



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:42 PM UTC

PDB ID : 5GUT / pdb_00005gut
Title : The crystal structure of mouse DNMT1 (731-1602) mutant - N1248A
Authors : Chen, S.J.; Ye, F.
Deposited on : 2016-08-31
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

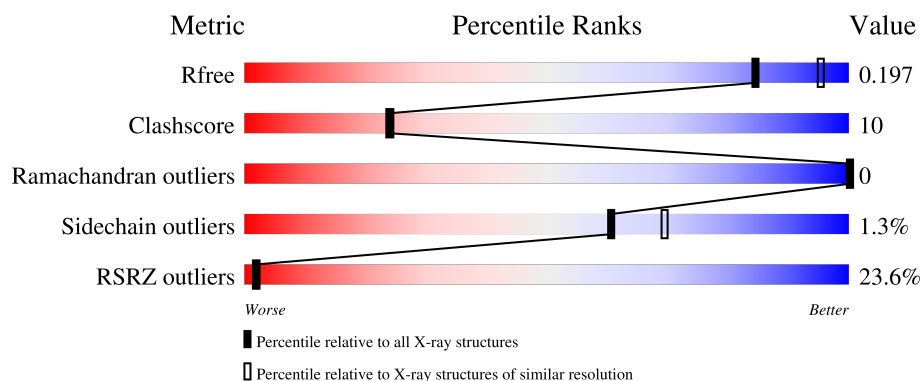
1 Overall quality at a glance

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	872	21% 73% 17% 9%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6962 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.

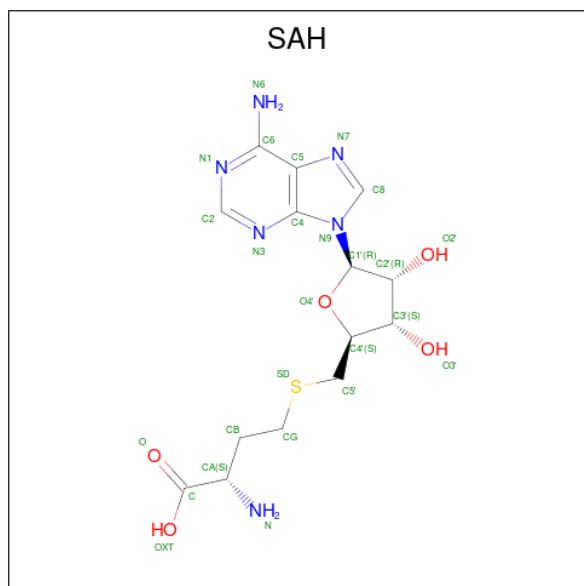
- Molecule 1 is a protein called DNA (cytosine-5)-methyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	794	6405	4071	1124	1168	42	0	7	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1248	ALA	ASN	engineered mutation	UNP P13864

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	479	Total 479	O 479	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.42Å 78.55Å 164.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.36 – 2.10 44.36 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.6 (44.36-2.10) 96.6 (44.36-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.36 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.200 , 0.231 (Not available) , 0.197	Depositor DCC
R_{free} test set	2839 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 60.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6962	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SAH, ZN, SO4

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	0.56	2/6593 (0.0%)	0.97	20/8925 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1279	ARG	C-N	6.82	1.43	1.33
1	A	1222	MET	SD-CE	-5.46	1.65	1.79

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	781	ARG	CG-CD-NE	-8.99	92.22	112.00
1	A	1343	GLN	CA-CB-CG	-7.79	98.52	114.10
1	A	752	LYS	N-CA-C	7.33	121.67	108.69
1	A	1537	LYS	CA-C-N	-7.10	112.99	122.85
1	A	1537	LYS	C-N-CA	-7.10	112.99	122.85
1	A	794	MET	CB-CG-SD	-6.95	91.85	112.70
1	A	1235	MET	CA-C-N	-6.84	108.33	122.07
1	A	1235	MET	C-N-CA	-6.84	108.33	122.07
1	A	1535	MET	CA-C-N	-6.83	111.31	121.01
1	A	1535	MET	C-N-CA	-6.83	111.31	121.01
1	A	1454	ILE	N-CA-C	5.80	116.24	108.11
1	A	1020	ARG	CG-CD-NE	5.62	124.36	112.00
1	A	1553	ARG	CB-CG-CD	5.60	124.17	111.30
1	A	761	GLU	CA-CB-CG	5.58	125.26	114.10
1	A	1411	ILE	N-CA-C	5.55	116.73	108.23
1	A	752	LYS	CA-C-N	5.46	131.44	122.64
1	A	752	LYS	C-N-CA	5.46	131.44	122.64
1	A	1537	LYS	N-CA-CB	5.42	118.06	109.82
1	A	1107	ARG	CB-CG-CD	-5.36	98.97	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	910	GLU	CA-CB-CG	-5.29	103.52	114.10

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	A	6405	0	6262	128	1
2	A	26	0	19	0	0
3	A	2	0	0	0	0
4	A	50	0	0	2	1
5	A	479	0	0	13	1
All	All	6962	0	6281	128	2

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 10.

All (128) 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:1222:MET:HE1	1:A:1594:ILE:HD13	1.44	0.98
1:A:1303:GLN:HE22	1:A:1313:ARG:H	1.11	0.94
1:A:1371:ARG:NH1	5:A:1804:HOH:O	2.01	0.93
1:A:1237:ARG:HH21	1:A:1279:ARG:HB2	1.39	0.88
1:A:1178:GLN:OE1	5:A:1802:HOH:O	1.91	0.88
1:A:741:MET:HG3	1:A:751:GLN:HG2	1.55	0.87
1:A:1303:GLN:HE21	1:A:1305:GLY:H	1.21	0.84
1:A:765:CYS:SG	1:A:781:ARG:NH1	2.52	0.82
1:A:1237:ARG:HE	1:A:1279:ARG:HD3	1.46	0.80
1:A:768:VAL:HG11	1:A:826:MET:HE1	1.62	0.80
1:A:789:LYS:O	5:A:1805:HOH:O	2.04	0.75
1:A:1237:ARG:HG2	1:A:1279:ARG:HH11	1.52	0.74
1:A:752:LYS:HG3	1:A:759:MET:HE2	1.70	0.74
1:A:1311:GLN:HE22	1:A:1313:ARG:HH11	1.36	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:772:ASP:OD1	1:A:774:SER:OG	2.10	0.67
1:A:752:LYS:HE3	1:A:759:MET:HE2	1.76	0.67
1:A:1067:TYR:CE1	1:A:1102:PRO:HG2	2.30	0.66
1:A:1237:ARG:NH2	5:A:1806:HOH:O	2.11	0.66
1:A:1178:GLN:NE2	5:A:1809:HOH:O	2.28	0.65
1:A:752:LYS:HG3	1:A:759:MET:CE	2.26	0.65
1:A:1303:GLN:NE2	1:A:1313:ARG:H	1.91	0.65
1:A:1096:THR:O	1:A:1098:ASN:ND2	2.29	0.65
1:A:1543:HIS:HD2	1:A:1545:GLU:H	1.45	0.64
1:A:1237:ARG:CG	1:A:1279:ARG:HH11	2.10	0.64
1:A:1311:GLN:NE2	1:A:1528:THR:H	1.95	0.64
1:A:1000:ILE:HG23	1:A:1019:LEU:HD12	1.81	0.62
1:A:780:ALA:HB2	1:A:799:TRP:CE3	2.34	0.62
1:A:914:VAL:HG23	1:A:1014:GLU:HG2	1.81	0.62
1:A:747:ARG:HD3	1:A:786:TRP:NE1	2.14	0.61
1:A:788:ASP:CG	1:A:792:GLN:HB2	2.27	0.60
1:A:761:GLU:HG2	1:A:764:ASP:CG	2.27	0.60
1:A:752:LYS:HG3	1:A:759:MET:SD	2.42	0.59
1:A:1343:GLN:NE2	5:A:1815:HOH:O	2.36	0.59
1:A:1181:ARG:HD2	5:A:1802:HOH:O	2.02	0.59
1:A:1050:GLU:OE1	1:A:1094:SER:HB2	2.03	0.58
1:A:766:VAL:HG13	1:A:831:ILE:HG23	1.86	0.58
1:A:1543:HIS:HE1	5:A:1882:HOH:O	1.86	0.58
1:A:1463:HIS:O	1:A:1483:GLU:HG2	2.04	0.56
1:A:1543:HIS:CD2	1:A:1545:GLU:H	2.23	0.56
1:A:747:ARG:HD3	1:A:786:TRP:CD1	2.41	0.56
1:A:741:MET:N	1:A:749:TYR:O	2.38	0.56
1:A:1207:THR:HG23	1:A:1208:ASN:O	2.05	0.56
1:A:1537:LYS:HD2	1:A:1537:LYS:O	2.05	0.55
1:A:1267:LEU:HD23	1:A:1319:LEU:HD23	1.89	0.55
1:A:995:TYR:OH	1:A:1359:ARG:HG2	2.07	0.55
1:A:788:ASP:OD1	1:A:792:GLN:HB2	2.05	0.55
1:A:1157:GLY:HA3	1:A:1587:ALA:HB3	1.87	0.55
1:A:1409:GLN:NE2	1:A:1411:ILE:O	2.40	0.54
1:A:1193:ASP:HB3	1:A:1196:VAL:HG13	1.89	0.54
1:A:1290:LEU:HA	1:A:1293:MET:HE3	1.89	0.54
1:A:1311:GLN:NE2	1:A:1313:ARG:HH11	2.05	0.54
1:A:1093:ASN:OD1	1:A:1095:LYS:HB2	2.08	0.54
1:A:1222:MET:HE1	1:A:1594:ILE:CD1	2.30	0.54
1:A:995:TYR:HH	1:A:1359:ARG:HG2	1.73	0.54
1:A:1267:LEU:HD23	1:A:1319:LEU:CD2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:918:ILE:HD11	1:A:928:SER:HB3	1.90	0.53
1:A:1543:HIS:CD2	1:A:1546:GLN:H	2.26	0.53
1:A:749:TYR:CD2	1:A:786:TRP:HB3	2.44	0.52
1:A:1537:LYS:HD2	1:A:1537:LYS:C	2.34	0.52
1:A:1009:LYS:HA	1:A:1009:LYS:HE2	1.91	0.52
1:A:761:GLU:HG2	1:A:764:ASP:OD2	2.10	0.51
1:A:1543:HIS:HD2	1:A:1546:GLN:H	1.58	0.51
1:A:795:PHE:CE1	1:A:826:MET:HB3	2.46	0.51
1:A:1378:PRO:HG3	1:A:1391:TYR:O	2.12	0.50
1:A:1141:LYS:HE3	5:A:1993:HOH:O	2.10	0.50
1:A:1205:GLU:O	5:A:1807:HOH:O	2.19	0.50
1:A:914:VAL:HG21	1:A:1012:VAL:HG11	1.93	0.49
1:A:1035:ASN:HA	1:A:1038:TYR:CZ	2.48	0.49
1:A:1516:TYR:CE2	1:A:1535:MET:HG3	2.47	0.49
1:A:747:ARG:CD	1:A:786:TRP:CD1	2.96	0.49
1:A:1103:PRO:HB2	1:A:1105:HIS:CE1	2.48	0.48
1:A:877:TYR:HA	1:A:1354:VAL:O	2.14	0.48
1:A:1266:PHE:HB3	1:A:1320:ALA:HB3	1.96	0.48
1:A:788:ASP:OD1	1:A:792:GLN:O	2.31	0.48
1:A:883:PRO:HD2	1:A:885:LYS:NZ	2.29	0.48
1:A:1007:LYS:HD2	1:A:1010:GLY:HA2	1.96	0.47
1:A:775:LYS:HD3	1:A:778:TYR:HE1	1.79	0.47
1:A:846:TRP:HH2	1:A:1295:TYR:CZ	2.33	0.47
1:A:1233:SER:HA	1:A:1277:TYR:CD2	2.50	0.47
1:A:1020:ARG:HH21	1:A:1053:VAL:HG21	1.80	0.47
1:A:761:GLU:O	1:A:764:ASP:HB2	2.15	0.47
1:A:1237:ARG:NE	1:A:1279:ARG:HD3	2.24	0.46
1:A:887:GLN:H	1:A:887:GLN:HG2	1.60	0.46
1:A:1515:LEU:HD11	1:A:1537:LYS:O	2.15	0.46
1:A:1516:TYR:HE2	1:A:1535:MET:HG3	1.81	0.46
1:A:775:LYS:HD3	1:A:778:TYR:CE1	2.51	0.46
1:A:1003:ILE:HG12	1:A:1019:LEU:HD13	1.98	0.45
1:A:1237:ARG:CD	1:A:1279:ARG:NH1	2.79	0.45
1:A:1303:GLN:NE2	1:A:1305:GLY:H	2.02	0.45
1:A:950:PHE:HA	4:A:1712:SO4:O3	2.17	0.45
1:A:894:HIS:CE1	1:A:895:LYS:HE3	2.51	0.45
1:A:769:ILE:HD13	1:A:777:LEU:CD2	2.47	0.45
1:A:915:LEU:HB2	1:A:929:SER:OG	2.17	0.44
1:A:1047:TRP:CG	1:A:1048:SER:N	2.85	0.44
1:A:1020:ARG:HH21	1:A:1053:VAL:CG2	2.30	0.44
1:A:1108:SER:HB3	1:A:1109:PRO:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1446:GLN:NE2	4:A:1706:SO4:O3	2.49	0.43
1:A:747:ARG:CZ	1:A:749:TYR:OH	2.67	0.43
1:A:743:ILE:HG22	1:A:748:THR:HG23	2.01	0.43
1:A:1011:LYS:HE3	1:A:1012:VAL:O	2.19	0.43
1:A:1537:LYS:NZ	5:A:1803:HOH:O	2.00	0.43
1:A:1237:ARG:CG	1:A:1279:ARG:NH1	2.81	0.43
1:A:751:GLN:O	1:A:785:LEU:HD12	2.19	0.42
1:A:1262:ARG:HA	1:A:1262:ARG:HD3	1.88	0.42
1:A:898:LEU:HD23	1:A:898:LEU:HA	1.87	0.42
1:A:1158:PHE:HB3	1:A:1164:SER:OG	2.19	0.42
1:A:1269:GLU:OE2	1:A:1315:ARG:NE	2.49	0.42
1:A:1021:LEU:O	1:A:1051:GLU:HA	2.20	0.42
1:A:783:THR:OG1	1:A:796:HIS:HB3	2.20	0.41
1:A:794:MET:SD	1:A:827:GLN:HG2	2.59	0.41
1:A:1311:GLN:HE22	1:A:1313:ARG:NH1	2.13	0.41
1:A:1303:GLN:HE22	1:A:1313:ARG:N	1.95	0.41
1:A:1012:VAL:HG12	1:A:1014:GLU:HG3	2.02	0.41
1:A:845:ASN:CG	1:A:845:ASN:O	2.62	0.41
1:A:826:MET:HE2	1:A:830:TYR:HB3	2.02	0.41
1:A:947:PRO:HA	1:A:996:ARG:HG2	2.03	0.41
1:A:980:TYR:HD1	1:A:980:TYR:HA	1.63	0.41
1:A:1280:SER:HA	5:A:1950:HOH:O	2.19	0.41
1:A:1237:ARG:HH21	1:A:1279:ARG:CB	2.19	0.41
1:A:1174:ASP:HB3	1:A:1175:PRO:HD3	2.02	0.41
1:A:1332:GLU:CD	1:A:1358:THR:H	2.28	0.41
1:A:1148:PHE:CE2	1:A:1227:PRO:HB3	2.56	0.40
1:A:803:GLY:HA3	1:A:812:SER:OG	2.22	0.40
1:A:1559:GLN:O	1:A:1584:PRO:HD2	2.21	0.40
1:A:804:THR:HA	1:A:809:GLY:O	2.22	0.40
1:A:1235:MET:HE3	1:A:1235:MET:HB3	1.94	0.40
1:A:1538:GLN:NE2	5:A:1819:HOH:O	2.54	0.40
1:A:925:VAL:O	1:A:1004:HIS:HA	2.21	0.40

All (2) 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)
5:A:2162:HOH:O	5:A:2196:HOH:O[4_455]	1.76	0.44
1:A:1095:LYS:NZ	4:A:1713:SO4:O2[3_554]	2.06	0.14

5.3 Torsion angles

5.3.1 Protein backbone

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	789/872 (90%)	756 (96%)	33 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	689/757 (91%)	680 (99%)	9 (1%)	61	69

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	752	LYS
1	A	759	MET
1	A	834	LYS
1	A	1196	VAL
1	A	1202	MET
1	A	1207	THR
1	A	1238	PHE
1	A	1270	ASN
1	A	1309	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	746	ASN
1	A	894	HIS
1	A	1039	HIS
1	A	1098	ASN
1	A	1195	ASN
1	A	1303	GLN
1	A	1311	GLN
1	A	1381	GLN
1	A	1543	HIS
1	A	1559	GLN

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 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	SO4	A	1707	-	4,4,4	0.24	0	6,6,6	0.25	0
4	SO4	A	1709	-	4,4,4	0.24	0	6,6,6	0.29	0
4	SO4	A	1710	-	4,4,4	0.23	0	6,6,6	0.21	0
4	SO4	A	1712	-	4,4,4	0.27	0	6,6,6	0.32	0
4	SO4	A	1711	-	4,4,4	0.28	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	1708	-	4,4,4	0.28	0	6,6,6	0.26	0
4	SO4	A	1706	-	4,4,4	0.23	0	6,6,6	0.13	0
4	SO4	A	1705	-	4,4,4	0.24	0	6,6,6	0.13	0
4	SO4	A	1713	-	4,4,4	0.20	0	6,6,6	0.12	0
2	SAH	A	1701	-	27,28,28	1.15	4 (14%)	36,40,40	2.01	8 (22%)
4	SO4	A	1704	-	4,4,4	0.21	0	6,6,6	0.23	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	SAH	A	1701	-	-	1/15/31/31	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1701	SAH	C2-N1	2.85	1.39	1.33
2	A	1701	SAH	C2-N3	2.65	1.38	1.33
2	A	1701	SAH	OXT-C	-2.43	1.22	1.30
2	A	1701	SAH	C8-N7	2.27	1.36	1.31

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1701	SAH	N3-C2-N1	-5.72	119.93	128.58
2	A	1701	SAH	N9-C8-N7	-4.68	107.30	113.94
2	A	1701	SAH	C5-N7-C8	4.03	109.78	103.45
2	A	1701	SAH	C5-C4-N3	-3.44	121.98	126.72
2	A	1701	SAH	C4-C5-N7	-3.35	106.75	110.58
2	A	1701	SAH	C2-N3-C4	2.99	119.14	111.83
2	A	1701	SAH	C4-N9-C8	2.67	108.54	105.74
2	A	1701	SAH	O4'-C1'-C2'	-2.50	101.27	106.62

There are no chirality outliers.

All (1) torsion outliers are listed below:

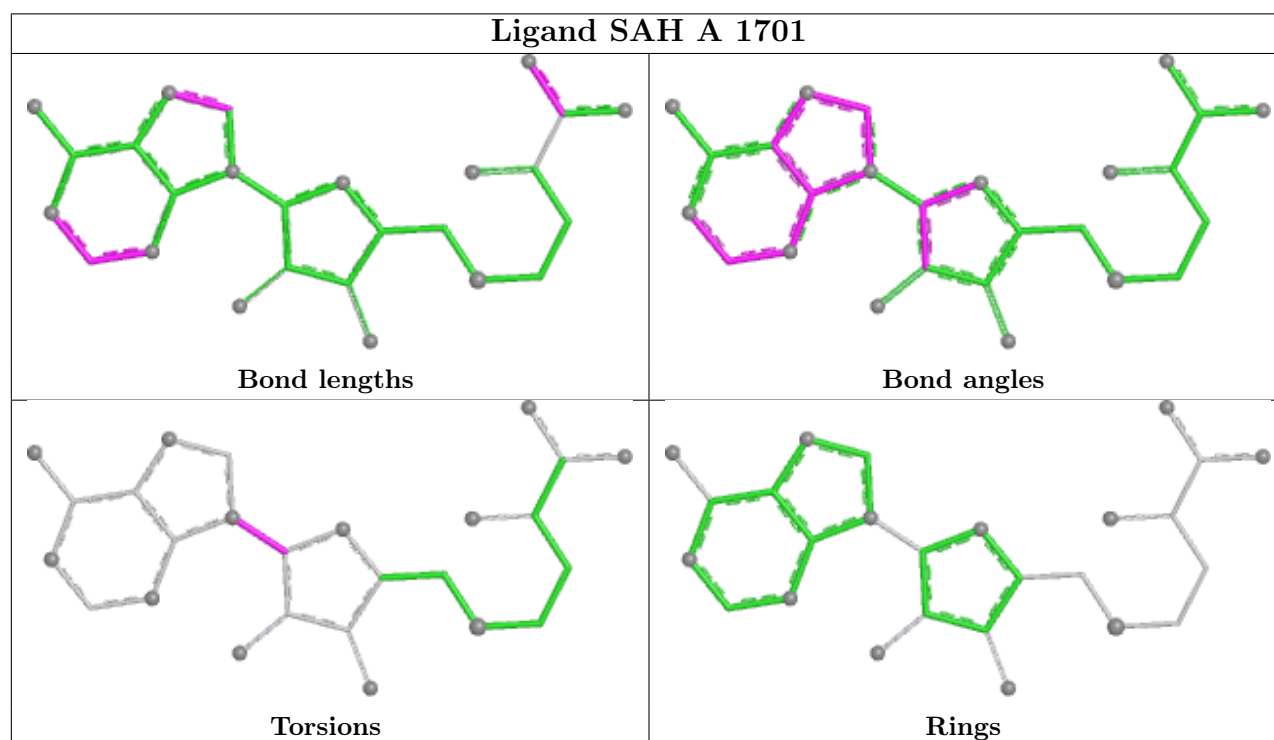
Mol	Chain	Res	Type	Atoms
2	A	1701	SAH	C2'-C1'-N9-C8

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1712	SO4	1	0
4	A	1706	SO4	1	0
4	A	1713	SO4	0	1

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	794/872 (91%)	0.87	187 (23%) 2 2	13, 32, 85, 130	7 (0%)

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	762	VAL	8.2
1	A	749	TYR	6.9
1	A	763	GLY	6.7
1	A	750	TYR	6.5
1	A	741	MET	6.1
1	A	760	LEU	6.1
1	A	786	TRP	6.0
1	A	755	ILE	5.7
1	A	785	LEU	5.7
1	A	743	ILE	5.7
1	A	748	THR	5.6
1	A	784	ALA	5.6
1	A	752	LYS	5.6
1	A	1406	SER	5.4
1	A	1453	VAL	5.2
1	A	894	HIS	5.2
1	A	753	VAL	5.1
1	A	751	GLN	5.1
1	A	957	ALA	5.0
1	A	1450	GLY	4.8
1	A	793	MET	4.8
1	A	789	LYS	4.8
1	A	742	LYS	4.8
1	A	1408	TYR	4.6
1	A	1452	GLY	4.6
1	A	830	TYR	4.6
1	A	1109	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	980	TYR	4.5
1	A	936	VAL	4.4
1	A	759	MET	4.3
1	A	795	PHE	4.3
1	A	928	SER	4.2
1	A	921	VAL	4.2
1	A	958	SER	4.2
1	A	895	LYS	4.2
1	A	959	PRO	4.1
1	A	915	LEU	4.1
1	A	1599	LEU	4.1
1	A	1012	VAL	4.1
1	A	747	ARG	4.1
1	A	923	GLY	4.1
1	A	838	ILE	4.1
1	A	1537	LYS	4.0
1	A	782	VAL	4.0
1	A	1067	TYR	4.0
1	A	768	VAL	3.9
1	A	896	PHE	3.9
1	A	757	GLU	3.9
1	A	833	SER	3.9
1	A	790	ASN	3.9
1	A	914	VAL	3.8
1	A	1139	LEU	3.8
1	A	766	VAL	3.8
1	A	794	MET	3.8
1	A	761	GLU	3.8
1	A	769	ILE	3.7
1	A	1072	LEU	3.7
1	A	926	TYR	3.7
1	A	1106	ALA	3.7
1	A	770	PRO	3.7
1	A	797	ALA	3.6
1	A	1017	ILE	3.6
1	A	900	CYS	3.6
1	A	791	GLY	3.5
1	A	783	THR	3.5
1	A	1053	VAL	3.5
1	A	918	ILE	3.4
1	A	1454	ILE	3.4
1	A	754	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	929	SER	3.4
1	A	1449	LEU	3.4
1	A	746	ASN	3.4
1	A	845	ASN	3.4
1	A	956	VAL	3.4
1	A	831	ILE	3.4
1	A	847	ALA	3.4
1	A	1015	ALA	3.4
1	A	1016	ASP	3.3
1	A	1405	GLY	3.3
1	A	779	LEU	3.3
1	A	1108	SER	3.3
1	A	1407	HIS	3.3
1	A	815	LEU	3.2
1	A	835	VAL	3.2
1	A	899	SER	3.2
1	A	1104	ASN	3.2
1	A	1020	ARG	3.1
1	A	1006	GLY	3.1
1	A	776	PRO	3.1
1	A	744	GLU	3.1
1	A	787	GLU	3.1
1	A	1105	HIS	3.1
1	A	1007	LYS	3.1
1	A	826	MET	3.1
1	A	1009	LYS	3.1
1	A	897	CYS	3.0
1	A	828	LEU	3.0
1	A	1021	LEU	3.0
1	A	954	ILE	3.0
1	A	1047	TRP	3.0
1	A	837	VAL	3.0
1	A	1089	LEU	3.0
1	A	927	CYS	3.0
1	A	1324	GLY	3.0
1	A	1538	GLN	2.9
1	A	780	ALA	2.9
1	A	1011	LYS	2.9
1	A	888	PRO	2.9
1	A	823	CYS	2.9
1	A	814	PRO	2.9
1	A	842	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	939	LEU	2.9
1	A	765	CYS	2.9
1	A	775	LYS	2.9
1	A	788	ASP	2.8
1	A	1350	ASP	2.8
1	A	912	PRO	2.8
1	A	938	ARG	2.8
1	A	887	GLN	2.8
1	A	773	SER	2.7
1	A	1000	ILE	2.7
1	A	1230	GLN	2.7
1	A	820	VAL	2.7
1	A	824	GLU	2.6
1	A	800	PHE	2.6
1	A	796	HIS	2.6
1	A	903	LEU	2.6
1	A	1451	ASP	2.6
1	A	799	TRP	2.6
1	A	904	ALA	2.6
1	A	1010	GLY	2.6
1	A	792	GLN	2.5
1	A	937	TYR	2.5
1	A	1008	LYS	2.5
1	A	745	GLU	2.5
1	A	1013	ASN	2.5
1	A	758	GLU	2.5
1	A	1088	PHE	2.5
1	A	756	ASP	2.5
1	A	908	GLN	2.5
1	A	1100	GLU	2.5
1	A	1434	PHE	2.5
1	A	778	TYR	2.4
1	A	829	SER	2.4
1	A	920	GLU	2.4
1	A	925	VAL	2.4
1	A	1005	CYS	2.4
1	A	1103	PRO	2.4
1	A	1004	HIS	2.4
1	A	913	LYS	2.4
1	A	1279	ARG	2.4
1	A	919	GLU	2.3
1	A	911	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	771	ASP	2.3
1	A	1240	SER	2.3
1	A	1068	GLY	2.3
1	A	767	SER	2.3
1	A	1094	SER	2.3
1	A	1448	ARG	2.3
1	A	764	ASP	2.3
1	A	867	TYR	2.3
1	A	832	HIS	2.2
1	A	1014	GLU	2.2
1	A	1409	GLN	2.2
1	A	1411	ILE	2.2
1	A	933	ASN	2.2
1	A	834	LYS	2.2
1	A	1019	LEU	2.2
1	A	781	ARG	2.2
1	A	1056	PHE	2.2
1	A	931	THR	2.2
1	A	841	ALA	2.2
1	A	945	LEU	2.2
1	A	827	GLN	2.2
1	A	1071	LEU	2.1
1	A	930	ILE	2.1
1	A	1003	ILE	2.1
1	A	1032	ARG	2.1
1	A	886	THR	2.1
1	A	1018	LYS	2.1
1	A	1070	ASP	2.1
1	A	1237	ARG	2.1
1	A	949	ALA	2.1
1	A	825	ASN	2.0
1	A	953	ASN	2.0
1	A	898	LEU	2.0
1	A	839	TYR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

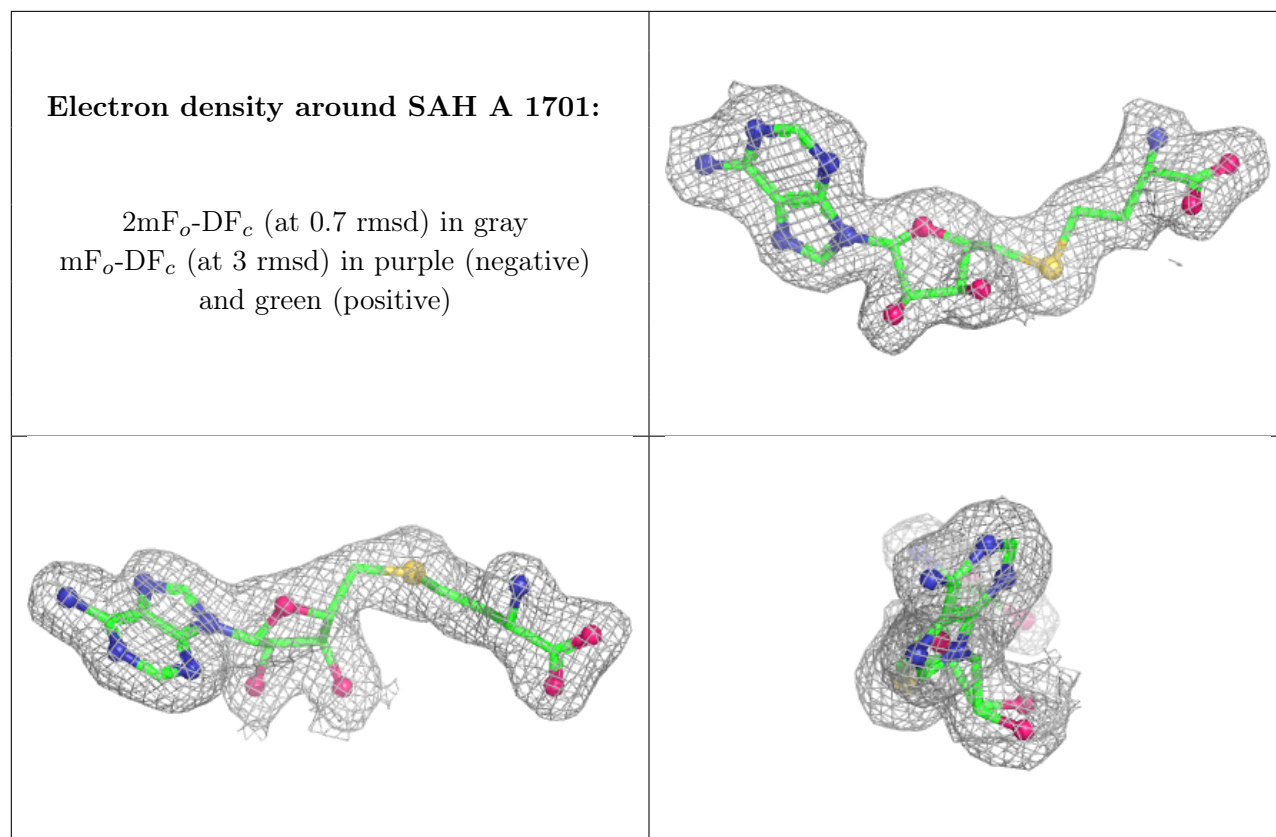
There are no oligosaccharides in this entry.

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
4	SO4	A	1712	5/5	0.67	0.14	81,83,89,95	0
4	SO4	A	1705	5/5	0.72	0.14	87,89,92,95	0
4	SO4	A	1713	5/5	0.75	0.14	73,79,81,82	0
4	SO4	A	1710	5/5	0.84	0.11	75,81,85,86	0
4	SO4	A	1706	5/5	0.85	0.11	48,67,71,71	0
4	SO4	A	1707	5/5	0.86	0.12	60,60,67,79	0
4	SO4	A	1711	5/5	0.92	0.18	47,50,59,60	0
4	SO4	A	1708	5/5	0.96	0.09	28,28,37,42	0
4	SO4	A	1704	5/5	0.97	0.10	29,32,36,38	0
4	SO4	A	1709	5/5	0.97	0.08	40,44,46,49	0
3	ZN	A	1702	1/1	0.98	0.06	50,50,50,50	0
3	ZN	A	1703	1/1	0.98	0.04	25,25,25,25	0
2	SAH	A	1701	26/26	0.98	0.05	12,15,17,20	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.