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

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ABSTRACT

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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 at Ref. 1. We also provide the full motion movies for the structures given in the main text in Fig. 1, namely the monomer of the SARS-Cov-2 spike ecto domain (6vxx)[?] and the trimer of main protease[3]. Similarly, for main text Fig. 2 we include the movies of the closed SARS-Cov-2 spike ecto domain trimer in side[4] and top view.[5] Last, for the open SARS-Cov-2 spike ecto domain trimer in main text Fig. 3, we again give the side[6] and top views.[7]

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	8	1st	1, 2, 3, 0.2	Main protease	cleavage of poly protein	dimer	
5r7z	8	1st	1, 2, 3	Main protease	icw. Z1220452176	dimer	
5r80	8	1st	1, 2, 3	Main protease	icw. Z18197050	dimer	
5r81	8	2nd	1, 2, 3	Main protease	icw. Z1367324110	dimer	
5r82	8	2nd	1, 2, 3	Main protease	icw. Z219104216	dimer	
5r83	8	1st	1, 2, 3	Main protease	icw. Z44592329	dimer	
5r84	8	1st	1, 2, 3, 2.5	Main protease	icw. Z31792168	dimer	
5r8t	8	1st	1, 2, 3	Main protease		dimer	
5re4	8	1st	1, 2, 3, 1.1	Main protease	icw. Z1129283193	dimer	
5re5	8	1st	1, 2, 3	Main protease	icw. Z1129283193	dimer	
5re6	8	1st	1, 2, 3	Main protease	icw. Z1129283193	dimer	
5re7	8		1, 2, 3	Main protease	icw. Z30932204	dimer	bond distance between intraresidue atoms 945 and 950 exceeds 6 Å
5re8	8	1st	1, 2, 3	Main protease	icw. Z2737076969	dimer	
5re9	8		1, 2, 3	Main protease	icw. Z2856434836	dimer	bond distance between intraresidue atoms 945 and 950 exceeds 6 Å
5rea	8		1, 2, 3	Main protease	icw. Z31432226	dimer	bond distance between intraresidue atoms 954 and 979 exceeds 6 Å
5reb	8	1st	1, 2, 3	Main protease	icw. Z2856434899	dimer	
5rec	8	1st	1, 2, 3, 0.4	Main protease	icw. Z1587220559	dimer	
5red	8		1, 2, 3	Main protease	icw. Z2856434865	dimer	bond distance between intraresidue atoms 952 and 957 exceeds 6 Å
5ree	8	1st	1, 2, 3	Main protease	icw. Z2217052426	dimer	
5ref	8	1st	1, 2, 3	Main protease	icw. Z24758179	dimer	
5reg	8		1, 2, 3	Main protease	icw. Z1545313172	dimer	bond distance between intraresidue atoms 947 and 972 exceeds 6 Å
5reh	8	1st	1, 2, 3, 1.8	Main protease	icw. Z111507846	dimer	
5rei	8	1st	1, 2, 3	Main protease	icw. Z2856434856	dimer	
5rej	8	1st	1, 2, 3	Main protease	icw. PCM-0102241	dimer	
5rek	8	1st	1, 2, 3	Main protease	icw. PCM-0102327	dimer	

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PDB code	Ref.	rigidity class.	E_{cut}'s (kcal/mol)	protein type	role	oligomeric state	error
5rel	8	2nd	1, 2, 3, 1.5	Main protease	icw. PCM-0102340	dimer	
5rem	8	1st	1, 2, 3	Main protease	icw. PCM-0103016	dimer	
5ren	8	1st	1, 2, 3	Main protease	icw. PCM-0102425	dimer	
5reo	8	1st	1, 2, 3, 1.7	Main protease	icw. PCM-0102578	dimer	
5rep	8	1st	1, 2, 3	Main protease	icw. PCM-0102201	dimer	
5rer	8	1st	1, 2, 3	Main protease	icw. PCM-0102615	dimer	
5res	8	1st	1, 2, 3	Main protease	icw. PCM-0102281	dimer	
5ret	8	1st	1, 2, 3	Main protease	icw. PCM-0102269	dimer	
5reu	8	1st	1, 2, 3	Main protease	icw. PCM-0102395	dimer	
5rev	8	1st	1, 2, 3	Main protease	icw. PCM-0103072	dimer	
5rew	8	1st	1, 2, 3	Main protease	icw. PCM-0102275	dimer	
5rex	8	1st	1, 2, 3	Main protease	icw. PCM-0102287	dimer	
5rey	8	1st	1, 2, 3, 0.5	Main protease	icw. PCM-0102911	dimer	
5rez	8	1st	1, 2, 3	Main protease	icw. POB0129	dimer	
5rf0	8	1st	1, 2, 3	Main protease	icw. POB0073	dimer	
5rf1	8	1st	1, 2, 3	Main protease	icw. NCL-00023830	dimer	
5rf2	8	1st	1, 2, 3	Main protease	icw. Z1741969146	dimer	
5rf3	8	1st	1, 2, 3	Main protease	icw. Z1741970824	dimer	
5rf4	8	1st	1, 2, 3	Main protease	icw. Z1741982125	dimer	
5rf5	8	1st	1, 2, 3, 1.5	Main protease	icw. Z3241250482	dimer	
5rf6	8	2nd	1, 2, 3	Main protease	icw. Z1348371854	dimer	
5rf7	8	1st	1, 2, 3	Main protease	icw. Z316425948_minor	dimer	
5rf8	8	1st	1, 2, 3	Main protease	icw. Z271004858	dimer	
5rf9	8	1st	1, 2, 3	Main protease	icw. Z217038356	dimer	
5rfa	8	1st	1, 2, 3	Main protease	icw. Z2643472210	dimer	
5rfb	8	1st	1, 2, 3	Main protease	icw. Z1271660837	dimer	
5rfc	8	1st	1, 2, 3	Main protease	icw. Z979145504	dimer	
5rfd	8	1st	1, 2, 3	Main protease	icw. Z126932614	dimer	
5rfe	8	1st	1, 2, 3	Main protease	icw. Z126932614	dimer	
5rff	8	1st	1, 2, 3	Main protease	icw. PCM-0102704	dimer	
5rfg	8	1st	1, 2, 3	Main protease	icw. PCM-0102372	dimer	
5rfh	8	1st	1, 2, 3	Main protease	icw. PCM-0102277	dimer	
5rfi	8	1st	1, 2, 3, 1.5	Main protease	icw. PCM-0102353	dimer	
5rfj	8	1st	1, 2, 3, 1.7	Main protease	icw. PCM-0103067	dimer	
5rfk	8	1st	1, 2, 3	Main protease	icw. PCM-0102575	dimer	
5rfl	8	1st	1, 2, 3	Main protease	icw. PCM-0102389	dimer	

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PDB code	Ref.	rigidity class.	E_{cut}'s (kcal/mol)	protein type	role	oligomeric state	error
5rfm	8	1st	1, 2, 3, 0.5	Main protease	icw. PCM-0102539	dimer	
5rfn	8	1st	1, 2, 3, 1.9	Main protease	icw. PCM-0102868	dimer	
5rfo	8	1st	1, 2, 3	Main protease	n complex with PCM-0102972	dimer	
5rfp	8	2nd	1, 2, 3	Main protease	icw. PCM-0102190	dimer	
5rfq	8	1st	1, 2, 3, 1.8	Main protease	icw. PCM-0102179	dimer	
5rfr	8	1st	1, 2, 3	Main protease	icw. PCM-0102169	dimer	
5rfs	8	1st	1, 2, 3	Main protease	icw. PCM-0102739	dimer	
5rft	8	1st	1, 2, 3	Main protease	icw. PCM-0102432	dimer	
5rfu	8	1st	1, 2, 3	Main protease	icw. PCM-0102121	dimer	
5rfv	8	1st	1, 2, 3	Main protease	icw. PCM-0102306	dimer	
5rfw	8	1st	1, 2, 3, 1.5	Main protease	icw. PCM-0102243	dimer	
5rfx	8	1st	1, 2, 3	Main protease	icw. PCM-0102254	dimer	
5rfy	8	1st	1, 2, 3, 0.5 1.5	Main protease	icw. PCM-0102974	dimer	
5rfz	8	1st	1, 2, 3	Main protease	icw. PCM-0102274	dimer	
5rg0	8	1st	1, 2, 3	Main protease	icw. PCM-0102535	dimer	
5rg1	8	1st	1, 2, 3, 1.5	Main protease	icw. NCL-00024905	dimer	
5rg2	8	2nd	1, 2, 3, 2.5	Main protease	icw. NCL-00025058	dimer	
5rg3	8	1st	1, 2, 3	Main protease	icw. NCL-00025412	dimer	
5rgg	8	1st	1, 2, 3, 1.5	Main protease	icw. Z2856434890 (Mpro-x0165)	dimer	
5rgh	8	1st	1, 2, 3	Main protease	icw. Z1619978933 (Mpro-x0395)	dimer	
5rgi	8	1st	1, 2, 3	Main protease	icw. Z369936976 (Mpro-x0397)	dimer	
5rgj	8	2nd	1, 2, 3, 1.5	Main protease	icw. Z1401276297 (Mpro-x0425)	dimer	
5rgk	8	1st	1, 2, 3	Main protease	icw. Z1310876699 (Mpro-x0426	dimer	
5rgl	8	1st	1, 2, 3, 1.6	Main protease	icw. PCM-0102962 (Mpro-x0705)	dimer	
5rgm	8	1st	1, 2, 3	Main protease	icw. PCM-0102142 (Mpro-x0708)	dimer	
5rgn	8	1st	1, 2, 3, 1.5	Main protease	icw. PCM-0102759 (Mpro-x0731)	dimer	

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PDB code	Ref.	rigidity class.	E_{cut}'s (kcal/mol)	protein type	role	oligomeric state	error
5rgo	8	1st	1, 2, 3	Main protease	icw. PCM-0102248 (Mpro-x0736)	dimer	
5rgp	8	1st	1, 2, 3	Main protease	icw. PCM-0102628 (Mpro-x0771)	dimer	
5rgq	8	1st	1, 2, 3, 1.75	Main protease	icw. Z1849009686 (Mpro-x1086)	dimer	
5rgr	8	1st	1, 2, 3	Main protease	icw. Z328695024 (Mpro-x1101)	dimer	
5rgs	8	1st	1, 2, 3	Main protease	icw. Z1259086950 (Mpro-x1163)	dimer	
6lu7	9	1st	1, 2, 3, 0.7 1.5	Main protease	icw. an inhibitor N3	dimer	
6lvn	10	brick	1, 2, 3	Spike protein HR2 domain	Spike protein does binding to receptor and involved in fusion of membranes	tetramer	
6lxt	11	1st	1, 2, 3, 3.3 3.6 4.6	Spike protein post fusion core	S2 subunit	trimer	
6lzg	12	1st	1, 2, 3	Spike protein domain icw. ace2		dimer	
6m03	13	1st	1, 2, 3	main protease	apoform	dimer	
6m0j	14		1, 2, 3	Spike protein domain icw. ace2		hetero-dimer	bond distance between intraresidue atoms 3327 and 3342 exceeds 6 Å
6m17	15	domain	1, 2, 3, 0.1 0.2 0.4 0.5 0.7	Ace2 icw. amino acid transporte and spike protein domain		hetero-hexamer	
6m18	15	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	15	2nd	1, 2, 3, 0.2 0.4 0.6	ace2 icw. amino acid transporter	This structure contains no viral protein	hetero-tetramer	
6m2n	16	2nd	1, 2, 3, 0.5	Protease	structure with ligand	dimer	
6m2q	17	2nd	1, 2, 3	Protease	apo protein	dimer	
6m3m	18	2nd	1, 2, 3, 0.15	Nucleocapside protein RNA binding domain		monomer	

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PDB code	Ref.	rigidity class.	E_{cut}'s (kcal/mol)	protein type	role	oligomeric state	error
6m71	19	2nd	1, 2, 3, 0.08 0.17 0.4 0.7	RNA polymerase	icw. cofactors	hetero-tetramer	
6vsb	20	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	21	1st	1, 2, 3, 0.5 4.0 4.5	Spike receptor binding domain with Ace2		hetero-dimer	
6vww	22		1, 2, 3	NSP15 endoribonuclease		hexamer	bond distance between intraresidue atoms 26 and 27 exceeds 6 Å
6vxs	23	domain	1, 2, 3, 1.3	ADP ribose phosphotase		monomer	
6vxx	24	domain	1, 2, 3, 0.001 0.08 0.5 1.5	Spike ecto domain	EM structure 2.8 angstrom closed	trimer	
6vyb	24	domain	1, 2, 3, 0.001 0.5	Spike ecto domain	Em structure open structure 3.2 angstrom	trimer	
6vyo	23	brick	1, 2, 3, 0.1 0.7	nucleocapside phosphoprotein		tetramer	
6w01	22		1, 2, 3	NSP15 endoribonuclease	in the Complex with a Citrate	hexamer	bond distance between intraresidue atoms 9 and 24 exceeds 6 Å
6w02	23		1, 2, 3	ADP ribose phosphotase	complex with ADP ribose	monomer	bond distance between intraresidue atoms 2095 and 2100 exceeds 6 Å
6w41	25		1, 2, 3	Spike receptor binding domain complexed with antibody	icw. human antibody CR3022	hetero-trimer	steric clashes
6w4b	23	1st	1, 2, 3, 0.1 0.4	NSP9 RNA binding protein		dimer	
6w4h	23		1, 2, 3	NSP16 - NSP10 Complex		hetero-dimer	bond distance between intraresidue atoms 430 and 453 exceeds 6 Å

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PDB code	Ref.	rigidity class.	E_{cut}'s (kcal/mol)	protein type	role	oligomeric state	error
6w61	23		1, 2, 3	NSP10 and NSP16 complex: methyltransferase stimulatory complex		hetero-dimer	bond distance between intraresidue atoms 320 and 345 exceeds 6 Å
6w63	23	2nd	1, 2, 3, 1.5	Main protease	bound to potent broad-spectrum non-covalent inhibitor X77	dimer	
6w6y	23	2nd	1, 2, 3	ADP ribose phosphotase	icw. AMP	monomer	
6w75	23		1, 2, 3	NSP10-NSP16 complex		hetero-dimer	bond distance between intraresidue atoms 322 and 323 exceeds 6 Å
6w9c	23	1st	1, 2, 3, 0.5	papain like protease		trimer	
6w9q	26	1st	1, 2, 3	NSP9 RNA replicase		dimer	
6wcf	23		1, 2, 3	ADP ribose phosphotase	icw. MES	monomer	bond distance between intraresidue atoms 1189 and 1214 exceeds 6 Å
6wen	23		1, 2, 3	ADP ribose phosphotase	apo form	monomer	bond distance between intraresidue atoms 1141 and 1147 exceeds 6 Å
6y2e	13	2nd	1, 2, 3	Main protease		dimer	
6y2f	13	1st	1, 2, 3	Main protease	monoclinic form	dimer	
6y2g	13	2nd	1, 2, 3, 0.5 1.5	Main protease	orthorhombic form	dimer	
6y84	27		1, 2, 3	Main protease	unliganded active site	dimer	bond distance between intraresidue atoms 4600 and 4603 exceeds 6 Å
6yb7	27	2nd	1, 2, 3, 2.5 4.0	Main protease	supercedes 6y84	dimer	
6yi3	28		1, 2, 3	nucleocapside phosphoprotein	NMR structure		bond distance between intraresidue atoms 4600 and 4603 exceeds 6 Å

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PDB code	Ref.	rigidity class.	E_{cut}'s (kcal/mol)	protein type	role	oligomeric state	error
6yla	29	2nd	1, 2, 3, 0.7 1.5	spike receptor binding domain with Fab fragment		hetero-trimer	
7btf	19	2nd	1, 2, 3, 0.1 0.3 0.4 0.8	RNA polymerase	icw. cofactors in reduced condition	hetero-tetramer	
The following PDB files were downloaded 19 May 2020							
3r24	18	1st	1, 2, 3	transferase	RNA maturation	hetero-dimer	
6lze	13	2nd	1, 2, 3, 1.7		icw. an inhibitor 11a	dimer	
6m0k	13	2nd	1, 2, 3	main protease	icw. an inhibitor 11b	dimer	
6w37	23	brick	1, 2, 3			monomer	
6w7y	18	domain	1, 2, 3, 0.015 0.15 0.4 0.6		SARS-CoV-2 reactive human antibody CR3022	dimer	
6wey	30	1, 2, 3, 2.5 4.0 5.0				monomer	
6wiq	23	"3,2"	1, 2, 3, 0.001 0.03 0.5 1.5			hetero-tetramer	
6wji	23	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	23		1, 2, 3			hetero-dimer	bond distance between intraresidue atoms 01952 and 01967 exceeds 6 Å
6wkp	23	brick	1, 2, 3, 0.08 0.5		monoclinic crystal form	tetramer	
6wkq	23	2nd	1, 2, 3		icw. Sinefungin	hetero-dimer	
6wks-bundle1	31	2nd	1, 2, 3, 0.01 0.2 0.5 1.5			hetero-tetramer	

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PDB code	Ref.	rigidity class.	E_{cut}'s (kcal/mol)	protein type	role	oligomeric state	error
6wlc	23		1, 2, 3		in the Complex with Uridine-5'-Monophosphate	hexamer	bond distance between intraresidue atoms 1 and 4 exceeds 6 Å
6wnp	23		1, 2, 3		bound to Boceprevir at 1.45 A	dimer	bond distance between intraresidue atoms 04378 and 04381 exceeds 6 Å
6woj	23	2nd	1, 2, 3, 4		icw. ADP-ribose	monomer	
6wq3	23		1, 2, 3		icw. 7-methyl-GpppA and S-adenosyl-L-homocysteine.	hetero-dimer	bond distance between intraresidue atoms 03495 and 03516 exceeds 6 Å
6wqd	23		1, 2, 3		Complex of NSP7 and the C-terminal Domain of NSP8 from SARS-CoV-2	hetero-tetramer	bond distance between intraresidue atoms 359 and 376 exceeds 6 Å
6wqf	32		1, 2, 3		Revealed by Room Temperature X-ray Crystallography	dimer	bond distance between intraresidue atoms 03306 and 03331 exceeds 6 Å
6wrh	23		1, 2, 3			monomer	bond distance between intraresidue atoms 02089 and 02110 exceeds 6 Å
6wrz	23		1, 2, 3			hetero-dimer	bond distance between intraresidue atoms 03491 and 03510 exceeds 6 Å
6wtc	23	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	
6wvn	23	2nd	1, 2, 3		icw. 7-methyl-GpppA and S-Adenosylmethionine.	hetero-dimer	

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PDB code	Ref.	rigidity class.	E_{cut}'s (kcal/mol)	protein type	role	oligomeric state	error
6y7m-bundle1	13	2nd	1, 2, 3, 0.3 0.4			dimer	
6yhu	33	domain	1, 2, 3	nsp7-nsp8 complex of SARS-CoV-2		hetero-dimer	
6ym0	34		1, 2, 3		icw. CR3022 Fab	hetero-trimer	steric clashes
6ynq	35		1, 2, 3	main protease	bound to 2-Methyl-1-tetralone	dimer	bond distance between intraresidue atoms 062 and 085 exceeds 6 Å
6yor	36	2nd	1, 2, 3, 0.26	SARS-CoV-2 spike S1 protein	icw. CR3022 Fab	hetero-trimer	
6yt8	37		1, 2, 3	main protease	bound to pyrithione zinc	dimer	bond distance between intraresidue atoms 079 and 082 exceeds 6 Å
6yva	38	1st	1, 2, 3, 0.15 0.3 1.5			hetero-dimer	
6ywk	39	domain	1, 2, 3, 1.5	SARS-CoV-2 (Covid-19) NSP3 macrodomain	icw. HEPES	monomer	
6ywl	39	domain	1, 2, 3, 1.5	SARS-CoV-2 (Covid-19) NSP3 macrodomain	icw. ADP-ribose	monomer	
6ywm	39	domain	1, 2, 3, 2.5 4.0	SARS-CoV-2 (Covid-19) NSP3 macrodomain	icw. MES	monomer	
6yyt	40	2nd	1, 2, 3, 0.004 0.15 0.3 0.4	replicating SARS-CoV-2 polymerase		hetero-tetramer	
6yz1	41		1, 2, 3		complex with Sinefungin	hetero-dimer	bond distance between intraresidue atoms 03770 and 03773 exceeds 6 Å
7bqy	9	2nd	1, 2, 3, 0.5 1.2	main protease	icw. AN INHIBITOR N3 at 1.7 angstrom	dimer	
7bro	42	2nd	1, 2, 3, 1.3 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
7brp	42	2nd	1, 2, 3, 0.5 0.75 1.3	main protease	complexed with Boceprevir	dimer	
7brr	42	1st	1, 2, 3, 1.5	main protease	complexed with GC376	dimer	
7buy	9	2nd	1, 2, 3, 0.5	main protease	icw. carmofur	dimer	
7bv1	43	2nd	1, 2, 3, 0.05 0.15 0.25 0.5 1.5	nsp12-nsp7-nsp8 complex	apo?	hetero-tetramer	
7bv2	43	2nd	1, 2, 3, 0.04 0.15 0.4	nsp12-nsp7-nsp8 complex	bound to the template-primer RNA and triphosphate form of Remdesivir(RTP)	hetero-trimer	
7bz5	44	brick	1, 2, 3	COVID-19 virus spike receptor-binding domain	complexed with a neutralizing antibody	hetero-trimer	
The following PDB files were downloaded 29 May 2020							
5rgt	8		1, 2, 3	main protease	icw. Z4439011607	dimer	The bond distance between intraresidue atoms 03302 and 03325 exceeds 6 Å
5rgu	8	1st	1, 2, 3, 2.5	main protease	icw. Z4444622180	dimer	
5rgv	8	1st	1, 2, 3	main protease	icw. Z4444622066	dimer	
5rgw	8	1st	1, 2, 3	main protease	icw. Z4444621910	dimer	
5rgx	8	1st	1, 2, 3	main protease	icw. Z1344037997	dimer	
5rgy	8	brick	1, 2, 3, 1.7 1.9	main protease	icw. Z1535580916	dimer	
5rgz	8	1st	1, 2, 3	main protease	icw. Z1343543528	dimer	
5rh0	8	1st	1, 2, 3	main protease	icw. Z1286870272	dimer	
5rh1	8	1st	1, 2, 3, 1.7	main protease	icw. Z2010253653	dimer	
5rh2	8	2nd	1, 2, 3	main protease	icw. Z1129289650	dimer	
5rh3	8		1, 2, 3	main protease	icw. Z1264525706	dimer	The bond distance between intraresidue atoms 03302 and 03325 exceeds 6 Å

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PDB code	Ref.	rigidity class.	E_{cut}'s (kcal/mol)	protein type	role	oligomeric state	error
5rh4	8		1, 2, 3	main protease	icw. Z1530425063	dimer	The bond distance between intraresidue atoms 02536 and 02551 exceeds 6 Å
5rh5	8	1st	1, 2, 3, 2.1 2.4	main protease	icw. Z4439011520	dimer	
5rh6	8	2nd	1, 2, 3	main protease	icw. Z4439011588	dimer	
5rh7	8		1, 2, 3	main protease	icw. Z4439011584	dimer	The bond distance between intraresidue atoms 03310 and 03333 exceeds 6 Å
5rh8	8	1st	1, 2, 3, 1.5	main protease	icw. Z4444621965	dimer	
5rh9	8		1, 2, 3	main protease	icw. Z4438424255	dimer	The bond distance between intraresidue atoms 03302 and 03325 exceeds 6 Å
5rha	8		1, 2, 3	main protease	icw. Z147647874	dimer	The bond distance between intraresidue atoms 03302 and 03327 exceeds 6 Å
6wps	45	domain	1, 2, 3	SARS-CoV-2 spike glycoprotein	icw. the S309 neutralizing antibody Fab fragment	Hetero-9-mer	
6wpt	45	domain	1, 2, 3	SARS-CoV-2 spike glycoprotein	icw. the S309 neutralizing antibody Fab fragment (open state)	Hetero-7-mer	
6wtj	46	2nd	1, 2, 3	main protease	Feline coronavirus drug inhibits	dimer	
6wtk	46	1st	1, 2, 3	main protease	Feline coronavirus drug inhibits	dimer	
6wtm	46	2nd	1, 2, 3	main protease	Feline coronavirus drug inhibits	dimer	
6wtt	47	2nd	1, 2, 3	main protease	with inhibitor GC-376	dimer	
6wuu	48	1st	1, 2, 3, 0.5	Papain-like protease	icw. peptide inhibitor VIR250	hetero-dimer	
6wx4	48		1, 2, 3	Papain-like protease	icw. peptide inhibitor VIR251	monomer	steric clashes

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PDB code	Ref.	rigidity class.	E_{cut}'s (kcal/mol)	protein type	role	oligomeric state	error
6wxc	23		1, 2, 3	NSP15 Endoribonuclease	n the Complex with potential repurposing drug Tipiracil	hexamer	The bond distance between intraresidue atoms 1 and 4 exceeds 6 Å
6wxd	49	brick	1, 2, 3	Nsp9 RNA-replicase		dimer	
6wzo	50	domain	1, 2, 3, 0.5	"Nucleocapsid dimerization domain, P1 form"		dimer	
6wzq	50	domain	1, 2, 3	"Nucleocapsid dimerization domain, P21 form"		dimer	
6wzu	23		1, 2, 3	Papain-Like Protease	P3221 space group	monomer	The bond distance between intraresidue atoms 02023 and 02026 exceeds 6 Å
6x1b	23		1, 2, 3	NSP15 Endoribonuclease	in the Complex with the Product Nucleotide GpU.	hexamer	The bond distance between intraresidue atoms 05377 and 05380 exceeds 6 Å
6x29	51	domain	1, 2, 3, 0.002 0.05 0.3			trimer	
6x2a	51	domain	1, 2, 3, 0.005 0.1			trimer	
6x2b	51	domain	1, 2, 3, 0.005 0.14 0.5			trimer	
6x2c	51	domain	1, 2, 3, 0.001 0.05 0.25 0.7			trimer	
6yun	52	domain	1, 2, 3	C-terminal Dimerization Domain of Nucleocapsid Phosphoprotein		dimer	The bond distance between intraresidue atoms 03404 and 03429 exceeds 6 Å
6yvf	35		1, 2, 3	Main Protease	bound to AZD6482	dimer	steric clashes

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PDB code	Ref.	rigidity class.	E_{cut}'s (kcal/mol)	protein type	role	oligomeric state	error
6yz6	35	1st	1, 2, 3		hemiacetal complex of Main Protease and Leupeptin	dimer	
7bw4	53	2nd	1, 2, 3, 0.015 0.15	RNA-dependent RNA polymerase		hetero-tetramer	
7c01	54	2nd	1, 2, 3		potent human neutralizing antibody targeting SARS-CoV-2 RBD	hetero-trimer	
7c22	55	domain	1, 2, 3, 0.5	C-terminal domain of SARS-CoV-2 nucleocapsid protein		dimer	
7c2i	56	2nd	1, 2, 3	nsp16-nsp10 heterodimer	icw. SAM (with additional SAM during crystallization)	hetero-dimer	
7c2j	56	2nd	1, 2, 3, 1.3	nsp16-nsp10 heterodimer	icw. SAM (with additional SAM during crystallization)	hetero-dimer	
wuhan_ace2_MD		domain	1, 2, 3, 0.001 0.1 0.2 0.3 0.4 0.5 0.8 1.5				
wuhan_ace2_min		domain	1, 2, 3, 0.001 0.1 0.2 0.3 0.4 0.5 0.8 1.5				
wuhan_E2_protein		"3,29	1, 2, 3, 0.2 0.5				
wuhan_spike (6vsb)		"3,1"	1, 2, 3, 0.001 0.1 0.2 0.3 0.4 0.5 0.8 1.5				

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 PANDDA[8] and CSGID[23]. 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 now motion result has been computed.

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