



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2025 – 08:03 AM EDT

PDB ID : 5S74 / pdb_00005s74
Title : PanDDA analysis group deposition of ground-state model of SARS-CoV-2 Nsp3 macrodomain
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Deposited on : 2020-11-23
Resolution : 0.96 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	:	NOT EXECUTED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

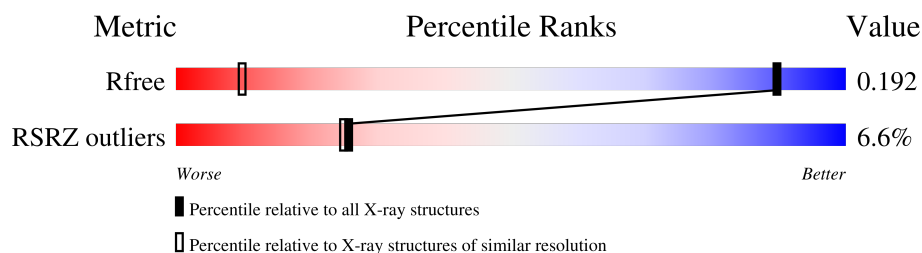
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 0.96 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}	164625	1192 (1.02-0.90)
RSRZ outliers	164620	1191 (1.02-0.90)

MolProbity was not executed - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2967 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.

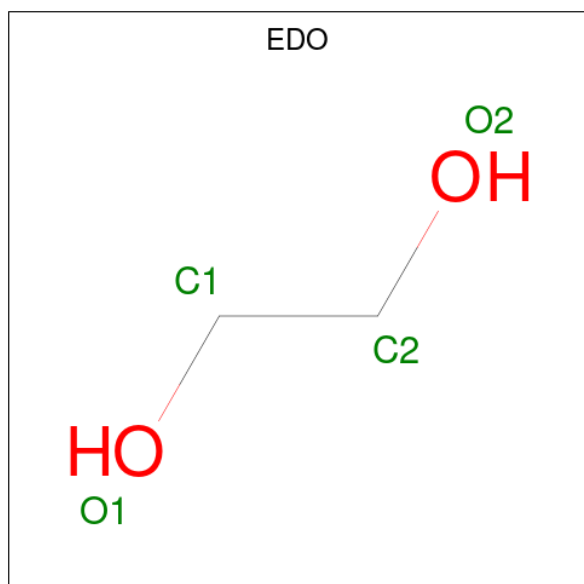
- Molecule 1 is a protein called Non-structural protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	8	0
			1302	829	221	248	4			
1	B	169	Total	C	N	O	S	0	4	0
			1303	826	223	249	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP P0DTD1
A	2	MET	-	expression tag	UNP P0DTD1
B	1	SER	-	expression tag	UNP P0DTD1
B	2	MET	-	expression tag	UNP P0DTD1

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	172	Total O 172 172	0	0
3	B	166	Total O 166 166	0	0

MolProbity was not executed - this section is therefore empty.

3 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	87.88Å 87.88Å 38.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.22 – 0.96 62.22 – 0.96	Depositor EDS
% Data completeness (in resolution range)	81.8 (62.22-0.96) 81.8 (62.22-0.96)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 0.96Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.176 , 0.185 0.182 , 0.192	Depositor DCC
R_{free} test set	8615 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	10.4	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 32.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	2967	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.31% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity was not executed - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity was not executed - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

MolProbity was not executed - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity was not executed - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

validation-pack was not executed - this section is therefore empty.

4.5 Carbohydrates [i](#)

validation-pack was not executed - this section is therefore empty.

4.6 Ligand geometry [i](#)

validation-pack was not executed - this section is therefore empty.

4.7 Other polymers [i](#)

validation-pack was not executed - this section is therefore empty.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 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	165/169 (97%)	0.41	7 (4%)	41	42	5, 10, 21, 40	8 (4%)
1	B	169/169 (100%)	0.54	15 (8%)	17	15	7, 11, 22, 36	4 (2%)
All	All	334/338 (98%)	0.48	22 (6%)	26	25	5, 10, 23, 40	12 (3%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	169	LEU	9.8
1	A	5	SER	5.5
1	A	156	PHE	4.2
1	B	103	GLY	3.5
1	B	166	SER	3.4
1	B	100	VAL	3.1
1	B	102	LYS	3.1
1	B	159	ASN	2.8
1	B	106	ILE	2.7
1	B	168	PHE	2.6
1	B	167	SER	2.5
1	A	7	SER	2.5
1	B	7[A]	SER	2.4
1	B	3	VAL	2.4
1	B	158	LYS	2.4
1	A	107	GLN	2.3
1	B	141	ARG	2.3
1	B	107	GLN	2.3
1	A	30	VAL	2.3
1	B	2	MET	2.3
1	B	104	GLU	2.2
1	A	10	LEU	2.1

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 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(\AA^2)	Q<0.9
2	EDO	B	303	4/4	0.61	0.28	20,33,35,40	0
2	EDO	A	302	4/4	0.65	0.28	48,50,51,51	0
2	EDO	B	302	4/4	0.68	0.24	40,45,46,47	0
2	EDO	A	301	4/4	0.75	0.26	47,48,50,50	0
2	EDO	B	301	4/4	0.80	0.15	20,29,29,33	0
2	EDO	B	304	4/4	0.83	0.14	21,26,29,32	0

5.5 Other polymers [i](#)

There are no such residues in this entry.