



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 08:08 AM EDT

PDB ID : 6W01
Title : The 1.9 Å Crystal Structure of NSP15 Endoribonuclease from SARS CoV-2 in the Complex with a Citrate
Authors : Kim, Y.; Jedrzejczak, R.; Maltseva, N.; Endres, M.; Godzik, A.; Michalska, K.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2020-02-28
Resolution : 1.90 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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : **FAILED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

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 1.90 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 6253 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 Uridylate-specific endoribonuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	347	2808	1802	456	538	12	0	9	0
1	B	347	2791	1791	455	533	12	0	7	0

There are 48 discrepancies between the modelled and reference sequences:

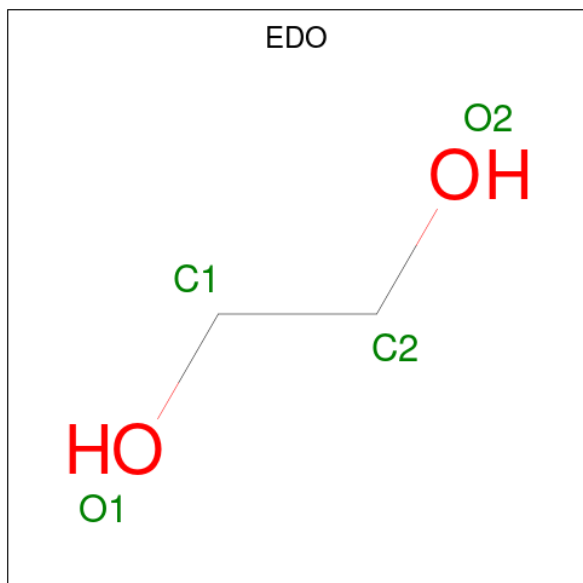
Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP P0DTD1
A	-21	HIS	-	expression tag	UNP P0DTD1
A	-20	HIS	-	expression tag	UNP P0DTD1
A	-19	HIS	-	expression tag	UNP P0DTD1
A	-18	HIS	-	expression tag	UNP P0DTD1
A	-17	HIS	-	expression tag	UNP P0DTD1
A	-16	HIS	-	expression tag	UNP P0DTD1
A	-15	SER	-	expression tag	UNP P0DTD1
A	-14	SER	-	expression tag	UNP P0DTD1
A	-13	GLY	-	expression tag	UNP P0DTD1
A	-12	VAL	-	expression tag	UNP P0DTD1
A	-11	ASP	-	expression tag	UNP P0DTD1
A	-10	LEU	-	expression tag	UNP P0DTD1
A	-9	GLY	-	expression tag	UNP P0DTD1
A	-8	THR	-	expression tag	UNP P0DTD1
A	-7	GLU	-	expression tag	UNP P0DTD1
A	-6	ASN	-	expression tag	UNP P0DTD1
A	-5	LEU	-	expression tag	UNP P0DTD1
A	-4	TYR	-	expression tag	UNP P0DTD1
A	-3	PHE	-	expression tag	UNP P0DTD1
A	-2	GLN	-	expression tag	UNP P0DTD1
A	-1	SER	-	expression tag	UNP P0DTD1
A	0	ASN	-	expression tag	UNP P0DTD1
A	1	MET	-	expression tag	UNP P0DTD1
B	-22	MET	-	initiating methionine	UNP P0DTD1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-21	HIS	-	expression tag	UNP P0DTD1
B	-20	HIS	-	expression tag	UNP P0DTD1
B	-19	HIS	-	expression tag	UNP P0DTD1
B	-18	HIS	-	expression tag	UNP P0DTD1
B	-17	HIS	-	expression tag	UNP P0DTD1
B	-16	HIS	-	expression tag	UNP P0DTD1
B	-15	SER	-	expression tag	UNP P0DTD1
B	-14	SER	-	expression tag	UNP P0DTD1
B	-13	GLY	-	expression tag	UNP P0DTD1
B	-12	VAL	-	expression tag	UNP P0DTD1
B	-11	ASP	-	expression tag	UNP P0DTD1
B	-10	LEU	-	expression tag	UNP P0DTD1
B	-9	GLY	-	expression tag	UNP P0DTD1
B	-8	THR	-	expression tag	UNP P0DTD1
B	-7	GLU	-	expression tag	UNP P0DTD1
B	-6	ASN	-	expression tag	UNP P0DTD1
B	-5	LEU	-	expression tag	UNP P0DTD1
B	-4	TYR	-	expression tag	UNP P0DTD1
B	-3	PHE	-	expression tag	UNP P0DTD1
B	-2	GLN	-	expression tag	UNP P0DTD1
B	-1	SER	-	expression tag	UNP P0DTD1
B	0	ASN	-	expression tag	UNP P0DTD1
B	1	MET	-	expression tag	UNP P0DTD1

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



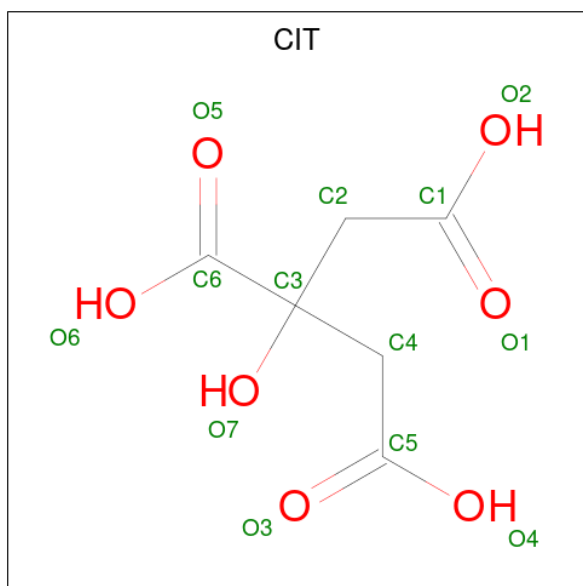
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
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
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
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 DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		
4	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	259	Total	O	0	0
			259	259		
5	B	260	Total	O	0	0
			260	260		

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics i

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	150.78Å 150.78Å 111.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.87 – 1.90	Depositor
% Data completeness (in resolution range)	98.7 (44.87-1.90)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 1.91Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.161 , 0.185	Depositor
Wilson B-factor (Å ²)	31.5	Xtrriage
Anisotropy	0.302	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.060 for h,-h-k,-l	Xtrriage
Total number of atoms	6253	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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 failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

27 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
3	PEG	A	406	-	6,6,6	0.11	0	5,5,5	0.21	0
2	EDO	A	404	-	3,3,3	0.56	0	2,2,2	0.38	0
2	EDO	B	410	-	3,3,3	0.51	0	2,2,2	0.13	0
2	EDO	A	410	-	3,3,3	0.41	0	2,2,2	0.59	0
2	EDO	A	402	-	3,3,3	0.70	0	2,2,2	0.37	0
2	EDO	A	409	-	3,3,3	0.47	0	2,2,2	0.46	0
2	EDO	A	414	-	3,3,3	0.54	0	2,2,2	0.11	0
3	PEG	A	405	-	6,6,6	0.23	0	5,5,5	0.14	0
2	EDO	B	412	-	3,3,3	0.53	0	2,2,2	0.26	0
4	CIT	B	408	-	12,12,12	0.99	0	17,17,17	1.78	4 (23%)
2	EDO	A	401	-	3,3,3	0.33	0	2,2,2	0.77	0
2	EDO	B	405	-	3,3,3	0.46	0	2,2,2	0.32	0
3	PEG	B	411	-	6,6,6	0.18	0	5,5,5	0.15	0
2	EDO	A	403	-	3,3,3	0.39	0	2,2,2	0.39	0
2	EDO	A	408	-	3,3,3	0.35	0	2,2,2	0.58	0
2	EDO	B	404	-	3,3,3	0.48	0	2,2,2	0.22	0
2	EDO	B	407	-	3,3,3	0.58	0	2,2,2	0.16	0
2	EDO	A	407	-	3,3,3	0.47	0	2,2,2	0.24	0
2	EDO	B	406	-	3,3,3	0.44	0	2,2,2	0.43	0
2	EDO	B	402	-	3,3,3	0.61	0	2,2,2	0.39	0
2	EDO	B	409	-	3,3,3	0.48	0	2,2,2	0.53	0
2	EDO	A	411	-	3,3,3	0.53	0	2,2,2	0.21	0
2	EDO	B	413	-	3,3,3	0.41	0	2,2,2	0.61	0
2	EDO	A	413	-	3,3,3	0.58	0	2,2,2	0.21	0
2	EDO	B	403	-	3,3,3	0.57	0	2,2,2	0.47	0
4	CIT	A	412	-	12,12,12	1.13	0	17,17,17	2.17	7 (41%)
2	EDO	B	401	-	3,3,3	0.71	0	2,2,2	0.10	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	A	406	-	-	0/4/4/4	-
2	EDO	A	404	-	-	0/1/1/1	-
2	EDO	B	410	-	-	0/1/1/1	-
2	EDO	A	410	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	402	-	-	1/1/1/1	-
2	EDO	A	409	-	-	0/1/1/1	-
2	EDO	A	414	-	-	1/1/1/1	-
3	PEG	A	405	-	-	2/4/4/4	-
2	EDO	B	412	-	-	0/1/1/1	-
4	CIT	B	408	-	-	0/16/16/16	-
2	EDO	A	401	-	-	0/1/1/1	-
2	EDO	B	405	-	-	1/1/1/1	-
3	PEG	B	411	-	-	2/4/4/4	-
2	EDO	A	403	-	-	1/1/1/1	-
2	EDO	A	408	-	-	0/1/1/1	-
2	EDO	B	404	-	-	0/1/1/1	-
2	EDO	B	407	-	-	1/1/1/1	-
2	EDO	A	407	-	-	1/1/1/1	-
2	EDO	B	406	-	-	0/1/1/1	-
2	EDO	B	402	-	-	1/1/1/1	-
2	EDO	B	409	-	-	0/1/1/1	-
2	EDO	A	411	-	-	0/1/1/1	-
2	EDO	B	413	-	-	1/1/1/1	-
2	EDO	A	413	-	-	1/1/1/1	-
2	EDO	B	403	-	-	0/1/1/1	-
4	CIT	A	412	-	-	7/16/16/16	-
2	EDO	B	401	-	-	1/1/1/1	-

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	412	CIT	O6-C6-C3	5.55	122.69	113.05
4	B	408	CIT	O6-C6-C3	4.50	120.86	113.05
4	A	412	CIT	O5-C6-C3	-3.37	117.47	122.25
4	A	412	CIT	C4-C3-C6	-2.88	103.91	110.11
4	A	412	CIT	C3-C4-C5	-2.77	107.10	113.81
4	A	412	CIT	C2-C3-C6	2.35	115.16	110.11
4	B	408	CIT	O2-C1-O1	-2.26	117.66	123.30
4	B	408	CIT	O2-C1-C2	2.20	121.40	114.35
4	A	412	CIT	O2-C1-C2	2.08	121.03	114.35
4	B	408	CIT	C3-C4-C5	-2.04	108.88	113.81
4	A	412	CIT	O2-C1-O1	-2.00	118.31	123.30

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	405	PEG	O1-C1-C2-O2
2	A	407	EDO	O1-C1-C2-O2
2	A	413	EDO	O1-C1-C2-O2
2	B	407	EDO	O1-C1-C2-O2
2	B	413	EDO	O1-C1-C2-O2
3	A	405	PEG	O2-C3-C4-O4
3	B	411	PEG	O2-C3-C4-O4
4	A	412	CIT	O1-C1-C2-C3
4	A	412	CIT	O2-C1-C2-C3
2	B	401	EDO	O1-C1-C2-O2
4	A	412	CIT	C4-C3-C6-O5
2	A	402	EDO	O1-C1-C2-O2
3	B	411	PEG	C4-C3-O2-C2
4	A	412	CIT	C2-C3-C6-O5
4	A	412	CIT	C4-C3-C6-O6
2	A	403	EDO	O1-C1-C2-O2
2	B	405	EDO	O1-C1-C2-O2
2	A	414	EDO	O1-C1-C2-O2
4	A	412	CIT	C3-C4-C5-O3
2	B	402	EDO	O1-C1-C2-O2
4	A	412	CIT	C3-C4-C5-O4

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.