



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2025 – 10:26 AM EDT

PDB ID : 7I2D
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 (DNV2_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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

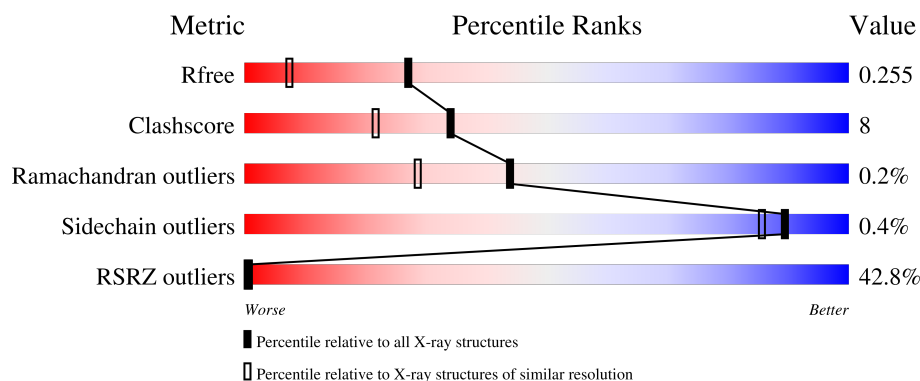
1 Overall quality at a glance

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}	164625	5161 (1.70-1.70)
Clashscore	180529	5671 (1.70-1.70)
Ramachandran outliers	177936	5594 (1.70-1.70)
Sidechain outliers	177891	5594 (1.70-1.70)
RSRZ outliers	164620	5159 (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) : 2.41.4

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 (three-letter code: 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 (three-letter code: 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 (three-letter code: DMS) (formula: C_2H_6OS).



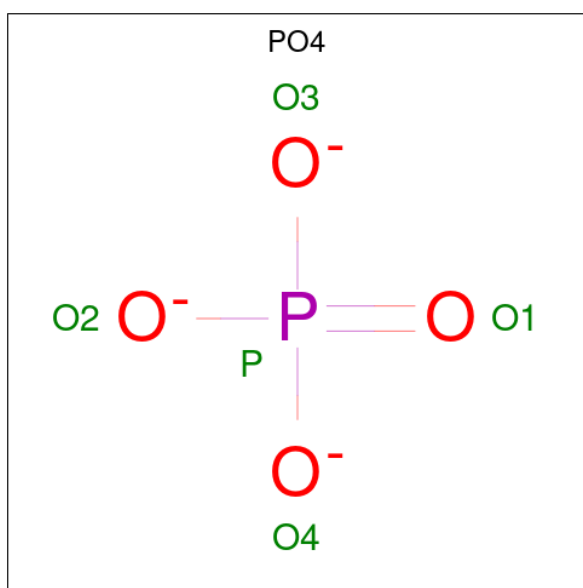
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



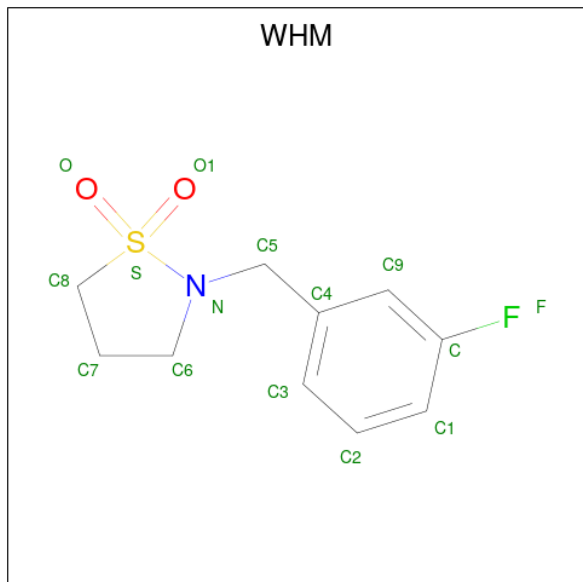
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is PHOSPHATE ION (three-letter code: 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]-1lambda 6 ,2-thiazolidine-1,1-dione (three-letter code: WHM) (formula: C₁₀H₁₂FNO₂S) (labeled as "Ligand of Interest" by depositor).



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

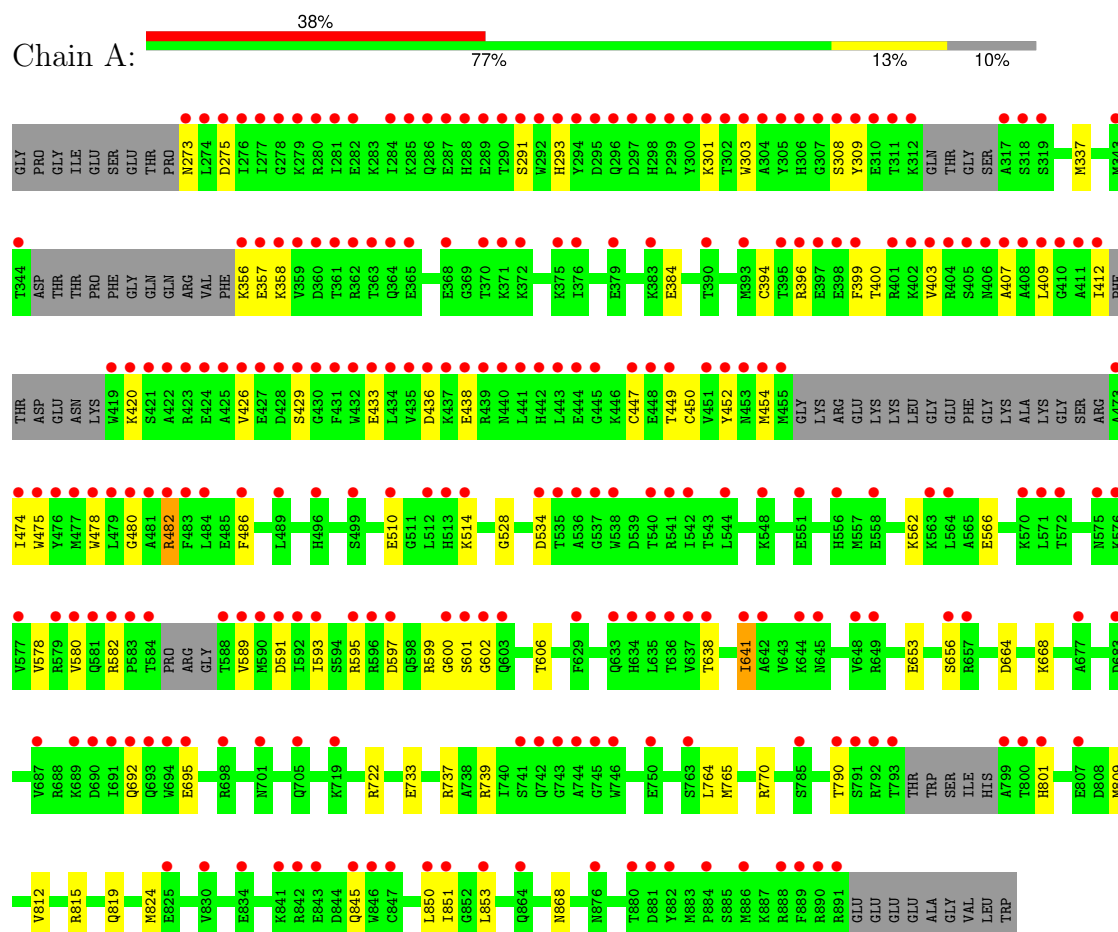
- Molecule 8 is water.

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

3 Residue-property plots [i](#)

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	4048 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: PEG, DMS, MES, ZN, PO4, WHM

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	0.79	0/4848	0.86	2/6537 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	739	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	A	815	ARG	NE-CZ-NH2	-5.09	117.75	120.30

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	70	0
2	A	2	0	0	0	0
3	A	24	0	26	0	0
4	A	12	0	18	2	0
5	A	14	0	20	1	0
6	A	10	0	0	4	0
7	A	15	0	0	1	0
8	A	414	0	0	7	2
All	All	5234	0	4707	72	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 8.

All (72) 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:357:GLU:N	1:A:357:GLU:OE2	2.11	0.83
1:A:664:ASP:OD1	6:A:1008:PO4:O4	1.97	0.82
1:A:273:ASN:O	1:A:275:ASP:OD1	2.03	0.76
1:A:303:TRP:CD1	1:A:595:ARG:NH1	2.59	0.71
1:A:653:GLU:O	1:A:656:SER:OG	2.12	0.68
1:A:595:ARG:NE	1:A:597:ASP:OD1	2.21	0.67
1:A:534:ASP:OD1	6:A:1008:PO4:O4	2.13	0.66
1:A:303:TRP:NE1	1:A:595:ARG:NH1	2.44	0.65
1:A:303:TRP:CZ2	1:A:595:ARG:HD2	2.32	0.65
1:A:664:ASP:OD1	6:A:1008:PO4:P	2.55	0.64
1:A:474:ILE:C	1:A:475:TRP:HD1	2.01	0.64
1:A:356:LYS:HE3	1:A:358:LYS:HB3	1.78	0.63
1:A:801[B]:HIS:H	1:A:801[B]:HIS:CD2	2.18	0.62
1:A:303:TRP:CE2	1:A:595:ARG:HD2	2.35	0.61
1:A:482:ARG:HH12	1:A:602:GLY:N	1.99	0.60
1:A:438:GLU:HG3	1:A:449:THR:OG1	2.02	0.59
1:A:475:TRP:CD1	1:A:475:TRP:N	2.70	0.58
1:A:638:THR:HA	1:A:641:ILE:HG22	1.85	0.58
1:A:638:THR:HA	1:A:641:ILE:CG2	2.34	0.57
1:A:510:GLU:OE1	1:A:514:LYS:HE2	2.04	0.57
1:A:638:THR:O	1:A:641:ILE:HG23	2.05	0.57
1:A:356:LYS:HE3	1:A:358:LYS:CB	2.36	0.55
1:A:478:TRP:CZ2	1:A:480:GLY:HA3	2.41	0.55
1:A:638:THR:O	1:A:641:ILE:CG2	2.55	0.55
1:A:407:ALA:O	1:A:409:LEU:HG	2.07	0.55
1:A:528:GLY:O	1:A:668:LYS:HE3	2.07	0.55
1:A:482:ARG:NH1	1:A:602:GLY:N	2.56	0.54
1:A:293:HIS:O	1:A:308:SER:HB2	2.08	0.54
1:A:454:MET:CB	1:A:580:VAL:HG22	2.38	0.53
1:A:770:ARG:HD2	1:A:851:ILE:HD13	1.90	0.53
1:A:412:ILE:O	1:A:412:ILE:HG13	2.09	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:510:GLU:OE1	1:A:510:GLU:HA	2.10	0.51
1:A:589:VAL:HG23	1:A:591:ASP:OD1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:A:1004:DMS:C1	8:A:1267:HOH:O	2.60	0.49
1:A:475:TRP:HD1	1:A:475:TRP:N	2.10	0.49
1:A:790:THR:HG22	8:A:1324:HOH:O	2.13	0.48
1:A:474:ILE:HD12	1:A:474:ILE:N	2.28	0.48
4:A:1004:DMS:H12	8:A:1271:HOH:O	2.14	0.48
1:A:400:THR:O	1:A:403:VAL:HG22	2.15	0.47
1:A:582:ARG:HB2	1:A:591:ASP:OD2	2.13	0.47
1:A:454:MET:HB3	1:A:580:VAL:HG22	1.97	0.46
1:A:429:SER:O	1:A:433:GLU:HG3	2.14	0.46
1:A:291:SER:O	1:A:309:TYR:HA	2.15	0.46
1:A:510:GLU:O	1:A:514:LYS:HG3	2.15	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:845:GLN:NE2	7:A:1011:WHM:O	2.49	0.45
1:A:599:ARG:HG2	1:A:606:THR:HG23	1.99	0.44
1:A:638:THR:CA	1:A:641:ILE:HG22	2.46	0.44
1:A:809:MET:HE1	1:A:812:VAL:HG21	1.98	0.44
1:A:692:GLN:HE21	1:A:695:GLU:HB2	1.82	0.43
1:A:850:LEU:HD22	1:A:853:LEU:HD12	2.01	0.43
1:A:764:LEU:HG	1:A:765:MET:HE2	2.01	0.43
1:A:454:MET:HB2	1:A:580:VAL:HG22	2.02	0.42
1:A:600:GLY:O	1:A:601:SER:OG	2.34	0.42
1:A:482:ARG:NH1	1:A:602:GLY:H	2.18	0.42
1:A:722:ARG:HD2	1:A:824:MET:SD	2.60	0.42
1:A:301:LYS:HA	1:A:301:LYS:HD2	1.82	0.42
1:A:394:CYS:HB3	1:A:486:PHE:CE2	2.56	0.41
1:A:337:MET:HG2	8:A:1347:HOH:O	2.21	0.41
1:A:357:GLU:N	1:A:357:GLU:CD	2.72	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:396:ARG:NH2	1:A:436:ASP:OD1	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	44 29

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%)	507 (100%)	2 (0%)	89 85

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	482	ARG
1	A	641	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	298	HIS
1	A	692	GLN
1	A	786	HIS

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, 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	$\# Z > 2$
4	DMS	A	1004	-	3,3,3	0.79	0	3,3,3	0.67	0
3	MES	A	1003[B]	-	12,12,12	0.69	0	15,16,16	0.29	0
6	PO4	A	1009	-	4,4,4	1.46	1 (25%)	6,6,6	0.52	0
5	PEG	A	1010	-	6,6,6	0.15	0	5,5,5	0.20	0
6	PO4	A	1008	-	4,4,4	5.20	3 (75%)	6,6,6	0.64	0
4	DMS	A	1006	-	3,3,3	0.31	0	3,3,3	0.39	0
5	PEG	A	1007	-	6,6,6	0.20	0	5,5,5	0.12	0
7	WHM	A	1011	-	15,16,16	0.19	0	19,23,23	0.47	0
4	DMS	A	1005	-	3,3,3	0.41	0	3,3,3	0.16	0
3	MES	A	1003[A]	-	12,12,12	0.85	0	15,16,16	0.75	1 (6%)

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
3	MES	A	1003[B]	-	-	5/6/14/14	0/1/1/1
5	PEG	A	1010	-	-	2/4/4/4	-
5	PEG	A	1007	-	-	0/4/4/4	-
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

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:

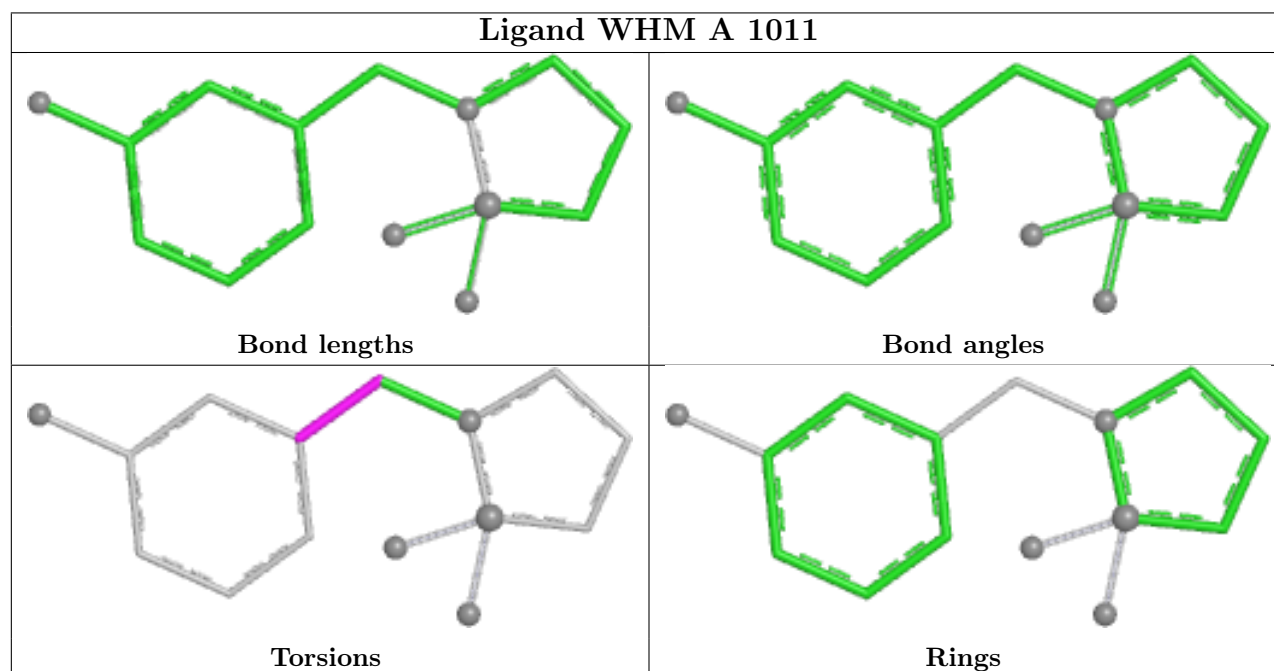
Mol	Chain	Res	Type	Atoms
3	A	1003[B]	MES	C8-C7-N4-C3
3	A	1003[B]	MES	C7-C8-S-O2S
3	A	1003[B]	MES	C7-C8-S-O3S
5	A	1010	PEG	O2-C3-C4-O4
3	A	1003[B]	MES	C8-C7-N4-C5
7	A	1011	WHM	C9-C4-C5-N
3	A	1003[B]	MES	C7-C8-S-O1S
5	A	1010	PEG	C4-C3-O2-C2
7	A	1011	WHM	C3-C4-C5-N

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1004	DMS	2	0
6	A	1008	PO4	4	0
5	A	1007	PEG	1	0
7	A	1011	WHM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	573/637 (89%)	2.60	245 (42%) 1 0	6, 34, 72, 120	142 (24%)

All (245) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	512[A]	LEU	12.3
1	A	637	VAL	11.8
1	A	409	LEU	11.8
1	A	801[A]	HIS	11.6
1	A	407	ALA	11.2
1	A	850	LEU	11.1
1	A	478	TRP	11.1
1	A	719[A]	LYS	10.9
1	A	641	ILE	10.7
1	A	635	LEU	10.6
1	A	441	LEU	10.6
1	A	636	THR	10.5
1	A	592	ILE	10.4
1	A	589	VAL	10.3
1	A	426	VAL	10.3
1	A	846	TRP	10.1
1	A	800	THR	10.0
1	A	274	LEU	9.8
1	A	853	LEU	9.7
1	A	851	ILE	9.7
1	A	479	LEU	9.6
1	A	638	THR	9.2
1	A	412	ILE	9.2
1	A	691	ILE	9.1
1	A	513	HIS	8.9
1	A	475	TRP	8.8
1	A	303	TRP	8.8

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Mol	Chain	Res	Type	RSRZ
1	A	304	ALA	8.7
1	A	294	TYR	8.6
1	A	575	ASN	8.6
1	A	847	CYS	8.5
1	A	480	GLY	8.5
1	A	656	SER	8.5
1	A	292	TRP	8.3
1	A	588	THR	8.3
1	A	408	ALA	8.2
1	A	580	VAL	8.1
1	A	763[A]	SER	8.1
1	A	741[A]	SER	8.0
1	A	551[A]	GLU	8.0
1	A	359	VAL	7.9
1	A	277	ILE	7.9
1	A	293	HIS	7.9
1	A	499	SER	7.8
1	A	319	SER	7.8
1	A	634	HIS	7.8
1	A	300	TYR	7.7
1	A	429	SER	7.6
1	A	474	ILE	7.6
1	A	514	LYS	7.6
1	A	687	VAL	7.6
1	A	657	ARG	7.6
1	A	305	TYR	7.5
1	A	451	VAL	7.4
1	A	425	ALA	7.3
1	A	601	SER	7.3
1	A	453	ASN	7.3
1	A	419	TRP	7.2
1	A	600	GLY	7.2
1	A	602	GLY	7.2
1	A	375	LYS	7.1
1	A	743	GLY	7.0
1	A	576	LYS	7.0
1	A	649	ARG	7.0
1	A	299	PRO	6.9
1	A	476	TYR	6.8
1	A	422	ALA	6.7
1	A	307	GLY	6.7
1	A	308	SER	6.7

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Mol	Chain	Res	Type	RSRZ
1	A	785[A]	SER	6.6
1	A	428	ASP	6.6
1	A	482	ARG	6.5
1	A	481	ALA	6.4
1	A	318	SER	6.4
1	A	891	ARG	6.4
1	A	477	MET	6.4
1	A	317	ALA	6.4
1	A	705	GLN	6.3
1	A	595	ARG	6.3
1	A	841	LYS	6.3
1	A	286	GLN	6.3
1	A	273	ASN	6.2
1	A	402	LYS	6.2
1	A	473	ALA	6.1
1	A	361	THR	6.1
1	A	864[A]	GLN	6.1
1	A	363	THR	6.0
1	A	411	ALA	6.0
1	A	591	ASP	6.0
1	A	842	ARG	6.0
1	A	689	LYS	6.0
1	A	583	PRO	5.9
1	A	590	MET	5.9
1	A	888	ARG	5.9
1	A	372	LYS	5.9
1	A	421	SER	5.9
1	A	633	GLN	5.8
1	A	295	ASP	5.8
1	A	358	LYS	5.8
1	A	584	THR	5.7
1	A	371	LYS	5.7
1	A	793	THR	5.7
1	A	692	GLN	5.7
1	A	698	ARG	5.7
1	A	845	GLN	5.7
1	A	603	GLN	5.6
1	A	298	HIS	5.6
1	A	799	ALA	5.6
1	A	889	PHE	5.5
1	A	290	THR	5.5
1	A	454	MET	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	279	LYS	5.5
1	A	364	GLN	5.5
1	A	403	VAL	5.5
1	A	596	ARG	5.5
1	A	309	TYR	5.5
1	A	360	ASP	5.4
1	A	510	GLU	5.4
1	A	548	LYS	5.4
1	A	742	GLN	5.4
1	A	455	MET	5.4
1	A	431	PHE	5.4
1	A	406	ASN	5.3
1	A	442	HIS	5.3
1	A	843	GLU	5.3
1	A	435	VAL	5.3
1	A	281	ILE	5.3
1	A	275	ASP	5.3
1	A	423	ARG	5.2
1	A	434	LEU	5.2
1	A	541	ARG	5.1
1	A	582	ARG	4.9
1	A	302	THR	4.9
1	A	312	LYS	4.8
1	A	410	GLY	4.8
1	A	287	GLU	4.8
1	A	379	GLU	4.8
1	A	597	ASP	4.7
1	A	289	GLU	4.6
1	A	571	LEU	4.6
1	A	288	HIS	4.5
1	A	484	LEU	4.5
1	A	311	THR	4.5
1	A	362	ARG	4.5
1	A	297	ASP	4.5
1	A	301	LYS	4.5
1	A	306	HIS	4.4
1	A	284	ILE	4.4
1	A	291	SER	4.4
1	A	356	LYS	4.4
1	A	424	GLU	4.4
1	A	581	GLN	4.3
1	A	282	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	357	GLU	4.3
1	A	644	LYS	4.3
1	A	693	GLN	4.2
1	A	445	GLY	4.2
1	A	694	TRP	4.1
1	A	744	ALA	4.1
1	A	296	GLN	4.0
1	A	745	GLY	4.0
1	A	401	ARG	4.0
1	A	399	PHE	3.9
1	A	420	LYS	3.8
1	A	564	LEU	3.8
1	A	677	ALA	3.8
1	A	690	ASP	3.8
1	A	792	ARG	3.7
1	A	430	GLY	3.7
1	A	427	GLU	3.6
1	A	791	SER	3.6
1	A	449	THR	3.6
1	A	452	TYR	3.5
1	A	365	GLU	3.5
1	A	876	ASN	3.5
1	A	310	GLU	3.4
1	A	439	ARG	3.4
1	A	544	LEU	3.4
1	A	538	TRP	3.4
1	A	443	LEU	3.4
1	A	880	THR	3.4
1	A	577	VAL	3.3
1	A	436	ASP	3.3
1	A	437	LYS	3.3
1	A	790	THR	3.2
1	A	344	THR	3.2
1	A	537	GLY	3.2
1	A	276	ILE	3.1
1	A	542	ILE	3.1
1	A	396	ARG	3.1
1	A	278	GLY	3.1
1	A	648	VAL	3.0
1	A	882	TYR	3.0
1	A	370	THR	3.0
1	A	376	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	558	GLU	3.0
1	A	280	ARG	2.9
1	A	447	CYS	2.9
1	A	563	LYS	2.9
1	A	395	THR	2.9
1	A	746	TRP	2.8
1	A	556	HIS	2.8
1	A	540	THR	2.8
1	A	645	ASN	2.8
1	A	483	PHE	2.8
1	A	570	LYS	2.8
1	A	404	ARG	2.8
1	A	629	PHE	2.8
1	A	890	ARG	2.8
1	A	881	ASP	2.7
1	A	701	ASN	2.7
1	A	393	MET	2.7
1	A	534	ASP	2.7
1	A	448	GLU	2.6
1	A	593	ILE	2.6
1	A	433	GLU	2.6
1	A	486	PHE	2.6
1	A	536	ALA	2.6
1	A	695	GLU	2.5
1	A	440	ASN	2.5
1	A	398	GLU	2.5
1	A	807	GLU	2.5
1	A	834	GLU	2.5
1	A	390	THR	2.5
1	A	438	GLU	2.4
1	A	444	GLU	2.4
1	A	884	PRO	2.3
1	A	489	LEU	2.3
1	A	405	SER	2.3
1	A	285	LYS	2.3
1	A	830	VAL	2.3
1	A	383	LYS	2.2
1	A	572	THR	2.2
1	A	683	ASP	2.2
1	A	642	ALA	2.2
1	A	886	MET	2.2
1	A	535	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	579	ARG	2.2
1	A	825	GLU	2.2
1	A	368	GLU	2.1
1	A	432	TRP	2.1
1	A	397	GLU	2.1
1	A	750	GLU	2.1
1	A	496	HIS	2.0
1	A	343	MET	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 monosaccharides in this entry.

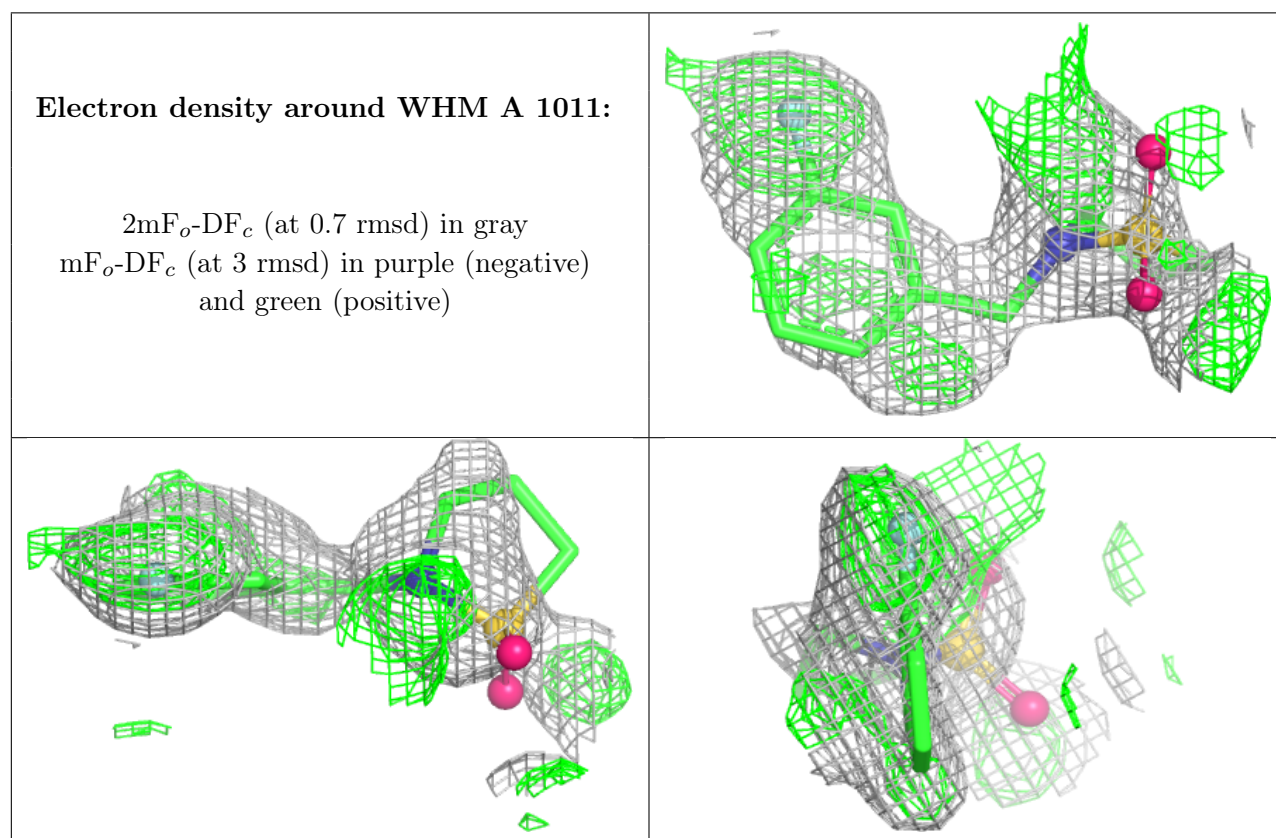
6.4 Ligands [i](#)

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
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.