



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 06:13 PM EDT

PDB ID : 7I29 / pdb_00007i29
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 Z48847594 (DNV2_NS5A-x0162)
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Deposited on : 2025-03-06
Resolution : 1.50 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)

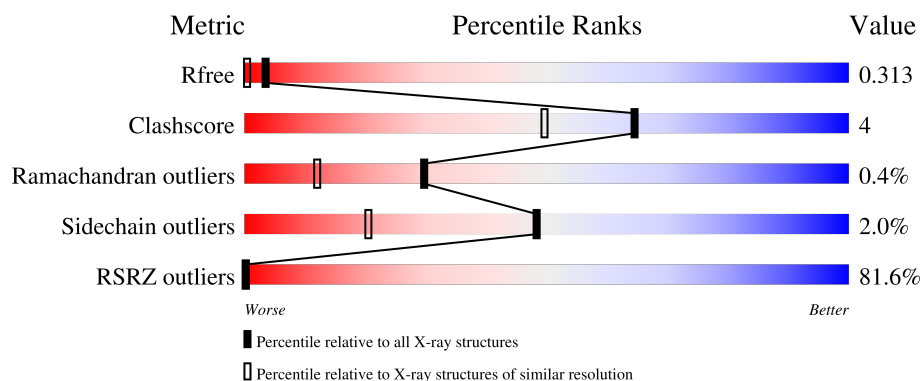
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	

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
4	DMS	A	1005	-	-	-	X
6	PO4	A	1007	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5068 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	561	Total	C	N	O	S	0	7	0
			4640	2924	832	850	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).



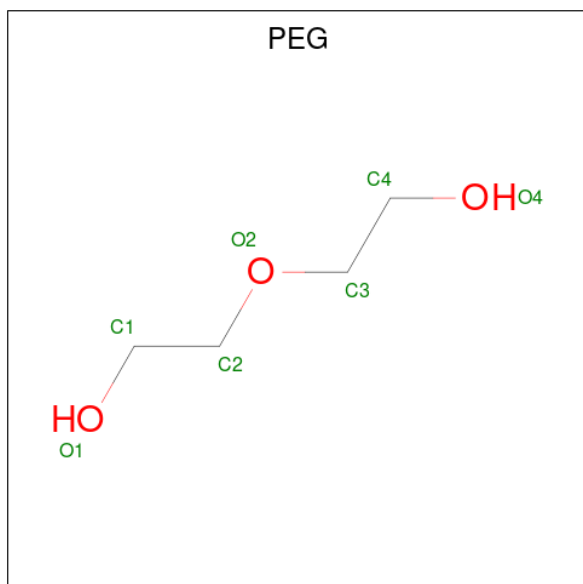
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			24	12	2	8	2		

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



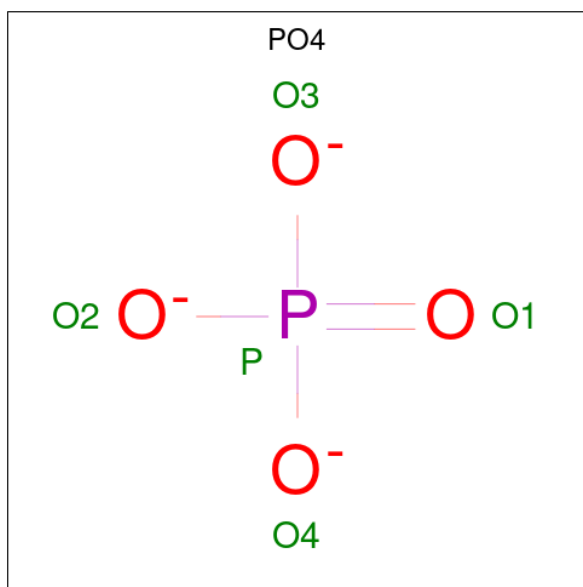
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

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



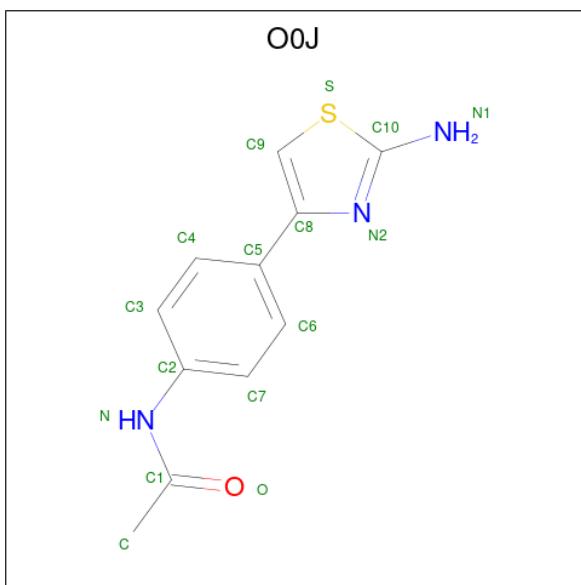
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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-[4-(2-amino-1,3-thiazol-4-yl)phenyl]acetamide (CCD ID: O0J) (formula: C₁₁H₁₁N₃OS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			16	11	3	1	1		

- 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		

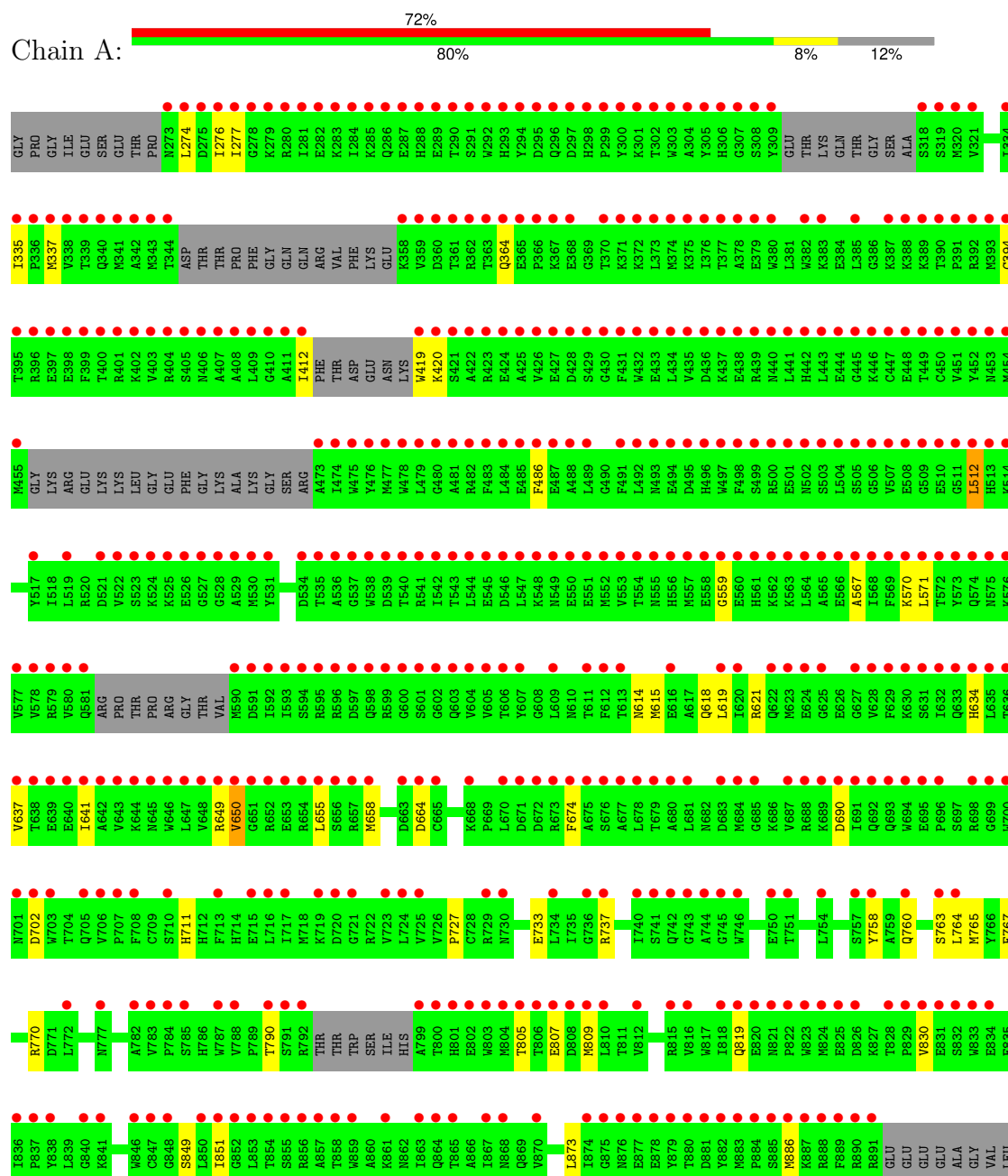
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	352	Total	O	0	1
			353	353		

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



TRP

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	82.28Å 117.42Å 148.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.46 – 1.50 74.46 – 1.50	Depositor EDS
% Data completeness (in resolution range)	95.1 (74.46-1.50) 95.1 (74.46-1.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC5	Depositor
R, R_{free}	0.255 , 0.291 0.298 , 0.313	Depositor DCC
R_{free} test set	5824 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	6.3	Xtriage
Anisotropy	1.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 379.0	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	0.82	EDS
Total number of atoms	5068	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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: DMS, O0J, PEG, ZN, MES, CL, 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	1.11	4/4744 (0.1%)	1.32	5/6396 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	711	HIS	CE1-NE2	6.25	1.38	1.32
1	A	650	VAL	N-CA	5.80	1.51	1.46
1	A	758	TYR	C-O	5.34	1.30	1.24
1	A	760	GLN	C-O	5.10	1.30	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	702	ASP	CA-CB-CG	6.71	119.31	112.60
1	A	559	GLY	CA-C-N	6.44	128.90	120.28
1	A	559	GLY	C-N-CA	6.44	128.90	120.28
1	A	702	ASP	CB-CA-C	5.58	118.72	110.14
1	A	615	MET	N-CA-C	-5.02	105.70	111.07

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	4640	0	4538	33	0
2	A	2	0	0	0	0
3	A	24	0	26	1	0
4	A	8	0	12	3	0
5	A	14	0	20	0	0
6	A	10	0	0	2	0
7	A	16	0	0	0	0
8	A	1	0	0	0	0
9	A	353	0	0	10	0
All	All	5068	0	4596	36	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 4.

All (36) 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)
4:A:1004:DMS:H11	9:A:1271:HOH:O	1.78	0.84
1:A:664:ASP:OD1	6:A:1007:PO4:O2	1.99	0.80
1:A:274:LEU:HA	1:A:277:ILE:HG12	1.74	0.68
1:A:807:GLU:HG3	9:A:1298:HOH:O	1.96	0.65
1:A:664:ASP:OD1	6:A:1007:PO4:P	2.55	0.64
1:A:770:ARG:HD2	1:A:851:ILE:HD13	1.80	0.63
1:A:819:GLN:HG3	9:A:1421:HOH:O	1.99	0.61
4:A:1004:DMS:H12	9:A:1274:HOH:O	2.01	0.60
1:A:849:SER:OG	1:A:851:ILE:HG12	2.02	0.59
1:A:276:ILE:O	9:A:1102:HOH:O	2.17	0.59
1:A:737:ARG:HB3	9:A:1385:HOH:O	2.06	0.56
1:A:337:MET:HG2	9:A:1309:HOH:O	2.08	0.54
1:A:733:GLU:O	1:A:737:ARG:HG3	2.10	0.51
1:A:764:LEU:O	1:A:765:MET:HE2	2.10	0.51
1:A:886:MET:HE1	9:A:1207:HOH:O	2.12	0.49
1:A:649:ARG:HG2	1:A:650:VAL:HG13	1.94	0.48
1:A:274:LEU:HD23	1:A:277:ILE:HG13	1.95	0.48
1:A:621:ARG:HG2	1:A:674:PHE:CE2	2.49	0.48
1:A:764:LEU:C	1:A:765:MET:HE2	2.40	0.47
1:A:619:LEU:HD11	1:A:655:LEU:HD21	1.96	0.47
1:A:873:LEU:HD13	3:A:1003[A]:MES:H62	1.97	0.47
4:A:1004:DMS:C1	9:A:1271:HOH:O	2.52	0.44
1:A:805:THR:CG2	1:A:809:MET:HE1	2.48	0.44
1:A:763[B]:SER:O	1:A:767:PHE:HB3	2.18	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	9:A:1327:HOH:O	2.18	0.43
1:A:764:LEU:HG	1:A:765:MET:CE	2.49	0.43
1:A:737:ARG:NH2	1:A:737:ARG:HG2	2.34	0.42
1:A:618:GLN:HB2	1:A:658:MET:SD	2.60	0.42
1:A:614:ASN:O	1:A:618:GLN:HG2	2.19	0.42
1:A:567:ALA:HB1	1:A:571:LEU:HD12	2.02	0.42
1:A:512[A]:LEU:HD12	1:A:512[A]:LEU:HA	1.82	0.41
1:A:274:LEU:C	1:A:276:ILE:N	2.76	0.41
1:A:274:LEU:C	1:A:276:ILE:H	2.28	0.41
1:A:512[A]:LEU:HG	1:A:727:PRO:CB	2.52	0.40
1:A:764:LEU:HG	1:A:765:MET:HE3	2.02	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	554/637 (87%)	532 (96%)	20 (4%)	2 (0%)	30 12

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	690	ASP
1	A	637	VAL

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	497/554 (90%)	486 (98%)	11 (2%)	45 17

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	335	ILE
1	A	364	GLN
1	A	412	ILE
1	A	419	TRP
1	A	420	LYS
1	A	512[A]	LEU
1	A	512[B]	LEU
1	A	570	LYS
1	A	634	HIS
1	A	641	ILE
1	A	830	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	603	GLN
1	A	705	GLN
1	A	742	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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 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
5	PEG	A	1006	-	6,6,6	0.19	0	5,5,5	0.10	0
4	DMS	A	1005	-	3,3,3	0.21	0	3,3,3	0.13	0
6	PO4	A	1007	-	4,4,4	2.29	1 (25%)	6,6,6	0.59	0
4	DMS	A	1004	-	3,3,3	1.11	0	3,3,3	0.54	0
5	PEG	A	1009	-	6,6,6	0.17	0	5,5,5	0.07	0
6	PO4	A	1008	-	4,4,4	1.12	1 (25%)	6,6,6	0.51	0
3	MES	A	1003[B]	-	12,12,12	0.71	0	15,16,16	0.30	0
3	MES	A	1003[A]	-	12,12,12	1.09	1 (8%)	15,16,16	1.07	2 (13%)
7	O0J	A	1010	-	17,17,17	0.22	0	23,23,23	0.21	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	1006	-	-	3/4/4/4	-
5	PEG	A	1009	-	-	2/4/4/4	-
3	MES	A	1003[B]	-	-	5/6/14/14	0/1/1/1
3	MES	A	1003[A]	-	-	0/6/14/14	0/1/1/1
7	O0J	A	1010	-	-	2/8/8/8	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1007	PO4	P-O1	4.19	1.60	1.50
3	A	1003[A]	MES	O1S-S	-2.50	1.38	1.45
6	A	1008	PO4	P-O1	2.04	1.55	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1003[A]	MES	O2S-S-C8	-3.26	101.81	106.73
3	A	1003[A]	MES	O3S-S-O1S	2.05	116.54	111.40

There are no chirality outliers.

All (12) torsion outliers are listed below:

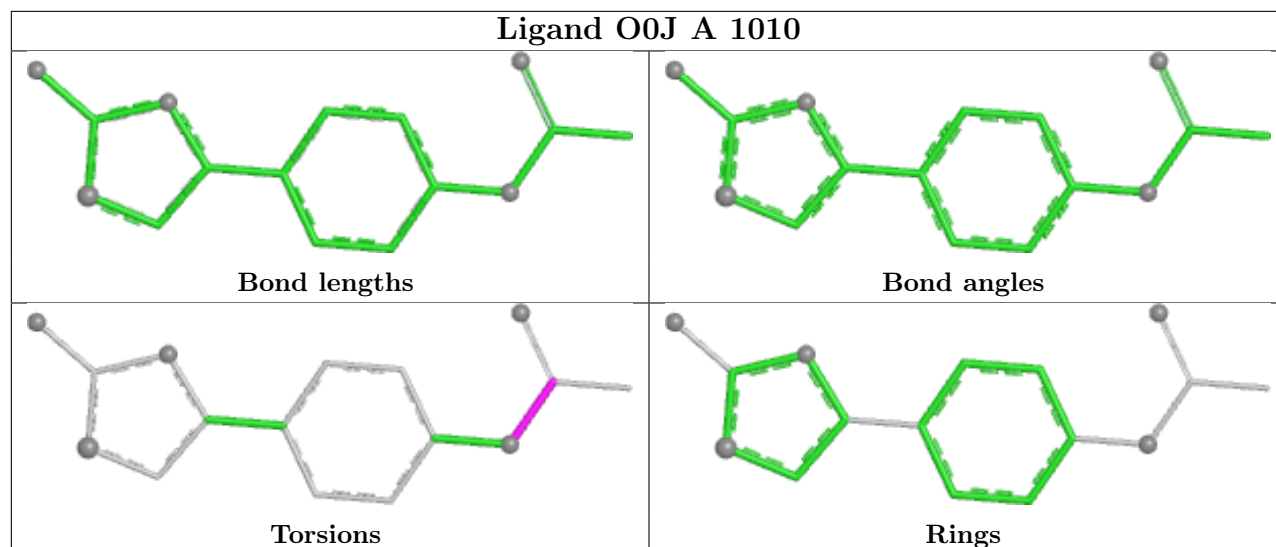
Mol	Chain	Res	Type	Atoms
3	A	1003[B]	MES	C8-C7-N4-C3
7	A	1010	O0J	C-C1-N-C2
7	A	1010	O0J	O-C1-N-C2
5	A	1006	PEG	O2-C3-C4-O4
3	A	1003[B]	MES	C7-C8-S-O3S
5	A	1009	PEG	O2-C3-C4-O4
5	A	1009	PEG	O1-C1-C2-O2
3	A	1003[B]	MES	C8-C7-N4-C5
3	A	1003[B]	MES	C7-C8-S-O1S
3	A	1003[B]	MES	C7-C8-S-O2S
5	A	1006	PEG	O1-C1-C2-O2
5	A	1006	PEG	C1-C2-O2-C3

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1007	PO4	2	0
4	A	1004	DMS	3	0
3	A	1003[A]	MES	1	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	561/637 (88%)	6.42	458 (81%) 0 0	6, 30, 55, 105	245 (43%)

All (458) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	412	ILE	26.0
1	A	411	ALA	22.1
1	A	294	TYR	20.6
1	A	403	VAL	20.3
1	A	292	TRP	17.5
1	A	419	TRP	17.3
1	A	409	LEU	17.1
1	A	293	HIS	16.9
1	A	284	ILE	16.9
1	A	305	TYR	16.9
1	A	299	PRO	16.7
1	A	474	ILE	16.7
1	A	435	VAL	16.4
1	A	432	TRP	16.2
1	A	303	TRP	16.1
1	A	431	PHE	15.9
1	A	309	TYR	15.8
1	A	281	ILE	15.5
1	A	800	THR	15.3
1	A	300	TYR	15.3
1	A	426	VAL	15.3
1	A	635	LEU	15.2
1	A	277	ILE	14.9
1	A	441	LEU	14.9
1	A	592	ILE	14.8
1	A	637	VAL	14.7
1	A	593	ILE	14.6

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Mol	Chain	Res	Type	RSRZ
1	A	302	THR	14.6
1	A	641	ILE	14.5
1	A	425	ALA	14.4
1	A	399	PHE	14.3
1	A	604	VAL	14.3
1	A	799	ALA	14.3
1	A	375	LYS	14.3
1	A	359	VAL	14.3
1	A	286	GLN	14.2
1	A	291	SER	14.2
1	A	443	LEU	14.2
1	A	434	LEU	14.1
1	A	364	GLN	14.1
1	A	578	VAL	14.0
1	A	407	ALA	14.0
1	A	404	ARG	13.9
1	A	859	TRP	13.8
1	A	362	ARG	13.8
1	A	422	ALA	13.7
1	A	298	HIS	13.5
1	A	577	VAL	13.5
1	A	544	LEU	13.4
1	A	687	VAL	13.3
1	A	600	GLY	13.2
1	A	483	PHE	13.2
1	A	304	ALA	13.2
1	A	452	TYR	12.9
1	A	446	LYS	12.9
1	A	307	GLY	12.8
1	A	891	ARG	12.8
1	A	476	TYR	12.6
1	A	451	VAL	12.6
1	A	580	VAL	12.6
1	A	648	VAL	12.6
1	A	420	LYS	12.6
1	A	638	THR	12.6
1	A	803	TRP	12.5
1	A	295	ASP	12.5
1	A	453	ASN	12.4
1	A	290	THR	12.4
1	A	297	ASP	12.3
1	A	408	ALA	12.3

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Mol	Chain	Res	Type	RSRZ
1	A	570	LYS	12.3
1	A	694	TRP	12.3
1	A	636	THR	12.3
1	A	361	THR	12.2
1	A	402	LYS	12.1
1	A	405	SER	12.1
1	A	447	CYS	12.1
1	A	575	ASN	12.1
1	A	410	GLY	12.0
1	A	889	PHE	11.9
1	A	473	ALA	11.9
1	A	406	ASN	11.9
1	A	288	HIS	11.9
1	A	479	LEU	11.9
1	A	850	LEU	11.9
1	A	401	ARG	11.8
1	A	367	LYS	11.8
1	A	319	SER	11.8
1	A	455	MET	11.8
1	A	857	ALA	11.7
1	A	536	ALA	11.7
1	A	478	TRP	11.6
1	A	484	LEU	11.6
1	A	851	ILE	11.5
1	A	475	TRP	11.5
1	A	400	THR	11.5
1	A	854	THR	11.4
1	A	512[A]	LEU	11.3
1	A	634	HIS	11.3
1	A	454	MET	11.2
1	A	283	LYS	11.2
1	A	449	THR	11.2
1	A	430	GLY	11.1
1	A	421	SER	11.1
1	A	573	TYR	11.0
1	A	450	CYS	11.0
1	A	647	LEU	11.0
1	A	318	SER	10.9
1	A	858	THR	10.9
1	A	547	LEU	10.8
1	A	691	ILE	10.8
1	A	279	LYS	10.8

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Mol	Chain	Res	Type	RSRZ
1	A	834	GLU	10.6
1	A	424	GLU	10.6
1	A	320	MET	10.5
1	A	287	GLU	10.5
1	A	274	LEU	10.5
1	A	498	PHE	10.5
1	A	301	LYS	10.4
1	A	366	PRO	10.4
1	A	363	THR	10.3
1	A	428	ASP	10.3
1	A	719[A]	LYS	10.3
1	A	395	THR	10.3
1	A	853	LEU	10.3
1	A	742	GLN	10.2
1	A	543	THR	10.1
1	A	289	GLU	10.1
1	A	480	GLY	10.0
1	A	538	TRP	10.0
1	A	429	SER	10.0
1	A	445	GLY	9.9
1	A	699	GLY	9.9
1	A	285	LYS	9.9
1	A	542	ILE	9.9
1	A	601	SER	9.8
1	A	477	MET	9.8
1	A	603	GLN	9.8
1	A	708	PHE	9.8
1	A	744	ALA	9.8
1	A	643	VAL	9.8
1	A	852	GLY	9.7
1	A	344	THR	9.7
1	A	282	GLU	9.7
1	A	308	SER	9.7
1	A	763[A]	SER	9.7
1	A	481	ALA	9.6
1	A	602	GLY	9.6
1	A	423	ARG	9.6
1	A	296	GLN	9.6
1	A	440	ASN	9.6
1	A	321	VAL	9.5
1	A	563	LYS	9.5
1	A	365	GLU	9.4

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Mol	Chain	Res	Type	RSRZ
1	A	649	ARG	9.4
1	A	879	TYR	9.2
1	A	654	ARG	9.1
1	A	741[A]	SER	9.1
1	A	383	LYS	9.0
1	A	594	SER	9.0
1	A	785[A]	SER	8.9
1	A	696	PRO	8.9
1	A	801[A]	HIS	8.9
1	A	655	LEU	8.9
1	A	280	ARG	8.8
1	A	595	ARG	8.8
1	A	864[A]	GLN	8.8
1	A	633	GLN	8.8
1	A	607	TYR	8.7
1	A	596	ARG	8.7
1	A	540	THR	8.7
1	A	524	LYS	8.6
1	A	535	THR	8.6
1	A	576	LYS	8.6
1	A	306	HIS	8.6
1	A	427	GLU	8.6
1	A	278	GLY	8.5
1	A	511	GLY	8.5
1	A	275	ASP	8.5
1	A	439	ARG	8.4
1	A	581	GLN	8.4
1	A	884	PRO	8.4
1	A	564	LEU	8.4
1	A	438	GLU	8.3
1	A	791	SER	8.2
1	A	790	THR	8.2
1	A	358	LYS	8.2
1	A	890	ARG	8.2
1	A	656	SER	8.2
1	A	448	GLU	8.1
1	A	396	ARG	8.1
1	A	506	GLY	8.1
1	A	579	ARG	8.0
1	A	688	ARG	8.0
1	A	360	ASP	8.0
1	A	482	ARG	7.9

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Mol	Chain	Res	Type	RSRZ
1	A	433	GLU	7.9
1	A	273	ASN	7.9
1	A	645	ASN	7.8
1	A	507	VAL	7.8
1	A	591	ASP	7.7
1	A	371	LYS	7.7
1	A	397	GLU	7.7
1	A	887	LYS	7.7
1	A	504	LEU	7.6
1	A	640	GLU	7.6
1	A	841	LYS	7.6
1	A	692	GLN	7.5
1	A	525	LYS	7.5
1	A	668	LYS	7.5
1	A	398	GLU	7.4
1	A	437	LYS	7.4
1	A	444	GLU	7.3
1	A	680	ALA	7.3
1	A	499	SER	7.3
1	A	436	ASP	7.2
1	A	856	ARG	7.2
1	A	505	SER	7.2
1	A	702	ASP	7.2
1	A	689	LYS	7.2
1	A	888	ARG	7.2
1	A	574	GLN	7.1
1	A	639	GLU	7.1
1	A	572	THR	7.0
1	A	276	ILE	6.9
1	A	598	GLN	6.8
1	A	541	ARG	6.8
1	A	599	ARG	6.8
1	A	804	MET	6.7
1	A	545	GLU	6.7
1	A	802	GLU	6.7
1	A	590	MET	6.7
1	A	551	GLU	6.7
1	A	693	GLN	6.7
1	A	529	ALA	6.6
1	A	559	GLY	6.5
1	A	743	GLY	6.5
1	A	556	HIS	6.5

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Mol	Chain	Res	Type	RSRZ
1	A	502	ASN	6.5
1	A	508	GLU	6.5
1	A	571	LEU	6.5
1	A	881	ASP	6.5
1	A	644	LYS	6.5
1	A	500	ARG	6.5
1	A	534	ASP	6.4
1	A	537	GLY	6.4
1	A	876	ASN	6.4
1	A	658	MET	6.4
1	A	539	ASP	6.4
1	A	652	ARG	6.4
1	A	509	GLY	6.3
1	A	886	MET	6.3
1	A	690	ASP	6.3
1	A	562	LYS	6.3
1	A	513	HIS	6.3
1	A	548	LYS	6.2
1	A	657	ARG	6.1
1	A	597	ASP	6.1
1	A	376	ILE	6.1
1	A	882	TYR	6.1
1	A	550	GLU	6.1
1	A	629	PHE	6.0
1	A	514	LYS	6.0
1	A	745	GLY	6.0
1	A	885	SER	6.0
1	A	823	TRP	6.0
1	A	503	SER	5.9
1	A	677	ALA	5.9
1	A	496	HIS	5.9
1	A	566	GLU	5.9
1	A	486	PHE	5.9
1	A	501	GLU	5.9
1	A	558	GLU	5.8
1	A	833	TRP	5.7
1	A	510	GLU	5.7
1	A	526	GLU	5.7
1	A	630	LYS	5.7
1	A	717	ILE	5.7
1	A	825	GLU	5.7
1	A	646	TRP	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	378	ALA	5.7
1	A	792	ARG	5.7
1	A	530	MET	5.7
1	A	605	VAL	5.7
1	A	663	ASP	5.7
1	A	338	VAL	5.6
1	A	701	ASN	5.5
1	A	746	TRP	5.5
1	A	695	GLU	5.5
1	A	390	THR	5.4
1	A	830	VAL	5.4
1	A	642	ALA	5.4
1	A	855	SER	5.3
1	A	393	MET	5.2
1	A	489	LEU	5.2
1	A	561	HIS	5.2
1	A	676	SER	5.2
1	A	877	GLU	5.2
1	A	442	HIS	5.1
1	A	653	GLU	5.1
1	A	683	ASP	5.1
1	A	880	THR	5.1
1	A	569	PHE	5.1
1	A	740	ILE	5.1
1	A	337	MET	5.0
1	A	368	GLU	4.9
1	A	674	PHE	4.9
1	A	628	VAL	4.8
1	A	568	ILE	4.8
1	A	819	GLN	4.8
1	A	370	THR	4.7
1	A	491	PHE	4.7
1	A	495	ASP	4.7
1	A	698	ARG	4.7
1	A	818	ILE	4.7
1	A	485	GLU	4.7
1	A	620	ILE	4.6
1	A	340	GLN	4.6
1	A	632	ILE	4.5
1	A	552	MET	4.5
1	A	878	GLU	4.5
1	A	493	ASN	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	379	GLU	4.4
1	A	549	ASN	4.4
1	A	387	LYS	4.4
1	A	664	ASP	4.3
1	A	391	PRO	4.3
1	A	723	VAL	4.3
1	A	750	GLU	4.2
1	A	373	LEU	4.2
1	A	625	GLY	4.2
1	A	555	ASN	4.0
1	A	546	ASP	4.0
1	A	807	GLU	4.0
1	A	883	MET	4.0
1	A	815	ARG	4.0
1	A	494	GLU	4.0
1	A	700	TRP	3.9
1	A	820	GLU	3.9
1	A	497	TRP	3.9
1	A	670	LEU	3.9
1	A	720	ASP	3.9
1	A	528	GLY	3.9
1	A	678	LEU	3.9
1	A	565	ALA	3.8
1	A	334	ILE	3.8
1	A	808	ASP	3.7
1	A	806	THR	3.7
1	A	631	SER	3.7
1	A	679	THR	3.7
1	A	560	GLU	3.7
1	A	831	GLU	3.7
1	A	810	LEU	3.6
1	A	828	THR	3.6
1	A	627	GLY	3.6
1	A	821	ASN	3.6
1	A	554	THR	3.6
1	A	764	LEU	3.6
1	A	826	ASP	3.5
1	A	703	TRP	3.5
1	A	829	PRO	3.5
1	A	816	VAL	3.5
1	A	488	ALA	3.5
1	A	716	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	567	ALA	3.5
1	A	737	ARG	3.4
1	A	377	THR	3.4
1	A	527	GLY	3.4
1	A	619	LEU	3.4
1	A	342	ALA	3.4
1	A	788	VAL	3.3
1	A	673	ARG	3.3
1	A	870	VAL	3.3
1	A	336	PRO	3.3
1	A	650	VAL	3.3
1	A	846	TRP	3.2
1	A	531	TYR	3.2
1	A	487	GLU	3.2
1	A	389	LYS	3.2
1	A	861	LYS	3.2
1	A	707	PRO	3.1
1	A	523	SER	3.1
1	A	832	SER	3.1
1	A	380	TRP	3.1
1	A	665	CYS	3.1
1	A	836	ILE	3.0
1	A	557	MET	3.0
1	A	681	LEU	3.0
1	A	706	VAL	2.9
1	A	372	LYS	2.9
1	A	840	GLY	2.9
1	A	343	MET	2.9
1	A	335	ILE	2.9
1	A	606	THR	2.9
1	A	613	THR	2.8
1	A	824	MET	2.8
1	A	838	TYR	2.8
1	A	822	PRO	2.8
1	A	710	SER	2.8
1	A	624	GLU	2.7
1	A	392	ARG	2.7
1	A	867	ILE	2.7
1	A	725	VAL	2.7
1	A	623	MET	2.7
1	A	616	GLU	2.7
1	A	374	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	754	LEU	2.6
1	A	705	GLN	2.6
1	A	684	MET	2.6
1	A	784	PRO	2.6
1	A	715	GLU	2.6
1	A	760	GLN	2.6
1	A	388	LYS	2.6
1	A	721	GLY	2.6
1	A	492	LEU	2.5
1	A	809	MET	2.5
1	A	612	PHE	2.5
1	A	757	SER	2.5
1	A	382	TRP	2.5
1	A	385	LEU	2.5
1	A	672	ASP	2.4
1	A	875	GLY	2.4
1	A	609	LEU	2.4
1	A	758	TYR	2.4
1	A	777	ASN	2.4
1	A	522	VAL	2.3
1	A	671	ASP	2.3
1	A	394	CYS	2.3
1	A	611	THR	2.3
1	A	837	PRO	2.3
1	A	553	VAL	2.3
1	A	734	LEU	2.3
1	A	730	ASN	2.2
1	A	736	GLY	2.2
1	A	805	THR	2.2
1	A	519	LEU	2.1
1	A	782	ALA	2.1
1	A	339	THR	2.1
1	A	517	TYR	2.1
1	A	751	THR	2.1
1	A	847	CYS	2.1
1	A	865	THR	2.1
1	A	675	ALA	2.1
1	A	863	ILE	2.1
1	A	787	TRP	2.1
1	A	651	GLY	2.1
1	A	685	GLY	2.1
1	A	812	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	724	LEU	2.1
1	A	772	LEU	2.1
1	A	874	ILE	2.1
1	A	521	ASP	2.1
1	A	848	GLY	2.1
1	A	713	PHE	2.0
1	A	729	ARG	2.0
1	A	622	GLN	2.0
1	A	783	VAL	2.0
1	A	341	MET	2.0
1	A	868	ASN	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](#)

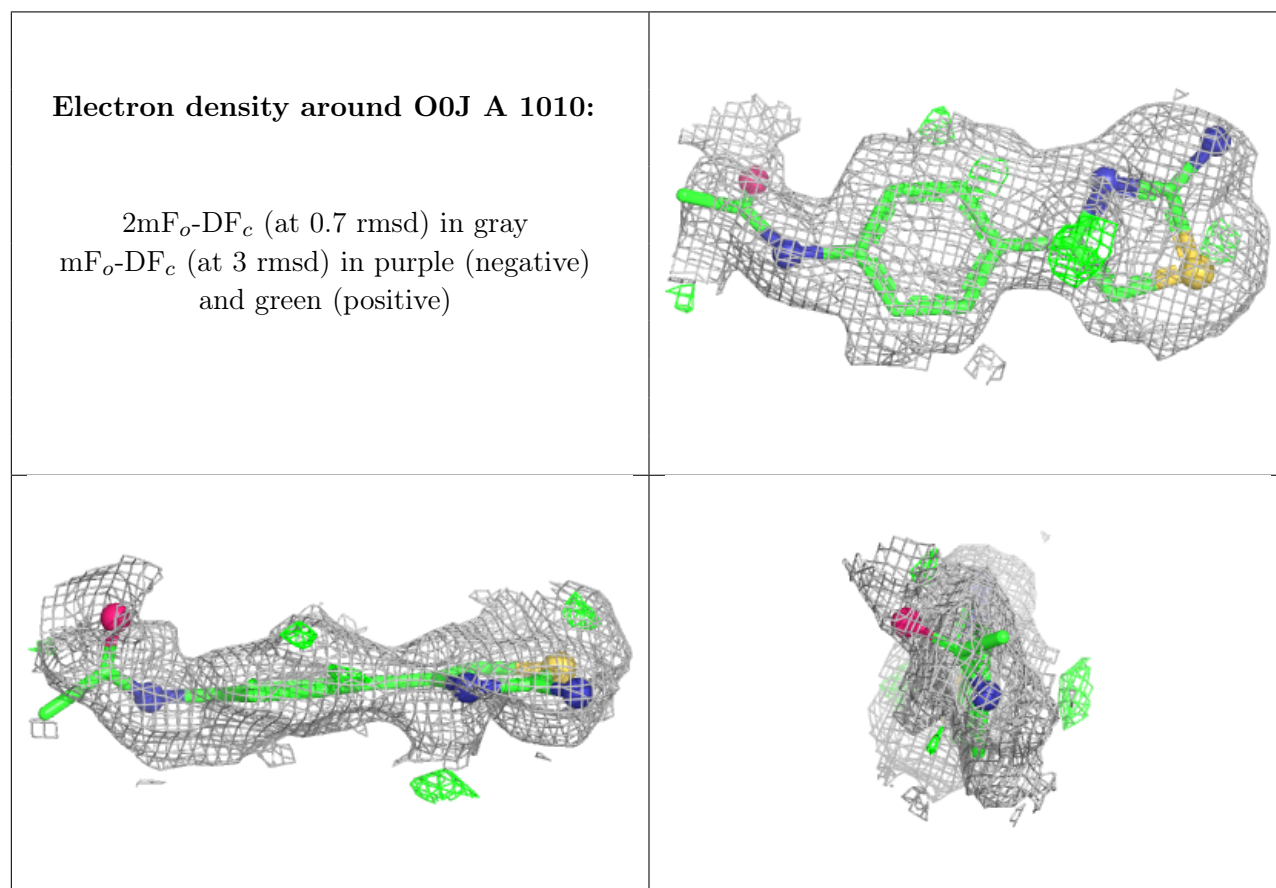
There are no oligosaccharides in this entry.

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
4	DMS	A	1005	4/4	0.53	0.64	52,57,58,58	4
6	PO4	A	1008	5/5	0.57	0.20	72,81,89,108	0
5	PEG	A	1006	7/7	0.58	0.36	46,48,50,50	7
7	O0J	A	1010	16/16	0.70	0.32	39,45,47,47	16
6	PO4	A	1007	5/5	0.72	0.23	28,29,33,36	5
5	PEG	A	1009	7/7	0.76	0.23	60,67,71,72	0
4	DMS	A	1004	4/4	0.88	0.18	41,46,47,52	0
2	ZN	A	1002	1/1	0.91	0.13	36,36,36,36	1
3	MES	A	1003[B]	12/12	0.96	0.31	504,516,534,537	12
3	MES	A	1003[A]	12/12	0.96	0.31	24,25,28,29	12
8	CL	A	1011	1/1	0.96	0.08	38,38,38,38	0
2	ZN	A	1001	1/1	1.00	0.04	21,21,21,21	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.