



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:54 AM UTC

PDB ID : 7I2L / pdb_00007i2l
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 Z1627772104 (DNV2_NS5A-x0566)
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 : 2.03 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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)

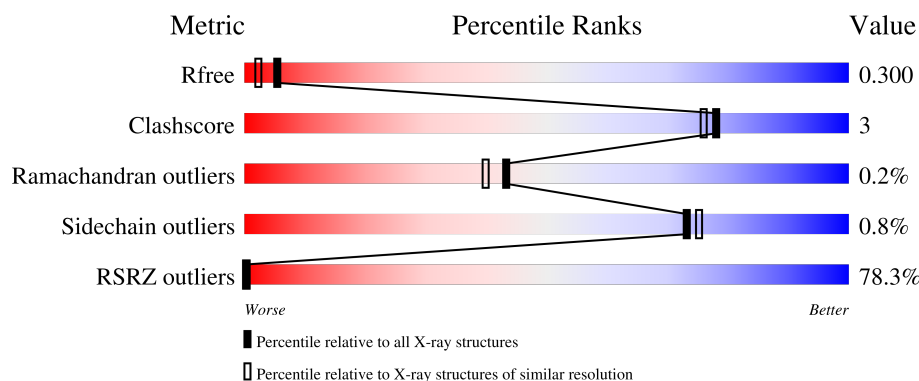
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	70% 83% 5% 11%

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	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 4990 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
1	A	566	Total	C	N	O	S	0	7	0
			4688	2951	839	864	34			

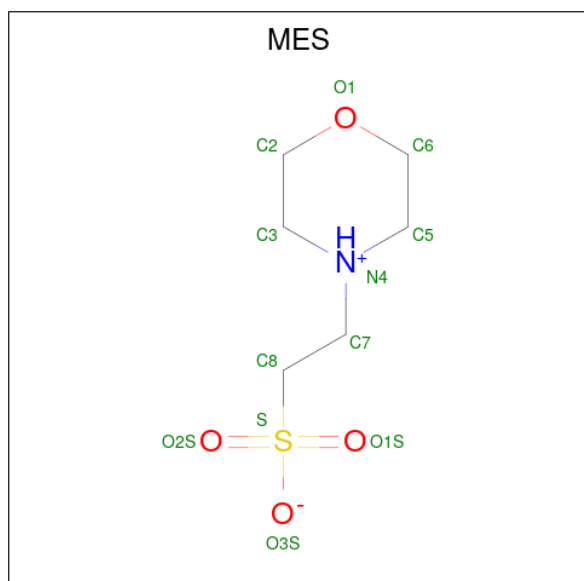
There are 2 discrepancies between the modelled and reference sequences:

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).

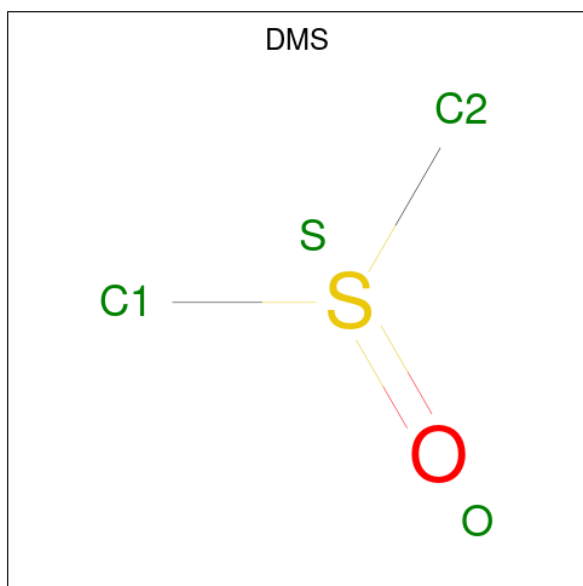
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

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



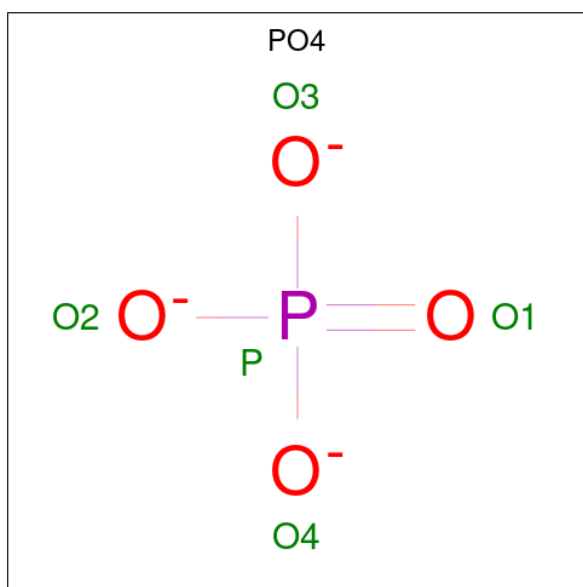
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			24	12	2	8	2		

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



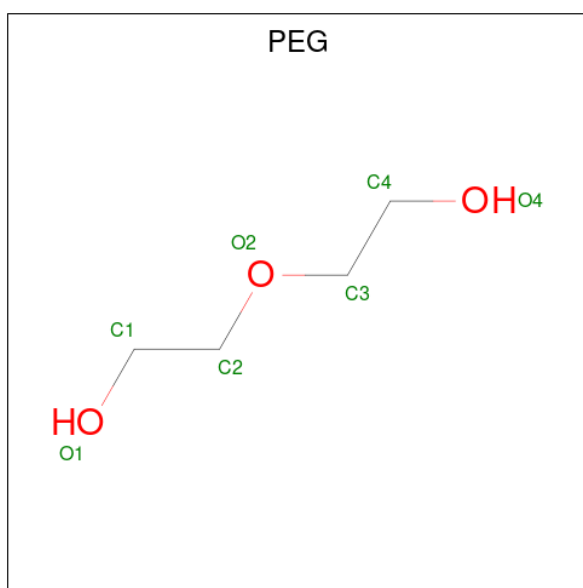
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

- 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		

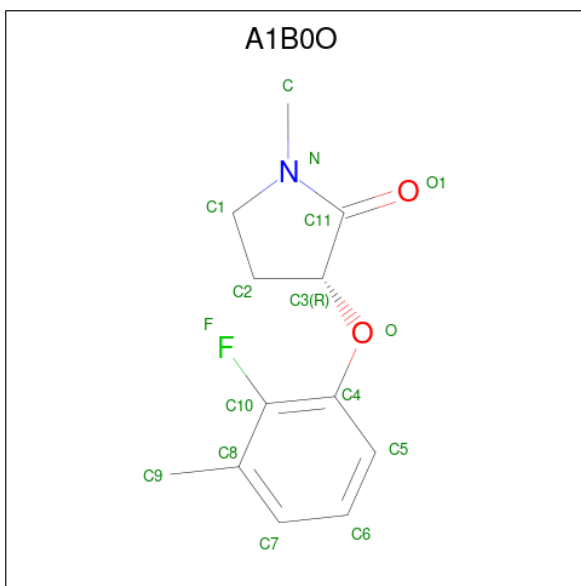
- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 7 is (3S)-3-(2-fluoro-3-methylphenoxy)-1-methylpyrrolidin-2-one (CCD ID:

A1B0O) (formula: C₁₂H₁₄FNO₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	F	N	O	0	0
			16	12	1	1	2		

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

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

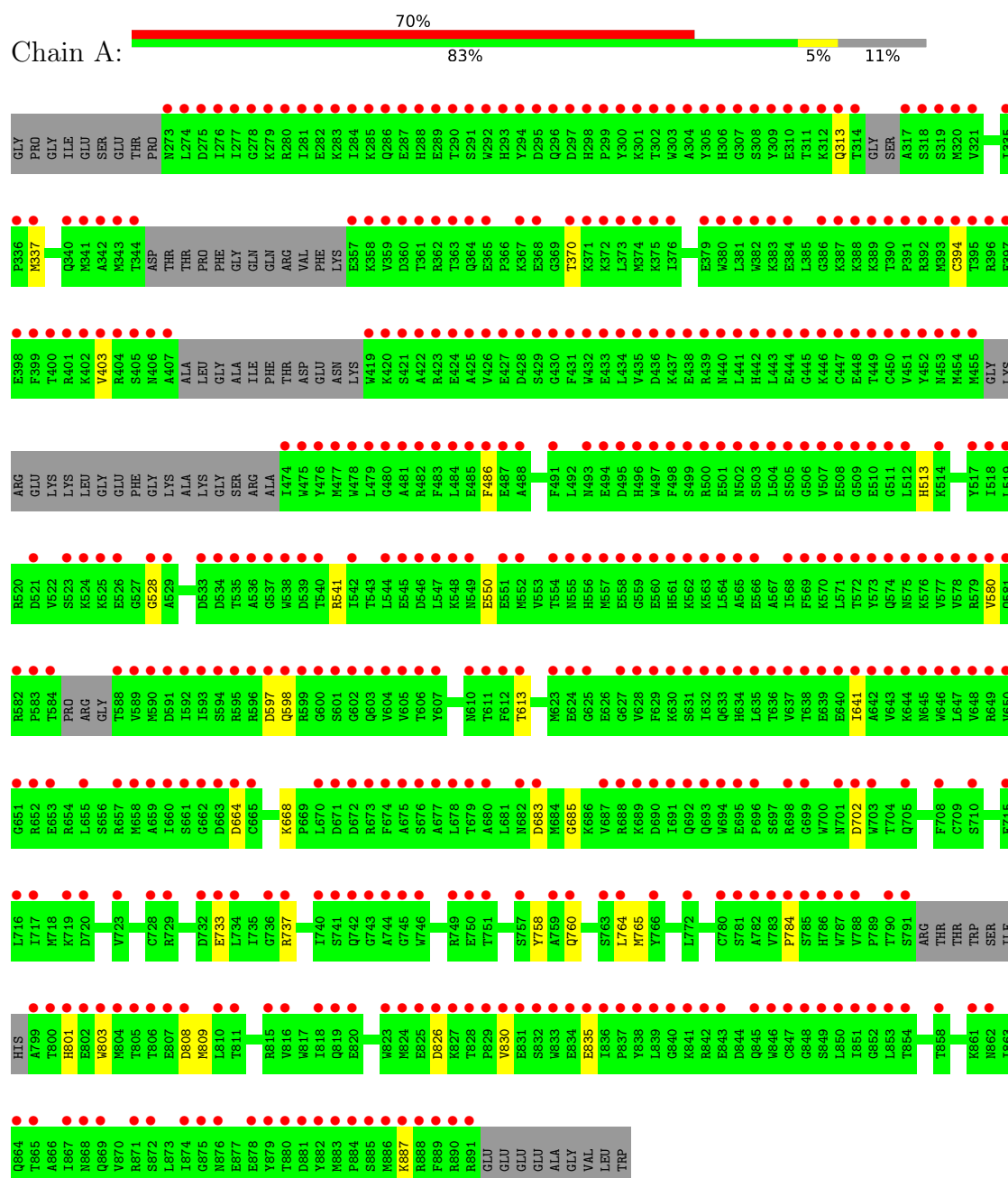
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	230	Total	O	0	0
			230	230		

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: NS5 RNA-dependent RNA polymerase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	82.38Å 116.32Å 147.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.29 – 2.03 91.29 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.8 (91.29-2.03) 99.7 (91.29-2.03)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.200 , 0.243 0.280 , 0.300	Depositor DCC
R_{free} test set	2329 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	41.2	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 494.9	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	0.81	EDS
Total number of atoms	4990	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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, PEG, A1B0O, PO4, CL, DMS, 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	0.99	0/4793	1.29	1/6464 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	702	ASP	CA-CB-CG	6.23	118.83	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	784	PRO	Mainchain

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	4688	0	4580	23	0
2	A	2	0	0	0	0
3	A	24	0	26	1	0
4	A	12	0	18	4	0
5	A	10	0	0	2	0
6	A	7	0	10	0	0
7	A	16	0	0	0	0
8	A	1	0	0	0	0
9	A	230	0	0	4	0
All	All	4990	0	4634	26	0

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 (26) 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:733:GLU:O	1:A:737:ARG:HG3	1.83	0.78
1:A:760:GLN:CD	1:A:809:MET:HE3	2.10	0.76
1:A:664:ASP:OD1	5:A:1007:PO4:O4	2.09	0.71
1:A:664:ASP:OD1	5:A:1007:PO4:P	2.53	0.67
4:A:1004:DMS:H12	9:A:1196:HOH:O	2.02	0.59
1:A:337:MET:HG2	9:A:1252:HOH:O	2.02	0.58
4:A:1004:DMS:H11	9:A:1169:HOH:O	2.03	0.57
1:A:765:MET:HA	1:A:765:MET:HE2	1.91	0.52
1:A:830:VAL:HG13	1:A:835:GLU:HB2	1.94	0.50
1:A:760:GLN:NE2	1:A:809:MET:HE3	2.27	0.49
1:A:826:ASP:OD1	1:A:826:ASP:C	2.56	0.47
1:A:764:LEU:O	1:A:765:MET:HE2	2.16	0.46
1:A:394:CYS:HB3	1:A:486:PHE:CE2	2.51	0.45
1:A:513:HIS:HB3	1:A:765:MET:HE1	1.97	0.45
1:A:808:ASP:HB3	9:A:1240:HOH:O	2.16	0.45
1:A:758:TYR:CD1	4:A:1006:DMS:H21	2.51	0.45
1:A:597:ASP:O	1:A:598:GLN:HB2	2.17	0.45
1:A:370:THR:OG1	1:A:683:ASP:OD2	2.32	0.44
1:A:758:TYR:CE1	4:A:1006:DMS:H21	2.53	0.43
1:A:550:GLU:OE2	1:A:613:THR:OG1	2.29	0.43
1:A:528:GLY:O	1:A:668:LYS:HE3	2.18	0.42
1:A:801[B]:HIS:CD2	1:A:801[B]:HIS:H	2.37	0.42
1:A:764:LEU:HD12	1:A:764:LEU:HA	1.83	0.42
3:A:1003[B]:MES:H32	3:A:1003[B]:MES:H81	1.91	0.41
1:A:541:ARG:HD2	1:A:685:GLY:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:760:GLN:NE2	1:A:803:TRP:O	2.54	0.40

There are no symmetry-related clashes.

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	559/637 (88%)	527 (94%)	31 (6%)	1 (0%)	43 40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	313	GLN

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	505/554 (91%)	501 (99%)	4 (1%)	73 75

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	403	VAL
1	A	580	VAL

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Mol	Chain	Res	Type
1	A	641	ILE
1	A	887	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	288	HIS
1	A	513	HIS
1	A	869	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 3 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	$\# Z > 2$
3	MES	A	1003[B]	-	12,12,12	0.71	0	15,16,16	0.29	0
4	DMS	A	1006	-	3,3,3	0.17	0	3,3,3	0.42	0
5	PO4	A	1007	-	4,4,4	2.35	1 (25%)	6,6,6	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MES	A	1003[A]	-	12,12,12	0.62	0	15,16,16	0.71	0
4	DMS	A	1005	-	3,3,3	0.28	0	3,3,3	0.09	0
7	A1B0O	A	1010	-	15,17,17	0.27	0	16,24,24	0.30	0
6	PEG	A	1009	-	6,6,6	0.13	0	5,5,5	0.17	0
5	PO4	A	1008	-	4,4,4	0.67	0	6,6,6	0.49	0
4	DMS	A	1004	-	3,3,3	0.44	0	3,3,3	0.28	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]	-	-	3/6/14/14	0/1/1/1
3	MES	A	1003[A]	-	-	0/6/14/14	0/1/1/1
6	PEG	A	1009	-	-	2/4/4/4	-
7	A1B0O	A	1010	-	-	0/4/17/17	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1007	PO4	P-O1	4.17	1.60	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1009	PEG	O2-C3-C4-O4
3	A	1003[B]	MES	C7-C8-S-O3S
3	A	1003[B]	MES	C7-C8-S-O1S
3	A	1003[B]	MES	C7-C8-S-O2S
6	A	1009	PEG	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 7 short contacts:

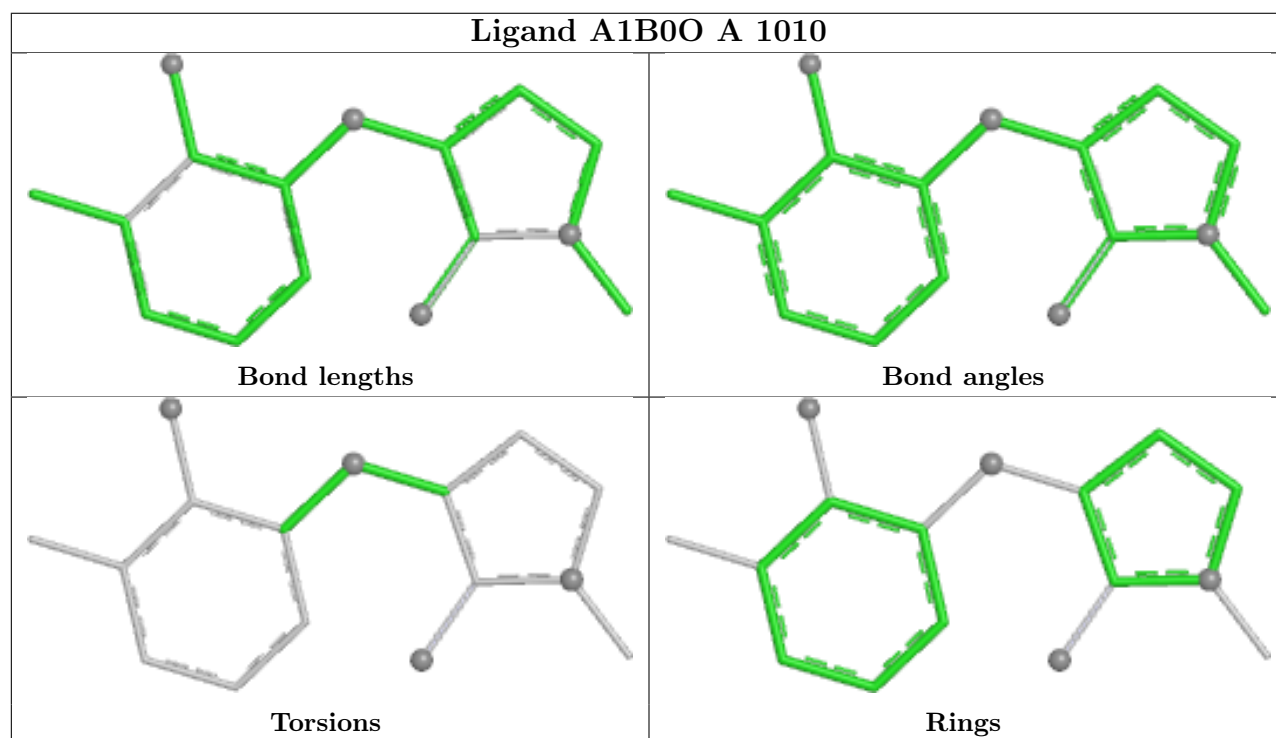
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003[B]	MES	1	0
4	A	1006	DMS	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1007	PO4	2	0
4	A	1004	DMS	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	566/637 (88%)	6.37	443 (78%) 0 0	7, 39, 71, 147	261 (46%)

All (443) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	344	THR	24.0
1	A	364	GLN	20.1
1	A	274	LEU	18.9
1	A	287	GLU	18.7
1	A	281	ILE	18.5
1	A	275	ASP	17.8
1	A	403	VAL	17.7
1	A	600	GLY	17.5
1	A	425	ALA	16.9
1	A	284	ILE	16.8
1	A	889	PHE	16.4
1	A	276	ILE	16.3
1	A	308	SER	16.0
1	A	589	VAL	15.8
1	A	359	VAL	15.7
1	A	282	GLU	15.6
1	A	474	ILE	15.6
1	A	431	PHE	15.1
1	A	584	THR	15.1
1	A	407	ALA	14.7
1	A	435	VAL	14.7
1	A	426	VAL	14.5
1	A	363	THR	14.1
1	A	289	GLU	14.1
1	A	294	TYR	14.1
1	A	278	GLY	14.1
1	A	441	LEU	13.9

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Mol	Chain	Res	Type	RSRZ
1	A	888	ARG	13.9
1	A	890	ARG	13.8
1	A	305	TYR	13.8
1	A	648	VAL	13.7
1	A	357	GLU	13.6
1	A	434	LEU	13.6
1	A	518	ILE	13.5
1	A	277	ILE	13.5
1	A	291	SER	13.4
1	A	405	SER	13.4
1	A	280	ARG	13.4
1	A	592	ILE	13.2
1	A	593	ILE	13.2
1	A	650	VAL	13.2
1	A	742	GLN	13.1
1	A	497	TRP	13.0
1	A	601	SER	12.9
1	A	309	TYR	12.8
1	A	286	GLN	12.7
1	A	443	LEU	12.7
1	A	744	ALA	12.7
1	A	406	ASN	12.6
1	A	453	ASN	12.6
1	A	317	ALA	12.6
1	A	571	LEU	12.6
1	A	825	GLU	12.5
1	A	312	LYS	12.5
1	A	544	LEU	12.5
1	A	836	ILE	12.5
1	A	288	HIS	12.5
1	A	481	ALA	12.5
1	A	646	TRP	12.5
1	A	314	THR	12.4
1	A	292	TRP	12.4
1	A	432	TRP	12.3
1	A	428	ASP	12.2
1	A	604	VAL	12.1
1	A	404	ARG	12.1
1	A	641	ILE	12.1
1	A	745	GLY	12.0
1	A	643	VAL	12.0
1	A	687	VAL	11.9

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Mol	Chain	Res	Type	RSRZ
1	A	399	PHE	11.9
1	A	603	GLN	11.9
1	A	478	TRP	11.9
1	A	476	TYR	11.9
1	A	475	TRP	11.9
1	A	511	GLY	11.8
1	A	886	MET	11.8
1	A	307	GLY	11.7
1	A	887	LYS	11.7
1	A	885	SER	11.6
1	A	519	LEU	11.6
1	A	651	GLY	11.6
1	A	649	ARG	11.5
1	A	283	LYS	11.5
1	A	602	GLY	11.5
1	A	302	THR	11.3
1	A	311	THR	11.3
1	A	763[A]	SER	11.3
1	A	423	ARG	11.3
1	A	582	ARG	11.1
1	A	483	PHE	11.1
1	A	493	ASN	11.1
1	A	572	THR	11.1
1	A	480	GLY	11.0
1	A	637	VAL	11.0
1	A	358	LYS	11.0
1	A	781	SER	10.9
1	A	583	PRO	10.9
1	A	438	GLU	10.9
1	A	290	THR	10.8
1	A	577	VAL	10.8
1	A	512[A]	LEU	10.8
1	A	801[A]	HIS	10.8
1	A	422	ALA	10.7
1	A	400	THR	10.7
1	A	498	PHE	10.6
1	A	430	GLY	10.6
1	A	303	TRP	10.6
1	A	846	TRP	10.6
1	A	631	SER	10.6
1	A	578	VAL	10.5
1	A	419	TRP	10.5

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Mol	Chain	Res	Type	RSRZ
1	A	833	TRP	10.5
1	A	636	THR	10.4
1	A	479	LEU	10.4
1	A	563	LYS	10.3
1	A	421	SER	10.3
1	A	647	LEU	10.3
1	A	558	GLU	10.2
1	A	452	TYR	10.2
1	A	642	ALA	10.2
1	A	635	LEU	10.1
1	A	383	LYS	10.1
1	A	891	ARG	10.1
1	A	791	SER	10.0
1	A	645	ASN	10.0
1	A	285	LYS	10.0
1	A	402	LYS	9.9
1	A	573	TYR	9.8
1	A	785[A]	SER	9.8
1	A	799	ALA	9.8
1	A	837	PRO	9.8
1	A	751	THR	9.8
1	A	361	THR	9.7
1	A	540	THR	9.7
1	A	606	THR	9.7
1	A	655	LEU	9.7
1	A	678	LEU	9.7
1	A	514	LYS	9.6
1	A	719[A]	LYS	9.6
1	A	420	LYS	9.6
1	A	433	GLU	9.5
1	A	437	LYS	9.5
1	A	477	MET	9.5
1	A	632	ILE	9.5
1	A	864[A]	GLN	9.4
1	A	362	ARG	9.4
1	A	273	ASN	9.3
1	A	708	PHE	9.3
1	A	424	GLU	9.3
1	A	449	THR	9.3
1	A	484	LEU	9.3
1	A	300	TYR	9.3
1	A	293	HIS	9.2

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Mol	Chain	Res	Type	RSRZ
1	A	851	ILE	9.2
1	A	657	ARG	9.2
1	A	499	SER	9.2
1	A	835	GLU	9.2
1	A	741[A]	SER	9.2
1	A	679	THR	9.1
1	A	539	ASP	9.1
1	A	395	THR	9.1
1	A	506	GLY	9.0
1	A	694	TRP	9.0
1	A	790	THR	9.0
1	A	304	ALA	9.0
1	A	659	ALA	9.0
1	A	675	ALA	8.9
1	A	538	TRP	8.9
1	A	337	MET	8.9
1	A	580	VAL	8.9
1	A	576	LYS	8.9
1	A	504	LEU	8.8
1	A	360	ASP	8.8
1	A	638	THR	8.8
1	A	429	SER	8.8
1	A	575	ASN	8.7
1	A	442	HIS	8.7
1	A	505	SER	8.7
1	A	501	GLU	8.6
1	A	279	LYS	8.6
1	A	691	ILE	8.5
1	A	629	PHE	8.5
1	A	447	CYS	8.5
1	A	581	GLN	8.5
1	A	556	HIS	8.4
1	A	546	ASP	8.4
1	A	507	VAL	8.4
1	A	450	CYS	8.4
1	A	850	LEU	8.3
1	A	548	LYS	8.3
1	A	839	LEU	8.3
1	A	591	ASP	8.3
1	A	436	ASP	8.3
1	A	536	ALA	8.2
1	A	455	MET	8.2

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Mol	Chain	Res	Type	RSRZ
1	A	594	SER	8.2
1	A	298	HIS	8.2
1	A	677	ALA	8.2
1	A	849	SER	8.2
1	A	800	THR	8.2
1	A	676	SER	8.2
1	A	640	GLU	8.1
1	A	660	ILE	8.0
1	A	876	ASN	8.0
1	A	296	GLN	8.0
1	A	644	LYS	8.0
1	A	788	VAL	8.0
1	A	633	GLN	7.9
1	A	838	TYR	7.9
1	A	693	GLN	7.9
1	A	295	ASP	7.9
1	A	852	GLY	7.9
1	A	688	ARG	7.9
1	A	834	GLU	7.8
1	A	808	ASP	7.8
1	A	627	GLY	7.8
1	A	701	ASN	7.7
1	A	652	ARG	7.7
1	A	545	GLU	7.7
1	A	365	GLU	7.6
1	A	301	LYS	7.6
1	A	427	GLU	7.6
1	A	588	THR	7.6
1	A	487	GLU	7.5
1	A	454	MET	7.5
1	A	661	SER	7.5
1	A	310	GLU	7.4
1	A	705	GLN	7.4
1	A	639	GLU	7.4
1	A	750	GLU	7.4
1	A	807	GLU	7.4
1	A	448	GLU	7.3
1	A	597	ASP	7.3
1	A	596	ARG	7.3
1	A	396	ARG	7.3
1	A	673	ARG	7.3
1	A	692	GLN	7.2

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Mol	Chain	Res	Type	RSRZ
1	A	318	SER	7.2
1	A	658	MET	7.2
1	A	595	ARG	7.1
1	A	535	THR	7.1
1	A	882	TYR	7.1
1	A	299	PRO	7.1
1	A	306	HIS	7.1
1	A	786	HIS	7.1
1	A	746	TRP	7.0
1	A	440	ASN	7.0
1	A	551	GLU	6.9
1	A	566	GLU	6.9
1	A	537	GLY	6.9
1	A	401	ARG	6.8
1	A	663	ASP	6.8
1	A	482	ARG	6.8
1	A	590	MET	6.8
1	A	398	GLU	6.8
1	A	510	GLU	6.8
1	A	806	THR	6.8
1	A	842	ARG	6.7
1	A	503	SER	6.6
1	A	840	GLY	6.6
1	A	880	THR	6.6
1	A	574	GLN	6.6
1	A	502	ASN	6.6
1	A	500	ARG	6.5
1	A	634	HIS	6.5
1	A	451	VAL	6.5
1	A	446	LYS	6.5
1	A	674	PHE	6.5
1	A	562	LYS	6.5
1	A	313	GLN	6.5
1	A	672	ASP	6.4
1	A	445	GLY	6.4
1	A	495	ASP	6.3
1	A	854	THR	6.3
1	A	743	GLY	6.3
1	A	579	ARG	6.3
1	A	749	ARG	6.3
1	A	393	MET	6.3
1	A	319	SER	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	717	ILE	6.2
1	A	534	ASP	6.2
1	A	802	GLU	6.2
1	A	552	MET	6.2
1	A	321	VAL	6.2
1	A	699	GLY	6.0
1	A	695	GLU	6.0
1	A	804	MET	6.0
1	A	367	LYS	6.0
1	A	570	LYS	6.0
1	A	861	LYS	6.0
1	A	858	THR	5.9
1	A	496	HIS	5.9
1	A	397	GLU	5.9
1	A	878	GLU	5.8
1	A	564	LEU	5.8
1	A	828	THR	5.8
1	A	716	LEU	5.8
1	A	486	PHE	5.8
1	A	524	LYS	5.7
1	A	815	ARG	5.7
1	A	494	GLU	5.7
1	A	689	LYS	5.7
1	A	372	LYS	5.6
1	A	485	GLU	5.5
1	A	555	ASN	5.5
1	A	630	LYS	5.4
1	A	690	ASP	5.4
1	A	881	ASP	5.4
1	A	625	GLY	5.4
1	A	371	LYS	5.3
1	A	831	GLU	5.3
1	A	368	GLU	5.2
1	A	845	GLN	5.2
1	A	703	TRP	5.1
1	A	820	GLU	5.1
1	A	841	LYS	5.1
1	A	444	GLU	5.1
1	A	559	GLY	5.0
1	A	375	LYS	5.0
1	A	569	PHE	4.9
1	A	653	GLU	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	843	GLU	4.9
1	A	680	ALA	4.9
1	A	811	THR	4.9
1	A	883	MET	4.8
1	A	764	LEU	4.8
1	A	376	ILE	4.8
1	A	379	GLU	4.7
1	A	827	LYS	4.6
1	A	394	CYS	4.5
1	A	819	GLN	4.5
1	A	698	ARG	4.5
1	A	565	ALA	4.5
1	A	390	THR	4.5
1	A	664	ASP	4.5
1	A	702	ASP	4.5
1	A	488	ALA	4.5
1	A	874	ILE	4.4
1	A	683	ASP	4.4
1	A	389	LYS	4.4
1	A	340	GLN	4.4
1	A	740	ILE	4.4
1	A	561	HIS	4.4
1	A	508	GLU	4.3
1	A	818	ILE	4.3
1	A	392	ARG	4.3
1	A	297	ASP	4.3
1	A	628	VAL	4.3
1	A	784	PRO	4.0
1	A	387	LYS	4.0
1	A	607	TYR	4.0
1	A	830	VAL	4.0
1	A	542	ILE	4.0
1	A	439	ARG	3.9
1	A	670	LEU	3.9
1	A	853	LEU	3.8
1	A	823	TRP	3.8
1	A	624	GLU	3.8
1	A	610	ASN	3.8
1	A	320	MET	3.8
1	A	343	MET	3.8
1	A	760	GLN	3.7
1	A	868	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	568	ILE	3.7
1	A	729	ARG	3.7
1	A	715	GLU	3.7
1	A	611	THR	3.7
1	A	529	ALA	3.6
1	A	867	ILE	3.6
1	A	381	LEU	3.6
1	A	720	ASP	3.5
1	A	865	THR	3.5
1	A	526	GLU	3.5
1	A	879	TYR	3.4
1	A	336	PRO	3.4
1	A	872	SER	3.4
1	A	521	ASP	3.3
1	A	805	THR	3.3
1	A	391	PRO	3.3
1	A	875	GLY	3.3
1	A	373	LEU	3.3
1	A	549	ASN	3.3
1	A	803	TRP	3.2
1	A	723	VAL	3.2
1	A	696	PRO	3.2
1	A	662	GLY	3.1
1	A	848	GLY	3.1
1	A	826	ASP	3.0
1	A	598	GLN	3.0
1	A	832	SER	3.0
1	A	370	THR	2.9
1	A	386	GLY	2.9
1	A	862	ASN	2.9
1	A	829	PRO	2.9
1	A	732	ASP	2.8
1	A	599	ARG	2.8
1	A	623	MET	2.7
1	A	665	CYS	2.7
1	A	523	SER	2.7
1	A	733	GLU	2.7
1	A	557	MET	2.7
1	A	772	LEU	2.7
1	A	560	GLU	2.6
1	A	782	ALA	2.6
1	A	554	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	380	TRP	2.6
1	A	491	PHE	2.6
1	A	533	ASP	2.5
1	A	671	ASP	2.5
1	A	869	GLN	2.5
1	A	388	LYS	2.5
1	A	517	TYR	2.5
1	A	847	CYS	2.5
1	A	810	LEU	2.5
1	A	341	MET	2.4
1	A	374	MET	2.4
1	A	547	LEU	2.4
1	A	605	VAL	2.4
1	A	736	GLY	2.4
1	A	824	MET	2.4
1	A	787	TRP	2.4
1	A	682	ASN	2.3
1	A	528	GLY	2.3
1	A	525	LYS	2.3
1	A	612	PHE	2.3
1	A	728	CYS	2.3
1	A	382	TRP	2.3
1	A	871	ARG	2.3
1	A	613	THR	2.3
1	A	884	PRO	2.3
1	A	509	GLY	2.2
1	A	384	GLU	2.2
1	A	710	SER	2.2
1	A	783	VAL	2.1
1	A	342	ALA	2.1
1	A	780	CYS	2.1
1	A	757	SER	2.1
1	A	737	ARG	2.1
1	A	766	TYR	2.1
1	A	335	ILE	2.1
1	A	816	VAL	2.1
1	A	759	ALA	2.1
1	A	734	LEU	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

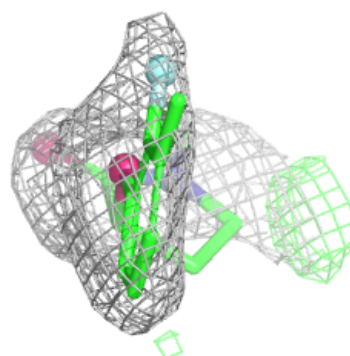
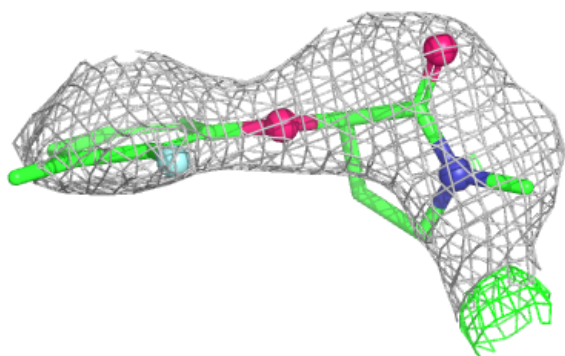
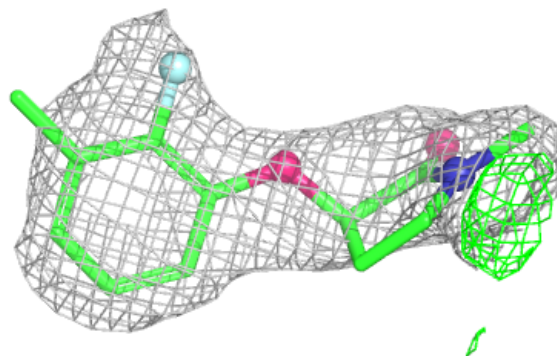
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	PO4	A	1007	5/5	0.70	0.19	53,56,61,86	0
5	PO4	A	1008	5/5	0.72	0.19	111,118,123,131	0
6	PEG	A	1009	7/7	0.73	0.22	73,76,82,83	0
7	A1B0O	A	1010	16/16	0.77	0.23	37,38,41,41	16
4	DMS	A	1005	4/4	0.81	0.20	93,104,108,111	0
4	DMS	A	1006	4/4	0.91	0.20	67,68,72,76	0
3	MES	A	1003[A]	12/12	0.95	0.24	15,19,21,21	12
3	MES	A	1003[B]	12/12	0.95	0.24	477,485,528,530	12
4	DMS	A	1004	4/4	0.95	0.23	52,57,60,61	0
8	CL	A	1011	1/1	0.95	0.16	26,26,26,26	1
2	ZN	A	1002	1/1	0.98	0.07	61,61,61,61	0
2	ZN	A	1001	1/1	1.00	0.04	30,30,30,30	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 A1B0O 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.