



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 10:57 AM UTC

PDB ID : 7I2J / pdb_00007i2j
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 Z1269139261 (DNV2_NS5A-x0479)
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Deposited on : 2025-03-06
Resolution : 1.98 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)

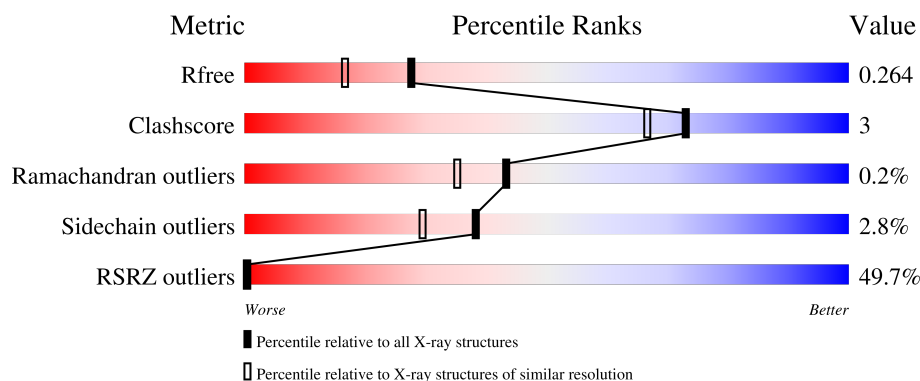
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	45% 81% 9% 10%

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	1007	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5194 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
1	A	571	Total	C	N	O	S	0	8	0
			4731	2979	848	870	34			

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).



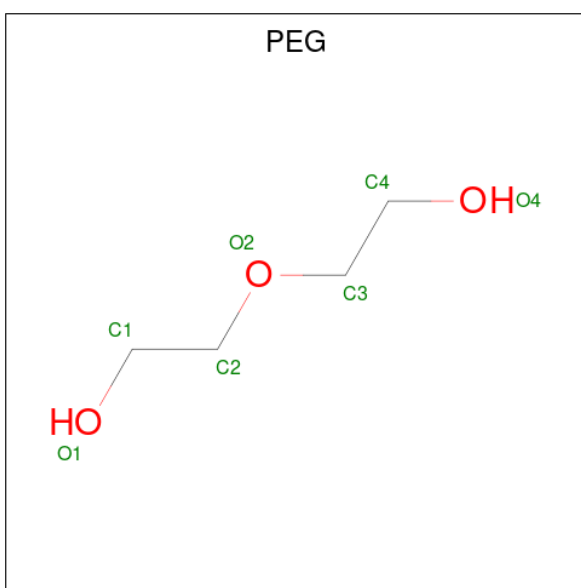
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

- 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		

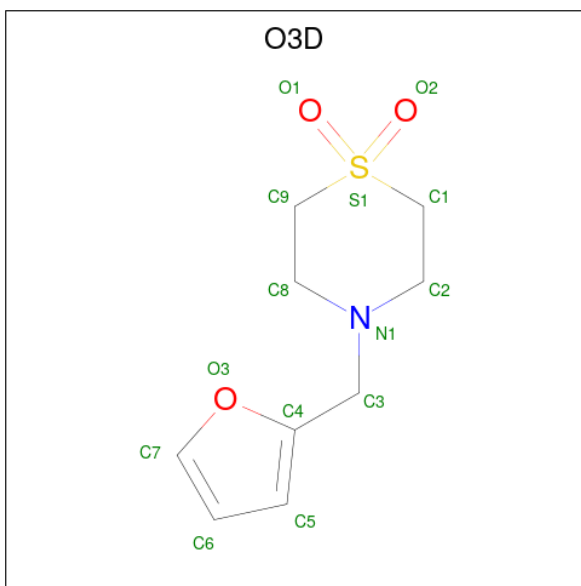
- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 7 is 4-[(furan-2-yl)methyl]-1λ⁶,4-thiazinane-1,1-dione (CCD ID: O3D)

(formula: C₉H₁₃NO₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			14	9	1	3	1		

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	393	Total	O	0	0
			393	393		

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	82.42Å 116.07Å 148.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.00 – 1.98 72.00 – 1.98	Depositor EDS
% Data completeness (in resolution range)	96.7 (72.00-1.98) 96.8 (72.00-1.98)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.183 , 0.227 (Not available) , 0.264	Depositor DCC
R_{free} test set	2560 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 171.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	5194	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% 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: O3D, MES, CL, PEG, PO4, DMS, ZN

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	1.14	2/4836 (0.0%)	1.38	7/6520 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	750	GLU	C-O	5.79	1.30	1.24
1	A	650	VAL	N-CA	5.37	1.51	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	702	ASP	CA-CB-CG	6.63	119.23	112.60
1	A	854	THR	CA-CB-OG1	-6.58	99.72	109.60
1	A	640	GLU	N-CA-C	-6.17	105.41	113.12
1	A	494	GLU	CA-C-O	-6.13	114.05	120.55
1	A	657	ARG	CG-CD-NE	-6.05	98.69	112.00
1	A	650	VAL	CA-C-O	-5.82	114.92	119.46
1	A	702	ASP	CB-CA-C	5.76	119.35	110.14

There are no chirality outliers.

There are no planarity outliers.

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	4731	0	4631	27	0
2	A	2	0	0	0	0
3	A	24	0	26	1	0
4	A	12	0	18	3	0
5	A	10	0	0	4	0
6	A	7	0	10	0	0
7	A	14	0	0	0	0
8	A	1	0	0	0	0
9	A	393	0	0	5	3
All	All	5194	0	4685	30	3

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 3.

All (30) 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:534:ASP:OD1	5:A:1007:PO4:O4	1.79	1.00
1:A:664:ASP:OD1	5:A:1007:PO4:O4	1.98	0.81
4:A:1004:DMS:H11	9:A:1264:HOH:O	1.83	0.77
1:A:809:MET:HA	1:A:809:MET:HE2	1.79	0.63
1:A:664:ASP:OD1	5:A:1007:PO4:P	2.57	0.62
4:A:1004:DMS:C1	9:A:1264:HOH:O	2.45	0.57
1:A:568:ILE:O	1:A:572:THR:OG1	2.22	0.56
1:A:599:ARG:HG2	1:A:606:THR:HG23	1.90	0.53
1:A:534:ASP:OD1	5:A:1007:PO4:P	2.67	0.53
1:A:311:THR:HG21	1:A:590:MET:HB2	1.92	0.52
1:A:562:LYS:O	1:A:566:GLU:HG3	2.11	0.51
1:A:428:ASP:OD1	1:A:428:ASP:C	2.55	0.49
1:A:815:ARG:HD2	9:A:1224:HOH:O	2.13	0.48
1:A:530:MET:HE2	1:A:706:VAL:HG21	1.95	0.48
4:A:1004:DMS:H12	9:A:1239:HOH:O	2.14	0.47
1:A:748:LEU:HD13	3:A:1003[B]:MES:H61	1.98	0.45
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.56	0.45
1:A:482:ARG:NH1	1:A:485:GLU:OE2	2.31	0.45
1:A:400:THR:HG23	1:A:426:VAL:CG1	2.47	0.44
1:A:321:VAL:HG11	1:A:326:ARG:CZ	2.48	0.43
1:A:807:GLU:HG3	9:A:1304:HOH:O	2.17	0.43
1:A:510:GLU:O	1:A:514:LYS:HG3	2.18	0.43
1:A:538:TRP:CD1	1:A:538:TRP:C	2.97	0.43
1:A:528:GLY:O	1:A:668:LYS:HE3	2.20	0.42
1:A:513:HIS:HB3	1:A:765:MET:HE1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512[B]:LEU:HD23	1:A:512[B]:LEU:HA	1.92	0.42
1:A:277:ILE:HD12	1:A:281:ILE:HD11	2.02	0.41
1:A:400:THR:HG23	1:A:426:VAL:HG11	2.02	0.41
1:A:550:GLU:OE2	1:A:613:THR:OG1	2.33	0.41
1:A:809:MET:HE1	1:A:812:VAL:HG21	2.02	0.40

All (3) 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:1147:HOH:O	9:A:1147:HOH:O[2_445]	1.44	0.76
9:A:1331:HOH:O	9:A:1331:HOH:O[4_545]	2.10	0.10
9:A:1349:HOH:O	9:A:1414:HOH:O[2_545]	2.12	0.08

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	565/637 (89%)	539 (95%)	25 (4%)	1 (0%)	43	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	406	ASN

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	508/554 (92%)	494 (97%)	14 (3%)	38 29

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	274	LEU
1	A	311	THR
1	A	356	LYS
1	A	409	LEU
1	A	412	ILE
1	A	482	ARG
1	A	499	SER
1	A	589	VAL
1	A	630	LYS
1	A	635	LEU
1	A	641	ILE
1	A	645	ASN
1	A	830	VAL
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	598	GLN
1	A	862	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 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 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	3.69	2 (50%)	6,6,6	0.60	0
4	DMS	A	1006	-	3,3,3	0.15	0	3,3,3	0.62	0
6	PEG	A	1009	-	6,6,6	0.16	0	5,5,5	0.06	0
3	MES	A	1003[B]	-	12,12,12	0.84	0	15,16,16	0.65	0
5	PO4	A	1008	-	4,4,4	1.49	1 (25%)	6,6,6	0.36	0
4	DMS	A	1005	-	3,3,3	0.29	0	3,3,3	0.06	0
3	MES	A	1003[A]	-	12,12,12	0.73	0	15,16,16	0.34	0
4	DMS	A	1004	-	3,3,3	0.43	0	3,3,3	0.59	0
7	O3D	A	1010	-	15,15,15	0.24	0	19,21,21	0.56	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
6	PEG	A	1009	-	-	2/4/4/4	-
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
7	O3D	A	1010	-	-	1/4/16/16	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1007	PO4	P-O1	6.73	1.66	1.50
5	A	1008	PO4	P-O1	2.96	1.57	1.50
5	A	1007	PO4	P-O2	2.39	1.61	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

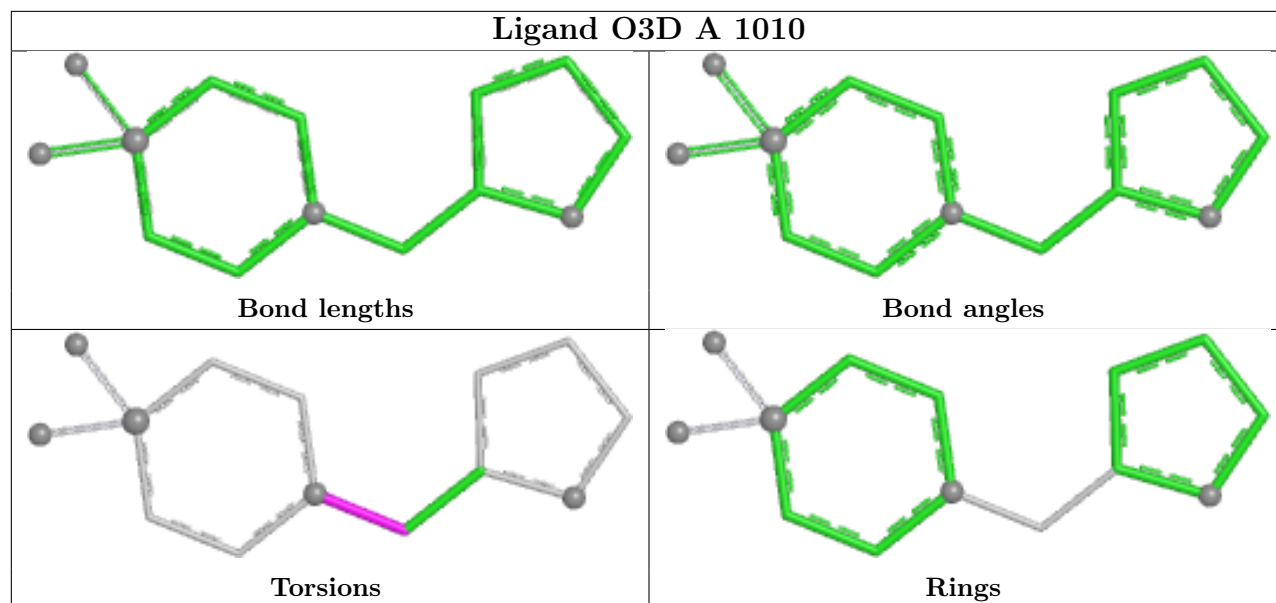
Mol	Chain	Res	Type	Atoms
3	A	1003[A]	MES	C7-C8-S-O1S
3	A	1003[A]	MES	C7-C8-S-O3S
3	A	1003[B]	MES	C8-C7-N4-C3
7	A	1010	O3D	C4-C3-N1-C2
6	A	1009	PEG	O2-C3-C4-O4
3	A	1003[B]	MES	C8-C7-N4-C5
3	A	1003[A]	MES	C7-C8-S-O2S
6	A	1009	PEG	C4-C3-O2-C2

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1007	PO4	4	0
3	A	1003[B]	MES	1	0
4	A	1004	DMS	3	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	571/637 (89%)	3.68	284 (49%) 0 0	6, 33, 69, 123	157 (27%)

All (284) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	292	TRP	17.4
1	A	600	GLY	16.8
1	A	741[A]	SER	15.0
1	A	294	TYR	14.4
1	A	366	PRO	14.4
1	A	635	LEU	14.2
1	A	305	TYR	13.8
1	A	637	VAL	13.7
1	A	304	ALA	13.6
1	A	303	TRP	13.5
1	A	281	ILE	13.5
1	A	403	VAL	13.4
1	A	641	ILE	13.3
1	A	409	LEU	13.1
1	A	632	ILE	13.0
1	A	407	ALA	13.0
1	A	431	PHE	12.9
1	A	425	ALA	12.9
1	A	801[A]	HIS	12.9
1	A	638	THR	12.7
1	A	478	TRP	12.5
1	A	359	VAL	12.5
1	A	426	VAL	12.4
1	A	435	VAL	12.3
1	A	691	ILE	12.0
1	A	449	THR	12.0
1	A	592	ILE	11.9

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Mol	Chain	Res	Type	RSRZ
1	A	535	THR	11.8
1	A	284	ILE	11.8
1	A	577	VAL	11.8
1	A	422	ALA	11.7
1	A	636	THR	11.6
1	A	367	LYS	11.6
1	A	373	LEU	11.5
1	A	300	TYR	11.5
1	A	580	VAL	11.4
1	A	411	ALA	11.4
1	A	542	ILE	11.3
1	A	601	SER	11.1
1	A	412	ILE	11.1
1	A	476	TYR	11.0
1	A	439	ARG	10.9
1	A	578	VAL	10.7
1	A	450	CYS	10.7
1	A	593	ILE	10.6
1	A	482	ARG	10.6
1	A	410	GLY	10.6
1	A	274	LEU	10.5
1	A	307	GLY	10.5
1	A	309	TYR	10.5
1	A	290	THR	10.5
1	A	640	GLU	10.4
1	A	363	THR	10.3
1	A	475	TRP	10.3
1	A	536	ALA	10.2
1	A	276	ILE	10.1
1	A	299	PRO	10.1
1	A	421	SER	10.1
1	A	477	MET	10.0
1	A	306	HIS	9.9
1	A	631	SER	9.9
1	A	551[A]	GLU	9.9
1	A	512[A]	LEU	9.9
1	A	639	GLU	9.9
1	A	401	ARG	9.8
1	A	649	ARG	9.8
1	A	293	HIS	9.8
1	A	408	ALA	9.7
1	A	644	LYS	9.7

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Mol	Chain	Res	Type	RSRZ
1	A	645	ASN	9.6
1	A	583	PRO	9.6
1	A	474	ILE	9.5
1	A	308	SER	9.5
1	A	402	LYS	9.4
1	A	419	TRP	9.3
1	A	575	ASN	9.2
1	A	541	ARG	9.1
1	A	375	LYS	9.1
1	A	280	ARG	9.0
1	A	311	THR	8.9
1	A	372	LYS	8.8
1	A	473	ALA	8.8
1	A	365	GLU	8.7
1	A	451	VAL	8.7
1	A	438	GLU	8.7
1	A	719[A]	LYS	8.7
1	A	452	TYR	8.6
1	A	453	ASN	8.5
1	A	548	LYS	8.5
1	A	695	GLU	8.5
1	A	291	SER	8.5
1	A	406	ASN	8.5
1	A	763[A]	SER	8.2
1	A	279	LYS	8.1
1	A	405	SER	8.1
1	A	356	LYS	8.0
1	A	589	VAL	8.0
1	A	591	ASP	8.0
1	A	745	GLY	7.9
1	A	273	ASN	7.9
1	A	283	LYS	7.9
1	A	692	GLN	7.9
1	A	277	ILE	7.9
1	A	441	LEU	7.8
1	A	744	ALA	7.8
1	A	582	ARG	7.8
1	A	634	HIS	7.7
1	A	705	GLN	7.7
1	A	576	LYS	7.6
1	A	423	ARG	7.6
1	A	302	THR	7.6

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Mol	Chain	Res	Type	RSRZ
1	A	455	MET	7.6
1	A	295	ASP	7.6
1	A	448	GLU	7.5
1	A	785[A]	SER	7.5
1	A	581	GLN	7.5
1	A	379	GLU	7.5
1	A	437	LYS	7.5
1	A	698	ARG	7.3
1	A	298	HIS	7.3
1	A	424	GLU	7.3
1	A	689	LYS	7.3
1	A	799	ALA	7.3
1	A	499	SER	7.3
1	A	598	GLN	7.3
1	A	358	LYS	7.2
1	A	834	GLU	7.2
1	A	584	THR	7.2
1	A	454	MET	7.1
1	A	404	ARG	7.1
1	A	513	HIS	7.0
1	A	288	HIS	7.0
1	A	427	GLU	7.0
1	A	286	GLN	7.0
1	A	885	SER	6.9
1	A	301	LYS	6.9
1	A	436	ASP	6.9
1	A	420	LYS	6.8
1	A	484	LEU	6.8
1	A	835	GLU	6.8
1	A	312	LYS	6.7
1	A	595	ARG	6.7
1	A	446	LYS	6.6
1	A	864[A]	GLN	6.6
1	A	596	ARG	6.6
1	A	275	ASP	6.5
1	A	481	ALA	6.3
1	A	287	GLU	6.3
1	A	856	ARG	6.2
1	A	886	MET	6.2
1	A	737	ARG	6.1
1	A	597	ASP	6.1
1	A	770	ARG	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	693	GLN	6.0
1	A	588	THR	6.0
1	A	579	ARG	5.9
1	A	479	LEU	5.9
1	A	357	GLU	5.7
1	A	285	LYS	5.6
1	A	800	THR	5.6
1	A	310	GLU	5.6
1	A	282	GLU	5.6
1	A	791	SER	5.5
1	A	296	GLN	5.5
1	A	399	PHE	5.4
1	A	318	SER	5.3
1	A	428	ASP	5.3
1	A	289	GLU	5.2
1	A	489	LEU	5.1
1	A	362	ARG	5.0
1	A	746	TRP	5.0
1	A	569	PHE	5.0
1	A	690	ASP	5.0
1	A	572	THR	4.8
1	A	605	VAL	4.7
1	A	890	ARG	4.7
1	A	297	ASP	4.6
1	A	888	ARG	4.6
1	A	887	LYS	4.5
1	A	699	GLY	4.5
1	A	278	GLY	4.4
1	A	590	MET	4.4
1	A	364	GLN	4.3
1	A	429	SER	4.3
1	A	568	ILE	4.3
1	A	337	MET	4.2
1	A	742	GLN	4.1
1	A	701	ASN	4.1
1	A	361	THR	4.1
1	A	880	THR	4.1
1	A	629	PHE	4.0
1	A	440	ASN	4.0
1	A	396	ARG	4.0
1	A	891	ARG	3.9
1	A	808	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	694	TRP	3.6
1	A	432	TRP	3.5
1	A	680	ALA	3.5
1	A	627	GLY	3.5
1	A	878	GLU	3.4
1	A	393	MET	3.4
1	A	743	GLY	3.4
1	A	564	LEU	3.4
1	A	556	HIS	3.3
1	A	444	GLU	3.3
1	A	790	THR	3.3
1	A	861	LYS	3.3
1	A	445	GLY	3.2
1	A	630	LYS	3.2
1	A	677	ALA	3.2
1	A	862	ASN	3.2
1	A	443	LEU	3.2
1	A	545	GLU	3.2
1	A	676	SER	3.1
1	A	497	TRP	3.1
1	A	571	LEU	3.1
1	A	383	LYS	3.1
1	A	442	HIS	3.1
1	A	360	ASP	3.0
1	A	882	TYR	3.0
1	A	319	SER	3.0
1	A	492	LEU	3.0
1	A	652	ARG	3.0
1	A	340	GLN	2.9
1	A	537	GLY	2.9
1	A	483	PHE	2.9
1	A	792	ARG	2.9
1	A	480	GLY	2.9
1	A	398	GLU	2.8
1	A	833	TRP	2.8
1	A	390	THR	2.8
1	A	558	GLU	2.8
1	A	594	SER	2.7
1	A	433	GLU	2.7
1	A	544	LEU	2.7
1	A	642	ALA	2.7
1	A	889	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	344	THR	2.7
1	A	430	GLY	2.6
1	A	820	GLU	2.6
1	A	570	LYS	2.6
1	A	628	VAL	2.6
1	A	674	PHE	2.5
1	A	559	GLY	2.5
1	A	561	HIS	2.5
1	A	540	THR	2.5
1	A	563	LYS	2.5
1	A	673	ARG	2.5
1	A	546	ASP	2.5
1	A	683	ASP	2.5
1	A	370	THR	2.5
1	A	486	PHE	2.4
1	A	376	ILE	2.4
1	A	377	THR	2.4
1	A	434	LEU	2.4
1	A	378	ALA	2.4
1	A	368	GLU	2.4
1	A	524	LYS	2.4
1	A	818	ILE	2.4
1	A	487	GLU	2.4
1	A	633	GLN	2.4
1	A	382	TRP	2.4
1	A	881	ASP	2.3
1	A	670	LEU	2.3
1	A	400	THR	2.3
1	A	602	GLY	2.3
1	A	854	THR	2.3
1	A	491	PHE	2.2
1	A	557	MET	2.2
1	A	625	GLY	2.2
1	A	603	GLN	2.2
1	A	574	GLN	2.2
1	A	687	VAL	2.1
1	A	343	MET	2.1
1	A	664	ASP	2.1
1	A	648	VAL	2.1
1	A	369	GLY	2.1
1	A	681	LEU	2.1
1	A	503	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	876	ASN	2.0
1	A	507	VAL	2.0
1	A	609	LEU	2.0
1	A	389	LYS	2.0
1	A	620	ILE	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](#)

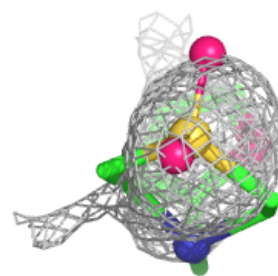
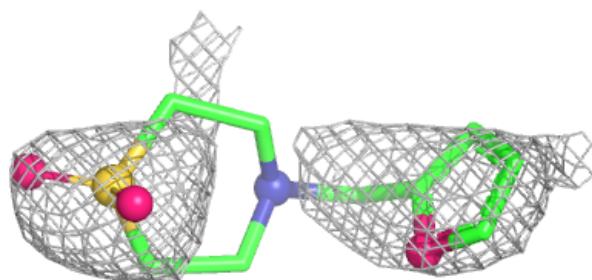
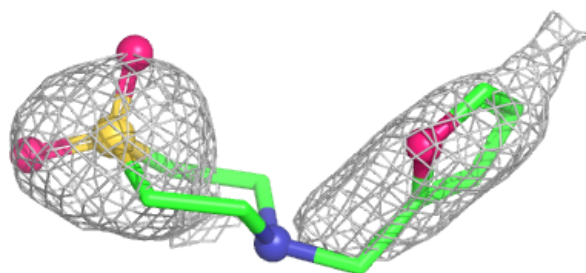
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PO4	A	1008	5/5	0.72	0.21	71,91,98,120	0
7	O3D	A	1010	14/14	0.77	0.24	51,52,55,55	14
6	PEG	A	1009	7/7	0.80	0.20	61,66,84,85	0
5	PO4	A	1007	5/5	0.80	0.14	35,44,54,67	0
4	DMS	A	1005	4/4	0.84	0.21	81,85,93,98	0
3	MES	A	1003[B]	12/12	0.95	0.23	25,30,31,32	12
3	MES	A	1003[A]	12/12	0.95	0.23	847,863,864,864	12
4	DMS	A	1004	4/4	0.96	0.14	43,45,46,49	0
4	DMS	A	1006	4/4	0.96	0.14	51,55,56,58	0
8	CL	A	1011	1/1	0.98	0.17	17,17,17,17	1
2	ZN	A	1002	1/1	0.99	0.03	56,56,56,56	0
2	ZN	A	1001	1/1	1.00	0.01	25,25,25,25	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.

Electron density around O3D A 1010:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.