



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 09:06 pm BST

PDB ID : 3AV5  
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](mailto: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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

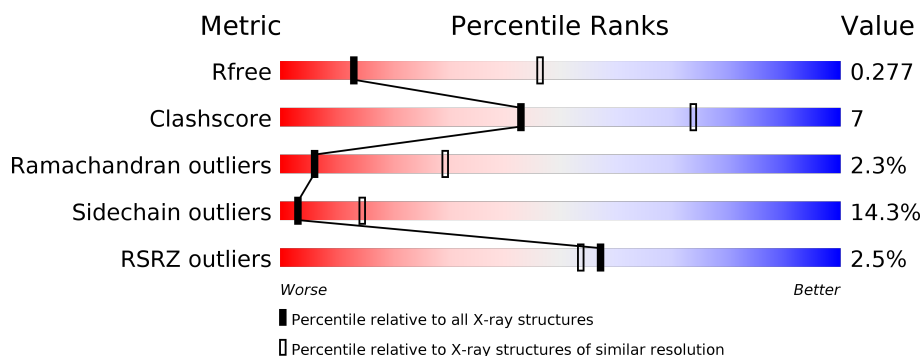
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>2%</div> <div>60%</div> <div>22%</div> <div>•</div> <div>14%</div> </div>

## 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.

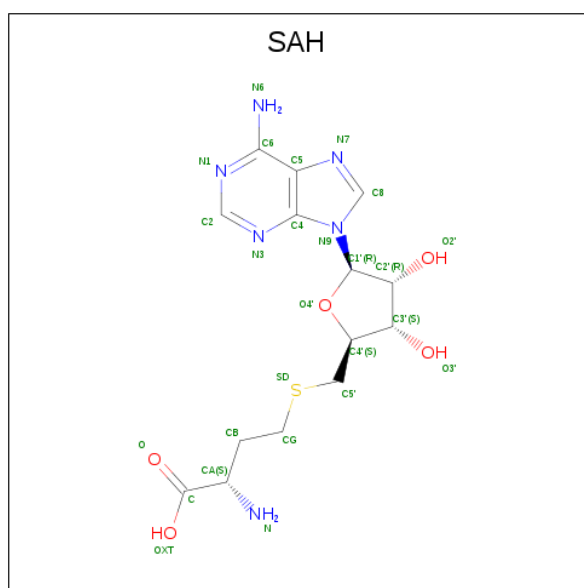
- Molecule 1 is a protein called DNA (cytosine-5)-methyltransferase 1.

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 (three-letter code: 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 (three-letter code: SAH) (formula:  $C_{14}H_{20}N_6O_5S$ ).

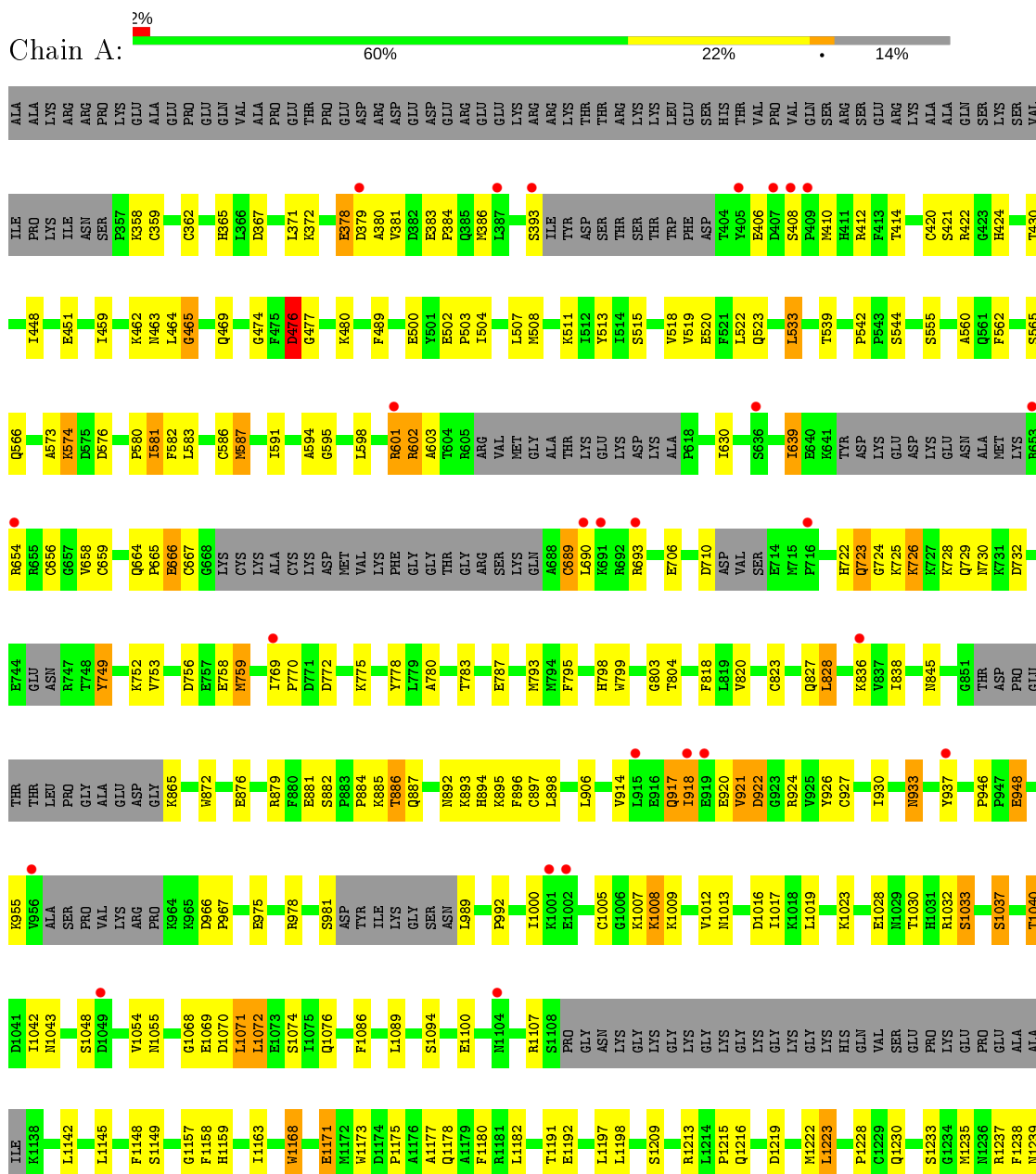


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 ( $\text{RSRZ} > 2$ ). 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



ALA	L1515	R1366	K1245
VAL	T1516	R1371	L1250
LYS	G1517	M1374	Y1257
ALA	R1518	S1375	Y1261
LYS	L1519	D1376	R1262
GLU	E1520	L1377	P1263
GLU	S1526	Q1402	F1266
ALA	T1527	P1410	L1267
ALA	T1528	I1411	N1270
THR	V1529	L1412	V1271
LYS	T1530	I1416	R1272
ASP	N1531	C1417	N1273
	P1532	K1418	F1274
	M1535	D1419	V1275
	Q1538	M1420	S1276
	V1541	A1425	Y1277
	L1542	A1426	R1292
	H1543	R1427	Q1296
	P1544	M1428	L1302
	E1545	R1429	L1302
	Q1546	H1430	V1309
	H1547	S1437	A1310
	R1548	D1438	Q1311
	V1549	W1439	T1312
	V1552	R1440	R1313
	R1553	R1448	A1320
	A1556	L1449	P1328
	R1557	G1450	L1329
	S1558	D1451	F1330
	I1571	G1452	P1331
	R1574	H1456	E1332
	H1575	K1457	P1333
	V1578	S1470	V1336
	P1585	V1478	F1337
	L1586	E1490	Q1343
	A1587	S1491	V1348
	K1588	R1492	D1349
	L1592	P1499	V1354
	E1593	W1500	S1355
	T1594	C1501	N1356
	C1597	L1502	R1359
	L1598	P1503	L1360
	S1601	A1513	S1361
	E1604	G1514	
	A1608		

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.99Å 96.92Å 130.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.66 – 3.25 40.81 – 3.25	Depositor EDS
% Data completeness (in resolution range)	(Not available) (38.66-3.25) 95.8 (40.81-3.25)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	59.9	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 72.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9135	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ZN, 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	0.52	0/9325	0.78	1/12607 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	1360	LEU	C-N-CA	6.83	138.78	121.70

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	9105	0	8877	123	0
2	A	4	0	0	0	0
3	A	26	0	19	0	0
All	All	9135	0	8896	123	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 (123) 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:1040:THR:CG2	1:A:1366:ARG:HH22	2.15	0.59
1:A:380:ALA:HB1	1:A:462:LYS:HB3	1.85	0.59
1:A:1456:HIS:CG	1:A:1457:LYS:H	2.21	0.59
1:A:992:PRO:HG2	1:A:1336:VAL:HG22	1.87	0.57
1:A:515:SER:O	1:A:519:VAL:HG23	2.04	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: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
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:H	1:A:1343:GLN:HE21	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: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:378:GLU:C	1:A:380:ALA:H	2.15	0.49
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:1332:GLU:HG3	1:A:1359:ARG:HD2	1.95	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:VAL:HG23	1:A:386:MET:HB3	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:1313:ARG:HH11	1:A:1528:THR:HG21	1.79	0.47
1:A:881:GLU:HG2	1:A:1296:GLN:HE21	1.79	0.47
1:A:667:CYS:HA	1:A:689:CYS:H	1.79	0.47
1:A:1546:GLN:HB3	1:A:1548:ARG:HG2	1.96	0.47
1:A:464:LEU:O	1:A:465:GLY:O	2.33	0.47
1:A:1274:PHE:HA	1:A:1277:TYR:CD1	2.49	0.47
1:A:1437:SER:O	1:A:1517:GLY:HA2	2.15	0.47
1:A:1416:ILE:HG12	1:A:1571:ILE:HD12	1.97	0.47
1:A:725:LYS:NZ	1:A:726:LYS:H	2.13	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: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:1348:VAL:HG12	1:A:1349:ASP:OD2	2.16	0.45
1:A:1309:VAL:HG23	1:A:1585:PRO:HG2	1.99	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:1556:ALA:HA	1:A:1578:VAL:HG11	1.99	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: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: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:476:ASP:HB3	1:A:477:GLY:H	1.56	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: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: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:566:GLN:HE22	1:A:603:ALA:HB3	1.83	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:1005:CYS:CB	1:A:1017:ILE:HA	2.49	0.42
1:A:1425:ALA:HA	1:A:1428:MET:HE2	2.02	0.42
1:A:1552:VAL:HG11	1:A:1574:ARG:HB3	2.01	0.42
1:A:1072:LEU:H	1:A:1072:LEU:HG	1.54	0.42
1:A:780:ALA:HB2	1:A:799:TRP:CE3	2.55	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:1418:LYS:HE2	1:A:1420:MET:HE3	2.01	0.41
1:A:1008:LYS:HB3	1:A:1013:ASN:HB2	2.02	0.41
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:1456:HIS:CG	1:A:1457:LYS:N	2.88	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:1439:TRP:CE2	1:A:1440:ARG:HG3	2.56	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:921:VAL:HG12	1:A:922:ASP:H	1.86	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:1429:ARG:HA	1:A:1547:HIS:CG	2.57	0.40
1:A:1068:GLY:HA3	1:A:1089:LEU:HD21	2.02	0.40
1:A:372:LYS:HD2	1:A:500:GLU:HB3	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

### 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	1117/1330 (84%)	992 (89%)	99 (9%)	26 (2%)	6	29

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	379	ASP
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%)	860 (86%)	143 (14%)	3 14

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	358	LYS
1	A	365	HIS
1	A	367	ASP
1	A	378	GLU
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	476	ASP
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	544	SER
1	A	555	SER
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	639	ILE
1	A	654	ARG
1	A	656	CYS
1	A	658	VAL
1	A	659	CYS
1	A	664	GLN
1	A	666	GLU
1	A	689	CYS
1	A	693	ARG
1	A	706	GLU
1	A	710	ASP
1	A	722	HIS
1	A	723	GLN
1	A	726	LYS
1	A	728	LYS
1	A	729	GLN
1	A	749	TYR
1	A	752	LYS
1	A	756	ASP
1	A	758	GLU
1	A	759	MET
1	A	769	ILE
1	A	795	PHE
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	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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	933	ASN
1	A	948	GLU
1	A	955	LYS
1	A	981	SER
1	A	989	LEU
1	A	1007	LYS
1	A	1008	LYS
1	A	1012	VAL
1	A	1016	ASP
1	A	1033	SER
1	A	1040	THR
1	A	1042	ILE
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	1148	PHE
1	A	1159	HIS
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	1213	ARG
1	A	1222	MET
1	A	1223	LEU
1	A	1230	GLN
1	A	1235	MET
1	A	1237	ARG
1	A	1238	PHE
1	A	1239	ASN
1	A	1245	LYS
1	A	1270	ASN
1	A	1271	VAL
1	A	1272	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1275	VAL
1	A	1309	VAL
1	A	1311	GLN
1	A	1312	THR
1	A	1313	ARG
1	A	1336	VAL
1	A	1337	PHE
1	A	1343	GLN
1	A	1354	VAL
1	A	1360	LEU
1	A	1361	SER
1	A	1374	MET
1	A	1385	SER
1	A	1412	LEU
1	A	1448	ARG
1	A	1451	ASP
1	A	1470	SER
1	A	1478	VAL
1	A	1490	GLU
1	A	1492	ARG
1	A	1520	GLU
1	A	1526	SER
1	A	1541	VAL
1	A	1546	GLN
1	A	1553	ARG
1	A	1558	SER
1	A	1597	CYS
1	A	1601	SER
1	A	1604	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	469	GLN
1	A	509	GLN
1	A	523	GLN
1	A	592	HIS
1	A	600	GLN
1	A	663	GLN
1	A	730	ASN
1	A	917	GLN
1	A	1029	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1043	ASN
1	A	1076	GLN
1	A	1159	HIS
1	A	1296	GLN
1	A	1311	GLN
1	A	1343	GLN
1	A	1356	ASN
1	A	1430	HIS
1	A	1446	GLN
1	A	1509	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 carbohydrates 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	-	21,28,28	1.38	3 (14%)	20,40,40	2.23	4 (20%)

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	-	-	1/7/31/31	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	SAH	C8-N7	-3.46	1.28	1.34
3	A	1	SAH	C2-N3	2.37	1.35	1.32
3	A	1	SAH	C2'-C3'	2.14	1.59	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	SAH	O4'-C1'-C2'	-6.89	96.85	106.93
3	A	1	SAH	N3-C2-N1	-4.65	121.41	128.68
3	A	1	SAH	C4-C5-N7	-2.75	106.53	109.40
3	A	1	SAH	N6-C6-N1	2.09	122.91	118.57

There are no chirality outliers.

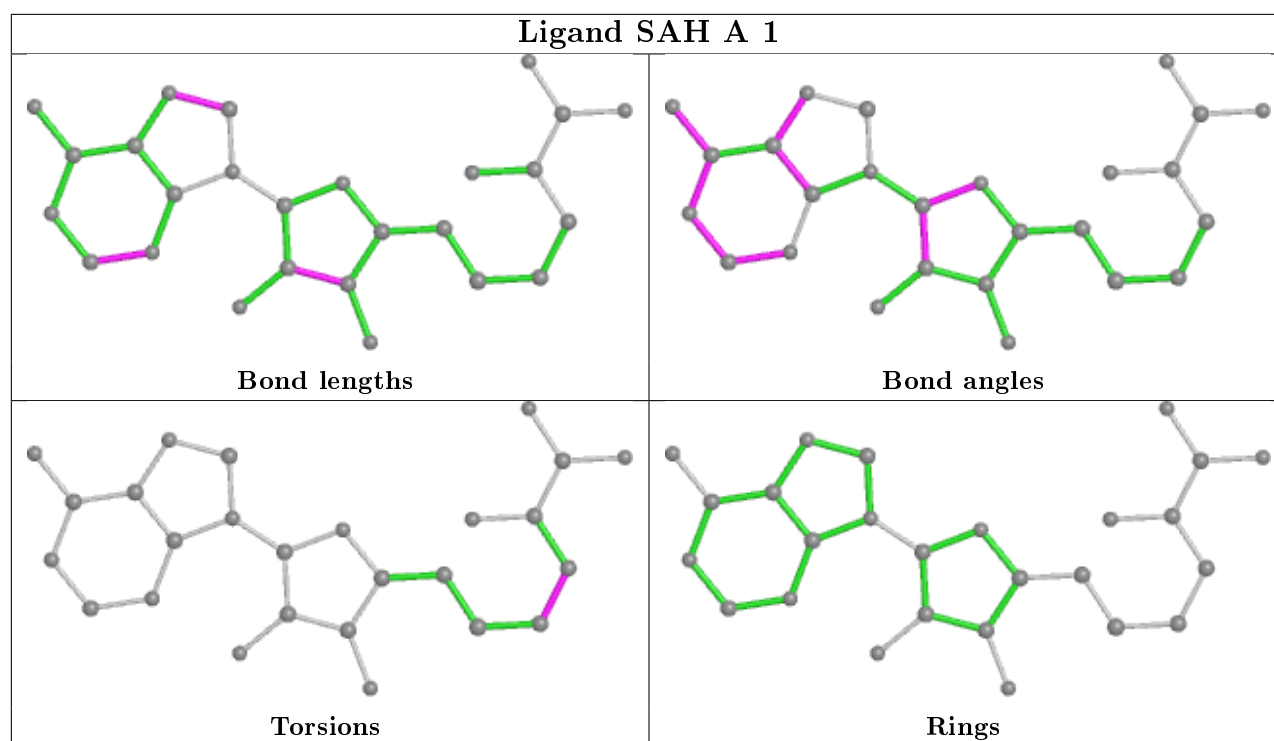
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	SAH	CA-CB-CG-SD

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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1139/1330 (85%)	-0.06	29 (2%) 57 53	16, 56, 103, 125	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	408	SER	4.5
1	A	379	ASP	4.1
1	A	716	PRO	3.2
1	A	405	TYR	3.2
1	A	690	LEU	3.0
1	A	653	ARG	3.0
1	A	393	SER	2.9
1	A	654	ARG	2.9
1	A	1451	ASP	2.9
1	A	636	SER	2.8
1	A	1001	LYS	2.8
1	A	1049	ASP	2.7
1	A	918	ILE	2.7
1	A	409	PRO	2.6
1	A	919	GLU	2.5
1	A	1452	GLY	2.4
1	A	769	ILE	2.3
1	A	693	ARG	2.3
1	A	1450	GLY	2.3
1	A	836	LYS	2.2
1	A	691	LYS	2.2
1	A	937	TYR	2.2
1	A	956	VAL	2.1
1	A	1002	GLU	2.1
1	A	601	ARG	2.1
1	A	915	LEU	2.1
1	A	387	LEU	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	407	ASP	2.1
1	A	1104	ASN	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](#)

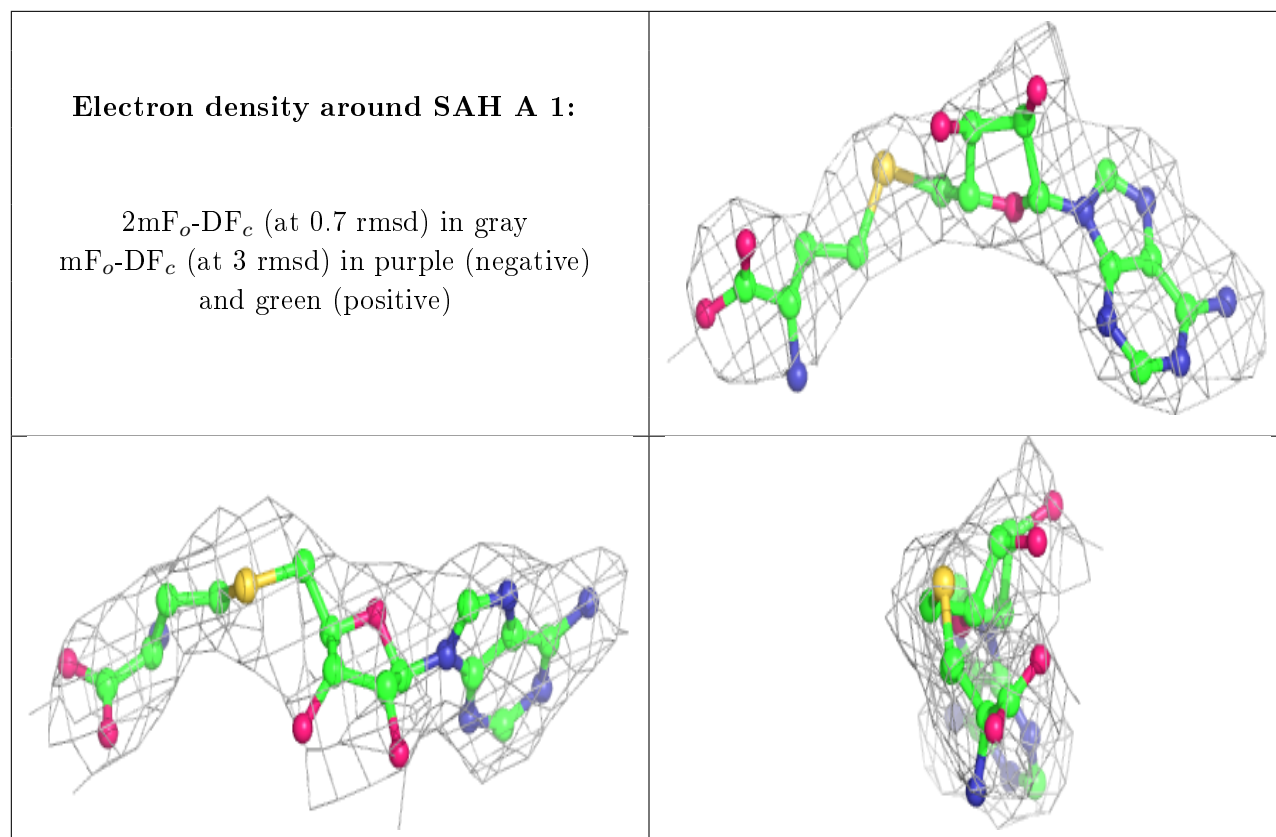
There are no carbohydrates in this entry.

## 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, 95<sup>th</sup> 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	0.19	38,41,51,52	0
2	ZN	A	2002	1/1	0.99	0.05	65,65,65,65	0
2	ZN	A	2001	1/1	0.99	0.12	56,56,56,56	0
2	ZN	A	2004	1/1	1.00	0.08	58,58,58,58	0
2	ZN	A	2005	1/1	1.00	0.10	34,34,34,34	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.