



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:42 AM UTC

PDB ID : 7I2D / pdb_00007i2d
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 Z729352906 (DENV2_NS5A-x0258)
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Deposited on : 2025-03-06
Resolution : 1.70 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)

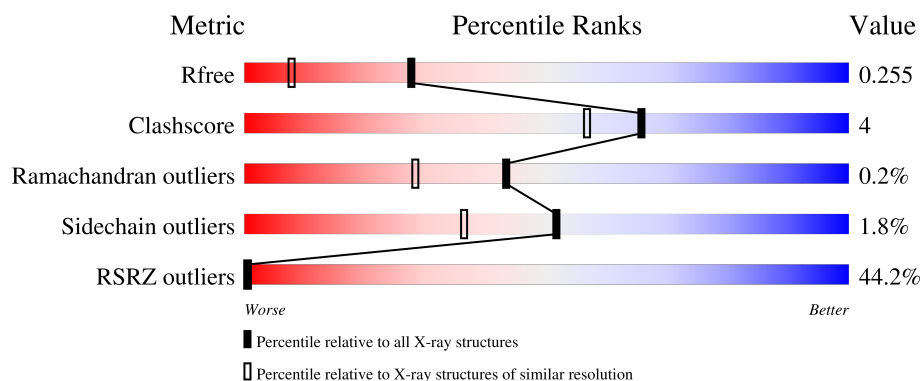
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	-
7	WHM	A	1011	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5234 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	573	Total	C	N	O	S	0	8	0
			4743	2986	850	873	34			

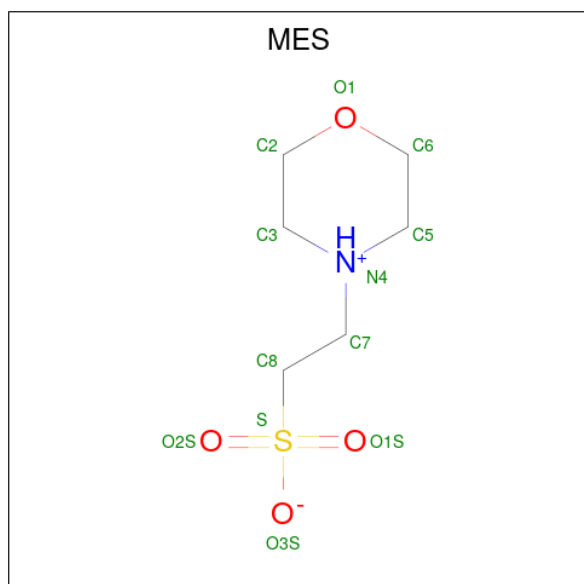
There are 2 discrepancies between the modelled and reference sequences:

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).

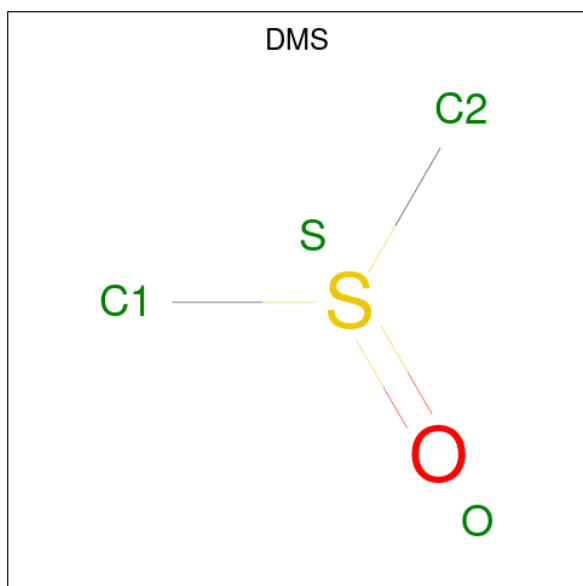
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- 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).



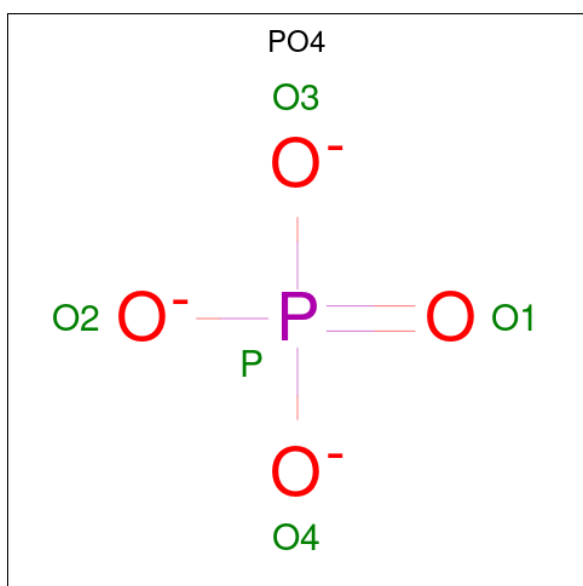
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



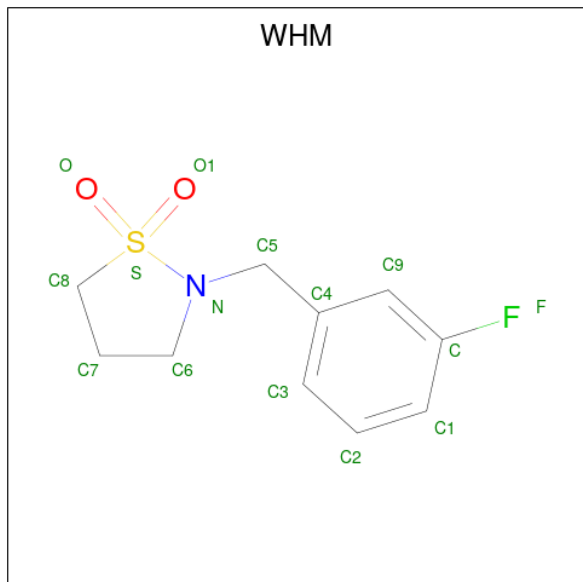
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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 2-[(3-fluorophenyl)methyl]-1λ⁶,2-thiazolidine-1,1-dione (CCD ID: WHM) (formula: C₁₀H₁₂FNO₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	A	1	Total	C	F	N	O	S	0	0
			15	10	1	1	2	1		

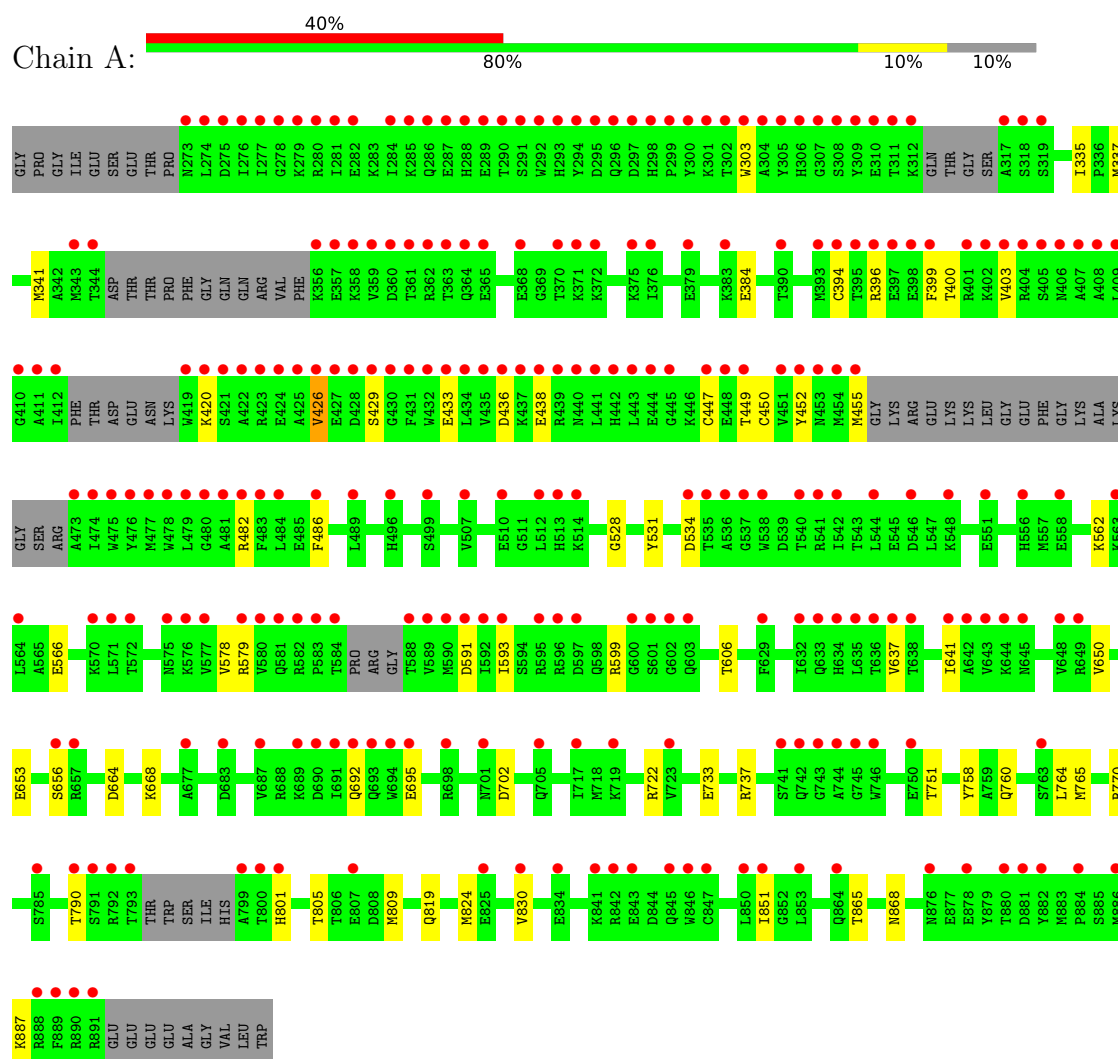
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	414	Total	O	0	0
			414	414		

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	82.47Å 116.82Å 148.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.91 – 1.70 49.91 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.91-1.70) 98.9 (49.91-1.70)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC5	Depositor
R, R_{free}	0.197 , 0.228 0.232 , 0.255	Depositor DCC
R_{free} test set	4052 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 75.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5234	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% 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 [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.13	4/4848 (0.1%)	1.33	5/6537 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	751	THR	C-O	6.45	1.31	1.24
1	A	531	TYR	C-O	6.09	1.31	1.23
1	A	760	GLN	C-O	5.25	1.30	1.24
1	A	650	VAL	N-CA	5.22	1.50	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	702	ASP	CA-CB-CG	5.93	118.53	112.60
1	A	650	VAL	CA-C-O	-5.18	115.42	119.46
1	A	579	ARG	CB-CA-C	5.17	118.73	110.16
1	A	702	ASP	CB-CA-C	5.13	118.98	109.70
1	A	865	THR	CA-CB-OG1	-5.09	101.96	109.60

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	4743	0	4643	34	0
2	A	2	0	0	0	0
3	A	24	0	26	0	0
4	A	12	0	18	3	0
5	A	14	0	20	1	0
6	A	10	0	0	4	0
7	A	15	0	0	0	0
8	A	414	0	0	7	2
All	All	5234	0	4707	36	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 (36) 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	1.97	0.82
4:A:1004:DMS:H11	8:A:1267:HOH:O	1.91	0.69
1:A:653:GLU:O	1:A:656:SER:OG	2.12	0.68
1:A:534:ASP:OD1	6:A:1008:PO4:O4	2.13	0.66
1:A:664:ASP:OD1	6:A:1008:PO4:P	2.55	0.64
1:A:801[B]:HIS:H	1:A:801[B]:HIS:CD2	2.18	0.62
1:A:438:GLU:HG3	1:A:449:THR:OG1	2.02	0.59
4:A:1004:DMS:H12	8:A:1271:HOH:O	2.02	0.58
1:A:528:GLY:O	1:A:668:LYS:HE3	2.07	0.55
1:A:770:ARG:HD2	1:A:851:ILE:HD13	1.90	0.53
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.49	0.52
1:A:403:VAL:HG21	1:A:426:VAL:HG21	1.91	0.52
1:A:733:GLU:O	1:A:737:ARG:HG3	2.10	0.52
1:A:303:TRP:CE3	1:A:593:ILE:HD12	2.45	0.51
1:A:764:LEU:O	1:A:765:MET:HE2	2.10	0.51
1:A:801[B]:HIS:CD2	5:A:1007:PEG:H42	2.46	0.50
1:A:562:LYS:HE3	1:A:566:GLU:OE2	2.11	0.49
1:A:790:THR:HG22	8:A:1324:HOH:O	2.13	0.48
1:A:400:THR:O	1:A:403:VAL:HG22	2.15	0.47
1:A:429:SER:O	1:A:433:GLU:HG3	2.14	0.46
1:A:819:GLN:NE2	8:A:1113:HOH:O	2.41	0.46
1:A:534:ASP:OD1	6:A:1008:PO4:P	2.73	0.45
1:A:384:GLU:OE2	8:A:1101:HOH:O	2.21	0.45
1:A:599:ARG:HG2	1:A:606:THR:HG23	1.99	0.44
1:A:692:GLN:HE21	1:A:695:GLU:HB2	1.82	0.43
1:A:722:ARG:HD2	1:A:824:MET:SD	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:758:TYR:CD1	4:A:1006:DMS:H21	2.54	0.42
1:A:394:CYS:HB3	1:A:486:PHE:CE2	2.56	0.41
1:A:764:LEU:C	1:A:765:MET:HE2	2.45	0.41
1:A:337:MET:HG2	8:A:1347:HOH:O	2.21	0.41
1:A:399:PHE:O	1:A:403:VAL:HG13	2.21	0.41
1:A:868:ASN:OD1	8:A:1102:HOH:O	2.22	0.40
1:A:452:TYR:HB2	1:A:578:VAL:HG22	2.03	0.40
1:A:341:MET:HE2	1:A:341:MET:HB3	1.88	0.40
1:A:396:ARG:NH2	1:A:436:ASP:OD1	2.47	0.40
1:A:805:THR:CG2	1:A:809:MET:HE1	2.52	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)
8:A:1160:HOH:O	8:A:1160:HOH:O[2_445]	1.70	0.50
8:A:1320:HOH:O	8:A:1378:HOH:O[2_545]	2.18	0.02

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	567/637 (89%)	550 (97%)	16 (3%)	1 (0%)	43 28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	420	LYS

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	509/554 (92%)	500 (98%)	9 (2%)	51 36

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

Mol	Chain	Res	Type
1	A	335	ILE
1	A	426	VAL
1	A	455	MET
1	A	482	ARG
1	A	591	ASP
1	A	637	VAL
1	A	641	ILE
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	288	HIS
1	A	298	HIS
1	A	692	GLN
1	A	701	ASN
1	A	786	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 12 ligands modelled in this entry, 2 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	PEG	A	1010	-	6,6,6	0.15	0	5,5,5	0.20	0
7	WHM	A	1011	-	15,16,16	0.19	0	19,23,23	0.47	0
6	PO4	A	1008	-	4,4,4	5.20	3 (75%)	6,6,6	0.64	0
3	MES	A	1003[A]	-	12,12,12	0.85	0	15,16,16	0.75	1 (6%)
4	DMS	A	1005	-	3,3,3	0.41	0	3,3,3	0.16	0
5	PEG	A	1007	-	6,6,6	0.20	0	5,5,5	0.12	0
3	MES	A	1003[B]	-	12,12,12	0.69	0	15,16,16	0.29	0
4	DMS	A	1006	-	3,3,3	0.31	0	3,3,3	0.39	0
4	DMS	A	1004	-	3,3,3	0.79	0	3,3,3	0.67	0
6	PO4	A	1009	-	4,4,4	1.46	1 (25%)	6,6,6	0.52	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
5	PEG	A	1010	-	-	2/4/4/4	-
7	WHM	A	1011	-	-	2/4/17/17	0/2/2/2
3	MES	A	1003[A]	-	-	0/6/14/14	0/1/1/1
5	PEG	A	1007	-	-	0/4/4/4	-
3	MES	A	1003[B]	-	-	5/6/14/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1008	PO4	P-O1	7.90	1.68	1.50
6	A	1008	PO4	P-O2	5.71	1.71	1.54
6	A	1008	PO4	P-O3	3.19	1.63	1.54
6	A	1009	PO4	P-O1	2.55	1.56	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1003[A]	MES	O2S-S-C8	-2.36	103.16	106.73

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1003[B]	MES	C8-C7-N4-C3
3	A	1003[B]	MES	C7-C8-S-O2S
3	A	1003[B]	MES	C7-C8-S-O3S
5	A	1010	PEG	O2-C3-C4-O4
3	A	1003[B]	MES	C8-C7-N4-C5
7	A	1011	WHM	C9-C4-C5-N
3	A	1003[B]	MES	C7-C8-S-O1S
5	A	1010	PEG	C4-C3-O2-C2
7	A	1011	WHM	C3-C4-C5-N

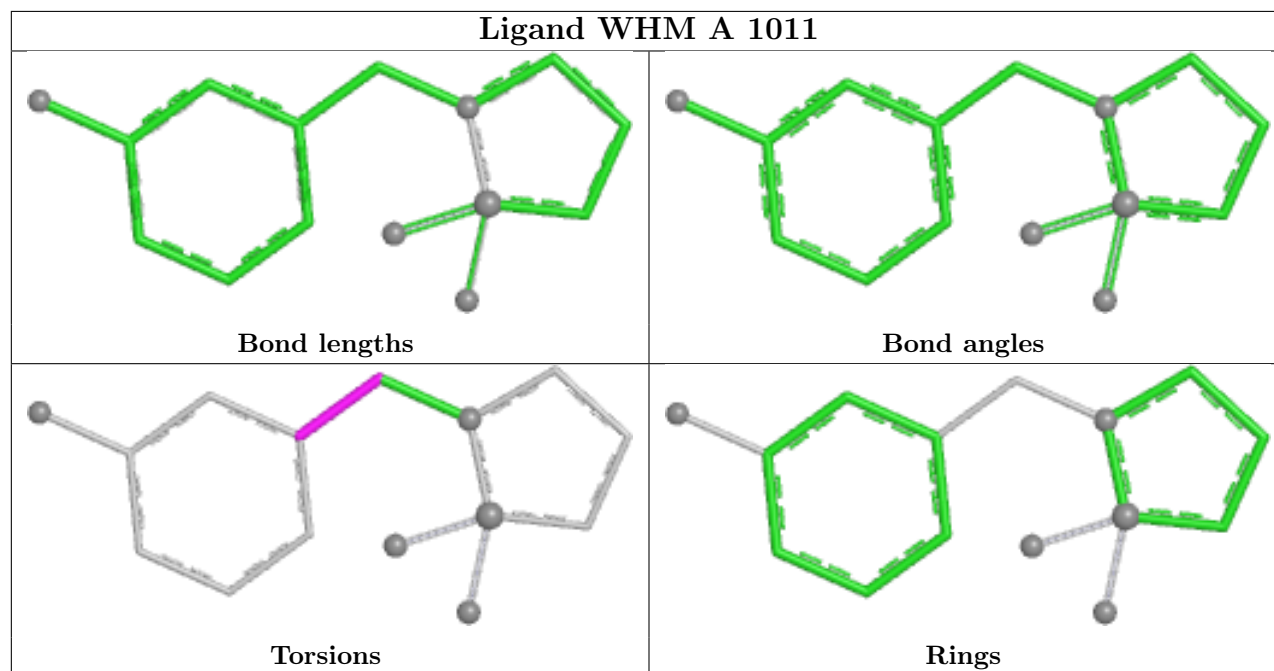
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1008	PO4	4	0
5	A	1007	PEG	1	0
4	A	1006	DMS	1	0
4	A	1004	DMS	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	573/637 (89%)	2.70	253 (44%) 0 0	6, 34, 72, 120	142 (24%)

All (253) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	512[A]	LEU	12.6
1	A	637	VAL	12.1
1	A	409	LEU	12.0
1	A	801[A]	HIS	11.8
1	A	407	ALA	11.5
1	A	850	LEU	11.4
1	A	478	TRP	11.3
1	A	641	ILE	11.0
1	A	719[A]	LYS	10.9
1	A	635	LEU	10.9
1	A	441	LEU	10.9
1	A	636	THR	10.8
1	A	592	ILE	10.7
1	A	589	VAL	10.7
1	A	426	VAL	10.6
1	A	846	TRP	10.3
1	A	800	THR	10.2
1	A	274	LEU	10.1
1	A	853	LEU	10.0
1	A	851	ILE	9.9
1	A	479	LEU	9.8
1	A	638	THR	9.4
1	A	412	ILE	9.4
1	A	691	ILE	9.4
1	A	513	HIS	9.1
1	A	475	TRP	9.0
1	A	304	ALA	9.0

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Mol	Chain	Res	Type	RSRZ
1	A	303	TRP	9.0
1	A	480	GLY	8.8
1	A	575	ASN	8.8
1	A	294	TYR	8.7
1	A	847	CYS	8.7
1	A	656	SER	8.6
1	A	292	TRP	8.5
1	A	588	THR	8.5
1	A	408	ALA	8.4
1	A	580	VAL	8.4
1	A	763[A]	SER	8.2
1	A	359	VAL	8.2
1	A	741[A]	SER	8.1
1	A	277	ILE	8.1
1	A	551[A]	GLU	8.1
1	A	293	HIS	8.0
1	A	499	SER	8.0
1	A	319	SER	7.9
1	A	634	HIS	7.9
1	A	687	VAL	7.9
1	A	474	ILE	7.8
1	A	300	TYR	7.8
1	A	429	SER	7.8
1	A	305	TYR	7.7
1	A	514	LYS	7.7
1	A	657	ARG	7.6
1	A	451	VAL	7.6
1	A	425	ALA	7.6
1	A	453	ASN	7.5
1	A	601	SER	7.5
1	A	419	TRP	7.4
1	A	600	GLY	7.4
1	A	602	GLY	7.4
1	A	743	GLY	7.3
1	A	375	LYS	7.1
1	A	299	PRO	7.0
1	A	649	ARG	7.0
1	A	576	LYS	7.0
1	A	422	ALA	7.0
1	A	476	TYR	7.0
1	A	307	GLY	6.9
1	A	308	SER	6.8

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Mol	Chain	Res	Type	RSRZ
1	A	785[A]	SER	6.8
1	A	428	ASP	6.7
1	A	481	ALA	6.7
1	A	317	ALA	6.6
1	A	482	ARG	6.6
1	A	318	SER	6.5
1	A	477	MET	6.5
1	A	891	ARG	6.4
1	A	705	GLN	6.4
1	A	286	GLN	6.4
1	A	273	ASN	6.4
1	A	595	ARG	6.4
1	A	473	ALA	6.4
1	A	841	LYS	6.3
1	A	361	THR	6.3
1	A	411	ALA	6.2
1	A	864[A]	GLN	6.2
1	A	402	LYS	6.2
1	A	363	THR	6.2
1	A	591	ASP	6.1
1	A	583	PRO	6.1
1	A	842	ARG	6.1
1	A	590	MET	6.0
1	A	689	LYS	6.0
1	A	888	ARG	6.0
1	A	421	SER	6.0
1	A	372	LYS	5.9
1	A	295	ASP	5.9
1	A	633	GLN	5.9
1	A	584	THR	5.9
1	A	793	THR	5.8
1	A	358	LYS	5.8
1	A	692	GLN	5.8
1	A	371	LYS	5.8
1	A	799	ALA	5.8
1	A	845	GLN	5.8
1	A	698	ARG	5.7
1	A	403	VAL	5.7
1	A	603	GLN	5.7
1	A	298	HIS	5.7
1	A	290	THR	5.7
1	A	889	PHE	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	454	MET	5.6
1	A	309	TYR	5.6
1	A	364	GLN	5.6
1	A	279	LYS	5.5
1	A	596	ARG	5.5
1	A	360	ASP	5.5
1	A	455	MET	5.5
1	A	431	PHE	5.5
1	A	742	GLN	5.5
1	A	510	GLU	5.5
1	A	435	VAL	5.5
1	A	406	ASN	5.5
1	A	548	LYS	5.5
1	A	281	ILE	5.4
1	A	442	HIS	5.4
1	A	843	GLU	5.4
1	A	434	LEU	5.4
1	A	275	ASP	5.4
1	A	423	ARG	5.3
1	A	541	ARG	5.1
1	A	582	ARG	5.0
1	A	410	GLY	5.0
1	A	302	THR	5.0
1	A	312	LYS	4.9
1	A	287	GLU	4.9
1	A	379	GLU	4.8
1	A	597	ASP	4.8
1	A	571	LEU	4.7
1	A	289	GLU	4.7
1	A	484	LEU	4.7
1	A	288	HIS	4.7
1	A	311	THR	4.6
1	A	284	ILE	4.6
1	A	297	ASP	4.6
1	A	306	HIS	4.5
1	A	362	ARG	4.5
1	A	301	LYS	4.5
1	A	291	SER	4.5
1	A	424	GLU	4.4
1	A	356	LYS	4.4
1	A	581	GLN	4.4
1	A	282	GLU	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	445	GLY	4.4
1	A	357	GLU	4.4
1	A	693	GLN	4.3
1	A	644	LYS	4.3
1	A	694	TRP	4.3
1	A	744	ALA	4.2
1	A	745	GLY	4.2
1	A	296	GLN	4.1
1	A	401	ARG	4.0
1	A	399	PHE	4.0
1	A	677	ALA	4.0
1	A	564	LEU	4.0
1	A	420	LYS	3.9
1	A	690	ASP	3.9
1	A	430	GLY	3.8
1	A	792	ARG	3.8
1	A	449	THR	3.8
1	A	791	SER	3.7
1	A	427	GLU	3.7
1	A	452	TYR	3.7
1	A	876	ASN	3.6
1	A	544	LEU	3.6
1	A	538	TRP	3.5
1	A	365	GLU	3.5
1	A	443	LEU	3.5
1	A	880	THR	3.5
1	A	310	GLU	3.5
1	A	439	ARG	3.5
1	A	577	VAL	3.5
1	A	436	ASP	3.4
1	A	790	THR	3.4
1	A	537	GLY	3.3
1	A	344	THR	3.3
1	A	437	LYS	3.3
1	A	276	ILE	3.3
1	A	542	ILE	3.3
1	A	278	GLY	3.2
1	A	648	VAL	3.2
1	A	396	ARG	3.2
1	A	882	TYR	3.1
1	A	376	ILE	3.1
1	A	370	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	558	GLU	3.0
1	A	280	ARG	3.0
1	A	447	CYS	3.0
1	A	746	TRP	3.0
1	A	395	THR	3.0
1	A	556	HIS	2.9
1	A	540	THR	2.9
1	A	563	LYS	2.9
1	A	645	ASN	2.9
1	A	483	PHE	2.9
1	A	701	ASN	2.9
1	A	629	PHE	2.8
1	A	404	ARG	2.8
1	A	570	LYS	2.8
1	A	881	ASP	2.8
1	A	890	ARG	2.8
1	A	393	MET	2.8
1	A	534	ASP	2.8
1	A	593	ILE	2.8
1	A	448	GLU	2.7
1	A	536	ALA	2.7
1	A	433	GLU	2.7
1	A	486	PHE	2.7
1	A	695	GLU	2.6
1	A	440	ASN	2.6
1	A	390	THR	2.6
1	A	398	GLU	2.6
1	A	807	GLU	2.6
1	A	834	GLU	2.6
1	A	438	GLU	2.5
1	A	884	PRO	2.5
1	A	489	LEU	2.4
1	A	444	GLU	2.4
1	A	405	SER	2.4
1	A	830	VAL	2.4
1	A	285	LYS	2.3
1	A	572	THR	2.3
1	A	642	ALA	2.3
1	A	383	LYS	2.3
1	A	683	ASP	2.3
1	A	535	THR	2.3
1	A	886	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	432	TRP	2.2
1	A	825	GLU	2.2
1	A	579	ARG	2.2
1	A	368	GLU	2.2
1	A	397	GLU	2.2
1	A	750	GLU	2.1
1	A	496	HIS	2.1
1	A	343	MET	2.1
1	A	632	ILE	2.1
1	A	717	ILE	2.1
1	A	507	VAL	2.0
1	A	878	GLU	2.0
1	A	546	ASP	2.0
1	A	394	CYS	2.0
1	A	643	VAL	2.0
1	A	723	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.

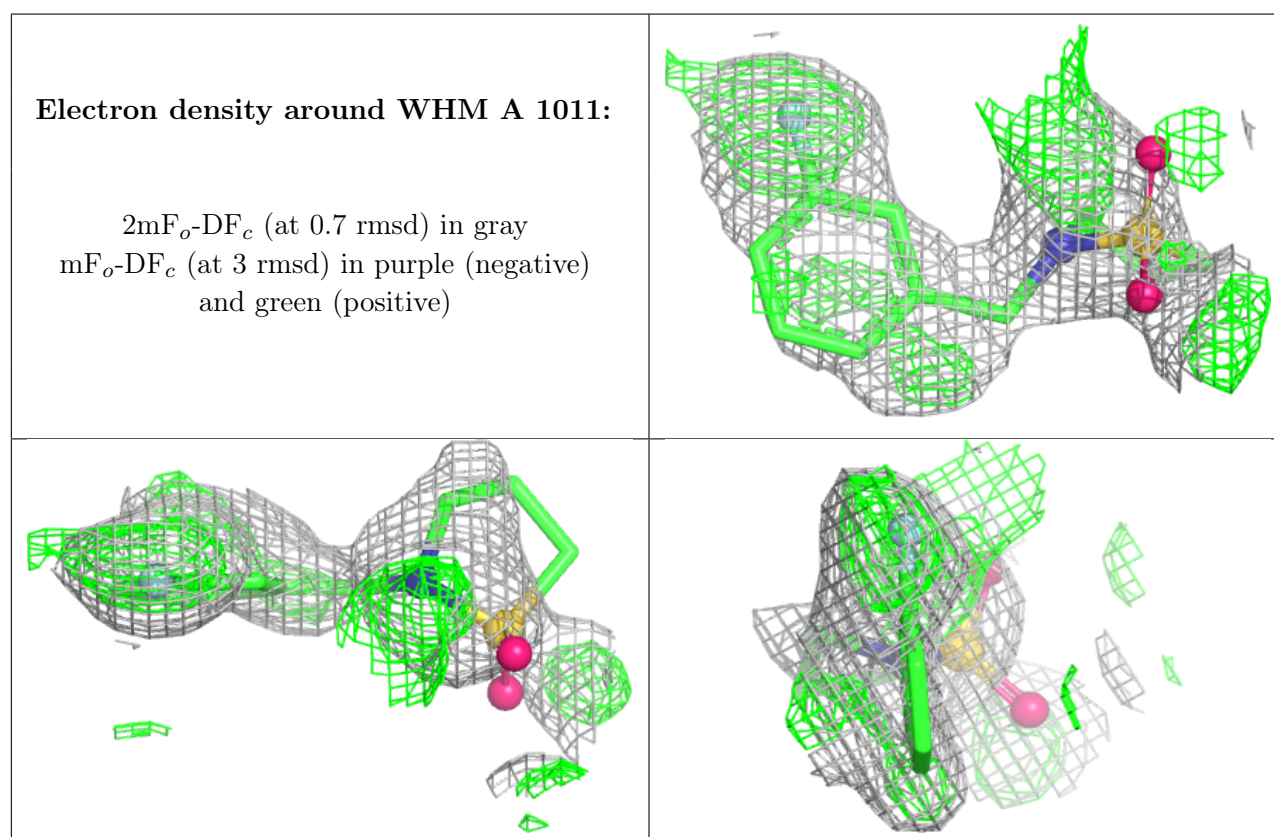
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PEG	A	1007	7/7	0.62	0.23	88,97,110,111	0
6	PO4	A	1009	5/5	0.63	0.17	66,71,89,106	0
4	DMS	A	1005	4/4	0.71	0.29	72,96,103,115	0
6	PO4	A	1008	5/5	0.77	0.15	34,38,58,61	0
7	WHM	A	1011	15/15	0.77	0.48	92,95,112,113	15
5	PEG	A	1010	7/7	0.82	0.18	61,69,76,81	0
4	DMS	A	1004	4/4	0.92	0.17	43,47,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	DMS	A	1006	4/4	0.96	0.09	47,54,55,58	0
3	MES	A	1003[A]	12/12	0.97	0.31	21,25,28,30	12
3	MES	A	1003[B]	12/12	0.97	0.31	630,652,728,732	12
2	ZN	A	1002	1/1	0.99	0.06	53,53,53,53	0
2	ZN	A	1001	1/1	1.00	0.02	21,21,21,21	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.