



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:00 PM UTC

PDB ID : 7I2U / pdb_00007i2u
Title : Group deposition for crystallographic fragment screening of the NS5 RNA-dependent RNA polymerase from Dengue virus serotype 2 – Crystal structure of the NS5 RNA-dependent RNA polymerase from Dengue virus serotype 2 in complex with Z32665176 (DNV2_NS5A-x0787)
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Deposited on : 2025-03-06
Resolution : 1.96 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	: 4-5-2 with Phenix2.0
Mogul	: 2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	: 2.0
EDS	: 3.0
Buster-report	: wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	: 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	: 9.0.010 (Gargrove)
Density-Fitness	: 1.0.12
Ideal geometry (proteins)	: Engh & Huber (2001)

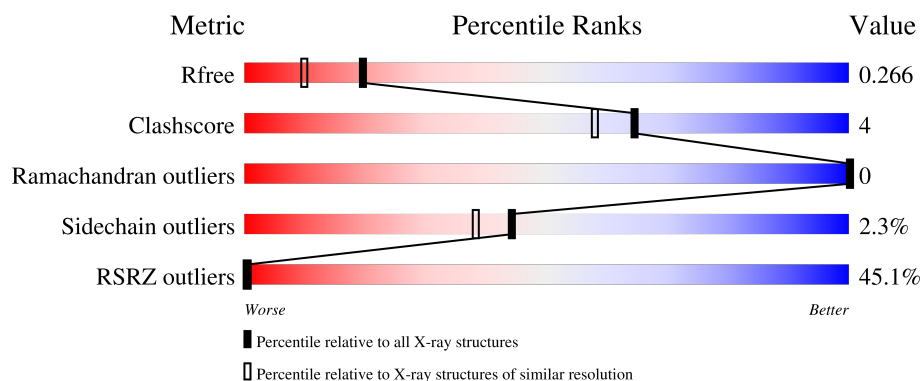
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	637	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PO4	A	1006	-	-	X	-
8	LQI	A	1010	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5173 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 NS5 RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	583	4811	3029	864	884	34	0	6	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	264	GLY	-	expression tag	UNP Q91H74
A	265	PRO	-	expression tag	UNP Q91H74

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



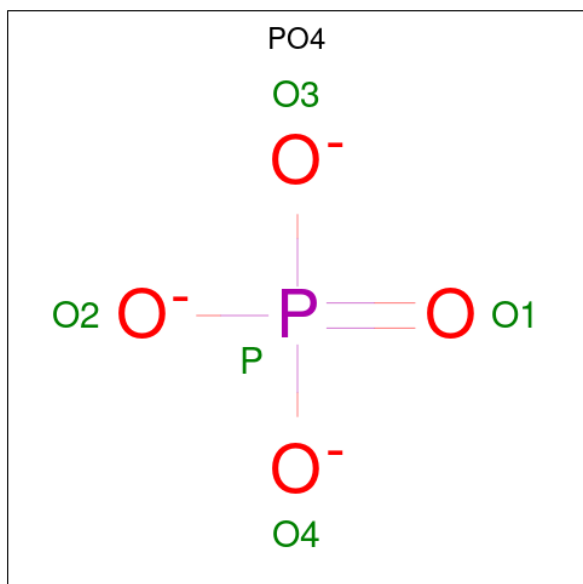
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			24	12	2	8	2		

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



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

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).

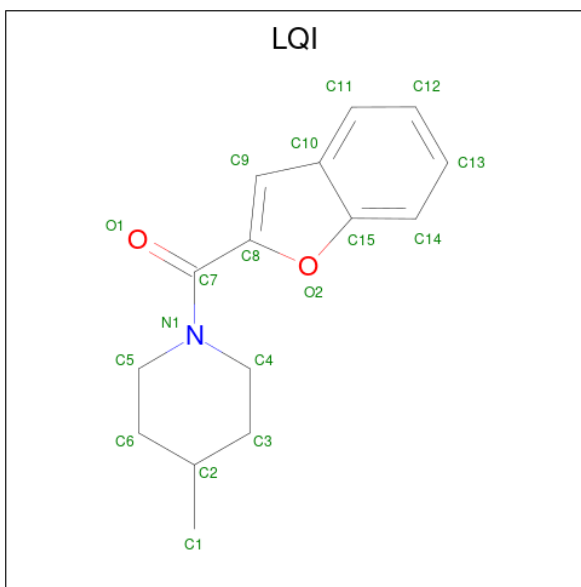


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		

- Molecule 8 is (1-benzofuran-2-yl)(4-methylpiperidin-1-yl)methanone (CCD ID: LQI) (formula: C₁₅H₁₇NO₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			18	15	1	2		

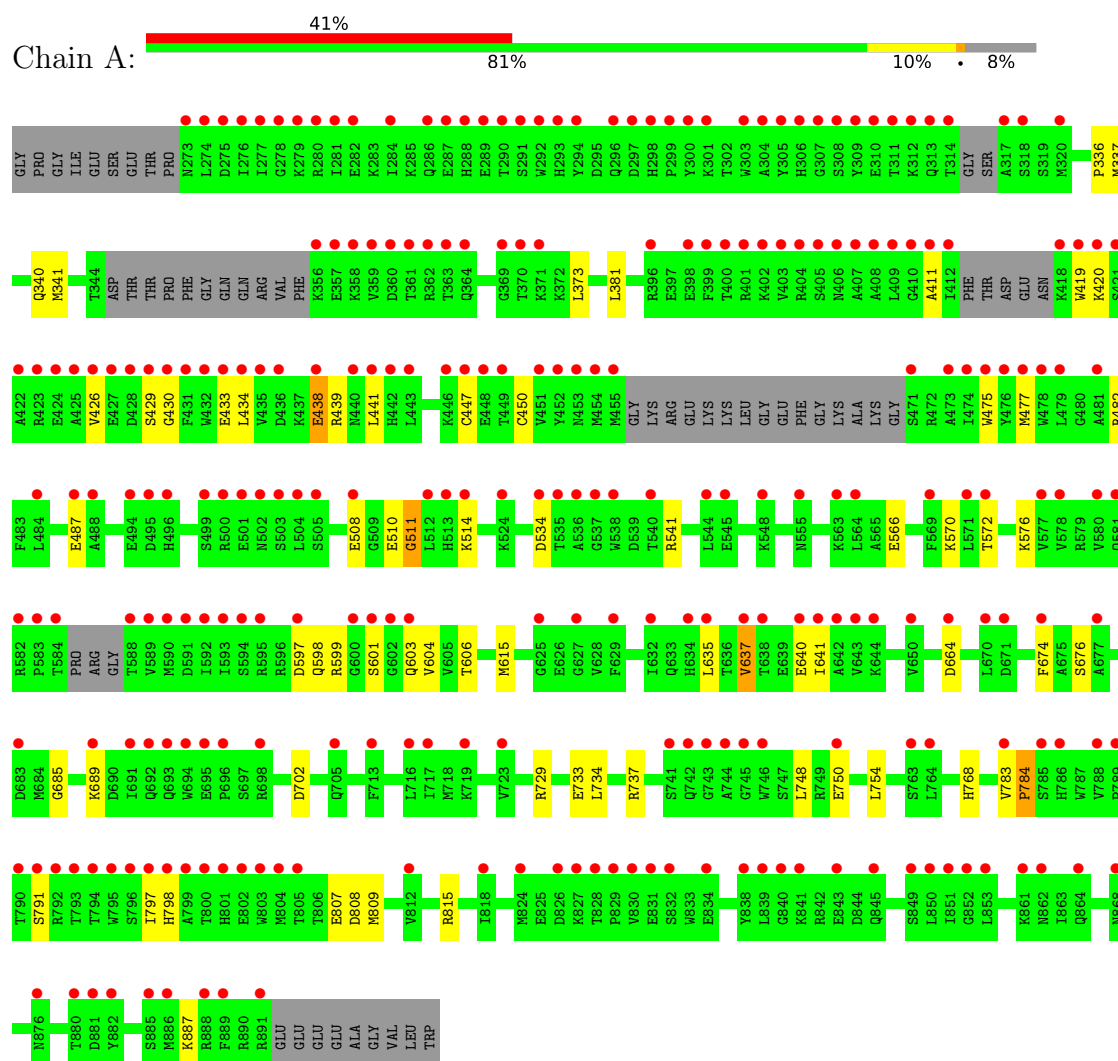
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	292	Total	O	0	0
			292	292		

3 Residue-property plots

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: NS5 RNA-dependent RNA polymerase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	82.62Å 115.81Å 145.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.50 – 1.96 49.50 – 1.96	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.50-1.96) 99.5 (49.50-1.96)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.194 , 0.240 0.244 , 0.266	Depositor DCC
R_{free} test set	2585 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 107.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5173	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, LQI, MES, PEG, CL, ZN, DMS

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	1.06	2/4919 (0.0%)	1.35	7/6635 (0.1%)

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
1	A	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	511	GLY	C-N	-6.82	1.24	1.33
1	A	768	HIS	CE1-NE2	5.38	1.38	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	511	GLY	CA-C-O	-6.16	117.07	121.88
1	A	373	LEU	CA-C-N	5.57	127.74	120.28
1	A	373	LEU	C-N-CA	5.57	127.74	120.28
1	A	572	THR	CB-CA-C	5.50	117.86	109.34
1	A	702	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	674	PHE	CA-C-N	5.04	127.03	120.28
1	A	674	PHE	C-N-CA	5.04	127.03	120.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	784	PRO	Mainchain

5.2 Too-close contacts

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	4811	0	4719	35	0
2	A	2	0	0	0	0
3	A	24	0	26	1	0
4	A	8	0	12	3	0
5	A	10	0	0	4	0
6	A	7	0	10	0	0
7	A	1	0	0	0	0
8	A	18	0	0	0	0
9	A	292	0	0	6	1
All	All	5173	0	4767	38	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 4.

All (38) 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)
4:A:1004:DMS:H11	9:A:1231:HOH:O	1.84	0.76
1:A:664:ASP:OD1	5:A:1006:PO4:O4	2.12	0.67
1:A:754:LEU:HD13	1:A:791:SER:HB3	1.77	0.65
1:A:635:LEU:HD23	1:A:640:GLU:HG2	1.79	0.64
1:A:664:ASP:OD1	5:A:1006:PO4:P	2.56	0.64
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.40	0.61
1:A:534:ASP:OD1	5:A:1006:PO4:O4	2.19	0.61
4:A:1004:DMS:C1	9:A:1231:HOH:O	2.48	0.54
1:A:340:GLN:OE1	9:A:1102:HOH:O	2.18	0.54
1:A:815:ARG:HD2	9:A:1152:HOH:O	2.08	0.54
1:A:429:SER:O	1:A:433:GLU:HG3	2.08	0.53
1:A:733:GLU:O	1:A:737:ARG:HG3	2.09	0.53
1:A:534:ASP:OD1	5:A:1006:PO4:P	2.68	0.52
1:A:510:GLU:O	1:A:514:LYS:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:ARG:HD2	1:A:685:GLY:O	2.13	0.48
1:A:337:MET:HG2	9:A:1306:HOH:O	2.14	0.48
1:A:807:GLU:CD	1:A:815:ARG:HH22	2.22	0.48
1:A:508:GLU:HG2	1:A:797:ILE:HG22	1.96	0.47
1:A:748:LEU:HD13	3:A:1003[B]:MES:H61	1.97	0.47
1:A:411:ALA:HA	1:A:477:MET:O	2.15	0.46
1:A:809:MET:HA	1:A:809:MET:HE2	1.97	0.45
1:A:381:LEU:HD11	1:A:615:MET:HE2	1.99	0.45
1:A:603:GLN:HG3	1:A:604:VAL:N	2.32	0.45
1:A:430:GLY:O	1:A:434:LEU:HG	2.17	0.44
1:A:576:LYS:NZ	1:A:597:ASP:O	2.37	0.44
1:A:599:ARG:HG2	1:A:606:THR:HG23	1.99	0.44
1:A:511:GLY:N	1:A:798:HIS:O	2.51	0.44
1:A:597:ASP:O	1:A:598:GLN:HB2	2.18	0.43
1:A:438:GLU:O	1:A:441:LEU:HB2	2.18	0.43
1:A:729:ARG:HD3	1:A:734:LEU:HD21	2.01	0.43
1:A:341:MET:HE2	1:A:341:MET:HB3	1.78	0.42
1:A:475:TRP:CD1	1:A:475:TRP:N	2.88	0.42
1:A:439:ARG:NH1	1:A:487:GLU:OE1	2.53	0.42
1:A:566:GLU:O	1:A:570:LYS:HB2	2.19	0.42
1:A:637:VAL:O	1:A:641:ILE:HG12	2.19	0.41
1:A:783:VAL:O	1:A:784:PRO:C	2.63	0.41
4:A:1004:DMS:H12	9:A:1255:HOH:O	2.19	0.40
1:A:336:PRO:O	1:A:340:GLN:HG2	2.21	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)
9:A:1133:HOH:O	9:A:1133:HOH:O[2_445]	1.05	1.15

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	577/637 (91%)	556 (96%)	21 (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	517/554 (93%)	505 (98%)	12 (2%)	44	38

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	419	TRP
1	A	420	LYS
1	A	426	VAL
1	A	438	GLU
1	A	482	ARG
1	A	601	SER
1	A	637	VAL
1	A	676	SER
1	A	689	LYS
1	A	750	GLU
1	A	808	ASP
1	A	887	LYS

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	298	HIS
1	A	701	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 for Mogul analysis.

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	$\# Z > 2$
5	PO4	A	1007	-	4,4,4	0.98	0	6,6,6	0.51	0
8	LQI	A	1010	-	20,20,20	0.29	0	26,28,28	0.51	0
6	PEG	A	1008	-	6,6,6	0.13	0	5,5,5	0.15	0
3	MES	A	1003[A]	-	12,12,12	0.74	0	15,16,16	0.40	0
4	DMS	A	1004	-	3,3,3	0.29	0	3,3,3	0.27	0
5	PO4	A	1006	-	4,4,4	2.95	2 (50%)	6,6,6	0.72	0
3	MES	A	1003[B]	-	12,12,12	0.73	0	15,16,16	0.52	0
4	DMS	A	1005	-	3,3,3	0.40	0	3,3,3	0.17	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
8	LQI	A	1010	-	-	0/8/18/18	0/3/3/3
6	PEG	A	1008	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MES	A	1003[A]	-	-	3/6/14/14	0/1/1/1
3	MES	A	1003[B]	-	-	2/6/14/14	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1006	PO4	P-O1	4.99	1.62	1.50
5	A	1006	PO4	P-O2	2.15	1.60	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1003[A]	MES	C7-C8-S-O1S
3	A	1003[A]	MES	C7-C8-S-O3S
3	A	1003[B]	MES	C8-C7-N4-C3
6	A	1008	PEG	O2-C3-C4-O4
3	A	1003[B]	MES	C8-C7-N4-C5
3	A	1003[A]	MES	C7-C8-S-O2S
6	A	1008	PEG	C4-C3-O2-C2

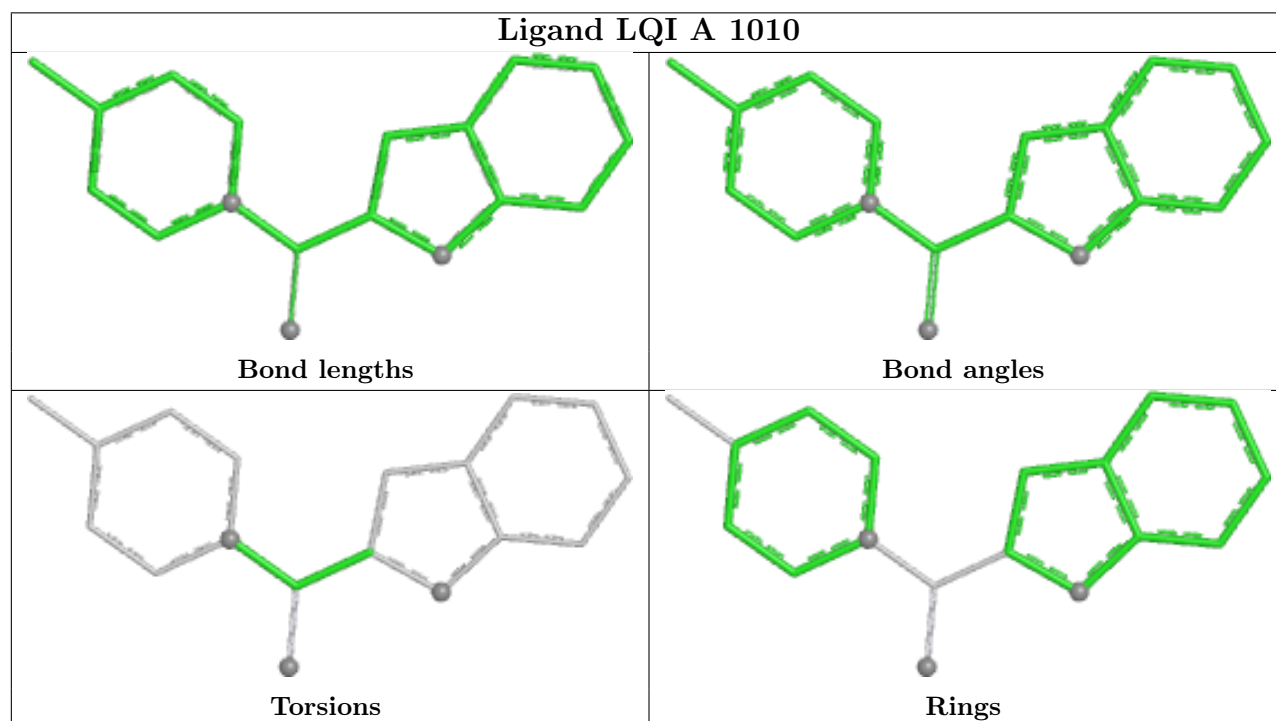
There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1004	DMS	3	0
5	A	1006	PO4	4	0
3	A	1003[B]	MES	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	583/637 (91%)	3.09	263 (45%) 0 0	7, 44, 95, 158	123 (21%)

All (263) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	512[A]	LEU	15.9
1	A	795	TRP	15.5
1	A	713	PHE	14.8
1	A	830	VAL	14.2
1	A	409	LEU	13.0
1	A	803	TRP	12.9
1	A	600	GLY	12.8
1	A	281	ILE	12.7
1	A	716	LEU	12.7
1	A	717	ILE	12.5
1	A	399	PHE	12.5
1	A	514	LYS	12.3
1	A	641	ILE	12.3
1	A	790	THR	12.0
1	A	838	TYR	12.0
1	A	593	ILE	11.9
1	A	793	THR	11.7
1	A	407	ALA	11.5
1	A	799	ALA	11.5
1	A	513	HIS	11.2
1	A	794	THR	11.2
1	A	719[A]	LYS	11.2
1	A	800	THR	11.1
1	A	801	HIS	11.1
1	A	850	LEU	11.0
1	A	403	VAL	10.9
1	A	426	VAL	10.8

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Mol	Chain	Res	Type	RSRZ
1	A	839	LEU	10.7
1	A	791	SER	10.7
1	A	580	VAL	10.7
1	A	488	ALA	10.6
1	A	840	GLY	10.6
1	A	797	ILE	10.5
1	A	504	LEU	10.4
1	A	832	SER	10.4
1	A	853	LEU	10.4
1	A	422	ALA	10.4
1	A	276	ILE	10.3
1	A	277	ILE	10.2
1	A	410	GLY	10.2
1	A	274	LEU	9.8
1	A	505	SER	9.8
1	A	851	ILE	9.8
1	A	829	PRO	9.7
1	A	400	THR	9.6
1	A	798	HIS	9.5
1	A	828	THR	9.5
1	A	278	GLY	9.5
1	A	885	SER	9.2
1	A	421	SER	9.2
1	A	594	SER	9.0
1	A	408	ALA	9.0
1	A	826	ASP	8.9
1	A	849	SER	8.9
1	A	792	ARG	8.9
1	A	309	TYR	8.8
1	A	311	THR	8.7
1	A	595	ARG	8.6
1	A	785[A]	SER	8.6
1	A	789	PRO	8.6
1	A	419	TRP	8.5
1	A	796	SER	8.5
1	A	696	PRO	8.5
1	A	788	VAL	8.4
1	A	582	ARG	8.3
1	A	589	VAL	8.3
1	A	314	THR	8.2
1	A	705	GLN	8.2
1	A	827	LYS	8.1

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Mol	Chain	Res	Type	RSRZ
1	A	763[A]	SER	8.0
1	A	805	THR	7.9
1	A	852	GLY	7.9
1	A	802	GLU	7.9
1	A	273	ASN	7.8
1	A	864[A]	GLN	7.8
1	A	280	ARG	7.8
1	A	786	HIS	7.7
1	A	289	GLU	7.6
1	A	487	GLU	7.6
1	A	279	LYS	7.5
1	A	500	ARG	7.3
1	A	356	LYS	7.3
1	A	298	HIS	7.3
1	A	288	HIS	7.2
1	A	431	PHE	7.2
1	A	361	THR	7.2
1	A	689	LYS	7.1
1	A	499	SER	7.1
1	A	398	GLU	7.1
1	A	584	THR	7.1
1	A	841	LYS	7.1
1	A	503	SER	7.1
1	A	405	SER	7.0
1	A	402	LYS	7.0
1	A	741[A]	SER	6.9
1	A	693	GLN	6.9
1	A	692	GLN	6.9
1	A	275	ASP	6.7
1	A	360	ASP	6.7
1	A	452	TYR	6.7
1	A	831	GLU	6.7
1	A	804	MET	6.7
1	A	429	SER	6.6
1	A	423	ARG	6.6
1	A	744	ALA	6.5
1	A	583	PRO	6.4
1	A	745	GLY	6.3
1	A	476	TYR	6.2
1	A	843	GLU	6.2
1	A	581	GLN	6.2
1	A	484	LEU	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	401	ARG	6.1
1	A	412	ILE	6.1
1	A	502	ASN	6.0
1	A	601	SER	6.0
1	A	434	LEU	6.0
1	A	406	ASN	5.9
1	A	296	GLN	5.8
1	A	284	ILE	5.8
1	A	698	ARG	5.7
1	A	293	HIS	5.7
1	A	424	GLU	5.6
1	A	282	GLU	5.6
1	A	357	GLU	5.5
1	A	695	GLU	5.5
1	A	312	LYS	5.5
1	A	442	HIS	5.5
1	A	420	LYS	5.4
1	A	882	TYR	5.4
1	A	290	THR	5.3
1	A	845	GLN	5.3
1	A	428	ASP	5.3
1	A	441	LEU	5.2
1	A	404	ARG	5.1
1	A	411	ALA	5.1
1	A	876	ASN	5.1
1	A	427	GLU	5.0
1	A	474	ILE	5.0
1	A	588	THR	5.0
1	A	362	ARG	5.0
1	A	418	LYS	4.9
1	A	435	VAL	4.9
1	A	292	TRP	4.8
1	A	501	GLU	4.8
1	A	455	MET	4.7
1	A	313	GLN	4.7
1	A	544	LEU	4.7
1	A	750	GLU	4.6
1	A	294	TYR	4.6
1	A	475	TRP	4.6
1	A	889	PHE	4.5
1	A	627	GLY	4.3
1	A	318	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	317	ALA	4.3
1	A	436	ASP	4.3
1	A	359	VAL	4.3
1	A	451	VAL	4.2
1	A	286	GLN	4.2
1	A	449	THR	4.1
1	A	880	THR	4.1
1	A	430	GLY	4.1
1	A	363	THR	4.0
1	A	305	TYR	4.0
1	A	591	ASP	3.9
1	A	861	LYS	3.9
1	A	742	GLN	3.9
1	A	297	ASP	3.9
1	A	473	ALA	3.9
1	A	545	GLU	3.9
1	A	310	GLU	3.9
1	A	664	ASP	3.9
1	A	308	SER	3.8
1	A	746	TRP	3.8
1	A	425	ALA	3.8
1	A	881	ASP	3.7
1	A	287	GLU	3.7
1	A	637	VAL	3.7
1	A	824	MET	3.6
1	A	670	LEU	3.6
1	A	370	THR	3.5
1	A	358	LYS	3.5
1	A	644	LYS	3.4
1	A	743	GLY	3.4
1	A	534	ASP	3.4
1	A	396	ARG	3.4
1	A	691	ILE	3.2
1	A	300	TYR	3.2
1	A	677	ALA	3.2
1	A	564	LEU	3.2
1	A	683	ASP	3.2
1	A	471	SER	3.1
1	A	299	PRO	3.1
1	A	479	LEU	3.1
1	A	537	GLY	3.1
1	A	592	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	438	GLU	3.1
1	A	496	HIS	3.0
1	A	303	TRP	3.0
1	A	674	PHE	3.0
1	A	635	LEU	3.0
1	A	307	GLY	2.9
1	A	447	CYS	2.9
1	A	453	ASN	2.9
1	A	634	HIS	2.9
1	A	783	VAL	2.9
1	A	432	TRP	2.8
1	A	364	GLN	2.7
1	A	643	VAL	2.7
1	A	304	ALA	2.7
1	A	454	MET	2.7
1	A	764	LEU	2.7
1	A	371	LYS	2.7
1	A	538	TRP	2.7
1	A	597	ASP	2.6
1	A	694	TRP	2.6
1	A	301	LYS	2.6
1	A	632	ILE	2.6
1	A	477	MET	2.6
1	A	478	TRP	2.6
1	A	642	ALA	2.6
1	A	603	GLN	2.6
1	A	481	ALA	2.6
1	A	590	MET	2.5
1	A	320	MET	2.5
1	A	536	ALA	2.5
1	A	446	LYS	2.5
1	A	888	ARG	2.5
1	A	495	ASP	2.4
1	A	625	GLY	2.4
1	A	723	VAL	2.4
1	A	572	THR	2.4
1	A	834	GLU	2.4
1	A	548	LYS	2.4
1	A	569	PHE	2.3
1	A	448	GLU	2.3
1	A	629	PHE	2.3
1	A	508	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	440	ASN	2.3
1	A	540	THR	2.3
1	A	291	SER	2.2
1	A	818	ILE	2.2
1	A	812	VAL	2.2
1	A	555	ASN	2.2
1	A	524	LYS	2.2
1	A	862	ASN	2.2
1	A	671	ASP	2.2
1	A	306	HIS	2.2
1	A	868	ASN	2.2
1	A	891	ARG	2.2
1	A	433	GLU	2.1
1	A	640	GLU	2.1
1	A	638	THR	2.1
1	A	650	VAL	2.1
1	A	602	GLY	2.1
1	A	535	THR	2.1
1	A	563	LYS	2.1
1	A	369	GLY	2.1
1	A	886	MET	2.1
1	A	443	LEU	2.1
1	A	571	LEU	2.0
1	A	494	GLU	2.0
1	A	577	VAL	2.0
1	A	578	VAL	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](#)

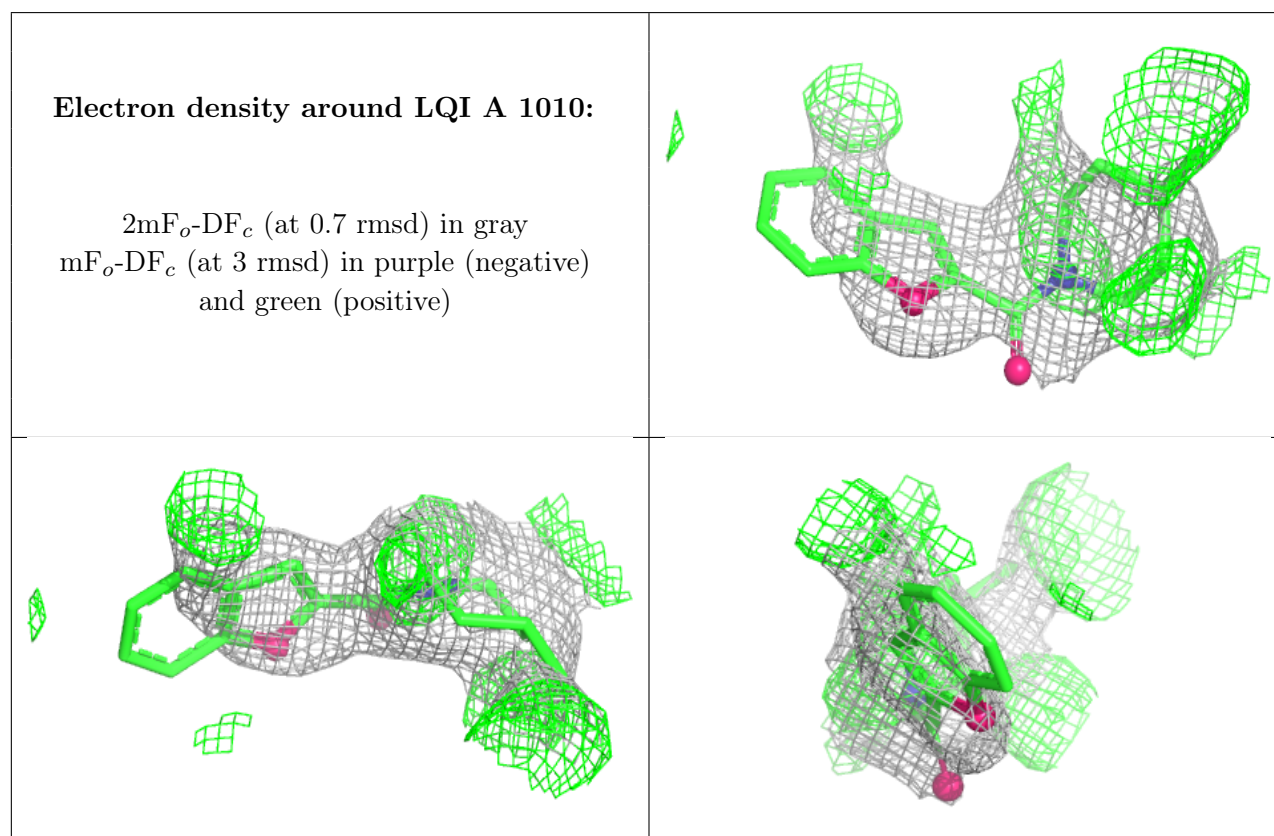
There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
8	LQI	A	1010	18/18	0.56	0.41	49,54,63,63	18
5	PO4	A	1007	5/5	0.76	0.11	77,83,91,110	0
4	DMS	A	1005	4/4	0.76	0.23	77,105,106,126	0
5	PO4	A	1006	5/5	0.80	0.12	43,48,58,79	0
6	PEG	A	1008	7/7	0.81	0.17	67,79,91,94	0
4	DMS	A	1004	4/4	0.82	0.22	66,69,70,71	0
3	MES	A	1003[A]	12/12	0.94	0.25	762,768,813,813	12
3	MES	A	1003[B]	12/12	0.94	0.25	30,36,41,44	12
7	CL	A	1009	1/1	0.96	0.44	51,51,51,51	1
2	ZN	A	1002	1/1	0.99	0.03	60,60,60,60	0
2	ZN	A	1001	1/1	1.00	0.01	29,29,29,29	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.