



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:29 PM UTC

PDB ID : 7I2P / pdb_00007i2p
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 Z221421630 (DNV2_NS5A-x0644)
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 : 1.76 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)

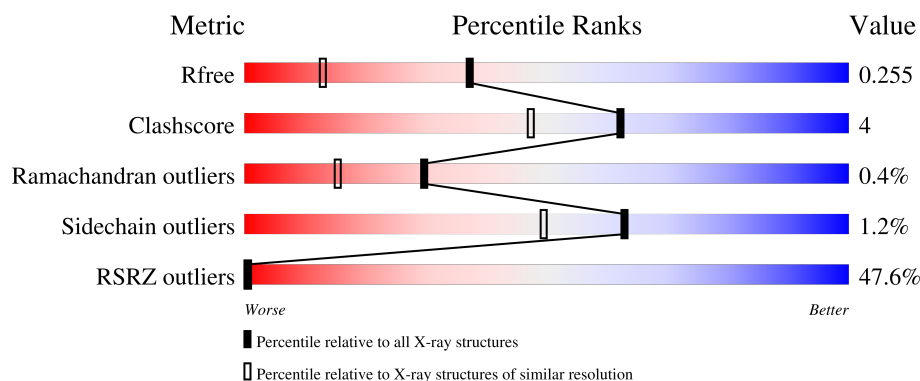
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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
6	PO4	A	1008	-	X	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 5159 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.

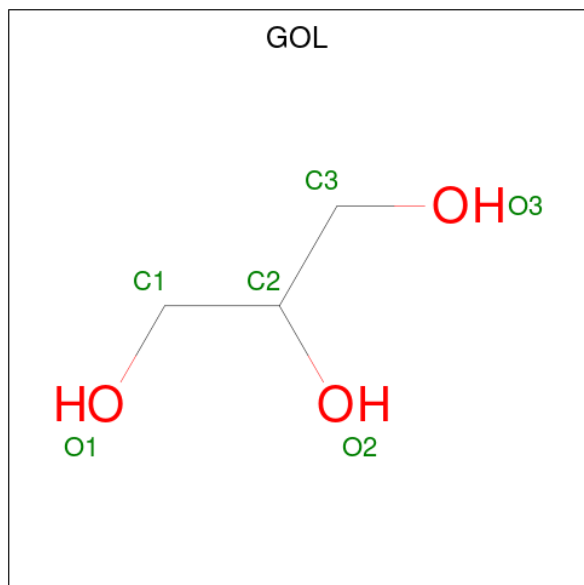
- Molecule 1 is a protein called NS5 RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	574	4740	2984	850	872	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 GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

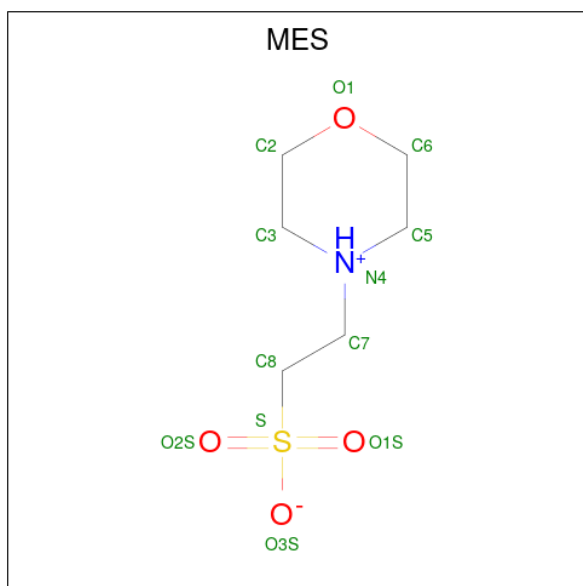


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	6	3	3	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

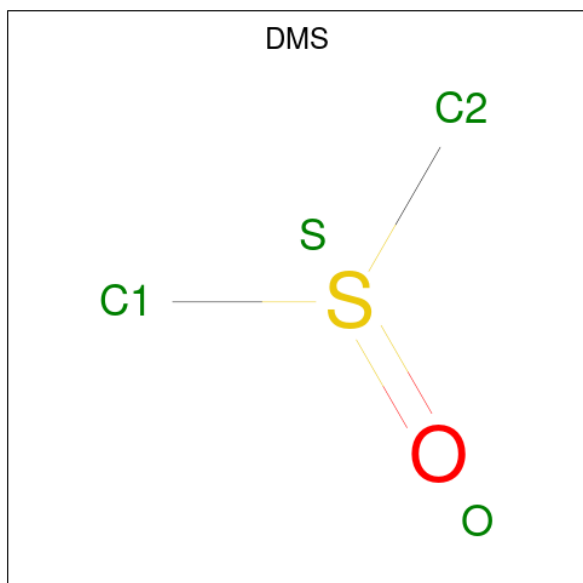
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Zn	0	0
			2	2		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



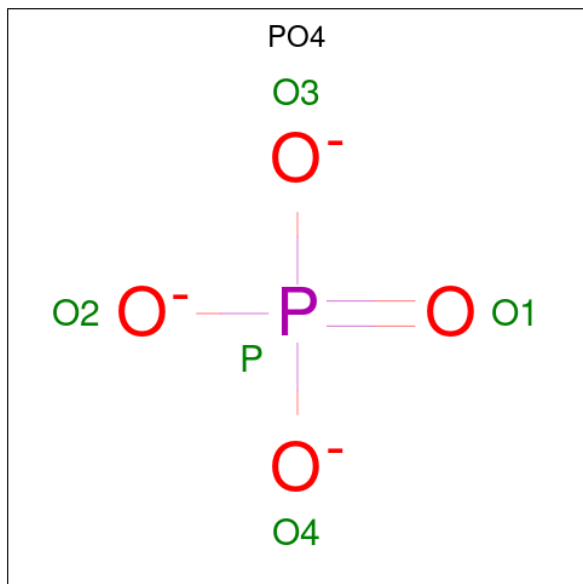
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	1
			24	12	2	8	2		

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



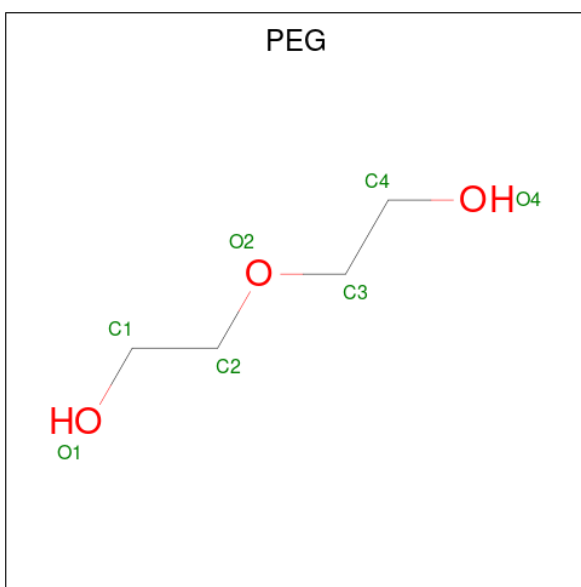
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



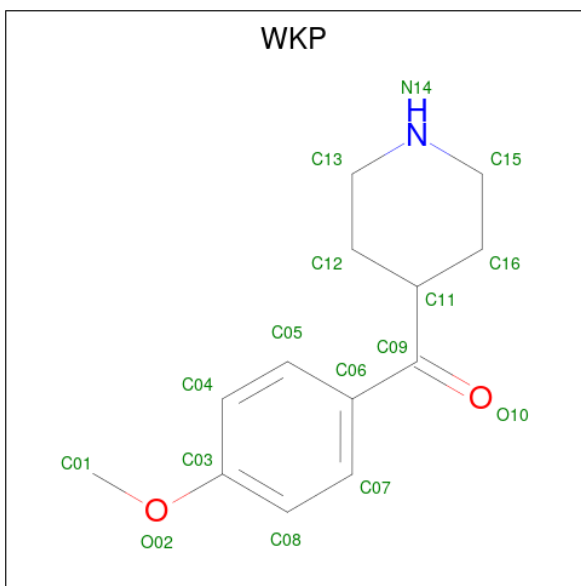
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 8 is (4-methoxyphenyl)(piperidin-4-yl)methanone (CCD ID: WKP) (formula: $C_{13}H_{17}NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			16	13	1	2		

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

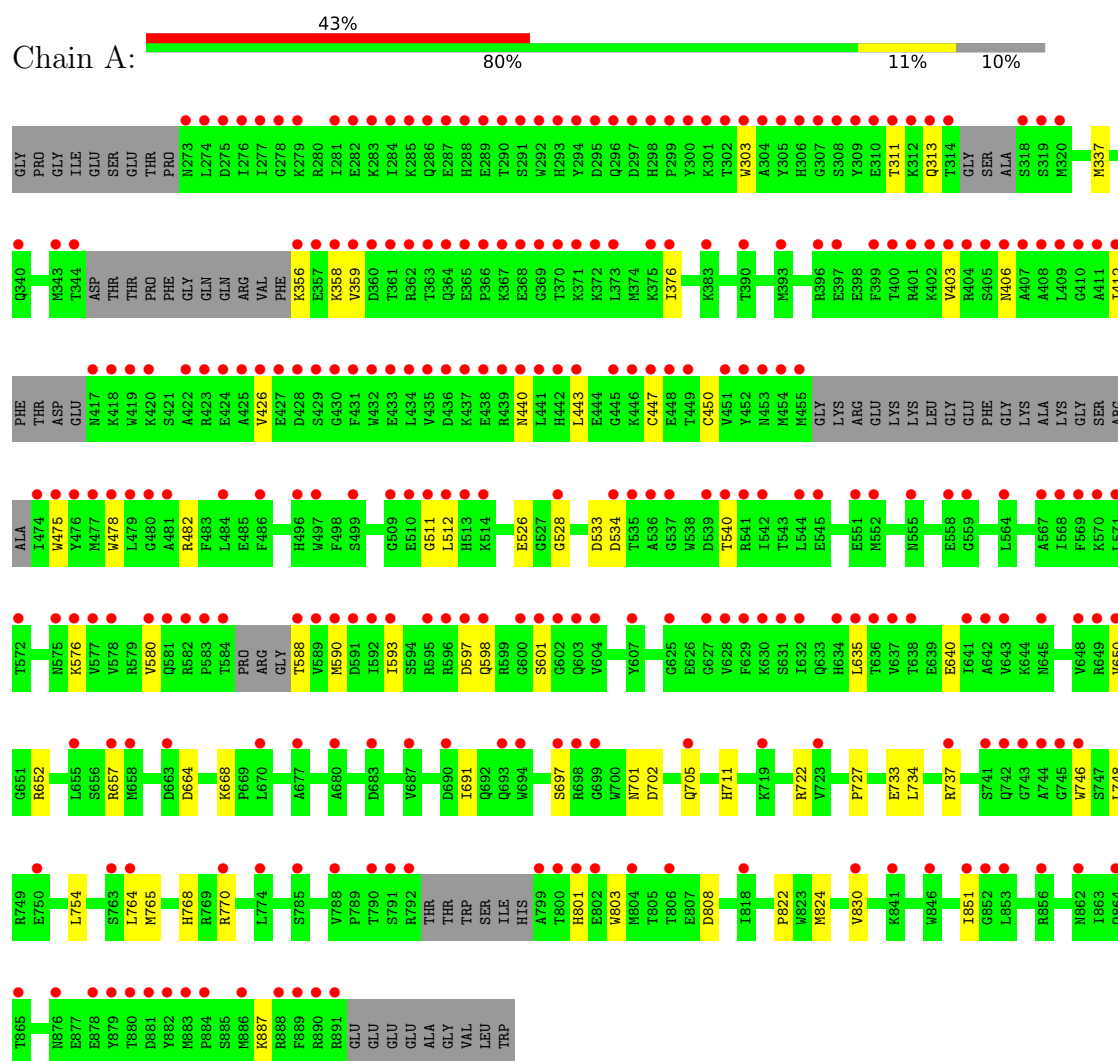
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	341	Total 341	O 341	0	0

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	82.38Å 115.92Å 146.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.90 – 1.76 57.90 – 1.76	Depositor EDS
% Data completeness (in resolution range)	98.8 (57.90-1.76) 98.9 (57.90-1.76)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.185 , 0.224 0.228 , 0.255	Depositor DCC
R_{free} test set	3570 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 80.7	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	0.92	EDS
Total number of atoms	5159	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.87% 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: PEG, WKP, DMS, PO4, CL, MES, ZN, GOL

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	1.11	5/4844 (0.1%)	1.34	6/6530 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	822	PRO	C-O	-5.54	1.16	1.24
1	A	768	HIS	CE1-NE2	5.28	1.37	1.32
1	A	376	ILE	C-O	5.12	1.29	1.24
1	A	734	LEU	C-O	5.10	1.30	1.24
1	A	650	VAL	N-CA	5.00	1.50	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	650	VAL	CA-C-N	6.14	126.93	119.99
1	A	650	VAL	C-N-CA	6.14	126.93	119.99
1	A	702	ASP	CA-CB-CG	5.59	118.19	112.60
1	A	511	GLY	CA-C-O	-5.36	117.16	121.77
1	A	691	ILE	CA-C-O	-5.17	116.61	120.96
1	A	652	ARG	N-CA-C	-5.01	105.89	111.36

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	4740	0	4649	36	0
2	A	6	0	8	0	0
3	A	2	0	0	0	0
4	A	24	0	26	1	0
5	A	12	0	18	3	0
6	A	10	0	0	3	0
7	A	7	0	10	0	0
8	A	16	0	0	0	0
9	A	1	0	0	0	0
10	A	341	0	0	5	2
All	All	5159	0	4711	39	2

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 (39) 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	6:A:1008:PO4:O4	1.91	0.87
5:A:1005:DMS:H11	10:A:1241:HOH:O	1.84	0.77
5:A:1005:DMS:H12	10:A:1262:HOH:O	1.91	0.71
1:A:534:ASP:OD1	6:A:1008:PO4:O4	2.14	0.65
1:A:403:VAL:HG21	1:A:426:VAL:HG21	1.80	0.63
1:A:664:ASP:OD1	6:A:1008:PO4:P	2.61	0.58
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.44	0.57
1:A:475:TRP:HZ3	1:A:576:LYS:HD3	1.69	0.57
1:A:764:LEU:O	1:A:765:MET:HE2	2.06	0.56
1:A:412:ILE:HG12	1:A:478:TRP:HA	1.87	0.55
1:A:311:THR:HG21	1:A:590:MET:HE2	1.87	0.55
1:A:580:VAL:HG21	1:A:593:ILE:HD11	1.89	0.54
1:A:748:LEU:HD13	4:A:1004[B]:MES:H61	1.89	0.53
1:A:311:THR:HG21	1:A:590:MET:HB2	1.90	0.53
1:A:440:ASN:HA	1:A:443:LEU:HD12	1.91	0.51
1:A:303:TRP:CE3	1:A:593:ILE:HD12	2.46	0.51
1:A:528:GLY:O	1:A:668:LYS:HE3	2.13	0.49
1:A:764:LEU:C	1:A:765:MET:HE2	2.38	0.48
1:A:512[B]:LEU:HD11	1:A:711:HIS:CE1	2.48	0.48
1:A:533:ASP:OD2	1:A:697:SER:OG	2.24	0.47
1:A:337:MET:HG2	10:A:1331:HOH:O	2.15	0.46
1:A:526:GLU:O	1:A:657:ARG:NH2	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:LEU:HD23	1:A:640:GLU:HG2	1.97	0.46
5:A:1005:DMS:C1	10:A:1241:HOH:O	2.53	0.45
1:A:356:LYS:O	1:A:359:VAL:HG12	2.16	0.45
1:A:801:HIS:CD2	1:A:803:TRP:CZ2	3.05	0.45
1:A:733:GLU:O	1:A:737:ARG:HG3	2.17	0.44
1:A:358:LYS:HG3	1:A:540:THR:HG21	2.00	0.44
1:A:512[B]:LEU:HD22	1:A:727:PRO:HB3	2.00	0.43
1:A:597:ASP:O	1:A:598:GLN:HB2	2.19	0.43
1:A:303:TRP:HE1	1:A:359:VAL:HG22	1.82	0.43
1:A:770:ARG:HD2	1:A:851:ILE:HD13	2.02	0.42
1:A:801:HIS:HD2	1:A:803:TRP:CZ2	2.38	0.41
1:A:311:THR:O	1:A:588:THR:HB	2.19	0.41
1:A:764:LEU:HD12	1:A:764:LEU:HA	1.87	0.41
1:A:701:ASN:ND2	10:A:1105:HOH:O	2.37	0.41
1:A:576:LYS:NZ	1:A:597:ASP:O	2.55	0.40
1:A:722:ARG:HB3	1:A:824:MET:SD	2.62	0.40
1:A:746:TRP:CH2	1:A:754:LEU:HD22	2.56	0.40

All (2) 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)
10:A:1283:HOH:O	10:A:1374:HOH:O[2_545]	1.84	0.36
10:A:1132:HOH:O	10:A:1132:HOH:O[2_445]	1.91	0.29

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	566/637 (89%)	546 (96%)	18 (3%)	2 (0%)	30 15

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	313	GLN
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	510/554 (92%)	504 (99%)	6 (1%)	63 49

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	482	ARG
1	A	601	SER
1	A	705	GLN
1	A	808	ASP
1	A	830	VAL
1	A	887	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	417	ASN
1	A	603	GLN
1	A	645	ASN
1	A	786	HIS
1	A	801	HIS

5.3.3 RNA [i](#)

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 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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	DMS	A	1005	-	3,3,3	0.95	0	3,3,3	0.40	0
2	GOL	A	1001	-	5,5,5	0.09	0	5,5,5	0.23	0
8	WKP	A	1011	-	17,17,17	0.59	1 (5%)	20,22,22	0.62	0
6	PO4	A	1009	-	4,4,4	1.12	1 (25%)	6,6,6	0.38	0
7	PEG	A	1010	-	6,6,6	0.20	0	5,5,5	0.21	0
4	MES	A	1004[B]	-	12,12,12	1.05	1 (8%)	15,16,16	0.76	0
4	MES	A	1004[A]	-	12,12,12	0.72	0	15,16,16	0.35	0
6	PO4	A	1008	-	4,4,4	6.61	4 (100%)	6,6,6	1.08	1 (16%)
5	DMS	A	1006	-	3,3,3	0.24	0	3,3,3	0.14	0
5	DMS	A	1007	-	3,3,3	0.03	0	3,3,3	0.36	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
2	GOL	A	1001	-	-	4/4/4/4	-
8	WKP	A	1011	-	-	9/10/18/18	0/2/2/2
7	PEG	A	1010	-	-	2/4/4/4	-
4	MES	A	1004[B]	-	-	2/6/14/14	0/1/1/1
4	MES	A	1004[A]	-	-	3/6/14/14	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1008	PO4	P-O1	9.61	1.72	1.50
6	A	1008	PO4	P-O4	-7.02	1.34	1.54
6	A	1008	PO4	P-O2	4.48	1.67	1.54
6	A	1008	PO4	P-O3	3.61	1.65	1.54
4	A	1004[B]	MES	C8-S	2.61	1.81	1.77
8	A	1011	WKP	C11-C09	2.33	1.57	1.51
6	A	1009	PO4	P-O1	2.17	1.55	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1008	PO4	O4-P-O1	-2.15	103.33	110.95

There are no chirality outliers.

All (20) torsion outliers are listed below:

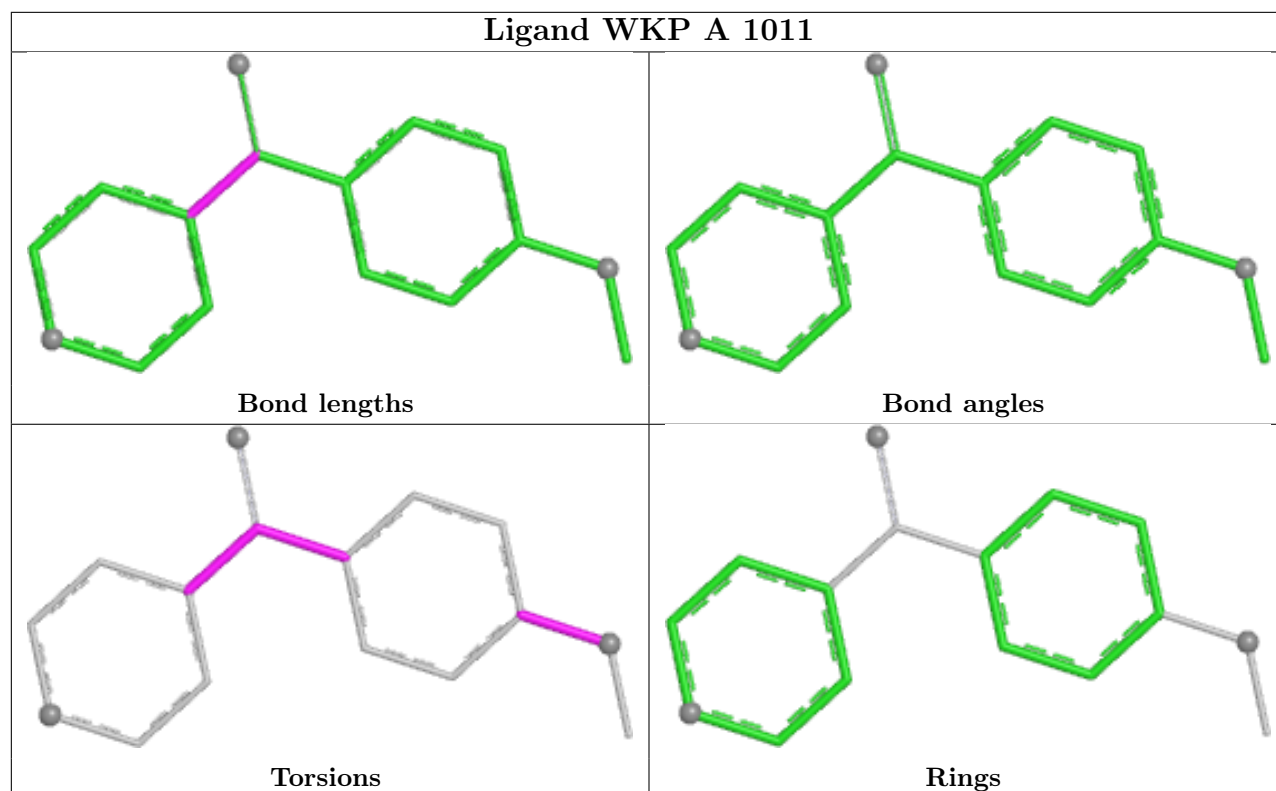
Mol	Chain	Res	Type	Atoms
2	A	1001	GOL	O1-C1-C2-O2
2	A	1001	GOL	O1-C1-C2-C3
2	A	1001	GOL	C1-C2-C3-O3
4	A	1004[A]	MES	C7-C8-S-O1S
4	A	1004[A]	MES	C7-C8-S-O3S
4	A	1004[B]	MES	C8-C7-N4-C3
8	A	1011	WKP	C06-C09-C11-C12
8	A	1011	WKP	O10-C09-C11-C12
8	A	1011	WKP	C05-C06-C09-C11
8	A	1011	WKP	C07-C06-C09-C11
8	A	1011	WKP	C05-C06-C09-O10
8	A	1011	WKP	C07-C06-C09-O10
7	A	1010	PEG	O2-C3-C4-O4
2	A	1001	GOL	O2-C2-C3-O3
4	A	1004[B]	MES	C8-C7-N4-C5
8	A	1011	WKP	C04-C03-O02-C01
4	A	1004[A]	MES	C7-C8-S-O2S
8	A	1011	WKP	C08-C03-O02-C01
7	A	1010	PEG	C4-C3-O2-C2
8	A	1011	WKP	C06-C09-C11-C16

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1005	DMS	3	0
4	A	1004[B]	MES	1	0
6	A	1008	PO4	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 ⓘ

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 ⓘ

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	574/637 (90%)	2.91	273 (47%) 0 0	7, 40, 89, 131	129 (22%)

All (273) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	475	TRP	14.6
1	A	637	VAL	13.5
1	A	432	TRP	13.0
1	A	799	ALA	12.9
1	A	512[A]	LEU	12.9
1	A	800	THR	12.8
1	A	419	TRP	12.7
1	A	281	ILE	12.1
1	A	441	LEU	12.0
1	A	719[A]	LYS	11.8
1	A	292	TRP	11.6
1	A	636	THR	11.5
1	A	511	GLY	11.1
1	A	655	LEU	10.9
1	A	276	ILE	10.9
1	A	426	VAL	10.9
1	A	412	ILE	10.7
1	A	474	ILE	10.7
1	A	407	ALA	10.6
1	A	774	LEU	10.6
1	A	542	ILE	10.6
1	A	580	VAL	10.2
1	A	435	VAL	10.2
1	A	431	PHE	10.2
1	A	476	TYR	10.1
1	A	277	ILE	10.1
1	A	851	ILE	9.9

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Mol	Chain	Res	Type	RSRZ
1	A	274	LEU	9.9
1	A	409	LEU	9.9
1	A	513	HIS	9.9
1	A	514	LYS	9.8
1	A	853	LEU	9.7
1	A	300	TYR	9.7
1	A	434	LEU	9.2
1	A	741[A]	SER	9.2
1	A	293	HIS	9.1
1	A	294	TYR	9.0
1	A	801	HIS	8.9
1	A	763[A]	SER	8.8
1	A	299	PRO	8.7
1	A	589	VAL	8.7
1	A	509	GLY	8.7
1	A	363	THR	8.6
1	A	451	VAL	8.6
1	A	852	GLY	8.6
1	A	600	GLY	8.5
1	A	405	SER	8.4
1	A	697	SER	8.2
1	A	400	THR	8.1
1	A	273	ASN	8.1
1	A	657	ARG	8.0
1	A	477	MET	7.9
1	A	410	GLY	7.9
1	A	430	GLY	7.8
1	A	510	GLU	7.8
1	A	537	GLY	7.7
1	A	303	TRP	7.7
1	A	588	THR	7.6
1	A	536	ALA	7.5
1	A	499	SER	7.5
1	A	453	ASN	7.4
1	A	439	ARG	7.4
1	A	705	GLN	7.3
1	A	411	ALA	7.3
1	A	602	GLY	7.3
1	A	449	THR	7.3
1	A	770	ARG	7.3
1	A	295	ASP	7.3
1	A	785[A]	SER	7.2

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Mol	Chain	Res	Type	RSRZ
1	A	540	THR	7.2
1	A	454	MET	7.1
1	A	698	ARG	7.1
1	A	601	SER	7.0
1	A	864[A]	GLN	7.0
1	A	408	ALA	6.9
1	A	658	MET	6.9
1	A	856	ARG	6.9
1	A	429	SER	6.8
1	A	744	ALA	6.7
1	A	308	SER	6.7
1	A	551	GLU	6.7
1	A	584	THR	6.7
1	A	298	HIS	6.7
1	A	418	LYS	6.6
1	A	802	GLU	6.6
1	A	541	ARG	6.6
1	A	402	LYS	6.6
1	A	404	ARG	6.5
1	A	288	HIS	6.5
1	A	367	LYS	6.5
1	A	406	ASN	6.5
1	A	396	ARG	6.5
1	A	302	THR	6.4
1	A	806	THR	6.4
1	A	291	SER	6.4
1	A	581	GLN	6.3
1	A	383	LYS	6.3
1	A	583	PRO	6.3
1	A	437	LYS	6.3
1	A	746	TRP	6.3
1	A	278	GLY	6.2
1	A	582	ARG	6.1
1	A	284	ILE	6.1
1	A	452	TYR	6.1
1	A	279	LYS	6.1
1	A	359	VAL	6.0
1	A	311	THR	6.0
1	A	534	ASP	5.9
1	A	275	ASP	5.9
1	A	591	ASP	5.9
1	A	590	MET	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	283	LYS	5.8
1	A	438	GLU	5.8
1	A	301	LYS	5.7
1	A	433	GLU	5.7
1	A	397	GLU	5.7
1	A	455	MET	5.5
1	A	423	ARG	5.5
1	A	880	THR	5.5
1	A	436	ASP	5.5
1	A	403	VAL	5.4
1	A	693	GLN	5.3
1	A	539	ASP	5.3
1	A	440	ASN	5.2
1	A	286	GLN	5.2
1	A	479	LEU	5.2
1	A	422	ALA	5.2
1	A	742	GLN	5.2
1	A	596	ARG	5.2
1	A	595	ARG	5.2
1	A	841	LYS	5.1
1	A	603	GLN	5.0
1	A	282	GLU	5.0
1	A	356	LYS	4.8
1	A	481	ALA	4.8
1	A	478	TRP	4.8
1	A	635	LEU	4.8
1	A	428	ASP	4.7
1	A	792	ARG	4.6
1	A	687	VAL	4.6
1	A	289	GLU	4.5
1	A	592	ILE	4.5
1	A	309	TYR	4.5
1	A	357	GLU	4.4
1	A	442	HIS	4.4
1	A	362	ARG	4.4
1	A	694	TRP	4.3
1	A	318	SER	4.3
1	A	366	PRO	4.3
1	A	745	GLY	4.2
1	A	364	GLN	4.2
1	A	641	ILE	4.2
1	A	791	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	420	LYS	4.2
1	A	544	LEU	4.1
1	A	677	ALA	4.0
1	A	305	TYR	4.0
1	A	572	THR	4.0
1	A	344	THR	4.0
1	A	648	VAL	4.0
1	A	287	GLU	3.9
1	A	889	PHE	3.9
1	A	290	THR	3.9
1	A	627	GLY	3.9
1	A	484	LEU	3.8
1	A	319	SER	3.8
1	A	634	HIS	3.7
1	A	593	ILE	3.7
1	A	882	TYR	3.7
1	A	629	PHE	3.7
1	A	638	THR	3.6
1	A	304	ALA	3.6
1	A	750	GLU	3.6
1	A	296	GLN	3.6
1	A	790	THR	3.6
1	A	571	LEU	3.6
1	A	443	LEU	3.5
1	A	312	LYS	3.4
1	A	314	THR	3.4
1	A	297	ASP	3.4
1	A	604	VAL	3.4
1	A	888	ARG	3.4
1	A	650	VAL	3.4
1	A	447	CYS	3.4
1	A	643	VAL	3.3
1	A	393	MET	3.3
1	A	804	MET	3.3
1	A	670	LEU	3.3
1	A	569	PHE	3.2
1	A	313	GLN	3.2
1	A	417	ASN	3.2
1	A	876	ASN	3.1
1	A	448	GLU	3.1
1	A	743	GLY	3.1
1	A	361	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	445	GLY	3.0
1	A	865	THR	3.0
1	A	425	ALA	3.0
1	A	879	TYR	2.9
1	A	373	LEU	2.9
1	A	564	LEU	2.9
1	A	597	ASP	2.9
1	A	649	ARG	2.9
1	A	555	ASN	2.9
1	A	570	LYS	2.9
1	A	884	PRO	2.9
1	A	699	GLY	2.8
1	A	642	ALA	2.8
1	A	567	ALA	2.8
1	A	545	GLU	2.8
1	A	764	LEU	2.8
1	A	399	PHE	2.7
1	A	497	TRP	2.7
1	A	632	ILE	2.7
1	A	575	ASN	2.7
1	A	368	GLU	2.7
1	A	578	VAL	2.6
1	A	830	VAL	2.6
1	A	663	ASP	2.6
1	A	558	GLU	2.6
1	A	343	MET	2.6
1	A	307	GLY	2.6
1	A	723	VAL	2.6
1	A	598	GLN	2.6
1	A	577	VAL	2.6
1	A	358	LYS	2.6
1	A	680	ALA	2.6
1	A	480	GLY	2.5
1	A	690	ASP	2.5
1	A	486	PHE	2.5
1	A	628	VAL	2.5
1	A	310	GLU	2.5
1	A	645	ASN	2.5
1	A	607	TYR	2.5
1	A	340	GLN	2.5
1	A	881	ASP	2.5
1	A	625	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	285	LYS	2.5
1	A	424	GLU	2.4
1	A	559	GLY	2.4
1	A	886	MET	2.4
1	A	862	ASN	2.3
1	A	360	ASP	2.3
1	A	372	LYS	2.3
1	A	883	MET	2.3
1	A	369	GLY	2.3
1	A	427	GLU	2.3
1	A	878	GLU	2.3
1	A	320	MET	2.3
1	A	631	SER	2.3
1	A	630	LYS	2.3
1	A	370	THR	2.3
1	A	535	THR	2.3
1	A	401	ARG	2.3
1	A	818	ILE	2.3
1	A	306	HIS	2.2
1	A	365	GLU	2.2
1	A	890	ARG	2.2
1	A	371	LYS	2.2
1	A	446	LYS	2.2
1	A	788	VAL	2.2
1	A	891	ARG	2.2
1	A	683	ASP	2.1
1	A	737	ARG	2.1
1	A	528	GLY	2.1
1	A	390	THR	2.1
1	A	375	LYS	2.1
1	A	552	MET	2.1
1	A	568	ILE	2.1
1	A	576	LYS	2.1
1	A	496	HIS	2.1
1	A	846	TRP	2.1
1	A	376	ILE	2.1

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

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

6.3 Carbohydrates ⓘ

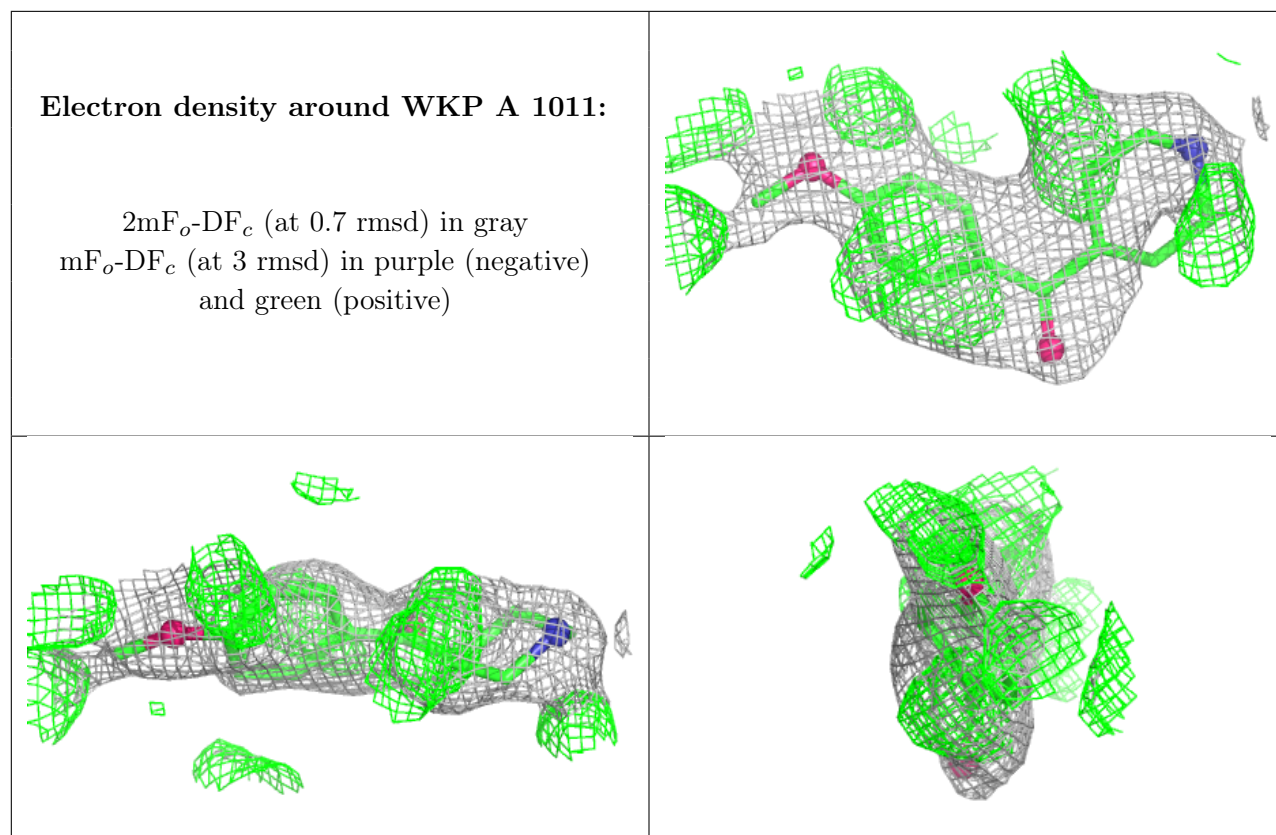
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
2	GOL	A	1001	6/6	0.60	0.32	52,52,56,59	6
6	PO4	A	1009	5/5	0.67	0.15	84,89,96,119	0
8	WKP	A	1011	16/16	0.70	0.31	48,58,62,63	16
6	PO4	A	1008	5/5	0.81	0.13	34,34,42,62	0
7	PEG	A	1010	7/7	0.83	0.15	64,70,80,86	0
5	DMS	A	1006	4/4	0.90	0.17	70,88,93,101	0
5	DMS	A	1005	4/4	0.93	0.14	42,46,47,47	0
4	MES	A	1004[A]	12/12	0.95	0.23	823,857,860,861	12
4	MES	A	1004[B]	12/12	0.95	0.23	26,30,38,38	12
9	CL	A	1012	1/1	0.97	0.06	45,45,45,45	0
5	DMS	A	1007	4/4	0.98	0.09	59,61,66,70	0
3	ZN	A	1003	1/1	0.99	0.04	57,57,57,57	0
3	ZN	A	1002	1/1	1.00	0.02	26,26,26,26	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 [i](#)

There are no such residues in this entry.