



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:26 PM UTC

PDB ID : 7I2R / pdb_00007i2r
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 Z31432226 (DNV2_NS5A-x0759)
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Deposited on : 2025-03-06
Resolution : 1.80 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)

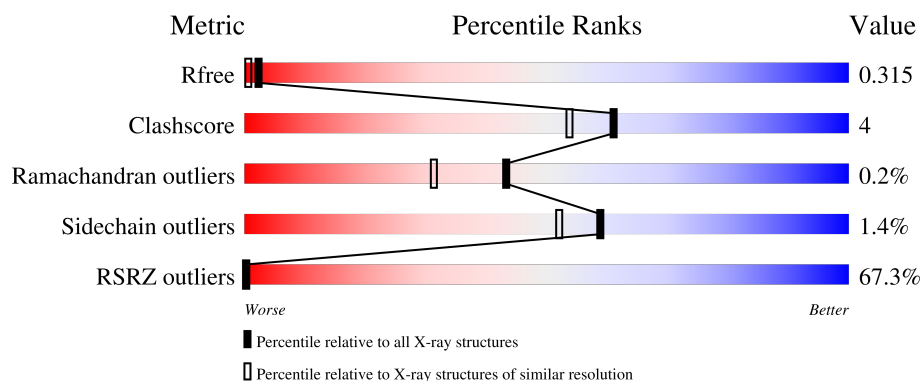
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	59% 78% 9% 12%

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	1006	-	-	X	-
5	PO4	A	1007	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5014 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	560	Total	C	N	O	S	0	6	0
			4641	2924	829	854	34			

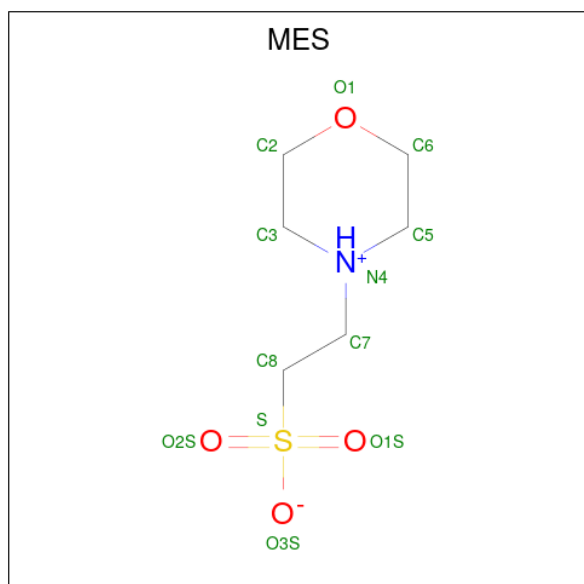
There are 2 discrepancies between the modelled and reference sequences:

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).

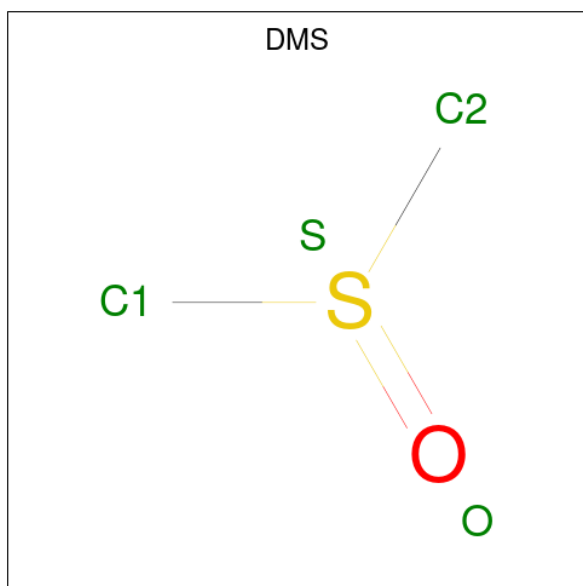
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

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



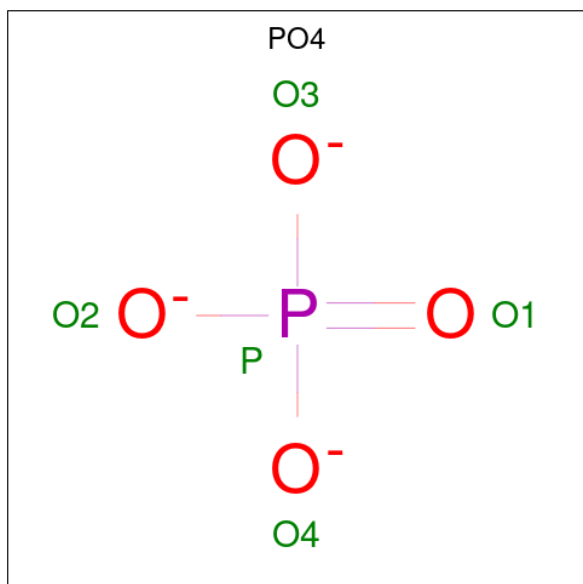
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			24	12	2	8	2		

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



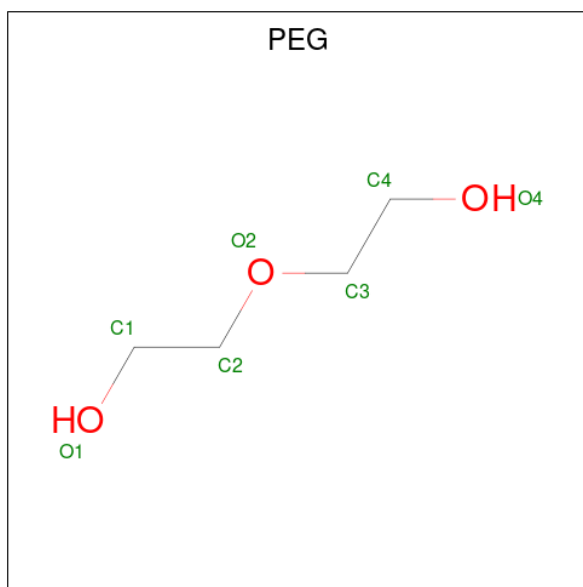
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is 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: C₄H₁₀O₃).

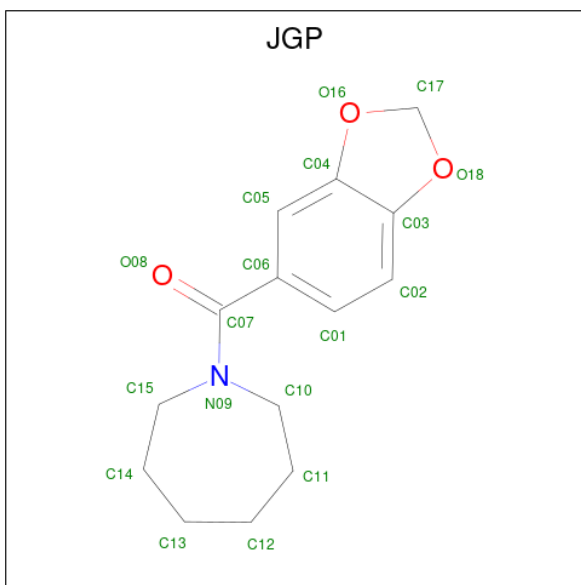


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 8 is (azepan-1-yl)(2H-1,3-benzodioxol-5-yl)methanone (CCD ID: JGP) (formula: C₁₄H₁₇NO₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			18	14	1	3		

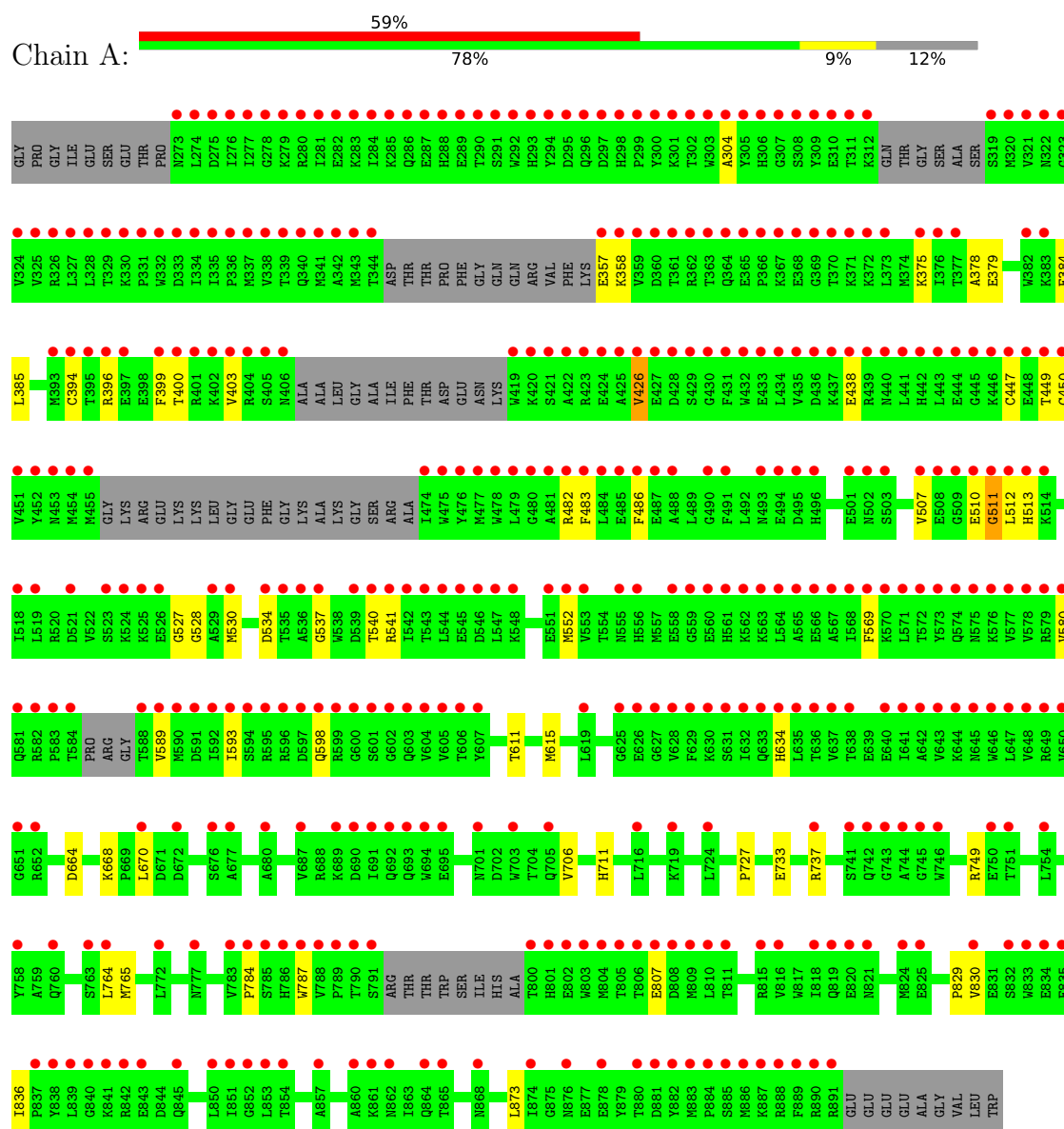
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	303	Total	O	0	0
			303	303		

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	81.93Å 115.96Å 148.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.75 – 1.80 45.75 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.6 (45.75-1.80) 97.6 (45.75-1.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.209 , 0.246 0.285 , 0.315	Depositor DCC
R_{free} test set	3391 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 194.8	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	0.85	EDS
Total number of atoms	5014	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.89% 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: PO4, CL, JGP, PEG, MES, ZN, DMS

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	1.02	1/4745 (0.0%)	1.30	4/6398 (0.1%)

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	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	378	ALA	C-O	5.65	1.30	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	511	GLY	CA-C-O	-6.54	116.78	121.88
1	A	569	PHE	CA-C-O	-5.11	115.64	121.00
1	A	836	ILE	CA-C-O	5.07	122.14	119.15
1	A	385	LEU	N-CA-C	-5.06	105.95	111.82

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	511	GLY	Mainchain
1	A	784	PRO	Mainchain

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	4641	0	4539	36	0
2	A	2	0	0	0	0
3	A	24	0	26	2	0
4	A	8	0	12	3	0
5	A	10	0	0	3	0
6	A	7	0	10	0	0
7	A	1	0	0	0	0
8	A	18	0	0	0	0
9	A	303	0	0	6	2
All	All	5014	0	4587	39	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 (39) 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:1305:HOH:O	1.92	0.69
1:A:664:ASP:OD1	5:A:1006:PO4:O4	2.10	0.68
1:A:438:GLU:HG3	1:A:449:THR:OG1	1.94	0.68
1:A:764:LEU:HG	1:A:765:MET:HE3	1.75	0.68
1:A:513:HIS:HB3	1:A:765:MET:HE1	1.75	0.68
1:A:580:VAL:HG21	1:A:593:ILE:HD11	1.78	0.65
1:A:873:LEU:HD13	3:A:1003[A]:MES:H62	1.82	0.60
1:A:530:MET:HE2	1:A:706:VAL:HG21	1.84	0.59
1:A:664:ASP:OD1	5:A:1006:PO4:P	2.62	0.58
1:A:733:GLU:O	1:A:737:ARG:HG3	2.08	0.54
1:A:396:ARG:HG2	1:A:483:PHE:CZ	2.44	0.53
1:A:358:LYS:HG3	1:A:540:THR:HG21	1.93	0.51
1:A:534:ASP:OD1	5:A:1006:PO4:O4	2.29	0.50
1:A:537:GLY:O	1:A:541:ARG:HG2	2.11	0.50
4:A:1004:DMS:C1	9:A:1305:HOH:O	2.55	0.48
1:A:304:ALA:O	1:A:593:ILE:HA	2.14	0.47
1:A:438:GLU:CG	1:A:449:THR:OG1	2.62	0.47
1:A:400:THR:HA	1:A:426:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.55	0.46
1:A:512[A]:LEU:HG	1:A:727:PRO:HB3	1.98	0.46
1:A:580:VAL:CG2	1:A:593:ILE:HD11	2.43	0.45
1:A:873:LEU:HD13	3:A:1003[B]:MES:H51	1.98	0.45
1:A:829:PRO:O	9:A:1103:HOH:O	2.21	0.45
1:A:394:CYS:HB3	1:A:486:PHE:CE2	2.52	0.44
1:A:512[A]:LEU:HG	1:A:727:PRO:CB	2.47	0.44
1:A:765:MET:HA	1:A:765:MET:HE2	1.99	0.44
1:A:528:GLY:O	1:A:668:LYS:HE3	2.18	0.44
1:A:399:PHE:O	1:A:403:VAL:HG13	2.17	0.44
1:A:749:ARG:HG3	1:A:787:TRP:CZ3	2.53	0.43
1:A:384:GLU:HG2	9:A:1107:HOH:O	2.18	0.43
1:A:807:GLU:OE2	9:A:1102:HOH:O	2.21	0.43
1:A:512[A]:LEU:HD21	1:A:711:HIS:NE2	2.35	0.42
1:A:379:GLU:HB2	1:A:552:MET:HE1	2.02	0.41
1:A:507:VAL:O	1:A:510:GLU:HG2	2.20	0.41
1:A:400:THR:O	1:A:403:VAL:HG22	2.19	0.41
4:A:1004:DMS:H12	9:A:1219:HOH:O	2.20	0.41
1:A:611:THR:O	1:A:615:MET:HG3	2.20	0.41
1:A:527:GLY:HA2	1:A:670:LEU:O	2.21	0.41
1:A:580:VAL:HG21	1:A:593:ILE:CD1	2.49	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)
9:A:1248:HOH:O	9:A:1342:HOH:O[2_545]	1.84	0.36
9:A:1131:HOH:O	9:A:1131:HOH:O[2_445]	1.98	0.22

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	552/637 (87%)	534 (97%)	17 (3%)	1 (0%)	43 31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	598	GLN

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	501/554 (90%)	494 (99%)	7 (1%)	59 52

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	357	GLU
1	A	375	LYS
1	A	426	VAL
1	A	482	ARG
1	A	589	VAL
1	A	634	HIS
1	A	830	VAL

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	298	HIS
1	A	575	ASN
1	A	603	GLN
1	A	760	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 11 ligands modelled in this entry, 3 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$
8	JGP	A	1010	-	20,20,20	0.30	0	27,27,27	0.51	0
4	DMS	A	1004	-	3,3,3	0.38	0	3,3,3	0.58	0
4	DMS	A	1005	-	3,3,3	0.22	0	3,3,3	0.07	0
3	MES	A	1003[B]	-	12,12,12	0.70	0	15,16,16	0.29	0
5	PO4	A	1006	-	4,4,4	4.05	3 (75%)	6,6,6	0.92	0
3	MES	A	1003[A]	-	12,12,12	0.70	0	15,16,16	0.30	0
6	PEG	A	1008	-	6,6,6	0.14	0	5,5,5	0.08	0
5	PO4	A	1007	-	4,4,4	0.71	0	6,6,6	0.46	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
8	JGP	A	1010	-	-	0/8/23/23	0/3/3/3
3	MES	A	1003[A]	-	-	0/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PEG	A	1008	-	-	2/4/4/4	-
3	MES	A	1003[B]	-	-	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	1006	PO4	P-O1	7.07	1.67	1.50
5	A	1006	PO4	P-O2	2.71	1.62	1.54
5	A	1006	PO4	P-O4	-2.42	1.47	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

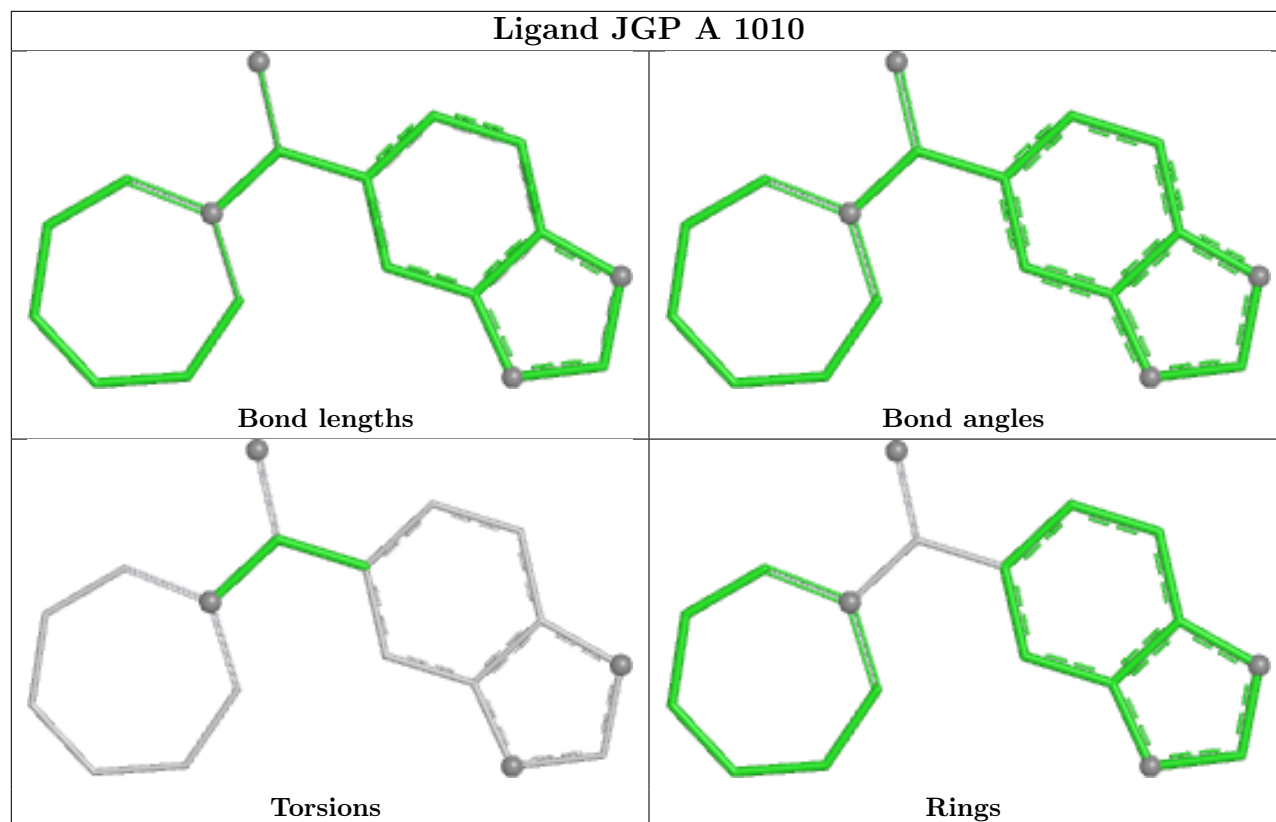
Mol	Chain	Res	Type	Atoms
6	A	1008	PEG	O2-C3-C4-O4
6	A	1008	PEG	C4-C3-O2-C2

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1004	DMS	3	0
3	A	1003[B]	MES	1	0
5	A	1006	PO4	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	560/637 (87%)	4.58	377 (67%) 0 0	5, 35, 63, 111	263 (46%)

All (377) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	292	TRP	13.4
1	A	403	VAL	13.2
1	A	512[A]	LEU	13.1
1	A	290	THR	13.1
1	A	600	GLY	13.0
1	A	478	TRP	12.3
1	A	300	TYR	12.2
1	A	589	VAL	12.2
1	A	476	TYR	12.2
1	A	542	ILE	12.0
1	A	299	PRO	12.0
1	A	293	HIS	11.8
1	A	763[A]	SER	11.8
1	A	294	TYR	11.5
1	A	431	PHE	11.4
1	A	309	TYR	11.3
1	A	641	ILE	11.1
1	A	441	LEU	11.1
1	A	291	SER	11.0
1	A	764	LEU	10.7
1	A	785[A]	SER	10.5
1	A	628	VAL	10.3
1	A	744	ALA	10.3
1	A	426	VAL	10.2
1	A	637	VAL	10.2
1	A	274	LEU	10.2
1	A	281	ILE	10.1

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Mol	Chain	Res	Type	RSRZ
1	A	425	ALA	10.0
1	A	363	THR	10.0
1	A	838	TYR	10.0
1	A	305	TYR	9.8
1	A	791	SER	9.7
1	A	480	GLY	9.7
1	A	578	VAL	9.6
1	A	359	VAL	9.5
1	A	479	LEU	9.5
1	A	583	PRO	9.4
1	A	277	ILE	9.4
1	A	435	VAL	9.3
1	A	298	HIS	9.3
1	A	367	LYS	9.3
1	A	788	VAL	9.3
1	A	276	ILE	9.3
1	A	839	LEU	9.2
1	A	366	PRO	9.2
1	A	575	ASN	9.2
1	A	443	LEU	9.2
1	A	629	PHE	9.1
1	A	519	LEU	9.1
1	A	636	THR	9.0
1	A	789	PRO	9.0
1	A	854	THR	9.0
1	A	518	ILE	9.0
1	A	475	TRP	9.0
1	A	325	VAL	9.0
1	A	474	ILE	9.0
1	A	311	THR	8.9
1	A	453	ASN	8.9
1	A	635	LEU	8.8
1	A	719[A]	LYS	8.8
1	A	810	LEU	8.7
1	A	423	ARG	8.7
1	A	742	GLN	8.7
1	A	419	TRP	8.6
1	A	530	MET	8.6
1	A	486	PHE	8.6
1	A	606	THR	8.6
1	A	803	TRP	8.5
1	A	790	THR	8.5

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Mol	Chain	Res	Type	RSRZ
1	A	551	GLU	8.5
1	A	432	TRP	8.5
1	A	565	ALA	8.5
1	A	541	ARG	8.5
1	A	627	GLY	8.5
1	A	604	VAL	8.4
1	A	809	MET	8.4
1	A	741[A]	SER	8.4
1	A	490	GLY	8.4
1	A	571	LEU	8.3
1	A	850	LEU	8.3
1	A	544	LEU	8.2
1	A	477	MET	8.2
1	A	580	VAL	8.2
1	A	584	THR	8.2
1	A	364	GLN	8.2
1	A	687	VAL	8.2
1	A	607	TYR	8.2
1	A	511	GLY	8.2
1	A	321	VAL	8.1
1	A	885	SER	8.1
1	A	334	ILE	8.1
1	A	601	SER	8.1
1	A	279	LYS	8.1
1	A	800	THR	8.1
1	A	484	LEU	8.0
1	A	332	TRP	8.0
1	A	552	MET	8.0
1	A	581	GLN	8.0
1	A	301	LYS	7.9
1	A	455	MET	7.9
1	A	327	LEU	7.9
1	A	889	PHE	7.9
1	A	808	ASP	7.9
1	A	488	ALA	7.8
1	A	596	ARG	7.8
1	A	328	LEU	7.8
1	A	864[A]	GLN	7.8
1	A	296	GLN	7.7
1	A	745	GLY	7.7
1	A	342	ALA	7.7
1	A	588	THR	7.7

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Mol	Chain	Res	Type	RSRZ
1	A	297	ASP	7.7
1	A	543	THR	7.7
1	A	853	LEU	7.7
1	A	452	TYR	7.7
1	A	884	PRO	7.6
1	A	852	GLY	7.6
1	A	582	ARG	7.6
1	A	525	LYS	7.6
1	A	401	ARG	7.6
1	A	599	ARG	7.6
1	A	481	ALA	7.6
1	A	851	ILE	7.5
1	A	323	GLY	7.5
1	A	579	ARG	7.5
1	A	338	VAL	7.5
1	A	434	LEU	7.4
1	A	406	ASN	7.4
1	A	405	SER	7.4
1	A	422	ALA	7.3
1	A	567	ALA	7.3
1	A	312	LYS	7.3
1	A	597	ASP	7.3
1	A	372	LYS	7.3
1	A	564	LEU	7.3
1	A	572	THR	7.3
1	A	746	TRP	7.2
1	A	306	HIS	7.2
1	A	358	LYS	7.2
1	A	598	GLN	7.2
1	A	645	ASN	7.2
1	A	638	THR	7.1
1	A	802	GLU	7.1
1	A	335	ILE	7.1
1	A	285	LYS	7.1
1	A	449	THR	7.0
1	A	649	ARG	7.0
1	A	811	THR	7.0
1	A	439	ARG	7.0
1	A	324	VAL	7.0
1	A	886	MET	7.0
1	A	303	TRP	6.9
1	A	524	LYS	6.9

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Mol	Chain	Res	Type	RSRZ
1	A	743	GLY	6.9
1	A	319	SER	6.8
1	A	805	THR	6.8
1	A	806	THR	6.8
1	A	343	MET	6.8
1	A	368	GLU	6.8
1	A	632	ILE	6.8
1	A	360	ASP	6.8
1	A	626	GLU	6.8
1	A	308	SER	6.8
1	A	329	THR	6.7
1	A	344	THR	6.7
1	A	331	PRO	6.6
1	A	424	GLU	6.6
1	A	801	HIS	6.6
1	A	446	LYS	6.6
1	A	737	ARG	6.5
1	A	320	MET	6.5
1	A	322	ASN	6.5
1	A	521	ASP	6.5
1	A	887	LYS	6.5
1	A	830	VAL	6.5
1	A	361	THR	6.4
1	A	602	GLY	6.4
1	A	556	HIS	6.4
1	A	562	LYS	6.4
1	A	555	ASN	6.4
1	A	483	PHE	6.4
1	A	845	GLN	6.4
1	A	339	THR	6.4
1	A	280	ARG	6.3
1	A	454	MET	6.3
1	A	396	ARG	6.3
1	A	548	LYS	6.3
1	A	284	ILE	6.3
1	A	428	ASP	6.3
1	A	275	ASP	6.2
1	A	393	MET	6.2
1	A	437	LYS	6.2
1	A	513	HIS	6.2
1	A	450	CYS	6.2
1	A	451	VAL	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	526	GLU	6.2
1	A	545	GLU	6.2
1	A	427	GLU	6.2
1	A	421	SER	6.2
1	A	840	GLY	6.2
1	A	333	ASP	6.1
1	A	295	ASP	6.1
1	A	336	PRO	6.1
1	A	304	ALA	6.0
1	A	440	ASN	6.0
1	A	694	TRP	6.0
1	A	634	HIS	6.0
1	A	509	GLY	6.0
1	A	326	ARG	6.0
1	A	890	ARG	6.0
1	A	307	GLY	6.0
1	A	330	LYS	6.0
1	A	341	MET	5.9
1	A	283	LYS	5.9
1	A	705	GLN	5.9
1	A	841	LYS	5.8
1	A	289	GLU	5.8
1	A	442	HIS	5.8
1	A	482	ARG	5.8
1	A	537	GLY	5.8
1	A	561	HIS	5.8
1	A	842	ARG	5.8
1	A	430	GLY	5.8
1	A	445	GLY	5.8
1	A	883	MET	5.8
1	A	760	GLN	5.7
1	A	404	ARG	5.7
1	A	357	GLU	5.7
1	A	286	GLN	5.7
1	A	595	ARG	5.7
1	A	508	GLU	5.7
1	A	485	GLU	5.6
1	A	577	VAL	5.6
1	A	523	SER	5.6
1	A	448	GLU	5.6
1	A	540	THR	5.6
1	A	880	THR	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	630	LYS	5.5
1	A	337	MET	5.5
1	A	282	GLU	5.5
1	A	288	HIS	5.5
1	A	310	GLU	5.5
1	A	278	GLY	5.4
1	A	689	LYS	5.4
1	A	891	ARG	5.4
1	A	514	LYS	5.4
1	A	546	ASP	5.4
1	A	568	ILE	5.4
1	A	365	GLU	5.3
1	A	383	LYS	5.3
1	A	494	GLU	5.3
1	A	302	THR	5.3
1	A	397	GLU	5.3
1	A	438	GLU	5.2
1	A	843	GLU	5.2
1	A	340	GLN	5.2
1	A	559	GLY	5.2
1	A	882	TYR	5.2
1	A	825	GLU	5.2
1	A	429	SER	5.2
1	A	576	LYS	5.1
1	A	362	ARG	5.1
1	A	563	LYS	5.0
1	A	804	MET	5.0
1	A	888	ARG	5.0
1	A	273	ASN	5.0
1	A	881	ASP	4.9
1	A	287	GLU	4.8
1	A	433	GLU	4.8
1	A	487	GLU	4.8
1	A	590	MET	4.8
1	A	591	ASP	4.7
1	A	593	ILE	4.7
1	A	566	GLU	4.7
1	A	693	GLN	4.7
1	A	510	GLU	4.6
1	A	648	VAL	4.6
1	A	501	GLU	4.5
1	A	647	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	436	ASP	4.5
1	A	876	ASN	4.5
1	A	820	GLU	4.5
1	A	400	THR	4.5
1	A	369	GLY	4.4
1	A	691	ILE	4.4
1	A	807	GLU	4.4
1	A	784	PRO	4.4
1	A	818	ILE	4.3
1	A	605	VAL	4.3
1	A	633	GLN	4.3
1	A	394	CYS	4.2
1	A	750	GLU	4.2
1	A	558	GLU	4.2
1	A	644	LYS	4.0
1	A	676	SER	4.0
1	A	815	ARG	3.9
1	A	399	PHE	3.9
1	A	819	GLN	3.8
1	A	677	ALA	3.8
1	A	640	GLU	3.8
1	A	547	LEU	3.8
1	A	373	LEU	3.7
1	A	670	LEU	3.7
1	A	603	GLN	3.7
1	A	695	GLU	3.7
1	A	529	ALA	3.6
1	A	493	ASN	3.5
1	A	534	ASP	3.5
1	A	376	ILE	3.4
1	A	420	LYS	3.4
1	A	370	THR	3.4
1	A	402	LYS	3.4
1	A	503	SER	3.3
1	A	701	ASN	3.3
1	A	444	GLU	3.3
1	A	377	THR	3.3
1	A	821	ASN	3.3
1	A	861	LYS	3.2
1	A	652	ARG	3.2
1	A	835	GLU	3.2
1	A	536	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	592	ILE	3.1
1	A	716	LEU	3.0
1	A	833	TRP	3.0
1	A	447	CYS	3.0
1	A	824	MET	3.0
1	A	495	ASP	2.9
1	A	680	ALA	2.9
1	A	786	HIS	2.9
1	A	560	GLU	2.9
1	A	569	PHE	2.9
1	A	646	TRP	2.9
1	A	754	LEU	2.9
1	A	570	LYS	2.8
1	A	642	ALA	2.8
1	A	787	TRP	2.8
1	A	783	VAL	2.8
1	A	816	VAL	2.8
1	A	507	VAL	2.8
1	A	573	TYR	2.7
1	A	491	PHE	2.7
1	A	496	HIS	2.7
1	A	703	TRP	2.7
1	A	692	GLN	2.6
1	A	868	ASN	2.6
1	A	672	ASP	2.6
1	A	395	THR	2.6
1	A	375	LYS	2.5
1	A	631	SER	2.5
1	A	535	THR	2.5
1	A	539	ASP	2.5
1	A	651	GLY	2.4
1	A	619	LEU	2.4
1	A	502	ASN	2.4
1	A	862	ASN	2.4
1	A	574	GLN	2.4
1	A	758	TYR	2.4
1	A	857	ALA	2.3
1	A	553	VAL	2.3
1	A	643	VAL	2.3
1	A	751	THR	2.3
1	A	777	ASN	2.3
1	A	625	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	832	SER	2.2
1	A	834	GLU	2.2
1	A	594	SER	2.2
1	A	382	TRP	2.2
1	A	650	VAL	2.2
1	A	860	ALA	2.2
1	A	371	LYS	2.2
1	A	865	THR	2.1
1	A	690	ASP	2.1
1	A	878	GLU	2.0
1	A	837	PRO	2.0
1	A	724	LEU	2.0
1	A	772	LEU	2.0
1	A	874	ILE	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.

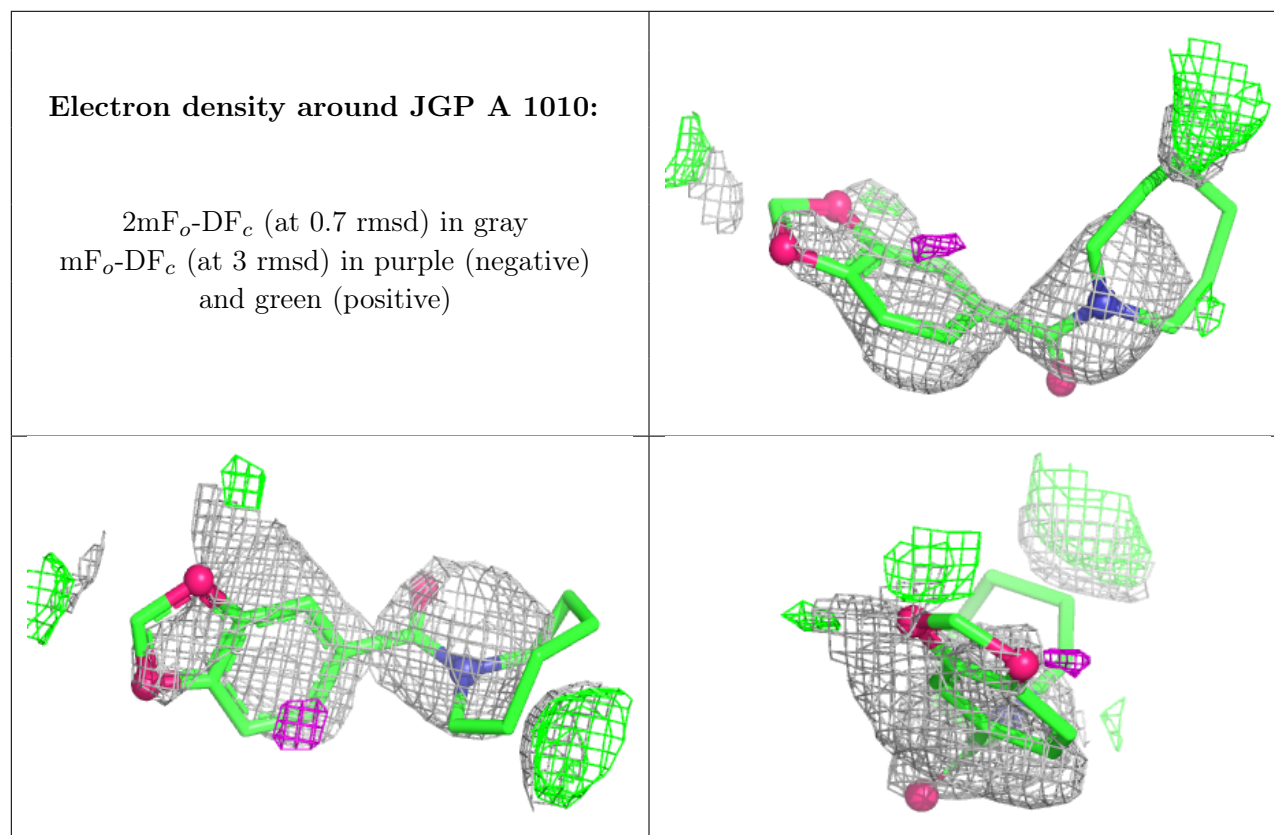
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	JGP	A	1010	18/18	0.61	0.37	57,64,67,69	18
5	PO4	A	1007	5/5	0.62	0.51	175,179,185,185	5
6	PEG	A	1008	7/7	0.73	0.30	54,59,61,61	7
5	PO4	A	1006	5/5	0.84	0.14	37,41,48,68	0
4	DMS	A	1005	4/4	0.85	0.44	93,95,98,99	4
3	MES	A	1003[B]	12/12	0.86	0.41	22,27,38,39	12
3	MES	A	1003[A]	12/12	0.86	0.41	744,999,999,999	12
4	DMS	A	1004	4/4	0.90	0.15	51,57,58,60	0
7	CL	A	1009	1/1	0.97	0.08	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	1002	1/1	0.99	0.06	58,58,58,58	0
2	ZN	A	1001	1/1	1.00	0.03	28,28,28,28	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.