



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:34 PM UTC

PDB ID : 7I2N / pdb_00007i2n
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 Z1685106505 (DNV2_NS5A-x0571)
Authors : Aschenbrenner, J.C.; Saini, M.; Chopra, A.; Marples, P.G.; Balcomb, B.H.; Lithgo, R.M.; Fearon, D.; von Delft, F.; Ruiz, F.X.; Arnold, E.
Deposited on : 2025-03-06
Resolution : 1.92 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)

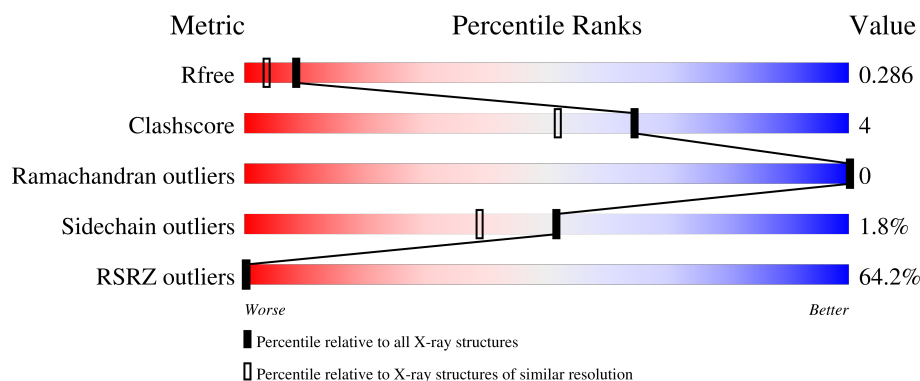
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	1007	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5034 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	565	4673	2945	836	858	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		
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		

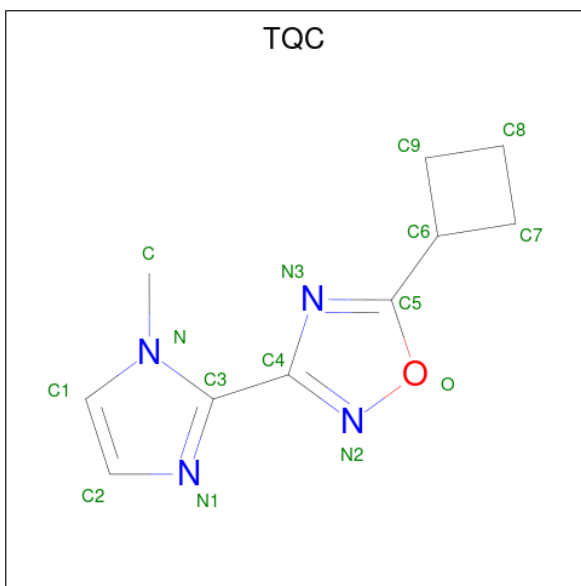
- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 7 is (3M)-5-cyclobutyl-3-(1-methyl-1H-imidazol-2-yl)-1,2,4-oxadiazole (CCD ID:

TQC) (formula: C₁₀H₁₂N₄O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			15	10	4	1		

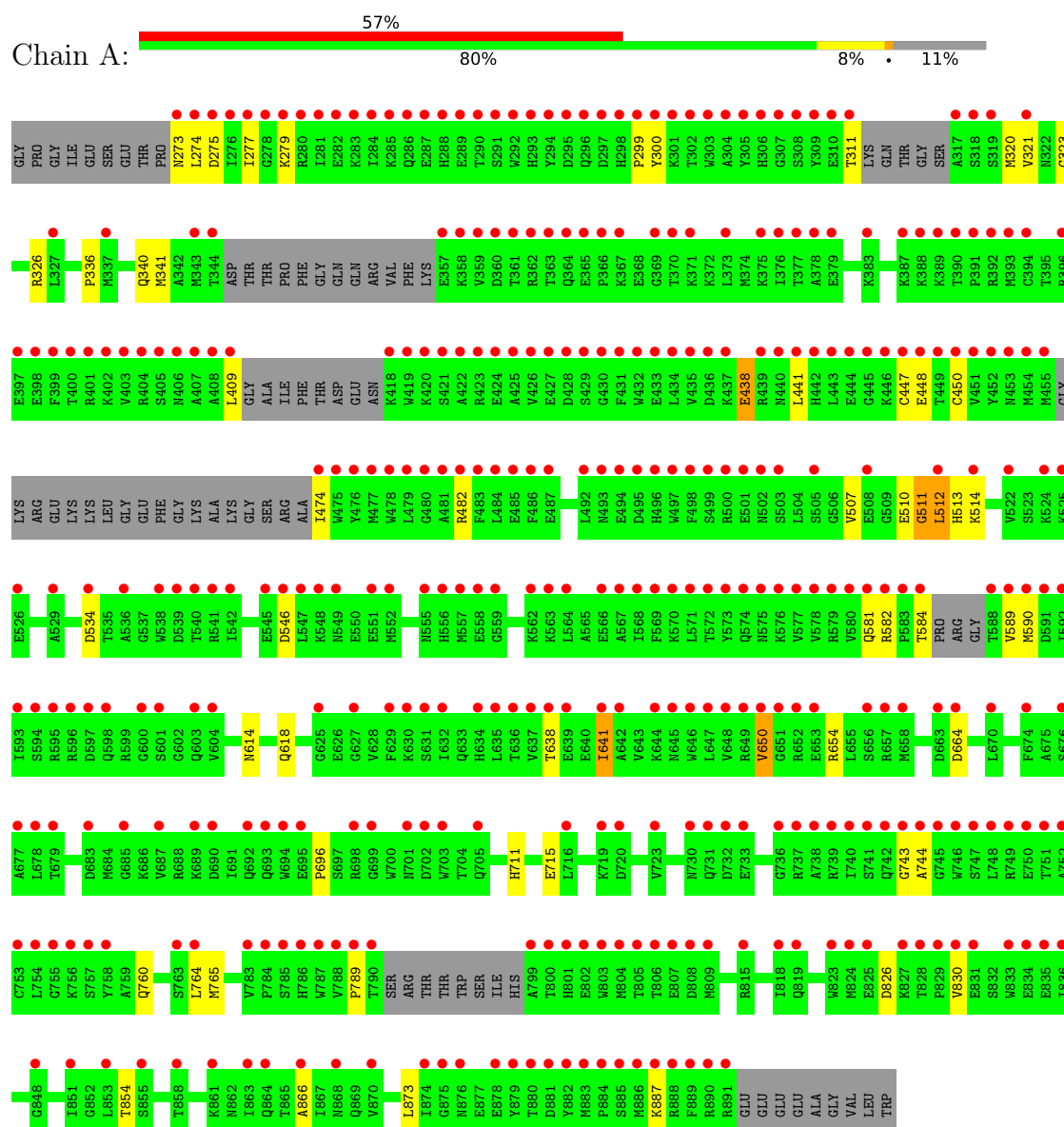
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	291	Total	O	0	0
			291	291		

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	82.76Å 116.49Å 147.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.39 – 1.92 91.39 – 1.92	Depositor EDS
% Data completeness (in resolution range)	98.1 (91.39-1.92) 98.2 (91.39-1.92)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 1.92Å)	Xtriage
Refinement program	REFMAC5	Depositor
R, R_{free}	0.200 , 0.247 0.273 , 0.286	Depositor DCC
R_{free} test set	2813 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	38.6	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 321.4	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	0.84	EDS
Total number of atoms	5034	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.01% 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, DMS, ZN, MES, PEG, TQC

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	2/4778 (0.0%)	1.37	4/6444 (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	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	696	PRO	C-O	-5.51	1.17	1.23
1	A	650	VAL	N-CA	5.17	1.50	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	511	GLY	CA-C-O	-7.06	116.37	121.88
1	A	854	THR	CA-CB-OG1	-5.71	101.04	109.60
1	A	866	ALA	N-CA-C	-5.16	105.35	111.69
1	A	546	ASP	CA-CB-CG	5.14	117.74	112.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	511	GLY	Mainchain

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Mol	Chain	Res	Type	Group
1	A	512[B]	LEU	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	4673	0	4572	37	0
2	A	2	0	0	0	0
3	A	24	0	26	2	0
4	A	12	0	18	0	0
5	A	10	0	0	3	0
6	A	7	0	10	0	0
7	A	15	0	0	0	0
8	A	291	0	0	3	1
All	All	5034	0	4626	37	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 (37) 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:664:ASP:OD1	5:A:1007:PO4:O4	2.00	0.78
1:A:323:GLY:HA3	3:A:1003[B]:MES:H71	1.66	0.77
1:A:638:THR:O	1:A:641:ILE:HG22	1.85	0.76
1:A:744:ALA:C	8:A:1133:HOH:O	2.40	0.65
1:A:664:ASP:OD1	5:A:1007:PO4:P	2.57	0.62
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.43	0.58
1:A:510:GLU:O	1:A:514:LYS:HG3	2.05	0.56
1:A:299:PRO:HD3	1:A:582:ARG:CZ	2.38	0.53
1:A:826:ASP:OD1	1:A:826:ASP:C	2.52	0.53
1:A:873:LEU:HD13	3:A:1003[B]:MES:H62	1.91	0.53
1:A:512[B]:LEU:HD11	1:A:711:HIS:CE1	2.44	0.52
1:A:409:LEU:HD22	8:A:1389:HOH:O	2.11	0.51
1:A:513:HIS:HB3	1:A:765:MET:HE1	1.93	0.50
1:A:336:PRO:O	1:A:340:GLN:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:PRO:HD2	1:A:300:TYR:CE2	2.47	0.49
1:A:274:LEU:HA	1:A:277:ILE:CG1	2.45	0.47
1:A:274:LEU:HA	1:A:277:ILE:HG12	1.97	0.47
1:A:438:GLU:HG2	8:A:1327:HOH:O	2.15	0.45
1:A:438:GLU:O	1:A:441:LEU:HB2	2.16	0.45
1:A:512[A]:LEU:HD21	1:A:711:HIS:NE2	2.31	0.45
1:A:764:LEU:O	1:A:765:MET:HE2	2.17	0.44
1:A:273:ASN:N	1:A:275:ASP:OD1	2.50	0.44
1:A:614:ASN:O	1:A:618:GLN:HG2	2.18	0.44
1:A:534:ASP:OD1	5:A:1007:PO4:O4	2.36	0.43
1:A:321:VAL:HG11	1:A:326:ARG:CZ	2.49	0.43
1:A:760:GLN:NE2	1:A:789:PRO:HG3	2.34	0.43
1:A:279:LYS:HE3	1:A:448:GLU:HB2	2.01	0.42
1:A:273:ASN:O	1:A:277:ILE:HG12	2.19	0.42
1:A:311:THR:HG21	1:A:590:MET:HE2	2.02	0.42
1:A:582:ARG:HG2	1:A:584:THR:OG1	2.19	0.42
1:A:507:VAL:C	1:A:510:GLU:HG2	2.45	0.41
1:A:341:MET:HE2	1:A:341:MET:HB3	1.80	0.41
1:A:299:PRO:HD3	1:A:582:ARG:NH1	2.35	0.41
1:A:650:VAL:O	1:A:654:ARG:HG2	2.20	0.40
1:A:320:MET:HG3	1:A:743:GLY:O	2.21	0.40
1:A:438:GLU:OE1	1:A:450:CYS:SG	2.79	0.40
1:A:275:ASP:OD1	1:A:275:ASP:N	2.54	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)
8:A:1279:HOH:O	8:A:1279:HOH:O[4_545]	2.16	0.04

5.3 Torsion angles

5.3.1 Protein backbone

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	557/637 (87%)	524 (94%)	33 (6%)	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	502/554 (91%)	493 (98%)	9 (2%)	51	39

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	438	GLU
1	A	474	ILE
1	A	482	ARG
1	A	581	GLN
1	A	589	VAL
1	A	641	ILE
1	A	715	GLU
1	A	830	VAL
1	A	887	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	819	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 2 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	$\# Z > 2$
4	DMS	A	1004	-	3,3,3	0.21	0	3,3,3	0.14	0
5	PO4	A	1007	-	4,4,4	2.77	2 (50%)	6,6,6	0.89	0
3	MES	A	1003[A]	-	12,12,12	0.72	0	15,16,16	0.29	0
4	DMS	A	1005	-	3,3,3	0.30	0	3,3,3	0.06	0
4	DMS	A	1006	-	3,3,3	0.18	0	3,3,3	0.29	0
7	TQC	A	1010	-	17,17,17	0.20	0	17,24,24	0.64	0
5	PO4	A	1008	-	4,4,4	0.83	0	6,6,6	0.43	0
6	PEG	A	1009	-	6,6,6	0.17	0	5,5,5	0.14	0
3	MES	A	1003[B]	-	12,12,12	0.70	0	15,16,16	0.28	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	-	-	3/4/4/4	-
7	TQC	A	1010	-	-	0/4/14/14	0/3/3/3
3	MES	A	1003[B]	-	-	0/6/14/14	0/1/1/1
3	MES	A	1003[A]	-	-	0/6/14/14	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1007	PO4	P-O1	4.18	1.60	1.50
5	A	1007	PO4	P-O2	2.94	1.63	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

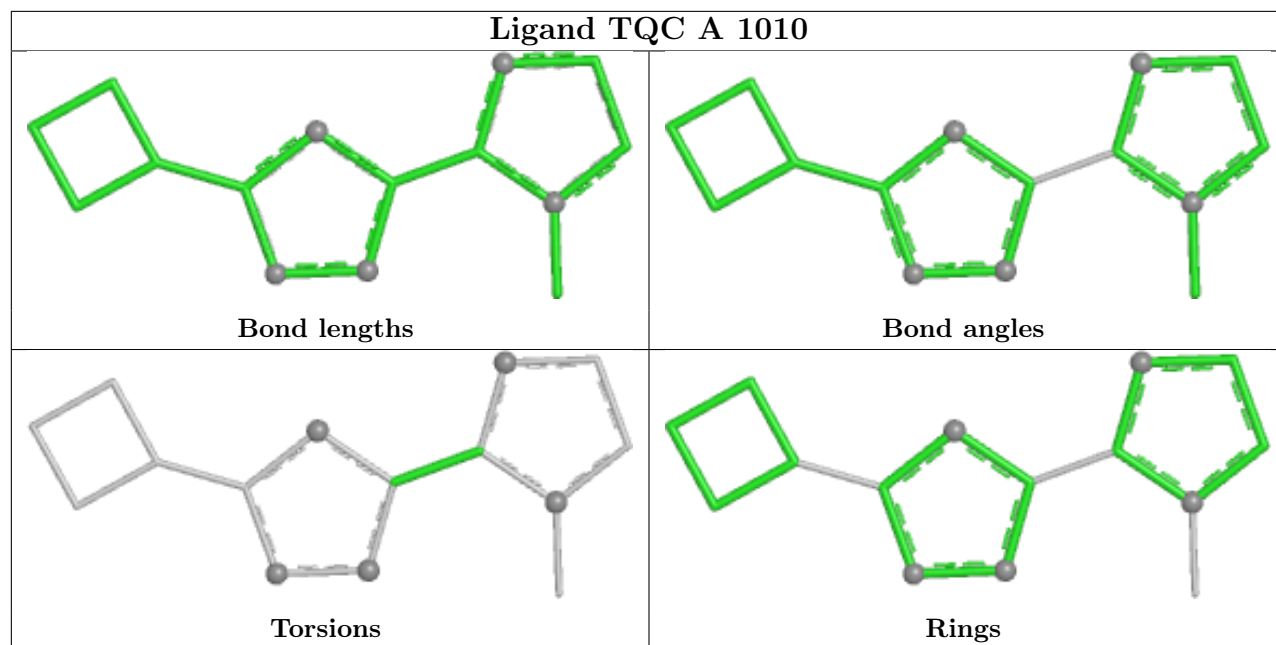
Mol	Chain	Res	Type	Atoms
6	A	1009	PEG	O2-C3-C4-O4
6	A	1009	PEG	C4-C3-O2-C2
6	A	1009	PEG	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1007	PO4	3	0
3	A	1003[B]	MES	2	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	565/637 (88%)	4.85	363 (64%) 0 0	6, 41, 99, 141	158 (27%)

All (363) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	309	TYR	17.0
1	A	284	ILE	16.8
1	A	292	TRP	16.5
1	A	425	ALA	16.4
1	A	426	VAL	16.0
1	A	592	ILE	15.6
1	A	801[A]	HIS	15.3
1	A	403	VAL	15.1
1	A	478	TRP	15.1
1	A	787	TRP	14.9
1	A	431	PHE	14.8
1	A	593	ILE	14.8
1	A	748	LEU	14.7
1	A	790	THR	14.4
1	A	303	TRP	14.3
1	A	311	THR	14.1
1	A	409	LEU	14.0
1	A	443	LEU	14.0
1	A	763[A]	SER	13.9
1	A	419	TRP	13.8
1	A	430	GLY	13.8
1	A	736	GLY	13.8
1	A	785[A]	SER	13.6
1	A	805	THR	13.6
1	A	746	TRP	13.5
1	A	578	VAL	13.5
1	A	400	THR	13.4

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Mol	Chain	Res	Type	RSRZ
1	A	486	PHE	13.2
1	A	738	ALA	13.1
1	A	758	TYR	13.0
1	A	294	TYR	13.0
1	A	755	GLY	12.9
1	A	589	VAL	12.8
1	A	321	VAL	12.8
1	A	359	VAL	12.8
1	A	452	TYR	12.6
1	A	474	ILE	12.5
1	A	542	ILE	12.5
1	A	391	PRO	12.3
1	A	291	SER	12.3
1	A	293	HIS	12.2
1	A	583	PRO	12.2
1	A	319	SER	12.1
1	A	283	LYS	12.1
1	A	740	ILE	11.9
1	A	806	THR	11.9
1	A	808	ASP	11.9
1	A	747	SER	11.9
1	A	367	LYS	11.9
1	A	751	THR	11.7
1	A	757	SER	11.7
1	A	512[A]	LEU	11.7
1	A	600	GLY	11.7
1	A	752	ALA	11.7
1	A	788	VAL	11.7
1	A	475	TRP	11.6
1	A	445	GLY	11.5
1	A	809	MET	11.4
1	A	753	CYS	11.4
1	A	591	ASP	11.4
1	A	789	PRO	11.4
1	A	505	SER	11.3
1	A	366	PRO	11.3
1	A	731	GLN	11.2
1	A	754	LEU	11.1
1	A	402	LYS	11.1
1	A	804	MET	11.1
1	A	318	SER	11.0
1	A	732	ASP	11.0

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Mol	Chain	Res	Type	RSRZ
1	A	594	SER	11.0
1	A	540	THR	10.9
1	A	302	THR	10.9
1	A	387	LYS	10.8
1	A	575	ASN	10.7
1	A	305	TYR	10.6
1	A	603	GLN	10.6
1	A	880	THR	10.6
1	A	304	ALA	10.6
1	A	388	LYS	10.6
1	A	499	SER	10.5
1	A	454	MET	10.5
1	A	401	ARG	10.4
1	A	498	PHE	10.4
1	A	656	SER	10.3
1	A	739	ARG	10.3
1	A	477	MET	10.3
1	A	595	ARG	10.3
1	A	636	THR	10.2
1	A	453	ASN	10.2
1	A	800	THR	10.2
1	A	576	LYS	10.1
1	A	306	HIS	10.1
1	A	485	GLU	10.0
1	A	481	ALA	10.0
1	A	737	ARG	10.0
1	A	392	ARG	9.9
1	A	694	TRP	9.8
1	A	745	GLY	9.7
1	A	807	GLU	9.6
1	A	429	SER	9.6
1	A	500	ARG	9.6
1	A	541	ARG	9.5
1	A	802	GLU	9.5
1	A	476	TYR	9.5
1	A	584	THR	9.5
1	A	744	ALA	9.5
1	A	424	GLU	9.5
1	A	298	HIS	9.5
1	A	389	LYS	9.5
1	A	539	ASP	9.4
1	A	730	ASN	9.4

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Mol	Chain	Res	Type	RSRZ
1	A	749	ARG	9.3
1	A	358	LYS	9.3
1	A	733	GLU	9.3
1	A	428	ASP	9.2
1	A	799	ALA	9.2
1	A	484	LEU	9.2
1	A	448	GLU	9.2
1	A	295	ASP	9.1
1	A	282	GLU	9.0
1	A	548	LYS	9.0
1	A	551	GLU	9.0
1	A	657	ARG	8.9
1	A	406	ASN	8.9
1	A	433	GLU	8.9
1	A	317	ALA	8.9
1	A	635	LEU	8.8
1	A	393	MET	8.8
1	A	503	SER	8.7
1	A	290	THR	8.7
1	A	285	LYS	8.7
1	A	364	GLN	8.6
1	A	719[A]	LYS	8.6
1	A	658	MET	8.5
1	A	756	LYS	8.5
1	A	741	SER	8.5
1	A	408	ALA	8.4
1	A	705	GLN	8.4
1	A	365	GLU	8.4
1	A	487	GLU	8.3
1	A	596	ARG	8.3
1	A	598	GLN	8.3
1	A	404	ARG	8.3
1	A	525	LYS	8.2
1	A	344	THR	8.2
1	A	441	LEU	8.1
1	A	884	PRO	8.1
1	A	502	ASN	8.1
1	A	423	ARG	7.9
1	A	286	GLN	7.9
1	A	455	MET	7.8
1	A	390	THR	7.8
1	A	310	GLU	7.8

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Mol	Chain	Res	Type	RSRZ
1	A	579	ARG	7.7
1	A	693	GLN	7.7
1	A	405	SER	7.5
1	A	882	TYR	7.5
1	A	275	ASP	7.5
1	A	362	ARG	7.4
1	A	300	TYR	7.4
1	A	690	ASP	7.3
1	A	864[A]	GLN	7.2
1	A	446	LYS	7.2
1	A	743	GLY	7.2
1	A	287	GLU	7.2
1	A	422	ALA	7.1
1	A	449	THR	7.0
1	A	420	LYS	7.0
1	A	418	LYS	7.0
1	A	296	GLN	7.0
1	A	597	ASP	6.8
1	A	649	ARG	6.8
1	A	639	GLU	6.7
1	A	653	GLU	6.7
1	A	297	ASP	6.7
1	A	274	LEU	6.7
1	A	750	GLU	6.6
1	A	692	GLN	6.6
1	A	299	PRO	6.6
1	A	891	ARG	6.5
1	A	427	GLU	6.3
1	A	279	LYS	6.3
1	A	742	GLN	6.2
1	A	881	ASP	6.2
1	A	588	THR	6.2
1	A	289	GLU	6.1
1	A	281	ILE	6.0
1	A	288	HIS	6.0
1	A	301	LYS	5.9
1	A	357	GLU	5.9
1	A	277	ILE	5.9
1	A	637	VAL	5.9
1	A	407	ALA	5.8
1	A	582	ARG	5.8
1	A	883	MET	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	648	VAL	5.8
1	A	641	ILE	5.8
1	A	630	LYS	5.7
1	A	701	ASN	5.7
1	A	568	ILE	5.6
1	A	363	THR	5.5
1	A	678	LEU	5.5
1	A	889	PHE	5.5
1	A	890	ARG	5.4
1	A	444	GLU	5.3
1	A	887	LYS	5.2
1	A	435	VAL	5.2
1	A	888	ARG	5.2
1	A	276	ILE	5.1
1	A	885	SER	5.1
1	A	501	GLU	5.0
1	A	571	LEU	5.0
1	A	563	LYS	5.0
1	A	564	LEU	4.9
1	A	434	LEU	4.9
1	A	644	LYS	4.9
1	A	825	GLU	4.8
1	A	440	ASN	4.8
1	A	555	ASN	4.8
1	A	570	LYS	4.7
1	A	534	ASP	4.7
1	A	677	ALA	4.6
1	A	876	ASN	4.6
1	A	396	ARG	4.5
1	A	494	GLU	4.5
1	A	879	TYR	4.5
1	A	830	VAL	4.4
1	A	634	HIS	4.3
1	A	558	GLU	4.3
1	A	670	LEU	4.3
1	A	886	MET	4.2
1	A	572	THR	4.1
1	A	432	TRP	4.0
1	A	689	LYS	4.0
1	A	480	GLY	4.0
1	A	642	ALA	3.9
1	A	833	TRP	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	307	GLY	3.8
1	A	360	ASP	3.8
1	A	383	LYS	3.8
1	A	853	LEU	3.8
1	A	549	ASN	3.7
1	A	421	SER	3.7
1	A	601	SER	3.7
1	A	538	TRP	3.7
1	A	647	LEU	3.7
1	A	577	VAL	3.7
1	A	398	GLU	3.6
1	A	399	PHE	3.6
1	A	308	SER	3.6
1	A	273	ASN	3.6
1	A	835	GLU	3.5
1	A	878	GLU	3.5
1	A	590	MET	3.5
1	A	663	ASP	3.5
1	A	361	THR	3.5
1	A	855	SER	3.4
1	A	638	THR	3.4
1	A	815	ARG	3.4
1	A	834	GLU	3.4
1	A	703	TRP	3.4
1	A	581	GLN	3.4
1	A	479	LEU	3.4
1	A	442	HIS	3.4
1	A	524	LYS	3.4
1	A	683	ASP	3.4
1	A	529	ALA	3.3
1	A	629	PHE	3.3
1	A	828	THR	3.3
1	A	861	LYS	3.3
1	A	559	GLY	3.3
1	A	625	GLY	3.3
1	A	343	MET	3.3
1	A	764	LEU	3.3
1	A	451	VAL	3.2
1	A	439	ARG	3.2
1	A	870	VAL	3.2
1	A	370	THR	3.2
1	A	562	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	631	SER	3.2
1	A	545	GLU	3.2
1	A	278	GLY	3.1
1	A	699	GLY	3.1
1	A	369	GLY	3.1
1	A	604	VAL	3.1
1	A	824	MET	3.1
1	A	394	CYS	3.1
1	A	556	HIS	3.1
1	A	698	ARG	3.0
1	A	547	LEU	3.0
1	A	674	PHE	3.0
1	A	493	ASN	3.0
1	A	508	GLU	3.0
1	A	379	GLU	2.9
1	A	566	GLU	2.9
1	A	514	LYS	2.9
1	A	803	TRP	2.9
1	A	863	ILE	2.8
1	A	377	THR	2.8
1	A	580	VAL	2.8
1	A	337	MET	2.8
1	A	492	LEU	2.8
1	A	632	ILE	2.8
1	A	375	LYS	2.8
1	A	831	GLU	2.8
1	A	818	ILE	2.8
1	A	646	TRP	2.7
1	A	627	GLY	2.7
1	A	376	ILE	2.7
1	A	397	GLU	2.7
1	A	695	GLU	2.7
1	A	496	HIS	2.7
1	A	436	ASP	2.6
1	A	645	ASN	2.6
1	A	866	ALA	2.6
1	A	437	LYS	2.6
1	A	497	TRP	2.6
1	A	784	PRO	2.6
1	A	868	ASN	2.6
1	A	569	PHE	2.6
1	A	819	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	522	VAL	2.6
1	A	447	CYS	2.5
1	A	482	ARG	2.5
1	A	676	SER	2.5
1	A	679	THR	2.5
1	A	526	GLU	2.5
1	A	829	PRO	2.5
1	A	573	TYR	2.4
1	A	652	ARG	2.4
1	A	851	ILE	2.4
1	A	327	LEU	2.4
1	A	567	ALA	2.4
1	A	650	VAL	2.4
1	A	858	THR	2.3
1	A	827	LYS	2.3
1	A	702	ASP	2.3
1	A	552	MET	2.3
1	A	651	GLY	2.3
1	A	687	VAL	2.3
1	A	720	ASP	2.3
1	A	280	ARG	2.3
1	A	786	HIS	2.3
1	A	716	LEU	2.3
1	A	685	GLY	2.2
1	A	848	GLY	2.2
1	A	495	ASP	2.2
1	A	783	VAL	2.2
1	A	546	ASP	2.2
1	A	723	VAL	2.2
1	A	378	ALA	2.2
1	A	371	LYS	2.2
1	A	483	PHE	2.1
1	A	373	LEU	2.1
1	A	823	TRP	2.1
1	A	574	GLN	2.1
1	A	874	ILE	2.1
1	A	450	CYS	2.1
1	A	557	MET	2.0
1	A	536	ALA	2.0
1	A	664	ASP	2.0
1	A	836	ILE	2.0
1	A	875	GLY	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](#)

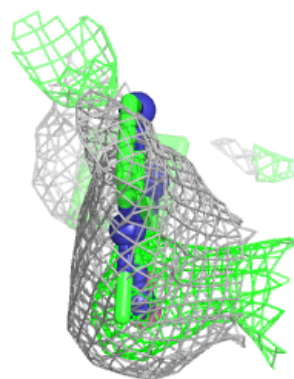
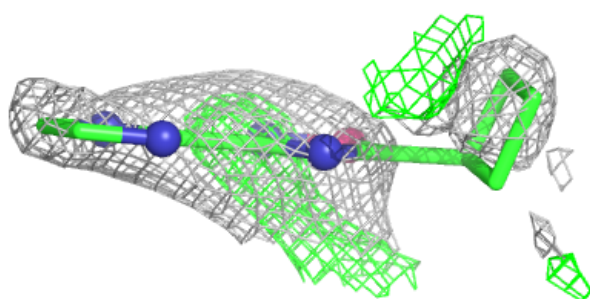
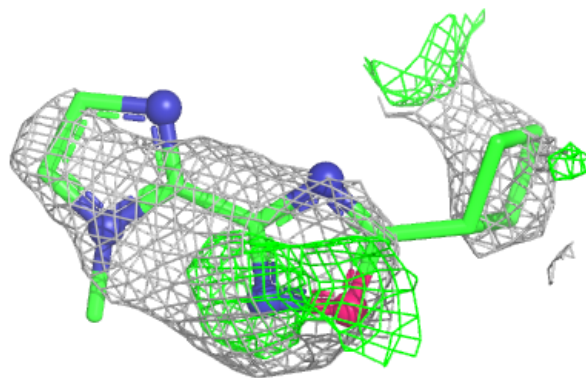
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PO4	A	1008	5/5	0.69	0.18	94,100,113,122	0
7	TQC	A	1010	15/15	0.74	0.37	47,49,50,52	15
4	DMS	A	1005	4/4	0.78	0.30	103,118,121,134	0
5	PO4	A	1007	5/5	0.79	0.17	48,51,74,88	0
6	PEG	A	1009	7/7	0.83	0.18	65,76,85,86	0
4	DMS	A	1006	4/4	0.89	0.14	65,72,72,80	0
3	MES	A	1003[A]	12/12	0.90	0.28	81,101,574,578	12
3	MES	A	1003[B]	12/12	0.90	0.28	3,27,40,45	12
4	DMS	A	1004	4/4	0.91	0.18	82,86,86,105	0
2	ZN	A	1002	1/1	0.99	0.03	64,64,64,64	0
2	ZN	A	1001	1/1	1.00	0.03	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.

Electron density around TQC 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 [i](#)

There are no such residues in this entry.