



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:46 AM UTC

PDB ID : 7VK0 / pdb_00007vk0
Title : Crystal Structure of SARS-CoV-2 Mpro at 2.10 Å resolution-6
Authors : DeMirici, H.; Cakilkaya, B.
Deposited on : 2021-09-29
Resolution : 2.10 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
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

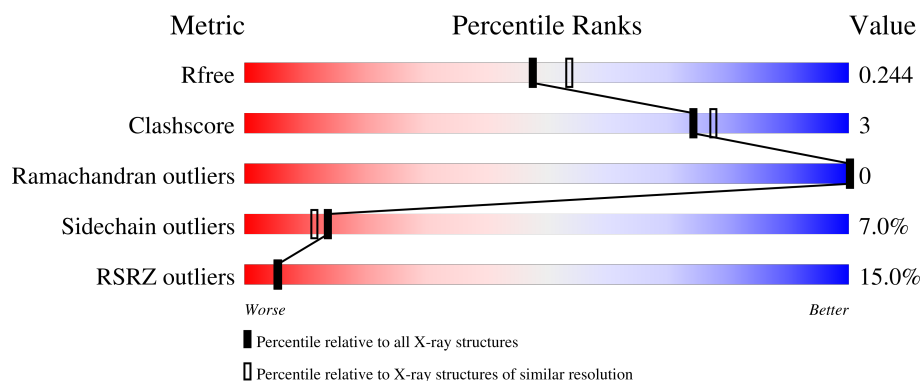
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	9% 87% 9% ..
1	B	306	20% 84% 12% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4746 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	300	Total	C	N	O	S	0	0	0
			2323	1471	395	435	22			
1	B	299	Total	C	N	O	S	0	0	0
			2319	1469	394	434	22			

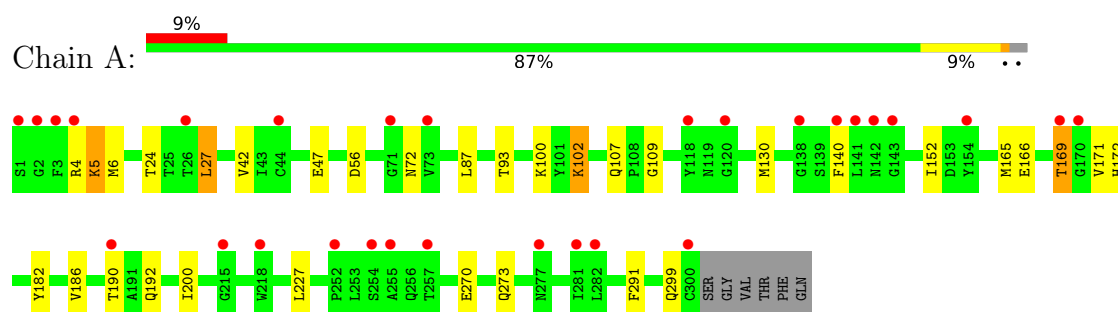
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	71	Total	O	0	0
			71	71		
2	B	33	Total	O	0	0
			33	33		

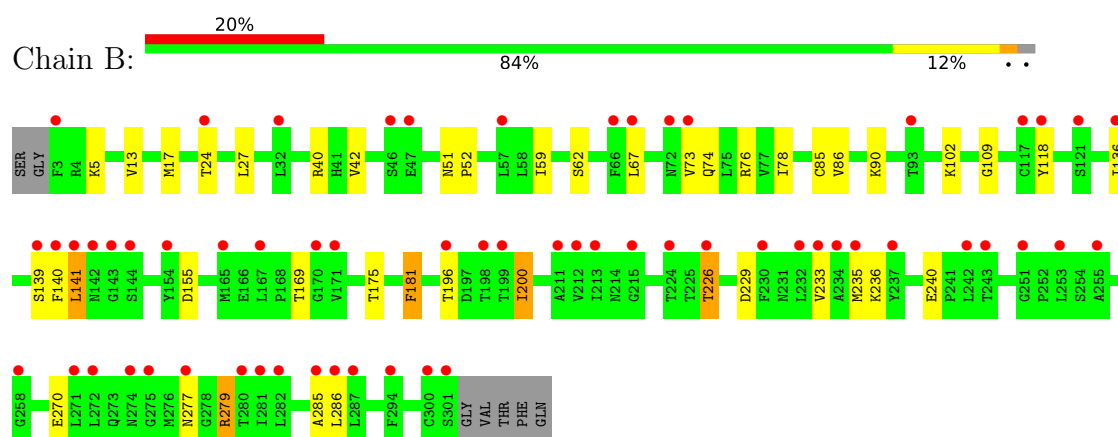
3 Residue-property plots [i](#)

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: 3C-like proteinase



• Molecule 1: 3C-like proteinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.20Å 104.30Å 105.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.77 – 2.10 46.77 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.77-2.10) 100.0 (46.77-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.237 , 0.242 0.239 , 0.244	Depositor DCC
R_{free} test set	2004 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å ²)	44.2	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 76.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.167 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4746	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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	A	0.77	1/2375 (0.0%)	1.10	3/3228 (0.1%)
1	B	0.79	0/2371	1.13	3/3223 (0.1%)
All	All	0.78	1/4746 (0.0%)	1.12	6/6451 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102	LYS	C-N	-6.83	1.23	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	285	ALA	N-CA-C	-6.48	105.41	113.38
1	B	52	PRO	N-CA-C	5.57	120.84	111.32
1	A	72	ASN	N-CA-C	-5.17	107.65	114.31
1	B	78	ILE	N-CA-C	-5.10	107.74	112.43
1	A	102	LYS	CA-C-N	5.03	130.09	123.05
1	A	102	LYS	C-N-CA	5.03	130.09	123.05

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	2323	0	2273	17	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2319	0	2267	11	1
2	A	71	0	0	5	0
2	B	33	0	0	1	0
All	All	4746	0	4540	28	1

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 3.

All (28) 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:A:56:ASP:OD1	2:A:401:HOH:O	1.93	0.85
1:A:169:THR:HG23	1:A:171:VAL:HG22	1.62	0.81
1:A:100:LYS:HE3	2:A:456:HOH:O	1.96	0.64
1:A:130:MET:HE1	1:A:182:TYR:HB3	1.80	0.62
1:A:299:GLN:NE2	2:A:402:HOH:O	2.36	0.56
1:B:13:VAL:HG12	1:B:17:MET:HE3	1.88	0.55
1:A:107:GLN:NE2	2:A:403:HOH:O	2.40	0.53
1:B:141:LEU:HA	2:B:422:HOH:O	2.07	0.53
1:A:190:THR:HG23	1:A:192:GLN:HG3	1.94	0.49
1:A:140:PHE:HB2	1:A:172:HIS:CE1	2.48	0.49
1:A:273:GLN:HB3	2:A:434:HOH:O	2.14	0.47
1:B:136:ILE:HD11	1:B:140:PHE:HE2	1.79	0.47
1:B:118:TYR:OH	1:B:141:LEU:HB2	2.14	0.47
1:A:5:LYS:HB2	1:A:5:LYS:HE3	1.78	0.46
1:A:270:GLU:HA	1:A:273:GLN:HG2	1.99	0.45
1:B:175:THR:HG22	1:B:181:PHE:HA	1.99	0.44
1:A:5:LYS:HG3	1:A:291:PHE:CZ	2.53	0.44
1:A:227:LEU:HD12	1:A:227:LEU:HA	1.89	0.44
1:A:27:LEU:HD21	1:A:42:VAL:HB	1.99	0.43
1:B:74:GLN:HB3	1:B:76:ARG:HH12	1.83	0.43
1:A:165:MET:HE3	1:A:165:MET:HB3	1.92	0.43
1:B:279:ARG:HE	1:B:279:ARG:HB2	1.34	0.42
1:A:186:VAL:H	1:A:192:GLN:NE2	2.17	0.42
1:B:27:LEU:HD21	1:B:42:VAL:HB	2.01	0.42
1:A:109:GLY:HA2	1:A:200:ILE:HD13	2.01	0.41
1:B:109:GLY:HA2	1:B:200:ILE:HD13	2.02	0.41
1:B:226:THR:HG22	1:B:229:ASP:HB2	2.03	0.40
1:B:40:ARG:HD3	1:B:85:CYS:HA	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LYS:NZ	1:B:270:GLU:OE1[3_554]	2.09	0.11

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	298/306 (97%)	290 (97%)	8 (3%)	0	100	100
1	B	297/306 (97%)	280 (94%)	17 (6%)	0	100	100
All	All	595/612 (97%)	570 (96%)	25 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	258/263 (98%)	247 (96%)	11 (4%)	26	27
1	B	258/263 (98%)	233 (90%)	25 (10%)	8	5
All	All	516/526 (98%)	480 (93%)	36 (7%)	14	11

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG

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Mol	Chain	Res	Type
1	A	5	LYS
1	A	6	MET
1	A	24	THR
1	A	27	LEU
1	A	47	GLU
1	A	87	LEU
1	A	93	THR
1	A	152	ILE
1	A	166	GLU
1	A	169	THR
1	B	5	LYS
1	B	24	THR
1	B	51	ASN
1	B	59	ILE
1	B	62	SER
1	B	67	LEU
1	B	73	VAL
1	B	86	VAL
1	B	90	LYS
1	B	102	LYS
1	B	139	SER
1	B	141	LEU
1	B	155	ASP
1	B	169	THR
1	B	181	PHE
1	B	196	THR
1	B	200	ILE
1	B	226	THR
1	B	233	VAL
1	B	235	MET
1	B	236	LYS
1	B	240	GLU
1	B	277	ASN
1	B	279	ARG
1	B	286	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	84	ASN
1	A	119	ASN

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Mol	Chain	Res	Type
1	A	142	ASN
1	A	172	HIS
1	A	180	ASN
1	A	192	GLN
1	A	299	GLN
1	B	72	ASN
1	B	83	GLN
1	B	107	GLN
1	B	163	HIS
1	B	256	GLN
1	B	274	ASN

5.3.3 RNA [i](#)

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 oligosaccharides 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

6.1 Protein, DNA and RNA chains

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	300/306 (98%)	0.82	29 (9%) 13 14	32, 51, 79, 107	0
1	B	299/306 (97%)	1.23	61 (20%) 3 3	34, 62, 95, 111	0
All	All	599/612 (97%)	1.02	90 (15%) 5 5	32, 55, 92, 111	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	140	PHE	5.1
1	B	232	LEU	4.7
1	B	253	LEU	4.2
1	A	3	PHE	3.6
1	A	118	TYR	3.6
1	B	141	LEU	3.6
1	B	287	LEU	3.5
1	B	142	ASN	3.5
1	A	140	PHE	3.4
1	B	251	GLY	3.4
1	B	275	GLY	3.4
1	B	143	GLY	3.3
1	B	212	VAL	3.3
1	A	252	PRO	3.2
1	B	118	TYR	3.2
1	A	281	ILE	3.2
1	B	139	SER	3.2
1	B	196	THR	3.2
1	B	242	LEU	3.2
1	A	141	LEU	3.1
1	B	67	LEU	3.1
1	B	215	GLY	3.0
1	B	47	GLU	2.9
1	A	170	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	255	ALA	2.9
1	B	258	GLY	2.9
1	A	215	GLY	2.8
1	B	170	GLY	2.8
1	B	136	ILE	2.8
1	B	46	SER	2.8
1	B	154	TYR	2.8
1	B	285	ALA	2.8
1	B	235	MET	2.7
1	B	3	PHE	2.7
1	B	199	THR	2.7
1	A	254	SER	2.7
1	B	117	CYS	2.7
1	A	143	GLY	2.7
1	A	71	GLY	2.6
1	B	226	THR	2.6
1	B	280	THR	2.6
1	A	1	SER	2.6
1	B	286	LEU	2.6
1	B	144	SER	2.6
1	A	257	THR	2.6
1	A	282	LEU	2.5
1	B	294	PHE	2.5
1	B	233	VAL	2.5
1	B	281	ILE	2.5
1	A	154	TYR	2.5
1	B	243	THR	2.5
1	B	255	ALA	2.5
1	B	230	PHE	2.5
1	B	167	LEU	2.4
1	B	271	LEU	2.3
1	B	274	ASN	2.3
1	B	300	CYS	2.3
1	B	234	ALA	2.3
1	A	73	VAL	2.3
1	B	171	VAL	2.3
1	A	44	CYS	2.3
1	A	300	CYS	2.3
1	B	237	TYR	2.3
1	B	73	VAL	2.2
1	A	142	ASN	2.2
1	A	190	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	57	LEU	2.2
1	B	121	SER	2.2
1	B	93	THR	2.2
1	B	224	THR	2.2
1	A	138	GLY	2.2
1	B	282	LEU	2.2
1	A	169	THR	2.2
1	B	165	MET	2.1
1	A	120	GLY	2.1
1	B	301	SER	2.1
1	B	72	ASN	2.1
1	B	277	ASN	2.1
1	A	26	THR	2.1
1	A	2	GLY	2.1
1	A	218	TRP	2.1
1	B	211	ALA	2.1
1	A	4	ARG	2.1
1	B	24	THR	2.1
1	B	213	ILE	2.1
1	A	277	ASN	2.0
1	B	66	PHE	2.0
1	B	32	LEU	2.0
1	B	272	LEU	2.0
1	B	198	THR	2.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.