



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2024 – 12:06 PM EDT

PDB ID : 7HKB
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 Z438067480 (DNV2_NS5A-x0135)
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Deposited on : 2024-10-15
Resolution : 1.61 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) : 1.20.1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)

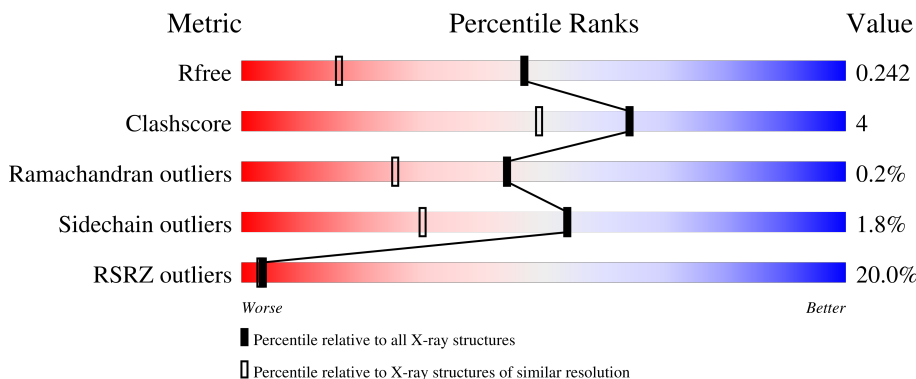
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.61 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	6077 (1.64-1.60)
Clashscore	180529	6617 (1.64-1.60)
Ramachandran outliers	177936	6498 (1.64-1.60)
Sidechain outliers	177891	6497 (1.64-1.60)
RSRZ outliers	164620	6075 (1.64-1.60)

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) : 2.39

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PO4	A	1008	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5345 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 Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	581	4811	3027	864	886	34	0	8	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 (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



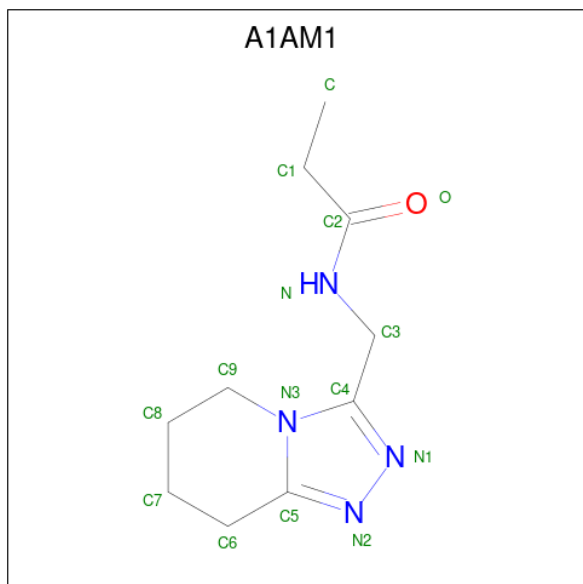
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 7 is N-{[(4R)-5,6,7,8-tetrahydro[1,2,4]triazolo[4,3-a]pyridin-3-yl]methyl}propanamide (three-letter code: A1AM1) (formula: C₁₀H₁₆N₄O) (labeled as "Ligand of Interest" by depositor).



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

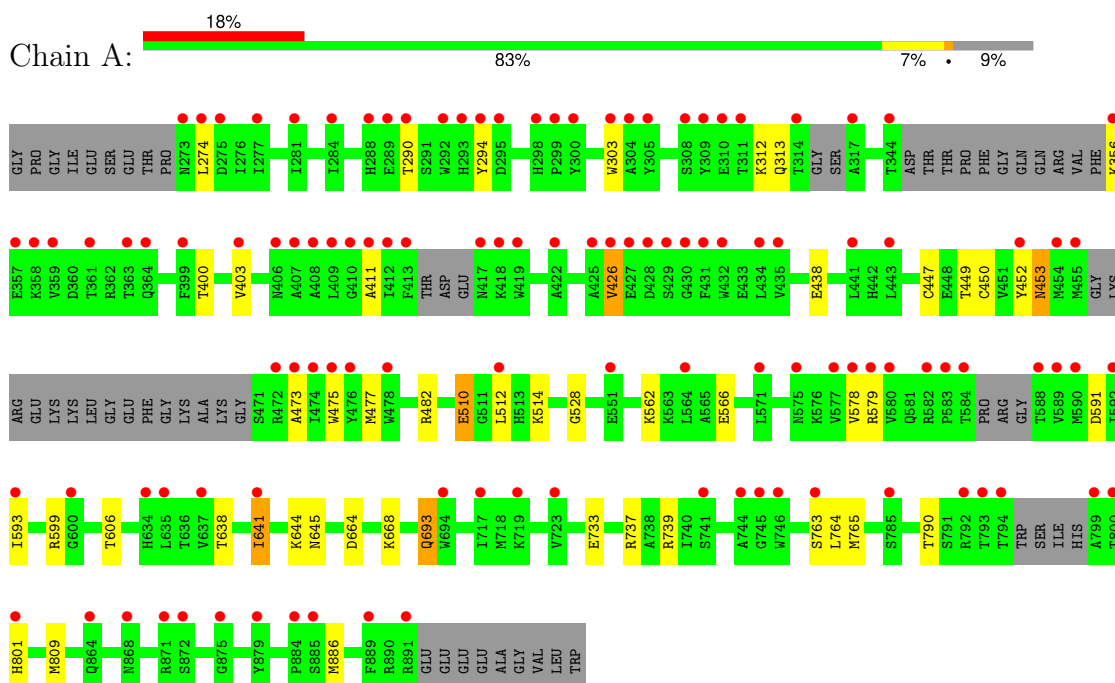
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	457	457	457	0	0

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: Genome polyprotein



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	82.55Å 116.85Å 148.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.42 – 1.61 74.42 – 1.61	Depositor EDS
% Data completeness (in resolution range)	97.2 (74.42-1.61) 97.2 (74.42-1.61)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 1.61Å)	Xtrriage
Refinement program	REFMAC 5.8.0267, REFMAC5	Depositor
R, R_{free}	0.202 , 0.236 0.214 , 0.242	Depositor DCC
R_{free} test set	4729 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtrriage
Anisotropy	0.241	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5345	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.56% 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: PO4, A1AM1, DMS, MES, PEG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.75	3/4917 (0.1%)	0.82	1/6629 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	510	GLU	CD-OE2	8.20	1.34	1.25
1	A	763[A]	SER	C-O	7.03	1.36	1.23
1	A	763[B]	SER	C-O	7.03	1.36	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	739	ARG	NE-CZ-NH1	5.93	123.27	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	4811	0	4711	35	0
2	A	2	0	0	0	0
3	A	24	0	26	0	0
4	A	12	0	18	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	14	0	20	0	0
6	A	10	0	0	2	0
7	A	15	0	0	0	0
8	A	457	0	0	7	1
All	All	5345	0	4775	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	6:A:1008:PO4:O4	2.09	0.71
1:A:356:LYS:O	1:A:356:LYS:HD3	1.93	0.68
1:A:403:VAL:HG21	1:A:426:VAL:HG21	1.83	0.61
1:A:664:ASP:OD1	6:A:1008:PO4:P	2.61	0.59
1:A:733:GLU:O	1:A:737:ARG:HG3	2.03	0.58
1:A:764:LEU:HG	1:A:765:MET:HE3	1.86	0.57
1:A:312:LYS:O	1:A:313:GLN:CG	2.53	0.57
1:A:764:LEU:HG	1:A:765:MET:CE	2.34	0.56
1:A:453:ASN:ND2	1:A:579:ARG:HD2	2.25	0.51
4:A:1004:DMS:C1	8:A:1323:HOH:O	2.58	0.51
1:A:411:ALA:HA	1:A:477:MET:O	2.11	0.50
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.52	0.50
1:A:356:LYS:O	1:A:356:LYS:CD	2.59	0.49
1:A:312:LYS:O	1:A:313:GLN:HG3	2.14	0.48
1:A:528:GLY:O	1:A:668:LYS:HE3	2.13	0.48
4:A:1004:DMS:H12	8:A:1305:HOH:O	2.14	0.48
1:A:886:MET:CE	8:A:1239:HOH:O	2.62	0.47
1:A:641:ILE:O	1:A:645:ASN:HB2	2.15	0.47
1:A:438:GLU:HG3	1:A:449:THR:OG1	2.15	0.47
1:A:638:THR:HA	1:A:641:ILE:HG22	1.98	0.46
1:A:809:MET:HA	1:A:809:MET:HE2	1.98	0.45
1:A:579:ARG:HA	1:A:591:ASP:O	2.18	0.44
1:A:638:THR:HA	1:A:641:ILE:CG2	2.48	0.44
1:A:303:TRP:CE3	1:A:593:ILE:HD12	2.53	0.43
1:A:801[B]:HIS:CD2	1:A:801[B]:HIS:H	2.36	0.43
1:A:599:ARG:HG2	1:A:606:THR:HG23	2.01	0.42
1:A:475:TRP:CD1	1:A:475:TRP:N	2.88	0.42
1:A:562:LYS:NZ	8:A:1119:HOH:O	2.49	0.42
1:A:790:THR:HG22	8:A:1398:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:886:MET:HE1	8:A:1239:HOH:O	2.19	0.41
1:A:452:TYR:HB2	1:A:578:VAL:HG22	2.02	0.41
1:A:562:LYS:HE3	1:A:566:GLU:OE2	2.20	0.41
1:A:510:GLU:O	1:A:514:LYS:HG3	2.19	0.41
1:A:512[B]:LEU:HD23	1:A:512[B]:LEU:HA	1.91	0.41
1:A:400:THR:HG23	1:A:426:VAL:CG1	2.50	0.41
1:A:303:TRP:CD2	1:A:593:ILE:HD12	2.56	0.40
1:A:693:GLN:HG3	8:A:1247:HOH:O	2.21	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:1158:HOH:O	8:A:1158:HOH:O[2_445]	1.56	0.64

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	575/637 (90%)	547 (95%)	27 (5%)	1 (0%)	44 25

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	473	ALA

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	517/554 (93%)	508 (98%)	9 (2%)	56 32

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

Mol	Chain	Res	Type
1	A	274	LEU
1	A	290	THR
1	A	294	TYR
1	A	426	VAL
1	A	453	ASN
1	A	482	ARG
1	A	641	ILE
1	A	644	LYS
1	A	693	GLN

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	693	GLN

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
3	MES	A	1003[B]	-	12,12,12	0.71	0	15,16,16	0.30	0
4	DMS	A	1004	-	3,3,3	0.61	0	3,3,3	0.41	0
4	DMS	A	1006	-	3,3,3	0.17	0	3,3,3	0.38	0
5	PEG	A	1007	-	6,6,6	0.24	0	5,5,5	0.12	0
3	MES	A	1003[A]	-	12,12,12	0.65	0	15,16,16	0.55	0
5	PEG	A	1010	-	6,6,6	0.12	0	5,5,5	0.13	0
6	PO4	A	1008	-	4,4,4	3.51	3 (75%)	6,6,6	0.68	0
4	DMS	A	1005	-	3,3,3	0.34	0	3,3,3	0.10	0
6	PO4	A	1009	-	4,4,4	1.01	0	6,6,6	0.53	0
7	A1AM1	A	1011	-	12,16,16	0.68	0	12,21,21	1.11	2 (16%)

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	1007	-	-	1/4/4/4	-
3	MES	A	1003[A]	-	-	0/6/14/14	0/1/1/1
5	PEG	A	1010	-	-	2/4/4/4	-
7	A1AM1	A	1011	-	-	2/5/14/14	0/1/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1008	PO4	P-O1	5.67	1.63	1.50
6	A	1008	PO4	P-O2	3.15	1.63	1.54
6	A	1008	PO4	P-O3	2.19	1.61	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1011	A1AM1	C9-N3-C4	2.67	130.81	125.38
7	A	1011	A1AM1	C4-N3-C5	-2.42	104.69	107.93

There are no chirality outliers.

All (10) torsion outliers are listed below:

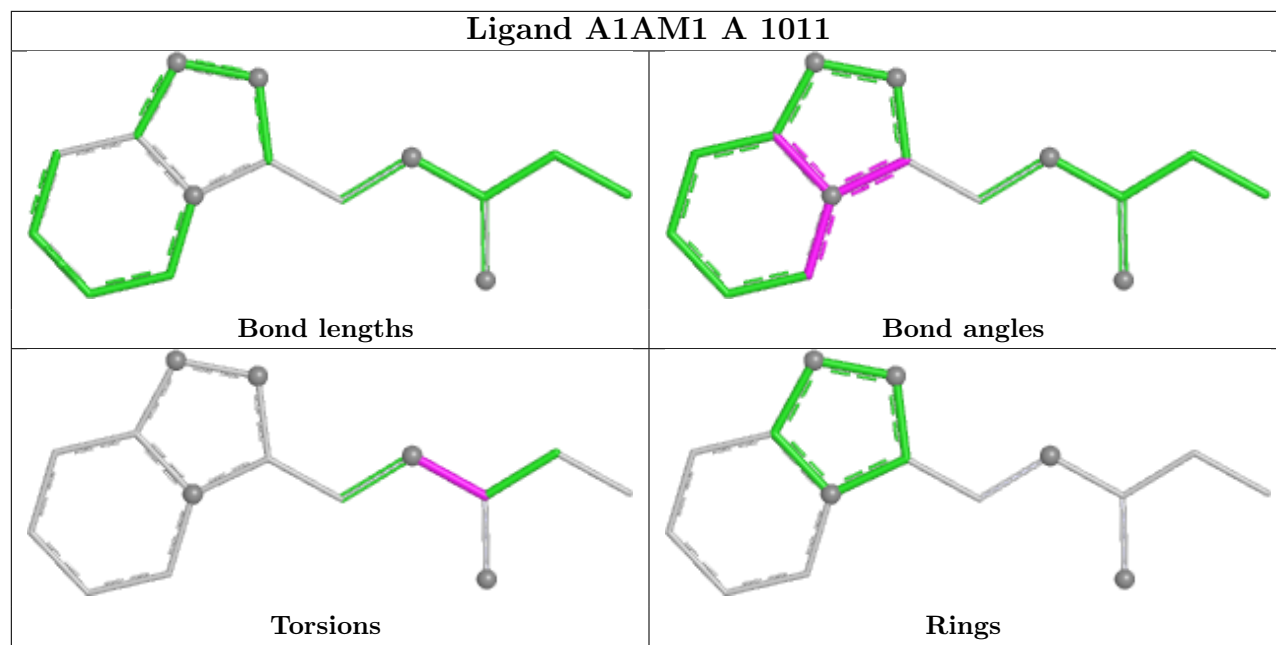
Mol	Chain	Res	Type	Atoms
3	A	1003[B]	MES	C8-C7-N4-C3
3	A	1003[B]	MES	C7-C8-S-O1S
7	A	1011	A1AM1	O-C2-N-C3
7	A	1011	A1AM1	C1-C2-N-C3
3	A	1003[B]	MES	C7-C8-S-O3S
5	A	1007	PEG	O2-C3-C4-O4
5	A	1010	PEG	O2-C3-C4-O4
3	A	1003[B]	MES	C8-C7-N4-C5
3	A	1003[B]	MES	C7-C8-S-O2S
5	A	1010	PEG	C4-C3-O2-C2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1004	DMS	2	0
6	A	1008	PO4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	581/637 (91%)	1.06	116 (19%) 3 3	6, 37, 98, 147	16 (2%)

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	359	VAL	17.0
1	A	512[A]	LEU	15.7
1	A	719[A]	LYS	14.1
1	A	801[A]	HIS	13.4
1	A	356	LYS	13.2
1	A	763[A]	SER	9.5
1	A	741[A]	SER	9.2
1	A	551[A]	GLU	9.1
1	A	589	VAL	8.0
1	A	413	PHE	6.1
1	A	799	ALA	5.5
1	A	475	TRP	4.7
1	A	600	GLY	4.6
1	A	294	TYR	4.6
1	A	407	ALA	4.5
1	A	409	LEU	4.2
1	A	281	ILE	4.1
1	A	363	THR	4.1
1	A	419	TRP	4.1
1	A	412	ILE	4.0
1	A	317	ALA	4.0
1	A	584	THR	4.0
1	A	889	PHE	3.8
1	A	311	THR	3.7
1	A	314	THR	3.7
1	A	284	ILE	3.7
1	A	571	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	588	THR	3.7
1	A	426	VAL	3.6
1	A	428	ASP	3.6
1	A	292	TRP	3.6
1	A	411	ALA	3.6
1	A	274	LEU	3.6
1	A	300	TYR	3.5
1	A	473	ALA	3.5
1	A	592	ILE	3.5
1	A	344	THR	3.4
1	A	583	PRO	3.3
1	A	635	LEU	3.3
1	A	879	TYR	3.3
1	A	427	GLU	3.2
1	A	309	TYR	3.2
1	A	593	ILE	3.2
1	A	875	GLY	3.2
1	A	578	VAL	3.2
1	A	290	THR	3.2
1	A	431	PHE	3.1
1	A	410	GLY	3.1
1	A	794	THR	3.1
1	A	454	MET	3.1
1	A	872	SER	3.0
1	A	293	HIS	3.0
1	A	637	VAL	3.0
1	A	305	TYR	2.9
1	A	358	LYS	2.9
1	A	793	THR	2.9
1	A	399	PHE	2.8
1	A	304	ALA	2.8
1	A	403	VAL	2.8
1	A	361	THR	2.8
1	A	785[A]	SER	2.7
1	A	580	VAL	2.7
1	A	864[A]	GLN	2.7
1	A	443	LEU	2.7
1	A	474	ILE	2.6
1	A	308	SER	2.6
1	A	577	VAL	2.6
1	A	694	TRP	2.6
1	A	435	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	800	THR	2.6
1	A	298	HIS	2.6
1	A	408	ALA	2.5
1	A	634	HIS	2.5
1	A	871	ARG	2.5
1	A	452	TYR	2.4
1	A	564	LEU	2.4
1	A	310	GLU	2.4
1	A	299	PRO	2.4
1	A	303	TRP	2.4
1	A	582	ARG	2.4
1	A	891	ARG	2.4
1	A	745	GLY	2.4
1	A	472	ARG	2.4
1	A	792	ARG	2.4
1	A	476	TYR	2.4
1	A	417	ASN	2.3
1	A	744	ALA	2.3
1	A	478	TRP	2.3
1	A	430	GLY	2.3
1	A	441	LEU	2.3
1	A	288	HIS	2.3
1	A	746	TRP	2.2
1	A	884	PRO	2.2
1	A	273	ASN	2.2
1	A	277	ILE	2.2
1	A	590	MET	2.2
1	A	295	ASP	2.2
1	A	575	ASN	2.2
1	A	425	ALA	2.2
1	A	723	VAL	2.2
1	A	422	ALA	2.2
1	A	641	ILE	2.2
1	A	406	ASN	2.2
1	A	434	LEU	2.2
1	A	455	MET	2.1
1	A	364	GLN	2.1
1	A	579	ARG	2.1
1	A	418	LYS	2.1
1	A	868	ASN	2.1
1	A	717	ILE	2.1
1	A	357	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	429	SER	2.1
1	A	885	SER	2.1
1	A	289	GLU	2.1
1	A	432	TRP	2.1
1	A	275	ASP	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](#)

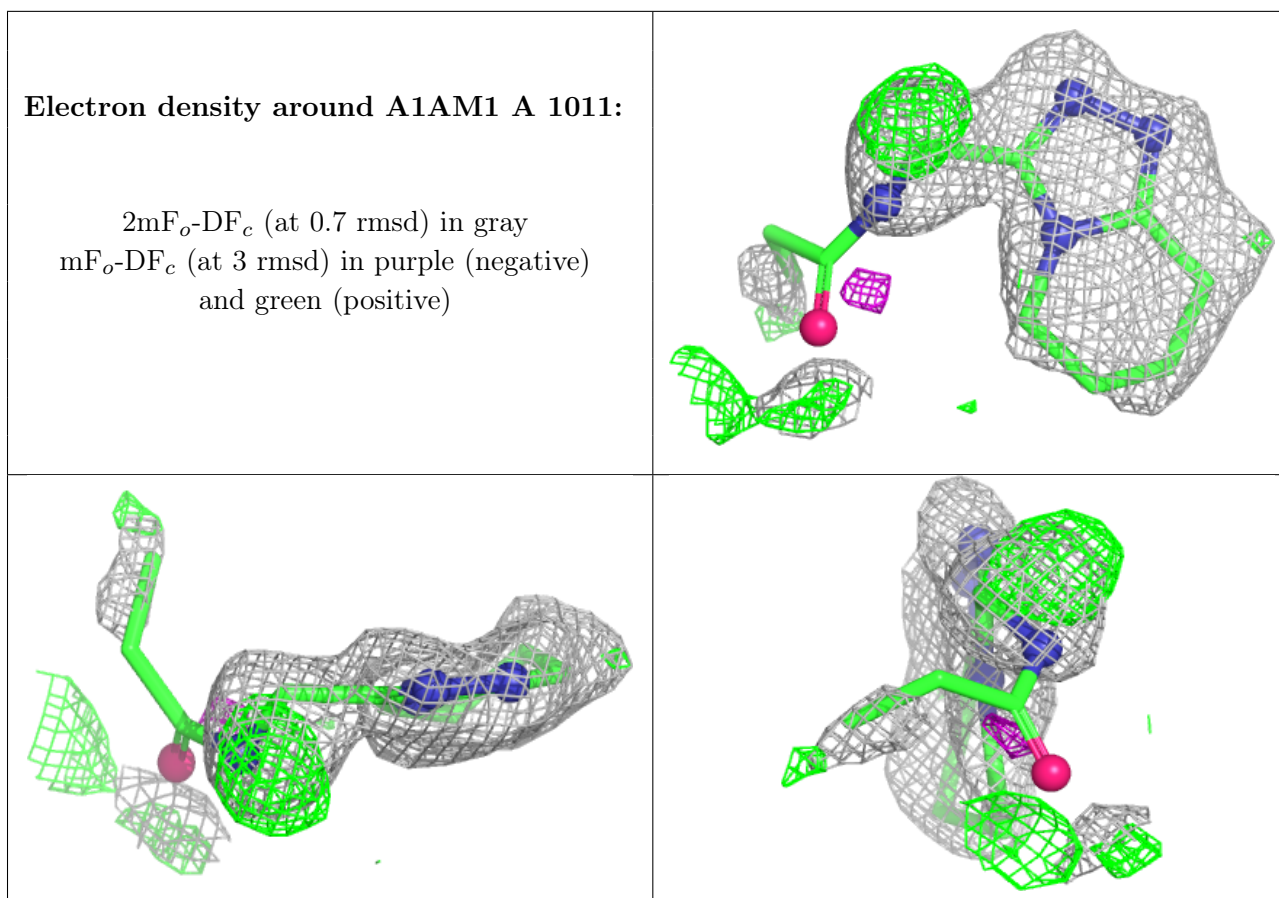
There are no monosaccharides in this entry.

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
6	PO4	A	1009	5/5	0.59	0.15	74,74,84,96	0
5	PEG	A	1007	7/7	0.65	0.20	78,84,89,91	0
7	A1AM1	A	1011	15/15	0.68	0.29	62,64,70,70	15
4	DMS	A	1005	4/4	0.71	0.30	74,100,101,115	0
6	PO4	A	1008	5/5	0.72	0.16	38,41,58,61	0
5	PEG	A	1010	7/7	0.86	0.15	59,67,72,74	0
4	DMS	A	1004	4/4	0.92	0.16	44,48,50,51	0
4	DMS	A	1006	4/4	0.94	0.13	54,56,56,59	0
3	MES	A	1003[A]	12/12	0.98	0.33	20,23,25,26	12
3	MES	A	1003[B]	12/12	0.98	0.33	530,547,576,578	12
2	ZN	A	1002	1/1	0.99	0.05	50,50,50,50	0
2	ZN	A	1001	1/1	1.00	0.01	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.