



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:52 AM UTC

PDB ID : 7SFD / pdb_00007sfd
Title : Human DNMT1(729-1600) Bound to Zebularine-Containing 12mer dsDNA and Inhibitor GSK3543105A
Authors : Horton, J.R.; Pathuri, S.; Cheng, X.
Deposited on : 2021-10-03
Resolution : 2.09 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

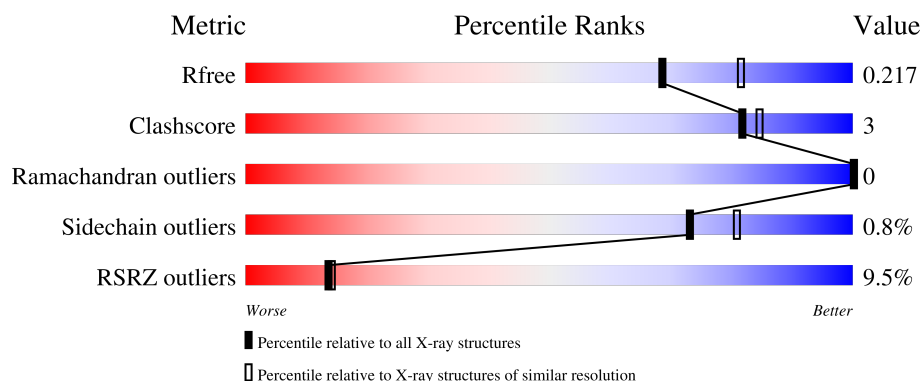
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	874	9% 91% 6% .
2	C	12	67% 33%
3	D	12	8% 67% 33%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7262 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 DNA (cytosine-5)-methyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	842	Total	C	N	O	S	0	4	0
			6439	4093	1127	1177	42			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	727	HIS	-	expression tag	UNP P26358
A	728	MET	-	expression tag	UNP P26358

- Molecule 2 is a DNA chain called DNA (12-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	12	Total	C	N	O	P	0	0	0
			244	116	47	70	11			

- Molecule 3 is a DNA chain called DNA (12-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	12	Total	C	N	O	P	0	0	0
			243	115	46	71	11			

- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C₁₄H₂₀N₆O₅S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			26	14	6	5		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



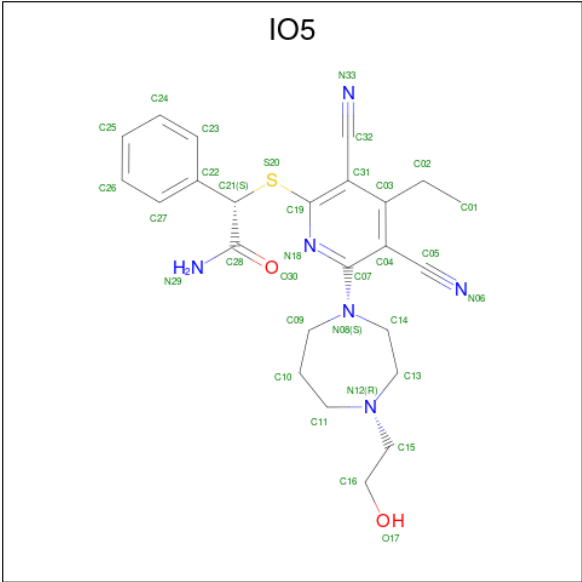
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 8 is (2S)-2-({3,5-dicyano-4-ethyl-6-[4-(2-hydroxyethyl)-1,4-diazepan-1-yl]pyridin-2-yl}sulfanyl)-2-phenylacetamide (CCD ID: IO5) (formula: C₂₄H₂₈N₆O₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	C	1	Total	C	N	O	S	0	0
			33	24	6	2	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	248	Total	O	0	0
			248	248		
9	C	2	Total	O	0	0
			2	2		
9	D	1	Total	O	0	0
			1	1		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	161.60Å 77.42Å 116.51Å 90.00° 125.76° 90.00°	Depositor
Resolution (Å)	41.81 – 2.09 41.81 – 2.09	Depositor EDS
% Data completeness (in resolution range)	96.1 (41.81-2.09) 88.5 (41.81-2.09)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.185 , 0.216 0.186 , 0.217	Depositor DCC
R_{free} test set	1968 reflections (2.85%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7262	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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: IO5, GOL, ZN, 5CM, PYO, EDO, SAH

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	0.22	0/6617	0.39	0/9013
2	C	0.23	0/250	0.39	0/382
3	D	0.22	0/250	0.38	0/382
All	All	0.22	0/7117	0.39	0/9777

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 [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	6439	0	6079	30	0
2	C	244	0	137	2	0
3	D	243	0	134	2	0
4	A	26	0	19	0	0
5	A	2	0	0	0	0
6	A	12	0	18	1	0
7	A	12	0	16	3	0
8	C	33	0	0	1	0
9	A	248	0	0	3	0
9	C	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	D	1	0	0	0	0
All	All	7262	0	6403	34	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 (34) 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:1446:LEU:HD12	1:A:1450:THR:HB	1.71	0.71
1:A:1266:GLU:OE2	1:A:1312[B]:ARG:HD2	2.00	0.60
1:A:1476:CYS:HB3	1:A:1478:CYS:SG	2.42	0.59
1:A:790:GLN:HB3	1:A:825:LEU:HD12	1.86	0.58
1:A:731:ILE:HG13	1:A:752:ILE:HG12	1.86	0.58
1:A:1187:PHE:HB3	1:A:1189:GLU:HG3	1.88	0.55
1:A:777:ALA:HB2	1:A:796:TRP:CE3	2.43	0.54
1:A:884:PRO:HB3	1:A:892:PHE:CG	2.43	0.54
2:C:2:DA:H2'	2:C:3:DG:C8	2.43	0.53
1:A:1497:PRO:O	1:A:1501:PRO:HD2	2.11	0.50
1:A:1333:VAL:HA	7:A:1707:GOL:H12	1.93	0.50
8:C:101:IO5:C05	8:C:101:IO5:C09	2.90	0.50
1:A:1533:MET:HE1	2:C:4:DG:H2'	1.95	0.49
1:A:1207[B]:ARG:NH1	9:A:1811:HOH:O	2.43	0.49
6:A:1704:EDO:H12	3:D:19:DG:H5'	1.94	0.49
1:A:1311:ARG:O	1:A:1312[A]:ARG:NH1	2.35	0.49
3:D:21:DC:H2''	3:D:22:DC:O5'	2.12	0.49
1:A:1232:MET:HE1	1:A:1273:SER:HB2	1.95	0.48
1:A:1098:ASP:CG	1:A:1099:PRO:HD2	2.39	0.48
1:A:921:VAL:HG21	1:A:1009:PRO:HG3	1.97	0.46
1:A:1168:GLU:O	1:A:1188:THR:HA	2.16	0.46
1:A:866:GLN:HG3	1:A:867:LEU:HG	1.98	0.46
1:A:1312[B]:ARG:HH22	7:A:1708:GOL:H31	1.80	0.46
1:A:847:GLY:HA3	1:A:1256:ASP:O	2.17	0.45
1:A:1454:LYS:HD2	1:A:1456:ARG:HH21	1.81	0.45
1:A:1459:HIS:O	1:A:1472:LEU:HB3	2.17	0.44
1:A:1020:LYS:O	1:A:1045:SER:HB3	2.17	0.43
1:A:1333:VAL:HA	7:A:1707:GOL:C1	2.48	0.43
1:A:1389:ASN:ND2	9:A:1812:HOH:O	2.43	0.43
1:A:1285:ARG:NE	9:A:1822:HOH:O	2.51	0.43
1:A:1087:GLU:HA	1:A:1099:PRO:HD3	2.00	0.42
1:A:776:LEU:HD22	1:A:832:VAL:HG21	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:792:PHE:CE2	1:A:794:ALA:HB2	2.56	0.40
1:A:1188:THR:C	1:A:1189:GLU:HG2	2.46	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	842/874 (96%)	817 (97%)	25 (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	657/753 (87%)	652 (99%)	5 (1%)	73	81

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1030	SER
1	A	1267	ASN
1	A	1450	THR
1	A	1494	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1536	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	829	HIS
1	A	871	GLN
1	A	1081	ASN
1	A	1157	GLN
1	A	1303	GLN
1	A	1340	GLN
1	A	1389	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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
2	5CM	C	6	2,3	18,21,22	1.70	6 (33%)	24,30,33	1.82	8 (33%)
3	PYO	D	18	2,3	16,20,21	1.26	3 (18%)	21,28,31	0.62	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	5CM	C	6	2,3	-	5/7/21/22	0/2/2/2
3	PYO	D	18	2,3	-	0/7/25/26	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	6	5CM	C2-N1	3.77	1.48	1.40
2	C	6	5CM	O2-C2	-3.60	1.17	1.23
3	D	18	PYO	C2-N1	3.24	1.46	1.40
3	D	18	PYO	O2-C2	-2.65	1.18	1.23
2	C	6	5CM	C6-C5	2.59	1.38	1.34
2	C	6	5CM	C5-C4	-2.33	1.42	1.44
2	C	6	5CM	C6-N1	2.14	1.41	1.38
3	D	18	PYO	C6-N1	-2.08	1.33	1.38
2	C	6	5CM	C4-N3	2.06	1.37	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	6	5CM	C6-N1-C2	-3.64	116.11	120.95
2	C	6	5CM	C1'-N1-C2	3.60	124.00	117.83
2	C	6	5CM	O4'-C1'-N1	3.59	114.24	107.86
2	C	6	5CM	C5A-C5-C6	-3.11	118.64	122.85
2	C	6	5CM	O2-C2-N3	-2.56	118.30	122.33
2	C	6	5CM	C4-N3-C2	-2.31	117.61	120.81
2	C	6	5CM	N1-C2-N3	2.22	122.66	118.80
2	C	6	5CM	C5-C6-N1	-2.04	121.10	123.31

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	6	5CM	C2'-C1'-N1-C6
2	C	6	5CM	O4'-C1'-N1-C6
2	C	6	5CM	C2'-C1'-N1-C2
2	C	6	5CM	O4'-C1'-N1-C2
2	C	6	5CM	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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
4	SAH	A	1701	-	27,28,28	1.15	3 (11%)	36,40,40	0.84	1 (2%)
7	GOL	A	1708	-	5,5,5	1.07	0	5,5,5	0.98	0
7	GOL	A	1707	-	5,5,5	0.80	0	5,5,5	1.14	0
8	IO5	C	101	-	33,35,35	0.97	1 (3%)	37,47,47	1.24	4 (10%)
6	EDO	A	1706	-	3,3,3	0.44	0	2,2,2	0.37	0
6	EDO	A	1705	-	3,3,3	0.49	0	2,2,2	0.28	0
6	EDO	A	1704	-	3,3,3	0.40	0	2,2,2	0.39	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	SAH	A	1701	-	-	1/15/31/31	0/3/3/3
7	GOL	A	1708	-	-	2/4/4/4	-
7	GOL	A	1707	-	-	0/4/4/4	-
8	IO5	C	101	-	-	2/19/36/36	0/3/3/3
6	EDO	A	1706	-	-	0/1/1/1	-
6	EDO	A	1705	-	-	0/1/1/1	-
6	EDO	A	1704	-	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1701	SAH	C8-N9	3.03	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	101	IO5	C04-C03	-3.02	1.37	1.40
4	A	1701	SAH	C8-N7	2.34	1.36	1.31
4	A	1701	SAH	C2'-C3'	2.01	1.58	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	101	IO5	N18-C07-N08	-3.13	110.88	116.77
8	C	101	IO5	C14-N08-C07	-2.92	113.97	120.19
8	C	101	IO5	C19-C31-C32	2.85	123.00	119.77
4	A	1701	SAH	O4'-C1'-N9	-2.19	103.88	108.09
8	C	101	IO5	C27-C22-C23	2.02	120.81	118.30

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	101	IO5	C16-C15-N12-C13
8	C	101	IO5	N12-C15-C16-O17
7	A	1708	GOL	C1-C2-C3-O3
7	A	1708	GOL	O2-C2-C3-O3
4	A	1701	SAH	C2'-C1'-N9-C8

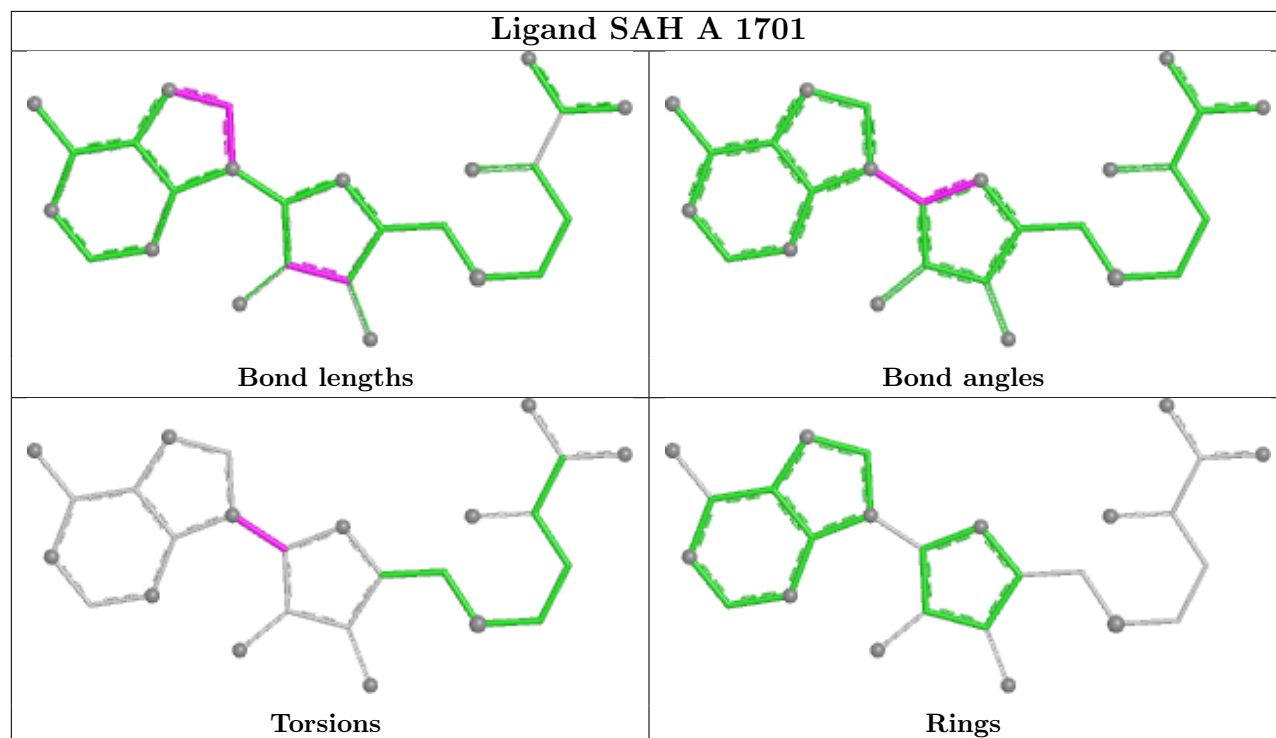
There are no ring outliers.

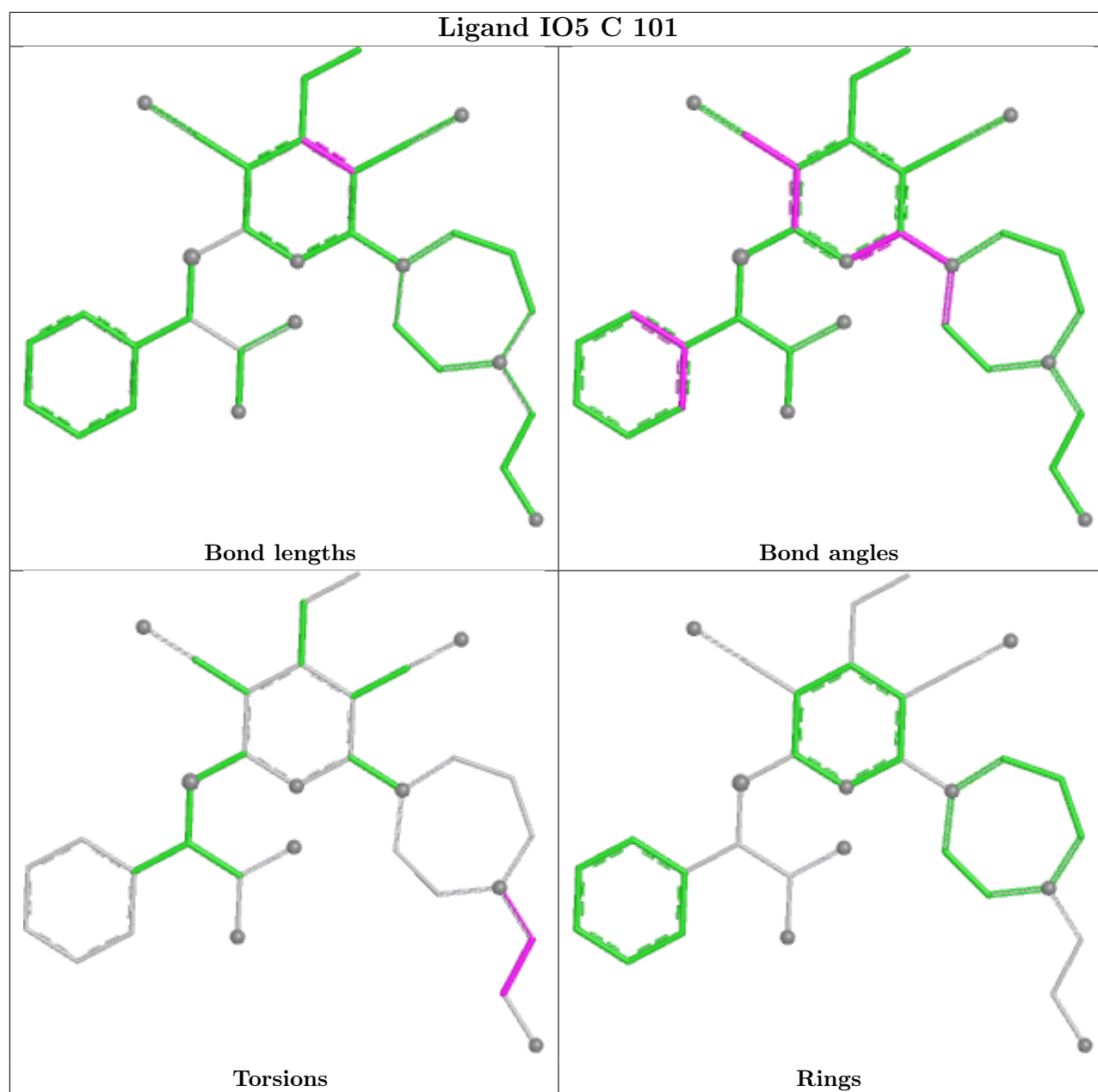
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1708	GOL	1	0
7	A	1707	GOL	2	0
8	C	101	IO5	1	0
6	A	1704	EDO	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	842/874 (96%)	0.48	81 (9%) 13 14	18, 52, 106, 142	4 (0%)
2	C	11/12 (91%)	0.61	0 100 100	82, 99, 150, 153	0
3	D	11/12 (91%)	0.99	1 (9%) 15 15	94, 107, 158, 174	0
All	All	864/898 (96%)	0.49	82 (9%) 14 14	18, 53, 109, 174	4 (0%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1229	PHE	5.5
1	A	1233	ASN	4.2
1	A	956	VAL	4.1
1	A	1484	ALA	3.7
1	A	860	GLY	3.6
1	A	1091	ALA	3.6
1	A	1103	ALA	3.5
1	A	850	ASP	3.5
1	A	1480	GLU	3.4
1	A	950	ILE	3.4
1	A	952	LEU	3.3
1	A	955	PRO	3.2
1	A	1064	TYR	3.2
1	A	738	VAL	3.2
1	A	1472	LEU	3.1
1	A	1230	SER	3.1
1	A	1231	GLY	3.1
1	A	1068	LEU	3.1
1	A	1464	ASN	3.1
1	A	958	ARG	3.0
1	A	737	ALA	3.0
1	A	849	MET	3.0
1	A	1483	LYS	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	957	LYS	2.9
1	A	1097	GLU	2.9
1	A	1237	SER	2.9
1	A	1498	TRP	2.9
1	A	954	SER	2.9
1	A	1600	ALA	2.9
1	A	1228	GLY	2.9
1	A	1227	GLN	2.8
1	A	1044	TRP	2.8
1	A	1104	ARG	2.8
1	A	1239	THR	2.8
1	A	1232	MET	2.8
1	A	918	ASP	2.8
1	A	1099	PRO	2.8
1	A	1096	PHE	2.7
1	A	1455	LEU	2.7
1	A	1457	TYR	2.7
1	A	788	ASN	2.6
1	A	754	ALA	2.6
1	A	1488	ALA	2.6
1	A	1226	CYS	2.5
1	A	1461	ASP	2.5
1	A	1234	ARG	2.5
1	A	1471	ALA	2.5
1	A	960	ARG	2.5
1	A	1088	ALA	2.4
1	A	1019	ASN	2.4
1	A	962	GLU	2.4
1	A	1072	VAL	2.4
1	A	753	ASP	2.4
1	A	1475	VAL	2.4
1	A	1470	GLY	2.3
1	A	731	ILE	2.3
1	A	1005	SER	2.3
1	A	729	ASN	2.3
1	A	1092	LYS	2.3
1	A	1235	PHE	2.3
1	A	853	SER	2.3
1	A	1460	HIS	2.3
1	A	907	ILE	2.3
1	A	1487	PRO	2.3
1	A	1462	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1006	ASN	2.2
1	A	748	LYS	2.2
1	A	947	THR	2.2
3	D	19	DG	2.2
1	A	854	LEU	2.2
1	A	1071	CYS	2.2
1	A	1465	GLY	2.1
1	A	1531	GLU	2.1
1	A	734	VAL	2.1
1	A	976	TYR	2.1
1	A	1492	PHE	2.0
1	A	757	LEU	2.0
1	A	922	LEU	2.0
1	A	1067	ASP	2.0
1	A	730	ARG	2.0
1	A	885	THR	2.0
1	A	970	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
3	PYO	D	18	19/20	0.77	0.17	111,119,131,136	0
2	5CM	C	6	20/21	0.94	0.11	73,81,87,92	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

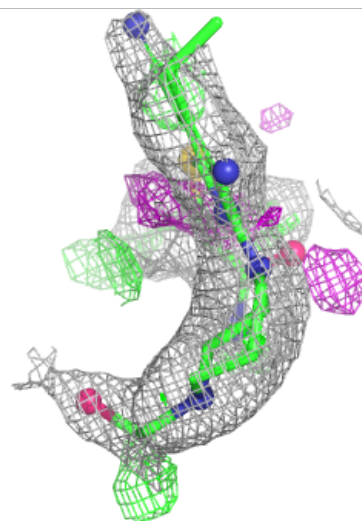
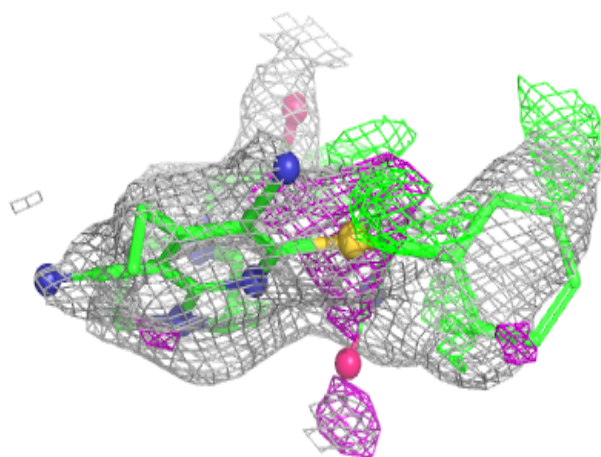
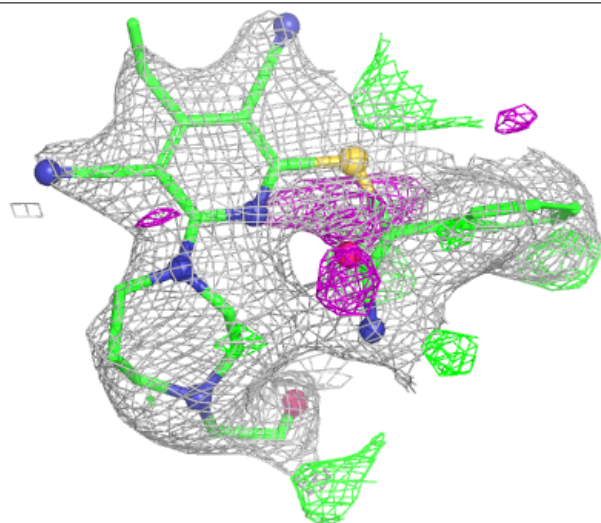
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

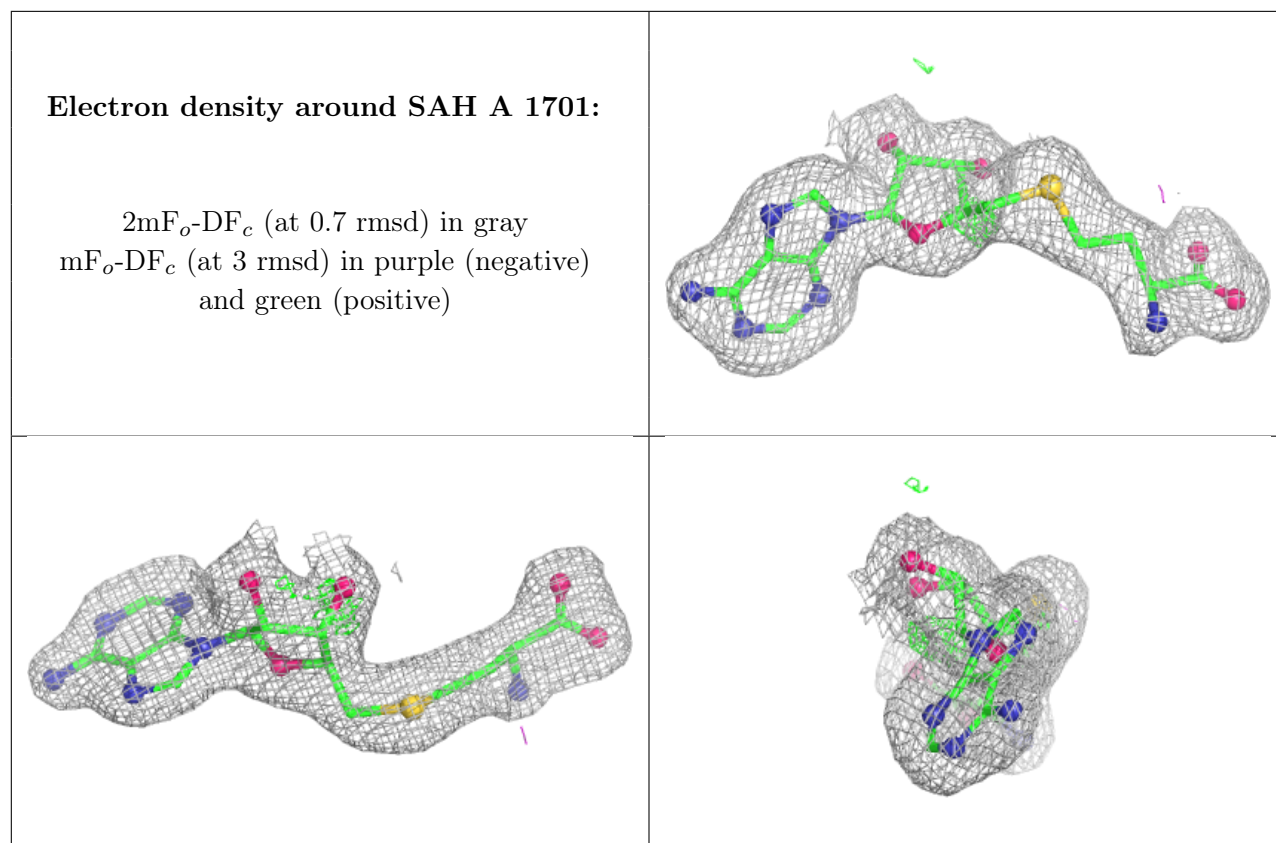
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	GOL	A	1708	6/6	0.67	0.20	58,60,65,72	0
8	IO5	C	101	33/33	0.76	0.20	69,86,102,104	0
6	EDO	A	1704	4/4	0.79	0.19	57,59,66,69	0
6	EDO	A	1706	4/4	0.81	0.16	79,88,88,91	0
7	GOL	A	1707	6/6	0.83	0.20	45,53,63,70	0
6	EDO	A	1705	4/4	0.93	0.14	46,54,55,55	0
5	ZN	A	1702	1/1	0.95	0.09	102,102,102,102	0
4	SAH	A	1701	26/26	0.97	0.06	25,34,39,41	0
5	ZN	A	1703	1/1	0.98	0.05	49,49,49,49	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 IO5 C 101:

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.