



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:34 AM UTC

PDB ID : 7HKD / pdb_00007hkd
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 Z53825479 (DNV2_NS5A-x0172)
Authors : Saini, M.; Chopra, A.; Aschenbrenner, J.C.; Marples, P.G.; Balcomb, B.H.; Fearon, D.; von Delft, F.; Ruiz, F.X.; Arnold, E.
Deposited on : 2024-10-15
Resolution : 1.66 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)

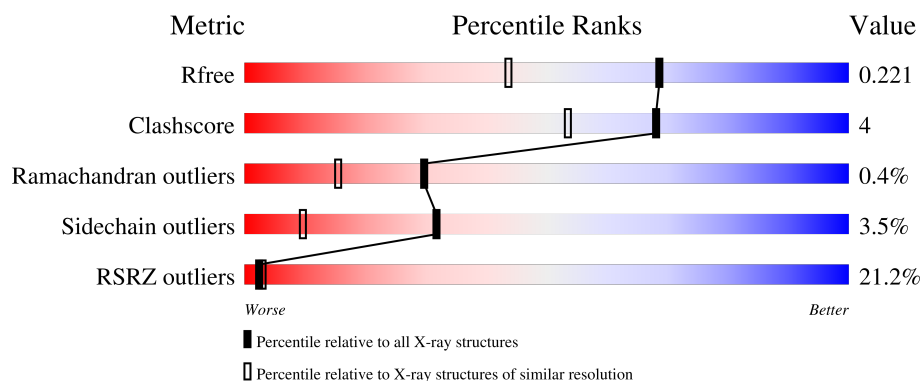
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.66 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	<div> <div>19%</div> <div>81%</div> <div>9%</div> <div>9%</div> </div>

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 8 unique types of molecules in this entry. The entry contains 5324 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 (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).



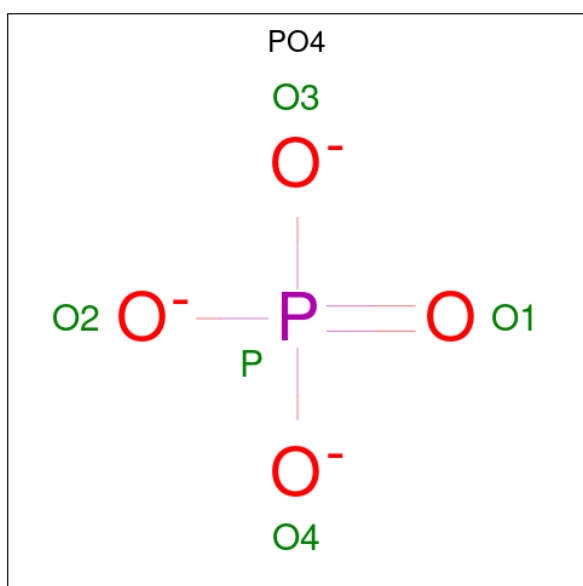
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

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



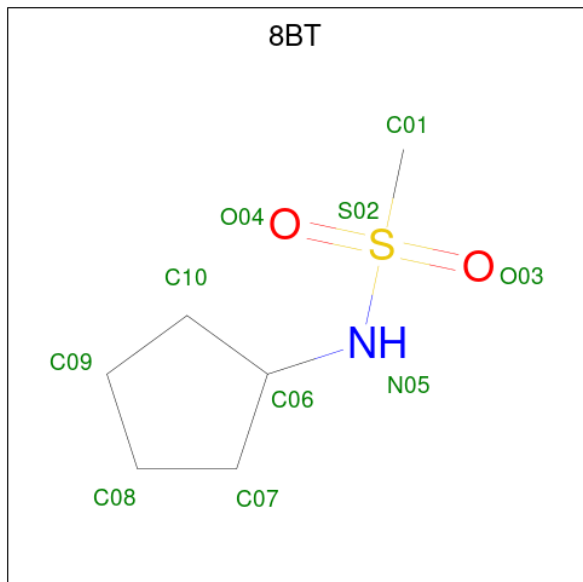
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		

- 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 N-cyclopentylmethanesulfonamide (CCD ID: 8BT) (formula: $C_6H_{13}NO_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			10	6	1	2	1		

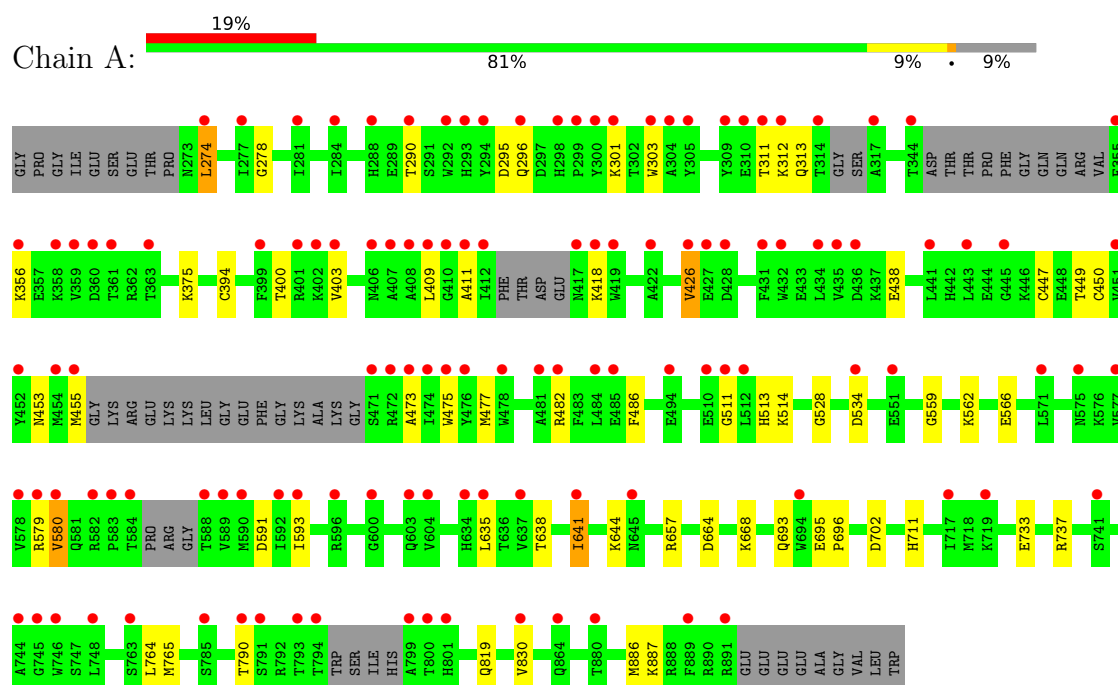
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	441	Total	O	0	0
			441	441		

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 polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	82.49Å 116.35Å 148.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.20 – 1.66 74.20 – 1.66	Depositor EDS
% Data completeness (in resolution range)	98.4 (74.20-1.66) 98.4 (74.20-1.66)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 1.66Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC5	Depositor
R, R_{free}	0.187 , 0.214 0.202 , 0.221	Depositor DCC
R_{free} test set	4317 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5324	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 4.97% 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: ZN, DMS, PO4, 8BT, PEG, MES

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	1.07	1/4917 (0.0%)	1.31	4/6629 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	711	HIS	CE1-NE2	5.20	1.37	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	702	ASP	CA-CB-CG	6.31	118.91	112.60
1	A	657	ARG	CG-CD-NE	-5.37	100.19	112.00
1	A	559	GLY	CA-C-N	5.34	127.75	120.54
1	A	559	GLY	C-N-CA	5.34	127.75	120.54

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	32	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	3	0
5	A	14	0	20	0	0
6	A	10	0	0	4	0
7	A	10	0	0	0	0
8	A	441	0	0	8	2
All	All	5324	0	4775	35	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 (35) 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	1.85	0.94
4:A:1004:DMS:H11	8:A:1281:HOH:O	1.82	0.79
1:A:534:ASP:OD1	6:A:1008:PO4:O4	2.06	0.73
1:A:664:ASP:OD1	6:A:1008:PO4:P	2.49	0.70
1:A:438:GLU:HG3	1:A:449:THR:OG1	1.98	0.62
4:A:1004:DMS:H12	8:A:1294:HOH:O	2.00	0.60
1:A:638:THR:HA	1:A:641:ILE:HG22	1.83	0.60
1:A:733:GLU:O	1:A:737:ARG:HG3	2.01	0.60
1:A:819:GLN:NE2	8:A:1106:HOH:O	2.30	0.58
1:A:886:MET:HE1	8:A:1252:HOH:O	2.03	0.58
1:A:534:ASP:OD1	6:A:1008:PO4:P	2.65	0.55
1:A:528:GLY:O	1:A:668:LYS:HE3	2.08	0.54
1:A:403:VAL:HG21	1:A:426:VAL:HG21	1.90	0.52
1:A:400:THR:O	1:A:403:VAL:HG22	2.11	0.51
1:A:886:MET:CE	8:A:1252:HOH:O	2.58	0.50
1:A:511:GLY:HA3	1:A:513:HIS:CE1	2.47	0.49
1:A:562:LYS:HE3	1:A:566:GLU:OE2	2.13	0.49
1:A:411:ALA:HA	1:A:477:MET:O	2.13	0.48
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.53	0.48
1:A:764:LEU:O	1:A:765:MET:HE2	2.12	0.48
1:A:475:TRP:CD1	1:A:475:TRP:N	2.80	0.48
1:A:580:VAL:HG21	1:A:593:ILE:HD11	1.95	0.48
1:A:303:TRP:CE3	1:A:593:ILE:HD12	2.50	0.47
1:A:312:LYS:O	1:A:313:GLN:CG	2.65	0.45
1:A:453:ASN:ND2	1:A:579:ARG:HD2	2.32	0.44
4:A:1004:DMS:C1	8:A:1281:HOH:O	2.55	0.44
1:A:295:ASP:OD1	1:A:296:GLN:N	2.51	0.43
1:A:394:CYS:HB3	1:A:486:PHE:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:790:THR:HG22	8:A:1376:HOH:O	2.18	0.43
1:A:274:LEU:O	1:A:278:GLY:N	2.53	0.42
1:A:562:LYS:NZ	8:A:1112:HOH:O	2.39	0.42
1:A:638:THR:HA	1:A:641:ILE:CG2	2.48	0.41
1:A:579:ARG:HA	1:A:591:ASP:O	2.21	0.41
1:A:695:GLU:HA	1:A:696:PRO:HD3	1.97	0.41
1:A:764:LEU:C	1:A:765:MET:HE2	2.46	0.41

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:1131:HOH:O	8:A:1131:HOH:O[2_445]	1.48	0.72
8:A:1310:HOH:O	8:A:1434:HOH:O[2_545]	2.15	0.05

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%)	550 (96%)	23 (4%)	2 (0%)	36 21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	418	LYS
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%)	499 (96%)	18 (4%)	32 10

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	274	LEU
1	A	290	THR
1	A	301	LYS
1	A	311	THR
1	A	356	LYS
1	A	375	LYS
1	A	409	LEU
1	A	426	VAL
1	A	455	MET
1	A	482	ARG
1	A	514	LYS
1	A	580	VAL
1	A	635	LEU
1	A	641	ILE
1	A	644	LYS
1	A	693	GLN
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	273	ASN
1	A	581	GLN
1	A	618	GLN
1	A	705	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 [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	$\# Z > 2$
4	DMS	A	1005	-	3,3,3	0.29	0	3,3,3	0.07	0
5	PEG	A	1010	-	6,6,6	0.17	0	5,5,5	0.13	0
6	PO4	A	1008	-	4,4,4	5.27	4 (100%)	6,6,6	0.73	0
4	DMS	A	1006	-	3,3,3	0.22	0	3,3,3	0.35	0
4	DMS	A	1004	-	3,3,3	0.64	0	3,3,3	0.54	0
5	PEG	A	1007	-	6,6,6	0.20	0	5,5,5	0.11	0
6	PO4	A	1009	-	4,4,4	1.20	1 (25%)	6,6,6	0.45	0
3	MES	A	1003[A]	-	12,12,12	0.68	0	15,16,16	0.72	0
3	MES	A	1003[B]	-	12,12,12	0.69	0	15,16,16	0.30	0
7	8BT	A	1011	-	10,10,10	0.20	0	13,14,14	0.30	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	-
5	PEG	A	1007	-	-	1/4/4/4	-
3	MES	A	1003[A]	-	-	3/6/14/14	0/1/1/1
3	MES	A	1003[B]	-	-	5/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	8BT	A	1011	-	-	0/5/12/12	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	8.15	1.69	1.50
6	A	1008	PO4	P-O2	4.66	1.68	1.54
6	A	1008	PO4	P-O3	4.20	1.66	1.54
6	A	1008	PO4	P-O4	-2.31	1.47	1.54
6	A	1009	PO4	P-O1	2.26	1.55	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1003[A]	MES	C7-C8-S-O2S
3	A	1003[A]	MES	C7-C8-S-O3S
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[A]	MES	C7-C8-S-O1S
3	A	1003[B]	MES	C7-C8-S-O1S
3	A	1003[B]	MES	C7-C8-S-O2S
5	A	1010	PEG	O1-C1-C2-O2

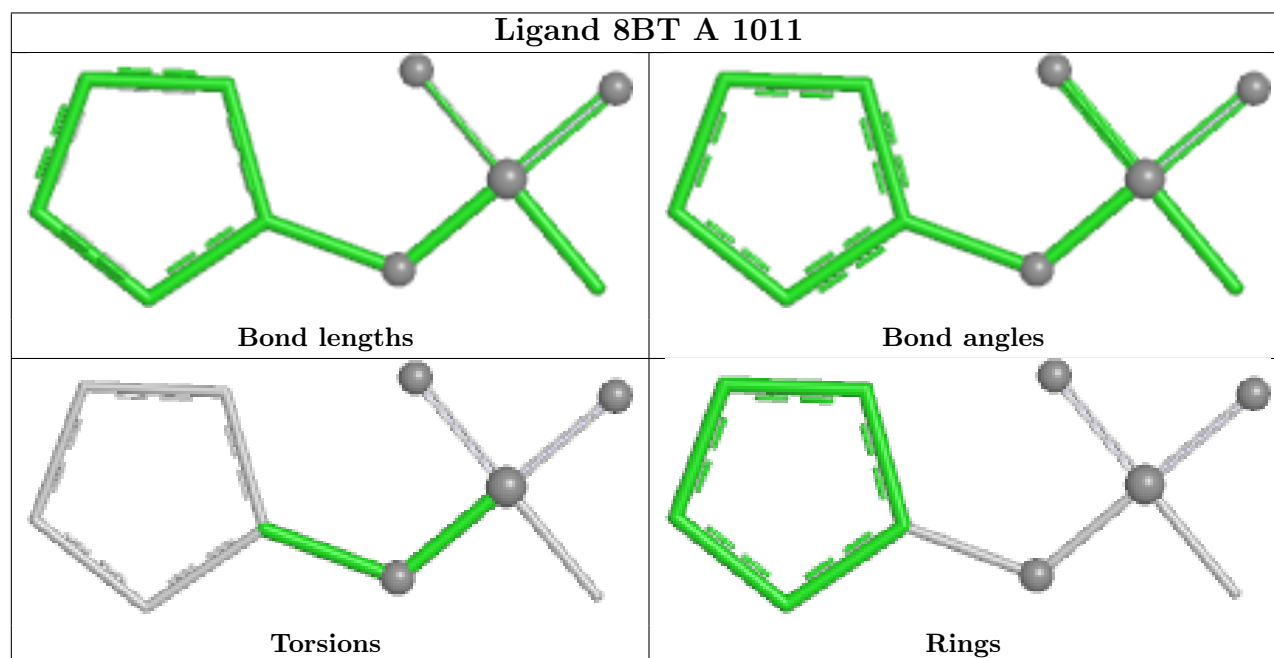
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1008	PO4	4	0
4	A	1004	DMS	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [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	581/637 (91%)	1.19	123 (21%) 2 3	6, 36, 105, 161	18 (3%)

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	409	LEU	16.1
1	A	512[A]	LEU	16.0
1	A	801[A]	HIS	14.2
1	A	719[A]	LYS	14.2
1	A	604	VAL	11.8
1	A	399	PHE	10.5
1	A	511	GLY	10.4
1	A	763[A]	SER	9.6
1	A	741[A]	SER	9.5
1	A	864[A]	GLN	9.0
1	A	785[A]	SER	8.8
1	A	551[A]	GLU	8.5
1	A	799	ALA	8.0
1	A	482	ARG	7.7
1	A	402	LYS	7.6
1	A	407	ALA	7.5
1	A	589	VAL	7.5
1	A	510	GLU	7.3
1	A	359	VAL	6.3
1	A	355	PHE	6.1
1	A	408	ALA	6.0
1	A	485	GLU	5.9
1	A	603	GLN	5.4
1	A	412	ILE	5.0
1	A	410	GLY	4.9
1	A	475	TRP	4.9
1	A	411	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	363	THR	4.4
1	A	794	THR	4.4
1	A	800	THR	4.3
1	A	294	TYR	4.2
1	A	344	THR	4.2
1	A	361	THR	4.2
1	A	637	VAL	4.0
1	A	292	TRP	3.9
1	A	317	ALA	3.8
1	A	419	TRP	3.8
1	A	793	THR	3.7
1	A	274	LEU	3.7
1	A	314	THR	3.7
1	A	441	LEU	3.6
1	A	600	GLY	3.6
1	A	584	THR	3.5
1	A	588	THR	3.5
1	A	284	ILE	3.5
1	A	745	GLY	3.5
1	A	435	VAL	3.5
1	A	583	PRO	3.5
1	A	309	TYR	3.3
1	A	880	THR	3.3
1	A	356	LYS	3.3
1	A	790	THR	3.2
1	A	300	TYR	3.2
1	A	311	THR	3.2
1	A	305	TYR	3.1
1	A	281	ILE	3.0
1	A	454	MET	3.0
1	A	494	GLU	3.0
1	A	290	THR	3.0
1	A	473	ALA	3.0
1	A	635	LEU	3.0
1	A	580	VAL	2.9
1	A	476	TYR	2.9
1	A	593	ILE	2.9
1	A	426	VAL	2.9
1	A	431	PHE	2.9
1	A	293	HIS	2.9
1	A	474	ILE	2.8
1	A	310	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	403	VAL	2.8
1	A	443	LEU	2.8
1	A	571	LEU	2.7
1	A	746	TRP	2.7
1	A	455	MET	2.7
1	A	422	ALA	2.7
1	A	744	ALA	2.7
1	A	427	GLU	2.6
1	A	298	HIS	2.6
1	A	452	TYR	2.6
1	A	590	MET	2.6
1	A	434	LEU	2.6
1	A	436	ASP	2.6
1	A	303	TRP	2.6
1	A	578	VAL	2.5
1	A	478	TRP	2.5
1	A	358	LYS	2.5
1	A	694	TRP	2.5
1	A	575	ASN	2.5
1	A	634	HIS	2.4
1	A	577	VAL	2.4
1	A	406	ASN	2.4
1	A	417	ASN	2.4
1	A	889	PHE	2.4
1	A	534	ASP	2.4
1	A	301	LYS	2.4
1	A	891	ARG	2.4
1	A	277	ILE	2.4
1	A	451	VAL	2.4
1	A	471	SER	2.3
1	A	641	ILE	2.3
1	A	645	ASN	2.3
1	A	401	ARG	2.2
1	A	472	ARG	2.2
1	A	428	ASP	2.2
1	A	288	HIS	2.2
1	A	582	ARG	2.2
1	A	592	ILE	2.2
1	A	304	ALA	2.2
1	A	312	LYS	2.2
1	A	579	ARG	2.1
1	A	484	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	445	GLY	2.1
1	A	360	ASP	2.1
1	A	432	TRP	2.1
1	A	717	ILE	2.1
1	A	830	VAL	2.1
1	A	791	SER	2.1
1	A	296	GLN	2.0
1	A	596	ARG	2.0
1	A	748	LEU	2.0
1	A	299	PRO	2.0
1	A	418	LYS	2.0
1	A	481	ALA	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.

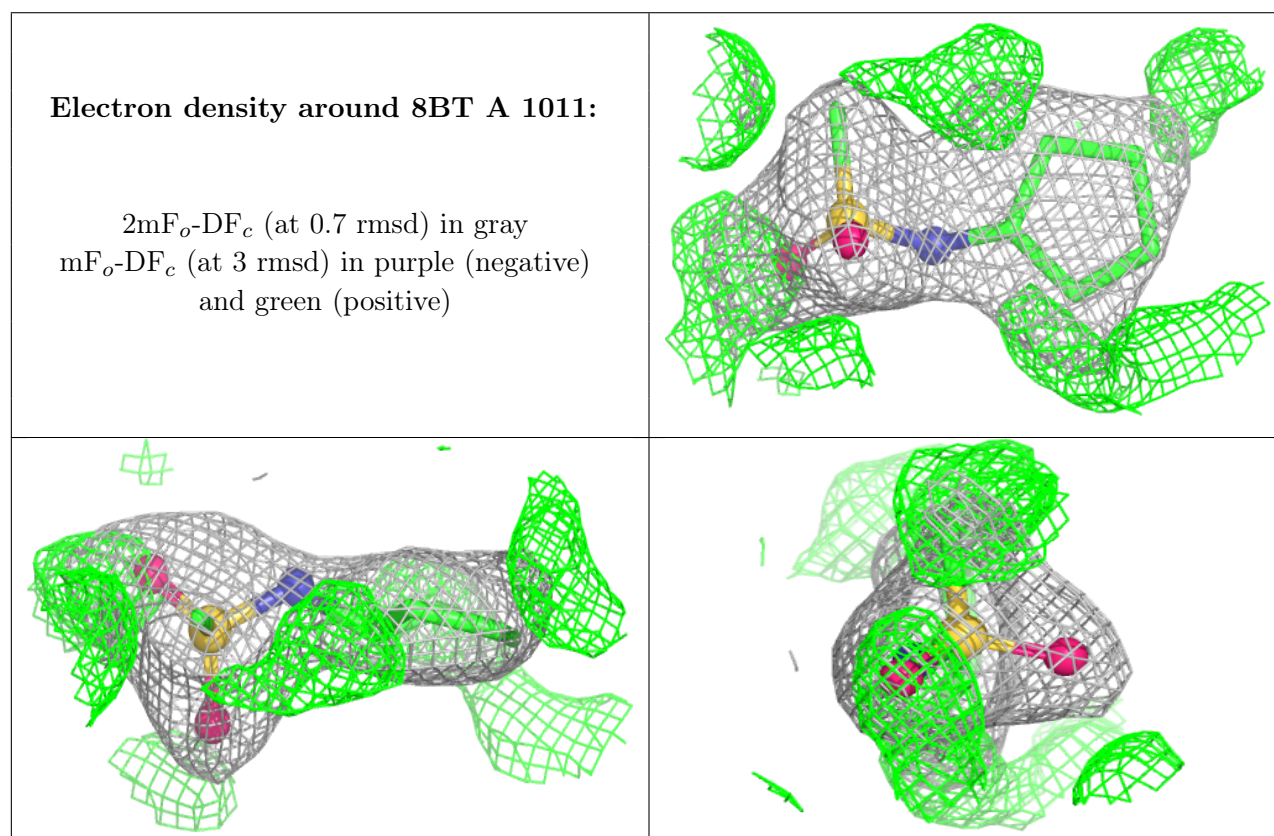
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PO4	A	1009	5/5	0.62	0.16	72,78,94,107	0
5	PEG	A	1007	7/7	0.68	0.20	76,80,87,88	0
6	PO4	A	1008	5/5	0.81	0.13	32,33,48,53	0
4	DMS	A	1005	4/4	0.83	0.21	70,82,88,96	0
5	PEG	A	1010	7/7	0.87	0.16	62,69,76,79	0
7	8BT	A	1011	10/10	0.87	0.21	51,52,53,54	10
4	DMS	A	1006	4/4	0.93	0.14	50,57,58,59	0
4	DMS	A	1004	4/4	0.94	0.12	38,43,45,47	0
3	MES	A	1003[B]	12/12	0.98	0.35	603,621,649,651	12
2	ZN	A	1002	1/1	0.98	0.06	48,48,48,48	0
3	MES	A	1003[A]	12/12	0.98	0.35	22,26,28,29	12

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	A	1001	1/1	1.00	0.01	20,20,20,20	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.