



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:36 AM UTC

PDB ID : 7HL4 / pdb_00007hl4
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 HL11 (DENV2_NS5A-x1094)
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 : 1.78 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)

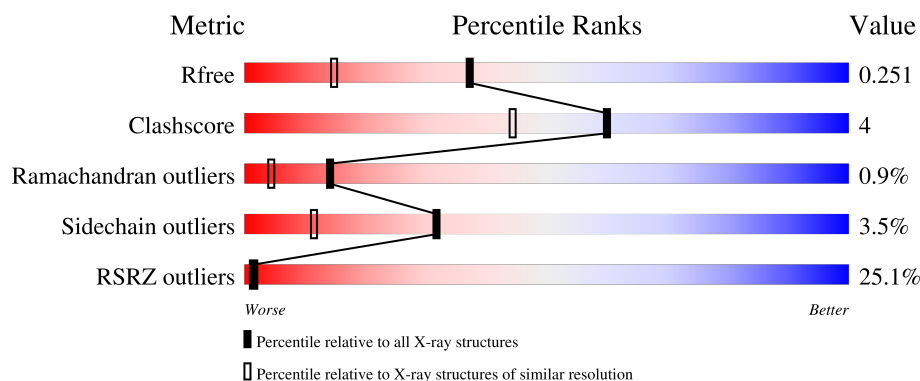
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	23% 80% 10% 9%

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
5	PO4	A	1007	-	-	X	-
7	A1BDM	A	1010	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5319 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
1	A	582	Total	C	N	O	S	0	8	0
			4822	3036	865	887	34			

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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



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

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



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

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

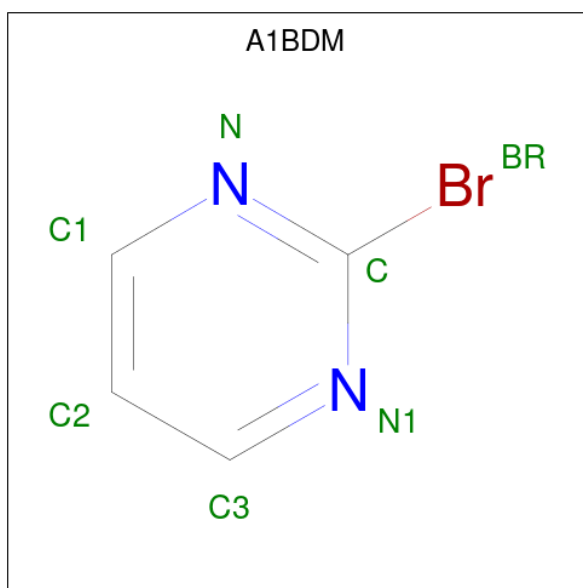
- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 7 is 2-bromopyrimidine (CCD ID: A1BDM) (formula: $C_4H_3BrN_2$) (labeled as "Lig-

and of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	Br	C	N	0	0
			7	1	4	2		

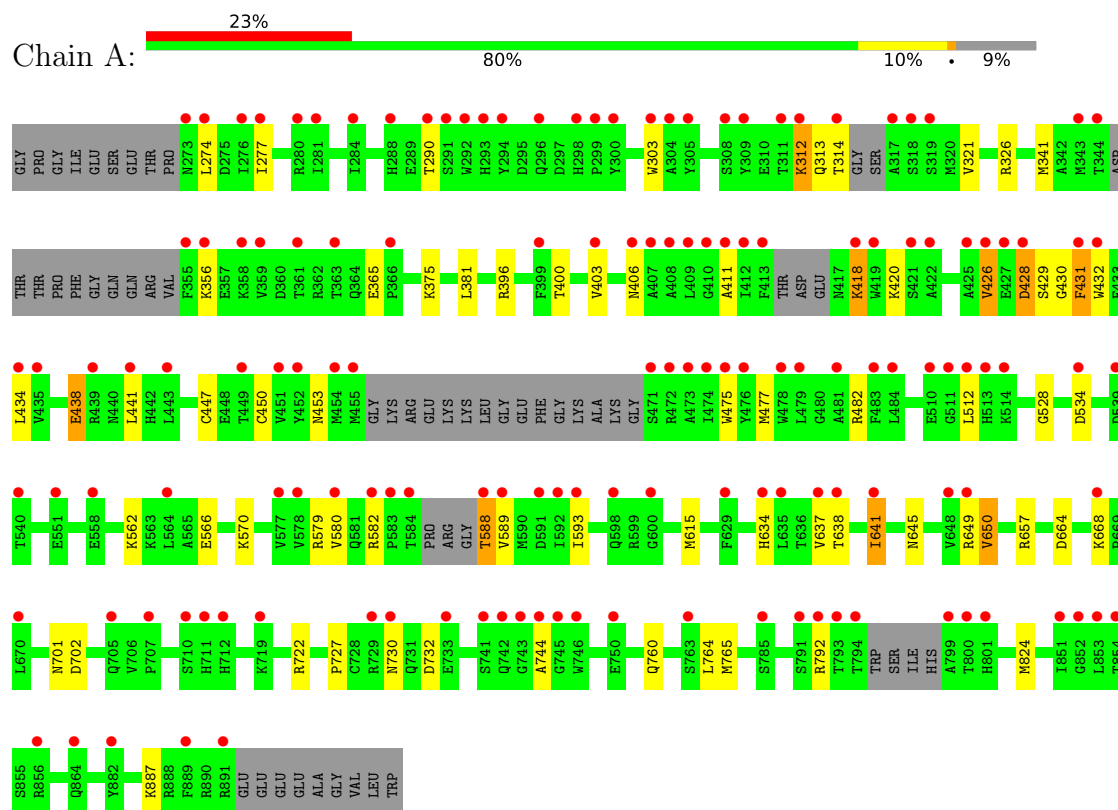
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	435	Total	O	0	1
			435	435		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 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	82.37Å 116.13Å 147.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.35 – 1.78 91.34 – 1.78	Depositor EDS
% Data completeness (in resolution range)	97.7 (91.35-1.78) 97.8 (91.34-1.78)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC5	Depositor
R, R_{free}	0.197 , 0.236 0.226 , 0.251	Depositor DCC
R_{free} test set	3487 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.9	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	0.94	EDS
Total number of atoms	5319	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% 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: MES, ZN, PEG, DMS, A1BDM, PO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.08	1/4929 (0.0%)	1.37	6/6645 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	760	GLN	C-O	5.88	1.31	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	657	ARG	CG-CD-NE	-6.35	98.03	112.00
1	A	650	VAL	CA-C-O	-5.80	114.94	119.46
1	A	702	ASP	CA-CB-CG	5.53	118.13	112.60
1	A	702	ASP	CB-CA-C	5.37	118.74	110.14
1	A	277	ILE	CA-C-N	5.13	125.78	120.03
1	A	277	ILE	C-N-CA	5.13	125.78	120.03

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	4822	0	4720	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
3	A	24	0	26	0	0
4	A	12	0	18	2	0
5	A	10	0	0	4	0
6	A	7	0	10	0	0
7	A	7	0	0	0	0
8	A	435	0	0	7	2
All	All	5319	0	4774	42	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 (42) 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:534:ASP:OD1	5:A:1007:PO4:O4	1.89	0.90
1:A:664:ASP:OD1	5:A:1007:PO4:O4	1.95	0.85
4:A:1004:DMS:H11	8:A:1273:HOH:O	1.88	0.72
4:A:1004:DMS:H12	8:A:1301:HOH:O	1.94	0.68
1:A:638:THR:O	1:A:641:ILE:HG22	1.97	0.65
1:A:664:ASP:OD1	5:A:1007:PO4:P	2.57	0.63
1:A:411:ALA:HA	1:A:477:MET:O	2.05	0.55
1:A:303:TRP:CE3	1:A:593:ILE:HD12	2.41	0.55
1:A:428:ASP:OD1	1:A:430:GLY:N	2.40	0.54
1:A:400:THR:O	1:A:403:VAL:HG22	2.07	0.53
1:A:764:LEU:O	1:A:765:MET:HE2	2.08	0.53
1:A:403:VAL:HG21	1:A:426:VAL:HG21	1.91	0.52
1:A:570:LYS:HG3	8:A:1278:HOH:O	2.11	0.51
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.51	0.50
1:A:534:ASP:OD1	5:A:1007:PO4:P	2.69	0.50
1:A:453:ASN:ND2	1:A:579:ARG:HD2	2.27	0.50
1:A:638:THR:HA	1:A:641:ILE:HG22	1.94	0.49
1:A:438:GLU:OE1	1:A:450:CYS:SG	2.71	0.49
1:A:792:ARG:NH1	8:A:1101:HOH:O	2.22	0.49
1:A:701:ASN:ND2	8:A:1108:HOH:O	2.35	0.48
1:A:438:GLU:O	1:A:441:LEU:HB2	2.14	0.48
1:A:303:TRP:CD2	1:A:593:ILE:HD12	2.49	0.47
1:A:730:ASN:OD1	1:A:732:ASP:HB2	2.16	0.46
1:A:764:LEU:C	1:A:765:MET:HE2	2.42	0.45
1:A:431:PHE:O	1:A:434:LEU:HB2	2.17	0.45
1:A:381:LEU:HD11	1:A:615:MET:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ARG:NH1	1:A:432:TRP:HB3	2.33	0.43
1:A:528:GLY:O	1:A:668:LYS:HE3	2.19	0.43
1:A:321:VAL:HG11	1:A:326:ARG:CZ	2.48	0.42
1:A:722:ARG:HB3	1:A:824:MET:SD	2.59	0.42
1:A:512[A]:LEU:HG	1:A:727:PRO:CB	2.50	0.42
1:A:638:THR:C	1:A:641:ILE:HG22	2.45	0.42
1:A:341:MET:HE2	1:A:341:MET:HB3	1.81	0.41
1:A:312:LYS:O	1:A:313:GLN:CG	2.68	0.41
1:A:562:LYS:O	1:A:566:GLU:HG3	2.20	0.41
1:A:649:ARG:HG2	1:A:650:VAL:HG13	2.03	0.41
1:A:637:VAL:HG13	8:A:1445:HOH:O	2.21	0.41
1:A:765:MET:HE2	1:A:765:MET:HA	2.03	0.41
1:A:475:TRP:CD1	1:A:475:TRP:N	2.88	0.41
1:A:313:GLN:O	1:A:314:THR:C	2.63	0.41
1:A:744:ALA:HA	8:A:1168:HOH:O	2.20	0.41
1:A:582:ARG:O	1:A:588:THR:HA	2.21	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:1169:HOH:O	8:A:1169:HOH:O[2_445]	1.63	0.57
8:A:1534:HOH:O	8:A:1534:HOH:O[2_545]	1.92	0.28

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	576/637 (90%)	548 (95%)	23 (4%)	5 (1%)	14 4

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	418	LYS
1	A	406	ASN
1	A	420	LYS
1	A	312	LYS
1	A	431	PHE

5.3.2 Protein sidechains ⓘ

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	518/554 (94%)	500 (96%)	18 (4%)	32 11

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	356	LYS
1	A	365	GLU
1	A	375	LYS
1	A	418	LYS
1	A	426	VAL
1	A	428	ASP
1	A	429	SER
1	A	438	GLU
1	A	482	ARG
1	A	580	VAL
1	A	588	THR
1	A	589	VAL
1	A	634	HIS
1	A	641	ILE
1	A	645	ASN
1	A	887	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	ASN
1	A	340	GLN
1	A	417	ASN
1	A	549	ASN
1	A	645	ASN
1	A	693	GLN
1	A	701	ASN
1	A	786	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	1006	-	3,3,3	0.14	0	3,3,3	0.39	0
6	PEG	A	1009	-	6,6,6	0.19	0	5,5,5	0.11	0
7	A1BDM	A	1010	-	4,7,7	0.16	0	6,8,8	0.67	0
3	MES	A	1003[A]	-	12,12,12	0.71	0	15,16,16	0.54	0
5	PO4	A	1008	-	4,4,4	0.87	0	6,6,6	0.42	0
3	MES	A	1003[B]	-	12,12,12	0.69	0	15,16,16	0.29	0
4	DMS	A	1004	-	3,3,3	0.41	0	3,3,3	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DMS	A	1005	-	3,3,3	0.26	0	3,3,3	0.04	0
5	PO4	A	1007	-	4,4,4	4.05	3 (75%)	6,6,6	0.63	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
3	MES	A	1003[B]	-	-	5/6/14/14	0/1/1/1
7	A1BDM	A	1010	-	-	-	0/1/1/1
6	PEG	A	1009	-	-	2/4/4/4	-
3	MES	A	1003[A]	-	-	0/6/14/14	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1007	PO4	P-O1	6.87	1.66	1.50
5	A	1007	PO4	P-O4	-2.94	1.46	1.54
5	A	1007	PO4	P-O2	2.61	1.62	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

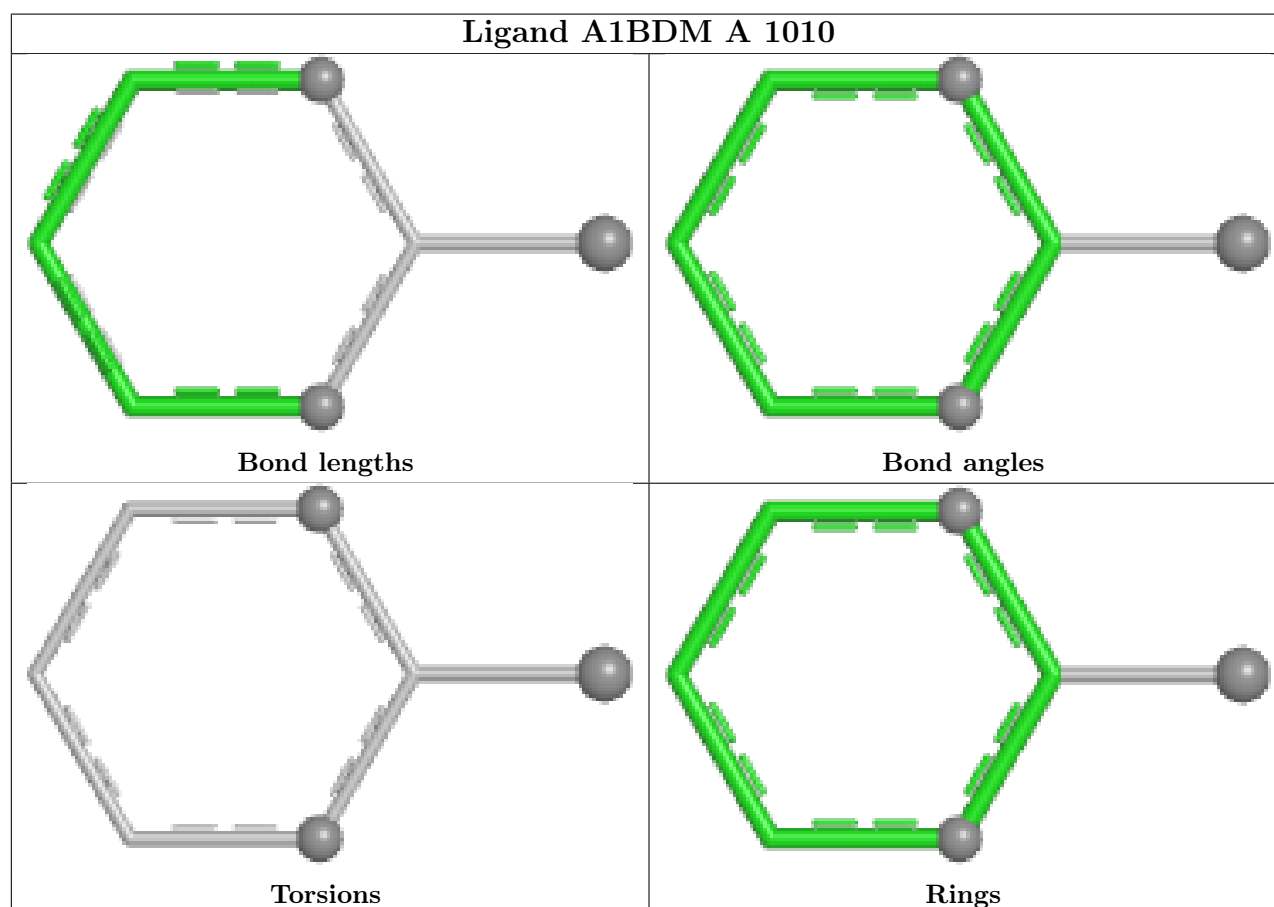
Mol	Chain	Res	Type	Atoms
3	A	1003[B]	MES	C8-C7-N4-C3
3	A	1003[B]	MES	C7-C8-S-O2S
3	A	1003[B]	MES	C7-C8-S-O3S
6	A	1009	PEG	O2-C3-C4-O4
3	A	1003[B]	MES	C8-C7-N4-C5
3	A	1003[B]	MES	C7-C8-S-O1S
6	A	1009	PEG	C4-C3-O2-C2

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
5	A	1007	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	582/637 (91%)	1.67	146 (25%) 1 1	7, 43, 116, 158	31 (5%)

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	512[A]	LEU	16.9
1	A	801[A]	HIS	16.0
1	A	511	GLY	14.3
1	A	648	VAL	13.9
1	A	853	LEU	13.7
1	A	851	ILE	13.6
1	A	719[A]	LYS	13.2
1	A	707	PRO	12.9
1	A	513	HIS	12.6
1	A	711	HIS	12.0
1	A	514	LYS	11.7
1	A	741[A]	SER	11.5
1	A	730	ASN	11.0
1	A	712	HIS	10.9
1	A	710	SER	10.5
1	A	540	THR	10.2
1	A	729	ARG	9.7
1	A	510	GLU	9.6
1	A	854	THR	9.6
1	A	733	GLU	9.2
1	A	705	GLN	9.2
1	A	551[A]	GLU	9.0
1	A	856	ARG	9.0
1	A	539	ASP	8.7
1	A	649	ARG	8.6
1	A	763[A]	SER	8.6
1	A	668	LYS	8.4

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Mol	Chain	Res	Type	RSRZ
1	A	785[A]	SER	8.3
1	A	598	GLN	8.1
1	A	864[A]	GLN	8.0
1	A	600	GLY	6.3
1	A	589	VAL	6.1
1	A	799	ALA	6.0
1	A	413	PHE	5.4
1	A	431	PHE	5.0
1	A	355	PHE	4.9
1	A	292	TRP	4.8
1	A	317	ALA	4.7
1	A	750	GLU	4.7
1	A	284	ILE	4.6
1	A	475	TRP	4.5
1	A	419	TRP	4.4
1	A	435	VAL	4.4
1	A	281	ILE	4.3
1	A	412	ILE	4.3
1	A	403	VAL	4.2
1	A	294	TYR	4.2
1	A	359	VAL	4.2
1	A	426	VAL	4.1
1	A	794	THR	4.1
1	A	407	ALA	4.1
1	A	637	VAL	4.1
1	A	791	SER	4.0
1	A	411	ALA	3.9
1	A	473	ALA	3.8
1	A	363	THR	3.8
1	A	314	THR	3.8
1	A	443	LEU	3.7
1	A	793	THR	3.7
1	A	800	THR	3.7
1	A	293	HIS	3.7
1	A	588	THR	3.6
1	A	634	HIS	3.6
1	A	635	LEU	3.5
1	A	409	LEU	3.4
1	A	474	ILE	3.4
1	A	584	THR	3.4
1	A	422	ALA	3.3
1	A	288	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	274	LEU	3.3
1	A	290	THR	3.3
1	A	410	GLY	3.1
1	A	593	ILE	3.1
1	A	303	TRP	3.1
1	A	277	ILE	3.0
1	A	399	PHE	3.0
1	A	792	ARG	3.0
1	A	441	LEU	3.0
1	A	534	ASP	3.0
1	A	478	TRP	3.0
1	A	319	SER	3.0
1	A	298	HIS	3.0
1	A	484	LEU	3.0
1	A	434	LEU	2.9
1	A	577	VAL	2.9
1	A	305	TYR	2.9
1	A	744	ALA	2.9
1	A	583	PRO	2.9
1	A	309	TYR	2.8
1	A	421	SER	2.8
1	A	358	LYS	2.7
1	A	406	ASN	2.7
1	A	425	ALA	2.7
1	A	455	MET	2.7
1	A	300	TYR	2.7
1	A	745	GLY	2.7
1	A	366	PRO	2.7
1	A	432	TRP	2.6
1	A	592	ILE	2.6
1	A	591	ASP	2.6
1	A	308	SER	2.6
1	A	418	LYS	2.6
1	A	746	TRP	2.6
1	A	299	PRO	2.6
1	A	454	MET	2.6
1	A	273	ASN	2.5
1	A	304	ALA	2.5
1	A	743	GLY	2.5
1	A	472	ARG	2.5
1	A	483	PHE	2.5
1	A	629	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	452	TYR	2.5
1	A	291	SER	2.5
1	A	311	THR	2.5
1	A	439	ARG	2.4
1	A	344	THR	2.4
1	A	641	ILE	2.4
1	A	670	LEU	2.4
1	A	889	PHE	2.4
1	A	356	LYS	2.3
1	A	471	SER	2.3
1	A	558	GLU	2.3
1	A	742	GLN	2.3
1	A	882	TYR	2.3
1	A	451	VAL	2.3
1	A	361	THR	2.3
1	A	408	ALA	2.2
1	A	481	ALA	2.2
1	A	582	ARG	2.2
1	A	427	GLU	2.2
1	A	476	TYR	2.2
1	A	580	VAL	2.2
1	A	428	ASP	2.2
1	A	318	SER	2.2
1	A	578	VAL	2.1
1	A	852	GLY	2.1
1	A	276	ILE	2.1
1	A	479	LEU	2.1
1	A	296	GLN	2.1
1	A	280	ARG	2.1
1	A	449	THR	2.1
1	A	343	MET	2.1
1	A	564	LEU	2.1
1	A	891	ARG	2.1
1	A	638	THR	2.0
1	A	312	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

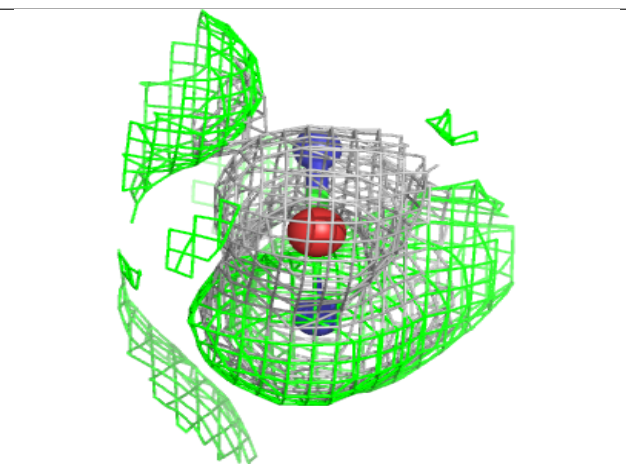
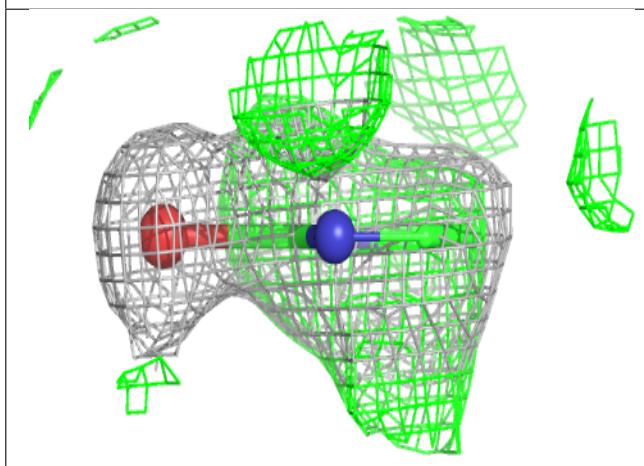
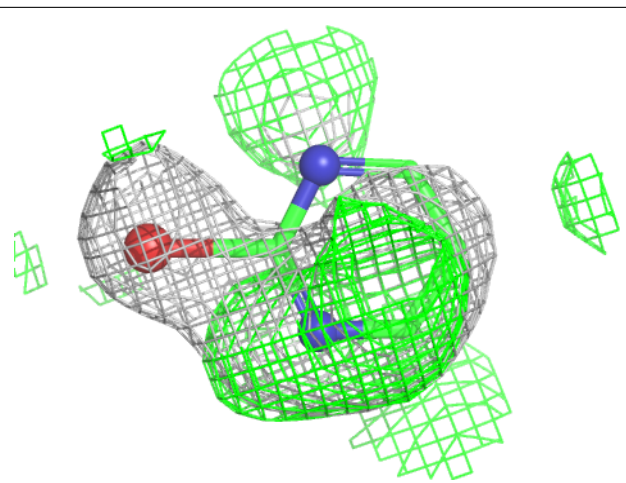
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	A1BDM	A	1010	7/7	0.62	0.44	49,51,54,54	7
5	PO4	A	1008	5/5	0.71	0.13	79,90,100,116	0
5	PO4	A	1007	5/5	0.76	0.13	37,40,47,64	0
4	DMS	A	1005	4/4	0.86	0.20	78,88,93,98	0
6	PEG	A	1009	7/7	0.87	0.15	65,68,72,78	0
4	DMS	A	1006	4/4	0.92	0.14	50,55,56,56	0
4	DMS	A	1004	4/4	0.95	0.11	43,45,47,50	0
3	MES	A	1003[B]	12/12	0.97	0.34	692,709,738,743	12
3	MES	A	1003[A]	12/12	0.97	0.34	23,27,30,30	12
2	ZN	A	1002	1/1	0.99	0.04	61,61,61,61	0
2	ZN	A	1001	1/1	1.00	0.02	25,25,25,25	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 A1BDM A 1010:

$2mF_o-DF_c$ (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.