

Supplemental Material for **Flexibility and Mobility of SARS-CoV-2-related protein structures**

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ABSTRACT

The supplemental material contains a list of all PDB structures used as well as links to some of the most important movie representations of the computed motions.

1 Sources and video links

In Table [S1](#) we give the complete list of all PDB codes used in our study, link their supporting publications as well as the list of modes and E_{cut} values used in computing the full motion movies available from Ref.¹. We also provide the full motion movies for the structures given in the main text in Fig. [3](#), namely the monomer of the SARS-Cov-2 spike ecto domain (6vxx)² and the dimer of the main protease³. Similarly, for main text Fig. [4](#) we include the movies of the closed SARS-Cov-2 spike ecto domain trimer in side⁴ and top view⁵. Last, for the open SARS-Cov-2 spike ecto domain trimer in main text Fig. [5](#), we again give the side⁶ and top views⁷. In addition, the rigidity dilution plots are given for the main protease (6lu7⁸), as well as the open and closed spike ecto domains, 6vxx⁹ and 6vyb¹⁰, respectively.

PDB code	Ref.	rigidity class.	E_{cut} 's (kcal/mol)	protein type	role	oligomeric state	error
The following PDB files were downloaded 18 April 2020							
5r7y	II	1st	1, 2, 3, 0.2	Main protease	cleavage of poly protein	dimer	
5r7z	II	1st	1, 2, 3	Main protease	icw. Z1220452176	dimer	
5r80	II	1st	1, 2, 3	Main protease	icw. Z18197050	dimer	
5r81	II	2nd	1, 2, 3	Main protease	icw. Z1367324110	dimer	
5r82	II	2nd	1, 2, 3	Main protease	icw. Z219104216	dimer	
5r83	II	1st	1, 2, 3	Main protease	icw. Z44592329	dimer	
5r84	II	1st	1, 2, 3, 2.5	Main protease	icw. Z31792168	dimer	
5r8t	II	1st	1, 2, 3	Main protease		dimer	
5re4	II	1st	1, 2, 3, 1.1	Main protease	icw. Z1129283193	dimer	
5re5	II	1st	1, 2, 3	Main protease	icw. Z1129283193	dimer	
5re6	II	1st	1, 2, 3	Main protease	icw. Z1129283193	dimer	
5re7	II		1, 2, 3	Main protease	icw. Z30932204	dimer	bond distance between intrasidue atoms 945 and 950 exceeds 6 Å
5re8	II	1st	1, 2, 3	Main protease	icw. Z2737076969	dimer	
5re9	II		1, 2, 3	Main protease	icw. Z2856434836	dimer	bond distance between intrasidue atoms 945 and 950 exceeds 6 Å
5rea	II		1, 2, 3	Main protease	icw. Z31432226	dimer	bond distance between intrasidue atoms 954 and 979 exceeds 6 Å
5reb	II	1st	1, 2, 3	Main protease	icw. Z2856434899	dimer	
5rec	II	1st	1, 2, 3, 0.4	Main protease	icw. Z1587220559	dimer	
5red	II		1, 2, 3	Main protease	icw. Z2856434865	dimer	bond distance between intrasidue atoms 952 and 957 exceeds 6 Å
5ree	II	1st	1, 2, 3	Main protease	icw. Z2217052426	dimer	
5ref	II	1st	1, 2, 3	Main protease	icw. Z24758179	dimer	
5reg	II		1, 2, 3	Main protease	icw. Z1545313172	dimer	bond distance between intrasidue atoms 947 and 972 exceeds 6 Å
5reh	II	1st	1, 2, 3, 1.8	Main protease	icw. Z111507846	dimer	
5rei	II	1st	1, 2, 3	Main protease	icw. Z2856434856	dimer	
5rej	II	1st	1, 2, 3	Main protease	icw. PCM-0102241	dimer	

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PDB code	Ref.	rigidity class.	E_{cut} 's (kcal/mol)	protein type	role	oligomeric state	error
5rek		1st	1, 2, 3	Main protease	icw. PCM-0102327	dimer	
5rel		2nd	1, 2, 3, 1.5	Main protease	icw. PCM-0102340	dimer	
5rem		1st	1, 2, 3	Main protease	icw. PCM-0103016	dimer	
5ren		1st	1, 2, 3	Main protease	icw. PCM-0102425	dimer	
5reo		1st	1, 2, 3, 1.7	Main protease	icw. PCM-0102578	dimer	
5rep		1st	1, 2, 3	Main protease	icw. PCM-0102201	dimer	
5rer		1st	1, 2, 3	Main protease	icw. PCM-0102615	dimer	
5res		1st	1, 2, 3	Main protease	icw. PCM-0102281	dimer	
5ret		1st	1, 2, 3	Main protease	icw. PCM-0102269	dimer	
5reu		1st	1, 2, 3	Main protease	icw. PCM-0102395	dimer	
5rev		1st	1, 2, 3	Main protease	icw. PCM-0103072	dimer	
5rew		1st	1, 2, 3	Main protease	icw. PCM-0102275	dimer	
5rex		1st	1, 2, 3	Main protease	icw. PCM-0102287	dimer	
5rey		1st	1, 2, 3, 0.5	Main protease	icw. PCM-0102911	dimer	
5rez		1st	1, 2, 3	Main protease	icw. POB0129	dimer	
5rf0		1st	1, 2, 3	Main protease	icw. POB0073	dimer	
5rf1		1st	1, 2, 3	Main protease	icw. NCL-00023830	dimer	
5rf2		1st	1, 2, 3	Main protease	icw. Z1741969146	dimer	
5rf3		1st	1, 2, 3	Main protease	icw. Z1741970824	dimer	
5rf4		1st	1, 2, 3	Main protease	icw. Z1741982125	dimer	
5rf5		1st	1, 2, 3, 1.5	Main protease	icw. Z3241250482	dimer	
5rf6		2nd	1, 2, 3	Main protease	icw. Z1348371854	dimer	
5rf7		1st	1, 2, 3	Main protease	icw. Z316425948_minor	dimer	
5rf8		1st	1, 2, 3	Main protease	icw. Z271004858	dimer	
5rf9		1st	1, 2, 3	Main protease	icw. Z217038356	dimer	
5rfa		1st	1, 2, 3	Main protease	icw. Z2643472210	dimer	
5rfb		1st	1, 2, 3	Main protease	icw. Z1271660837	dimer	
5rfc		1st	1, 2, 3	Main protease	icw. Z979145504	dimer	
5rfd		1st	1, 2, 3	Main protease	icw. Z126932614	dimer	
5rfe		1st	1, 2, 3	Main protease	icw. Z126932614	dimer	
5rff		1st	1, 2, 3	Main protease	icw. PCM-0102704	dimer	
5rfg		1st	1, 2, 3	Main protease	icw. PCM-0102372	dimer	
5rfh		1st	1, 2, 3	Main protease	icw. PCM-0102277	dimer	
5rfi		1st	1, 2, 3, 1.5	Main protease	icw. PCM-0102353	dimer	
5rfj		1st	1, 2, 3, 1.7	Main protease	icw. PCM-0103067	dimer	

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PDB code	Ref.	rigidity class.	E_{cut} 's (kcal/mol)	protein type	role	oligomeric state	error
5rfk	11	1st	1, 2, 3	Main protease	icw. PCM-0102575	dimer	
5rfl	11	1st	1, 2, 3	Main protease	icw. PCM-0102389	dimer	
5rfm	11	1st	1, 2, 3, 0.5	Main protease	icw. PCM-0102539	dimer	
5rfn	11	1st	1, 2, 3, 1.9	Main protease	icw. PCM-0102868	dimer	
5rfo	11	1st	1, 2, 3	Main protease	n complex with PCM-0102972	dimer	
5rfp	11	2nd	1, 2, 3	Main protease	icw. PCM-0102190	dimer	
5rfq	11	1st	1, 2, 3, 1.8	Main protease	icw. PCM-0102179	dimer	
5rfr	11	1st	1, 2, 3	Main protease	icw. PCM-0102169	dimer	
5rfs	11	1st	1, 2, 3	Main protease	icw. PCM-0102739	dimer	
5rft	11	1st	1, 2, 3	Main protease	icw. PCM-0102432	dimer	
5rfu	11	1st	1, 2, 3	Main protease	icw. PCM-0102121	dimer	
5rfv	11	1st	1, 2, 3	Main protease	icw. PCM-0102306	dimer	
5rfw	11	1st	1, 2, 3, 1.5	Main protease	icw. PCM-0102243	dimer	
5rfx	11	1st	1, 2, 3	Main protease	icw. PCM-0102254	dimer	
5rfy	11	1st	1, 2, 3, 0.5 1.5	Main protease	icw. PCM-0102974	dimer	
5rfz	11	1st	1, 2, 3	Main protease	icw. PCM-0102274	dimer	
5rg0	11	1st	1, 2, 3	Main protease	icw. PCM-0102535	dimer	
5rg1	11	1st	1, 2, 3, 1.5	Main protease	icw. NCL-00024905	dimer	
5rg2	11	2nd	1, 2, 3, 2.5	Main protease	icw. NCL-00025058	dimer	
5rg3	11	1st	1, 2, 3	Main protease	icw. NCL-00025412	dimer	
5rgg	11	1st	1, 2, 3, 1.5	Main protease	icw. Z2856434890 (Mpro-x0165)	dimer	
5rgh	11	1st	1, 2, 3	Main protease	icw. Z1619978933 (Mpro-x0395)	dimer	
5rgi	11	1st	1, 2, 3	Main protease	icw. Z369936976 (Mpro-x0397)	dimer	
5rgj	11	2nd	1, 2, 3, 1.5	Main protease	icw. Z1401276297 (Mpro-x0425)	dimer	
5rgk	11	1st	1, 2, 3	Main protease	icw. Z1310876699 (Mpro-x0426)	dimer	
5rgl	11	1st	1, 2, 3, 1.6	Main protease	icw. PCM-0102962 (Mpro-x0705)	dimer	
5rgm	11	1st	1, 2, 3	Main protease	icw. PCM-0102142 (Mpro-x0708)	dimer	

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PDB code	Ref.	rigidity class.	E_{cut} 's (kcal/mol)	protein type	role	oligomeric state	error
5rgn	11	1st	1, 2, 3, 1.5	Main protease	icw. PCM-0102759 (Mpro-x0731)	dimer	
5rgo	11	1st	1, 2, 3	Main protease	icw. PCM-0102248 (Mpro-x0736)	dimer	
5rgp	11	1st	1, 2, 3	Main protease	icw. PCM-0102628 (Mpro-x0771)	dimer	
5rgq	11	1st	1, 2, 3, 1.75	Main protease	icw. Z1849009686 (Mpro-x1086)	dimer	
5rgr	11	1st	1, 2, 3	Main protease	icw. Z328695024 (Mpro-x1101)	dimer	
5rgs	11	1st	1, 2, 3	Main protease	icw. Z1259086950 (Mpro-x1163)	dimer	
6lu7	12	1st	1, 2, 3, 0.7, 1.5	Main protease	icw. an inhibitor N3	dimer	
6lvn	13	brick	1, 2, 3	Spike protein HR2 domain	Spike protein does binding to receptor and involved in fusion of membranes	tetramer	
6lxt	14	1st	1, 2, 3, 3.3, 3.6, 4.6	Spike protein post fusion core	S2 subunit	trimer	
6lzg	15	1st	1, 2, 3	Spike protein domain icw. ace2		dimer	
6m03	16	1st	1, 2, 3	main protease	apoform	dimer	
6m0j	17		1, 2, 3	Spike protein domain icw. ace2		hetero-dimer	bond distance between intrasidue atoms 3327 and 3342 exceeds 6 Å
6m17	18	domain	1, 2, 3, 0.1, 0.2, 0.4, 0.5, 0.7	Ace2 icw. amino acid transport and spike protein domain		hetero-hexamer	
6m18	18	domain	1, 2, 3, 0.03, 0.06, 0.2, 0.5	ace2 icw. amino acid transporter	This structure contains no viral protein	hetero-tetramer	
6m1d	18	2nd	1, 2, 3, 0.2, 0.4, 0.6	ace2 icw. amino acid transporter	This structure contains no viral protein	hetero-tetramer	
6m2n	19	2nd	1, 2, 3, 0.5	Protease	structure with ligand	dimer	
6m2q	20	2nd	1, 2, 3	Protease	apo protein	dimer	

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PDB code	Ref.	rigidity class.	E_{cut} 's (kcal/mol)	protein type	role	oligomeric state	error
6m3m	21	2nd	1, 2, 3, 0.15	Nucleocapsid protein RNA binding domain		monomer	
6m71	22	2nd	1, 2, 3, 0.08 0.17 0.4 0.7	RNA polymerase	icw. cofactors	hetero-tetramer	
6vsb	23	domain	1, 2, 3, 0.005 0.04 0.1 0.35 0.8 1.5	Spike ecto domain	EM structure 3.5 angstrom	trimer	
6vw1	24	1st	1, 2, 3, 0.5 4.0 4.5	Spike receptor binding domain with Ace2		hetero-dimer	
6vww	25		1, 2, 3	NSP15 endoribonuclease		hexamer	bond distance between intrasidue atoms 26 and 27 exceeds 6 Å
6vxs	26	domain	1, 2, 3, 1.3	ADP ribose phosphatase		monomer	
6vxx	27	domain	1, 2, 3, 0.001 0.08 0.5 1.5	Spike ecto domain	EM structure 2.8 angstrom closed	trimer	
6vyb	27	domain	1, 2, 3, 0.001 0.5	Spike ecto domain	Em structure open structure 3.2 angstrom	trimer	
6vyo	26	brick	1, 2, 3, 0.1 0.7	nucleocapsid phosphoprotein		tetramer	
6w01	25		1, 2, 3	NSP15 endoribonuclease	in the Complex with a Citrate	hexamer	bond distance between intrasidue atoms 9 and 24 exceeds 6 Å
6w02	26		1, 2, 3	ADP ribose phosphatase	complex with ADP ribose	monomer	bond distance between intrasidue atoms 2095 and 2100 exceeds 6 Å
6w41	28		1, 2, 3	Spike receptor binding domain complexed with antibody	icw. human antibody CR3022	hetero-trimer	steric clashes
6w4b	26	1st	1, 2, 3, 0.1 0.4	NSP9 RNA binding protein		dimer	

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PDB code	Ref.	rigidity class.	E_{cut} 's (kcal/mol)	protein type	role	oligomeric state	error
6w4h	²⁶		1, 2, 3	NSP16 - NSP10 Complex		hetero-dimer	bond distance between intrasidue atoms 430 and 453 exceeds 6 Å
6w61	²⁶		1, 2, 3	NSP10 and NSP16 complex: methyltransferase stimulatory complex		hetero-dimer	bond distance between intrasidue atoms 320 and 345 exceeds 6 Å
6w63	²⁶	2nd	1, 2, 3, 1.5	Main protease	bound to potent broad-spectrum non-covalent inhibitor X77	dimer	
6w6y	²⁶	2nd	1, 2, 3	ADP ribose phosphatase	icw. AMP	monomer	
6w75	²⁶		1, 2, 3	NSP10-NSP16 complex		hetero-dimer	bond distance between intrasidue atoms 322 and 323 exceeds 6 Å
6w9c	²⁶	1st	1, 2, 3, 0.5	papain like protease		trimer	
6w9q	²⁹	1st	1, 2, 3	NSP9 RNA replicase		dimer	
6wcf	²⁶		1, 2, 3	ADP ribose phosphatase	icw. MES	monomer	bond distance between intrasidue atoms 1189 and 1214 exceeds 6 Å
6wen	²⁶		1, 2, 3	ADP ribose phosphatase	apo form	monomer	bond distance between intrasidue atoms 1141 and 1147 exceeds 6 Å
6y2e	¹⁶	2nd	1, 2, 3	Main protease		dimer	
6y2f	¹⁶	1st	1, 2, 3	Main protease	monoclinic form	dimer	
6y2g	¹⁶	2nd	1, 2, 3, 0.5, 1.5	Main protease	orthorhombic form	dimer	
6y84	³⁰		1, 2, 3	Main protease	unliganded active site	dimer	bond distance between intrasidue atoms 4600 and 4603 exceeds 6 Å
6yb7	³⁰	2nd	1, 2, 3, 2.5, 4.0	Main protease	supercedes 6y84	dimer	

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PDB code	Ref.	rigidity class.	E_{cut} 's (kcal/mol)	protein type	role	oligomeric state	error
6yi3	31		1, 2, 3	nucleocapsid phosphoprotein	NMR structure		bond distance between intrasidue atoms 4600 and 4603 exceeds 6 Å
6yla	32	2nd	1, 2, 3, 0.7 1.5	spike receptor binding domain with Fab fragment		heterotrimer	
7btf	22	2nd	1, 2, 3, 0.1 0.3 0.4 0.8	RNA polymerase	icw. cofactors in reduced condition	heterotetramer	

The following PDB files were downloaded 19 May 2020

3r24	21	1st	1, 2, 3	transferase	RNA maturation	heterodimer	
6lze	16	2nd	1, 2, 3, 1.7		icw. an inhibitor 11a	dimer	
6m0k	16	2nd	1, 2, 3	main protease	icw. an inhibitor 11b	dimer	
6w37	26	brick	1, 2, 3			monomer	
6w7y	21	domain	1, 2, 3, 0.015 0.15 0.4 0.6		SARS-CoV-2 reactive human antibody CR3022	dimer	
6wey	33	1, 2, 3, 2.5 4.0 5.0				monomer	
6wiq	26	"3,2"	1, 2, 3, 0.001 0.03 0.5 1.5			heterotetramer	
6wji	26	domain	1, 2, 3, 0.001 0.13 0.6 1.7		Crystal Structure of C-terminal Dimerization Domain of Nucleocapsid Phosphoprotein from SARS-CoV-2	dimer	
6wjt	26		1, 2, 3			heterodimer	bond distance between intrasidue atoms 01952 and 01967 exceeds 6 Å
6wkp	26	brick	1, 2, 3, 0.08 0.5		monoclinic crystal form	tetramer	
6wkq	26	2nd	1, 2, 3		icw. Sinefungin	heterodimer	

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PDB code	Ref.	rigidity class.	E_{cut} 's (kcal/mol)	protein type	role	oligomeric state	error
6wks-bundle1	³⁴	2nd	1, 2, 3, 0.01 0.2 0.5 1.5			hetero-tetramer	
6wlc	²⁶		1, 2, 3		in the Complex with Uridine-5'-Monophosphate	hexamer	bond distance between intrasidue atoms 1 and 4 exceeds 6 Å
6wnp	²⁶		1, 2, 3		bound to Boceprevir at 1.45 Å	dimer	bond distance between intrasidue atoms 04378 and 04381 exceeds 6 Å
6woj	²⁶	2nd	1, 2, 3, 4		icw. ADP-ribose	monomer	
6wq3	²⁶		1, 2, 3		icw. 7-methyl-GpppA and S-adenosyl-L-homocysteine.	hetero-dimer	bond distance between intrasidue atoms 03495 and 03516 exceeds 6 Å
6wqd	²⁶		1, 2, 3		Complex of NSP7 and the C-terminal Domain of NSP8 from SARS-CoV-2	hetero-tetramer	bond distance between intrasidue atoms 359 and 376 exceeds 6 Å
6wqf	³⁵		1, 2, 3		Revealed by Room Temperature X-ray Crystallography	dimer	bond distance between intrasidue atoms 03306 and 03331 exceeds 6 Å
6wrh	²⁶		1, 2, 3			monomer	bond distance between intrasidue atoms 02089 and 02110 exceeds 6 Å
6wrz	²⁶		1, 2, 3			hetero-dimer	bond distance between intrasidue atoms 03491 and 03510 exceeds 6 Å
6wtc	²⁶	domain	1, 2, 3, 4		Second Form of the Co-factor Complex of NSP7 and the C-terminal Domain of NSP8 from SARS CoV-2	hetero-tetramer	

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PDB code	Ref.	rigidity class.	E_{cut} 's (kcal/mol)	protein type	role	oligomeric state	error
6wvn	26	2nd	1, 2, 3		icw. 7-methyl-GpppA and S-Adenosylmethionine.	hetero-dimer	
6y7m-bundle1	16	2nd	1, 2, 3, 0.3 0.4			dimer	
6yhu	36	domain	1, 2, 3	nsp7-nsp8 complex of SARS-CoV-2		hetero-dimer	
6ym0	32		1, 2, 3		icw. CR3022 Fab	hetero-trimer	steric clashes
6ynq	37		1, 2, 3	main protease	bound to 2-Methyl-1-tetralone	dimer	bond distance between intrasidue atoms 062 and 085 exceeds 6 Å
6yor	38	2nd	1, 2, 3, 0.26	SARS-CoV-2 spike S1 protein	icw. CR3022 Fab	hetero-trimer	
6yt8	39		1, 2, 3	main protease	bound to pyrithione zinc	dimer	bond distance between intrasidue atoms 079 and 082 exceeds 6 Å
6yva	40	1st	1, 2, 3, 0.15 0.3 1.5			hetero-dimer	
6ywk	41	domain	1, 2, 3, 1.5	SARS-CoV-2 (Covid-19) NSP3 macrodomain	icw. HEPES	monomer	
6ywl	41	domain	1, 2, 3, 1.5	SARS-CoV-2 (Covid-19) NSP3 macrodomain	icw. ADP-ribose	monomer	
6ywm	41	domain	1, 2, 3, 2.5 4.0	SARS-CoV-2 (Covid-19) NSP3 macrodomain	icw. MES	monomer	
6yyt	42	2nd	1, 2, 3, 0.004 0.15 0.3 0.4	replicating SARS-CoV-2 polymerase		hetero-tetramer	
6yz1	43		1, 2, 3		complex with Sinefungin	hetero-dimer	bond distance between intrasidue atoms 03770 and 03773 exceeds 6 Å

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PDB code	Ref.	rigidity class.	E_{cut} 's (kcal/mol)	protein type	role	oligomeric state	error
7bqy	12	2nd	1, 2, 3, 0.5 1.2	main protease	icw. AN INHIBITOR N3 at 1.7 angstrom	dimer	
7bro	44	2nd	1, 2, 3, 1.3 1.5	main protease		dimer	
7brp	44	2nd	1, 2, 3, 0.5 0.75 1.3	main protease	complexed with Bo- ceprevir	dimer	
7brr	44	1st	1, 2, 3, 1.5	main protease	complexed with GC376	dimer	
7buy	12	2nd	1, 2, 3, 0.5	main protease	icw. carmofur	dimer	
7bv1	45	2nd	1, 2, 3, 0.05 0.15 0.25 0.5 1.5	nsp12-nsp7-nsp8 com- plex	apo?	hetero- tetramer	
7bv2	45	2nd	1, 2, 3, 0.04 0.15 0.4	nsp12-nsp7-nsp8 com- plex	bound to the template- primer RNA and triphosphate form of Remdesivir(RTP)	hetero- trimer	
7bz5	46	brick	1, 2, 3	COVID-19 virus spike receptor-binding domain	complexed with a neu- tralizing antibody	hetero- trimer	
The following PDB files were downloaded 29 May 2020							
5rgt	11		1, 2, 3	main protease	icw. Z4439011607	dimer	bond distance between intraresidue atoms 03302 and 03325 exceeds 6 Å
5rgu	11	1st	1, 2, 3, 2.5	main protease	icw. Z4444622180	dimer	
5rgv	11	1st	1, 2, 3	main protease	icw. Z4444622066	dimer	
5rgw	11	1st	1, 2, 3	main protease	icw. Z4444621910	dimer	
5rgx	11	1st	1, 2, 3	main protease	icw. Z1344037997	dimer	
5rgy	11	brick	1, 2, 3, 1.7 1.9	main protease	icw. Z1535580916	dimer	
5rgz	11	1st	1, 2, 3	main protease	icw. Z1343543528	dimer	
5rh0	11	1st	1, 2, 3	main protease	icw. Z1286870272	dimer	
5rh1	11	1st	1, 2, 3, 1.7	main protease	icw. Z2010253653	dimer	
5rh2	11	2nd	1, 2, 3	main protease	icw. Z1129289650	dimer	

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PDB code	Ref.	rigidity class.	E_{cut} 's (kcal/mol)	protein type	role	oligomeric state	error
5rh3	11		1, 2, 3	main protease	icw. Z1264525706	dimer	bond distance between intrasidue atoms 03302 and 03325 exceeds 6 Å
5rh4	11		1, 2, 3	main protease	icw. Z1530425063	dimer	bond distance between intrasidue atoms 02536 and 02551 exceeds 6 Å
5rh5	11	1st	1, 2, 3, 2.1 2.4	main protease	icw. Z4439011520	dimer	
5rh6	11	2nd	1, 2, 3	main protease	icw. Z4439011588	dimer	
5rh7	11		1, 2, 3	main protease	icw. Z4439011584	dimer	bond distance between intrasidue atoms 03310 and 03333 exceeds 6 Å
5rh8	11	1st	1, 2, 3, 1.5	main protease	icw. Z4444621965	dimer	
5rh9	11		1, 2, 3	main protease	icw. Z4438424255	dimer	bond distance between intrasidue atoms 03302 and 03325 exceeds 6 Å
5rha	11		1, 2, 3	main protease	icw. Z147647874	dimer	bond distance between intrasidue atoms 03302 and 03327 exceeds 6 Å
6wps	47	domain	1, 2, 3	SARS-CoV-2 spike glycoprotein	icw. the S309 neutralizing antibody Fab fragment	Hetero-9-mer	
6wpt	47	domain	1, 2, 3	SARS-CoV-2 spike glycoprotein	icw. the S309 neutralizing antibody Fab fragment (open state)	Hetero-7-mer	
6wtj	48	2nd	1, 2, 3	main protease	Feline coronavirus drug inhibits	dimer	
6wtk	48	1st	1, 2, 3	main protease	Feline coronavirus drug inhibits	dimer	
6wtm	48	2nd	1, 2, 3	main protease	Feline coronavirus drug inhibits	dimer	
6wtt	49	2nd	1, 2, 3	main protease	with inhibitor GC-376	dimer	

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PDB code	Ref.	rigidity class.	E_{cut} 's (kcal/mol)	protein type	role	oligomeric state	error
6wuu	50	1st	1, 2, 3, 0.5	Papain-like protease	icw. peptide inhibitor VIR250	hetero-dimer	
6wx4	50		1, 2, 3	Papain-like protease	icw. peptide inhibitor VIR251	monomer	steric clashes
6wxc	26		1, 2, 3	NSP15 Endoribonuclease	n the Complex with potential repurposing drug Tipiracil	hexamer	bond distance between intrasidue atoms 1 and 4 exceeds 6 Å
6wxd	51	brick	1, 2, 3	Nsp9 RNA-replicase		dimer	
6wzo	52	domain	1, 2, 3, 0.5	"Nucleocapsid dimerization domain, P1 form"		dimer	
6wzq	52	domain	1, 2, 3	"Nucleocapsid dimerization domain, P21 form"		dimer	
6wzu	26		1, 2, 3	Papain-Like Protease	P3221 space group	monomer	bond distance between intrasidue atoms 02023 and 02026 exceeds 6 Å
6x1b	26		1, 2, 3	NSP15 Endoribonuclease	in the Complex with the Product Nucleotide GpU.	hexamer	bond distance between intrasidue atoms 05377 and 05380 exceeds 6 Å
6x29	53	domain	1, 2, 3, 0.002 0.05 0.3			trimer	
6x2a	53	domain	1, 2, 3, 0.005 0.1			trimer	
6x2b	53	domain	1, 2, 3, 0.005 0.14 0.5			trimer	
6x2c	53	domain	1, 2, 3, 0.001 0.05 0.25 0.7			trimer	
6yun	54	domain	1, 2, 3	C-terminal Dimerization Domain of Nucleocapsid Phosphoprotein		dimer	bond distance between intrasidue atoms 03404 and 03429 exceeds 6 Å

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PDB code	Ref.	rigidity class.	E_{cut} 's (kcal/mol)	protein type	role	oligomeric state	error
6yvf	37		1, 2, 3	Main Protease	bound to AZD6482	dimer	steric clashes
6yz6	37	1st	1, 2, 3		hemiacetal complex of Main Protease and Leupeptin	dimer	
7bw4	35	2nd	1, 2, 3, 0.015	RNA-dependent RNA polymerase		hetero-tetramer	
7c01	36	2nd	1, 2, 3		potent human neutralizing antibody targeting SARS-CoV-2 RBD	hetero-trimer	
7c22	37	domain	1, 2, 3, 0.5	C-terminal domain of SARS-CoV-2 nucleocapsid protein		dimer	
7c2i	38	2nd	1, 2, 3	nsp16-nsp10 heterodimer	icw. SAM (with additional SAM during crystallization)	hetero-dimer	
7c2j	38	2nd	1, 2, 3, 1.3	nsp16-nsp10 heterodimer	icw. SAM (with additional SAM during crystallization)	hetero-dimer	

The following PDB files were downloaded 27 July 2020

5rhb	11	1st	1, 2, 3	main protease		dimer	
5rhc	11	1st	1, 2, 3	main protease		dimer	
5rhd	11	1st	1, 2, 3, 3.2	main protease		dimer	
5rhe	11	1st	1, 2, 3	main protease		dimer	
5rhf	11	1st	1, 2, 3	main protease		dimer	
6m1v	59	domain, brick	1, 2, 3, 4.6, 5.05	post fusion core of S2 of spike protein	part of the spike protein	trimer	
6m5i	60	domain	1, 2, 3, 0.1	nsp7-nsp8c complex	potentially interesting as involved in RNA replication	dimer	
6x4i	26		1, 2, 3	endoribonuclease		6-mer	bond distance between intrasidue atoms 00003 and 00018 exceeds 6 Å
6x6p	61	domain	1, 2, 3, 0.01, 0.15, 0.25, 0.5	spike	another spike structure, determined via EM at 3.2 Å resolution	trimer	
6xa4	62	2nd	1, 2, 3, 1.5	main protease		dimer	

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PDB code	Ref.	rigidity class.	E_{cut} 's (kcal/mol)	protein type	role	oligomeric state	error
6xa9	63		1, 2, 3	another protease (not the main one)		hetero-dimer	bond distance between intrasidue atoms 04000 and 04003 exceeds 6 Å
6xaa	64		1, 2, 3	same protease as 6xa9 but different complex		hetero-dimer	bond distance between intrasidue atoms 01520 and 01523 exceeds 6 Å
6xb0	65		1, 2, 3	main protease		dimer	bond distance between intrasidue atoms 03354 and 03381 exceeds 6 Å
6xb1	66	1st	1, 2, 3	main protease		dimer	
6xb2	67	2nd	1, 2, 3, 0.5	main protease		dimer	
6xbg	68	2nd	1, 2, 3	main protease		dimer	
6xbh	69		1, 2, 3	main protease		dimer	bond distance between intrasidue atoms 04558 and 04563 exceeds 6 Å
6xbi	70	2nd	1, 2, 3	main protease		dimer	
6xc2	71	2nd, brick	1, 2, 3	part of the spike protein		hetero-trimer	
6xc3	71	brick	1, 2, 3, 0.5	part of the spike protein		hetero-5-mer	
6xc4	71	3 0	1, 2, 3	part of the spike protein		hetero-trimer	
6xc7	71	2nd	1, 2, 3, 0.5, 1.5	part of the spike protein		hetero-5-mer	
6xch	72	1 2?	1, 2, 3, 0.5, 1.5	main protease		dimer	
6xcm	73	domain	1, 2, 3, 0.005, 0.05, 0.2, 0.5	spike protein		hetero-7-mer	

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PDB code	Ref.	rigidity class.	E_{cut} 's (kcal/mol)	protein type	role	oligomeric state	error
6xcn	⁷³	domain	1, 2, 3, 0.001, 0.02, 0.08, 0.5	spike protein		hetero-9-mer	"missing residues, steric clashes"
6xdc	⁷⁴	domain	1, 2, 3, 0.08, 0.25, 0.5	protein from open reading frame 3	protein may be part important in the inflammatory response which is critical to understanding why some patients get very ill and others not	dimer	
6xdg	⁷⁵	domain	1, 2, 3, 0.008, 0.04, 0.2	spike protein		hetero-5-mer	
6xdh	⁴⁷	1st	1, 2, 3, 0.5, 0.75	another endoribonuclease		trimer	
6xe1	⁷⁶		1, 2, 3		part of the spike protein	hetero-trimer	no chain A
6xfn	⁷⁷	2nd	1, 2, 3, 0.75	main protease		dimer	
6xg3	²⁶		1, 2, 3	This is a protease but not the main one		monomer	bond distance between intrasidue atoms 02024 and 02045 exceeds 6 Å
6xhm	⁷⁸	1st, 2nd	1, 2, 3, 1.5	main protease		dimer	
6xhu	⁷⁹	1st, 2nd	1, 2, 3, 0.5	main protease		dimer	
6xip	²⁶	2nd	1, 2, 3, 3.5, 4.5	nsp7 and 8	similar to 6m5i structure but at low resolution	hetero-tetramer	
6xkf	⁸⁰	1st, 2nd	1, 2, 3, 0.25	nsp7 and 9	similar to 6m5i structure but at low resolution	homo-dimer	
6xkh	⁸¹	2nd	1, 2, 3, 3.5	main protease		dimer	
6xkl	⁸²	domain	1, 2, 3, 0.05, 0.15, 0.5	spike protein		trimer	

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PDB code	Ref.	rigidity class.	E_{cut} 's (kcal/mol)	protein type	role	oligomeric state	error
6xkm	26	2nd	1, 2, 3, 0.25, 1.5	nsp10/nsp16 methyl transferase		hetero-dimer	
6xmk	83	2nd	1, 2, 3	main protease	low resolution structure	dimer	
6xoa	84	1st, 2nd	1, 2, 3, 0.2	main protease		dimer	
6yz5	85		1, 2, 3	part of the spike protein		hetero-dimer	no chain A
6z2m	86	2 0	1, 2, 3, 0.4, 1.5	part of the spike protein		hetero-tetramer	
6z43	87	domain	1, 2, 3, 0.05, 0.25	spike protein		hetero-6-mer	
6z4u	88	domain	1, 2, 3, 0.001, 0.5	Orf9b	protein may be involved in immune regulation which is important in understanding the different responses of different patients to infection	homo-dimer	
6z97	32	domain	1, 2, 3, 0.001, 0.01, 0.07, 0.25, 0.5	spike protein		trimer	
6zco	89		1, 2, 3	spike protein		dimer	bond distance between intraresidue atoms 00202 and 00225 exceeds 6 Å
6zct	90	1 0	1, 2, 3, 0.5	nsp10	forms part of the methyl transferase complex	monomer	
6zcz	91		1, 2, 3	part of the spike protein		hetero-tetramer	no chain A
6zdh	91	domain	1, 2, 3, 0.002, 0.05, 0.2, 0.5	spike protein		hetero-9-mer	

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PDB code	Ref.	rigidity class.	E_{cut} 's (kcal/mol)	protein type	role	oligomeric state	error
6zer	91	1st, 2nd	1, 2, 3, 0.05, 0.25, 0.75	part of the spike protein		heterotrimer	
6zfo	91	2nd	1, 2, 3, 0.1, 0.5	part of the spike protein		heterotrimer	
6zge	92		1, 2, 3	spike protein		trimer	bond distance between intrasidue atoms 12073 and 12092 exceeds 6 Å
6zgg	93	domain	1, 2, 3, 0.002, 0.02, 0.03, 0.1, 0.25	spike protein		trimer	
6zgh	94	domain	1, 2, 3, 0.001, 0.03, 0.075, 0.2, 4.2	spike protein		trimer	
6zgi	95	2nd	1, 2, 3	spike protein		trimer	bond distance between intrasidue atoms 12073 and 12092 exceeds 6 Å
7bq7	96	domain	1, 2, 3, 0.25	nsp10/nsp16 methyl transferase		heterodimer	
7bwj	97		1, 2, 3	part of the spike protein		heterotrimer	no chain A
7byr	98	domain	1, 2, 3, 0.001, 0.03, 0.07, 0.15, 0.5	spike protein		hetero-5-mer	
7bzf	15	2nd, domain	1, 2, 3, 0.02, 0.1, 0.25, 0.5	RNA polymerase	important for replication	heterotetramer	
7c2k	15	1st, 2nd	1, 2, 3, 0.15, 0.25, 0.4	Complex of proteins needed in replication	chain A is the RNA polymerase which is the important one	heterotetramer	

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PDB code	Ref.	rigidity class.	E_{cut} 's (kcal/mol)	protein type	role	oligomeric state	error
7c2l	99	domain	1, 2, 3, 0.003, 0.08, 0.15, 0.5	spike protein		hetero-9-mer	
7c8r	100	1st, 2hd	1, 2, 3	main protease		dimer	
7c8t	101	1st, 2hd	1, 2, 3	main protease		dimer	
7c8u	102	1st, 2hd	1, 2, 3, 0.5	main protease		dimer	
7c8v	103	brick	1, 2, 3	part of the spike protein		hetero-dimer	
7c8w	104		1, 2, 3	art of the spike protein		hetero-dimer	bond distance between intrasidue atoms 00965 and 00966 exceeds 6 Å
7can	105		1, 2, 3	part of the spike protein		hetero-dimer	bond distance between intrasidue atoms 00966 and 00989 exceeds 6 Å

Table S1. List of all SARS-Cov-2-related structures investigated in this study. The relevant references have been provided if they had been listed on the PDB download pages for each PDB code at the time of download access. The abbreviation "icw." stands for "in complex with". Two large scale collaborations have been labelled by acronyms PANDDA¹¹ and CSGID²⁶. The rigidity association into solid "brick", 1st and 2nd order as well as rigidity domains are given on column 3. Values for E_{cut} are given explicitly whereas all results have been computed for all 6 modes m_7 to m_{12} . Protein description, role and oligomeric state are as written of from the information in each PDB entry or in the referenced publication. The last column indicates the computational error encountered when no motion result has been computed.

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