



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:03 AM UTC

PDB ID : 7I2C / pdb_00007i2c
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 Z71308235 (DNV2_NS5A-x0253)
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 : 1.63 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)

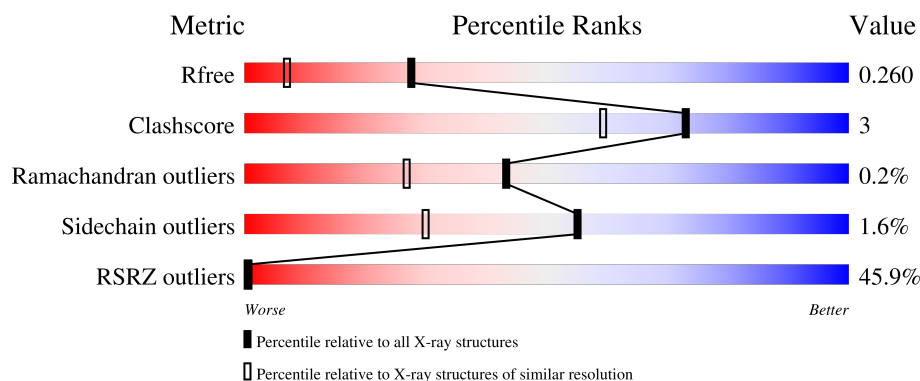
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.63 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	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

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	41% 82% 8% 10%

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 9 unique types of molecules in this entry. The entry contains 5216 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	573	4736	2982	849	871	34	0	7	0

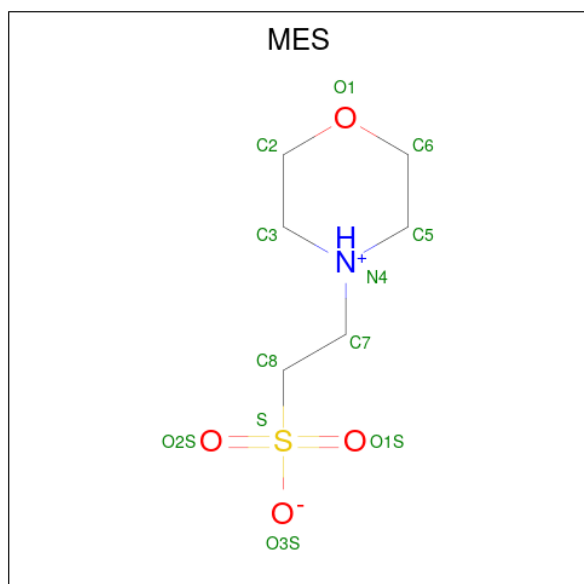
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	264	GLY	-	expression tag	UNP Q91H74
A	265	PRO	-	expression tag	UNP Q91H74

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

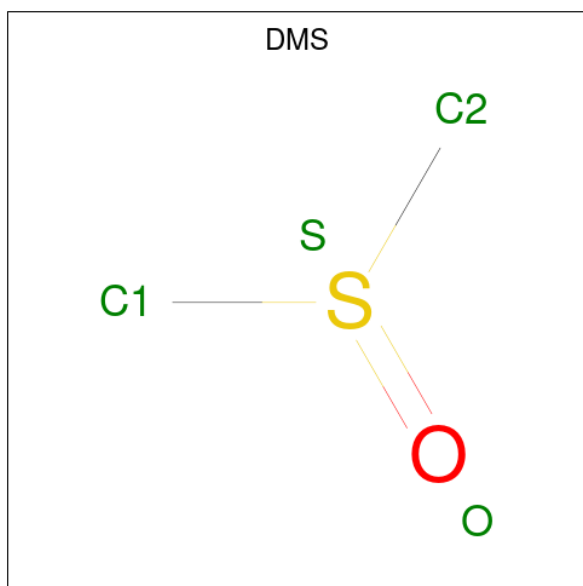
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



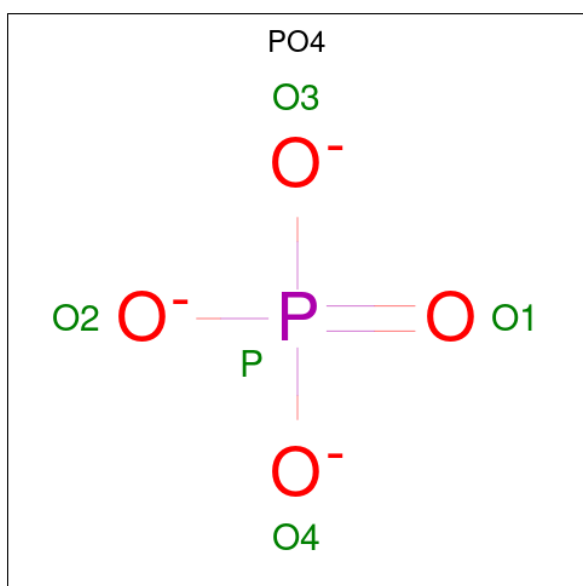
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

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



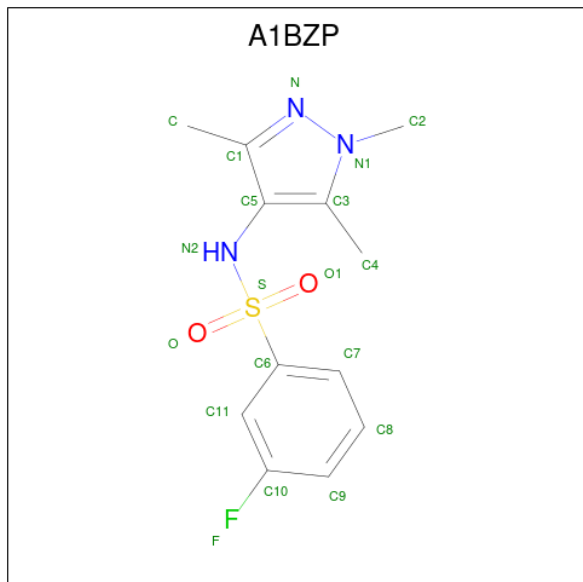
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		

- 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 3-fluoro-N-(1,3,5-trimethyl-1H-pyrazol-4-yl)benzene-1-sulfonamide (CCD ID: A1BZP) (formula: $C_{12}H_{14}FN_3O_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	F	N	O	S	
			19	12	1	3	2	1	0

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	398	Total	O		
			398	398	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	82.64Å 117.01Å 149.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.55 – 1.63 74.55 – 1.63	Depositor EDS
% Data completeness (in resolution range)	97.7 (74.55-1.63) 97.7 (74.55-1.63)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 1.63Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC5	Depositor
R, R_{free}	0.193 , 0.226 0.236 , 0.260	Depositor DCC
R_{free} test set	4581 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 76.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5216	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.63% 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, PEG, CL, A1BZP, MES, DMS, 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	1.09	2/4841 (0.0%)	1.31	3/6528 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	751	THR	C-O	6.03	1.31	1.24
1	A	711	HIS	CE1-NE2	5.35	1.38	1.32

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	702	ASP	CB-CA-C	5.60	118.77	110.14
1	A	702	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	483	PHE	CA-CB-CG	-5.11	108.69	113.80

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	4736	0	4640	28	0
2	A	2	0	0	0	0
3	A	24	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	12	0	18	2	0
5	A	14	0	20	0	0
6	A	10	0	0	4	0
7	A	19	0	0	0	0
8	A	1	0	0	0	0
9	A	398	0	0	6	1
All	All	5216	0	4704	30	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 3.

All (30) 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	2.00	0.79
4:A:1004:DMS:H11	9:A:1245:HOH:O	1.82	0.78
4:A:1004:DMS:H12	9:A:1259:HOH:O	1.97	0.64
1:A:886:MET:HE1	9:A:1234:HOH:O	2.04	0.57
1:A:801[B]:HIS:H	1:A:801[B]:HIS:CD2	2.22	0.56
1:A:664:ASP:OD1	6:A:1008:PO4:P	2.63	0.56
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.47	0.55
1:A:733:GLU:O	1:A:737:ARG:HG3	2.07	0.55
1:A:562:LYS:NZ	9:A:1110:HOH:O	2.41	0.54
1:A:534:ASP:OD1	6:A:1008:PO4:O4	2.26	0.53
1:A:400:THR:HG23	1:A:426:VAL:HG11	1.92	0.52
1:A:438:GLU:HG3	1:A:449:THR:OG1	2.09	0.52
1:A:764:LEU:HG	1:A:765:MET:CE	2.41	0.51
1:A:303:TRP:CE3	1:A:593:ILE:HD12	2.45	0.51
1:A:805:THR:CG2	1:A:809:MET:HE1	2.40	0.51
1:A:834:GLU:OE2	1:A:890:ARG:NE	2.44	0.47
1:A:429:SER:O	1:A:433:GLU:HG3	2.14	0.46
1:A:452:TYR:CZ	1:A:600:GLY:O	2.68	0.46
1:A:528:GLY:O	1:A:668:LYS:HE3	2.15	0.46
1:A:886:MET:CE	9:A:1234:HOH:O	2.62	0.46
1:A:285:LYS:HG3	1:A:292:TRP:CE2	2.51	0.46
1:A:599:ARG:HG2	1:A:606:THR:HG23	1.99	0.44
1:A:719[A]:LYS:NZ	1:A:834:GLU:O	2.51	0.44
1:A:649:ARG:HG2	1:A:650:VAL:HG13	2.00	0.43
1:A:400:THR:HG23	1:A:426:VAL:CG1	2.49	0.43
1:A:888:ARG:HD2	9:A:1268:HOH:O	2.18	0.42
1:A:321:VAL:HG11	1:A:326:ARG:CZ	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:ASP:OD1	6:A:1008:PO4:P	2.78	0.41
1:A:341:MET:HE2	1:A:341:MET:HB3	1.84	0.40
1:A:562:LYS:HE3	1:A:566:GLU:OE2	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)
9:A:1175:HOH:O	9:A:1175:HOH:O[2_445]	1.68	0.52

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	566/637 (89%)	545 (96%)	20 (4%)	1 (0%)	43 27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	509/554 (92%)	501 (98%)	8 (2%)	55 30

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	290	THR
1	A	455	MET
1	A	633	GLN
1	A	635	LEU
1	A	641	ILE
1	A	830	VAL
1	A	854	THR
1	A	887	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	645	ASN
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 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
6	PO4	A	1009	-	4,4,4	1.58	1 (25%)	6,6,6	0.54	0
5	PEG	A	1010	-	6,6,6	0.13	0	5,5,5	0.12	0
3	MES	A	1003[A]	-	12,12,12	0.91	0	15,16,16	0.67	0
7	A1BZP	A	1011	-	19,20,20	0.20	0	27,30,30	0.79	1 (3%)
4	DMS	A	1004	-	3,3,3	0.91	0	3,3,3	0.54	0
4	DMS	A	1006	-	3,3,3	0.28	0	3,3,3	0.27	0
6	PO4	A	1008	-	4,4,4	5.36	4 (100%)	6,6,6	0.96	0
4	DMS	A	1005	-	3,3,3	0.46	0	3,3,3	0.14	0
5	PEG	A	1007	-	6,6,6	0.22	0	5,5,5	0.11	0
3	MES	A	1003[B]	-	12,12,12	0.70	0	15,16,16	0.32	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
7	A1BZP	A	1011	-	-	0/11/11/11	0/2/2/2
5	PEG	A	1010	-	-	2/4/4/4	-
3	MES	A	1003[A]	-	-	0/6/14/14	0/1/1/1
5	PEG	A	1007	-	-	1/4/4/4	-
3	MES	A	1003[B]	-	-	5/6/14/14	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1008	PO4	P-O1	8.30	1.69	1.50
6	A	1008	PO4	P-O2	4.98	1.69	1.54
6	A	1008	PO4	P-O3	3.86	1.65	1.54
6	A	1009	PO4	P-O1	2.74	1.57	1.50
6	A	1008	PO4	P-O4	-2.56	1.47	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1011	A1BZP	C5-C3-N1	3.65	106.20	104.79

There are no chirality outliers.

All (8) torsion outliers are listed below:

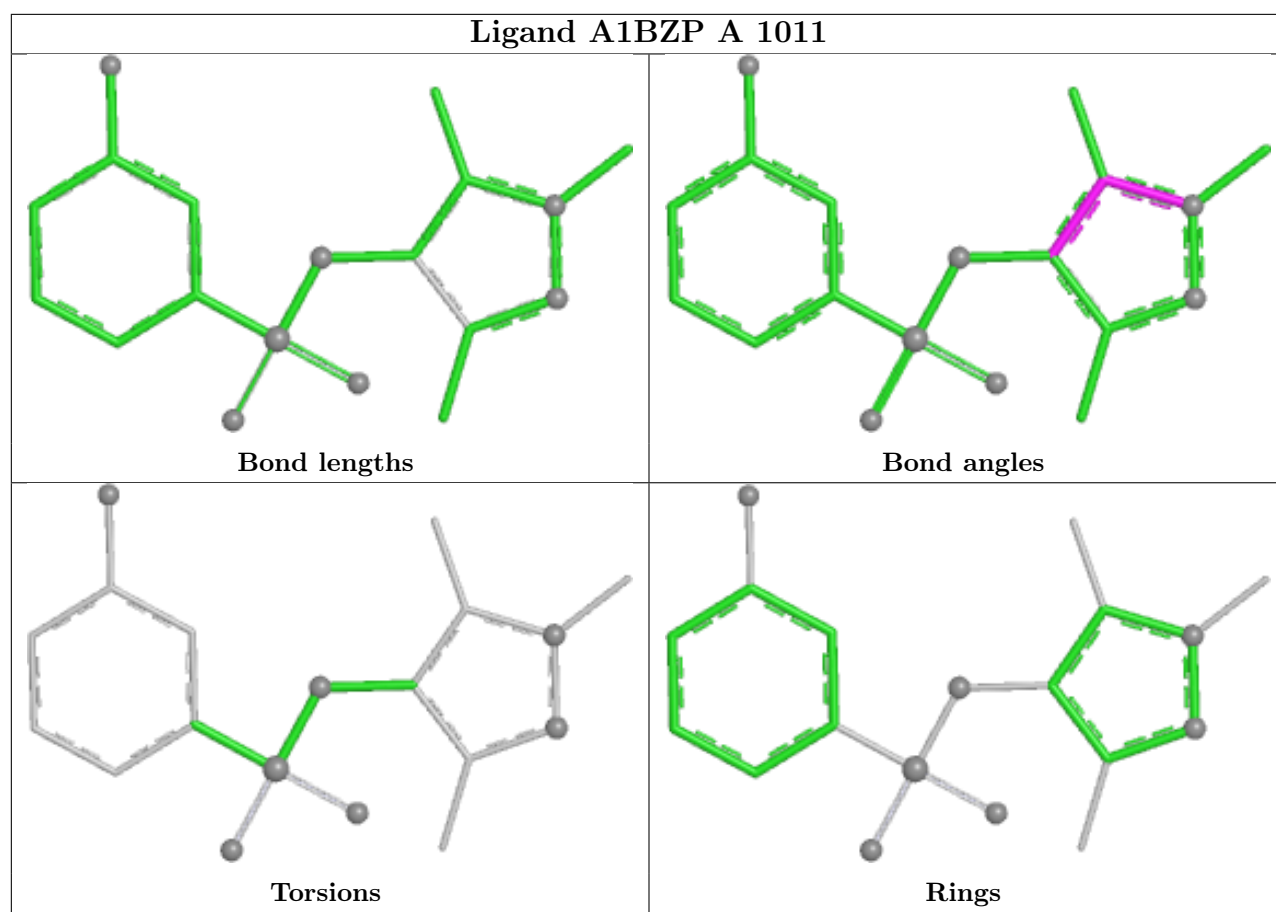
Mol	Chain	Res	Type	Atoms
3	A	1003[B]	MES	C8-C7-N4-C3
3	A	1003[B]	MES	C7-C8-S-O3S
5	A	1007	PEG	O2-C3-C4-O4
5	A	1010	PEG	O2-C3-C4-O4
3	A	1003[B]	MES	C8-C7-N4-C5
3	A	1003[B]	MES	C7-C8-S-O1S
3	A	1003[B]	MES	C7-C8-S-O2S
5	A	1010	PEG	C4-C3-O2-C2

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1004	DMS	2	0
6	A	1008	PO4	4	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%)	3.05	263 (45%) 0 1	6, 33, 82, 158	135 (23%)

All (263) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	850	LEU	16.5
1	A	846	TRP	15.5
1	A	853	LEU	15.5
1	A	851	ILE	14.7
1	A	854	THR	13.9
1	A	852	GLY	13.7
1	A	848	GLY	13.2
1	A	512[A]	LEU	12.2
1	A	304	ALA	12.2
1	A	303	TRP	12.1
1	A	641	ILE	11.9
1	A	411	ALA	11.8
1	A	844	ASP	11.7
1	A	409	LEU	11.7
1	A	700	TRP	11.6
1	A	801[A]	HIS	11.5
1	A	580	VAL	11.3
1	A	478	TRP	11.3
1	A	719[A]	LYS	11.3
1	A	426	VAL	11.2
1	A	281	ILE	11.2
1	A	589	VAL	11.0
1	A	309	TYR	10.8
1	A	399	PHE	10.8
1	A	451	VAL	10.6
1	A	475	TRP	10.2
1	A	588	THR	10.2

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Mol	Chain	Res	Type	RSRZ
1	A	274	LEU	10.0
1	A	600	GLY	10.0
1	A	403	VAL	10.0
1	A	511	GLY	9.5
1	A	601	SER	9.2
1	A	474	ILE	9.2
1	A	800	THR	9.2
1	A	308	SER	9.0
1	A	429	SER	9.0
1	A	743	GLY	9.0
1	A	842	ARG	8.6
1	A	410	GLY	8.6
1	A	841	LYS	8.6
1	A	311	THR	8.6
1	A	476	TYR	8.5
1	A	845	GLN	8.5
1	A	277	ILE	8.5
1	A	408	ALA	8.5
1	A	359	VAL	8.5
1	A	656	SER	8.5
1	A	638	THR	8.5
1	A	843	GLU	8.5
1	A	544	LEU	8.4
1	A	602	GLY	8.3
1	A	412	ILE	8.3
1	A	480	GLY	8.2
1	A	422	ALA	8.1
1	A	741[A]	SER	8.1
1	A	276	ILE	8.1
1	A	473	ALA	8.0
1	A	513	HIS	8.0
1	A	319	SER	8.0
1	A	481	ALA	8.0
1	A	575	ASN	8.0
1	A	509	GLY	7.9
1	A	499	SER	7.8
1	A	280	ARG	7.8
1	A	552	MET	7.8
1	A	549	ASN	7.7
1	A	421	SER	7.7
1	A	576	LYS	7.6
1	A	540	THR	7.6

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Mol	Chain	Res	Type	RSRZ
1	A	419	TRP	7.6
1	A	484	LEU	7.5
1	A	785[A]	SER	7.5
1	A	425	ALA	7.4
1	A	763[A]	SER	7.4
1	A	479	LEU	7.3
1	A	356	LYS	7.3
1	A	402	LYS	7.3
1	A	273	ASN	7.2
1	A	375	LYS	7.2
1	A	423	ARG	7.2
1	A	453	ASN	7.1
1	A	649	ARG	7.1
1	A	742	GLN	7.0
1	A	864[A]	GLN	7.0
1	A	320	MET	7.0
1	A	371	LYS	6.9
1	A	541	ARG	6.9
1	A	372	LYS	6.9
1	A	302	THR	6.9
1	A	361	THR	6.9
1	A	401	ARG	6.9
1	A	595	ARG	6.9
1	A	639	GLU	6.9
1	A	279	LYS	6.9
1	A	318	SER	6.8
1	A	294	TYR	6.8
1	A	485	GLU	6.8
1	A	300	TYR	6.8
1	A	358	LYS	6.8
1	A	502	ASN	6.7
1	A	640	GLU	6.7
1	A	428	ASP	6.7
1	A	514	LYS	6.7
1	A	794	THR	6.5
1	A	441	LEU	6.5
1	A	292	TRP	6.4
1	A	477	MET	6.4
1	A	582	ARG	6.4
1	A	305	TYR	6.4
1	A	551	GLU	6.4
1	A	591	ASP	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	705	GLN	6.3
1	A	635	LEU	6.3
1	A	482	ARG	6.2
1	A	791	SER	6.2
1	A	590	MET	6.1
1	A	284	ILE	6.1
1	A	597	ASP	6.0
1	A	397	GLU	6.0
1	A	298	HIS	6.0
1	A	363	THR	6.0
1	A	362	ARG	5.9
1	A	880	THR	5.9
1	A	548	LYS	5.9
1	A	581	GLN	5.9
1	A	698	ARG	5.9
1	A	889	PHE	5.9
1	A	287	GLU	5.8
1	A	282	GLU	5.8
1	A	407	ALA	5.8
1	A	644	LYS	5.7
1	A	431	PHE	5.7
1	A	793	THR	5.7
1	A	888	ARG	5.6
1	A	297	ASP	5.5
1	A	275	ASP	5.5
1	A	634	HIS	5.5
1	A	290	THR	5.5
1	A	418	LYS	5.4
1	A	510	GLU	5.4
1	A	487	GLU	5.4
1	A	501	GLU	5.4
1	A	596	ARG	5.4
1	A	364	GLN	5.3
1	A	379	GLU	5.3
1	A	442	HIS	5.3
1	A	357	GLU	5.3
1	A	286	GLN	5.2
1	A	398	GLU	5.2
1	A	583	PRO	5.2
1	A	653	GLU	5.2
1	A	434	LEU	5.1
1	A	645	ASN	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	310	GLU	5.0
1	A	420	LYS	5.0
1	A	293	HIS	5.0
1	A	444	GLU	5.0
1	A	545	GLU	5.0
1	A	289	GLU	5.0
1	A	424	GLU	5.0
1	A	360	ASP	5.0
1	A	790	THR	4.9
1	A	799	ALA	4.8
1	A	603	GLN	4.8
1	A	452	TYR	4.7
1	A	890	ARG	4.6
1	A	427	GLU	4.6
1	A	288	HIS	4.5
1	A	299	PRO	4.5
1	A	629	PHE	4.4
1	A	435	VAL	4.4
1	A	430	GLY	4.3
1	A	556	HIS	4.3
1	A	564	LEU	4.2
1	A	886	MET	4.2
1	A	881	ASP	4.2
1	A	584	THR	4.0
1	A	604	VAL	4.0
1	A	571	LEU	4.0
1	A	882	TYR	3.9
1	A	404	ARG	3.8
1	A	792	ARG	3.8
1	A	637	VAL	3.8
1	A	448	GLU	3.8
1	A	891	ARG	3.7
1	A	406	ASN	3.7
1	A	443	LEU	3.7
1	A	694	TRP	3.7
1	A	825	GLU	3.6
1	A	445	GLY	3.5
1	A	368	GLU	3.5
1	A	344	THR	3.4
1	A	291	SER	3.4
1	A	592	ILE	3.3
1	A	455	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	593	ILE	3.3
1	A	677	ALA	3.2
1	A	439	ARG	3.2
1	A	746	TRP	3.2
1	A	750	GLU	3.2
1	A	884	PRO	3.1
1	A	296	GLN	3.1
1	A	570	LYS	3.0
1	A	695	GLU	3.0
1	A	307	GLY	3.0
1	A	432	TRP	3.0
1	A	437	LYS	3.0
1	A	744	ALA	3.0
1	A	301	LYS	3.0
1	A	438	GLU	2.8
1	A	834	GLU	2.8
1	A	436	ASP	2.8
1	A	396	ARG	2.8
1	A	876	ASN	2.8
1	A	764	LEU	2.7
1	A	285	LYS	2.6
1	A	830	VAL	2.6
1	A	717	ILE	2.6
1	A	558	GLU	2.6
1	A	440	ASN	2.6
1	A	524	LYS	2.6
1	A	559	GLY	2.6
1	A	693	GLN	2.6
1	A	648	VAL	2.6
1	A	393	MET	2.6
1	A	454	MET	2.5
1	A	295	ASP	2.5
1	A	579	ARG	2.5
1	A	633	GLN	2.5
1	A	572	THR	2.5
1	A	433	GLU	2.4
1	A	643	VAL	2.4
1	A	577	VAL	2.4
1	A	691	ILE	2.4
1	A	642	ALA	2.4
1	A	370	THR	2.4
1	A	578	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	605	VAL	2.4
1	A	808	ASP	2.3
1	A	278	GLY	2.3
1	A	450	CYS	2.3
1	A	405	SER	2.3
1	A	486	PHE	2.3
1	A	534	ASP	2.3
1	A	449	THR	2.2
1	A	447	CYS	2.2
1	A	676	SER	2.2
1	A	885	SER	2.2
1	A	701	ASN	2.2
1	A	483	PHE	2.2
1	A	879	TYR	2.2
1	A	636	THR	2.2
1	A	878	GLU	2.1
1	A	395	THR	2.1
1	A	383	LYS	2.1
1	A	365	GLU	2.1
1	A	663	ASP	2.1
1	A	400	THR	2.1
1	A	535	THR	2.1
1	A	807	GLU	2.0
1	A	683	ASP	2.0
1	A	394	CYS	2.0
1	A	446	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

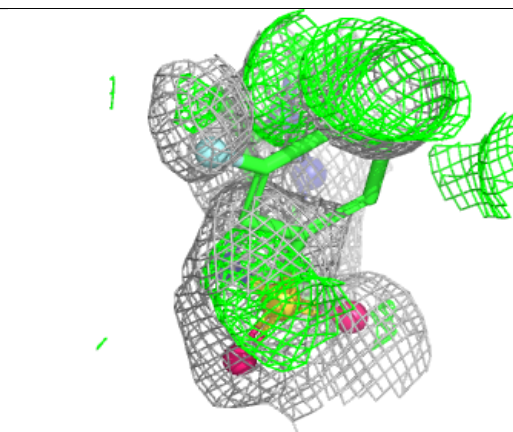
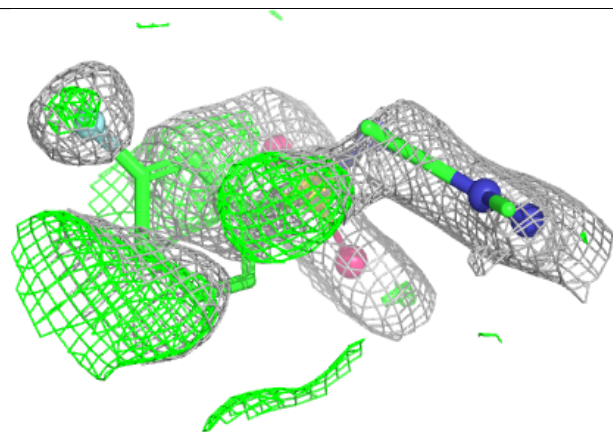
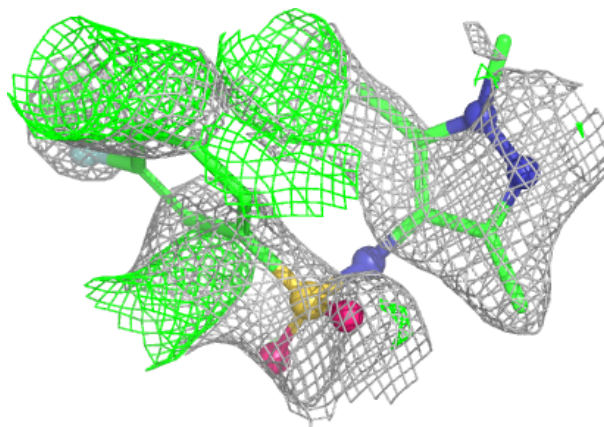
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	A1BZP	A	1011	19/19	0.48	0.40	45,48,51,52	19
6	PO4	A	1009	5/5	0.54	0.20	66,70,79,108	0
5	PEG	A	1007	7/7	0.54	0.24	91,101,108,109	0
4	DMS	A	1005	4/4	0.60	0.34	70,95,99,119	0
6	PO4	A	1008	5/5	0.72	0.17	36,37,55,58	0
5	PEG	A	1010	7/7	0.81	0.19	65,68,75,76	0
4	DMS	A	1006	4/4	0.91	0.14	45,54,61,62	0
4	DMS	A	1004	4/4	0.91	0.17	39,46,50,51	0
3	MES	A	1003[A]	12/12	0.97	0.32	21,25,29,30	12
3	MES	A	1003[B]	12/12	0.97	0.32	621,639,661,664	12
2	ZN	A	1002	1/1	0.98	0.06	50,50,50,50	0
8	CL	A	1012	1/1	0.98	0.06	40,40,40,40	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.

Electron density around A1BZP A 1011:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.