



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:03 PM UTC

PDB ID : 7HKF / pdb_00007hkf
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 Z55669204 (DNV2_NS5A-x0191)
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 : 1.58 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)

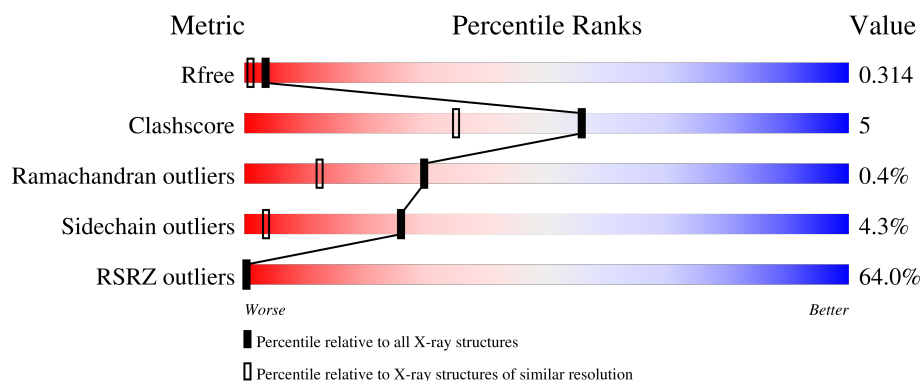
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.58 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	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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>59%</div> <div>81% 9% 8%</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
3	DMS	A	1003	-	-	-	X
3	DMS	A	1004	-	-	-	X
3	DMS	A	1005	-	-	-	X
4	PO4	A	1006	-	-	X	X
5	PEG	A	1008	-	-	-	X
7	MES	A	1010	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5316 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	583	Total	C	N	O	S	0	7	0
			4823	3038	865	886	34			

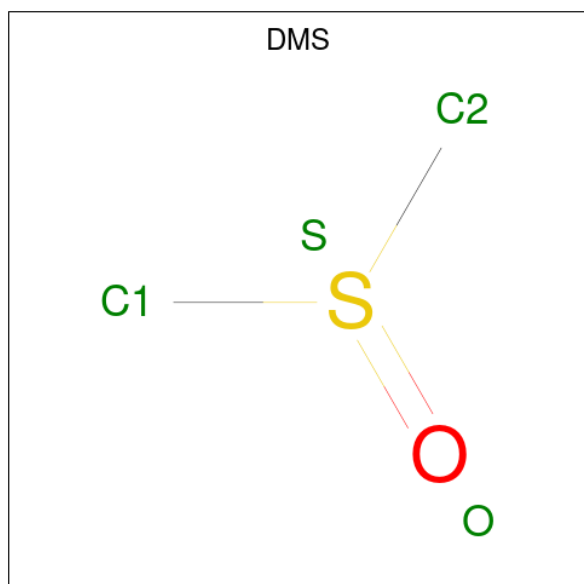
There are 2 discrepancies between the modelled and reference sequences:

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 DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



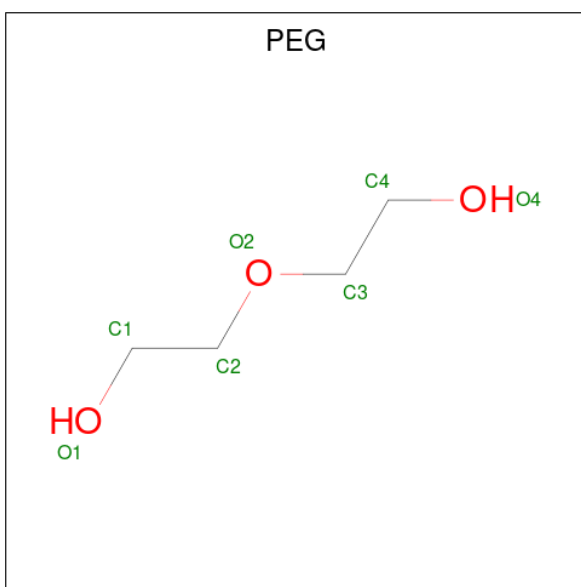
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



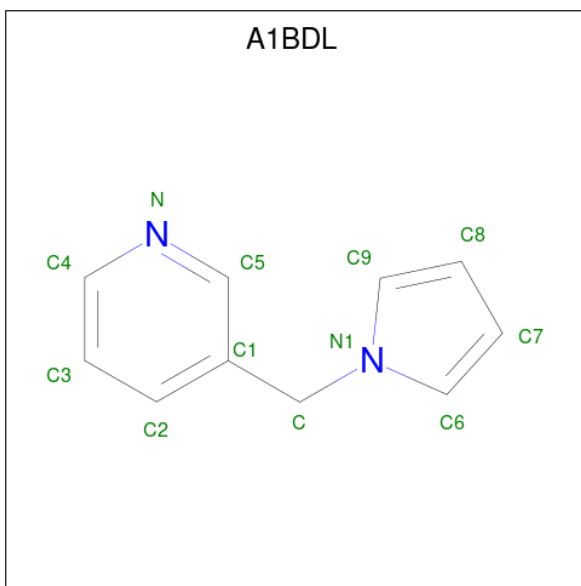
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		

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



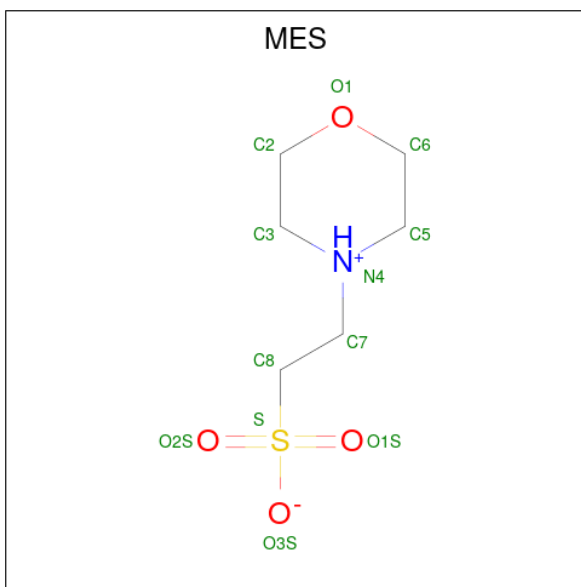
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is 3-[(1H-pyrrol-1-yl)methyl]pyridine (CCD ID: A1BDL) (formula: $C_{10}H_{10}N_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	N	0	0
			12	10	2		

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

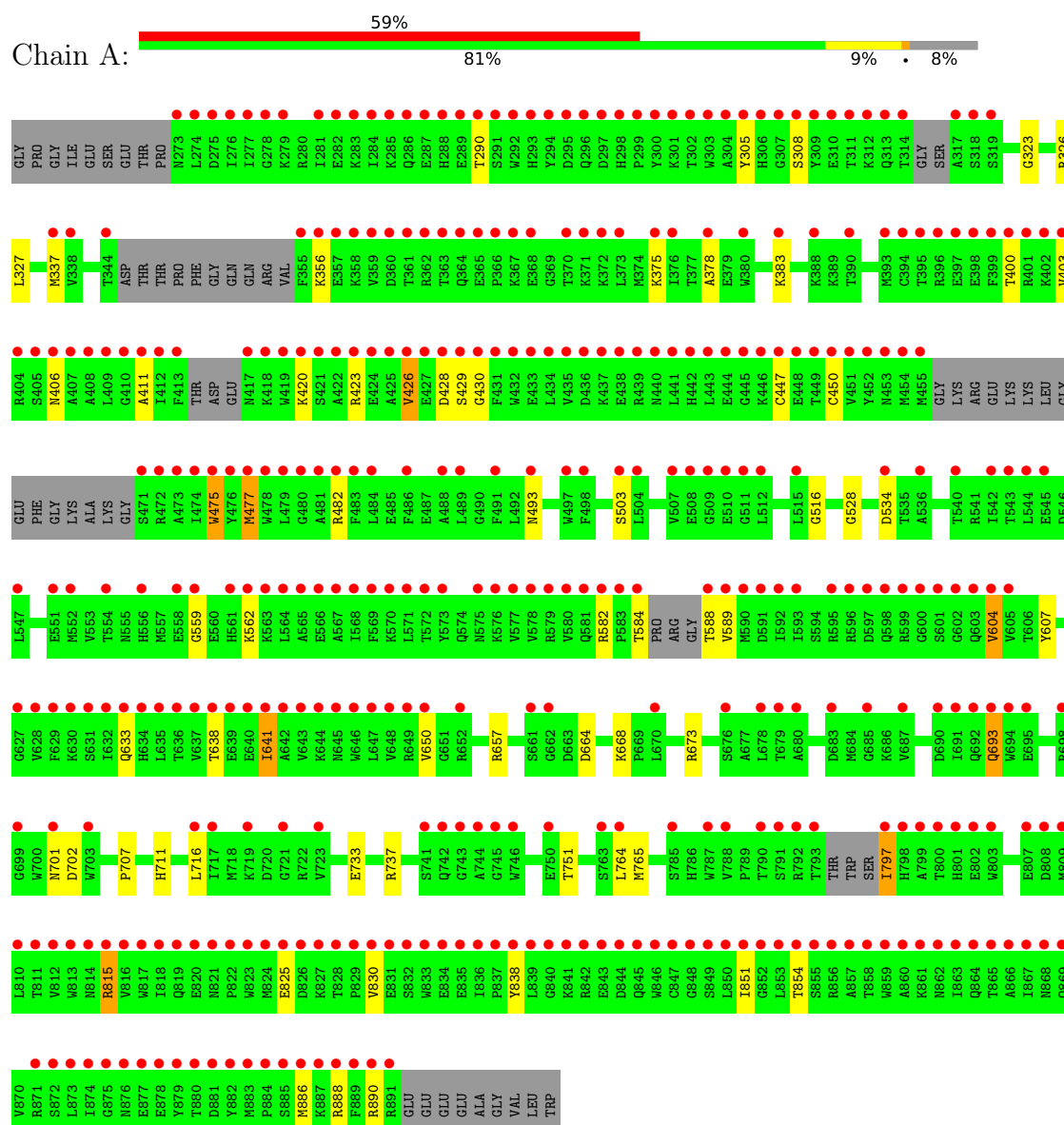
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	438	Total	O	0	1
			438	438		

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 polyprotein



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	82.41Å 117.35Å 148.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.53 – 1.58 67.53 – 1.58	Depositor EDS
% Data completeness (in resolution range)	98.5 (67.53-1.58) 98.6 (67.53-1.58)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 1.58Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC5	Depositor
R, R_{free}	0.211 , 0.247 0.290 , 0.314	Depositor DCC
R_{free} test set	5018 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 104.5	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	0.87	EDS
Total number of atoms	5316	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 4.78% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, DMS, MES, A1BDL, PO4, 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	1.10	5/4930 (0.1%)	1.35	9/6646 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	516	GLY	C-O	6.52	1.31	1.23
1	A	751	THR	C-O	5.98	1.30	1.24
1	A	711	HIS	CE1-NE2	5.09	1.37	1.32
1	A	378	ALA	C-O	5.09	1.29	1.24
1	A	604	VAL	C-O	5.06	1.29	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	650	VAL	CA-C-O	-5.36	115.28	119.46
1	A	559	GLY	CA-C-N	5.32	127.67	120.65
1	A	559	GLY	C-N-CA	5.32	127.67	120.65
1	A	673	ARG	CA-C-N	5.31	127.65	120.38
1	A	673	ARG	C-N-CA	5.31	127.65	120.38
1	A	657	ARG	CG-CD-NE	-5.22	100.52	112.00
1	A	702	ASP	CB-CA-C	5.11	118.02	110.14
1	A	503	SER	CA-C-N	5.03	131.15	121.54
1	A	503	SER	C-N-CA	5.03	131.15	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	4823	0	4725	45	0
2	A	2	0	0	0	0
3	A	12	0	18	0	0
4	A	10	0	0	3	0
5	A	7	0	10	0	0
6	A	12	0	0	0	0
7	A	12	0	13	13	0
8	A	438	0	0	7	1
All	All	5316	0	4766	45	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 5.

All (45) 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:327:LEU:HG	7:A:1010:MES:H71	1.57	0.84
1:A:327:LEU:HD12	7:A:1010:MES:H32	1.59	0.84
1:A:323:GLY:HA2	7:A:1010:MES:H82	1.77	0.66
1:A:327:LEU:CG	7:A:1010:MES:H71	2.24	0.66
1:A:305:TYR:OH	1:A:308:SER:OG	2.03	0.66
1:A:638:THR:HA	1:A:641:ILE:HG22	1.79	0.65
1:A:323:GLY:CA	7:A:1010:MES:H82	2.28	0.63
1:A:733:GLU:O	1:A:737:ARG:HG3	1.98	0.63
1:A:327:LEU:HD11	7:A:1010:MES:H52	1.81	0.62
1:A:534:ASP:OD1	4:A:1006:PO4:O3	2.18	0.62
1:A:562:LYS:NZ	8:A:1112:HOH:O	2.35	0.60
1:A:411:ALA:HA	1:A:477:MET:O	2.03	0.59
1:A:693:GLN:HG3	8:A:1448:HOH:O	2.03	0.59
1:A:638:THR:HA	1:A:641:ILE:CG2	2.34	0.57
1:A:327:LEU:CD1	7:A:1010:MES:H71	2.34	0.57
1:A:400:THR:O	1:A:403:VAL:HG22	2.04	0.56
1:A:607:TYR:CD2	1:A:797:ILE:HD12	2.41	0.56
1:A:815:ARG:NH1	8:A:1114:HOH:O	2.39	0.55
1:A:825:GLU:HB3	8:A:1314:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:LEU:HG	7:A:1010:MES:C7	2.34	0.55
1:A:528:GLY:O	1:A:668:LYS:HE3	2.08	0.54
1:A:764:LEU:HG	1:A:765:MET:CE	2.38	0.54
1:A:428:ASP:OD1	1:A:430:GLY:N	2.41	0.53
1:A:493:ASN:ND2	1:A:797:ILE:HD13	2.23	0.53
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.48	0.52
1:A:327:LEU:CD1	7:A:1010:MES:H32	2.37	0.51
1:A:764:LEU:HG	1:A:765:MET:HE3	1.93	0.50
1:A:327:LEU:CD1	7:A:1010:MES:C7	2.89	0.50
1:A:475:TRP:CD1	1:A:475:TRP:N	2.80	0.48
1:A:327:LEU:HD11	7:A:1010:MES:C7	2.45	0.47
1:A:707:PRO:O	4:A:1006:PO4:O4	2.35	0.45
1:A:428:ASP:OD1	1:A:428:ASP:C	2.60	0.45
1:A:764:LEU:C	1:A:765:MET:HE2	2.42	0.44
1:A:326:ARG:NE	7:A:1010:MES:O1S	2.40	0.44
1:A:716:LEU:HD11	1:A:838:TYR:O	2.18	0.43
1:A:337:MET:HG2	8:A:1345:HOH:O	2.19	0.43
1:A:733:GLU:O	1:A:737:ARG:CG	2.67	0.43
1:A:764:LEU:O	1:A:765:MET:HE2	2.18	0.43
1:A:582:ARG:HG2	1:A:584:THR:OG1	2.19	0.42
1:A:604:VAL:HA	1:A:797:ILE:CG1	2.50	0.42
1:A:403:VAL:HG21	1:A:426:VAL:HG21	2.01	0.41
1:A:327:LEU:CG	7:A:1010:MES:C7	2.96	0.41
1:A:664:ASP:OD1	4:A:1006:PO4:O3	2.39	0.40
1:A:701:ASN:ND2	8:A:1111:HOH:O	2.35	0.40
1:A:888:ARG:HD2	8:A:1395: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:1245:HOH:O	8:A:1245:HOH:O[2_445]	1.75	0.45

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%)	549 (95%)	25 (4%)	2 (0%)	36	20

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	420	LYS
1	A	406	ASN

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%)	496 (96%)	22 (4%)	26	4

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	290	THR
1	A	356	LYS
1	A	375	LYS
1	A	383	LYS
1	A	423	ARG
1	A	426	VAL
1	A	429	SER
1	A	475	TRP
1	A	477	MET
1	A	482	ARG
1	A	588	THR
1	A	589	VAL
1	A	633	GLN
1	A	641	ILE
1	A	693	GLN
1	A	797	ILE
1	A	815	ARG

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Mol	Chain	Res	Type
1	A	830	VAL
1	A	851	ILE
1	A	854	THR
1	A	886	MET
1	A	890	ARG

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	417	ASN
1	A	701	ASN
1	A	705	GLN
1	A	786	HIS
1	A	801	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 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	PO4	A	1007	-	4,4,4	0.54	0	6,6,6	0.53	0
3	DMS	A	1005	-	3,3,3	0.22	0	3,3,3	0.18	0
7	MES	A	1010	-	12,12,12	1.87	1 (8%)	15,16,16	1.05	1 (6%)
3	DMS	A	1004	-	3,3,3	0.23	0	3,3,3	0.03	0
6	A1BDL	A	1009	-	13,13,13	0.20	0	16,16,16	0.25	0
5	PEG	A	1008	-	6,6,6	0.16	0	5,5,5	0.13	0
4	PO4	A	1006	-	4,4,4	0.83	0	6,6,6	0.44	0
3	DMS	A	1003	-	3,3,3	0.21	0	3,3,3	0.12	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	MES	A	1010	-	-	6/6/14/14	0/1/1/1
6	A1BDL	A	1009	-	-	0/4/4/4	0/2/2/2
5	PEG	A	1008	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1010	MES	C8-S	5.96	1.85	1.77

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1010	MES	O2S-S-C8	2.88	111.08	106.73

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1010	MES	C7-C8-S-O1S
7	A	1010	MES	C7-C8-S-O2S
7	A	1010	MES	C7-C8-S-O3S
5	A	1008	PEG	O1-C1-C2-O2
5	A	1008	PEG	O2-C3-C4-O4
7	A	1010	MES	C8-C7-N4-C3
7	A	1010	MES	C8-C7-N4-C5

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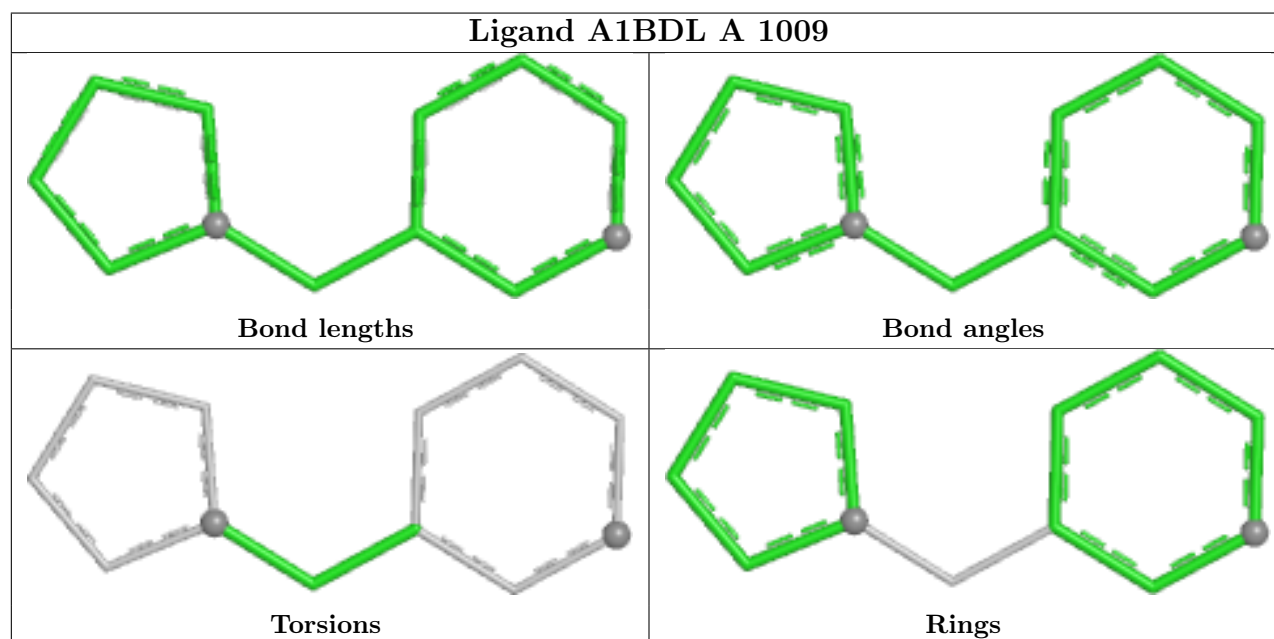
Mol	Chain	Res	Type	Atoms
5	A	1008	PEG	C4-C3-O2-C2
7	A	1010	MES	N4-C7-C8-S
5	A	1008	PEG	C1-C2-O2-C3

There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1010	MES	13	0
4	A	1006	PO4	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	583/637 (91%)	4.17	373 (63%) 0 0	5, 35, 93, 150	139 (23%)

All (373) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	889	PHE	18.2
1	A	409	LEU	16.9
1	A	426	VAL	16.3
1	A	882	TYR	16.2
1	A	407	ALA	15.6
1	A	859	TRP	15.4
1	A	813	TRP	14.8
1	A	851	ILE	14.5
1	A	823	TRP	14.3
1	A	846	TRP	14.1
1	A	810	LEU	14.1
1	A	512[A]	LEU	13.9
1	A	413	PHE	13.9
1	A	359	VAL	13.9
1	A	873	LEU	13.7
1	A	830	VAL	13.7
1	A	857	ALA	13.7
1	A	885	SER	13.6
1	A	879	TYR	13.5
1	A	803	TRP	13.5
1	A	874	ILE	13.5
1	A	836	ILE	13.1
1	A	860	ALA	13.1
1	A	858	THR	13.0
1	A	589	VAL	12.9
1	A	812	VAL	12.9
1	A	833	TRP	12.9

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Mol	Chain	Res	Type	RSRZ
1	A	515	LEU	12.6
1	A	839	LEU	12.5
1	A	355	PHE	12.4
1	A	867	ILE	12.3
1	A	817	TRP	12.1
1	A	884	PRO	12.1
1	A	866	ALA	12.0
1	A	408	ALA	11.9
1	A	886	MET	11.8
1	A	850	LEU	11.6
1	A	838	TYR	11.6
1	A	853	LEU	11.4
1	A	816	VAL	11.4
1	A	811	THR	11.1
1	A	852	GLY	11.1
1	A	865	THR	11.1
1	A	797	ILE	11.0
1	A	863	ILE	10.9
1	A	880	THR	10.9
1	A	603	GLN	10.8
1	A	453	ASN	10.7
1	A	828	THR	10.5
1	A	822	PRO	10.4
1	A	763[A]	SER	10.4
1	A	887	LYS	10.3
1	A	507	VAL	10.3
1	A	875	GLY	10.3
1	A	356	LYS	10.3
1	A	719[A]	LYS	10.2
1	A	872	SER	10.2
1	A	883	MET	10.2
1	A	551[A]	GLU	10.1
1	A	826	ASP	10.1
1	A	888	ARG	10.1
1	A	840	GLY	10.0
1	A	818	ILE	9.9
1	A	829	PRO	9.9
1	A	847	CYS	9.7
1	A	600	GLY	9.7
1	A	815	ARG	9.6
1	A	837	PRO	9.5
1	A	849	SER	9.4

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Mol	Chain	Res	Type	RSRZ
1	A	854	THR	9.3
1	A	511	GLY	9.3
1	A	661	SER	9.2
1	A	832	SER	9.1
1	A	861	LYS	9.1
1	A	869	GLN	9.0
1	A	412	ILE	8.8
1	A	827	LYS	8.7
1	A	834	GLU	8.7
1	A	431	PHE	8.5
1	A	848	GLY	8.5
1	A	862	ASN	8.5
1	A	844	ASP	8.4
1	A	785[A]	SER	8.3
1	A	856	ARG	8.3
1	A	841	LYS	8.3
1	A	809	MET	8.2
1	A	855	SER	8.2
1	A	845	GLN	8.2
1	A	799	ALA	8.0
1	A	825	GLU	8.0
1	A	808	ASP	8.0
1	A	294	TYR	7.9
1	A	410	GLY	7.9
1	A	814	ASN	7.8
1	A	290	THR	7.8
1	A	878	GLU	7.7
1	A	791	SER	7.7
1	A	881	ASP	7.7
1	A	842	ARG	7.6
1	A	584	THR	7.6
1	A	383	LYS	7.6
1	A	876	ASN	7.6
1	A	583	PRO	7.5
1	A	357	GLU	7.5
1	A	289	GLU	7.4
1	A	292	TRP	7.4
1	A	831	GLU	7.4
1	A	890	ARG	7.3
1	A	877	GLU	7.3
1	A	891	ARG	7.3
1	A	821	ASN	7.3

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Mol	Chain	Res	Type	RSRZ
1	A	824	MET	7.3
1	A	361	THR	7.3
1	A	864[A]	GLN	7.2
1	A	298	HIS	7.2
1	A	441	LEU	7.2
1	A	835	GLU	7.1
1	A	741[A]	SER	7.1
1	A	843	GLU	7.1
1	A	303	TRP	7.1
1	A	868	ASN	7.1
1	A	807	GLU	7.1
1	A	317	ALA	7.0
1	A	800	THR	7.0
1	A	281	ILE	7.0
1	A	591	ASP	7.0
1	A	801	HIS	6.9
1	A	424	GLU	6.9
1	A	637	VAL	6.9
1	A	422	ALA	6.9
1	A	599	ARG	6.8
1	A	509	GLY	6.8
1	A	645	ASN	6.7
1	A	570	LYS	6.7
1	A	474	ILE	6.7
1	A	475	TRP	6.7
1	A	798	HIS	6.6
1	A	411	ALA	6.6
1	A	295	ASP	6.6
1	A	746	TRP	6.6
1	A	305	TYR	6.6
1	A	793	THR	6.6
1	A	284	ILE	6.6
1	A	427	GLU	6.4
1	A	476	TYR	6.4
1	A	820	GLU	6.3
1	A	406	ASN	6.3
1	A	419	TRP	6.3
1	A	286	GLN	6.3
1	A	275	ASP	6.0
1	A	802	GLU	6.0
1	A	871	ARG	5.9
1	A	428	ASP	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	508	GLU	5.9
1	A	358	LYS	5.9
1	A	309	TYR	5.8
1	A	274	LEU	5.8
1	A	314	THR	5.8
1	A	399	PHE	5.8
1	A	273	ASN	5.8
1	A	698	ARG	5.7
1	A	742	GLN	5.7
1	A	435	VAL	5.6
1	A	405	SER	5.6
1	A	448	GLU	5.6
1	A	403	VAL	5.6
1	A	451	VAL	5.6
1	A	432	TRP	5.5
1	A	434	LEU	5.5
1	A	297	ASP	5.4
1	A	635	LEU	5.4
1	A	819	GLN	5.4
1	A	300	TYR	5.4
1	A	452	TYR	5.3
1	A	634	HIS	5.3
1	A	277	ILE	5.2
1	A	601	SER	5.2
1	A	588	THR	5.2
1	A	288	HIS	5.2
1	A	478	TRP	5.2
1	A	638	THR	5.2
1	A	693	GLN	5.1
1	A	318	SER	5.1
1	A	473	ALA	5.1
1	A	282	GLU	5.1
1	A	563	LYS	5.1
1	A	593	ILE	5.0
1	A	454	MET	5.0
1	A	425	ALA	5.0
1	A	580	VAL	4.9
1	A	792	ARG	4.9
1	A	446	LYS	4.9
1	A	471	SER	4.9
1	A	311	THR	4.9
1	A	510	GLU	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	544	LEU	4.8
1	A	571	LEU	4.8
1	A	363	THR	4.8
1	A	417	ASN	4.8
1	A	279	LYS	4.8
1	A	443	LEU	4.7
1	A	790	THR	4.7
1	A	694	TRP	4.6
1	A	308	SER	4.6
1	A	429	SER	4.6
1	A	592	ILE	4.6
1	A	745	GLY	4.6
1	A	418	LYS	4.6
1	A	479	LEU	4.6
1	A	558	GLU	4.5
1	A	293	HIS	4.5
1	A	312	LYS	4.4
1	A	582	ARG	4.4
1	A	287	GLU	4.3
1	A	310	GLU	4.3
1	A	604	VAL	4.3
1	A	296	GLN	4.3
1	A	596	ARG	4.2
1	A	649	ARG	4.2
1	A	404	ARG	4.2
1	A	484	LEU	4.2
1	A	313	GLN	4.2
1	A	455	MET	4.2
1	A	644	LYS	4.2
1	A	304	ALA	4.1
1	A	643	VAL	4.1
1	A	362	ARG	4.1
1	A	472	ARG	4.1
1	A	590	MET	4.1
1	A	278	GLY	4.0
1	A	301	LYS	4.0
1	A	744	ALA	4.0
1	A	421	SER	4.0
1	A	670	LEU	4.0
1	A	695	GLU	4.0
1	A	648	VAL	3.9
1	A	442	HIS	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	360	ASP	3.9
1	A	650	VAL	3.9
1	A	691	ILE	3.9
1	A	302	THR	3.9
1	A	344	THR	3.9
1	A	481	ALA	3.8
1	A	577	VAL	3.8
1	A	433	GLU	3.8
1	A	641	ILE	3.8
1	A	564	LEU	3.8
1	A	647	LEU	3.8
1	A	562	LYS	3.8
1	A	401	ARG	3.8
1	A	567	ALA	3.7
1	A	581	GLN	3.7
1	A	679	THR	3.6
1	A	299	PRO	3.6
1	A	423	ARG	3.6
1	A	449	THR	3.6
1	A	319	SER	3.6
1	A	365	GLU	3.5
1	A	578	VAL	3.5
1	A	393	MET	3.5
1	A	447	CYS	3.5
1	A	632	ILE	3.5
1	A	717	ILE	3.5
1	A	285	LYS	3.4
1	A	370	THR	3.4
1	A	636	THR	3.4
1	A	482	ARG	3.4
1	A	750	GLU	3.4
1	A	364	GLN	3.4
1	A	439	ARG	3.3
1	A	430	GLY	3.3
1	A	436	ASP	3.3
1	A	337	MET	3.3
1	A	402	LYS	3.2
1	A	307	GLY	3.2
1	A	575	ASN	3.2
1	A	367	LYS	3.2
1	A	629	PHE	3.2
1	A	642	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	291	SER	3.2
1	A	276	ILE	3.2
1	A	394	CYS	3.2
1	A	602	GLY	3.2
1	A	692	GLN	3.1
1	A	646	TRP	3.1
1	A	368	GLU	3.1
1	A	445	GLY	3.1
1	A	395	THR	3.1
1	A	486	PHE	3.1
1	A	543	THR	3.0
1	A	703	TRP	3.0
1	A	373	LEU	3.0
1	A	699	GLY	3.0
1	A	483	PHE	3.0
1	A	450	CYS	3.0
1	A	438	GLU	3.0
1	A	396	ARG	3.0
1	A	420	LYS	3.0
1	A	480	GLY	3.0
1	A	556	HIS	2.9
1	A	534	ASP	2.9
1	A	652	ARG	2.9
1	A	633	GLN	2.9
1	A	437	LYS	2.9
1	A	566	GLU	2.9
1	A	489	LEU	2.9
1	A	680	ALA	2.9
1	A	283	LYS	2.9
1	A	477	MET	2.9
1	A	683	ASP	2.8
1	A	687	VAL	2.8
1	A	568	ILE	2.8
1	A	559	GLY	2.7
1	A	440	ASN	2.7
1	A	400	THR	2.7
1	A	572	THR	2.7
1	A	630	LYS	2.7
1	A	676	SER	2.7
1	A	788	VAL	2.6
1	A	605	VAL	2.5
1	A	723	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	565	ALA	2.5
1	A	579	ARG	2.5
1	A	631	SER	2.5
1	A	444	GLU	2.5
1	A	627	GLY	2.5
1	A	366	PRO	2.5
1	A	569	PHE	2.5
1	A	376	ILE	2.4
1	A	380	TRP	2.4
1	A	721	GLY	2.4
1	A	540	THR	2.4
1	A	388	LYS	2.4
1	A	488	ALA	2.4
1	A	597	ASP	2.3
1	A	397	GLU	2.3
1	A	716	LEU	2.3
1	A	764	LEU	2.3
1	A	375	LYS	2.3
1	A	573	TYR	2.3
1	A	595	ARG	2.3
1	A	552	MET	2.3
1	A	662	GLY	2.3
1	A	787	TRP	2.3
1	A	306	HIS	2.3
1	A	542	ILE	2.3
1	A	378	ALA	2.2
1	A	598	GLN	2.2
1	A	561	HIS	2.2
1	A	628	VAL	2.2
1	A	545	GLU	2.2
1	A	493	ASN	2.2
1	A	536	ALA	2.2
1	A	639	GLU	2.2
1	A	498	PHE	2.2
1	A	690	ASP	2.2
1	A	398	GLU	2.2
1	A	504	LEU	2.1
1	A	678	LEU	2.1
1	A	743	GLY	2.1
1	A	372	LYS	2.1
1	A	491	PHE	2.1
1	A	685	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	554	THR	2.1
1	A	701	ASN	2.1
1	A	371	LYS	2.1
1	A	576	LYS	2.0
1	A	338	VAL	2.0
1	A	547	LEU	2.0
1	A	640	GLU	2.0
1	A	503	SER	2.0
1	A	390	THR	2.0
1	A	497	TRP	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.

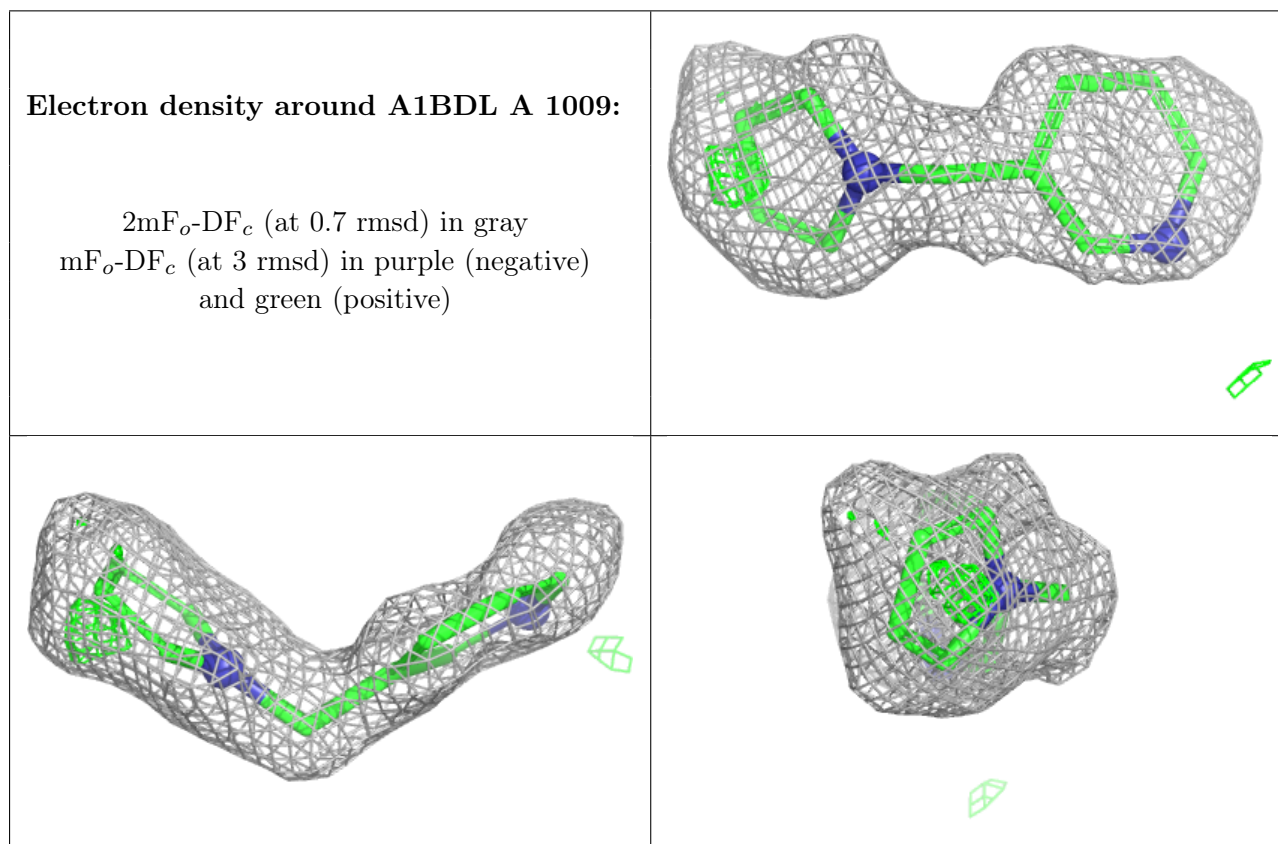
6.4 Ligands [i](#)

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
3	DMS	A	1004	4/4	0.08	0.56	81,85,85,86	4
3	DMS	A	1005	4/4	0.50	0.55	47,51,52,52	4
4	PO4	A	1006	5/5	0.54	0.52	60,68,70,75	5
4	PO4	A	1007	5/5	0.58	0.26	47,48,52,56	5
5	PEG	A	1008	7/7	0.59	0.46	42,44,47,48	7
3	DMS	A	1003	4/4	0.73	0.60	88,91,91,92	4
6	A1BDL	A	1009	12/12	0.78	0.18	18,19,20,21	12
7	MES	A	1010	12/12	0.93	0.25	17,71,78,793	12
2	ZN	A	1001	1/1	0.97	0.40	25,25,25,25	1
2	ZN	A	1002	1/1	0.99	0.05	51,51,51,51	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 ⓘ

There are no such residues in this entry.