



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:27 PM UTC

PDB ID : 7I2A / pdb_00007i2a
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 Z54226095 (DNV2_NS5A-x0176)
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Deposited on : 2025-03-06
Resolution : 1.51 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)

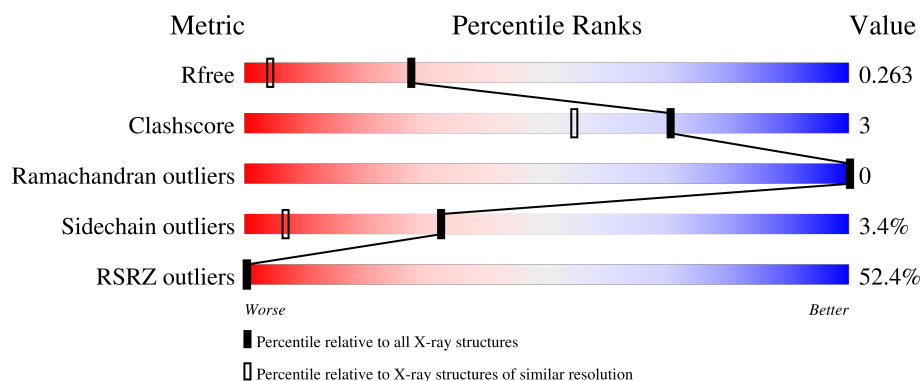
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.51 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	5890 (1.54-1.50)
Clashscore	190562	6116 (1.54-1.50)
Ramachandran outliers	187476	6002 (1.54-1.50)
Sidechain outliers	187428	5999 (1.54-1.50)
RSRZ outliers	180081	5891 (1.54-1.50)

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	-
7	WLJ	A	1010	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5244 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	574	Total	C	N	O	S	0	7	0
			4743	2989	848	872	34			

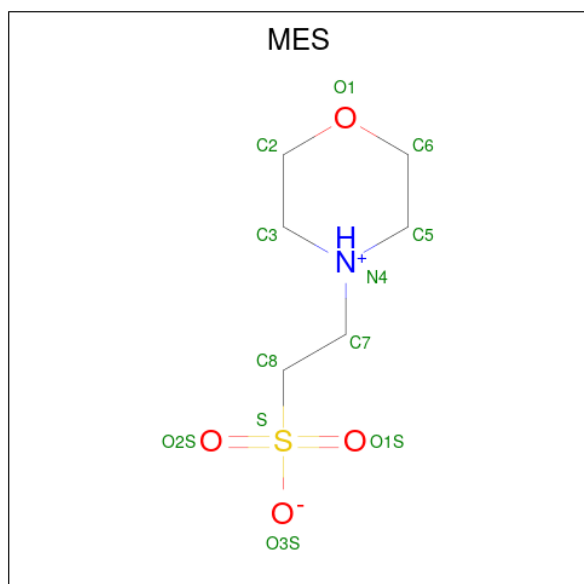
There are 2 discrepancies between the modelled and reference sequences:

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).

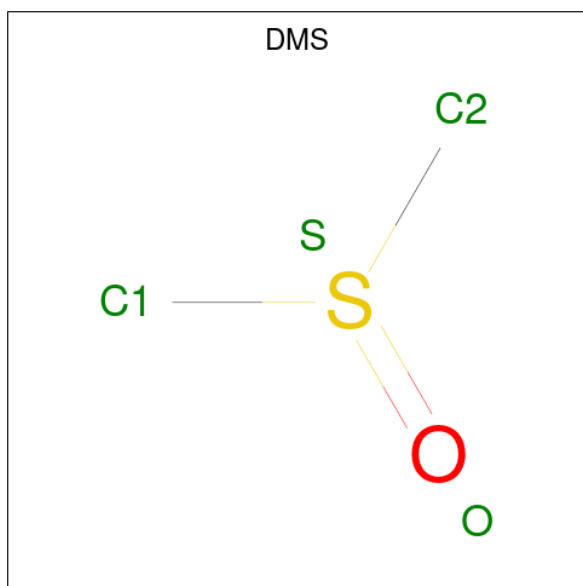
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

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



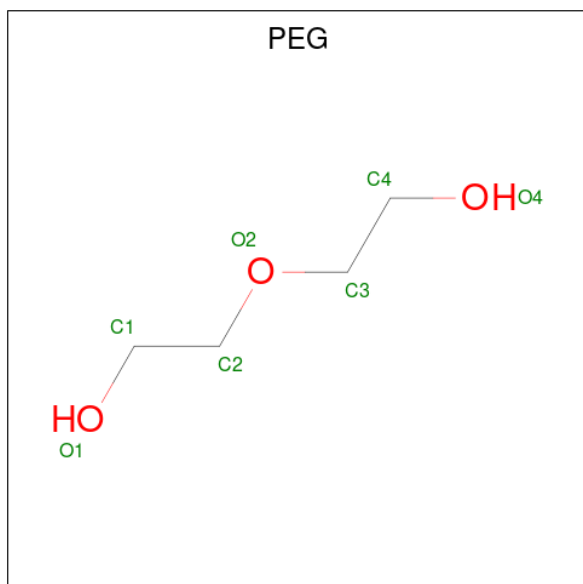
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			24	12	2	8	2		

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



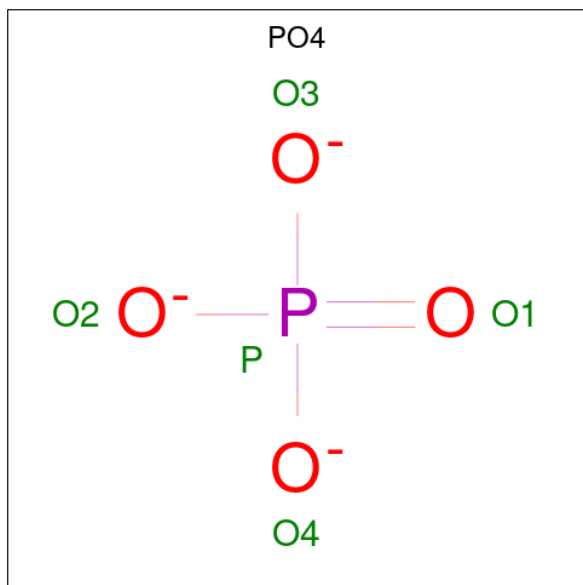
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

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



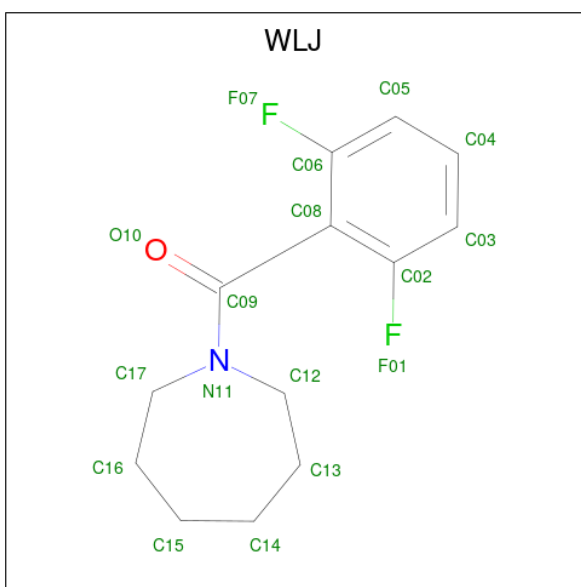
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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 (azepan-1-yl)(2,6-difluorophenyl)methanone (CCD ID: WLJ) (formula: C₁₃H₁₅F₂NO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	F	N	O	0	0
			17	13	2	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		

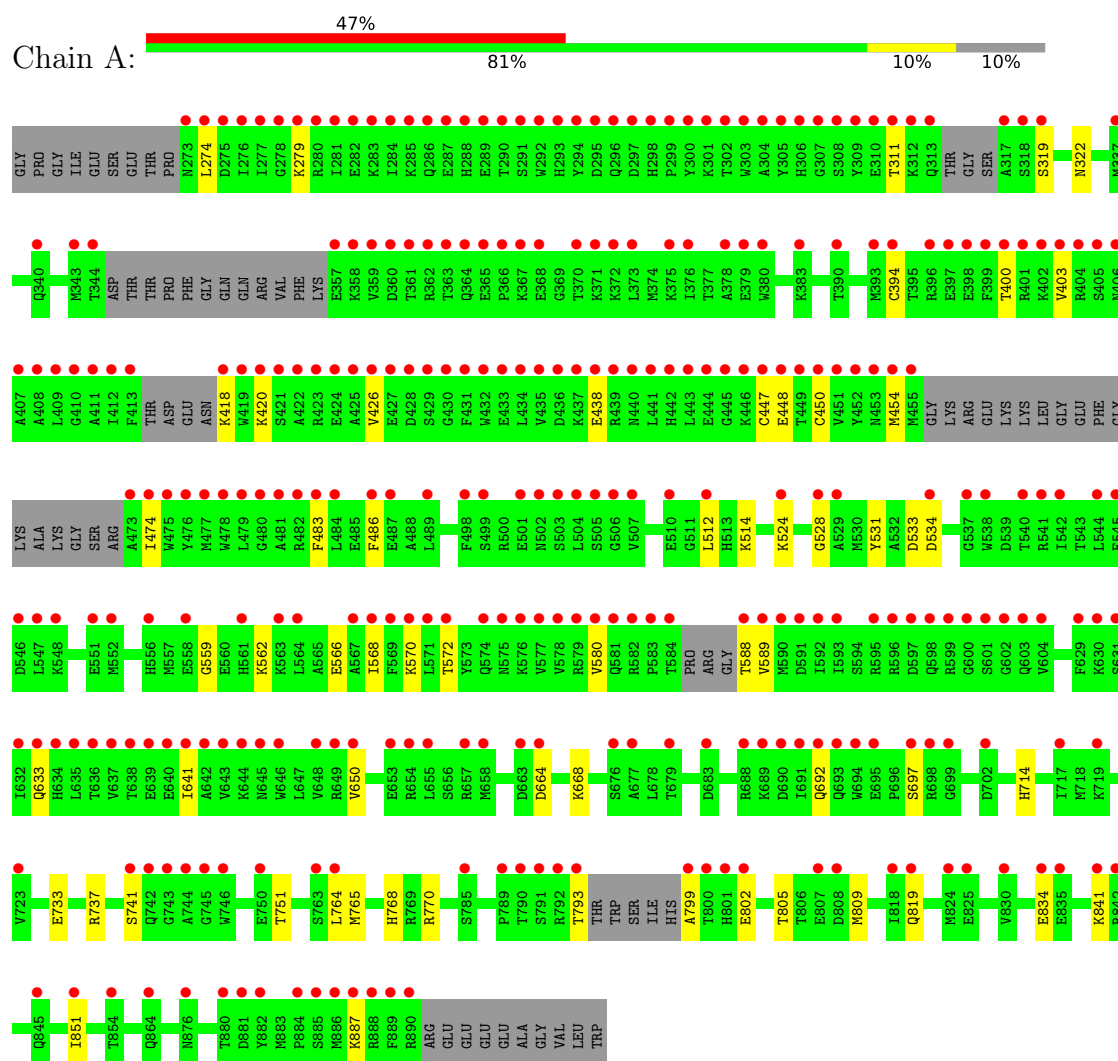
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	425	Total	O	0	0
			425	425		

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	82.48Å 116.71Å 148.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.06 – 1.51 74.06 – 1.51	Depositor EDS
% Data completeness (in resolution range)	96.2 (74.06-1.51) 96.3 (74.06-1.51)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.95 (at 1.51Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC5	Depositor
R, R_{free}	0.202 , 0.231 0.243 , 0.263	Depositor DCC
R_{free} test set	5682 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 106.0	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	0.90	EDS
Total number of atoms	5244	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% 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, PEG, ZN, CL, WLJ, PO4, 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	1.09	3/4849 (0.1%)	1.27	7/6539 (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	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	531	TYR	C-O	6.61	1.31	1.23
1	A	751	THR	C-O	5.67	1.30	1.24
1	A	768	HIS	CE1-NE2	5.38	1.38	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	714	HIS	CE1-NE2-CD2	-5.82	103.18	109.00
1	A	650	VAL	CA-C-O	-5.78	114.95	119.46
1	A	322	ASN	CA-C-N	5.16	125.71	119.98
1	A	322	ASN	C-N-CA	5.16	125.71	119.98
1	A	559	GLY	CA-C-N	5.08	127.40	120.54
1	A	559	GLY	C-N-CA	5.08	127.40	120.54
1	A	483	PHE	CA-CB-CG	-5.01	108.79	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	741[B]	SER	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	4743	0	4642	29	0
2	A	2	0	0	0	0
3	A	24	0	26	0	0
4	A	8	0	12	3	0
5	A	14	0	20	0	0
6	A	10	0	0	4	0
7	A	17	0	0	0	0
8	A	1	0	0	0	0
9	A	425	0	0	8	1
All	All	5244	0	4700	32	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 3.

All (32) 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:664:ASP:OD1	6:A:1007:PO4:O4	1.93	0.85
4:A:1004:DMS:H11	9:A:1289:HOH:O	1.84	0.78
1:A:664:ASP:OD1	6:A:1007:PO4:P	2.46	0.73
1:A:524:LYS:NZ	9:A:1104:HOH:O	2.27	0.67
1:A:279:LYS:HE3	1:A:448:GLU:HB2	1.77	0.65
1:A:534:ASP:OD1	6:A:1007:PO4:O4	2.17	0.61
1:A:764:LEU:HG	1:A:765:MET:CE	2.31	0.61
1:A:403:VAL:HG21	1:A:426:VAL:HG11	1.82	0.61
4:A:1004:DMS:H12	9:A:1292:HOH:O	2.01	0.60
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.43	0.58
1:A:454:MET:HB3	1:A:580:VAL:HG22	1.85	0.58
1:A:400:THR:O	1:A:403:VAL:HG22	2.05	0.56
1:A:568:ILE:O	1:A:572:THR:OG1	2.22	0.56
1:A:809:MET:HA	1:A:809:MET:HE2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:GLY:O	1:A:668:LYS:HE3	2.12	0.50
1:A:770:ARG:HD2	1:A:851:ILE:HD13	1.94	0.49
1:A:733:GLU:O	1:A:737:ARG:HG3	2.13	0.48
1:A:805:THR:CG2	1:A:809:MET:HE1	2.44	0.47
1:A:841:LYS:HE3	9:A:1474:HOH:O	2.15	0.47
1:A:514:LYS:NZ	9:A:1121:HOH:O	2.49	0.46
1:A:394:CYS:HB3	1:A:486:PHE:CE2	2.52	0.45
1:A:764:LEU:HG	1:A:765:MET:HE2	1.99	0.45
1:A:512[B]:LEU:HD23	1:A:512[B]:LEU:HA	1.90	0.44
1:A:805:THR:HG23	1:A:809:MET:HE1	1.99	0.44
1:A:819:GLN:NE2	9:A:1109:HOH:O	2.40	0.43
1:A:533:ASP:OD2	1:A:697:SER:OG	2.30	0.42
1:A:764:LEU:C	1:A:765:MET:HE2	2.45	0.42
1:A:534:ASP:OD1	6:A:1007:PO4:P	2.78	0.41
1:A:562:LYS:HE3	1:A:566:GLU:OE2	2.20	0.41
1:A:799:ALA:N	9:A:1129:HOH:O	2.54	0.40
1:A:764:LEU:HG	1:A:765:MET:HE3	2.03	0.40
4:A:1004:DMS:C1	9:A:1289:HOH:O	2.58	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)
9:A:1159:HOH:O	9:A:1159:HOH:O[2_445]	1.60	0.60

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	567/637 (89%)	548 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	509/554 (92%)	492 (97%)	17 (3%)	33 7

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	274	LEU
1	A	311	THR
1	A	319	SER
1	A	418	LYS
1	A	420	LYS
1	A	438	GLU
1	A	474	ILE
1	A	570	LYS
1	A	588	THR
1	A	589	VAL
1	A	633	GLN
1	A	641	ILE
1	A	692	GLN
1	A	793	THR
1	A	802	GLU
1	A	834	GLU
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	575	ASN
1	A	618	GLN
1	A	701	ASN

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	$\# Z > 2$
6	PO4	A	1007	-	4,4,4	5.89	3 (75%)	6,6,6	0.96	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	0.76	0	15,16,16	0.96	1 (6%)
6	PO4	A	1008	-	4,4,4	0.56	0	6,6,6	0.55	0
5	PEG	A	1009	-	6,6,6	0.15	0	5,5,5	0.07	0
4	DMS	A	1004	-	3,3,3	0.75	0	3,3,3	0.55	0
4	DMS	A	1005	-	3,3,3	0.21	0	3,3,3	0.09	0
5	PEG	A	1006	-	6,6,6	0.15	0	5,5,5	0.12	0
7	WLJ	A	1010	-	18,18,18	0.13	0	24,24,24	0.58	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MES	A	1003[B]	-	-	5/6/14/14	0/1/1/1
3	MES	A	1003[A]	-	-	3/6/14/14	0/1/1/1
5	PEG	A	1009	-	-	2/4/4/4	-
5	PEG	A	1006	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	WLJ	A	1010	-	-	0/8/17/17	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	9.26	1.72	1.50
6	A	1007	PO4	P-O2	6.07	1.72	1.54
6	A	1007	PO4	P-O3	3.80	1.65	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1010	WLJ	C06-C08-C09	2.30	125.02	121.54
3	A	1003[A]	MES	O1S-S-C8	-2.26	103.31	106.73

There are no chirality outliers.

All (13) torsion outliers are listed below:

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

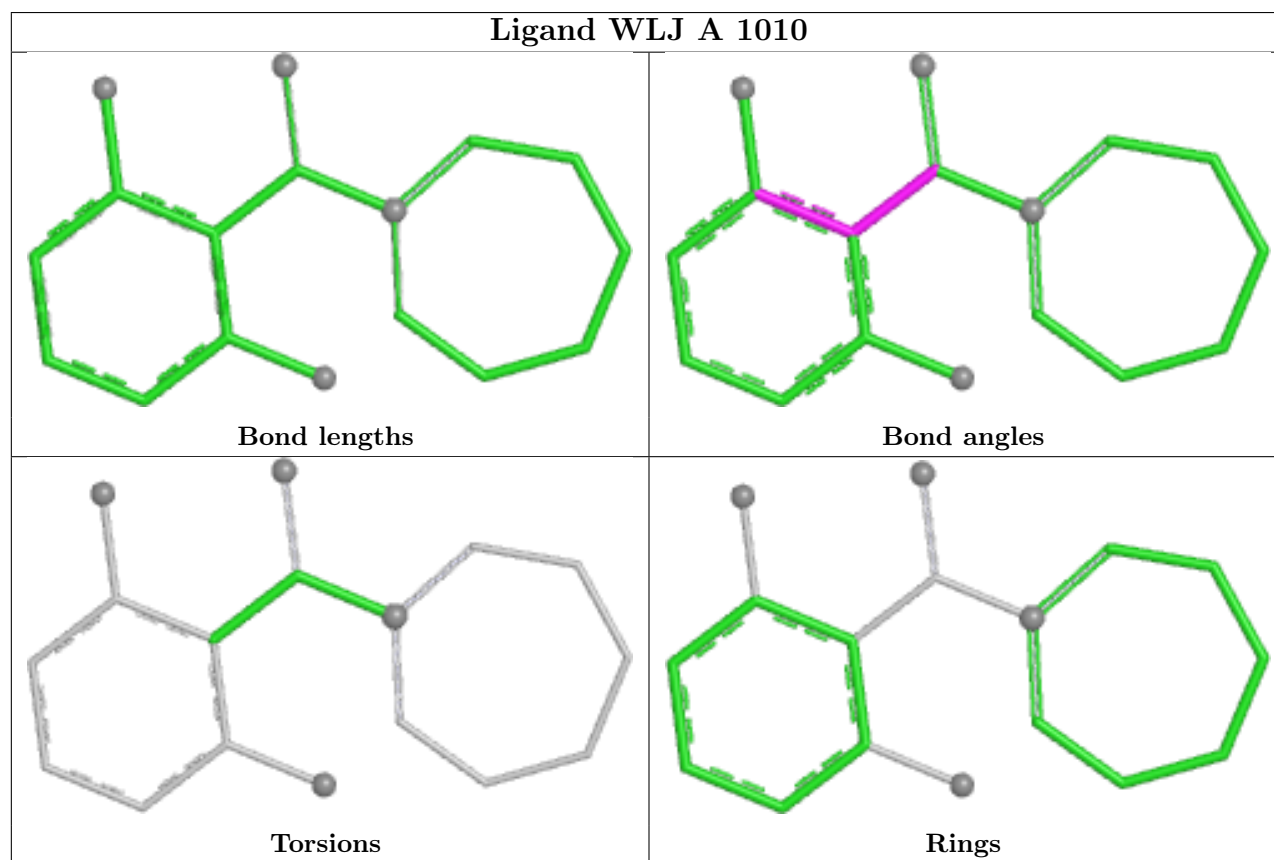
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1007	PO4	4	0
4	A	1004	DMS	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	574/637 (90%)	3.59	301 (52%) 0 0	3, 27, 60, 116	192 (33%)

All (301) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	589	VAL	15.6
1	A	851	ILE	14.9
1	A	884	PRO	13.7
1	A	885	SER	13.6
1	A	719[A]	LYS	13.2
1	A	763[A]	SER	12.9
1	A	512[A]	LEU	12.7
1	A	294	TYR	12.4
1	A	435	VAL	12.3
1	A	412	ILE	12.3
1	A	800	THR	12.2
1	A	407	ALA	12.1
1	A	635	LEU	12.0
1	A	886	MET	12.0
1	A	319	SER	11.5
1	A	604	VAL	11.3
1	A	284	ILE	11.2
1	A	637	VAL	11.1
1	A	411	ALA	10.9
1	A	380	TRP	10.8
1	A	318	SER	10.8
1	A	478	TRP	10.7
1	A	413	PHE	10.6
1	A	864[A]	GLN	10.6
1	A	304	ALA	10.5
1	A	281	ILE	10.5
1	A	547	LEU	10.4

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Mol	Chain	Res	Type	RSRZ
1	A	292	TRP	10.4
1	A	441	LEU	10.4
1	A	311	THR	10.4
1	A	431	PHE	10.3
1	A	303	TRP	10.3
1	A	432	TRP	10.3
1	A	578	VAL	10.1
1	A	582	ARG	10.0
1	A	451	VAL	10.0
1	A	842	ARG	9.9
1	A	475	TRP	9.9
1	A	600	GLY	9.8
1	A	835	GLU	9.7
1	A	409	LEU	9.7
1	A	434	LEU	9.7
1	A	274	LEU	9.6
1	A	655	LEU	9.6
1	A	887	LYS	9.6
1	A	641	ILE	9.6
1	A	452	TYR	9.5
1	A	845	GLN	9.5
1	A	305	TYR	9.5
1	A	636	THR	9.5
1	A	694	TRP	9.4
1	A	544	LEU	9.3
1	A	317	ALA	9.2
1	A	276	ILE	9.1
1	A	888	ARG	9.1
1	A	498	PHE	9.0
1	A	834	GLU	8.9
1	A	277	ILE	8.9
1	A	510	GLU	8.9
1	A	801[A]	HIS	8.9
1	A	359	VAL	8.8
1	A	448	GLU	8.8
1	A	293	HIS	8.8
1	A	506	GLY	8.7
1	A	479	LEU	8.7
1	A	841	LYS	8.7
1	A	799	ALA	8.6
1	A	741[A]	SER	8.5
1	A	742	GLN	8.5

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Mol	Chain	Res	Type	RSRZ
1	A	473	ALA	8.5
1	A	638	THR	8.4
1	A	697	SER	8.3
1	A	629	PHE	8.3
1	A	588	THR	8.3
1	A	542	ILE	8.2
1	A	476	TYR	8.2
1	A	298	HIS	8.1
1	A	419	TRP	8.1
1	A	474	ILE	8.1
1	A	400	THR	8.0
1	A	300	TYR	7.9
1	A	744	ALA	7.9
1	A	645	ASN	7.9
1	A	602	GLY	7.9
1	A	299	PRO	7.9
1	A	484	LEU	7.8
1	A	309	TYR	7.7
1	A	283	LYS	7.7
1	A	453	ASN	7.7
1	A	785[A]	SER	7.6
1	A	679	THR	7.6
1	A	363	THR	7.5
1	A	505	SER	7.4
1	A	789	PRO	7.4
1	A	601	SER	7.4
1	A	403	VAL	7.4
1	A	426	VAL	7.3
1	A	504	LEU	7.3
1	A	890	ARG	7.3
1	A	290	THR	7.3
1	A	572	THR	7.2
1	A	634	HIS	7.2
1	A	691	ILE	7.2
1	A	402	LYS	7.1
1	A	631	SER	7.1
1	A	575	ASN	7.0
1	A	405	SER	7.0
1	A	430	GLY	6.9
1	A	291	SER	6.9
1	A	499	SER	6.9
1	A	439	ARG	6.9

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Mol	Chain	Res	Type	RSRZ
1	A	425	ALA	6.9
1	A	401	ARG	6.8
1	A	408	ALA	6.8
1	A	275	ASP	6.8
1	A	551	GLU	6.7
1	A	422	ALA	6.7
1	A	524	LYS	6.6
1	A	576	LYS	6.6
1	A	410	GLY	6.6
1	A	437	LYS	6.5
1	A	584	THR	6.5
1	A	396	ARG	6.5
1	A	438	GLU	6.5
1	A	436	ASP	6.5
1	A	791	SER	6.5
1	A	282	GLU	6.5
1	A	429	SER	6.4
1	A	406	ASN	6.4
1	A	455	MET	6.4
1	A	280	ARG	6.4
1	A	595	ARG	6.4
1	A	583	PRO	6.4
1	A	454	MET	6.3
1	A	482	ARG	6.3
1	A	296	GLN	6.3
1	A	790	THR	6.3
1	A	692	GLN	6.2
1	A	654	ARG	6.2
1	A	597	ASP	6.2
1	A	793	THR	6.2
1	A	658	MET	6.2
1	A	657	ARG	6.2
1	A	372	LYS	6.2
1	A	288	HIS	6.2
1	A	640	GLU	6.1
1	A	302	THR	6.1
1	A	301	LYS	6.1
1	A	279	LYS	6.0
1	A	295	ASP	6.1
1	A	579	ARG	6.0
1	A	358	LYS	5.9
1	A	599	ARG	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	548	LYS	5.9
1	A	591	ASP	5.9
1	A	361	THR	5.8
1	A	397	GLU	5.8
1	A	603	GLN	5.8
1	A	273	ASN	5.8
1	A	503	SER	5.8
1	A	580	VAL	5.8
1	A	630	LYS	5.8
1	A	593	ILE	5.7
1	A	433	GLU	5.7
1	A	477	MET	5.7
1	A	442	HIS	5.7
1	A	644	LYS	5.7
1	A	423	ARG	5.7
1	A	598	GLN	5.7
1	A	889	PHE	5.7
1	A	688	ARG	5.6
1	A	364	GLN	5.6
1	A	689	LYS	5.6
1	A	421	SER	5.6
1	A	802	GLU	5.5
1	A	366	PRO	5.5
1	A	633	GLN	5.5
1	A	570	LYS	5.5
1	A	574	GLN	5.4
1	A	310	GLU	5.4
1	A	297	ASP	5.4
1	A	399	PHE	5.4
1	A	375	LYS	5.4
1	A	344	THR	5.4
1	A	502	ASN	5.2
1	A	362	ARG	5.2
1	A	286	GLN	5.2
1	A	285	LYS	5.2
1	A	541	ARG	5.2
1	A	312	LYS	5.1
1	A	564	LEU	5.1
1	A	695	GLU	5.1
1	A	367	LYS	5.0
1	A	590	MET	5.0
1	A	596	ARG	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	278	GLY	4.9
1	A	371	LYS	4.9
1	A	443	LEU	4.8
1	A	653	GLU	4.7
1	A	746	TRP	4.7
1	A	698	ARG	4.7
1	A	446	LYS	4.7
1	A	632	ILE	4.7
1	A	428	ASP	4.7
1	A	571	LEU	4.7
1	A	501	GLU	4.7
1	A	357	GLU	4.6
1	A	745	GLY	4.6
1	A	289	GLU	4.6
1	A	581	GLN	4.6
1	A	449	THR	4.6
1	A	308	SER	4.5
1	A	424	GLU	4.4
1	A	404	ARG	4.4
1	A	313	GLN	4.4
1	A	639	GLU	4.4
1	A	444	GLU	4.2
1	A	563	LYS	4.2
1	A	379	GLU	4.2
1	A	825	GLU	4.2
1	A	445	GLY	4.2
1	A	287	GLU	4.1
1	A	882	TYR	4.1
1	A	693	GLN	4.0
1	A	420	LYS	4.0
1	A	393	MET	3.9
1	A	481	ALA	3.9
1	A	538	TRP	3.9
1	A	390	THR	3.9
1	A	418	LYS	3.8
1	A	880	THR	3.8
1	A	545	GLU	3.7
1	A	486	PHE	3.6
1	A	360	ASP	3.6
1	A	398	GLU	3.5
1	A	556	HIS	3.5
1	A	568	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	440	ASN	3.4
1	A	592	ILE	3.4
1	A	365	GLU	3.4
1	A	717	ILE	3.4
1	A	427	GLU	3.4
1	A	643	VAL	3.3
1	A	792	ARG	3.3
1	A	764	LEU	3.3
1	A	743	GLY	3.2
1	A	676	SER	3.2
1	A	370	THR	3.2
1	A	690	ASP	3.2
1	A	376	ILE	3.2
1	A	677	ALA	3.2
1	A	881	ASP	3.1
1	A	723	VAL	3.1
1	A	807	GLU	3.0
1	A	373	LEU	3.0
1	A	487	GLU	3.0
1	A	528	GLY	3.0
1	A	480	GLY	3.0
1	A	577	VAL	3.0
1	A	561	HIS	3.0
1	A	569	PHE	3.0
1	A	649	ARG	2.9
1	A	552	MET	2.9
1	A	450	CYS	2.9
1	A	483	PHE	2.9
1	A	307	GLY	2.9
1	A	854	THR	2.8
1	A	368	GLU	2.8
1	A	394	CYS	2.8
1	A	824	MET	2.8
1	A	750	GLU	2.7
1	A	383	LYS	2.7
1	A	830	VAL	2.7
1	A	683	ASP	2.6
1	A	337	MET	2.6
1	A	540	THR	2.5
1	A	699	GLY	2.5
1	A	819	GLN	2.5
1	A	447	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	534	ASP	2.5
1	A	558	GLU	2.4
1	A	378	ALA	2.4
1	A	876	ASN	2.4
1	A	567	ALA	2.3
1	A	489	LEU	2.3
1	A	340	GLN	2.3
1	A	529	ALA	2.3
1	A	546	ASP	2.3
1	A	664	ASP	2.2
1	A	702	ASP	2.2
1	A	663	ASP	2.2
1	A	808	ASP	2.2
1	A	642	ALA	2.2
1	A	646	TRP	2.2
1	A	537	GLY	2.2
1	A	650	VAL	2.2
1	A	818	ILE	2.1
1	A	306	HIS	2.1
1	A	648	VAL	2.1
1	A	507	VAL	2.1
1	A	343	MET	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.

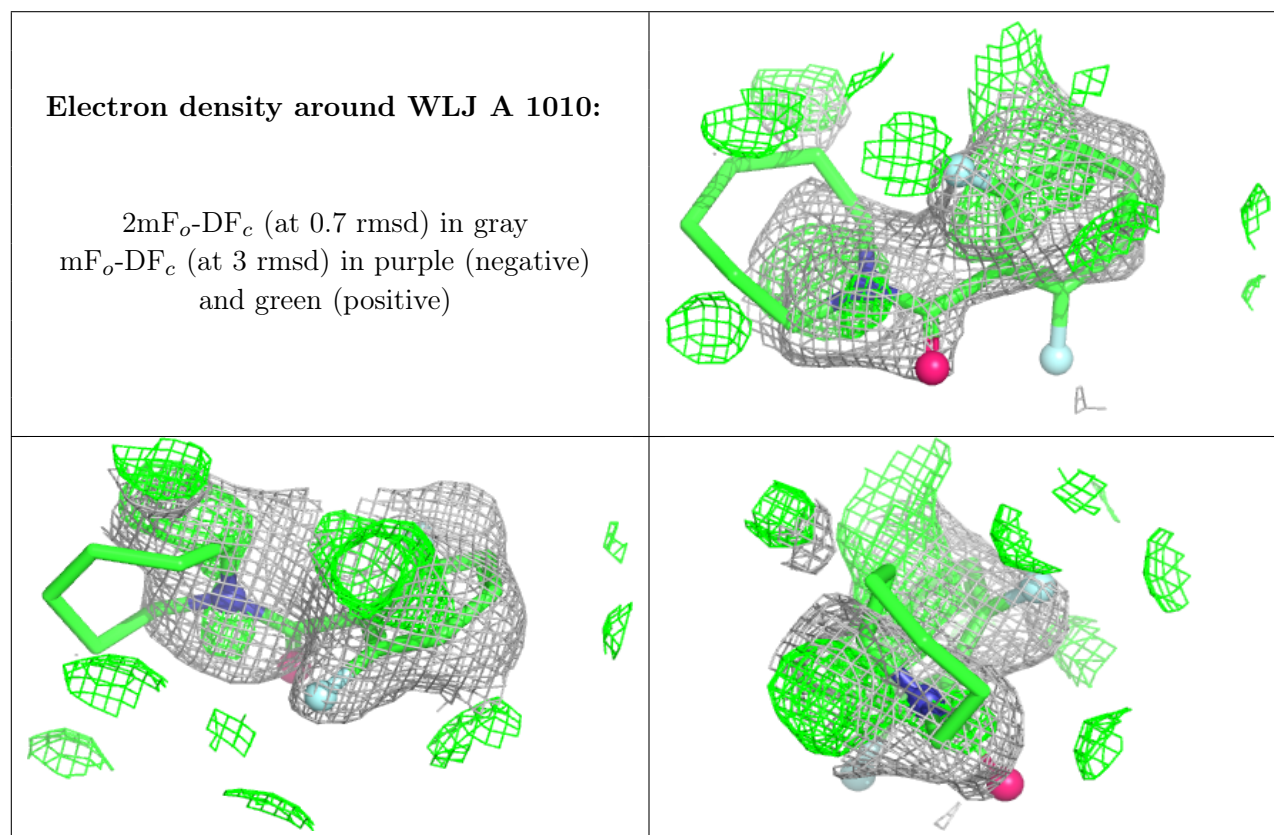
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PO4	A	1008	5/5	0.47	0.32	46,47,54,56	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	WLJ	A	1010	17/17	0.64	0.46	41,49,51,52	17
4	DMS	A	1005	4/4	0.75	0.61	68,70,72,73	4
6	PO4	A	1007	5/5	0.76	0.18	30,31,44,59	0
5	PEG	A	1006	7/7	0.79	0.19	47,47,47,48	7
5	PEG	A	1009	7/7	0.83	0.17	61,68,72,75	0
4	DMS	A	1004	4/4	0.87	0.18	38,40,42,45	0
3	MES	A	1003[B]	12/12	0.96	0.32	502,519,540,541	12
3	MES	A	1003[A]	12/12	0.96	0.32	19,23,25,27	12
2	ZN	A	1002	1/1	0.98	0.06	45,45,45,45	0
8	CL	A	1011	1/1	0.98	0.09	34,34,34,34	0
2	ZN	A	1001	1/1	1.00	0.02	18,18,18,18	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.