



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 7KEG
Title : Crystal structure from SARS-COV2 NendoU NSP15
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Deposited on : 2020-10-10
Resolution : 2.90 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 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)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
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) : 2.14.6

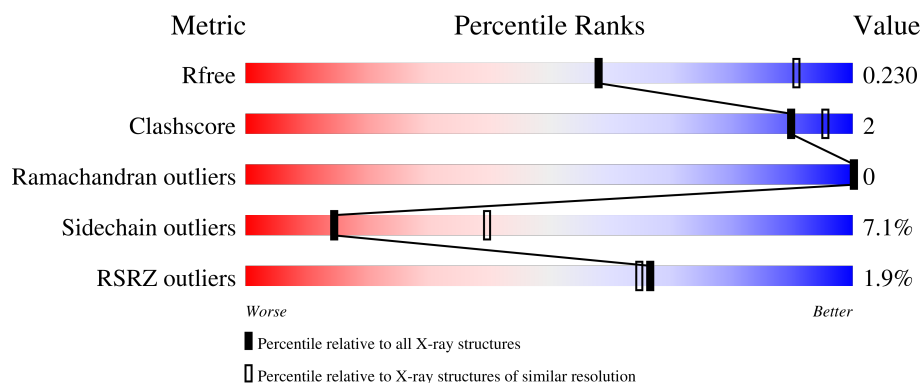
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


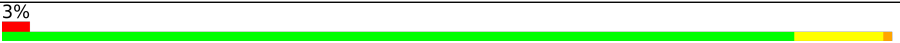
The reported resolution of this entry is 2.90 Å.

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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on 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	349	 90% 9% .
1	B	349	 3% 89% 10% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5883 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
1	A	348	Total	C	N	O	S	0	1	0
			2758	1771	449	527	11			
1	B	348	Total	C	N	O	S	0	1	0
			2758	1771	449	527	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P0DTD1
A	-1	ALA	-	expression tag	UNP P0DTD1
A	0	MET	-	expression tag	UNP P0DTD1
B	-2	GLY	-	expression tag	UNP P0DTD1
B	-1	ALA	-	expression tag	UNP P0DTD1
B	0	MET	-	expression tag	UNP P0DTD1

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

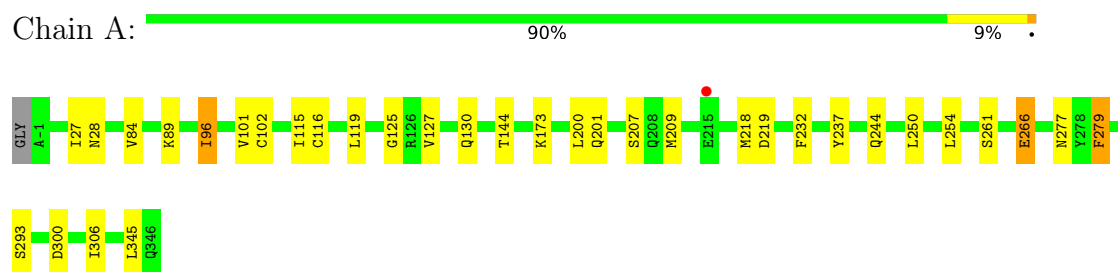
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	185	Total	O	0	0
			185	185		
3	B	172	Total	O	0	0
			172	172		

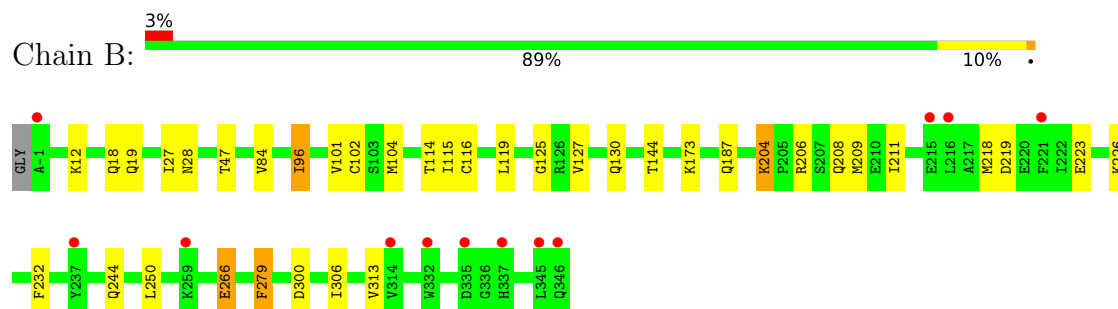
3 Residue-property plots [i](#)

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: Uridylate-specific endoribonuclease



- Molecule 1: Uridylate-specific endoribonuclease



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	150.68Å 150.68Å 110.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.32 – 2.90 45.03 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.32-2.90) 99.1 (45.03-2.90)	Depositor EDS
R_{merge}	0.57	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.175 , 0.218 0.194 , 0.230	Depositor DCC
R_{free} test set	1560 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.040 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5883	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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: PO4

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	0.47	0/2815	0.70	2/3817 (0.1%)
1	B	0.46	0/2815	0.69	0/3817
All	All	0.46	0/5630	0.69	2/7634 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28[A]	ASN	C-N-CA	5.45	135.31	121.70
1	A	28[B]	ASN	C-N-CA	5.45	135.31	121.70

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	2758	0	2750	10	0
1	B	2758	0	2750	10	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	185	0	0	0	0
3	B	172	0	0	0	0
All	All	5883	0	5500	20	0

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 2.

All (20) 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:127:VAL:HB	1:A:130:GLN:HG3	1.64	0.79
1:B:127:VAL:HB	1:B:130:GLN:HG3	1.64	0.79
1:A:84:VAL:HG23	1:A:101:VAL:HG11	1.87	0.55
1:B:84:VAL:HG23	1:B:101:VAL:HG11	1.89	0.53
1:B:204:LYS:HE2	1:B:206:ARG:HE	1.73	0.52
1:A:84:VAL:CG2	1:A:101:VAL:HG11	2.42	0.49
1:B:125:GLY:HA3	1:B:144:THR:HG22	1.94	0.49
1:B:266:GLU:HB3	1:B:279:PHE:HB3	1.95	0.48
1:A:125:GLY:HA3	1:A:144:THR:HG22	1.95	0.48
1:B:84:VAL:CG2	1:B:101:VAL:HG11	2.43	0.48
1:A:266:GLU:HB3	1:A:279:PHE:HB3	1.95	0.47
1:A:116:CYS:HA	1:A:119:LEU:HD12	1.97	0.46
1:B:12:LYS:NZ	1:B:18:GLN:HG3	2.32	0.44
1:B:116:CYS:HA	1:B:119:LEU:HD12	1.99	0.44
1:A:277:ASN:HD22	1:A:293:SER:HA	1.83	0.43
1:B:96:ILE:HG13	1:B:96:ILE:H	1.67	0.43
1:A:218:MET:HG3	1:A:237:TYR:CZ	2.55	0.42
1:B:208:GLN:HA	1:B:211:ILE:HD12	2.02	0.41
1:A:200:LEU:HD13	1:A:254:LEU:HB3	2.03	0.41
1:A:96:ILE:H	1:A:96:ILE:HG13	1.70	0.40

There are no symmetry-related clashes.

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	347/349 (99%)	334 (96%)	13 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	347/349 (99%)	335 (96%)	12 (4%)	0	100	100
All	All	694/698 (99%)	669 (96%)	25 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	310/309 (100%)	291 (94%)	19 (6%)	18	48
1	B	310/309 (100%)	284 (92%)	26 (8%)	11	31
All	All	620/618 (100%)	575 (93%)	45 (7%)	14	38

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ILE
1	A	89	LYS
1	A	96	ILE
1	A	102	CYS
1	A	115	ILE
1	A	173	LYS
1	A	201	GLN
1	A	207	SER
1	A	209	MET
1	A	219	ASP
1	A	232	PHE
1	A	244	GLN
1	A	250	LEU
1	A	261	SER
1	A	266	GLU
1	A	279	PHE
1	A	300	ASP
1	A	306	ILE

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Mol	Chain	Res	Type
1	A	345	LEU
1	B	19	GLN
1	B	27	ILE
1	B	28[A]	ASN
1	B	28[B]	ASN
1	B	47	THR
1	B	96	ILE
1	B	102	CYS
1	B	104	MET
1	B	114	THR
1	B	115	ILE
1	B	173	LYS
1	B	187	GLN
1	B	204	LYS
1	B	209	MET
1	B	218	MET
1	B	219	ASP
1	B	223	GLU
1	B	226	LYS
1	B	232	PHE
1	B	244	GLN
1	B	250	LEU
1	B	266	GLU
1	B	279	PHE
1	B	300	ASP
1	B	306	ILE
1	B	313	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	ASN
1	A	199	ASN
1	A	201	GLN
1	B	188	GLN

5.3.3 RNA ⓘ

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](#)

2 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	$\# Z > 2$
2	PO4	A	401	-	4,4,4	2.47	1 (25%)	6,6,6	0.47	0
2	PO4	B	401	-	4,4,4	2.50	1 (25%)	6,6,6	0.41	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	PO4	P-O1	4.15	1.60	1.50
2	A	401	PO4	P-O1	4.09	1.60	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	348/349 (99%)	-0.40	1 (0%) 94 94	24, 43, 71, 97	0
1	B	348/349 (99%)	-0.10	12 (3%) 45 40	26, 53, 110, 136	0
All	All	696/698 (99%)	-0.25	13 (1%) 66 65	24, 48, 97, 136	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	345	LEU	5.0
1	B	215	GLU	3.5
1	B	314	VAL	3.0
1	B	237	TYR	2.8
1	A	215	GLU	2.8
1	B	216	LEU	2.6
1	B	346	GLN	2.5
1	B	-1	ALA	2.4
1	B	335	ASP	2.2
1	B	332	TRP	2.1
1	B	337	HIS	2.1
1	B	221	PHE	2.1
1	B	259	LYS	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 monosaccharides in this entry.

6.4 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	PO4	B	401	5/5	0.85	0.18	115,115,116,116	0
2	PO4	A	401	5/5	0.99	0.12	60,63,64,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.