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Supplementary Material

The Role of Molecular Modeling and Bioinformatics in Treating a Pandemic Disease: The Case of COVID-19

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Table S1. 3D structures of the SARS-CoV-2 proteins obtained using X-ray crystallography.

Protein	Code	Resolution	R Value	Ligand Complexed
Mpro	6LU7	2.16 Å	0.235	inhibitor N3
Mpro	7BQY	1.70 Å	0.226	inhibitor N3
Mpro	6M2N	2.20 Å	0.254	novel inhibtor (5,6,7-trihydroxy-2-phenyl-4H-chromen-4-one)
Mpro	6M2Q	1.70 Å	0.204	
Mpro	7BUY	1.60 Å	0.201	carmofur
Mpro	6Y84	1.39 Å	0.2	
Mpro	6Y2G	2.20 Å	0.247	alpha-ketoamide 13b
Mpro	6Y2E	1.75 Å	0.222	
Mpro	6Y2F	1.95 Å	0.219	alpha-ketoamide 13b
Mpro	6M0K	1.50 Å	0.193	inhibitor 11b
Mpro	6LZE	1.50 Å	0.199	inhibitor 11a
Mpro	6WQF	2.30 Å	0.23	
Mpro	6YNQ	1.80 Å	0.226	2-Methyl-1-tetralone
Mpro	6YT8	2.05 Å	0.233	pyrithione zinc
Mpro	6YVF	1.60 Å	0.208	AZD6482
Mpro	6WNP	1.44 Å	0.196	Boceprevir
Mpro	7BRR	1.40 Å	0.197	GC376
Mpro	7BRO	2.00 Å	0.259	
Mpro	7BRP	1.80 Å	0.240	Boceprevir
Mpro	7C8U	2.35 Å	0.273	GC376
Mpro	6YB7	1.25 Å	0.192	
Mpro	6XA4	1.65 Å	0.239	UAW241
Mpro	6WTT	2.15 Å	0.3	GC376
Mpro	7C8R	2.30 Å	0.261	TG-0203770
Mpro	7C8T	2.05 Å	0.243	TG-0205221

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(Table S1) contd.....

Protein	Code	Resolution	R Value	Ligand Complexed
Mpro	6XFN	1.70 Å	0.228	UAW243
Mpro	6XCH	2.20 Å	0.237	Leupeptin
Mpro	6W63	2.10 Å	0.221	broad-spectrum non-covalent inhibitor X77
Mpro	6XBI	1.70 Å	0.217	UAW248 inhibitor
Mpro	6XBH	1.60 Å	0.221	UAW247 inhibitor
Mpro	6XBG	1.45 Å	0.206	UAW246 inhibitor
PLpro	6WX4	1.66 Å	0.196	peptide inhibitor VIR251
PLpro	6WUU	2.79 Å	0.23	peptide inhibitor VIR250
PLpro	6XAA	2.70 Å	0.26	ubiquitin propargylamide
PLpro	6XA9	2.90 Å	0.231	ISG15 C-terminal domain propargylamide
PLpro	6W9C	2.70 Å	0.309	
PLpro	6WZU	1.79 Å	0.174	
PLpro	6XG3	2.48 Å	0.193	
PLpro(C111S mutant)	6WRH	1.60 Å	0.164	
PLpro(C111S mutant)	6YVA	3.18 Å	0.315	mISG15
NSP3	6WOJ	2.20 Å	0.252	ADP-ribose
NSP3	6WEY	0.95 Å	0.136	
NSP3	6YWM	2.16 Å	0.229	MES
NSP3	6YWL	2.50 Å	0.223	ADP-ribose
NSP3	6YWK	2.20 Å	0.214	HEPES
NSP3 (ADP ribose phosphatase)	6W6Y	1.45 Å	0.189	AMP
NSP3 (ADP ribose phosphatase)	6W02	1.50 Å	0.173	ADP ribose
NSP3 (ADP ribose phosphatase)	6VXS	2.03 Å	0.234	
NSP3 (ADP ribose phosphatase)	6WCF	1.06 Å	0.154	MES
NSP3 (ADP ribose phosphatase)	6WEN	1.35 Å	0.144	
NSP7-NSP8 Complex	6WIQ	2.85 Å	0.252	
NSP7-NSP8 Complex	6WQD	1.95 Å	0.229	
NSP7-NSP8 Complex	6WTC	1.85 Å	0.214	
NSP7-NSP8 Complex	6YHU	2.00 Å	0.239	
NSP7-NSP8 Complex	6M5I	2.50 Å	0.292	
NSP9	6W9Q	2.05 Å	0.246	
NSP9	6W4B	2.95 Å	0.276	
NSP9	6WXD	2.00 Å	0.253	
NSP10	6ZCT	2.55 Å	0.195	
NSP16 - NSP10 Complex	6W4H	1.80 Å	0.163	
NSP16 - NSP10 Complex	6WKQ	1.98 Å	0.180	
NSP16 - NSP10 Complex	6WVN	2.00 Å	0.178	
NSP16 - NSP10 Complex	7C2I	2.50 Å	0.209	
NSP16 - NSP10 Complex	7C2J	2.80 Å	0.235	
NSP16 - NSP10 Complex	6WQ3	2.10 Å	0.186	
NSP16 - NSP10 Complex	6WRZ	2.25 Å	0.190	
NSP16 - NSP10 Complex	7BQ7	2.37 Å	0.208	
NSP16 - NSP10 Complex	6WKS	1.80 Å	0.187	
NSP16 - NSP10 Complex	6WJT	2.00 Å	0.191	
NSP10 - NSP16 Complex	6W75	1.95 Å	0.174	
NSP10 - NSP16 Complex	6YZ1	2.40 Å	0.226	
Nsp15	6W01	1.90 Å	0.185	
NSP15	6VWW	2.20 Å	0.178	
NSP15	6WLC	1.82 Å	0.195	
Nsp15	6XDH	2.35 Å	0.182	
NSP15	6X1B	1.97 Å	0.185	
NSP15	6X4I	1.85 Å	0.189	
NSP15	6WXC	1.85 Å	0.194	
ORF7A	6W37	2.90 Å	0.268	

(Table S1) contd.....

Protein	Code	Resolution	R Value	Ligand Complexed
ORF9B	6Z4U	1.95 Å	0.257	
S (RBD)	6W41	3.08 Å	0.243	human antibody CR3022
S (RBD)	6M0J	2.45 Å	0.227	human ACE2
S (RBD)	6LZG	2.50 Å	0.216	human ACE2
S (RBD)	6VW1	2.68 Å	0.229	human ACE2
S (RBD)	6YM0	4.36 Å	0.319	CR3022 Fab
S (RBD)	6YZ5	1.80 Å	0.193	Nanobody H11-D4
S (RBD)	6YLA	2.42 Å	0.237	CR3022 Fab
S (RBD)	6ZCZ	2.65 Å	0.260	EY6A Fab and a nanobody
S (RBD)	6ZER	3.80 Å	0.251	EY6A Fab
S (RBD)	6Z2M	2.71 Å	0.241	Nanobody H11-D4 and CR3022
S (RBD)	6YZ7	3.30 Å	0.269	Nanobody H11-D4 and CR3022
S (RBD)	7BZ5	1.84 Å	0.191	neutralizing antibody
N	6M3M	2.70 Å	0.293	
N	6WZQ	1.45 Å	0.18	
N	6WZO	1.42 Å	0.173	
N	6WJI	2.05 Å	0.228	
N (C terminal domain)	7C22	2.00 Å	0.238	
N (C terminal domain)	6YUN	1.44 Å	0.189	
N (RNA binding domain)	6WKP	2.67 Å	0.248	
N (RNA binding domain)	6VYO	1.70 Å	0.205	

Table S2. 3D structures of the SARS-CoV-2 proteins obtained using Cryogenic electron microscope.

Protein	Code	Resolution	Ligand Complexed
S	6WPT	3.70 Å	S309 neutralizing antibody Fab fragment
S	6WPS	3.10 Å	S309 neutralizing antibody Fab fragment
S	6X6P	3.22 Å	
S	6VSB	3.46 Å	
S	6X29	2.70 Å	
S	6Z43	3.30 Å	H11-D4 Nanobody
S (Close State)	6VXX	2.80 Å	
S (Open State)	6VYB	3.20 Å	
S (RBD)	6XDG	3.90 Å	Fab fragments of two neutralizing antibodies
S (RBD)	6X2A	3.30 Å	
S (RBD)	6X2C	3.20 Å	
S (RBD)	6X2B	3.60 Å	
S (RBD)	6M17	2.90 Å	ACE2-B0AT1
S (S1)	6YOR	3.30 Å, 3.90 Å	CR3022 Fab
RdRp	7BTF	2.95 Å	Cofactors
RdRp	6M71	2.90 Å	Cofactors
RdRp	7BW4	3.70 Å	
RdRp/RNA complex	6X2G	3.53 Å	
NSP12-NSP7-NSP8 Complex	7BV2	2.50 Å	template-primer RNA and triphosphate form of Remdesivir(RTP)
NSP12-NSP7-NSP8 Complex	7BV1	2.80 Å	
ORF3a	6XDC	2.90 Å	
ORF7A	6WPT	3.70 Å	S309 neutralizing antibody Fab fragment
ORF9B	6WPS	3.10 Å	S309 neutralizing antibody Fab fragment