



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:19 PM UTC

PDB ID : 4DRU / pdb_00004dru
Title : HCV NS5B in complex with macrocyclic INDOLE INHIBITOR
Authors : Cummings, M.D.; Vendeville, S.
Deposited on : 2012-02-17
Resolution : 2.10 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)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

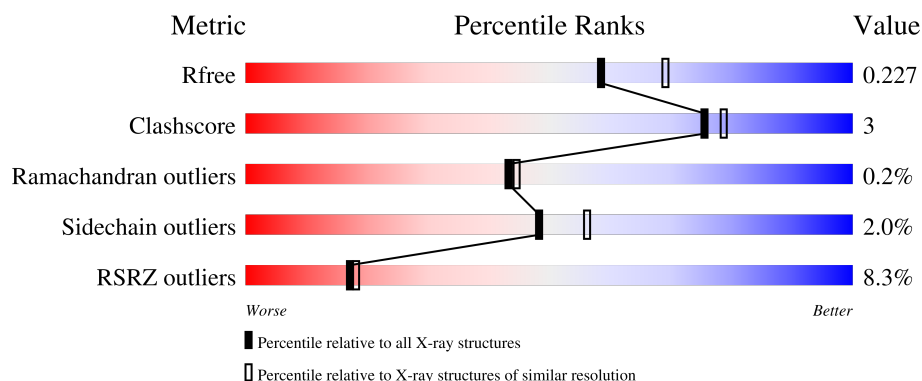
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	563	14% 88% 9% ..
1	B	563	2% 92% 6% ..

2 Entry composition [i](#)

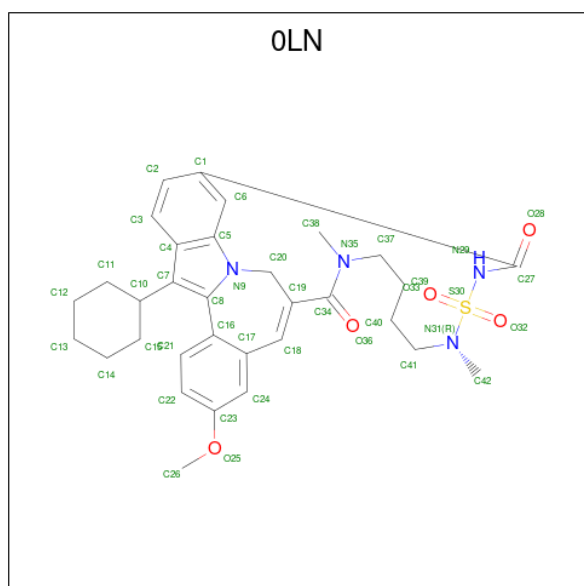
There are 5 unique types of molecules in this entry. The entry contains 9474 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	27	1	0
			4286	2698	756	800	32			
1	B	559	Total	C	N	O	S	14	6	0
			4403	2768	778	824	33			

- Molecule 2 is 13-cyclohexyl-3-methoxy-17,22-dimethyl-7H-10,6-(methanoiminothioiminobutanoiminomethano)indolo[2,1-a][2]benzazepine-14,23-dione 16,16-dioxide (CCD ID: 0LN) (formula: C₃₂H₃₈N₄O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			42	32	4	5	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	250	Total	O	0	0
			250	250		

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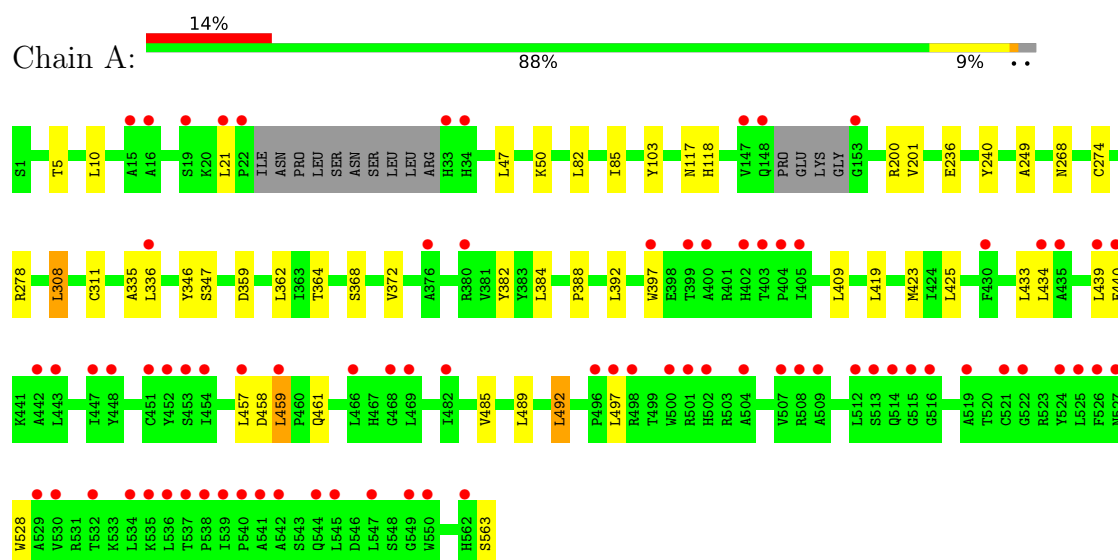
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	376	Total	O	0	0
			376	376		

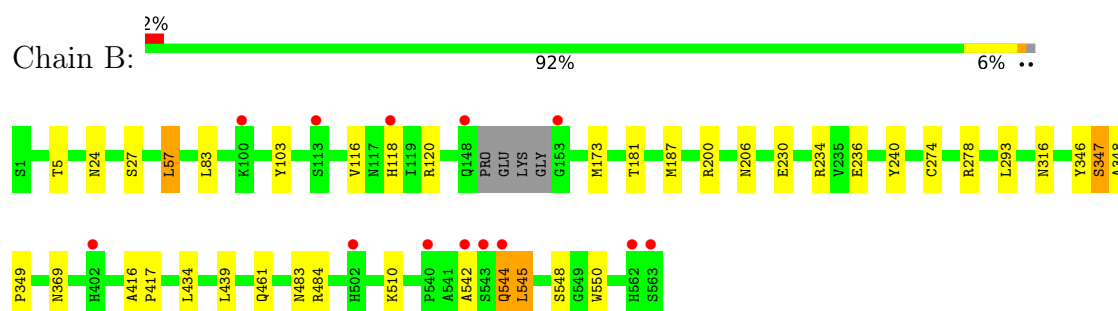
3 Residue-property plots [i](#)

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: RNA-directed RNA polymerase



• Molecule 1: RNA-directed RNA polymerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.13Å 106.64Å 133.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.63 – 2.10 41.63 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.9 (41.63-2.10) 98.8 (41.63-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.185 , 0.226 0.194 , 0.227	Depositor DCC
R_{free} test set	990 reflections (1.14%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9474	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 0LN, SO4, GOL

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	0.67	0/4378	0.81	0/5938
1	B	0.75	0/4498	0.83	2/6103 (0.0%)
All	All	0.71	0/8876	0.82	2/12041 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	550	TRP	N-CA-C	6.37	118.02	111.14
1	B	548	SER	N-CA-C	-5.14	102.77	110.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4286	0	4285	23	0
1	B	4403	0	4394	30	0
2	A	42	0	38	1	0
3	A	20	0	0	0	0
3	B	55	0	0	0	0
4	A	12	0	16	1	0
4	B	30	0	40	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	250	0	0	1	0
5	B	376	0	0	5	0
All	All	9474	0	8773	53	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (53) 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:B:369:ASN:HD21	1:B:484:ARG:HH22	1.26	0.80
1:A:117:ASN:HB3	5:A:909:HOH:O	1.95	0.66
1:A:21:LEU:HD21	1:A:397:TRP:HA	1.84	0.60
1:A:236[A]:GLU:OE1	1:A:240:TYR:OH	2.15	0.60
1:B:544:GLN:HE21	1:B:544:GLN:HA	1.69	0.58
1:A:308:LEU:HB3	1:A:311:CYS:SG	2.45	0.57
1:A:82:LEU:HD13	1:A:249:ALA:HB2	1.89	0.55
1:B:236[B]:GLU:OE2	1:B:240:TYR:OH	2.11	0.54
1:B:103:TYR:OH	1:B:118[B]:HIS:HD2	1.91	0.54
1:B:230:GLU:HG3	1:B:234:ARG:HH11	1.74	0.53
1:A:103:TYR:OH	1:A:118:HIS:HD2	1.92	0.53
1:A:458:ASP:HA	1:A:461:GLN:HE22	1.74	0.53
1:B:542:ALA:O	1:B:545:LEU:HB2	2.09	0.52
1:B:200:ARG:HH12	1:B:316:ASN:HD21	1.58	0.50
1:B:544:GLN:HE21	1:B:544:GLN:CA	2.23	0.50
1:A:10:LEU:HD23	4:A:607:GOL:H11	1.93	0.50
1:B:230:GLU:HG3	1:B:234:ARG:NH1	2.27	0.49
1:A:268:ASN:HB3	1:A:274:CYS:SG	2.54	0.48
1:B:483:ASN:HB3	5:B:1024:HOH:O	2.14	0.47
1:B:173:MET:CE	5:B:1074:HOH:O	2.62	0.47
1:B:116:VAL:O	1:B:120:ARG:HG3	2.15	0.47
1:B:347:SER:O	1:B:349:PRO:CD	2.63	0.47
1:B:200:ARG:HH12	1:B:316:ASN:ND2	2.14	0.46
1:B:346:TYR:O	1:B:347:SER:CB	2.63	0.46
1:B:206:ASN:HB3	5:B:995:HOH:O	2.16	0.46
1:B:230:GLU:CG	1:B:234:ARG:HH11	2.30	0.45
1:A:492:LEU:HG	2:A:601:OLN:H22	1.99	0.45
1:B:230:GLU:CG	1:B:234:ARG:NH1	2.80	0.45
1:B:483:ASN:ND2	5:B:1025:HOH:O	2.49	0.45
1:B:24:ASN:HB3	1:B:27:SER:OG	2.17	0.45
1:A:200:ARG:HD3	1:A:384:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:GLU:HG2	1:A:457:LEU:HD12	1.98	0.44
1:A:5:THR:HG23	1:A:278:ARG:HH12	1.83	0.44
1:B:347:SER:O	1:B:349:PRO:HD3	2.17	0.43
1:B:236[B]:GLU:HG2	1:B:240:TYR:CZ	2.54	0.43
1:A:388:PRO:O	1:A:392:LEU:HG	2.18	0.42
1:A:372:VAL:HG22	1:A:382:TYR:CD1	2.54	0.42
1:B:5:THR:HG23	1:B:278:ARG:HH22	1.85	0.42
1:B:57:LEU:C	1:B:57:LEU:HD12	2.44	0.42
1:A:308:LEU:CD1	1:A:335:ALA:HB1	2.50	0.42
1:B:181:THR:HG21	5:B:978:HOH:O	2.19	0.42
1:B:461:GLN:HB2	1:B:542:ALA:HA	2.01	0.42
1:A:359:ASP:HB3	1:A:362:LEU:HD12	2.01	0.42
1:B:434:LEU:HD21	1:B:510:LYS:HB2	2.02	0.42
1:A:346:TYR:O	1:A:347:SER:CB	2.67	0.41
1:A:364:THR:HA	1:A:368:SER:O	2.20	0.41
1:A:439:LEU:HB3	1:A:457:LEU:HD11	2.03	0.41
1:A:419:LEU:CD2	1:A:485:VAL:HG11	2.50	0.41
1:B:416:ALA:N	1:B:417:PRO:CD	2.84	0.41
1:A:409:LEU:HD11	1:A:459:LEU:HD11	2.02	0.41
1:A:423:MET:HA	1:A:528:TRP:CZ2	2.54	0.41
1:B:187:MET:HE2	1:B:293:LEU:HD23	2.04	0.40
1:B:83:LEU:HB2	1:B:173:MET:HA	2.03	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	544/563 (97%)	533 (98%)	11 (2%)	0	100	100
1	B	561/563 (100%)	546 (97%)	13 (2%)	2 (0%)	30	28
All	All	1105/1126 (98%)	1079 (98%)	24 (2%)	2 (0%)	43	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	347	SER
1	B	348	ALA

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	467/479 (98%)	453 (97%)	14 (3%)	36	41
1	B	482/479 (101%)	477 (99%)	5 (1%)	68	76
All	All	949/958 (99%)	930 (98%)	19 (2%)	48	56

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LEU
1	A	50	LYS
1	A	85	ILE
1	A	201	VAL
1	A	308	LEU
1	A	336	LEU
1	A	425	LEU
1	A	433	LEU
1	A	434	LEU
1	A	459	LEU
1	A	489	LEU
1	A	492	LEU
1	A	497	LEU
1	A	563	SER
1	B	57	LEU
1	B	274	CYS
1	B	439	LEU
1	B	544	GLN
1	B	545	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	HIS
1	A	194	GLN
1	A	273	ASN
1	A	316	ASN
1	A	438	GLN
1	A	461	GLN
1	A	514	GLN
1	B	28	ASN
1	B	110	ASN
1	B	194	GLN
1	B	316	ASN
1	B	369	ASN
1	B	411	ASN
1	B	483	ASN
1	B	514	GLN
1	B	544	GLN

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 ⓘ

23 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	602	-	4,4,4	0.24	0	6,6,6	0.54	0
4	GOL	A	606	-	5,5,5	0.50	0	5,5,5	0.51	0
3	SO4	B	601	-	4,4,4	0.24	0	6,6,6	0.73	0
3	SO4	A	603	-	4,4,4	0.30	0	6,6,6	0.26	0
4	GOL	B	614	-	5,5,5	0.55	0	5,5,5	0.49	0
3	SO4	A	604	-	4,4,4	0.25	0	6,6,6	0.13	0
3	SO4	B	602	-	4,4,4	0.30	0	6,6,6	0.46	0
3	SO4	B	609	-	4,4,4	0.24	0	6,6,6	0.22	0
3	SO4	B	603	-	4,4,4	0.49	0	6,6,6	0.66	0
3	SO4	B	604	-	4,4,4	0.25	0	6,6,6	0.21	0
3	SO4	B	605	-	4,4,4	0.31	0	6,6,6	0.58	0
4	GOL	B	615	-	5,5,5	0.62	0	5,5,5	0.77	0
3	SO4	B	610	-	4,4,4	0.28	0	6,6,6	0.39	0
4	GOL	B	613	-	5,5,5	0.43	0	5,5,5	0.33	0
4	GOL	A	607	-	5,5,5	0.53	0	5,5,5	1.23	1 (20%)
4	GOL	B	612	-	5,5,5	0.41	0	5,5,5	0.53	0
3	SO4	A	605	-	4,4,4	0.21	0	6,6,6	0.21	0
4	GOL	B	616	-	5,5,5	0.58	0	5,5,5	0.79	0
3	SO4	B	606	-	4,4,4	0.24	0	6,6,6	0.14	0
2	OLN	A	601	-	43,47,47	1.63	10 (23%)	57,70,70	1.51	8 (14%)
3	SO4	B	608	-	4,4,4	0.35	0	6,6,6	0.18	0
3	SO4	B	607	-	4,4,4	0.42	0	6,6,6	0.83	0
3	SO4	B	611	-	4,4,4	0.32	0	6,6,6	0.38	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
4	GOL	A	606	-	-	2/4/4/4	-
4	GOL	B	616	-	-	2/4/4/4	-
2	OLN	A	601	-	-	15/32/56/56	0/4/6/6
4	GOL	B	615	-	-	2/4/4/4	-
4	GOL	B	613	-	-	2/4/4/4	-
4	GOL	B	614	-	-	0/4/4/4	-
4	GOL	A	607	-	-	2/4/4/4	-
4	GOL	B	612	-	-	1/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	0LN	C4-C7	-4.19	1.37	1.44
2	A	601	0LN	C8-N9	-3.84	1.33	1.39
2	A	601	0LN	C4-C5	-3.39	1.36	1.41
2	A	601	0LN	C5-N9	-3.21	1.33	1.39
2	A	601	0LN	C41-N31	3.13	1.49	1.47
2	A	601	0LN	C34-N35	2.94	1.40	1.35
2	A	601	0LN	C8-C7	2.51	1.40	1.37
2	A	601	0LN	C18-C19	2.28	1.36	1.34
2	A	601	0LN	C20-C19	2.17	1.54	1.51
2	A	601	0LN	C10-C7	2.17	1.53	1.49

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	0LN	O33-S30-O32	-5.65	109.71	119.80
2	A	601	0LN	O36-C34-N35	-3.87	117.25	122.54
2	A	601	0LN	C18-C19-C34	-2.81	113.11	119.39
2	A	601	0LN	C41-N31-S30	-2.77	112.52	117.97
2	A	601	0LN	C11-C10-C7	-2.70	107.50	113.00
2	A	601	0LN	C42-N31-S30	-2.38	109.90	117.72
2	A	601	0LN	C37-N35-C34	2.38	125.68	120.28
2	A	601	0LN	C39-C37-N35	2.34	119.97	112.53
4	A	607	GOL	O3-C3-C2	2.16	120.08	110.38

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	0LN	C18-C19-C34-O36
2	A	601	0LN	C39-C37-N35-C38
2	A	601	0LN	C40-C41-N31-C42
2	A	601	0LN	C42-N31-S30-O32
2	A	601	0LN	C42-N31-S30-N29
2	A	601	0LN	C27-N29-S30-N31
2	A	601	0LN	C27-N29-S30-O32
4	B	615	GOL	O1-C1-C2-C3
2	A	601	0LN	C22-C23-O25-C26
2	A	601	0LN	C24-C23-O25-C26
4	B	615	GOL	O1-C1-C2-O2
4	A	606	GOL	O1-C1-C2-C3
4	A	607	GOL	C1-C2-C3-O3
4	B	613	GOL	O1-C1-C2-C3

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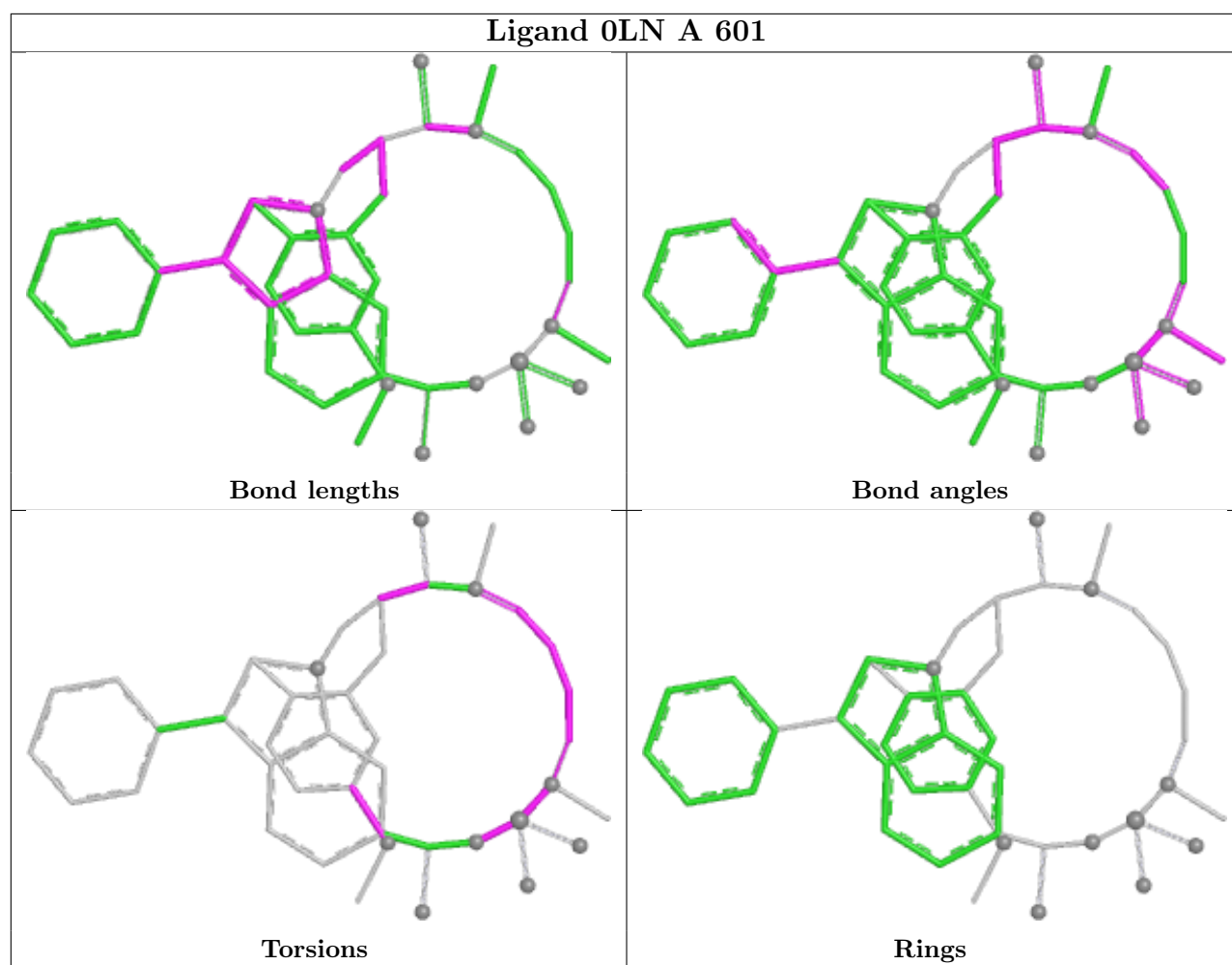
Mol	Chain	Res	Type	Atoms
4	B	616	GOL	O1-C1-C2-C3
4	A	607	GOL	O2-C2-C3-O3
4	B	616	GOL	O1-C1-C2-O2
2	A	601	0LN	C37-C39-C40-C41
2	A	601	0LN	N35-C37-C39-C40
4	A	606	GOL	O1-C1-C2-O2
4	B	613	GOL	O1-C1-C2-O2
4	B	612	GOL	C1-C2-C3-O3
2	A	601	0LN	C39-C37-N35-C34
2	A	601	0LN	C27-N29-S30-O33
2	A	601	0LN	C39-C40-C41-N31
2	A	601	0LN	C41-N31-S30-O32

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	607	GOL	1	0
2	A	601	0LN	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	549/563 (97%)	0.63	79 (14%) 6 6	12, 44, 94, 110	8 (1%)
1	B	559/563 (99%)	-0.10	13 (2%) 61 64	10, 29, 53, 78	10 (1%)
All	All	1108/1126 (98%)	0.26	92 (8%) 17 18	10, 34, 84, 110	18 (1%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	547	LEU	4.4
1	A	550	TRP	4.4
1	A	457	LEU	4.2
1	A	542	ALA	4.1
1	A	22	PRO	3.8
1	A	541	ALA	3.7
1	A	434	LEU	3.7
1	A	430	PHE	3.6
1	A	498	ARG	3.6
1	A	435	ALA	3.4
1	A	540	PRO	3.4
1	A	400	ALA	3.3
1	A	405	ILE	3.3
1	A	439	LEU	3.3
1	A	442	ALA	3.3
1	B	544	GLN	3.3
1	B	153	GLY	3.2
1	A	404	PRO	3.2
1	A	153	GLY	3.2
1	A	16	ALA	3.1
1	A	447	ILE	3.1
1	A	466	LEU	3.1
1	A	545	LEU	3.1
1	B	563	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	440	GLU	3.0
1	A	443	LEU	3.0
1	A	507	VAL	3.0
1	A	539	ILE	2.9
1	A	403	THR	2.9
1	A	33	HIS	2.9
1	A	147	VAL	2.8
1	A	537	THR	2.8
1	A	549	GLY	2.8
1	A	525	LEU	2.8
1	B	402	HIS	2.8
1	B	502	HIS	2.8
1	A	509	ALA	2.8
1	A	21	LEU	2.8
1	A	469	LEU	2.8
1	A	148	GLN	2.7
1	A	544	GLN	2.7
1	A	534	LEU	2.7
1	A	34	HIS	2.7
1	A	402	HIS	2.7
1	A	502	HIS	2.6
1	A	536	LEU	2.6
1	A	451	CYS	2.6
1	A	516	GLY	2.6
1	B	542	ALA	2.6
1	A	500	TRP	2.6
1	A	513	SER	2.5
1	A	459	LEU	2.5
1	A	497	LEU	2.5
1	A	512	LEU	2.5
1	A	397	TRP	2.5
1	A	538	PRO	2.5
1	A	452	TYR	2.5
1	A	522	GLY	2.4
1	A	454	ILE	2.4
1	A	19	SER	2.4
1	A	519	ALA	2.4
1	A	515	GLY	2.4
1	B	148	GLN	2.4
1	A	399	THR	2.4
1	B	118[A]	HIS	2.4
1	A	482	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	540	PRO	2.4
1	A	501	ARG	2.3
1	A	530	VAL	2.3
1	A	535	LYS	2.3
1	A	526	PHE	2.3
1	B	562	HIS	2.3
1	A	504	ALA	2.3
1	B	113	SER	2.2
1	A	380	ARG	2.2
1	A	529	ALA	2.2
1	B	543	SER	2.2
1	A	514	GLN	2.2
1	A	448	TYR	2.2
1	A	496	PRO	2.1
1	A	376	ALA	2.1
1	A	15	ALA	2.1
1	A	524	TYR	2.1
1	A	532	THR	2.1
1	A	453	SER	2.1
1	A	508	ARG	2.1
1	B	100	LYS	2.1
1	A	336	LEU	2.0
1	A	527	ASN	2.0
1	A	562	HIS	2.0
1	A	468	GLY	2.0
1	A	521	CYS	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](#)

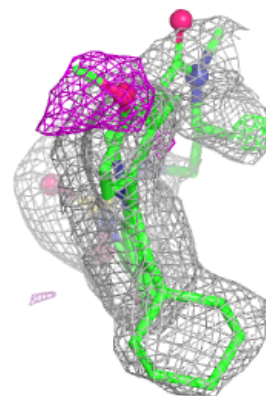
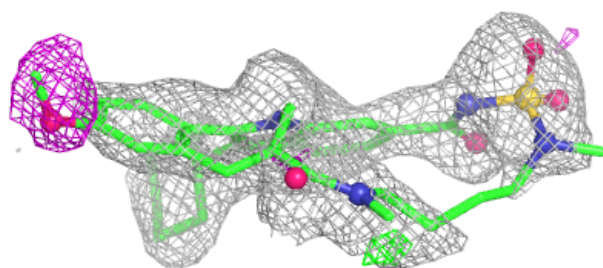
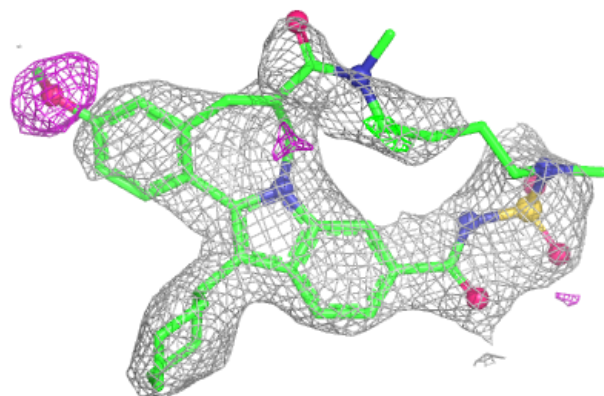
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	B	606	5/5	0.72	0.11	104,104,106,107	0
3	SO4	B	607	5/5	0.76	0.17	40,59,65,75	0
3	SO4	B	610	5/5	0.77	0.12	74,79,83,84	0
3	SO4	B	604	5/5	0.78	0.14	79,83,90,93	0
3	SO4	A	604	5/5	0.78	0.10	92,96,97,99	0
3	SO4	B	608	5/5	0.79	0.11	56,60,69,76	0
4	GOL	A	607	6/6	0.80	0.18	47,58,63,65	0
4	GOL	B	615	6/6	0.81	0.15	44,56,59,61	0
2	OLN	A	601	42/42	0.82	0.20	75,91,104,107	0
3	SO4	B	611	5/5	0.82	0.17	56,65,79,83	0
4	GOL	B	613	6/6	0.84	0.20	56,61,65,65	0
4	GOL	A	606	6/6	0.85	0.17	48,58,59,68	0
3	SO4	B	609	5/5	0.85	0.16	85,88,91,91	0
3	SO4	A	605	5/5	0.86	0.20	88,92,94,98	0
3	SO4	A	602	5/5	0.86	0.11	59,60,64,64	0
4	GOL	B	614	6/6	0.88	0.18	44,53,59,60	0
4	GOL	B	616	6/6	0.89	0.15	41,45,53,53	0
3	SO4	A	603	5/5	0.90	0.14	68,76,80,85	0
3	SO4	B	603	5/5	0.91	0.20	42,53,63,69	0
3	SO4	B	605	5/5	0.92	0.16	49,55,62,62	0
3	SO4	B	601	5/5	0.96	0.08	37,39,46,47	0
4	GOL	B	612	6/6	0.96	0.07	29,34,40,42	0
3	SO4	B	602	5/5	0.97	0.13	37,42,48,53	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 0LN A 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.