	-27.10	-2.74	-1.44	-17.34	45.46	-67.53	44.71
		11M7	-6.6	-49.22	-31.83	-3.35	-16.14	51.02	-70.27	25.62
		11M8	-6.4	-23.60	-18.81	-2.37	-15.06	47.09	-53.49	43.34
		11M9	-6.4	-54.41	-11.12	-2.79	-17.08	33.56	-65.77	32.16
		11M10	-6.3	-54.16	-17.77	-2.30	-12.49	39.34	-65.03	3.82
		12M1	-6.1	-43.26	-10.27	-3.06	-24.41	49.16	-67.74	36.28
		12M2	-6.1	-33.82	-14.29	-4.56	-28.21	46.29	-56.82	61.07
		12M3	-5.9	-57.60	-12.61	-2.42	-30.13	34.62	-75.40	37.34
13	Nsp7	12M4	-5.6	-47.68	-32.35	-3.44	-18.10	49.46	-61.22	33.35
		12M5	-5.5	-51.61	-17.26	-3.03	-21.12	43.16	-61.40	26.87
		12M6	-5.4	-42.97	-11.89	-1.94	-26.85	34.94	-62.88	38.08
		12M7	-5.3	-43.63	-27.19	-2.99	-22.22	40.83	-50.56	28.24
		12M8	-5.2	-48.37	-29.98	-4.36	-25.62	42.04	-52.37	39.95
		12M9	-5.2	-36.15	-25.57	-4.74	-15.39	35.39	-47.63	38.73
		12M10	-5.1	-43.33	-3.25	-1.54	-20.34	30.26	-65.38	25.17
		13M1	-5.2	-26.63	-25.65	-1.50	-13.13	50.89	-50.83	18.66
		13M2	-4.9	-42.29	-34.84	-2.81	-19.73	56.40	-58.37	18.41
		13M3	-4.7	-7.18	-5.28	-3.28	-13.07	46.38	-51.46	52.87
		13M4	-4.4	-66.61	-54.39	-4.15	-19.17	55.49	-60.78	8.43
		13M5	-4.1	-19.64	-29.42	-3.42	-12.66	47.18	-45.67	40.05

14	Nsp8	13M6	-3.9	-4.02	2.55	-1.97	-11.15	37.51	-58.47	46.14
		13M7	-3.9	-32.59	-16.95	-2.77	-14.77	45.27	-47.03	13.64
		13M8	-3.9	-44.20	-35.42	-3.37	-21.33	66.94	-65.69	22.09
		13M9	-3.8	-22.57	-15.52	-3.78	-14.77	46.48	-57.15	34.62
		13M10	-3.7	-21.10	-31.49	-3.31	-17.03	54.38	-60.19	49.76
		14M1	-7	-40.86	8.45	-1.97	-27.19	24.42	-68.20	44.83
		14M2	-6.7	-10.97	21.42	-1.77	-14.58	28.08	-62.69	58.04
		14M3	-6.2	-64.46	-19.68	-3.01	-27.43	34.13	-54.25	31.30
		14M4	-6.2	-32.48	9.13	-1.54	-20.01	30.57	-57.92	38.90
		14M5	-6.1	-43.84	3.97	-0.85	-21.39	31.97	-63.54	29.91
15	Nsp9	14M6	-6.1	-58.54	-1.60	-3.21	-23.07	23.68	-68.72	35.54
		14M7	-6	-56.07	-3.84	-1.92	-30.28	21.53	-59.84	29.46
		14M8	-5.9	-67.93	-10.55	-2.28	-25.51	28.75	-68.85	16.42
		14M9	-5.9	-9.80	-0.87	-1.50	-21.33	34.71	-46.76	48.31
		14M10	-5.9	-57.18	-23.05	-2.39	-22.58	42.24	-67.22	29.99
		15M1	-5	-65.41	-44.21	-5.05	-20.94	61.63	-68.43	26.18
		15M2	-4.6	-29.70	-12.43	-3.27	-15.18	52.94	-66.93	26.23
		15M3	-4.5	-66.83	-43.87	-3.59	-19.55	46.75	-57.02	10.15
		15M4	-4.3	0.66	5.02	-1.54	-7.59	29.09	-46.72	41.15
		15M5	-4	-58.92	-33.40	-3.73	-17.80	55.27	-67.12	10.53
16	Nsp10	15M6	-3.8	-22.74	-31.88	-2.38	-12.94	54.98	-45.30	29.37
		15M7	-3.4	-32.33	-34.35	-3.32	-13.73	46.62	-48.05	40.14
		15M8	-3.4	-24.26	-19.53	-2.80	-11.71	49.97	-59.36	39.80
		15M9	-3.3	-35.83	-8.80	-2.65	-17.22	49.54	-63.28	25.47
		15M10	-3.1	-25.58	-13.79	-3.74	-9.18	42.58	-51.15	32.35
		16M1	-4.4	-11.29	-5.33	-4.47	-16.23	61.45	-60.16	56.98
		16M2	-2.8	-16.01	-15.59	-3.35	-9.32	54.52	-52.29	13.19
		16M3	-2.6	-25.83	-30.15	-4.77	-11.85	54.10	-53.85	40.00
		16M4	-2.3	-35.50	-21.16	-3.83	-11.13	44.07	-52.46	18.57
		16M5	-2.2	-47.56	-29.62	-2.47	-23.97	57.87	-62.53	40.47
17	Nsp12	16M6	-1.7	-34.50	-42.90	-2.76	-12.47	54.17	-43.17	9.41
		16M7	-1.6	-22.69	-19.80	-3.29	-20.89	56.23	-53.17	40.06
		16M8	-1.6	-31.33	-7.44	-0.60	-13.64	35.27	-54.00	0.49
		16M9	-1.4	-13.16	-24.80	-4.55	-0.46	56.80	-39.61	32.66
		16M10	-1.1	-44.10	-27.82	-2.80	-11.34	45.56	-52.31	9.99
		17M1	-8	-69.05	-39.13	-6.34	-18.19	79.99	-102.58	36.33
		17M2	-8	-68.41	-46.76	-5.99	-23.37	89.68	-106.35	35.49
		17M3	-7.8	-87.84	-96.33	-8.48	-19.26	135.75	-108.20	8.52
		17M4	-7.4	-11.32	-40.30	-4.84	-19.48	109.74	-94.39	50.76
		17M5	-7.2	-24.57	-49.55	-7.52	-23.55	126.72	-90.20	52.20
18	Nsp13 (hel- icase ADP site)	17M6	-7.1	-8.66	-45.04	-6.20	-22.82	96.19	-69.71	49.76
		17M7	-7.1	23.00	-15.87	-5.08	-9.41	74.06	-52.53	62.29
		17M8	-7.1	8.76	-25.15	-6.14	-19.96	91.35	-63.61	54.27
		17M9	-7	-34.11	-29.02	-8.72	-12.57	67.09	-76.06	47.50
		17M10	-7	67.78	-21.66	-5.26	-17.41	102.26	-45.75	83.32
		18M1	-6.6	10.59	-48.06	-6.21	-14.26	89.32	-41.34	54.40
		18M2	-6.6	2.60	-30.10	-5.03	-14.48	68.84	-51.54	42.07
		18M3	-6.5	-41.57	-63.94	-7.00	-19.36	88.70	-53.79	16.23
		18M4	-6.4	-0.80	-10.63	-3.93	-12.45	54.81	-46.29	41.87
		18M5	-6.2	-29.82	-2.92	-3.60	-8.18	44.81	-62.99	13.90
		18M6	-6.2	-20.65	-38.92	-4.12	-12.96	69.06	-58.74	26.05
		18M7	-6.2	-22.47	-54.76	-6.55	-5.06	78.91	-43.44	39.00

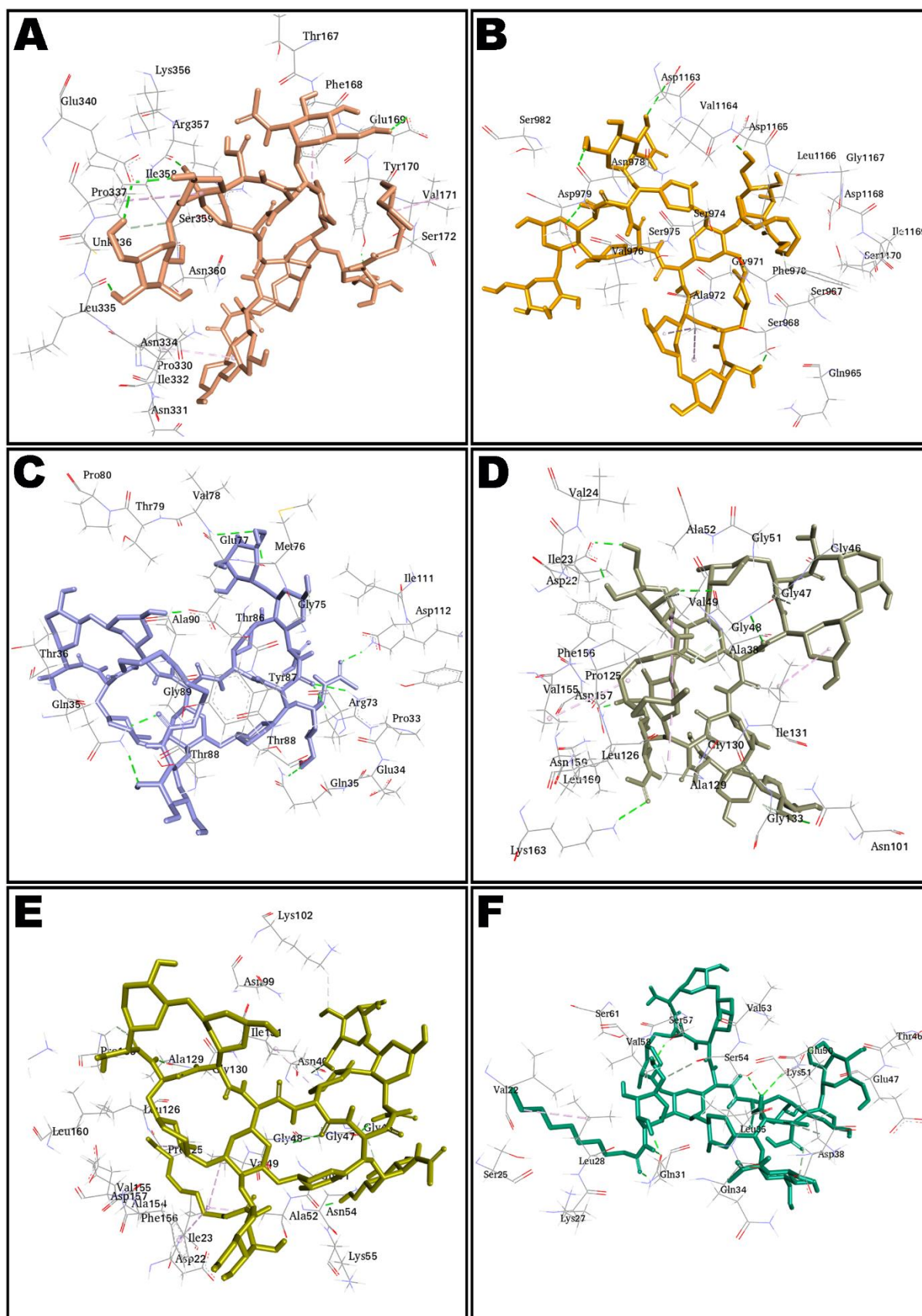
19	Nsp13 (hel- icase NCB site)	18M8	-6.1	1.47	-15.95	-6.03	-13.33	69.21	-51.47	27.64
		18M9	-6	-35.99	-36.54	-2.79	-12.01	65.42	-57.06	12.82
		18M10	-5.9	-16.45	-15.80	-1.71	-8.68	54.10	-48.38	15.65
		19M1	-6.4	-20.11	-50.92	-4.46	-23.73	92.54	-62.00	40.26
		19M2	-6.4	0.74	-37.44	-4.95	-26.35	95.39	-75.95	67.99
		19M3	-6.4	-13.41	-45.41	-6.32	-20.53	75.40	-46.06	52.14
		19M4	-6.2	68.15	-46.42	-5.18	-28.20	109.29	-39.46	96.50
		19M5	-6.2	-47.55	-66.12	-6.54	-23.12	118.38	-88.16	39.58
		19M6	-6.2	5.63	-53.23	-5.76	-29.98	108.00	-58.60	60.71
		19M7	-5.8	-7.70	-34.37	-5.17	-31.20	97.76	-80.37	59.34
20	Nsp14 (ExoN)	19M8	-5.8	38.83	-20.52	-5.42	-10.76	81.06	-37.82	86.41
		19M9	-5.4	1.18	-28.99	-6.39	-22.58	107.15	-89.89	72.11
		19M10	-5.4	-53.99	-42.21	-4.05	-26.40	87.73	-78.57	7.39
		20M1	-7.7	-42.32	-30.48	-5.45	-21.60	75.61	-69.32	35.82
		20M2	-7.5	-34.92	-13.94	-3.89	-21.66	65.02	-72.26	26.70
		20M3	-7.2	-21.01	-45.14	-4.11	-20.07	96.24	-74.89	46.00
		20M4	-7.1	-49.41	-32.04	-4.56	-20.91	64.52	-80.34	28.66
		20M5	-7.1	-36.77	-17.60	-3.11	-19.90	48.46	-66.01	28.16
		20M6	-7.1	-22.00	-23.15	-4.84	-14.02	59.35	-57.56	43.03
		20M7	-7	-31.05	-1.35	-3.48	-23.24	59.98	-83.91	30.18
21	Nsp14 (N7mtase)	20M8	-7	-20.73	-29.69	-5.58	-12.41	72.45	-70.50	49.47
		20M9	-7	-32.55	-29.75	-3.85	-15.35	61.67	-57.88	25.24
		20M10	-6.8	-46.01	-45.55	-5.37	-16.52	85.23	-74.48	25.38
		21M1	-3.5	5.75	-30.70	-5.41	-9.54	69.16	-43.23	58.57
		21M2	-3.1	-38.04	-33.66	-5.47	-18.33	58.77	-48.87	11.98
		21M3	-3	-38.83	-21.49	-4.69	-15.49	47.57	-44.45	1.51
		21M4	-3	47.17	-4.40	-3.33	-31.26	83.37	-33.08	65.62
		21M5	-2.9	5.80	-25.73	-4.61	-15.36	84.18	-61.67	51.06
		21M6	-2.8	41.53	-27.06	-3.52	-31.61	82.10	-32.35	74.56
		21M7	-2.7	50.56	-19.24	-4.96	-10.93	55.34	-11.77	84.78
22	Nsp15 (Exori- bonuclease)	21M8	-2.7	35.99	-9.50	-3.58	-14.53	66.28	-56.46	94.42
		21M9	-2.5	-29.13	-40.06	-3.58	-19.41	64.24	-46.76	27.06
		21M10	-2.3	37.93	-29.19	-3.74	-30.66	86.65	-30.51	70.73
		22M1	-6.9	-1.36	-20.15	-3.34	-24.02	55.24	-56.15	68.84
		22M2	-6.5	-64.40	-48.67	-6.39	-23.20	47.29	-55.77	43.43
		22M3	-6.5	-30.47	-27.83	-4.04	-16.11	53.97	-63.06	55.29
		22M4	-6.2	-50.93	-31.21	-4.28	-24.49	53.94	-61.55	34.98
		22M5	-6.2	-36.69	-17.40	-2.31	-20.42	47.15	-57.56	15.21
		22M6	-6.2	-51.59	-17.90	-4.66	-16.32	38.59	-51.78	33.42
		22M7	-6.2	-24.27	-9.37	-3.55	-16.98	41.12	-49.74	36.83
23	Nsp16 (GTA site)	22M8	-6.1	-42.00	-17.19	-2.07	-24.85	54.74	-68.53	24.68
		22M9	-6.1	-32.71	-20.04	-2.52	-18.38	53.65	-60.22	24.93
		22M10	-6.1	-28.17	-13.10	-2.82	-20.57	50.66	-67.83	37.73
		23M1	-6.8	-29.16	-33.10	-6.55	-14.60	66.25	-59.58	37.56
		23M2	-6.8	-38.00	-39.20	-6.48	-15.13	71.97	-66.32	32.38
		23M3	-6.7	-61.01	-49.28	-5.73	-17.72	70.05	-72.02	11.41
		23M4	-6.6	-42.54	-34.27	-6.25	-16.08	59.88	-65.91	19.52
		23M5	-6.4	-39.88	-33.92	-4.20	-12.48	62.05	-69.89	24.58
		23M6	-6.4	-39.16	-38.61	-4.72	-13.99	68.11	-68.73	30.44
		23M7	-6.3	-23.60	-11.17	-4.25	-12.17	49.51	-59.45	41.12
		23M8	-6.2	-63.57	-55.69	-5.17	-12.18	65.46	-62.63	8.44
		23M9	-6.1	6.44	-11.41	-2.63	-14.96	36.65	-50.62	61.06

24	Nsp16 (MGP site)	23M10	-6.1	-2.47	-5.32	-3.15	-10.65	49.08	-61.57	54.52
		24M1	-7.8	-29.24	-23.42	-3.94	-29.01	76.00	-72.54	39.15
		24M2	-7.6	-50.73	-16.98	-2.81	-31.66	58.93	-79.64	34.11
		24M3	-7.6	-33.03	-19.24	-1.91	-23.32	64.57	-74.99	27.54
		24M4	-7.5	-56.44	-45.38	-2.03	-22.08	64.42	-70.91	15.40
		24M5	-7.4	-51.13	-41.60	-1.88	-23.11	70.23	-65.10	17.51
		24M6	-7.4	-58.04	-31.42	-3.89	-22.67	59.61	-79.15	30.67
		24M7	-7.4	-49.36	-35.59	-3.11	-17.92	59.18	-63.75	22.72
		24M8	-7.3	-21.15	-19.03	-3.79	-22.04	50.95	-52.36	29.91
		24M9	-7.3	-50.94	-31.21	-1.90	-24.62	72.08	-77.65	14.32
25	Nsp16 (SAM site)	24M10	-7.3	-52.64	-42.04	-3.38	-22.67	61.26	-72.16	28.20
		25M1	-6.5	-54.88	-34.65	-4.69	-21.69	74.67	-74.43	15.52
		25M2	-6.3	-18.25	-32.58	-4.97	-22.72	73.90	-62.01	41.63
		25M3	-6	-38.31	-39.18	-5.27	-21.22	84.23	-72.94	36.95
		25M4	-5.8	-33.63	-38.97	-3.81	-10.99	59.25	-57.26	27.18
		25M5	-5.7	-41.14	-54.00	-4.02	-12.58	71.47	-57.64	21.71
		25M6	-5.7	-3.99	8.06	-2.61	-8.92	43.72	-64.09	52.14
		25M7	-5.7	-36.30	-20.54	-3.35	-13.22	46.06	-59.81	16.72
		25M8	-5.6	-10.92	-27.47	-2.55	-18.62	52.91	-33.00	25.68
		25M9	-5.6	-10.55	-21.28	-3.22	-20.16	56.94	-43.15	27.36
		25M10	-5.6	11.03	-9.91	-3.45	-18.12	63.59	-42.51	58.90

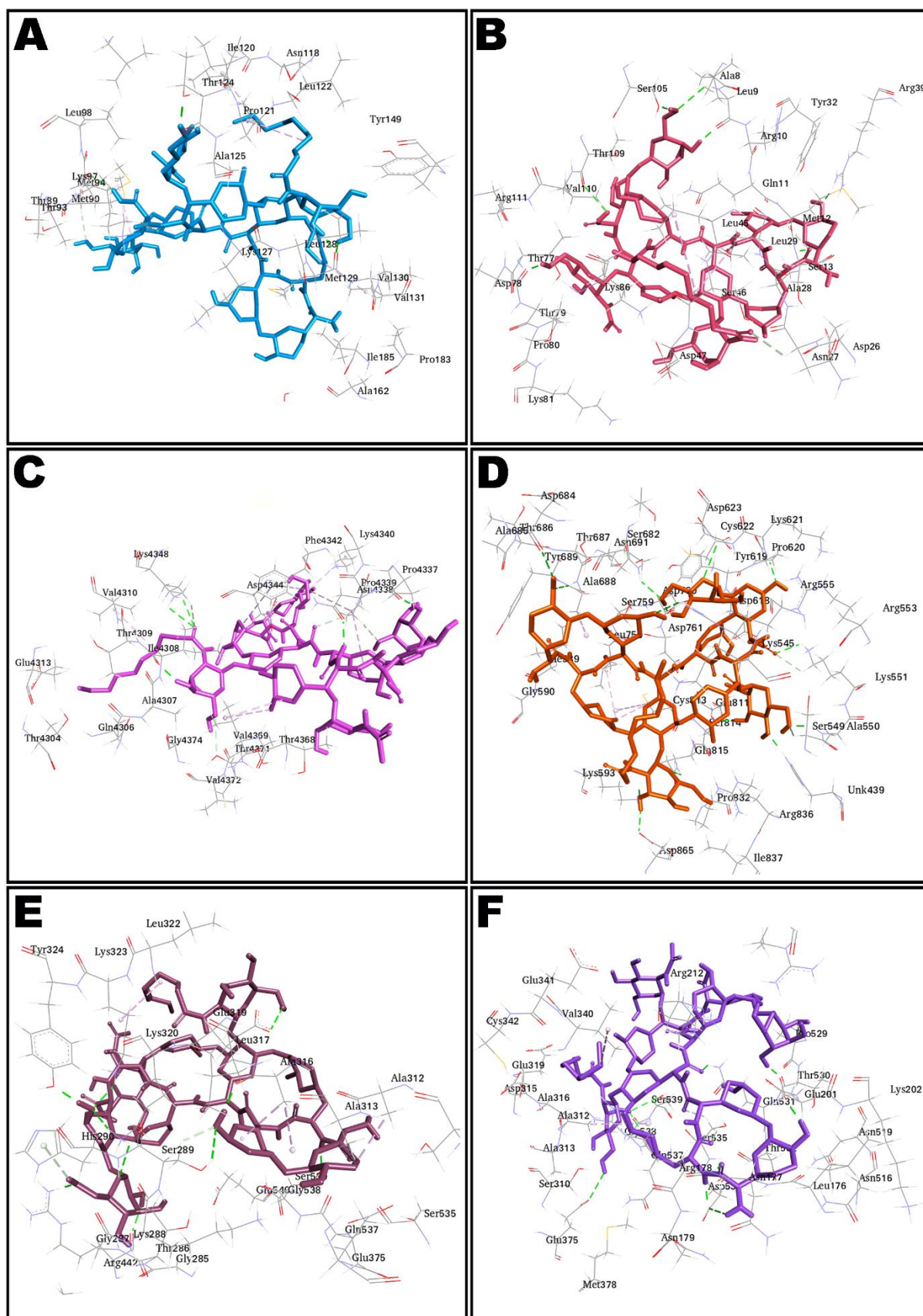


**Figure S1.** MM/GBSA optimized complexes of teicoplanin (displayed as stick) showing non-bond interactions with main protease (A), papain-like protease (B), RdRp-RTP site (C), RdRp-RNA site (D), spike protein-RBD (E), and spike monomer (F). Broken green lines enumerate hydrogen bonds whereas purple lines justify hydrophobic interactions.



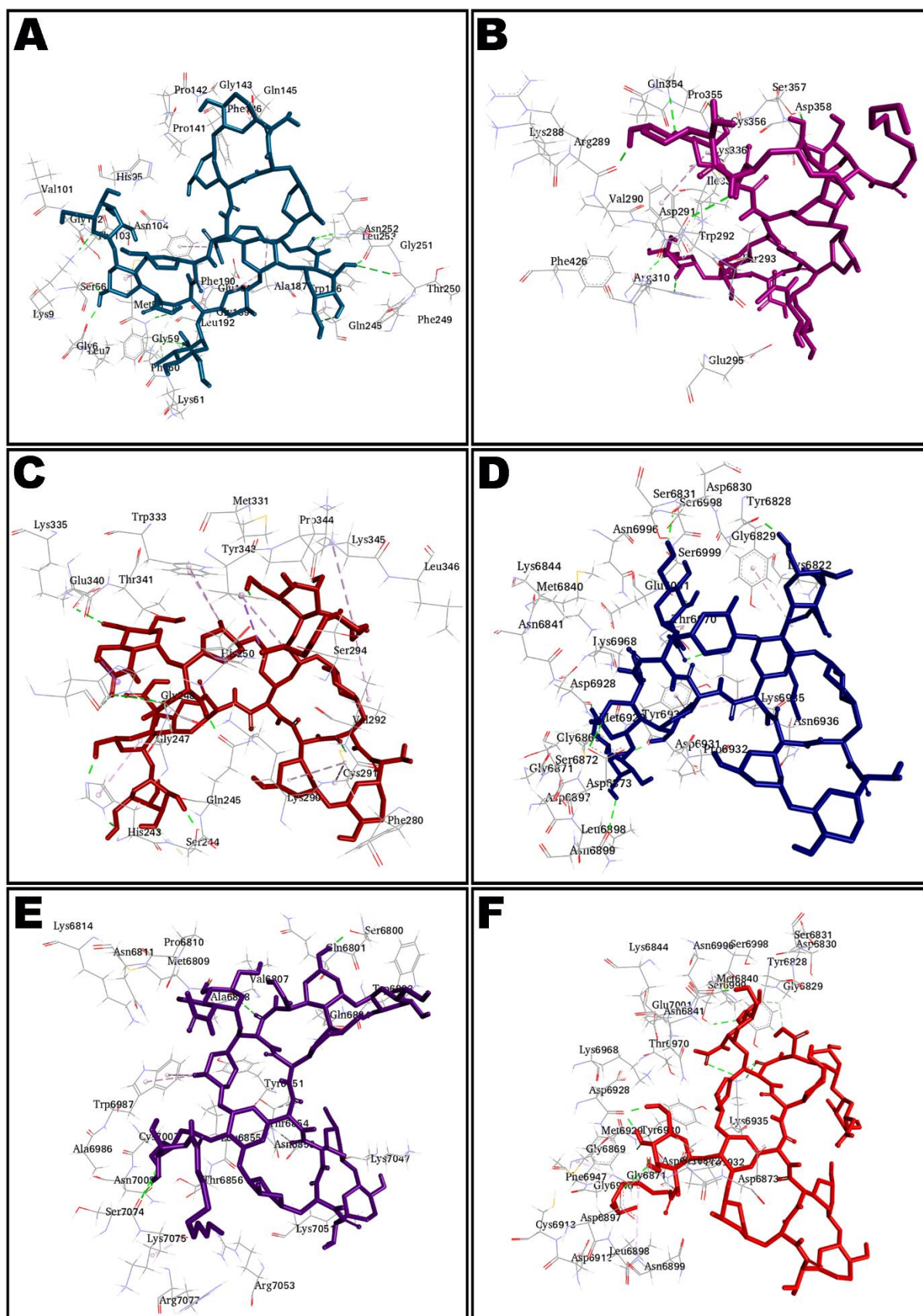


**Figure S2.** Non-bond interactions of teicoplanin (portrayed as stick style) with spike trimer (A), S2 protein-post fusion state (B), N-protein-C domain (C), Nsp3-AMP site (D), Nsp3-MES site (E), and Nsp7 (E) in MM/GBSA optimized complexes. Hydrogen bonds are shown by broken green lines and purple lines enumerate hydrophobic interactions.



**Figure S3.** Intermolecular interactions of teicoplanin (shown in stick style) with Nsp8 (A), Nsp9 (B), Nsp10 (C), Nsp12 (D), Nsp13 helicase-ADP site (E), and Nsp13 helicase-NCB site (E) after MM/GBSA computations. Hydrogen bonds are represented by broken green lines and purple lines specify non-polar interactions.





**Figure S4.** Intermolecular complexes of teicoplanin (shown as sticks) with Nsp14 N-exoribonuclease (A), Nsp14 N7-methyl transferase (B), Nsp15 exoribonuclease (C), Nsp16-GTA site (D), Nsp16-MGP site (E), and Nsp16-SAM site (E) resulted after MM-GBSA analysis showing hydrogen bonds (broken green lines) and non-polar contacts (purple lines).