Full wwPDB X-ray Structure Validation Report (i)

Mar 27, 2025 – 11:33 AM EDT

PDB ID	:	7I2U
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 Z32665176 (DNV2_NS5A-x0787)
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	:	1.96 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 (i) 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 (i)) were used in the production of this report:

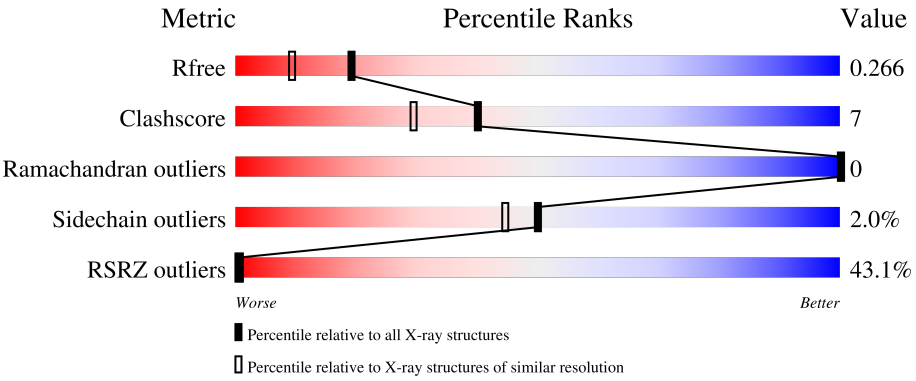
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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}	164625	3187 (1.96-1.96)
Clashscore	180529	3412 (1.96-1.96)
Ramachandran outliers	177936	3390 (1.96-1.96)
Sidechain outliers	177891	3390 (1.96-1.96)
RSRZ outliers	164620	3186 (1.96-1.96)

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 <=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	39% 78% 13% • 8%

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) : 2.41.4

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PO4	A	1006	-	-	X	-
8	LQI	A	1010	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5173 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
			Total	C	N	O	S			
1	A	583	4811	3029	864	884	34	0	6	0

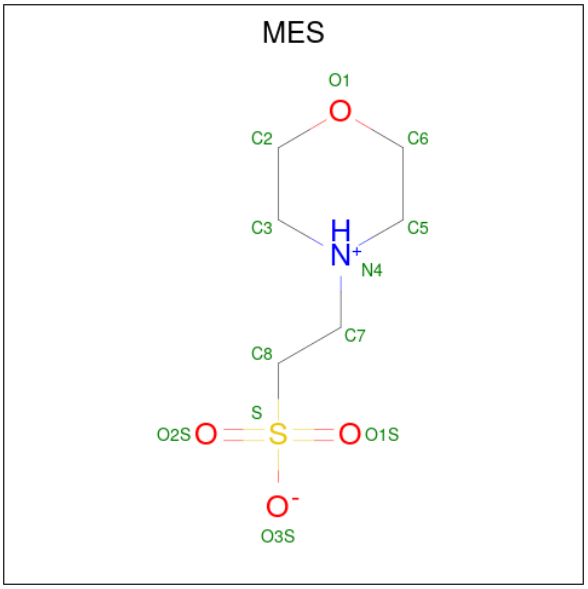
There are 2 discrepancies between the modelled and reference sequences:

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 (three-letter code: ZN) (formula: Zn).

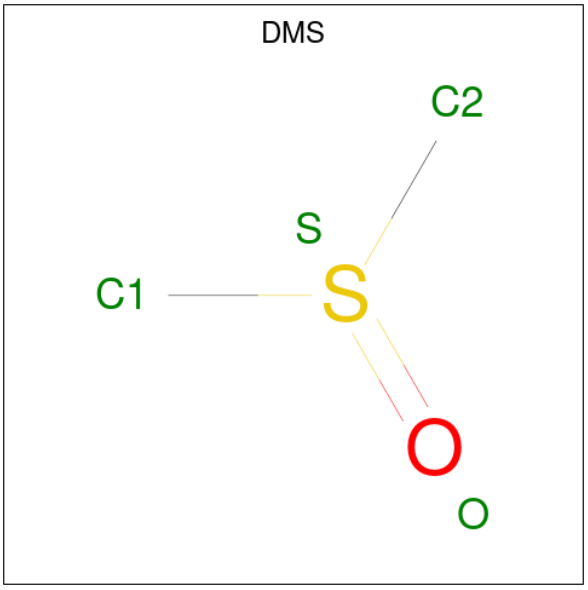
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	2	2	2	0	0

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



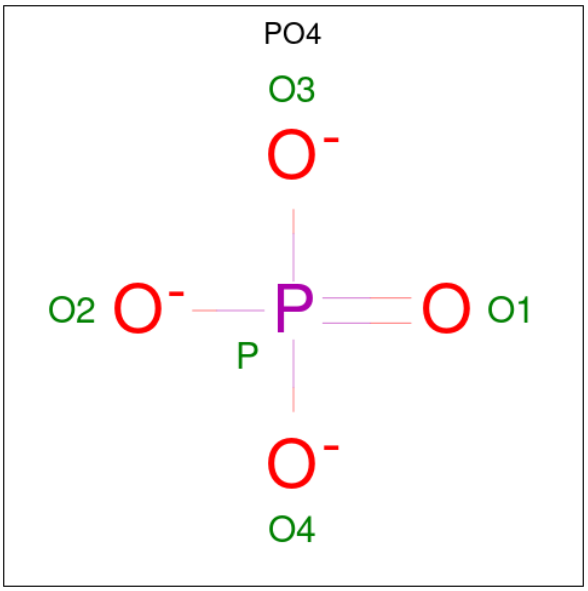
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			24	12	2	8	2		

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



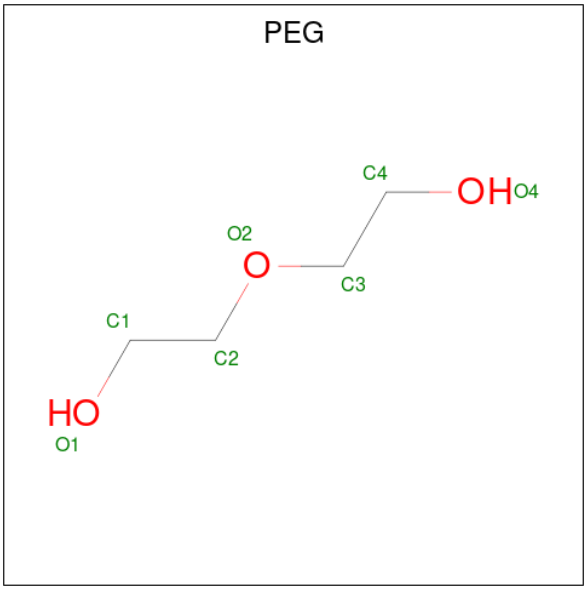
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

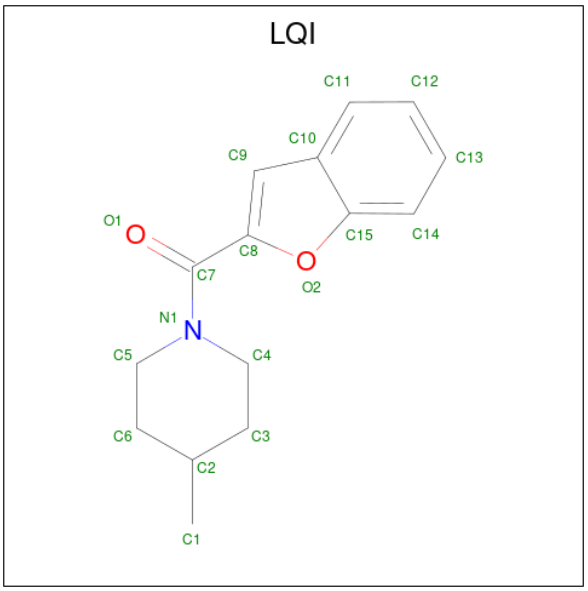


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 8 is (1-benzofuran-2-yl)(4-methylpiperidin-1-yl)methanone (three-letter code: LQI) (formula: $C_{15}H_{17}NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O 18 15 1 2	0	0

- Molecule 9 is water.

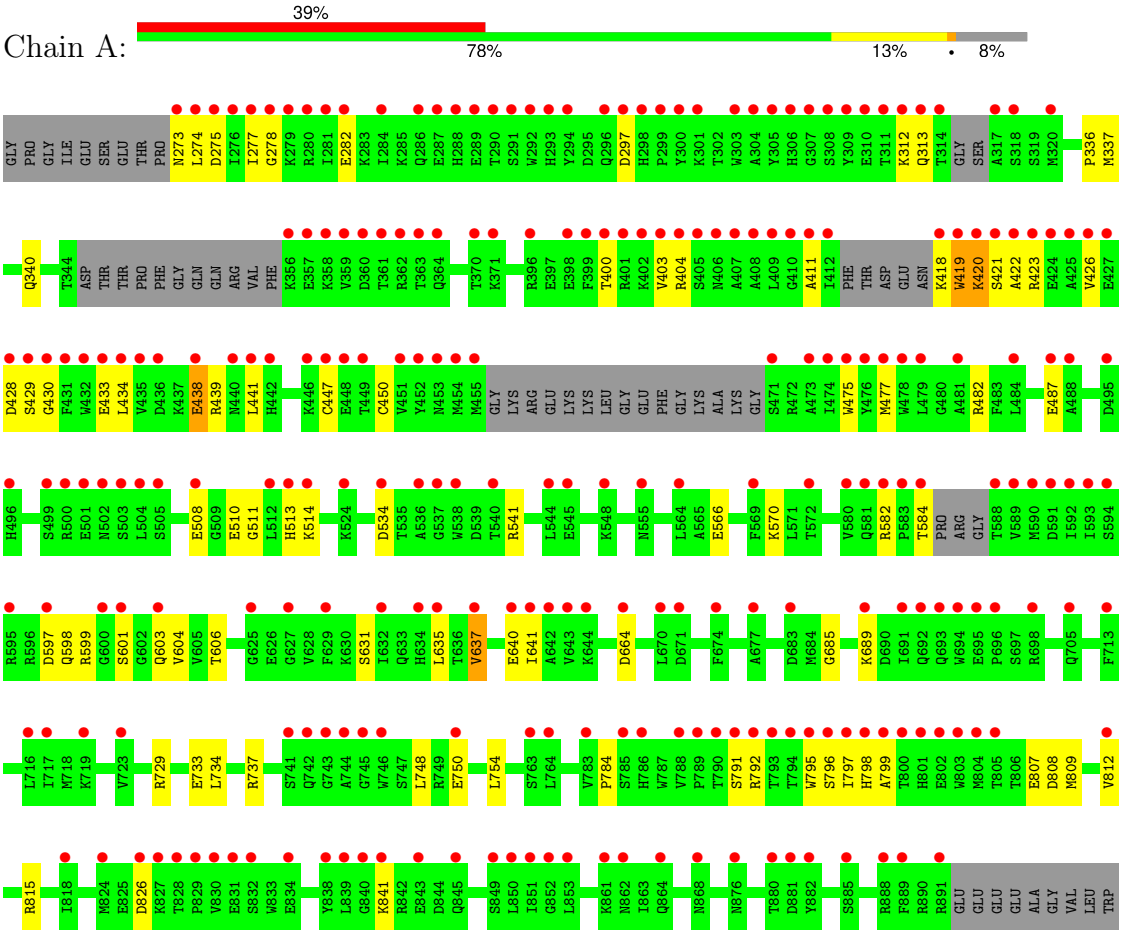
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	292	Total O 292 292	0	0

3 Residue-property plots (i)

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

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	82.62Å 115.81Å 145.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.50 – 1.96 49.50 – 1.96	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.50-1.96) 99.5 (49.50-1.96)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.194 , 0.240 0.244 , 0.266	Depositor DCC
R_{free} test set	2579 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	37.2	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 107.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5173	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN, LQI, MES, PEG, CL, DMS, 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	0.72	0/4919	0.82	0/6635

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.

There are no bond angle outliers.

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

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	4811	0	4719	60	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	24	0	26	1	0
4	A	8	0	12	2	0
5	A	10	0	0	4	0
6	A	7	0	10	0	0
7	A	1	0	0	0	0
8	A	18	0	0	2	0
9	A	292	0	0	7	1
All	All	5173	0	4767	63	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 7.

All (63) 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:513:HIS:O	9:A:1101:HOH:O	1.67	1.12
1:A:403:VAL:HG21	1:A:426:VAL:HG21	1.56	0.88
4:A:1004:DMS:H13	9:A:1231:HOH:O	1.92	0.70
1:A:664:ASP:OD1	5:A:1006:PO4:O4	2.12	0.67
1:A:754:LEU:HD13	1:A:791:SER:HB3	1.77	0.65
1:A:635:LEU:HD23	1:A:640:GLU:HG2	1.79	0.64
1:A:664:ASP:OD1	5:A:1006:PO4:P	2.56	0.64
1:A:312:LYS:O	1:A:313:GLN:HG2	2.00	0.61
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.40	0.61
1:A:534:ASP:OD1	5:A:1006:PO4:O4	2.19	0.61
4:A:1004:DMS:C1	9:A:1231:HOH:O	2.48	0.61
1:A:278:GLY:O	1:A:282:GLU:HG2	2.01	0.61
1:A:273:ASN:N	1:A:275:ASP:OD1	2.37	0.58
1:A:841:LYS:HD3	8:A:1010:LQI:C5	2.35	0.56
1:A:340:GLN:OE1	9:A:1102:HOH:O	2.18	0.54
1:A:792:ARG:NH2	1:A:795:TRP:HA	2.23	0.54
1:A:815:ARG:HD2	9:A:1152:HOH:O	2.08	0.54
1:A:420:LYS:HD2	1:A:421:SER:N	2.23	0.54
1:A:792:ARG:HH21	1:A:795:TRP:HA	1.73	0.54
1:A:429:SER:O	1:A:433:GLU:HG3	2.08	0.53
1:A:733:GLU:O	1:A:737:ARG:HG3	2.09	0.53
1:A:534:ASP:OD1	5:A:1006:PO4:P	2.68	0.52
1:A:274:LEU:O	1:A:278:GLY:HA3	2.12	0.50
1:A:420:LYS:HD2	1:A:421:SER:HB3	1.94	0.50
1:A:510:GLU:O	1:A:514:LYS:HG3	2.11	0.50
1:A:826:ASP:OD1	1:A:826:ASP:C	2.50	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:ARG:HD2	1:A:685:GLY:O	2.13	0.48
1:A:404:ARG:HG3	1:A:423:ARG:NH2	2.28	0.48
1:A:337:MET:HG2	9:A:1306:HOH:O	2.14	0.48
1:A:508:GLU:HG2	1:A:797:ILE:HG22	1.96	0.47
1:A:748:LEU:HD13	3:A:1003[B]:MES:H61	1.97	0.47
1:A:411:ALA:HA	1:A:477:MET:O	2.15	0.46
1:A:419:TRP:HE1	1:A:428:ASP:CG	2.19	0.46
1:A:582:ARG:HG2	1:A:584:THR:OG1	2.16	0.46
1:A:791:SER:OG	1:A:792:ARG:N	2.48	0.46
1:A:422:ALA:O	1:A:426:VAL:HG23	2.15	0.46
1:A:689:LYS:HE3	1:A:689:LYS:HB3	1.63	0.46
1:A:809:MET:HE1	1:A:812:VAL:HG21	1.99	0.45
8:A:1010:LQI:C5	8:A:1010:LQI:C9	2.94	0.45
1:A:603:GLN:HG3	1:A:604:VAL:N	2.32	0.45
1:A:796:SER:O	1:A:799:ALA:HB3	2.16	0.45
1:A:430:GLY:O	1:A:434:LEU:HG	2.17	0.44
1:A:841:LYS:HE3	9:A:1356:HOH:O	2.16	0.44
1:A:599:ARG:HG2	1:A:606:THR:HG23	1.99	0.44
1:A:511:GLY:N	1:A:798:HIS:O	2.51	0.44
1:A:597:ASP:O	1:A:598:GLN:HB2	2.18	0.43
1:A:438:GLU:O	1:A:441:LEU:HB2	2.18	0.43
1:A:807:GLU:CD	1:A:815:ARG:HH22	2.22	0.43
1:A:729:ARG:HD3	1:A:734:LEU:HD21	2.01	0.43
1:A:513:HIS:CD2	1:A:514:LYS:HG2	2.54	0.42
1:A:475:TRP:CD1	1:A:475:TRP:N	2.88	0.42
1:A:809:MET:HA	1:A:809:MET:HE2	2.02	0.42
1:A:274:LEU:HA	1:A:277:ILE:HG12	2.01	0.42
1:A:419:TRP:HE1	1:A:428:ASP:CB	2.32	0.42
1:A:439:ARG:NH1	1:A:487:GLU:OE1	2.53	0.42
1:A:274:LEU:HA	1:A:277:ILE:CG1	2.50	0.42
1:A:566:GLU:O	1:A:570:LYS:HB2	2.19	0.42
1:A:275:ASP:OD1	1:A:275:ASP:N	2.51	0.42
1:A:637:VAL:O	1:A:641:ILE:HG12	2.19	0.41
1:A:403:VAL:CG2	1:A:426:VAL:HG21	2.40	0.41
1:A:418:LYS:HD3	1:A:418:LYS:C	2.42	0.40
1:A:336:PRO:O	1:A:340:GLN:HG2	2.21	0.40
1:A:400:THR:O	1:A:403:VAL:HG22	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1133:HOH:O	9:A:1133:HOH:O[2_445]	1.05	1.15

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	577/637 (91%)	556 (96%)	21 (4%)	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	517/554 (93%)	507 (98%)	10 (2%)	52 47

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	297	ASP
1	A	419	TRP
1	A	420	LYS
1	A	438	GLU
1	A	482	ARG
1	A	601	SER
1	A	631	SER
1	A	637	VAL

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Mol	Chain	Res	Type
1	A	750	GLU
1	A	808	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
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 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	$\#\|Z\| > 2$
5	PO4	A	1006	-	4,4,4	2.95	2 (50%)	6,6,6	0.72	0
4	DMS	A	1005	-	3,3,3	0.40	0	3,3,3	0.17	0
3	MES	A	1003[A]	-	12,12,12	0.74	0	15,16,16	0.40	0
8	LQI	A	1010	-	18,20,20	1.04	2 (11%)	20,28,28	0.57	0
4	DMS	A	1004	-	3,3,3	0.29	0	3,3,3	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PO4	A	1007	-	4,4,4	0.98	0	6,6,6	0.51	0
6	PEG	A	1008	-	6,6,6	0.13	0	5,5,5	0.15	0
3	MES	A	1003[B]	-	12,12,12	0.73	0	15,16,16	0.52	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[A]	-	-	3/6/14/14	0/1/1/1
8	LQI	A	1010	-	-	0/4/18/18	0/3/3/3
6	PEG	A	1008	-	-	2/4/4/4	-
3	MES	A	1003[B]	-	-	2/6/14/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1006	PO4	P-O1	4.99	1.62	1.50
8	A	1010	LQI	C9-C8	-3.20	1.35	1.38
5	A	1006	PO4	P-O2	2.15	1.60	1.54
8	A	1010	LQI	C10-C15	-2.07	1.39	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (7) 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-O3S
3	A	1003[B]	MES	C8-C7-N4-C3
6	A	1008	PEG	O2-C3-C4-O4
3	A	1003[B]	MES	C8-C7-N4-C5
3	A	1003[A]	MES	C7-C8-S-O2S
6	A	1008	PEG	C4-C3-O2-C2

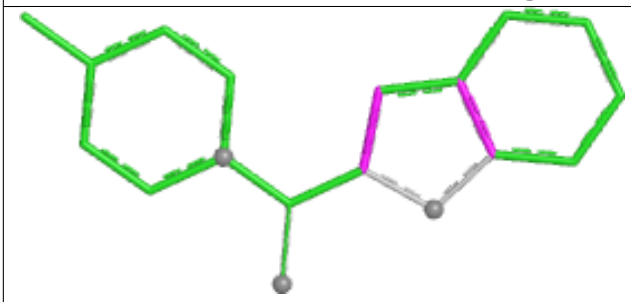
There are no ring outliers.

4 monomers are involved in 9 short contacts:

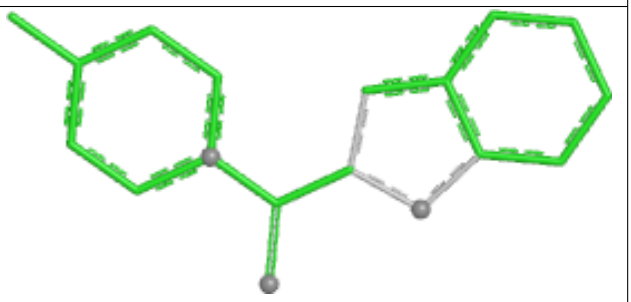
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1006	PO4	4	0
8	A	1010	LQI	2	0
4	A	1004	DMS	2	0
3	A	1003[B]	MES	1	0

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 then 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.

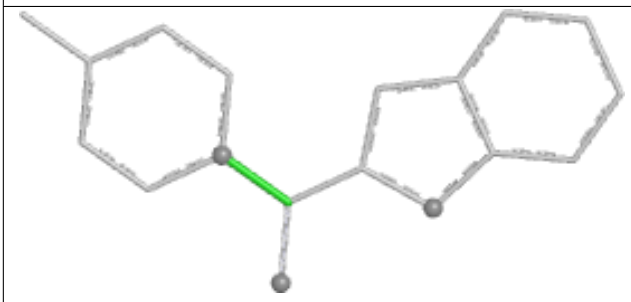
Ligand LQI A 1010



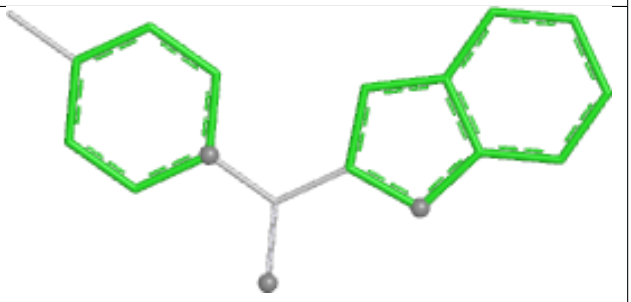
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	583/637 (91%)	2.94	251 (43%) 1 0	7, 44, 95, 158	123 (21%)

All (251) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	512[A]	LEU	15.4
1	A	795	TRP	14.8
1	A	713	PHE	14.3
1	A	830	VAL	13.7
1	A	409	LEU	12.6
1	A	803	TRP	12.3
1	A	281	ILE	12.3
1	A	600	GLY	12.3
1	A	514	LYS	12.3
1	A	716	LEU	12.3
1	A	717	ILE	12.1
1	A	399	PHE	12.1
1	A	641	ILE	11.9
1	A	790	THR	11.7
1	A	838	TYR	11.6
1	A	593	ILE	11.5
1	A	793	THR	11.4
1	A	719[A]	LYS	11.2
1	A	407	ALA	11.0
1	A	799	ALA	11.0
1	A	513	HIS	11.0
1	A	794	THR	10.9
1	A	800	THR	10.8
1	A	801	HIS	10.8
1	A	850	LEU	10.6
1	A	403	VAL	10.5
1	A	791	SER	10.5

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Mol	Chain	Res	Type	RSRZ
1	A	426	VAL	10.4
1	A	839	LEU	10.4
1	A	580	VAL	10.3
1	A	840	GLY	10.2
1	A	488	ALA	10.2
1	A	797	ILE	10.1
1	A	832	SER	10.1
1	A	504	LEU	10.0
1	A	276	ILE	10.0
1	A	853	LEU	10.0
1	A	422	ALA	9.9
1	A	277	ILE	9.9
1	A	410	GLY	9.8
1	A	505	SER	9.6
1	A	274	LEU	9.5
1	A	851	ILE	9.5
1	A	829	PRO	9.5
1	A	400	THR	9.3
1	A	798	HIS	9.3
1	A	828	THR	9.2
1	A	278	GLY	9.1
1	A	885	SER	9.0
1	A	421	SER	9.0
1	A	792	ARG	8.8
1	A	826	ASP	8.8
1	A	594	SER	8.7
1	A	849	SER	8.7
1	A	408	ALA	8.6
1	A	595	ARG	8.5
1	A	309	TYR	8.5
1	A	311	THR	8.4
1	A	785[A]	SER	8.4
1	A	789	PRO	8.3
1	A	796	SER	8.3
1	A	696	PRO	8.2
1	A	582	ARG	8.2
1	A	419	TRP	8.1
1	A	788	VAL	8.1
1	A	827	LYS	8.1
1	A	705	GLN	8.0
1	A	314	THR	8.0
1	A	589	VAL	8.0

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Mol	Chain	Res	Type	RSRZ
1	A	802	GLU	7.8
1	A	763[A]	SER	7.8
1	A	805	THR	7.7
1	A	280	ARG	7.7
1	A	864[A]	GLN	7.6
1	A	273	ASN	7.6
1	A	852	GLY	7.6
1	A	289	GLU	7.6
1	A	487	GLU	7.5
1	A	786	HIS	7.5
1	A	279	LYS	7.4
1	A	500	ARG	7.2
1	A	356	LYS	7.2
1	A	298	HIS	7.1
1	A	689	LYS	7.1
1	A	288	HIS	7.0
1	A	398	GLU	7.0
1	A	841	LYS	7.0
1	A	361	THR	6.9
1	A	431	PHE	6.9
1	A	499	SER	6.9
1	A	402	LYS	6.9
1	A	503	SER	6.9
1	A	584	THR	6.9
1	A	405	SER	6.8
1	A	693	GLN	6.8
1	A	741[A]	SER	6.7
1	A	692	GLN	6.7
1	A	831	GLU	6.6
1	A	275	ASP	6.6
1	A	360	ASP	6.6
1	A	423	ARG	6.5
1	A	804	MET	6.5
1	A	452	TYR	6.4
1	A	429	SER	6.4
1	A	744	ALA	6.2
1	A	583	PRO	6.2
1	A	843	GLU	6.2
1	A	581	GLN	6.1
1	A	745	GLY	6.1
1	A	401	ARG	6.0
1	A	476	TYR	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	484	LEU	5.9
1	A	502	ASN	5.9
1	A	412	ILE	5.8
1	A	601	SER	5.8
1	A	406	ASN	5.8
1	A	434	LEU	5.8
1	A	296	GLN	5.7
1	A	698	ARG	5.6
1	A	424	GLU	5.6
1	A	282	GLU	5.5
1	A	284	ILE	5.5
1	A	293	HIS	5.5
1	A	357	GLU	5.5
1	A	695	GLU	5.5
1	A	312	LYS	5.4
1	A	420	LYS	5.4
1	A	442	HIS	5.3
1	A	845	GLN	5.2
1	A	882	TYR	5.2
1	A	290	THR	5.2
1	A	428	ASP	5.1
1	A	404	ARG	5.0
1	A	441	LEU	5.0
1	A	876	ASN	4.9
1	A	427	GLU	4.9
1	A	362	ARG	4.9
1	A	418	LYS	4.9
1	A	411	ALA	4.8
1	A	588	THR	4.8
1	A	474	ILE	4.8
1	A	501	GLU	4.7
1	A	435	VAL	4.6
1	A	313	GLN	4.6
1	A	455	MET	4.6
1	A	292	TRP	4.6
1	A	750	GLU	4.6
1	A	544	LEU	4.5
1	A	294	TYR	4.4
1	A	475	TRP	4.3
1	A	889	PHE	4.3
1	A	318	SER	4.2
1	A	436	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	627	GLY	4.1
1	A	359	VAL	4.1
1	A	317	ALA	4.1
1	A	286	GLN	4.1
1	A	451	VAL	4.0
1	A	449	THR	4.0
1	A	880	THR	4.0
1	A	363	THR	3.9
1	A	430	GLY	3.9
1	A	861	LYS	3.9
1	A	545	GLU	3.8
1	A	591	ASP	3.8
1	A	742	GLN	3.8
1	A	310	GLU	3.8
1	A	297	ASP	3.8
1	A	305	TYR	3.8
1	A	664	ASP	3.7
1	A	308	SER	3.7
1	A	473	ALA	3.7
1	A	287	GLU	3.7
1	A	881	ASP	3.6
1	A	425	ALA	3.6
1	A	746	TRP	3.6
1	A	637	VAL	3.5
1	A	824	MET	3.5
1	A	358	LYS	3.4
1	A	670	LEU	3.4
1	A	370	THR	3.4
1	A	644	LYS	3.3
1	A	396	ARG	3.3
1	A	534	ASP	3.3
1	A	743	GLY	3.2
1	A	691	ILE	3.1
1	A	300	TYR	3.0
1	A	683	ASP	3.0
1	A	677	ALA	3.0
1	A	471	SER	3.0
1	A	564	LEU	3.0
1	A	438	GLU	3.0
1	A	299	PRO	2.9
1	A	479	LEU	2.9
1	A	592	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	496	HIS	2.9
1	A	537	GLY	2.9
1	A	674	PHE	2.8
1	A	635	LEU	2.8
1	A	453	ASN	2.8
1	A	447	CYS	2.8
1	A	303	TRP	2.8
1	A	634	HIS	2.8
1	A	307	GLY	2.8
1	A	783	VAL	2.7
1	A	432	TRP	2.6
1	A	364	GLN	2.6
1	A	371	LYS	2.6
1	A	454	MET	2.6
1	A	301	LYS	2.5
1	A	643	VAL	2.5
1	A	764	LEU	2.5
1	A	597	ASP	2.5
1	A	304	ALA	2.5
1	A	477	MET	2.5
1	A	538	TRP	2.5
1	A	632	ILE	2.5
1	A	603	GLN	2.5
1	A	694	TRP	2.4
1	A	590	MET	2.4
1	A	478	TRP	2.4
1	A	642	ALA	2.4
1	A	320	MET	2.4
1	A	446	LYS	2.4
1	A	888	ARG	2.4
1	A	481	ALA	2.4
1	A	495	ASP	2.3
1	A	536	ALA	2.3
1	A	834	GLU	2.3
1	A	548	LYS	2.3
1	A	448	GLU	2.3
1	A	625	GLY	2.2
1	A	572	THR	2.2
1	A	723	VAL	2.2
1	A	508	GLU	2.2
1	A	569	PHE	2.2
1	A	440	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	629	PHE	2.2
1	A	540	THR	2.1
1	A	291	SER	2.1
1	A	524	LYS	2.1
1	A	555	ASN	2.1
1	A	818	ILE	2.1
1	A	862	ASN	2.1
1	A	891	ARG	2.1
1	A	812	VAL	2.1
1	A	671	ASP	2.1
1	A	433	GLU	2.1
1	A	640	GLU	2.1
1	A	868	ASN	2.1
1	A	306	HIS	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 monosaccharides 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, 95^{th} 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	LQI	A	1010	18/18	0.56	0.41	49,54,63,63	18
5	PO4	A	1007	5/5	0.76	0.11	77,83,91,110	0
4	DMS	A	1005	4/4	0.76	0.23	77,105,106,126	0
5	PO4	A	1006	5/5	0.80	0.12	43,48,58,79	0
6	PEG	A	1008	7/7	0.81	0.17	67,79,91,94	0
4	DMS	A	1004	4/4	0.82	0.22	66,69,70,71	0
3	MES	A	1003[A]	12/12	0.94	0.25	762,768,813,813	12
3	MES	A	1003[B]	12/12	0.94	0.25	30,36,41,44	12
7	CL	A	1009	1/1	0.96	0.44	51,51,51,51	1

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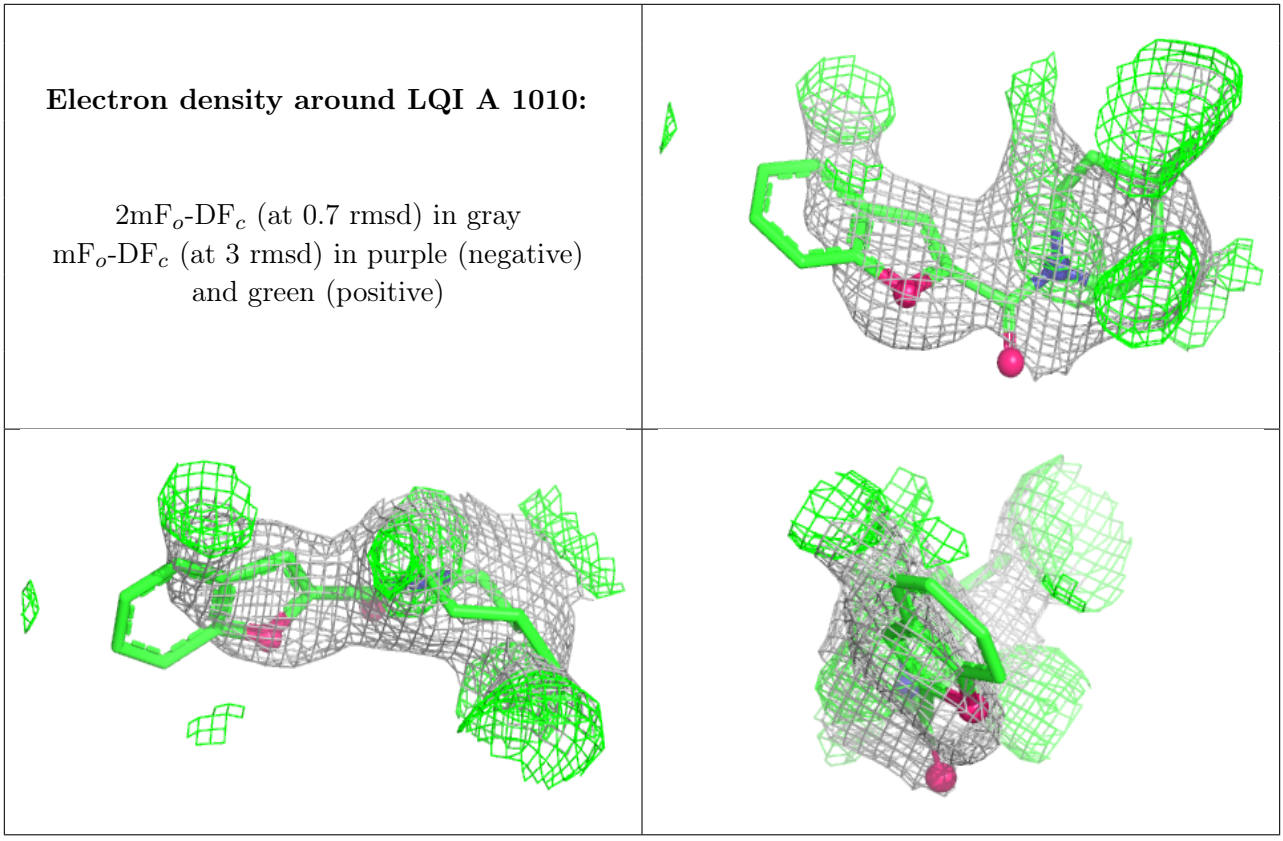
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	A	1002	1/1	0.99	0.03	60,60,60,60	0
2	ZN	A	1001	1/1	1.00	0.01	29,29,29,29	0

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 LQI 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.