



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 02:21 PM UTC

PDB ID : 7MBG / pdb_00007mbg
Title : SARS-CoV-2 Main protease in orthorhombic space group
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Deposited on : 2021-03-31
Resolution : 1.86 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 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 : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

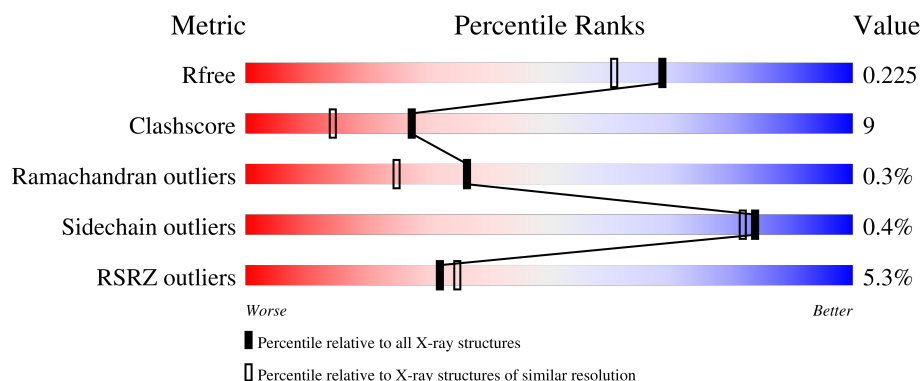
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	A	306	3% 83% 15% ..
1	B	306	7% 77% 20% ...

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5097 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 3C-like proteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	1	0
			2338	1480	397	438	23			
1	B	302	Total	C	N	O	S	0	2	0
			2350	1491	400	437	22			

- Molecule 2 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 1	S 1	0	0
2	A	1	Total 4	C 2	O 1	S 1	0	0
2	A	1	Total 4	C 2	O 1	S 1	0	0
2	B	1	Total 4	C 2	O 1	S 1	0	0
2	B	1	Total 4	C 2	O 1	S 1	0	0
2	B	1	Total 4	C 2	O 1	S 1	0	0
2	B	1	Total 4	C 2	O 1	S 1	0	0
2	B	1	Total 4	C 2	O 1	S 1	0	0
2	B	1	Total 4	C 2	O 1	S 1	0	0
2	B	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	215	Total 215	O 215	0	0
3	B	138	Total 138	O 138	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.25Å 98.16Å 102.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.19 – 1.86 56.19 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.4 (56.19-1.86) 99.4 (56.19-1.86)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 1.86Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.195 , 0.222 0.196 , 0.225	Depositor DCC
R_{free} test set	2918 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5097	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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: DMS

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	0.60	4/2393 (0.2%)	0.64	2/3251 (0.1%)
1	B	0.72	8/2408 (0.3%)	0.72	7/3270 (0.2%)
All	All	0.66	12/4801 (0.2%)	0.68	9/6521 (0.1%)

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	270[A]	GLU	CA-C	6.64	1.61	1.52
1	B	270[B]	GLU	CA-C	6.64	1.61	1.52
1	B	269	LYS	C-O	-6.42	1.16	1.24
1	B	138	GLY	C-O	-6.38	1.17	1.23
1	A	128	CYS	C-O	-6.28	1.15	1.23

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	270[A]	GLU	CA-C-O	9.04	130.39	120.63
1	B	270[B]	GLU	CA-C-O	9.04	130.39	120.63
1	B	54	TYR	N-CA-C	6.84	119.32	111.11
1	B	51	ASN	N-CA-C	-6.30	95.88	109.81
1	B	50	LEU	N-CA-C	6.15	121.56	113.20

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	A	2338	0	2290	33	0
1	B	2350	0	2306	50	0
2	A	28	0	42	6	0
2	B	28	0	42	9	0
3	A	215	0	0	12	0
3	B	138	0	0	16	0
All	All	5097	0	4680	86	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 9.

The worst 5 of 86 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)
1:B:298:ARG:HH11	2:B:401:DMS:H13	1.38	0.88
1:B:263:ASP:OD1	3:B:501:HOH:O	1.93	0.87
1:B:145:CYS:SG	3:B:583:HOH:O	2.33	0.85
1:B:102:LYS:NZ	1:B:156:CYS:SG	2.53	0.81
1:A:56:ASP:OD1	3:A:501:HOH:O	2.00	0.79

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	A	301/306 (98%)	296 (98%)	4 (1%)	1 (0%)	36	25
1	B	300/306 (98%)	293 (98%)	6 (2%)	1 (0%)	36	25
All	All	601/612 (98%)	589 (98%)	10 (2%)	2 (0%)	36	25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	49	MET
1	A	154	TYR

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	A	260/263 (99%)	260 (100%)	0	100	100
1	B	261/263 (99%)	259 (99%)	2 (1%)	73	67
All	All	521/526 (99%)	519 (100%)	2 (0%)	84	82

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	50	LEU
1	B	51	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	107	GLN
1	A	119	ASN
1	B	172	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 ligands are 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	DMS	A	402	-	3,3,3	0.73	0	3,3,3	0.43	0
2	DMS	A	407	-	3,3,3	0.77	0	3,3,3	0.55	0
2	DMS	B	407	-	3,3,3	0.77	0	3,3,3	0.45	0
2	DMS	A	405	-	3,3,3	0.75	0	3,3,3	0.60	0
2	DMS	B	403	-	3,3,3	0.79	0	3,3,3	0.81	0
2	DMS	B	402	-	3,3,3	0.74	0	3,3,3	0.50	0
2	DMS	B	405	-	3,3,3	0.70	0	3,3,3	0.55	0
2	DMS	B	406	-	3,3,3	0.64	0	3,3,3	0.29	0
2	DMS	A	404	-	3,3,3	0.63	0	3,3,3	0.67	0
2	DMS	A	403	-	3,3,3	0.73	0	3,3,3	0.52	0
2	DMS	A	406	-	3,3,3	0.68	0	3,3,3	0.69	0
2	DMS	A	401	-	3,3,3	0.66	0	3,3,3	0.46	0
2	DMS	B	401	-	3,3,3	0.63	0	3,3,3	0.61	0
2	DMS	B	404	-	3,3,3	0.67	0	3,3,3	0.57	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	403	DMS	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	405	DMS	1	0
2	B	406	DMS	3	0
2	A	406	DMS	3	0
2	A	401	DMS	3	0
2	B	401	DMS	3	0

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	A	302/306 (98%)	0.10	10 (3%) 49 53	20, 32, 52, 79	1 (0%)
1	B	302/306 (98%)	0.41	22 (7%) 21 23	22, 35, 67, 108	2 (0%)
All	All	604/612 (98%)	0.25	32 (5%) 32 35	20, 33, 59, 108	3 (0%)

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	305	PHE	5.2
1	B	59	ILE	4.8
1	B	50	LEU	4.6
1	A	154	TYR	4.0
1	B	154	TYR	3.9

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DMS	B	407	4/4	0.67	0.24	62,62,70,85	0
2	DMS	B	406	4/4	0.68	0.19	51,61,70,78	0
2	DMS	A	403	4/4	0.68	0.23	50,53,59,70	0
2	DMS	B	405	4/4	0.69	0.18	48,57,67,91	0
2	DMS	B	403	4/4	0.73	0.24	52,57,66,74	0
2	DMS	A	406	4/4	0.76	0.20	51,52,56,71	0
2	DMS	A	401	4/4	0.83	0.15	43,51,66,77	0
2	DMS	A	407	4/4	0.83	0.19	43,46,54,61	0
2	DMS	B	402	4/4	0.84	0.17	53,60,63,80	0
2	DMS	A	402	4/4	0.86	0.18	46,51,54,62	0
2	DMS	A	404	4/4	0.89	0.14	42,48,52,54	0
2	DMS	B	404	4/4	0.92	0.14	47,50,52,57	0
2	DMS	A	405	4/4	0.95	0.12	37,38,39,50	0
2	DMS	B	401	4/4	0.96	0.10	35,41,41,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.