



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 02:48 PM JST

PDB ID : 7VK8
Title : Crystal structure of SARS-CoV-2 Mpro at 2.4 Å Resolution
Authors : DeMirci, H.; Usta, G.
Deposited on : 2021-09-29
Resolution : 2.40 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

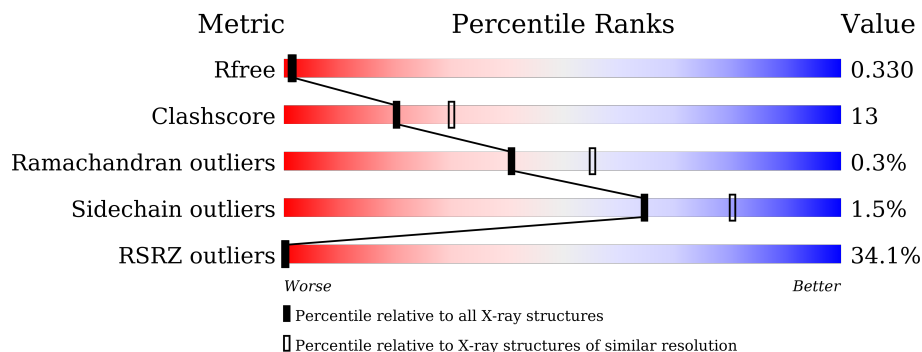
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2502 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
			Total	C	N	O	S			
1	A	305	2435	1536	415	460	24	15	10	0

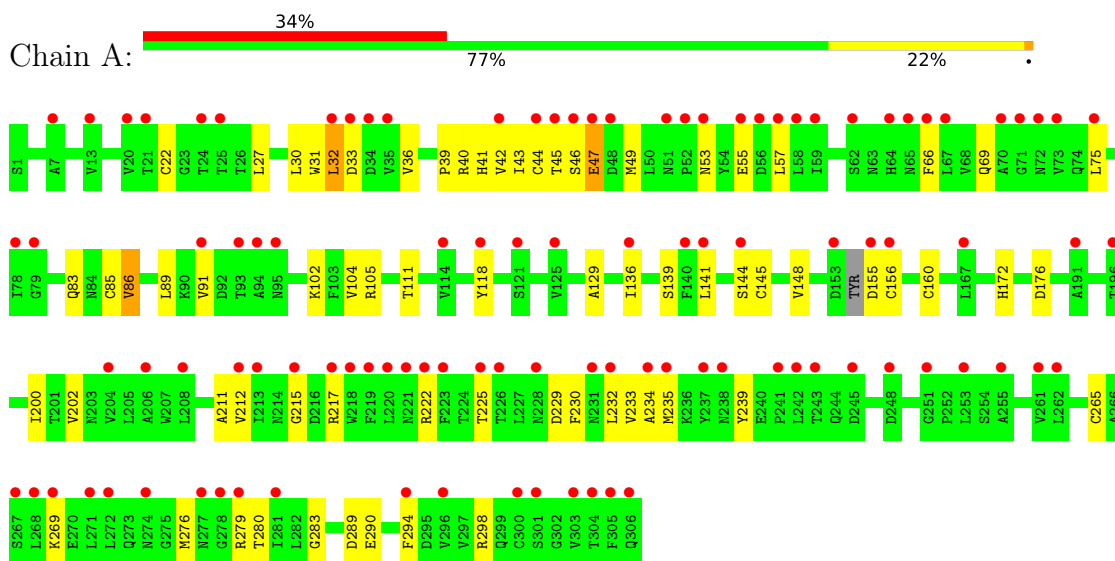
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	67	Total	O	0	0
			67	67		

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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	115.30Å 55.20Å 45.70Å 90.00° 101.30° 90.00°	Depositor
Resolution (Å)	31.92 – 2.40 31.92 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.0 (31.92-2.40) 99.0 (31.92-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.39Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.272 , 0.329 0.270 , 0.330	Depositor DCC
R_{free} test set	1103 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.7	Xtrriage
Anisotropy	0.145	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 97.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	2502	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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	0.31	0/2486	0.54	0/3374

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	A	2435	0	2372	60	0
2	A	67	0	0	25	2
All	All	2502	0	2372	60	2

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 13.

All (60) 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:49:MET:HG2	2:A:403:HOH:O	1.10	1.26
1:A:155:ASP:HA	2:A:414:HOH:O	1.53	1.09
1:A:49:MET:N	2:A:403:HOH:O	2.00	0.93
1:A:45:THR:OG1	2:A:401:HOH:O	1.88	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ASN:OD1	2:A:402:HOH:O	1.95	0.81
1:A:279:ARG:HE	1:A:280:THR:H	1.29	0.80
1:A:232:LEU:O	2:A:404:HOH:O	2.02	0.77
1:A:49:MET:CG	2:A:403:HOH:O	1.88	0.71
1:A:215:GLY:HA2	1:A:217:ARG:HH11	1.54	0.71
1:A:290:GLU:OE2	2:A:406:HOH:O	2.09	0.70
1:A:212:VAL:O	1:A:217:ARG:NH1	2.25	0.69
1:A:129:ALA:HB3	1:A:290:GLU:HG2	1.75	0.68
1:A:139:SER:O	2:A:408:HOH:O	2.14	0.65
1:A:283:GLY:O	2:A:409:HOH:O	2.15	0.65
1:A:202:VAL:N	2:A:405:HOH:O	2.07	0.64
1:A:75:LEU:HD23	1:A:91:VAL:HG21	1.80	0.62
1:A:111:THR:HG22	1:A:129:ALA:HB2	1.80	0.62
1:A:49:MET:CB	2:A:403:HOH:O	2.36	0.62
1:A:46[A]:SER:HB3	2:A:456:HOH:O	2.02	0.59
1:A:235:MET:HB3	2:A:404:HOH:O	2.03	0.58
1:A:145:CYS:SG	2:A:435:HOH:O	2.31	0.56
1:A:294:PHE:O	1:A:298:ARG:HG3	2.07	0.55
1:A:233:VAL:HG21	1:A:269:LYS:NZ	2.22	0.55
1:A:47[A]:GLU:N	2:A:401:HOH:O	2.42	0.53
1:A:31:TRP:CZ2	1:A:75:LEU:HD21	2.46	0.51
1:A:43:ILE:HG22	1:A:66:PHE:HE1	1.76	0.50
1:A:233:VAL:HG21	1:A:269:LYS:HZ3	1.76	0.50
1:A:105:ARG:NH1	1:A:176:ASP:OD2	2.44	0.50
1:A:46[B]:SER:HB2	2:A:456:HOH:O	2.11	0.50
1:A:47[B]:GLU:N	2:A:401:HOH:O	2.42	0.49
1:A:27:LEU:HD13	1:A:39:PRO:HD2	1.95	0.49
1:A:230:PHE:CD2	1:A:265:CYS:HB3	2.48	0.48
1:A:55[A]:GLU:N	2:A:402:HOH:O	2.46	0.48
1:A:234:ALA:HB1	1:A:239:TYR:HB2	1.95	0.48
1:A:276:MET:HB2	2:A:410:HOH:O	2.14	0.47
1:A:55[B]:GLU:N	2:A:402:HOH:O	2.47	0.47
1:A:118:TYR:CE2	1:A:141:LEU:HB2	2.50	0.47
1:A:69:GLN:OE1	2:A:413:HOH:O	2.20	0.47
1:A:104:VAL:HG23	1:A:160:CYS:HB3	1.97	0.47
1:A:129:ALA:CB	1:A:290:GLU:HG2	2.44	0.46
1:A:32:LEU:HD12	1:A:32:LEU:HA	1.80	0.46
1:A:141:LEU:O	1:A:144:SER:OG	2.27	0.46
1:A:279:ARG:NE	1:A:280:THR:H	2.07	0.46
1:A:102:LYS:HD3	1:A:156:CYS:SG	2.56	0.45
1:A:30:LEU:HD13	1:A:148:VAL:HG11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ASN:C	2:A:402:HOH:O	2.55	0.45
1:A:200:ILE:HB	1:A:289:ASP:HB2	1.99	0.44
1:A:118:TYR:HE2	1:A:141:LEU:HB2	1.83	0.44
1:A:136:ILE:HG13	1:A:172:HIS:HB2	2.00	0.43
1:A:83:GLN:HB3	1:A:86:VAL:HG12	2.00	0.43
1:A:49:MET:CA	2:A:403:HOH:O	2.40	0.43
1:A:40:ARG:HD3	1:A:85:CYS:HA	1.99	0.43
1:A:22:CYS:SG	1:A:43:ILE:HA	2.59	0.43
1:A:43:ILE:HD12	1:A:57:LEU:HB3	2.01	0.43
1:A:211:ALA:O	1:A:215:GLY:N	2.52	0.42
1:A:22:CYS:HB3	1:A:42:VAL:HG22	2.01	0.42
1:A:41:HIS:O	1:A:44:CYS:HB2	2.20	0.42
1:A:36:VAL:HB	1:A:89:LEU:HB2	2.02	0.41
1:A:298:ARG:NH1	2:A:420:HOH:O	2.49	0.41
1:A:225:THR:OG1	1:A:229:ASP:HB3	2.21	0.41

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:453:HOH:O	2:A:457:HOH:O[1_556]	1.83	0.37
2:A:439:HOH:O	2:A:447:HOH:O[4_555]	2.05	0.15

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	311/306 (102%)	295 (95%)	15 (5%)	1 (0%)	41 55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	ASP

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	272/263 (103%)	266 (98%)	6 (2%)	52 71

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	47[A]	GLU
1	A	47[B]	GLU
1	A	86	VAL
1	A	222[A]	ARG
1	A	222[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	273	GLN

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 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

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	305/306 (99%)	1.71	104 (34%) 0 0	9, 30, 54, 68	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	222[A]	ARG	6.4
1	A	234	ALA	6.0
1	A	153	ASP	5.1
1	A	95	ASN	5.1
1	A	232	LEU	5.0
1	A	46[A]	SER	4.8
1	A	226	THR	4.8
1	A	72	ASN	4.5
1	A	24	THR	4.5
1	A	220	LEU	4.5
1	A	238	ASN	4.4
1	A	305	PHE	4.2
1	A	21	THR	4.1
1	A	228	ASN	4.1
1	A	45	THR	4.0
1	A	303	VAL	3.9
1	A	67	LEU	3.9
1	A	58	LEU	3.8
1	A	274	ASN	3.8
1	A	223	PHE	3.7
1	A	59	ILE	3.7
1	A	304	THR	3.7
1	A	306	GLN	3.6
1	A	221	ASN	3.6
1	A	65[A]	ASN	3.6
1	A	48	ASP	3.5
1	A	155	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	277	ASN	3.5
1	A	278	GLY	3.5
1	A	79	GLY	3.4
1	A	167	LEU	3.2
1	A	237	TYR	3.2
1	A	212	VAL	3.2
1	A	42	VAL	3.1
1	A	191	ALA	3.0
1	A	217	ARG	2.9
1	A	57	LEU	2.9
1	A	269	LYS	2.9
1	A	62	SER	2.9
1	A	196	THR	2.9
1	A	141	LEU	2.8
1	A	114	VAL	2.8
1	A	262[A]	LEU	2.8
1	A	64	HIS	2.8
1	A	300	CYS	2.7
1	A	235	MET	2.7
1	A	294	PHE	2.7
1	A	71	GLY	2.7
1	A	245	ASP	2.7
1	A	156	CYS	2.6
1	A	51	ASN	2.6
1	A	53	ASN	2.6
1	A	91	VAL	2.6
1	A	225	THR	2.6
1	A	25	THR	2.6
1	A	70	ALA	2.6
1	A	34	ASP	2.6
1	A	94	ALA	2.6
1	A	66	PHE	2.6
1	A	219	PHE	2.6
1	A	268	LEU	2.6
1	A	231	ASN	2.6
1	A	118	TYR	2.6
1	A	144	SER	2.5
1	A	301[A]	SER	2.5
1	A	56	ASP	2.5
1	A	261	VAL	2.5
1	A	296	VAL	2.4
1	A	121	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	267	SER	2.4
1	A	279	ARG	2.4
1	A	272	LEU	2.4
1	A	35	VAL	2.4
1	A	78	ILE	2.4
1	A	213	ILE	2.4
1	A	44	CYS	2.4
1	A	13	VAL	2.4
1	A	32	LEU	2.4
1	A	75	LEU	2.3
1	A	255	ALA	2.3
1	A	204	VAL	2.3
1	A	136	ILE	2.3
1	A	253	LEU	2.3
1	A	248	ASP	2.3
1	A	52	PRO	2.3
1	A	55[A]	GLU	2.3
1	A	251	GLY	2.3
1	A	73	VAL	2.2
1	A	281	ILE	2.2
1	A	93	THR	2.2
1	A	215	GLY	2.2
1	A	47[A]	GLU	2.2
1	A	242	LEU	2.2
1	A	208	LEU	2.2
1	A	7	ALA	2.1
1	A	33	ASP	2.1
1	A	206	ALA	2.1
1	A	241	PRO	2.1
1	A	271	LEU	2.1
1	A	20	VAL	2.0
1	A	125	VAL	2.0
1	A	218	TRP	2.0
1	A	243	THR	2.0
1	A	140	PHE	2.0

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

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.