



Full wwPDB EM Validation Report ⓘ

May 17, 2026 – 12:11 AM JST

PDB ID : 9V7N / pdb_00009v7n
EMDB ID : EMD-64818
Title : Cryo-EM structures of the Azoarcus pre-tRNA(ILE) conformation a undergoing the first-step self-splicing
Authors : Hong, Y.; Liu, J.; Zhang, X.; Liu, J.; Li, S.; Zhang, K.
Deposited on : 2025-05-28
Resolution : 3.11 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

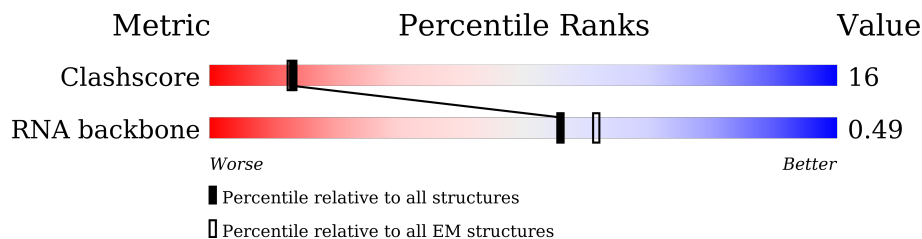
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

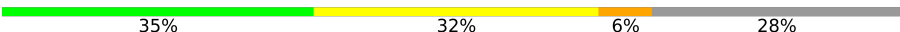
The reported resolution of this entry is 3.11 Å.

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)	EM structures (#Entries)
Clashscore	229148	23984
RNA backbone	8273	3508

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	B	284	 35% 32% 6% 28%
1	D	284	 • 5% 7% 86%
1	E	284	 • 11% • 86%

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:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GMP	B	301	-	-	X	-

2 Entry composition [i](#)

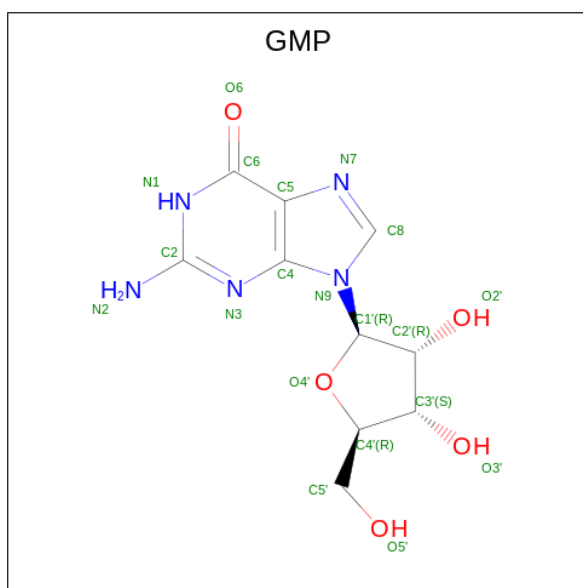
There are 3 unique types of molecules in this entry. The entry contains 6109 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 RNA chain called RNA (284-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	205	Total	C	N	O	P	0	0
			4401	1963	821	1412	205		
1	D	39	Total	C	N	O	P	0	0
			831	370	145	277	39		
1	E	40	Total	C	N	O	P	0	0
			851	379	150	282	40		

- Molecule 2 is GUANOSINE (CCD ID: GMP) (formula: $C_{10}H_{13}N_5O_5$).



Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C	N	O	0
			20	10	5	5	

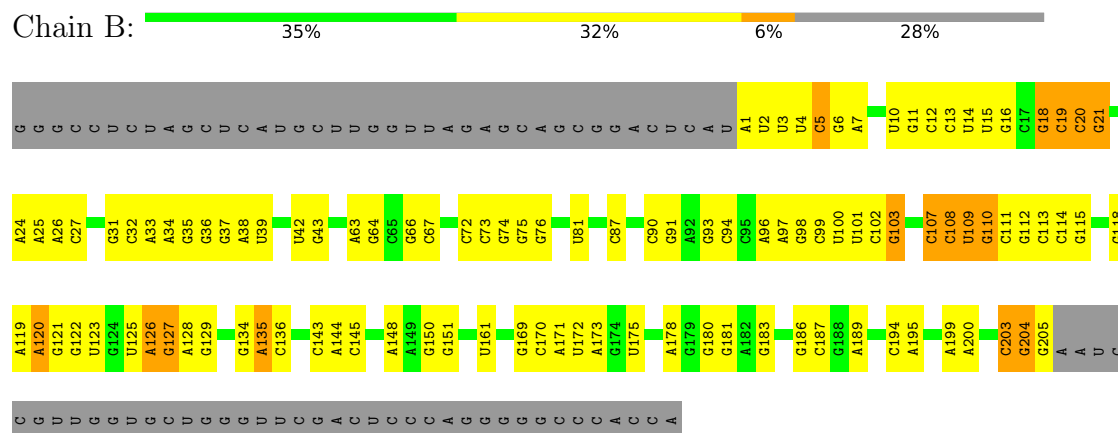
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
3	B	6	Total	Mg	0
			6	6	

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. 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. 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 (284-MER)



C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	105746	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GMP

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	B	0.39	0/4928	0.41	0/7686
1	D	0.21	0/927	0.39	0/1441
1	E	0.11	0/949	0.26	0/1477
All	All	0.35	0/6804	0.39	0/10604

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4401	0	2225	87	0
1	D	831	0	419	34	0
1	E	851	0	433	38	0
2	B	20	0	11	12	0
3	B	6	0	0	0	0
All	All	6109	0	3088	148	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 16.

All (148) 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:126:A:H1'	2:B:301:GMP:N2	1.40	1.32
1:B:126:A:C1'	2:B:301:GMP:N2	1.97	1.27
1:B:126:A:O2'	2:B:301:GMP:N2	1.68	1.23
1:B:126:A:C2'	2:B:301:GMP:HN22	1.60	1.14
1:B:126:A:C2'	2:B:301:GMP:N2	2.15	1.07
1:B:126:A:H1'	2:B:301:GMP:C2	1.91	1.06
1:B:126:A:N3	2:B:301:GMP:N1	2.14	0.95
1:D:30:G:H1	1:E:46:U:H3	1.19	0.88
1:D:25:G:H2'	1:D:26:A:C8	2.24	0.72
1:B:126:A:C1'	2:B:301:GMP:HN21	2.05	0.69
1:B:111:C:H2'	1:B:112:G:H8	1.57	0.69
1:B:143:C:H2'	1:B:144:A:H8	1.59	0.68
1:B:126:A:HO2'	2:B:301:GMP:HN22	1.41	0.68
1:B:111:C:H2'	1:B:112:G:C8	2.29	0.67
1:B:33:A:H2'	1:B:34:A:C8	2.31	0.66
1:D:6:U:H3	1:E:70:G:H1	1.44	0.65
1:B:12:C:H2'	1:B:13:C:C6	2.31	0.65
1:D:25:G:H2'	1:D:26:A:H8	1.62	0.65
1:E:66:C:H2'	1:E:67:A:H8	1.62	0.64
1:E:71:G:H2'	1:E:72:G:H8	1.61	0.64
1:D:31:C:H2'	1:D:32:G:H8	1.64	0.63
1:D:31:C:H2'	1:D:32:G:C8	2.34	0.63
1:B:118:G:H2'	1:B:119:A:H8	1.63	0.62
1:B:33:A:H2'	1:B:34:A:H8	1.67	0.59
1:E:66:C:H2'	1:E:67:A:C8	2.39	0.58
1:D:8:U:H5'	1:E:52:C:H5''	1.87	0.57
1:B:42:U:H2'	1:B:43:G:H8	1.71	0.56
1:D:11:C:H2'	1:D:12:U:C6	2.41	0.56
1:E:63:U:H5''	1:E:64:C:C5	2.42	0.55
1:B:25:A:H2'	1:B:26:A:C8	2.41	0.55
1:B:143:C:H2'	1:B:144:A:C8	2.40	0.55
1:D:26:A:H2'	1:D:27:G:C8	2.42	0.54
1:E:69:G:H2'	1:E:70:G:H8	1.73	0.54
1:D:2:G:H2'	1:D:3:G:H8	1.72	0.54
1:B:24:A:H2'	1:B:25:A:C8	2.43	0.54
1:E:71:G:H2'	1:E:72:G:C8	2.41	0.54
1:B:144:A:H2'	1:B:145:C:H6	1.73	0.53
1:E:70:G:H2'	1:E:71:G:H8	1.74	0.53
1:E:65:C:H2'	1:E:66:C:H6	1.74	0.53
1:D:21:G:H4'	1:D:22:U:O5'	2.10	0.52
1:B:118:G:H2'	1:B:119:A:C8	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:C:H2'	1:B:14:U:C6	2.45	0.52
1:B:90:C:H2'	1:B:91:G:H8	1.75	0.52
1:B:109:U:H4'	1:B:110:G:C8	2.46	0.51
1:B:10:U:H2'	1:B:11:G:H8	1.75	0.51
1:B:96:A:H2'	1:B:97:A:C8	2.45	0.51
1:B:19:C:O2'	1:B:20:C:H5'	2.11	0.51
1:D:30:G:N2	1:E:46:U:O2	2.38	0.51
1:B:144:A:H2'	1:B:145:C:C6	2.46	0.51
1:E:65:C:H2'	1:E:66:C:C6	2.46	0.50
1:B:75:G:H2'	1:B:76:G:H8	1.77	0.50
1:B:31:G:H2'	1:B:32:C:C6	2.46	0.50
1:E:68:G:H2'	1:E:69:G:H8	1.77	0.50
1:B:110:G:H2'	1:B:111:C:O4'	2.11	0.50
1:B:18:G:H2'	1:B:19:C:H5'	1.94	0.50
1:D:25:G:N7	1:E:49:G:O6	2.45	0.50
1:B:108:C:H2'	1:B:110:G:C2	2.47	0.49
1:B:13:C:H2'	1:B:14:U:H6	1.78	0.49
1:B:26:A:H2'	1:B:27:C:O4'	2.13	0.49
1:B:75:G:H2'	1:B:76:G:C8	2.46	0.49
1:D:38:A:H2'	1:D:39:U:C6	2.48	0.49
1:B:126:A:C3'	2:B:301:GMP:HN22	2.23	0.49
1:B:172:U:H2'	1:B:173:A:C8	2.48	0.49
1:B:63:A:H2'	1:B:64:G:O4'	2.13	0.49
1:B:42:U:H2'	1:B:43:G:C8	2.47	0.48
1:E:67:A:H2'	1:E:68:G:H8	1.78	0.48
1:B:134:G:O2'	1:B:135:A:H8	1.96	0.48
1:D:8:U:H2'	1:D:13:C:H41	1.79	0.48
1:D:2:G:H2'	1:D:3:G:C8	2.47	0.48
1:B:1:A:C8	1:D:39:U:H2'	2.49	0.47
1:B:126:A:N3	2:B:301:GMP:C2	2.82	0.47
1:D:18:U:O4'	1:E:64:C:H4'	2.14	0.47
1:D:10:G:H2'	1:D:11:C:C6	2.48	0.47
1:E:77:C:H2'	1:E:78:C:C6	2.50	0.47
1:B:113:C:H2'	1:B:114:C:C6	2.49	0.47
1:B:172:U:H2'	1:B:173:A:H8	1.79	0.47
1:E:53:U:H2'	1:E:54:G:C8	2.50	0.46
1:E:53:U:H2'	1:E:54:G:H8	1.80	0.46
1:E:75:C:H2'	1:E:76:A:C8	2.50	0.46
1:D:1:G:H2'	1:D:2:G:C8	2.50	0.46
1:B:113:C:H2'	1:B:114:C:H6	1.81	0.46
1:B:203:C:H3'	1:B:204:G:N2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:C:H2'	1:B:110:G:N1	2.31	0.46
1:B:180:G:H2'	1:B:181:G:O4'	2.16	0.46
1:E:69:G:H2'	1:E:70:G:C8	2.51	0.46
1:E:78:C:H2'	1:E:79:A:O4'	2.15	0.46
1:B:127:G:H5''	2:B:301:GMP:O4'	2.15	0.46
1:B:38:A:H8	1:B:38:A:O5'	1.99	0.46
1:E:68:G:H2'	1:E:69:G:C8	2.52	0.46
1:B:120:A:H5'	1:B:121:G:OP2	2.17	0.45
1:B:189:A:H8	1:B:189:A:P	2.39	0.45
1:D:22:U:H5''	1:D:23:U:H2'	1.97	0.45
1:E:40:A:C2	1:E:41:A:H1'	2.51	0.45
1:B:66:G:H2'	1:B:67:C:C6	2.51	0.45
1:B:107:C:H4'	1:B:108:C:H5	1.82	0.45
1:E:70:G:H2'	1:E:71:G:C8	2.51	0.45
1:D:22:U:H3'	1:D:23:U:H2'	1.97	0.45
1:D:1:G:H2'	1:D:2:G:H8	1.82	0.45
1:B:72:C:H2'	1:B:73:C:C5	2.52	0.44
1:D:29:A:C4	1:D:30:G:C8	3.05	0.44
1:B:18:G:C2'	1:B:19:C:H5'	2.46	0.44
1:B:127:G:N2	1:B:178:A:H1'	2.32	0.44
1:B:72:C:H2'	1:B:73:C:C6	2.53	0.44
1:B:73:C:H3'	1:B:74:G:H8	1.81	0.44
1:B:114:C:H2'	1:B:115:G:C8	2.53	0.44
1:B:96:A:H2'	1:B:97:A:H8	1.82	0.44
1:E:42:U:H2'	1:E:43:C:H6	1.82	0.44
1:D:6:U:H2'	1:D:7:C:C6	2.53	0.43
1:B:101:U:H2'	1:B:102:C:C6	2.53	0.43
1:B:63:A:C8	1:B:189:A:N1	2.86	0.43
1:B:93:G:C6	1:B:94:C:C4	3.07	0.43
1:D:9:A:H1'	1:E:48:G:H2'	2.00	0.43
1:B:150:G:C6	1:B:151:G:C5	3.07	0.43
1:B:20:C:C4	1:B:21:G:H1'	2.54	0.43
1:B:98:G:C5	1:B:99:C:C5	3.07	0.43
1:B:122:G:C5	1:B:123:U:C5	3.06	0.43
1:B:24:A:OP1	1:B:24:A:H8	2.01	0.43
1:D:11:C:H2'	1:D:12:U:H6	1.83	0.43
1:D:15:U:O2	1:D:24:A:H1'	2.19	0.43
1:E:42:U:H2'	1:E:43:C:C6	2.53	0.43
1:B:25:A:C6	1:B:26:A:C6	3.07	0.42
1:B:34:A:H2'	1:B:35:G:C8	2.54	0.42
1:B:31:G:H2'	1:B:32:C:H6	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:G:H2'	1:B:67:C:H6	1.83	0.42
1:B:38:A:O2'	1:B:39:U:H5'	2.18	0.42
1:B:194:C:H2'	1:B:195:A:H8	1.85	0.42
1:E:47:U:H2'	1:E:48:G:C8	2.54	0.42
1:B:5:C:C4	1:E:41:A:H8	2.37	0.42
1:B:32:C:H2'	1:B:33:A:C8	2.55	0.41
1:B:103:G:C6	1:B:115:G:N1	2.88	0.41
1:B:15:U:H2'	1:B:16:G:C8	2.55	0.41
1:B:194:C:H2'	1:B:195:A:C8	2.54	0.41
1:E:52:C:H2'	1:E:53:U:H6	1.85	0.41
1:E:67:A:H2'	1:E:68:G:C8	2.54	0.41
1:D:14:A:C6	1:D:25:G:C6	3.08	0.41
1:D:34:A:H5'	1:D:35:C:C5	2.56	0.41
1:B:114:C:H2'	1:B:115:G:H8	1.86	0.41
1:B:134:G:C8	1:B:135:A:C8	3.09	0.41
1:D:38:A:H2'	1:D:39:U:H6	1.84	0.41
1:E:43:C:H2'	1:E:44:C:C6	2.56	0.41
1:E:52:C:H2'	1:E:53:U:C6	2.56	0.41
1:E:66:C:C2	1:E:67:A:C8	3.09	0.41
1:E:73:C:H2'	1:E:74:C:C6	2.56	0.41
1:B:1:A:H8	1:D:39:U:H2'	1.84	0.40
1:B:99:C:N3	1:B:100:U:C5	2.89	0.40
1:D:10:G:OP1	1:E:49:G:H5'	2.20	0.40
1:B:186:G:H2'	1:B:187:C:H6	1.87	0.40
1:D:35:C:O2'	1:D:36:U:H5''	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	204/284 (71%)	38 (18%)	2 (0%)
1	D	38/284 (13%)	22 (57%)	2 (5%)
1	E	39/284 (13%)	13 (33%)	1 (2%)
All	All	281/852 (32%)	73 (25%)	5 (1%)

All (73) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	2	U
1	B	3	U
1	B	4	U
1	B	5	C
1	B	6	G
1	B	7	A
1	B	18	G
1	B	19	C
1	B	20	C
1	B	21	G
1	B	37	G
1	B	81	U
1	B	87	C
1	B	103	G
1	B	107	C
1	B	108	C
1	B	109	U
1	B	110	G
1	B	120	A
1	B	125	U
1	B	126	A
1	B	127	G
1	B	128	A
1	B	129	G
1	B	135	A
1	B	136	C
1	B	148	A
1	B	161	U
1	B	169	G
1	B	170	C
1	B	171	A
1	B	175	U
1	B	183	G
1	B	199	A
1	B	200	A

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Mol	Chain	Res	Type
1	B	203	C
1	B	204	G
1	B	205	G
1	D	7	C
1	D	8	U
1	D	10	G
1	D	11	C
1	D	13	C
1	D	14	A
1	D	17	C
1	D	18	U
1	D	19	U
1	D	20	G
1	D	21	G
1	D	22	U
1	D	23	U
1	D	24	A
1	D	25	G
1	D	26	A
1	D	27	G
1	D	28	C
1	D	32	G
1	D	34	A
1	D	35	C
1	D	36	U
1	E	41	A
1	E	42	U
1	E	45	G
1	E	49	G
1	E	50	U
1	E	51	G
1	E	52	C
1	E	55	G
1	E	56	G
1	E	57	U
1	E	62	C
1	E	63	U
1	E	64	C

All (5) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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Mol	Chain	Res	Type
1	B	4	U
1	B	36	G
1	D	21	G
1	D	31	C
1	E	62	C

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 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 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
2	GMP	B	301	3	22,22,22	0.38	0	33,33,33	0.41	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
2	GMP	B	301	3	-	2/6/22/22	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

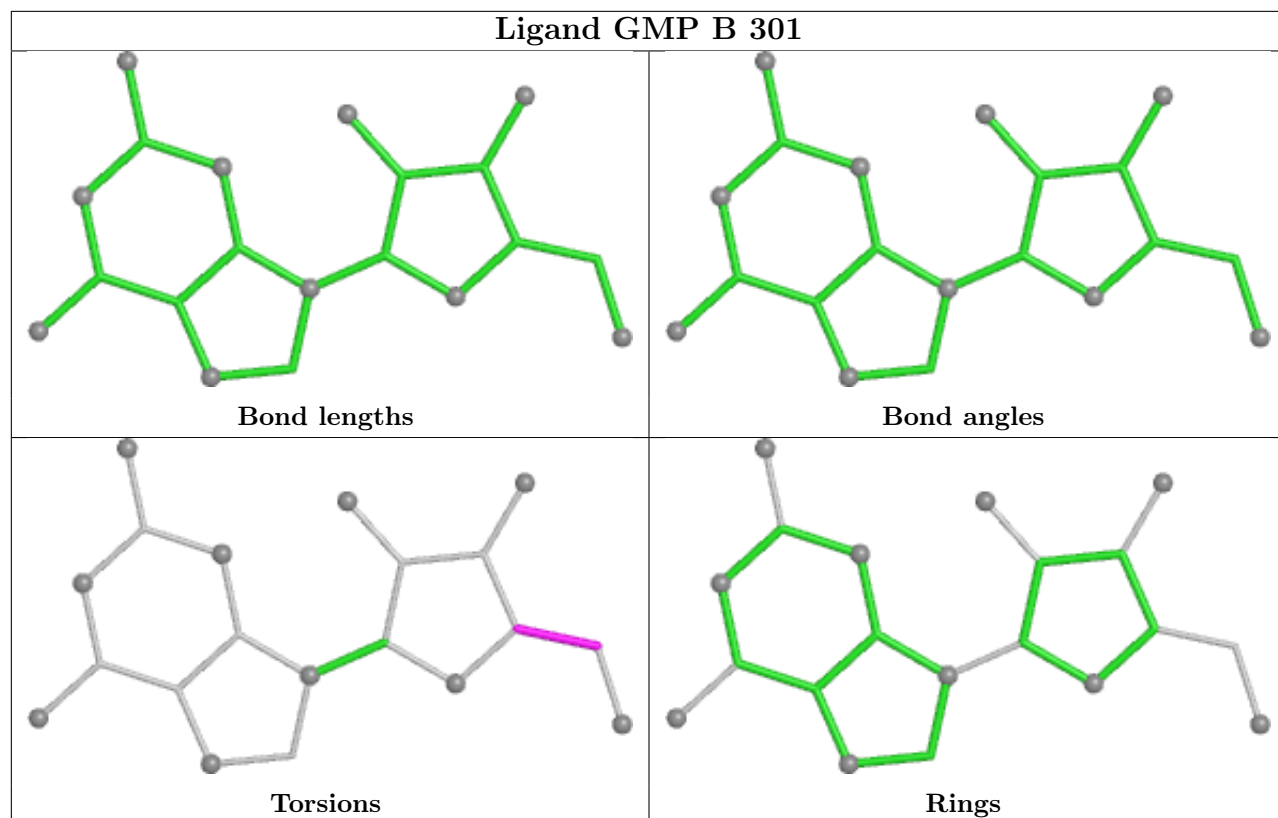
Mol	Chain	Res	Type	Atoms
2	B	301	GMP	C3'-C4'-C5'-O5'
2	B	301	GMP	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	GMP	12	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.