



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2024 – 02:03 PM EDT

PDB ID : 8TQU
Title : MPI51 bound to Mpro of SARS-CoV-2
Authors : Blankenship, L.R.; Liu, W.R.
Deposited on : 2023-08-08
Resolution : 1.85 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.37.1
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) : 2.37.1

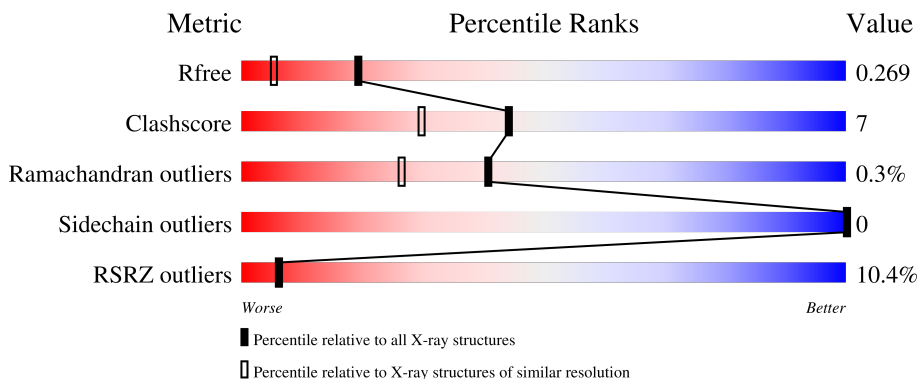
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

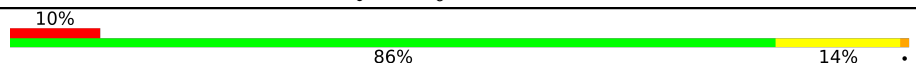

The reported resolution of this entry is 1.85 Å.

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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (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	
2	B	3	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2582 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 nsp5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	306	2363	1497	402	442	22	0	0	0

- Molecule 2 is a protein called UAW247.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	3	32	24	3	5	0	0	0

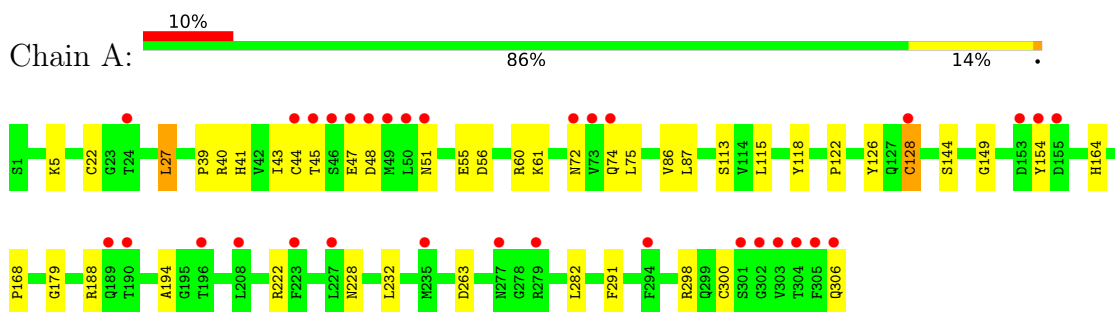
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	186	186	186	0	0
3	B	1	1	1	0	0

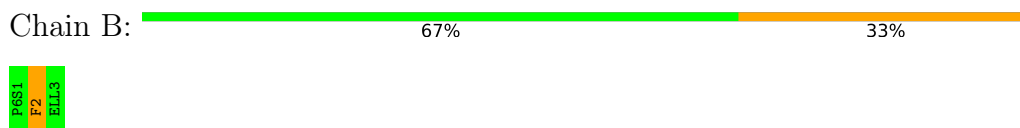
3 Residue-property plots [i](#)

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 nsp5



- Molecule 2: UAW247



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	54.55Å 81.10Å 86.91Å 90.00° 97.31° 90.00°	Depositor
Resolution (Å)	24.18 – 1.85 24.35 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.1 (24.18-1.85) 99.1 (24.35-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 1.85Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.235 , 0.269 0.235 , 0.269	Depositor DCC
R_{free} test set	1558 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtrriage
Anisotropy	0.380	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2582	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.49% 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: P6S, ELL

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	0.48	1/2416 (0.0%)	0.71	4/3284 (0.1%)
2	B	6.18	6/11 (54.5%)	8.03	7/13 (53.8%)
All	All	0.63	7/2427 (0.3%)	0.87	11/3297 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	PHE	CG-CD2	9.70	1.53	1.38
2	B	2	PHE	CG-CD1	9.50	1.52	1.38
2	B	2	PHE	CE1-CZ	8.32	1.53	1.37
2	B	2	PHE	CE2-CZ	7.99	1.52	1.37
2	B	2	PHE	CD2-CE2	7.11	1.53	1.39
2	B	2	PHE	CD1-CE1	7.00	1.53	1.39
1	A	128	CYS	CB-SG	-5.89	1.72	1.81

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	PHE	CB-CG-CD1	-15.65	109.84	120.80
2	B	2	PHE	CB-CG-CD2	-14.99	110.31	120.80
2	B	2	PHE	CG-CD1-CE1	-9.61	110.23	120.80
2	B	2	PHE	CG-CD2-CE2	-8.93	110.98	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	PHE	CD1-CE1-CZ	-8.71	109.65	120.10
1	A	222	ARG	NE-CZ-NH1	-7.86	116.37	120.30
2	B	2	PHE	CD1-CG-CD2	-7.01	109.18	118.30
2	B	2	PHE	CZ-CE2-CD2	-6.79	111.95	120.10
1	A	27	LEU	CB-CG-CD2	-6.58	99.81	111.00
1	A	27	LEU	CB-CG-CD1	5.77	120.81	111.00
1	A	87	LEU	CA-CB-CG	5.28	127.43	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	2	PHE	Sidechain

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	2363	0	2309	31	0
2	B	32	0	8	0	0
3	A	186	0	0	11	1
3	B	1	0	0	0	0
All	All	2582	0	2317	31	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 7.

All (31) 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:44:CYS:SG	3:A:542:HOH:O	2.02	1.17
1:A:55:GLU:OE2	3:A:401:HOH:O	1.84	0.95
1:A:306:GLN:NE2	3:A:405:HOH:O	2.16	0.77
1:A:194:ALA:O	3:A:402:HOH:O	2.05	0.75
1:A:300:CYS:O	3:A:403:HOH:O	2.10	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ARG:NH1	3:A:411:HOH:O	2.28	0.67
1:A:75:LEU:O	3:A:404:HOH:O	2.14	0.66
1:A:115:LEU:HD11	1:A:122:PRO:HB3	1.77	0.66
1:A:27:LEU:HD13	1:A:39:PRO:HD2	1.80	0.63
1:A:45:THR:H	1:A:48:ASP:HB2	1.62	0.62
1:A:22:CYS:SG	1:A:61:LYS:NZ	2.65	0.61
1:A:51:ASN:OD1	1:A:188:ARG:HD3	2.03	0.58
1:A:22:CYS:HG	1:A:61:LYS:HZ1	1.47	0.57
1:A:86:VAL:HG13	1:A:179:GLY:HA2	1.88	0.54
1:A:74:GLN:NE2	3:A:404:HOH:O	2.40	0.54
1:A:126:TYR:HE1	1:A:128:CYS:SG	2.32	0.52
1:A:5:LYS:HE2	3:A:436:HOH:O	2.13	0.48
1:A:263:ASP:OD2	3:A:407:HOH:O	2.20	0.48
1:A:168:PRO:HA	3:A:564:HOH:O	2.13	0.47
1:A:5:LYS:HG3	1:A:291:PHE:CZ	2.51	0.46
1:A:47:GLU:OE1	1:A:47:GLU:N	2.46	0.44
1:A:72:ASN:OD1	1:A:72:ASN:N	2.50	0.44
1:A:118:TYR:CE1	1:A:144:SER:HB3	2.53	0.44
1:A:56:ASP:O	1:A:60:ARG:HG3	2.18	0.43
1:A:40:ARG:O	1:A:43:ILE:HG12	2.18	0.43
1:A:228:ASN:O	1:A:232:LEU:HD23	2.19	0.43
1:A:41:HIS:O	1:A:44:CYS:HB2	2.20	0.41
1:A:39:PRO:HB3	1:A:164:HIS:CE1	2.56	0.41
1:A:113:SER:O	1:A:149:GLY:HA2	2.20	0.41
1:A:282:LEU:HD23	1:A:282:LEU:HA	1.82	0.41
1:A:86:VAL:HG13	1:A:179:GLY:CA	2.51	0.40

All (1) 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)
3:A:570:HOH:O	3:A:570:HOH:O[2_455]	1.80	0.40

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	304/306 (99%)	297 (98%)	6 (2%)	1 (0%)	41	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	TYR

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	262/263 (100%)	262 (100%)	0	100	100
2	B	1/1 (100%)	1 (100%)	0	100	100
All	All	263/264 (100%)	263 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	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	306/306 (100%)	0.72	32 (10%) 6 6	11, 28, 50, 78	0
2	B	1/3 (33%)	-0.03	0 100 100	27, 27, 27, 27	0
All	All	307/309 (99%)	0.72	32 (10%) 6 6	11, 28, 50, 78	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	50	LEU	13.1
1	A	306	GLN	7.2
1	A	72	ASN	6.1
1	A	46	SER	6.0
1	A	305	PHE	5.8
1	A	154	TYR	5.8
1	A	304	THR	5.7
1	A	303	VAL	5.5
1	A	223	PHE	5.5
1	A	45	THR	4.6
1	A	48	ASP	4.5
1	A	47	GLU	4.3
1	A	49	MET	4.2
1	A	44	CYS	4.0
1	A	302	GLY	3.1
1	A	301	SER	3.0
1	A	189	GLN	3.0
1	A	196	THR	3.0
1	A	51	ASN	3.0
1	A	294	PHE	2.9
1	A	153	ASP	2.8
1	A	227	LEU	2.7
1	A	74	GLN	2.6
1	A	277	ASN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	155	ASP	2.6
1	A	235	MET	2.5
1	A	190	THR	2.4
1	A	73	VAL	2.4
1	A	128	CYS	2.3
1	A	24	THR	2.2
1	A	279	ARG	2.1
1	A	208	LEU	2.1

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.