



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 8, 2021 – 08:02 AM EDT

PDB ID : 7LMC
Title : Structure of SARS CoV-2 main protease shows simultaneous processing of its N- and C-terminii
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Deposited on : 2021-02-05
Resolution : 2.98 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.18
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.18

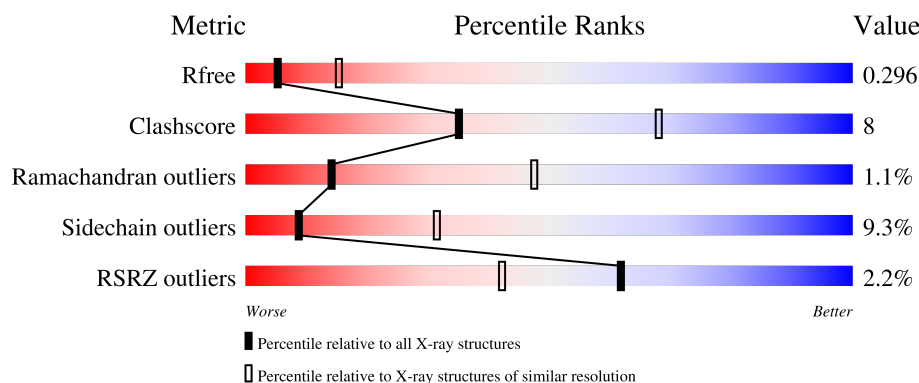
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	E	6	<div> <div>67%</div> <div>33%</div> </div>
1	F	6	<div> <div>17%</div> <div>50%</div> <div>33%</div> <div>17%</div> </div>
2	A	306	<div> <div>%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
2	B	306	<div> <div>%</div> <div>74%</div> <div>25%</div> <div>.</div> </div>
2	C	306	<div> <div>4%</div> <div>71%</div> <div>28%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	306	<div><div></div><div>3%</div><div>70%</div><div>27%</div><div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9539 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Non-structural protein 4 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	E	6	Total	C	N	O	0	0	0
			42	26	7	9			
1	F	6	Total	C	N	O	0	0	0
			42	26	7	9			

- Molecule 2 is a protein called 3C-like proteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	306	Total	C	N	O	S	0	0	0
			2366	1499	402	444	21			
2	B	306	Total	C	N	O	S	0	0	0
			2366	1499	402	444	21			
2	C	306	Total	C	N	O	S	0	0	0
			2366	1499	402	444	21			
2	D	305	Total	C	N	O	S	0	0	0
			2357	1494	400	442	21			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	145	ALA	CYS	engineered mutation	UNP P0DTD1
B	145	ALA	CYS	engineered mutation	UNP P0DTD1
C	145	ALA	CYS	engineered mutation	UNP P0DTD1
D	145	ALA	CYS	engineered mutation	UNP P0DTD1

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Non-structural protein 4 peptide

Chain E: 




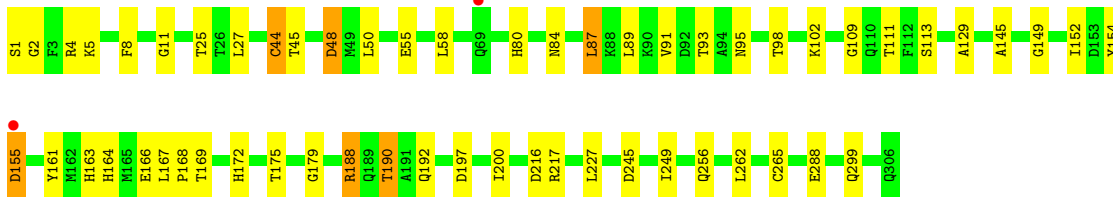
- Molecule 1: Non-structural protein 4 peptide

Chain F: 




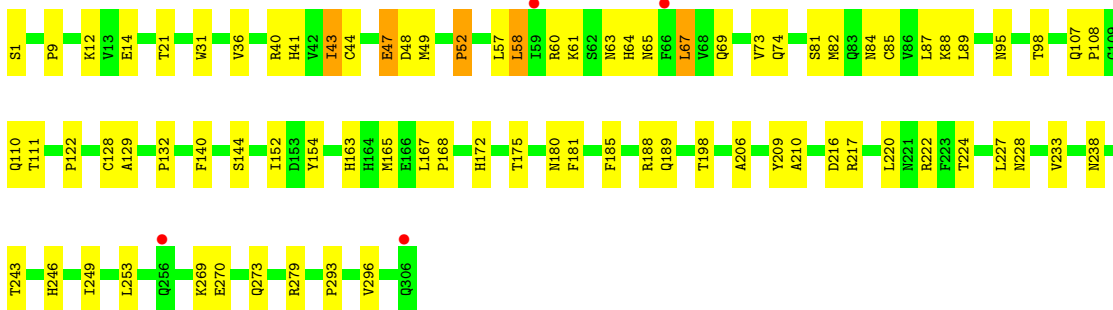
- Molecule 2: 3C-like proteinase

Chain A: 



- Molecule 2: 3C-like proteinase

Chain B: 



Chain C:

Chain D:

Category	Value
Red	3%
Green	70%
Yellow	27%

Label	Category
S1	Yellow
M6	Yellow
S10	Red
G11	Green
K12	Green
V13	Green
E14	Yellow
M17	Yellow
L27	Yellow
L30	Yellow
P39	Yellow
R40	Yellow
H41	Yellow
V42	Green
I43	Yellow
C44	Green
T45	Yellow
S46	Yellow
E47	Yellow
D48	Red
M49	Red
L50	Green
N51	Green
P52	Green
N53	Yellow
Y54	Yellow
E55	Yellow
D56	Yellow
L57	Yellow
P66	Yellow
V73	Red
I78	Yellow
M82	Yellow
C85	Yellow
V86	Green
L87	Green
P99	Yellow
K100	Yellow
Q107	Yellow
T111	Yellow
C117	Yellow
S121	Yellow
C128	Yellow
R131	Green
T135	Yellow
G138	Yellow
S139	Yellow
N142	Red
A145	Yellow
V149	Yellow
I152	Yellow
D153	Yellow
V154	Red
D155	Green
C156	Yellow
V157	Green
S158	Yellow
Y161	Yellow
H162	Green
H163	Yellow
H164	Yellow
M165	Yellow
P168	Green
H172	Yellow
A173	Green
G174	Yellow
T175	Yellow
F181	Yellow
V186	Red
D187	Green
R188	Red
Q189	Yellow
T190	Yellow
A191	Yellow
Q192	Yellow
L200	Yellow
T201	Red
T202	Green
V204	Yellow
L205	Yellow
L208	Yellow
D216	Yellow
R222	Red
F223	Yellow
T224	Yellow
T225	Yellow
T226	Yellow
L227	Yellow
V233	Yellow
V237	Red
E240	Yellow
P241	Red
T242	Red
L243	Yellow
Q244	Green
D245	Yellow
D248	Yellow
I249	Yellow
D153	Yellow
D263	Yellow
K289	Yellow
E270	Yellow
L271	Yellow
L272	Yellow
N276	Yellow
I281	Yellow
S284	Yellow
A285	Red
L286	Green
D289	Yellow
T292	Yellow
P293	Yellow
F294	Yellow
R298	Yellow
Q299	Yellow
T304	Yellow
F305	Yellow
GLN	Grey

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.77Å 66.30Å 80.26Å 80.52° 89.46° 70.55°	Depositor
Resolution (Å)	79.07 – 2.98 79.07 – 2.98	Depositor EDS
% Data completeness (in resolution range)	88.7 (79.07-2.98) 88.6 (79.07-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.96Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.208 , 0.288 0.217 , 0.296	Depositor DCC
R_{free} test set	1095 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	63.2	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9539	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	E	0.45	0/41	0.41	0/55
1	F	0.38	0/41	0.67	0/55
2	A	0.46	0/2419	0.68	0/3288
2	B	0.40	0/2419	0.63	0/3288
2	C	0.42	0/2419	0.68	0/3288
2	D	0.42	0/2410	0.64	0/3276
All	All	0.42	0/9749	0.66	0/13250

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	42	0	47	3	0
1	F	42	0	47	7	0
2	A	2366	0	2314	24	0
2	B	2366	0	2314	46	0
2	C	2366	0	2314	41	0
2	D	2357	0	2306	51	0
All	All	9539	0	9342	154	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 154 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:51:ASN:HB2	2:D:188:ARG:HE	1.43	0.82
2:B:84:ASN:ND2	2:B:180:ASN:ND2	2.28	0.81
2:B:58:LEU:HD13	2:B:82:MET:HB2	1.63	0.81
2:C:40:ARG:HD3	2:C:85:CYS:HA	1.70	0.73
2:C:285:ALA:H	2:D:286:LEU:HD11	1.53	0.73

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	4/6 (67%)	4 (100%)	0	0	100	100
1	F	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
2	A	304/306 (99%)	280 (92%)	19 (6%)	5 (2%)	9	38
2	B	304/306 (99%)	274 (90%)	26 (9%)	4 (1%)	12	43
2	C	304/306 (99%)	265 (87%)	36 (12%)	3 (1%)	15	50
2	D	303/306 (99%)	264 (87%)	38 (12%)	1 (0%)	41	74
All	All	1223/1236 (99%)	1090 (89%)	120 (10%)	13 (1%)	14	47

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	154	TYR
2	B	47	GLU
2	C	154	TYR
2	B	63	ASN
2	A	155	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	5/5 (100%)	4 (80%)	1 (20%)	1	6
1	F	5/5 (100%)	4 (80%)	1 (20%)	1	6
2	A	262/262 (100%)	242 (92%)	20 (8%)	13	41
2	B	262/262 (100%)	245 (94%)	17 (6%)	17	48
2	C	262/262 (100%)	234 (89%)	28 (11%)	6	24
2	D	261/262 (100%)	230 (88%)	31 (12%)	5	21
All	All	1057/1058 (100%)	959 (91%)	98 (9%)	9	31

5 of 98 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	128	CYS
2	D	78	ILE
2	C	217	ARG
2	C	291	PHE
2	D	128	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	80	HIS
2	C	214	ASN
2	D	299	GLN
2	D	41	HIS
2	B	180	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	E	6/6 (100%)	0.44	0 100 100	81, 82, 83, 83	0
1	F	6/6 (100%)	0.94	1 (16%) 1 1	74, 78, 84, 85	0
2	A	306/306 (100%)	-0.11	2 (0%) 87 74	30, 48, 67, 79	0
2	B	306/306 (100%)	-0.02	4 (1%) 77 59	33, 59, 88, 99	0
2	C	306/306 (100%)	0.34	11 (3%) 42 26	45, 71, 92, 103	0
2	D	305/306 (99%)	0.21	9 (2%) 50 31	41, 65, 94, 108	0
All	All	1235/1236 (99%)	0.11	27 (2%) 62 42	30, 61, 90, 108	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	266	ALA	4.5
2	A	155	ASP	4.0
2	D	237	TYR	3.9
2	C	224	THR	3.7
2	D	154	TYR	3.6

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.