



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:21 PM UTC

PDB ID : 3AV5 / pdb_00003av5
Title : Crystal structure of mouse DNA methyltransferase 1 with AdoHcy
Authors : Takeshita, K.; Suetake, I.; Yamashita, E.; Suga, M.; Narita, H.; Nakagawa, A.; Tajima, S.
Deposited on : 2011-02-22
Resolution : 3.25 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

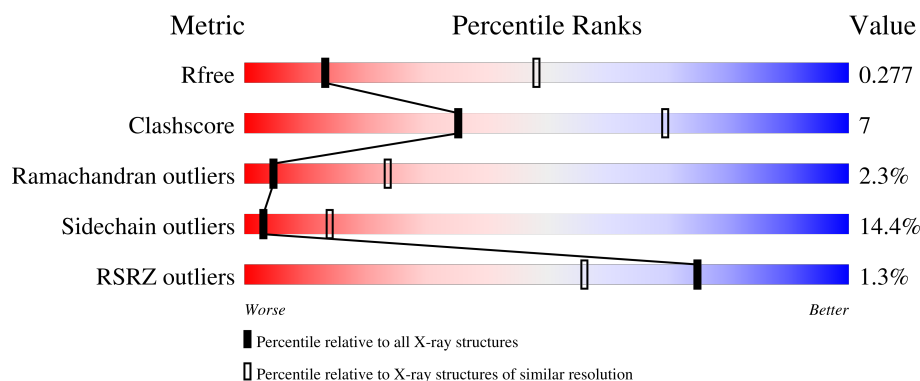
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	1330	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9135 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.

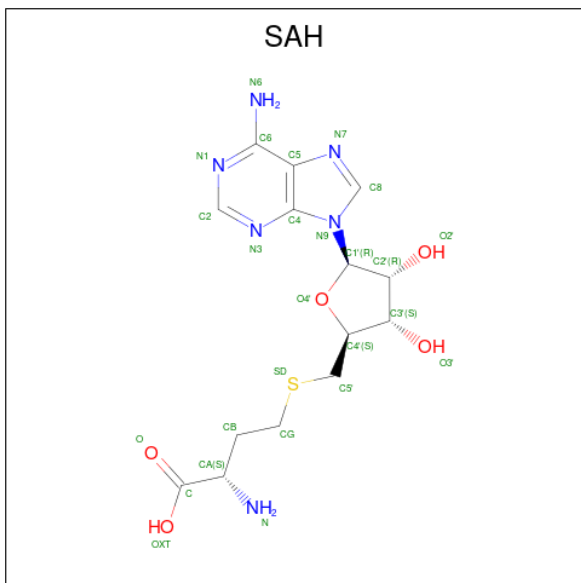
- Molecule 1 is a protein called DNA (cytosine-5)-methyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1139	Total	C	N	O	S	0	0	0
			9105	5760	1584	1701	60			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Zn	0	0
			4	4		

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).

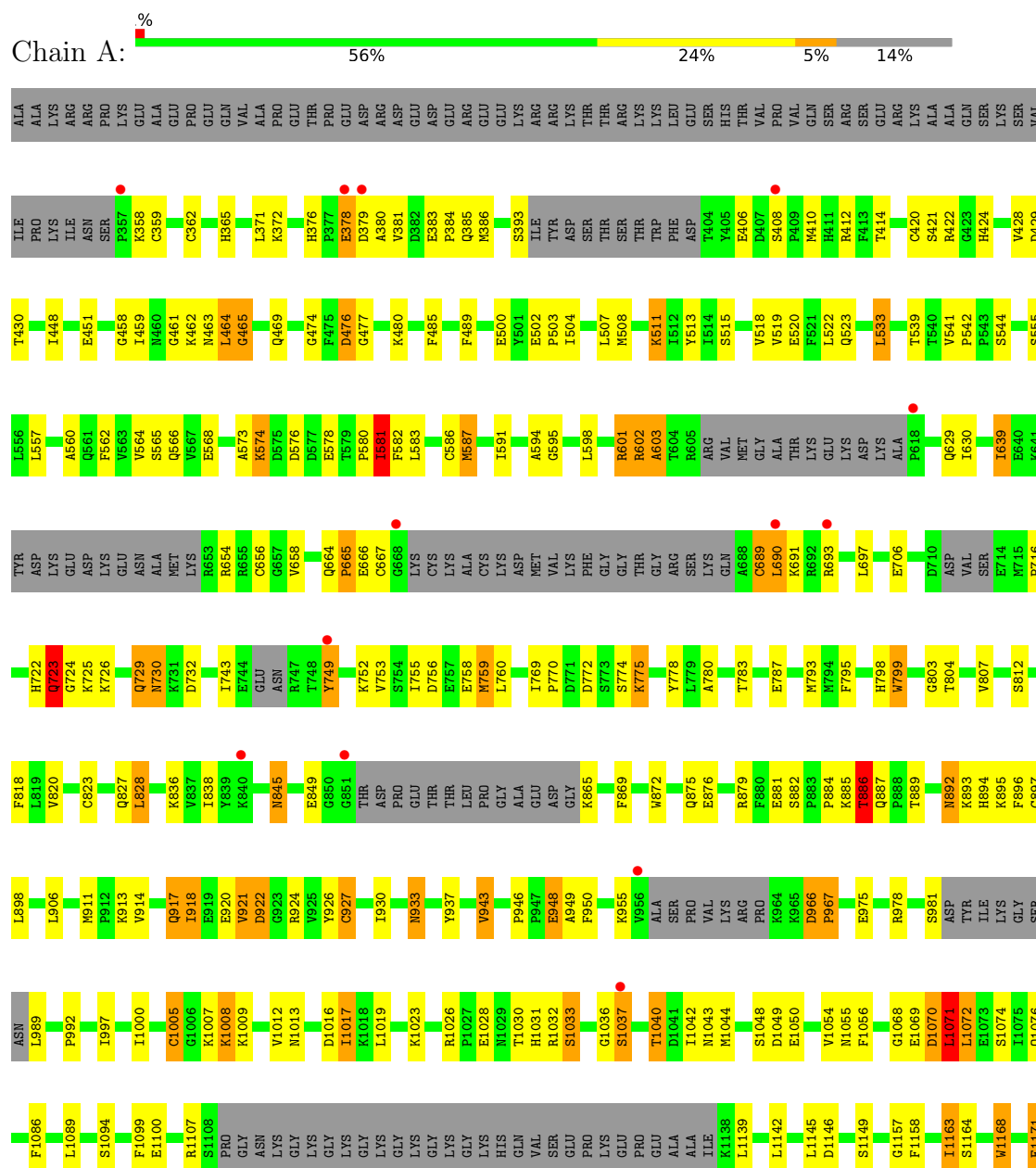


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

3 Residue-property plots

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: DNA (cytosine-5)-methyltransferase 1



LYS	GLI517	P1410	R1292	WI172
ALA	RI518	TI411	M1293	WI173
LYS	L1519	LI412	G1294	DI174
GLU	E1520	RI413	Y1295	P1175
GLU	F1525	DI414	Q1296	A1176
ALA		HI415	L1302	A1177
ALA		TI416	V1309	Q1178
THR	TI528	CI417	A1310	AI179
LYS	VI529	DI418	Q1311	F1180
ASP	TI530	DI419	TI312	LI182
	TI531	M1420	TI311	
	PI532		RI515	TI191
		VI424	LI313	E1192
	MI535	A1425	TI317	
		A1426	LI197	
	Q1538	RI427	LI198	
	GI539	M1428	A1320	
	RI540	RI429	P1328	
	VI541	HI430	LI329	S1209
	LI542		P1330	P1215
	HI543	LI433	P1331	Q1216
	PI544		P1332	
	E1545	SI437	P1333	DI219
	Q1546	DI438		
	HI547	WI439		M1222
	RI548	RI440	VI336	LI223
	VI549		C1342	
		DI451	Q1343	P1228
	VI552	G1452	VI348	G1229
	A1556	VI453	DI349	Q1230
		HI456	VI354	GI231
	TI571	K1457	M1355	F1232
	RI574	TI461		SI233
	HI575	VI465	RI359	
	VI578		LI360	RI237
		SI470	SI361	F1238
	VI582	VI478	SI362	NI239
			RI366	K1245
	PI585	PI489	RI371	LI250
	LI586	SI491	M1374	Y1257
	AI587	RI492	SI375	Y1261
	K1588		DI376	RI262
		TI498	LI377	P1263
	LI592	PI499	SI385	F1266
	E1593	WI500	NI386	LI267
	TI594	CI501		
		LI502		N1270
	CI597	PI503		VI271
	LI598			RI272
	SI601			NI273
	E1604	VI512		F1274
		AI513		VI275
	AI608	GI514		SI276
	ALA	LI515	Q1400	Y1277
	VAL	Y1516	RI401	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	134.99Å 96.92Å 130.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.66 – 3.25 38.66 – 3.25	Depositor EDS
% Data completeness (in resolution range)	(Not available) (38.66-3.25) 95.7 (38.66-3.25)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.11 (at 3.25Å)	Xtriage
Refinement program	BUSTER-TNT, BUSTER 2.8.0	Depositor
R, R_{free}	0.183 , 0.264 0.192 , 0.277	Depositor DCC
R_{free} test set	1367 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å ²)	59.9	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 80.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9135	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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

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	0.89	2/9325 (0.0%)	1.43	93/12607 (0.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	690	LEU	CA-C	5.65	1.59	1.52
1	A	1430	HIS	C-N	5.20	1.37	1.33

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1360	LEU	N-CA-C	9.82	123.92	111.24
1	A	1360	LEU	CA-C-N	9.49	138.78	121.70
1	A	1360	LEU	C-N-CA	9.49	138.78	121.70
1	A	376	HIS	N-CA-C	7.56	120.72	110.29
1	A	1491	SER	N-CA-C	-7.41	104.24	113.28
1	A	1070	ASP	CA-CB-CG	7.33	119.93	112.60
1	A	967	PRO	N-CA-C	7.22	122.64	110.95
1	A	1342	CYS	N-CA-C	6.93	120.62	112.72
1	A	485	PHE	CA-CB-CG	6.76	120.56	113.80
1	A	730	ASN	N-CA-C	6.68	118.93	110.24
1	A	755	ILE	N-CA-C	6.65	116.30	106.85
1	A	1071	LEU	CA-C-N	6.64	129.50	120.54
1	A	1071	LEU	C-N-CA	6.64	129.50	120.54
1	A	1071	LEU	N-CA-C	6.63	119.74	109.07
1	A	1377	LEU	N-CA-C	6.55	117.91	109.72
1	A	1146	ASP	CA-CB-CG	6.49	119.09	112.60
1	A	665	PRO	CA-C-N	6.47	133.34	121.70
1	A	665	PRO	C-N-CA	6.47	133.34	121.70
1	A	1031	HIS	CA-C-N	6.37	128.71	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1031	HIS	C-N-CA	6.37	128.71	120.44
1	A	729	GLN	CA-C-N	6.25	130.01	120.82
1	A	729	GLN	C-N-CA	6.25	130.01	120.82
1	A	775	LYS	N-CA-C	6.23	123.57	109.81
1	A	1541	VAL	CB-CA-C	6.14	116.67	110.65
1	A	1005	CYS	N-CA-C	6.13	120.60	109.32
1	A	886	THR	CA-C-N	6.10	132.69	121.70
1	A	886	THR	C-N-CA	6.10	132.69	121.70
1	A	892	ASN	CA-CB-CG	6.08	118.68	112.60
1	A	1336	VAL	CB-CA-C	6.04	119.00	111.15
1	A	1026	ARG	N-CA-C	-6.04	102.54	110.39
1	A	1512	TRP	CA-C-N	6.03	133.05	121.54
1	A	1512	TRP	C-N-CA	6.03	133.05	121.54
1	A	774	SER	N-CA-C	-5.91	99.17	108.63
1	A	1313	ARG	N-CA-C	5.89	117.99	107.80
1	A	1180	PHE	CA-C-N	5.86	128.40	120.38
1	A	1180	PHE	C-N-CA	5.86	128.40	120.38
1	A	723	GLN	N-CA-C	5.74	117.33	110.44
1	A	1540	ARG	CB-CA-C	5.70	118.81	110.26
1	A	1461	THR	N-CA-C	5.67	120.26	113.23
1	A	1362	SER	N-CA-C	5.67	117.22	110.19
1	A	849	GLU	N-CA-C	5.64	120.03	113.20
1	A	428	VAL	CA-C-N	5.61	127.74	120.44
1	A	428	VAL	C-N-CA	5.61	127.74	120.44
1	A	812	SER	N-CA-C	5.52	118.01	110.55
1	A	603	ALA	N-CA-C	5.52	118.54	109.76
1	A	875	GLN	CA-C-N	5.50	127.91	120.38
1	A	875	GLN	C-N-CA	5.50	127.91	120.38
1	A	807	VAL	CA-C-N	5.47	127.92	120.54
1	A	807	VAL	C-N-CA	5.47	127.92	120.54
1	A	1017	ILE	N-CA-CB	5.47	116.78	110.49
1	A	568	GLU	CA-C-N	5.45	127.58	120.28
1	A	568	GLU	C-N-CA	5.45	127.58	120.28
1	A	1049	ASP	CA-C-N	5.45	128.97	120.75
1	A	1049	ASP	C-N-CA	5.45	128.97	120.75
1	A	1164	SER	CA-C-N	5.41	130.34	121.58
1	A	1164	SER	C-N-CA	5.41	130.34	121.58
1	A	949	ALA	N-CA-C	5.39	117.91	111.71
1	A	1452	GLY	CA-C-N	5.38	127.71	120.50
1	A	1452	GLY	C-N-CA	5.38	127.71	120.50
1	A	1498	ILE	N-CA-C	-5.36	102.69	107.56
1	A	1191	THR	CB-CA-C	5.35	117.86	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	458	GLY	N-CA-C	5.35	119.09	111.12
1	A	378	GLU	CB-CG-CD	5.30	121.61	112.60
1	A	464	LEU	CA-C-N	5.30	130.19	121.87
1	A	464	LEU	C-N-CA	5.30	130.19	121.87
1	A	845	ASN	CA-CB-CG	5.26	117.86	112.60
1	A	1525	PHE	N-CA-C	-5.25	101.15	109.96
1	A	943	VAL	N-CA-C	5.24	116.27	108.46
1	A	869	PHE	CA-CB-CG	5.24	119.04	113.80
1	A	966	ASP	CA-CB-CG	5.24	117.83	112.60
1	A	511	LYS	CA-C-N	5.20	127.87	120.53
1	A	511	LYS	C-N-CA	5.20	127.87	120.53
1	A	795	PHE	CA-CB-CG	5.20	119.00	113.80
1	A	1528	THR	CB-CA-C	5.19	119.83	111.05
1	A	799	TRP	N-CA-C	5.19	117.81	110.50
1	A	581	ILE	CB-CA-C	5.17	120.18	112.16
1	A	1036	GLY	N-CA-C	-5.17	106.24	112.49
1	A	429	ASP	CA-C-N	5.14	131.36	121.54
1	A	429	ASP	C-N-CA	5.14	131.36	121.54
1	A	1099	PHE	N-CA-C	5.13	117.78	107.41
1	A	1582	VAL	N-CA-C	-5.12	97.82	108.88
1	A	1257	TYR	CA-C-N	5.11	127.08	120.44
1	A	1257	TYR	C-N-CA	5.11	127.08	120.44
1	A	950	PHE	CA-CB-CG	5.10	118.90	113.80
1	A	578	GLU	CA-C-N	5.10	127.50	120.67
1	A	578	GLU	C-N-CA	5.10	127.50	120.67
1	A	691	LYS	CA-C-N	5.09	127.91	119.35
1	A	691	LYS	C-N-CA	5.09	127.91	119.35
1	A	1056	PHE	CA-CB-CG	5.06	118.86	113.80
1	A	716	PRO	CA-C-N	5.04	127.82	120.51
1	A	716	PRO	C-N-CA	5.04	127.82	120.51
1	A	1491	SER	CA-C-N	5.04	128.00	120.95
1	A	1491	SER	C-N-CA	5.04	128.00	120.95

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	9105	0	8877	133	0
2	A	4	0	0	0	0
3	A	26	0	19	0	0
All	All	9135	0	8896	133	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 7.

All (133) 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:1543:HIS:HD2	1:A:1546:GLN:H	1.18	0.85
1:A:1330:PHE:H	1:A:1356:ASN:HD21	1.24	0.83
1:A:885:LYS:HA	1:A:886:THR:HG23	1.61	0.80
1:A:1068:GLY:HA2	1:A:1071:LEU:HD12	1.62	0.79
1:A:1223:LEU:HB2	1:A:1263:PRO:HG3	1.66	0.77
1:A:383:GLU:HG3	1:A:464:LEU:HD23	1.67	0.77
1:A:975:GLU:OE1	1:A:978:ARG:HD2	1.90	0.72
1:A:1157:GLY:HA3	1:A:1587:ALA:HB3	1.71	0.71
1:A:1028:GLU:HG3	1:A:1037:SER:HB3	1.71	0.71
1:A:1543:HIS:CD2	1:A:1546:GLN:H	2.06	0.71
1:A:966:ASP:HB2	1:A:967:PRO:HD2	1.73	0.70
1:A:783:THR:HG21	1:A:897:CYS:HB2	1.75	0.69
1:A:886:THR:HG22	1:A:898:LEU:HD21	1.75	0.68
1:A:503:PRO:HG2	1:A:504:ILE:HD12	1.79	0.65
1:A:522:LEU:HB3	1:A:581:ILE:HG13	1.76	0.65
1:A:1371:ARG:O	1:A:1375:SER:HB3	1.99	0.63
1:A:1000:ILE:HG12	1:A:1019:LEU:HD23	1.81	0.62
1:A:1171:GLU:HB3	1:A:1177:ALA:HB2	1.81	0.61
1:A:1266:PHE:HB3	1:A:1320:ALA:HB3	1.83	0.61
1:A:1030:THR:HG22	1:A:1032:ARG:H	1.67	0.60
1:A:380:ALA:HB1	1:A:462:LYS:HB3	1.85	0.59
1:A:1040:THR:CG2	1:A:1366:ARG:HH22	2.15	0.59
1:A:1456:HIS:CG	1:A:1457:LYS:H	2.21	0.59
1:A:515:SER:O	1:A:519:VAL:HG23	2.04	0.57
1:A:992:PRO:HG2	1:A:1336:VAL:HG22	1.87	0.57
1:A:1028:GLU:O	1:A:1033:SER:HA	2.06	0.56
1:A:1478:VAL:HG13	1:A:1500:TRP:NE1	2.20	0.56
1:A:1543:HIS:CD2	1:A:1545:GLU:H	2.24	0.55
1:A:378:GLU:C	1:A:380:ALA:H	2.15	0.55
1:A:753:VAL:HG11	1:A:759:MET:SD	2.48	0.54
1:A:1173:TRP:CD1	1:A:1175:PRO:HD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1076:GLN:HE22	1:A:1402:GLN:HE22	1.56	0.53
1:A:1426:ALA:O	1:A:1430:HIS:HD2	1.91	0.53
1:A:1343:GLN:HE21	1:A:1343:GLN:H	1.58	0.52
1:A:1302:LEU:HD21	1:A:1330:PHE:HD2	1.74	0.51
1:A:1588:LYS:HG2	1:A:1592:LEU:HD23	1.93	0.51
1:A:1397:SER:HG	1:A:1400:GLN:H	1.58	0.50
1:A:1216:GLN:O	1:A:1219:ASP:HB2	2.10	0.50
1:A:894:HIS:CD2	1:A:895:LYS:HG3	2.47	0.50
1:A:793:MET:HB3	1:A:828:LEU:HD13	1.93	0.50
1:A:582:PHE:HA	1:A:587:MET:HG3	1.93	0.49
1:A:602:ARG:HH11	1:A:603:ALA:H	1.59	0.49
1:A:381:VAL:HG23	1:A:386:MET:HB3	1.95	0.49
1:A:1332:GLU:HG3	1:A:1359:ARG:HD2	1.95	0.49
1:A:917:GLN:HA	1:A:927:CYS:HA	1.95	0.48
1:A:1532:PRO:HB2	1:A:1549:VAL:HG13	1.95	0.48
1:A:1515:LEU:HD22	1:A:1535:MET:HA	1.95	0.48
1:A:1171:GLU:O	1:A:1191:THR:HA	2.14	0.48
1:A:723:GLN:N	1:A:724:GLY:HA3	2.29	0.48
1:A:881:GLU:HG2	1:A:1296:GLN:HE21	1.79	0.47
1:A:1313:ARG:HH11	1:A:1528:THR:HG21	1.79	0.47
1:A:667:CYS:HA	1:A:689:CYS:H	1.79	0.47
1:A:464:LEU:O	1:A:465:GLY:O	2.33	0.47
1:A:1546:GLN:HB3	1:A:1548:ARG:HG2	1.96	0.47
1:A:1274:PHE:HA	1:A:1277:TYR:CD1	2.49	0.47
1:A:1424:VAL:HG12	1:A:1428:MET:HE2	1.96	0.47
1:A:725:LYS:NZ	1:A:726:LYS:H	2.13	0.47
1:A:1416:ILE:HG12	1:A:1571:ILE:HD12	1.97	0.47
1:A:1437:SER:O	1:A:1517:GLY:HA2	2.15	0.47
1:A:1023:LYS:O	1:A:1048:SER:HB3	2.14	0.47
1:A:1149:SER:HB2	1:A:1180:PHE:CE1	2.50	0.47
1:A:1293:MET:HE2	1:A:1295:TYR:CD1	2.50	0.46
1:A:1333:PRO:HD2	1:A:1359:ARG:HB2	1.97	0.46
1:A:630:ILE:HD11	1:A:1292:ARG:HG2	1.97	0.46
1:A:879:ARG:NH2	1:A:1328:PRO:O	2.49	0.46
1:A:1309:VAL:HG23	1:A:1585:PRO:HG2	1.99	0.45
1:A:1348:VAL:HG12	1:A:1349:ASP:OD2	2.16	0.45
1:A:1223:LEU:HD11	1:A:1257:TYR:HB3	1.98	0.45
1:A:1500:TRP:O	1:A:1503:PRO:HD2	2.16	0.45
1:A:591:ILE:HG12	1:A:598:LEU:HD21	1.98	0.45
1:A:798:HIS:HA	1:A:823:CYS:HB3	1.99	0.45
1:A:1556:ALA:HA	1:A:1578:VAL:HG11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:946:PRO:HB2	1:A:948:GLU:HG2	1.98	0.45
1:A:1142:LEU:HD11	1:A:1598:LEU:HD21	1.99	0.45
1:A:580:PRO:HD2	1:A:583:LEU:HD12	1.99	0.45
1:A:476:ASP:HB3	1:A:477:GLY:H	1.56	0.44
1:A:1068:GLY:O	1:A:1071:LEU:HB2	2.17	0.44
1:A:1530:THR:O	1:A:1575:HIS:HB3	2.18	0.44
1:A:689:CYS:HB2	1:A:690:LEU:H	1.60	0.44
1:A:885:LYS:HA	1:A:886:THR:CG2	2.40	0.44
1:A:1374:MET:HE2	1:A:1374:MET:HB3	1.79	0.44
1:A:511:LYS:HB3	1:A:562:PHE:CD2	2.53	0.44
1:A:886:THR:CB	1:A:887:GLN:HA	2.47	0.44
1:A:1499:PRO:HB2	1:A:1502:LEU:HG	2.00	0.44
1:A:566:GLN:HE22	1:A:603:ALA:HB3	1.83	0.44
1:A:1228:PRO:HD2	1:A:1250:LEU:HD13	2.00	0.44
1:A:1519:LEU:HB2	1:A:1544:PRO:HD3	1.99	0.44
1:A:359:CYS:SG	1:A:422:ARG:HD2	2.58	0.43
1:A:384:PRO:HG3	1:A:489:PHE:CE1	2.52	0.43
1:A:911:MET:HE3	1:A:913:LYS:HB2	2.00	0.43
1:A:1418:LYS:HB3	1:A:1420:MET:HE3	2.00	0.43
1:A:1158:PHE:HZ	1:A:1267:LEU:HD13	1.83	0.43
1:A:730:ASN:HD21	1:A:732:ASP:HB2	1.83	0.43
1:A:594:ALA:HB1	1:A:1492:ARG:HH21	1.83	0.43
1:A:770:PRO:HB3	1:A:778:TYR:CE1	2.53	0.43
1:A:1043:ASN:HD22	1:A:1086:PHE:HA	1.84	0.43
1:A:513:TYR:HE2	1:A:542:PRO:HB3	1.84	0.43
1:A:914:VAL:HA	1:A:930:ILE:HG22	2.01	0.43
1:A:386:MET:HE3	1:A:461:GLY:HA3	2.01	0.43
1:A:1145:LEU:HA	1:A:1168:TRP:O	2.19	0.43
1:A:1311:GLN:HE21	1:A:1313:ARG:HB2	1.84	0.42
1:A:1414:ASP:C	1:A:1416:ILE:H	2.26	0.42
1:A:520:GLU:HA	1:A:523:GLN:NE2	2.34	0.42
1:A:1215:PRO:O	1:A:1261:TYR:OH	2.27	0.42
1:A:1425:ALA:HA	1:A:1428:MET:HE3	2.01	0.42
1:A:1005:CYS:CB	1:A:1017:ILE:HA	2.49	0.42
1:A:1552:VAL:HG11	1:A:1574:ARG:HB3	2.01	0.42
1:A:1489:PRO:C	1:A:1491:SER:H	2.28	0.42
1:A:780:ALA:HB2	1:A:799:TRP:CE3	2.55	0.42
1:A:1072:LEU:H	1:A:1072:LEU:HG	1.54	0.42
1:A:518:VAL:HG22	1:A:533:LEU:HD21	2.02	0.42
1:A:924:ARG:HG3	1:A:926:TYR:HE1	1.85	0.42
1:A:1008:LYS:HB3	1:A:1013:ASN:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:PRO:HB2	1:A:666:GLU:HB2	2.02	0.41
1:A:371:LEU:HD11	1:A:424:HIS:HD2	1.86	0.41
1:A:803:GLY:HA2	1:A:818:PHE:HE1	1.85	0.41
1:A:371:LEU:HD11	1:A:424:HIS:CD2	2.56	0.41
1:A:749:TYR:HD2	1:A:787:GLU:HB3	1.85	0.41
1:A:1456:HIS:CG	1:A:1457:LYS:N	2.88	0.41
1:A:1439:TRP:CE2	1:A:1440:ARG:HG3	2.56	0.41
1:A:921:VAL:HG12	1:A:922:ASP:H	1.86	0.41
1:A:1163:ILE:HD13	1:A:1594:ILE:HB	2.01	0.41
1:A:1377:LEU:HD22	1:A:1412:LEU:HD11	2.01	0.41
1:A:362:CYS:HB3	1:A:420:CYS:HB3	2.03	0.41
1:A:522:LEU:HD21	1:A:586:CYS:SG	2.61	0.41
1:A:930:ILE:HG13	1:A:937:TYR:HB2	2.02	0.41
1:A:557:LEU:HD11	1:A:1535:MET:HE1	2.04	0.40
1:A:1429:ARG:HA	1:A:1547:HIS:CG	2.57	0.40
1:A:372:LYS:HD2	1:A:500:GLU:HB3	2.02	0.40
1:A:1068:GLY:HA3	1:A:1089:LEU:HD21	2.02	0.40
1:A:522:LEU:HD11	1:A:587:MET:HE3	2.02	0.40
1:A:1070:ASP:HB3	1:A:1107:ARG:HH21	1.86	0.40
1:A:1530:THR:H	1:A:1538:GLN:NE2	2.20	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	1117/1330 (84%)	992 (89%)	99 (9%)	26 (2%)	5 24

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	379	ASP

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Mol	Chain	Res	Type
1	A	408	SER
1	A	465	GLY
1	A	573	ALA
1	A	896	PHE
1	A	1233	SER
1	A	1513	ALA
1	A	430	THR
1	A	476	ASP
1	A	574	LYS
1	A	639	ILE
1	A	772	ASP
1	A	1361	SER
1	A	775	LYS
1	A	1009	LYS
1	A	1037	SER
1	A	601	ARG
1	A	463	ASN
1	A	560	ALA
1	A	595	GLY
1	A	921	VAL
1	A	933	ASN
1	A	474	GLY
1	A	884	PRO
1	A	918	ILE
1	A	1410	PRO

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	1003/1162 (86%)	859 (86%)	144 (14%)	3 14

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	358	LYS

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Mol	Chain	Res	Type
1	A	365	HIS
1	A	385	GLN
1	A	393	SER
1	A	406	GLU
1	A	410	MET
1	A	412	ARG
1	A	414	THR
1	A	421	SER
1	A	448	ILE
1	A	451	GLU
1	A	459	ILE
1	A	469	GLN
1	A	480	LYS
1	A	502	GLU
1	A	507	LEU
1	A	508	MET
1	A	533	LEU
1	A	539	THR
1	A	541	VAL
1	A	544	SER
1	A	555	SER
1	A	564	VAL
1	A	565	SER
1	A	574	LYS
1	A	576	ASP
1	A	581	ILE
1	A	587	MET
1	A	601	ARG
1	A	602	ARG
1	A	629	GLN
1	A	639	ILE
1	A	654	ARG
1	A	656	CYS
1	A	658	VAL
1	A	664	GLN
1	A	689	CYS
1	A	693	ARG
1	A	697	LEU
1	A	706	GLU
1	A	722	HIS
1	A	723	GLN
1	A	729	GLN

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Mol	Chain	Res	Type
1	A	743	ILE
1	A	749	TYR
1	A	752	LYS
1	A	756	ASP
1	A	758	GLU
1	A	759	MET
1	A	760	LEU
1	A	769	ILE
1	A	804	THR
1	A	820	VAL
1	A	827	GLN
1	A	828	LEU
1	A	836	LYS
1	A	838	ILE
1	A	845	ASN
1	A	865	LYS
1	A	872	TRP
1	A	876	GLU
1	A	882	SER
1	A	886	THR
1	A	889	THR
1	A	892	ASN
1	A	893	LYS
1	A	906	LEU
1	A	917	GLN
1	A	918	ILE
1	A	920	GLU
1	A	922	ASP
1	A	927	CYS
1	A	933	ASN
1	A	943	VAL
1	A	948	GLU
1	A	955	LYS
1	A	981	SER
1	A	989	LEU
1	A	997	ILE
1	A	1007	LYS
1	A	1008	LYS
1	A	1012	VAL
1	A	1016	ASP
1	A	1033	SER
1	A	1040	THR

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Mol	Chain	Res	Type
1	A	1042	ILE
1	A	1044	MET
1	A	1050	GLU
1	A	1054	VAL
1	A	1055	ASN
1	A	1069	GLU
1	A	1071	LEU
1	A	1072	LEU
1	A	1074	SER
1	A	1094	SER
1	A	1100	GLU
1	A	1139	LEU
1	A	1163	ILE
1	A	1168	TRP
1	A	1171	GLU
1	A	1178	GLN
1	A	1182	LEU
1	A	1192	GLU
1	A	1197	LEU
1	A	1198	LEU
1	A	1209	SER
1	A	1222	MET
1	A	1223	LEU
1	A	1230	GLN
1	A	1237	ARG
1	A	1239	ASN
1	A	1245	LYS
1	A	1270	ASN
1	A	1271	VAL
1	A	1272	ARG
1	A	1275	VAL
1	A	1309	VAL
1	A	1311	GLN
1	A	1312	THR
1	A	1313	ARG
1	A	1317	ILE
1	A	1336	VAL
1	A	1343	GLN
1	A	1354	VAL
1	A	1360	LEU
1	A	1361	SER
1	A	1374	MET

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Mol	Chain	Res	Type
1	A	1385	SER
1	A	1386	ASN
1	A	1412	LEU
1	A	1433	LEU
1	A	1451	ASP
1	A	1453	VAL
1	A	1465	VAL
1	A	1470	SER
1	A	1478	VAL
1	A	1490	GLU
1	A	1520	GLU
1	A	1541	VAL
1	A	1546	GLN
1	A	1549	VAL
1	A	1597	CYS
1	A	1601	SER
1	A	1604	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	374	GLN
1	A	375	GLN
1	A	376	HIS
1	A	452	ASN
1	A	469	GLN
1	A	509	GLN
1	A	523	GLN
1	A	600	GLN
1	A	663	GLN
1	A	696	ASN
1	A	723	GLN
1	A	729	GLN
1	A	739	GLN
1	A	832	HIS
1	A	917	GLN
1	A	1029	ASN
1	A	1035	ASN
1	A	1043	ASN
1	A	1060	GLN
1	A	1076	GLN
1	A	1105	HIS

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Mol	Chain	Res	Type
1	A	1159	HIS
1	A	1160	GLN
1	A	1184	ASN
1	A	1273	ASN
1	A	1296	GLN
1	A	1311	GLN
1	A	1343	GLN
1	A	1356	ASN
1	A	1409	GLN
1	A	1430	HIS
1	A	1463	HIS
1	A	1543	HIS

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 5 ligands modelled in this entry, 4 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
3	SAH	A	1	-	27,28,28	1.17	2 (7%)	36,40,40	2.56	15 (41%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SAH	A	1	-	-	3/15/31/31	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	SAH	C6-N6	2.75	1.41	1.34
3	A	1	SAH	C2'-C3'	2.15	1.59	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	SAH	C5-C4-N3	-5.84	118.68	126.72
3	A	1	SAH	N3-C4-N9	5.63	136.74	127.17
3	A	1	SAH	N3-C2-N1	-4.74	121.41	128.58
3	A	1	SAH	O4'-C1'-C2'	-4.56	96.85	106.62
3	A	1	SAH	C5-N7-C8	4.26	110.14	103.45
3	A	1	SAH	C2-N3-C4	3.73	120.95	111.83
3	A	1	SAH	C4-C5-N7	-3.54	106.53	110.58
3	A	1	SAH	O4'-C1'-N9	-3.25	101.84	108.09
3	A	1	SAH	CB-CA-N	2.91	117.71	110.12
3	A	1	SAH	C4-N9-C8	2.79	108.67	105.74
3	A	1	SAH	N9-C8-N7	-2.78	109.99	113.94
3	A	1	SAH	C4'-O4'-C1'	-2.53	103.89	109.47
3	A	1	SAH	C2'-C1'-N9	2.42	119.33	113.30
3	A	1	SAH	C6-C5-C4	2.08	120.01	117.18
3	A	1	SAH	N6-C6-N1	2.03	122.91	118.38

There are no chirality outliers.

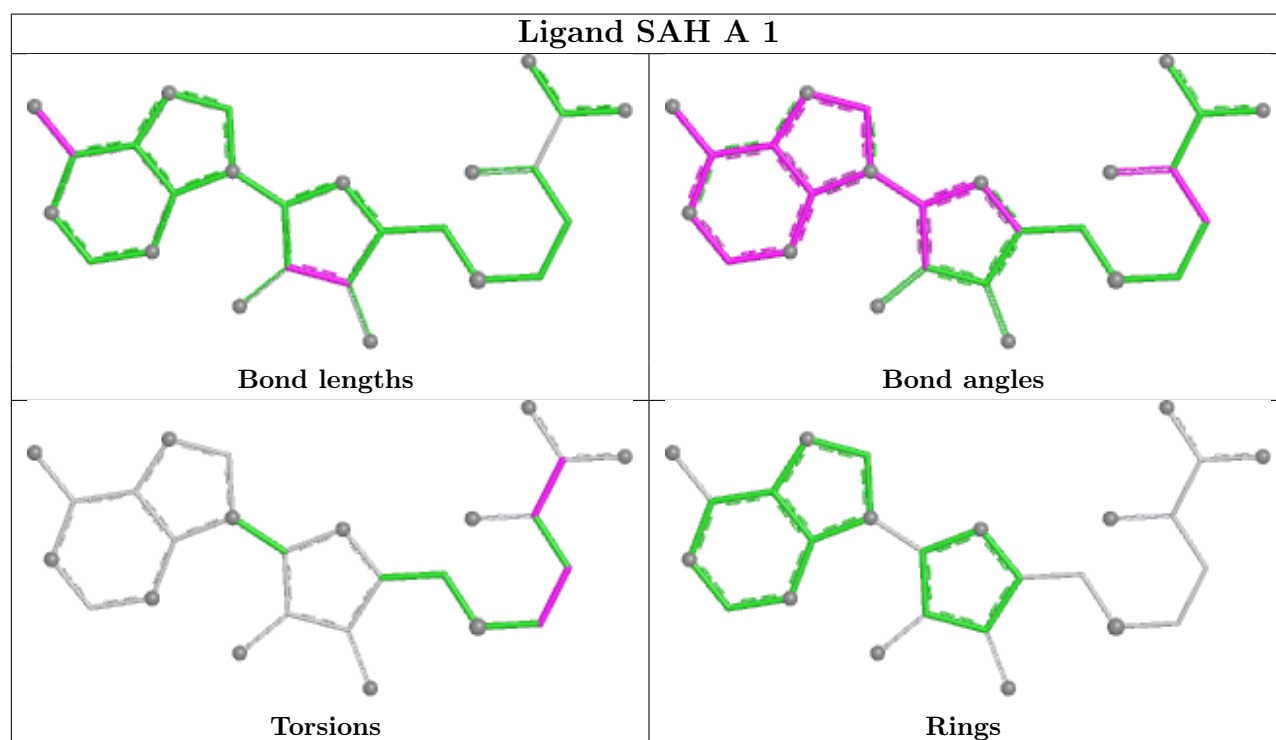
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	SAH	CA-CB-CG-SD
3	A	1	SAH	O-C-CA-N
3	A	1	SAH	OXT-C-CA-N

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1139/1330 (85%)	-0.09	15 (1%) 75 56	16, 56, 103, 125	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1608	ALA	5.4
1	A	851	GLY	4.4
1	A	690	LEU	3.9
1	A	408	SER	3.1
1	A	668	GLY	3.1
1	A	379	ASP	2.6
1	A	618	PRO	2.6
1	A	693	ARG	2.6
1	A	956	VAL	2.5
1	A	378	GLU	2.3
1	A	1231	GLY	2.2
1	A	840	LYS	2.2
1	A	1037	SER	2.1
1	A	749	TYR	2.0
1	A	357	PRO	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](#)

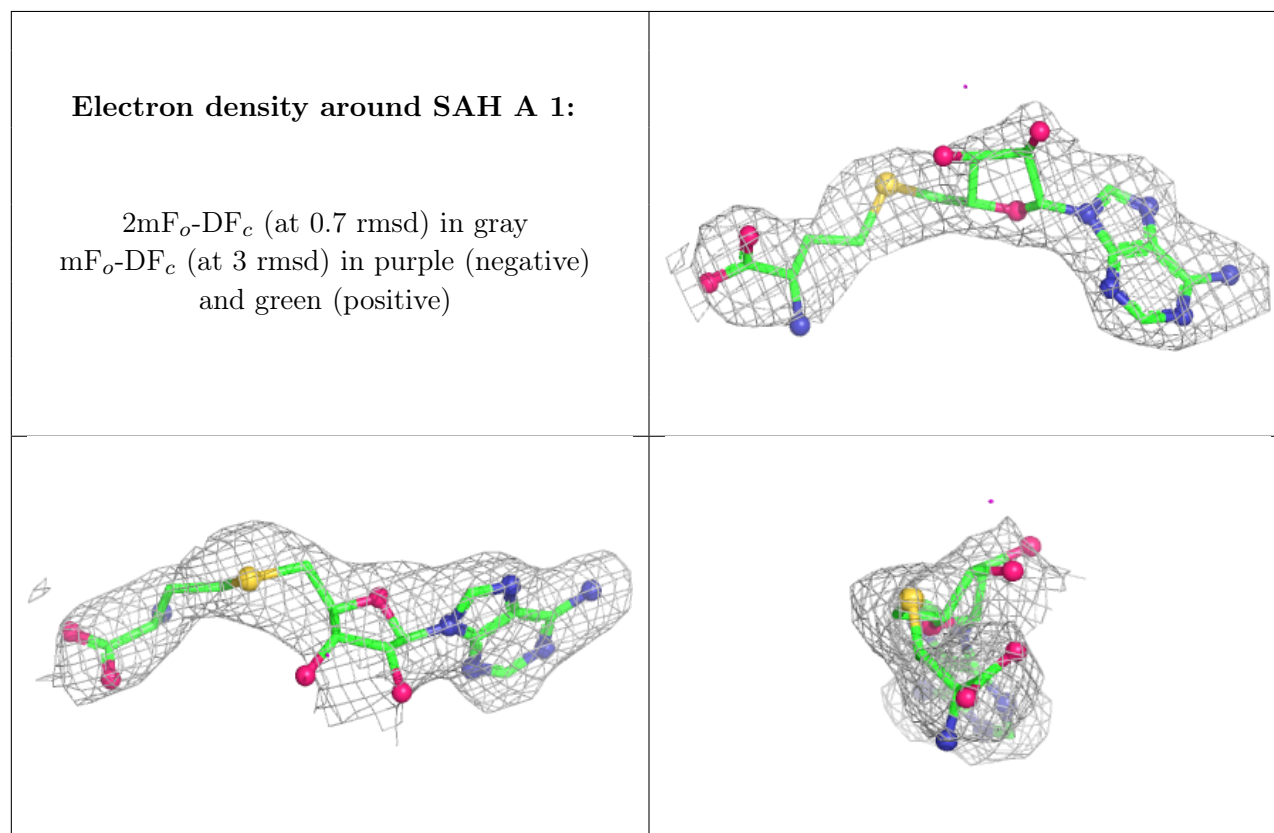
There are no oligosaccharides in this entry.

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	SAH	A	1	26/26	0.98	0.07	38,41,51,52	0
2	ZN	A	2002	1/1	1.00	0.02	65,65,65,65	0
2	ZN	A	2004	1/1	1.00	0.02	58,58,58,58	0
2	ZN	A	2005	1/1	1.00	0.01	34,34,34,34	0
2	ZN	A	2001	1/1	1.00	0.03	56,56,56,56	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.