



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 09:03 PM UTC

PDB ID : 7LB7 / pdb_00007lb7
Title : Joint X-ray/neutron structure of SARS-CoV-2 main protease (3CL Mpro) in complex with Telaprevir
Authors : Kovalevsky, A.Y.; Kneller, D.W.; Coates, L.
Deposited on : 2021-01-07
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	FAILED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

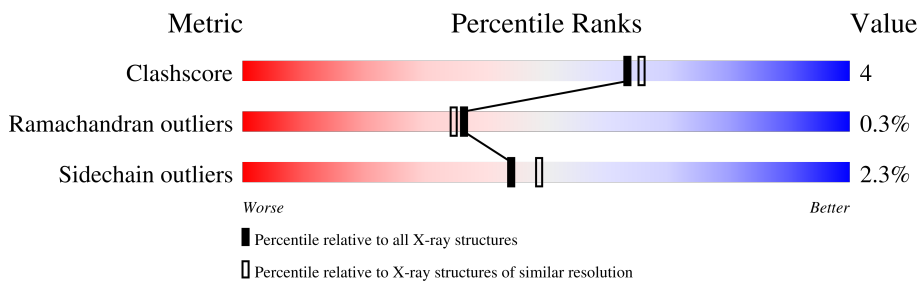
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION, NEUTRON DIFFRACTION

The reported resolution of this entry is 2.00 Å.

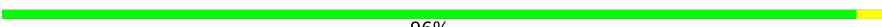
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	306	 96% .

2 Entry composition [i](#)

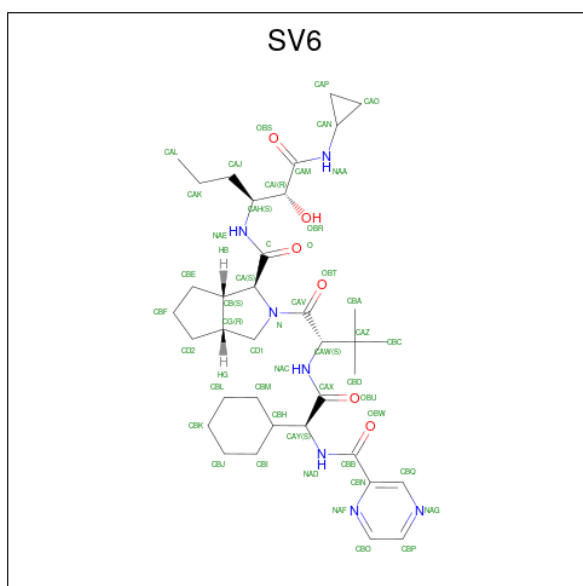
There are 3 unique types of molecules in this entry. The entry contains 6783 atoms, of which 1817 are hydrogens and 2454 are deuteriums.

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 3C-like proteinase.

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
			Total	C	D	H	N	O	S				
1	A	306	6395	1499	2259	1768	402	445	22		0	303	0

- Molecule 2 is (1S,3aR,6aS)-2-[(2S)-2-({(2S)-2-cyclohexyl-2-[(pyrazin-2-ylcarbonyl)amino]acetyl}amino)-3,3-dimethylbutanoyl]-N-[(2R,3S)-1-(cyclopropylamino)-2-hydroxy-1-oxohexan-3-yl]octahydrocyclopenta[c]pyrrole-1-carboxamide (CCD ID: SV6) (formula: C₃₆H₅₅N₇O₆).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	D	H	N	O		
2	A	1	103	36	5	49	7	6	0	0

- Molecule 3 is water.

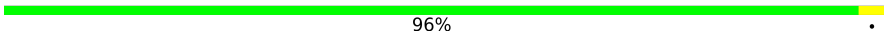
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	95	Total	D	O	0	0
			285	190	95		

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. 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. 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.

Note EDS failed to run properly.

- Molecule 1: 3C-like proteinase

Chain A:  96%



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	110.56Å 55.69Å 48.81Å 90.00° 101.31° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00	Depositor
% Data completeness (in resolution range)	97.5 (40.00-2.00)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	14.40 (at 2.00Å)	Xtriage
Refinement program	nCNS 1.0.0	Depositor
R, R_{free}	0.204 , 0.225	Depositor
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.169	Xtriage
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
Total number of atoms	6783	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.41% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SV6, DOD

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	A	0.54	0/4826	0.90	8/6557 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	182[A]	TYR	N-CA-C	-6.96	97.90	109.24
1	A	182[B]	TYR	N-CA-C	-6.96	97.90	109.24
1	A	45[A]	THR	N-CA-C	-5.76	101.93	110.46
1	A	45[B]	THR	N-CA-C	-5.76	101.93	110.46
1	A	165[A]	MET	N-CA-C	5.61	115.95	108.38
1	A	165[B]	MET	N-CA-C	5.61	115.95	108.38
1	A	176[A]	ASP	N-CA-C	-5.24	102.23	110.36
1	A	176[B]	ASP	N-CA-C	-5.24	102.23	110.36

There are no chirality outliers.

There are no planarity outliers.

CLOSE-CONTACTS INFOmissingINFO

5.2 Torsion angles [i](#)

5.2.1 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	A	605/306 (198%)	585 (97%)	18 (3%)	2 (0%)	36	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154[A]	TYR
1	A	154[B]	TYR

5.2.2 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	A	524/263 (199%)	512 (98%)	12 (2%)	44	49

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50[A]	LEU
1	A	50[B]	LEU
1	A	67[A]	LEU
1	A	67[B]	LEU
1	A	107[A]	GLN
1	A	107[B]	GLN
1	A	165[A]	MET
1	A	165[B]	MET
1	A	222[A]	ARG
1	A	222[B]	ARG
1	A	238[A]	ASN
1	A	238[B]	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.2.3 RNA ⓘ

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.4 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.5 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	SV6	A	401	1	53,53,53	1.28	4 (7%)	69,76,76	1.22	6 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SV6	A	401	1	-	8/57/89/89	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	SV6	CAH-NAE	4.33	1.53	1.46
2	A	401	SV6	OBT-CAV	2.76	1.27	1.22
2	A	401	SV6	CAW-CAV	2.30	1.57	1.53
2	A	401	SV6	CA-C	2.08	1.56	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	SV6	CAY-NAD-CBB	4.54	130.68	121.53
2	A	401	SV6	C-CA-N	-3.64	103.59	112.01
2	A	401	SV6	CAI-CAH-NAE	2.79	115.12	109.93
2	A	401	SV6	CA-C-NAE	2.78	120.60	115.59
2	A	401	SV6	CAI-CAM-NAA	-2.32	113.08	116.22
2	A	401	SV6	CB-CA-N	2.25	106.53	103.21

There are no chirality outliers.

All (8) torsion outliers are listed below:

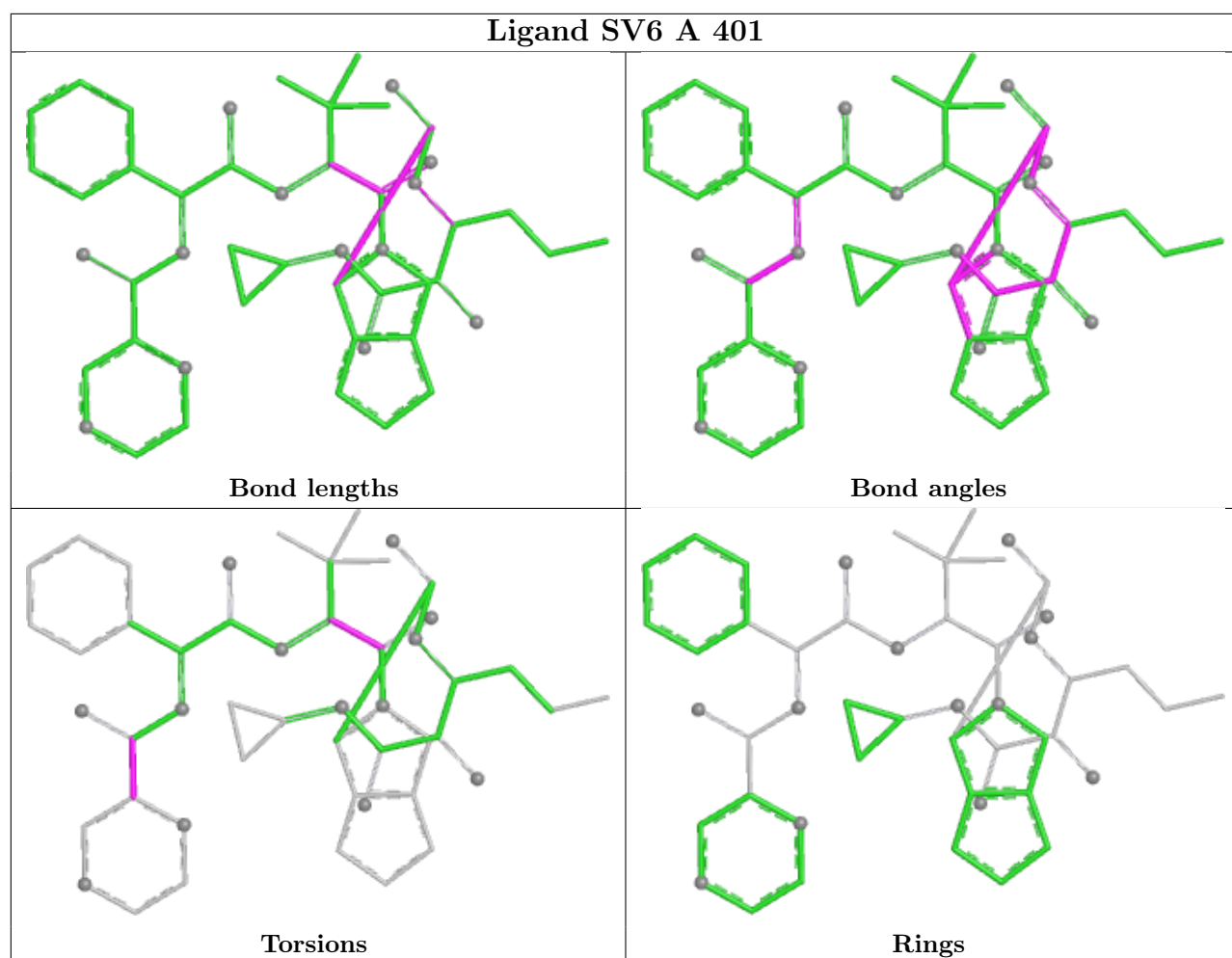
Mol	Chain	Res	Type	Atoms
2	A	401	SV6	OBW-CBB-CBN-NAF
2	A	401	SV6	NAD-CBB-CBN-NAF
2	A	401	SV6	OBW-CBB-CBN-CBQ
2	A	401	SV6	NAD-CBB-CBN-CBQ
2	A	401	SV6	N-CAV-CAW-NAC
2	A	401	SV6	N-CAV-CAW-CAZ
2	A	401	SV6	OBT-CAV-CAW-NAC
2	A	401	SV6	OBT-CAV-CAW-CAZ

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	SV6	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.6 Other polymers [i](#)

There are no such residues in this entry.

5.7 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.