



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:53 PM UTC

PDB ID : 3AV6 / pdb_00003av6
Title : Crystal structure of mouse DNA methyltransferase 1 with AdoMet
Authors : Takeshita, K.; Suetake, I.; Yamashita, E.; Suga, M.; Narita, H.; Nakagawa, A.; Tajima, S.
Deposited on : 2011-02-22
Resolution : 3.09 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

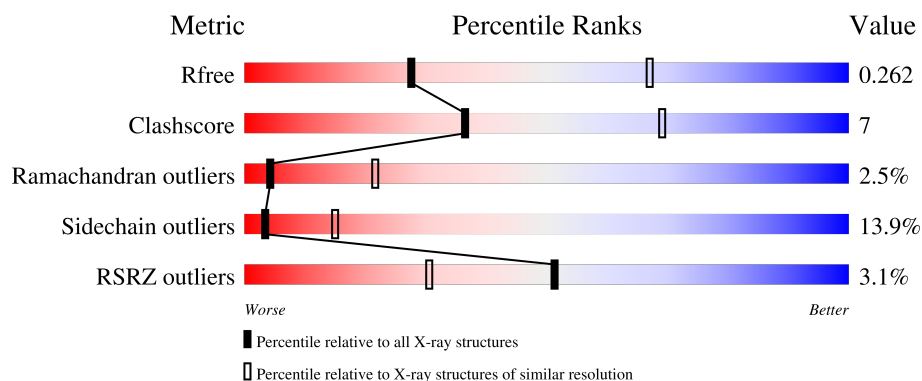
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	1330	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9110 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.

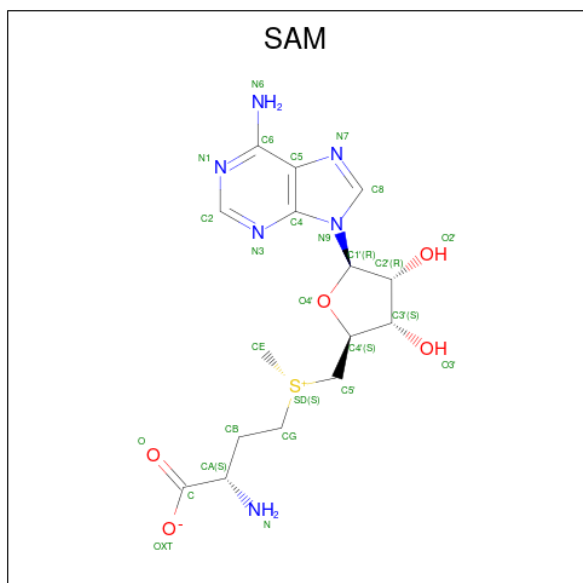
- Molecule 1 is a protein called DNA (cytosine-5)-methyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1135	Total	C	N	O	S	0	0	0
			9079	5744	1579	1697	59			

- 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-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: C₁₅H₂₂N₆O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	135.00Å 97.14Å 130.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.14 – 3.09 43.14 – 3.09	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.14-3.09) 99.6 (43.14-3.09)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.02 (at 3.12Å)	Xtriage
Refinement program	BUSTER-TNT, BUSTER 2.8.0	Depositor
R, R_{free}	0.191 , 0.255 0.198 , 0.262	Depositor DCC
R_{free} test set	1626 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	54.2	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 67.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9110	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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: ZN, SAM

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	2/9299 (0.0%)	1.44	102/12573 (0.8%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1505	THR	CA-C	6.56	1.61	1.52
1	A	1428	MET	SD-CE	-5.37	1.66	1.79

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1360	LEU	CA-C-N	10.02	139.73	121.70
1	A	1360	LEU	C-N-CA	10.02	139.73	121.70
1	A	1042	ILE	CA-C-N	8.91	137.34	121.66
1	A	1042	ILE	C-N-CA	8.91	137.34	121.66
1	A	379	ASP	CA-CB-CG	8.03	120.63	112.60
1	A	1491	SER	N-CA-C	-7.96	101.66	113.61
1	A	845	ASN	CA-CB-CG	7.14	119.75	112.60
1	A	1541	VAL	CB-CA-C	6.76	118.37	110.93
1	A	885	LYS	N-CA-C	6.56	120.41	111.17
1	A	691	LYS	N-CA-C	6.54	118.94	108.41
1	A	844	GLU	N-CA-C	-6.51	104.26	111.36
1	A	1193	ASP	CA-CB-CG	6.50	119.11	112.60
1	A	886	THR	CA-C-N	6.45	133.31	121.70
1	A	886	THR	C-N-CA	6.45	133.31	121.70
1	A	892	ASN	CA-CB-CG	6.45	119.05	112.60
1	A	1149	SER	N-CA-C	6.44	119.99	111.75
1	A	1261	TYR	N-CA-C	6.43	118.29	111.28
1	A	885	LYS	CA-C-N	6.36	133.15	121.70
1	A	885	LYS	C-N-CA	6.36	133.15	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	368	ASP	CA-CB-CG	6.36	118.95	112.60
1	A	577	ASP	N-CA-C	-6.31	105.05	114.64
1	A	658	VAL	N-CA-C	6.25	116.41	110.53
1	A	875	GLN	CA-C-N	6.12	128.49	120.28
1	A	875	GLN	C-N-CA	6.12	128.49	120.28
1	A	812	SER	N-CA-C	6.11	118.80	110.55
1	A	1070	ASP	CA-CB-CG	6.07	118.67	112.60
1	A	468	ASN	CA-CB-CG	6.04	118.64	112.60
1	A	464	LEU	CA-C-N	6.00	131.30	121.87
1	A	464	LEU	C-N-CA	6.00	131.30	121.87
1	A	1548	ARG	CA-C-N	5.91	129.40	120.95
1	A	1548	ARG	C-N-CA	5.91	129.40	120.95
1	A	428	VAL	CA-C-N	5.88	128.63	120.29
1	A	428	VAL	C-N-CA	5.88	128.63	120.29
1	A	529	VAL	N-CA-CB	-5.87	101.64	111.38
1	A	1491	SER	CA-C-N	5.84	129.85	121.50
1	A	1491	SER	C-N-CA	5.84	129.85	121.50
1	A	950	PHE	N-CA-C	5.79	115.75	108.45
1	A	1456	HIS	N-CA-C	5.76	119.05	110.52
1	A	527	ASP	CA-CB-CG	5.72	118.32	112.60
1	A	1056	PHE	CA-CB-CG	5.70	119.50	113.80
1	A	450	ASP	CA-CB-CG	5.66	118.25	112.60
1	A	1270	ASN	CA-C-N	5.65	128.29	120.49
1	A	1270	ASN	C-N-CA	5.65	128.29	120.49
1	A	804	THR	N-CA-C	-5.64	100.99	109.79
1	A	1313	ARG	N-CA-C	5.63	117.82	108.13
1	A	516	LYS	CA-C-N	5.57	127.79	120.60
1	A	516	LYS	C-N-CA	5.57	127.79	120.60
1	A	1026	ARG	N-CA-C	-5.56	102.12	110.24
1	A	661	VAL	N-CA-C	-5.55	105.69	111.58
1	A	1434	PHE	N-CA-C	5.51	115.94	109.60
1	A	428	VAL	CB-CA-C	5.50	116.04	110.65
1	A	1416	ILE	CA-CB-CG2	5.49	119.83	110.50
1	A	1490	GLU	CA-C-N	5.49	130.85	122.29
1	A	1490	GLU	C-N-CA	5.49	130.85	122.29
1	A	1201	VAL	CA-C-N	5.46	127.60	120.28
1	A	1201	VAL	C-N-CA	5.46	127.60	120.28
1	A	1452	GLY	CA-C-N	5.46	127.81	120.50
1	A	1452	GLY	C-N-CA	5.46	127.81	120.50
1	A	764	ASP	CA-CB-CG	5.44	118.04	112.60
1	A	1528	THR	CB-CA-C	5.43	119.56	110.88
1	A	873	TYR	N-CA-C	5.42	117.58	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	624	THR	N-CA-C	-5.41	100.87	109.96
1	A	1541	VAL	N-CA-CB	-5.41	105.33	112.36
1	A	1549	VAL	N-CA-C	-5.41	104.15	110.05
1	A	952	PHE	CA-CB-CG	5.41	119.21	113.80
1	A	795	PHE	CA-CB-CG	5.40	119.20	113.80
1	A	729	GLN	CA-C-N	5.40	131.85	121.54
1	A	729	GLN	C-N-CA	5.40	131.85	121.54
1	A	1412	LEU	N-CA-C	-5.40	99.93	108.73
1	A	1288	ARG	CA-C-N	5.38	127.80	120.54
1	A	1288	ARG	C-N-CA	5.38	127.80	120.54
1	A	639	ILE	N-CA-C	5.36	115.31	107.37
1	A	659	CYS	N-CA-C	5.32	117.40	110.43
1	A	1180	PHE	CA-C-N	5.32	127.67	120.38
1	A	1180	PHE	C-N-CA	5.32	127.67	120.38
1	A	1607	SER	N-CA-C	5.32	115.05	108.19
1	A	458	GLY	N-CA-C	5.31	118.96	111.42
1	A	572	GLU	N-CA-C	-5.30	105.19	110.97
1	A	896	PHE	N-CA-C	5.29	122.07	110.80
1	A	837	VAL	CA-C-N	5.29	130.96	122.50
1	A	837	VAL	C-N-CA	5.29	130.96	122.50
1	A	692	ARG	N-CA-C	-5.27	105.13	112.30
1	A	1152	GLY	N-CA-C	5.26	123.66	115.72
1	A	1581	ALA	N-CA-C	5.22	117.45	110.35
1	A	964	LYS	CA-C-N	5.21	131.48	121.54
1	A	964	LYS	C-N-CA	5.21	131.48	121.54
1	A	1148	PHE	CA-C-N	5.20	127.97	120.38
1	A	1148	PHE	C-N-CA	5.20	127.97	120.38
1	A	654	ARG	CA-C-N	5.19	129.04	121.31
1	A	654	ARG	C-N-CA	5.19	129.04	121.31
1	A	602	ARG	CA-C-N	5.17	131.42	121.54
1	A	602	ARG	C-N-CA	5.17	131.42	121.54
1	A	1360	LEU	N-CA-C	5.16	121.78	110.80
1	A	1251	VAL	CA-C-N	5.05	127.38	120.46
1	A	1251	VAL	C-N-CA	5.05	127.38	120.46
1	A	1296	GLN	N-CA-C	-5.05	101.74	109.76
1	A	1191	THR	CB-CA-C	5.04	120.12	112.00
1	A	849	GLU	N-CA-C	5.04	119.14	112.89
1	A	884	PRO	N-CA-C	5.04	120.45	113.65
1	A	1374	MET	N-CA-C	5.04	121.14	113.19
1	A	1233	SER	N-CA-C	5.00	121.46	110.80
1	A	1452	GLY	N-CA-C	-5.00	107.74	114.25

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	9079	0	8847	130	0
2	A	4	0	0	0	0
3	A	27	0	22	0	0
All	All	9110	0	8869	130	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 (130) 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	1.21	0.88
1:A:885:LYS:HA	1:A:886:THR:HG23	1.60	0.82
1:A:975:GLU:OE1	1:A:978:ARG:HD2	1.81	0.80
1:A:886:THR:H	1:A:887:GLN:HG2	1.50	0.77
1:A:1543:HIS:CD2	1:A:1546:GLN:H	2.02	0.76
1:A:1488:ASP:O	1:A:1491:SER:HB3	1.88	0.73
1:A:1159:HIS:HE1	1:A:1166:THR:H	1.37	0.72
1:A:1543:HIS:CD2	1:A:1545:GLU:H	2.10	0.70
1:A:1043:ASN:ND2	1:A:1085:ARG:O	2.23	0.66
1:A:1541:VAL:HG13	1:A:1549:VAL:HG22	1.78	0.65
1:A:1428:MET:HE2	1:A:1542:LEU:HD22	1.79	0.65
1:A:1234:GLY:HA3	1:A:1278:ARG:HH21	1.62	0.63
1:A:783:THR:HG21	1:A:897:CYS:HB2	1.80	0.63
1:A:412:ARG:HD2	1:A:495:MET:HE3	1.81	0.63
1:A:753:VAL:HG22	1:A:761:GLU:HB3	1.81	0.62
1:A:1023:LYS:O	1:A:1048:SER:HB3	1.99	0.62
1:A:1333:PRO:HD2	1:A:1359:ARG:HB2	1.82	0.61
1:A:1478:VAL:HG13	1:A:1500:TRP:NE1	2.17	0.60
1:A:1374:MET:HE1	1:A:1525:PHE:HZ	1.68	0.59
1:A:445:ALA:O	1:A:458:GLY:HA3	2.02	0.59
1:A:522:LEU:HD11	1:A:587:MET:HE3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:929:SER:HB3	1:A:938:ARG:HG2	1.83	0.58
1:A:1157:GLY:HA3	1:A:1587:ALA:HB3	1.85	0.58
1:A:992:PRO:HD2	1:A:1336:VAL:HG22	1.86	0.58
1:A:1543:HIS:HD2	1:A:1545:GLU:H	1.53	0.57
1:A:1385:SER:C	1:A:1416:ILE:HD11	2.30	0.56
1:A:1530:THR:O	1:A:1575:HIS:HB3	2.05	0.56
1:A:1229:CYS:O	1:A:1231:GLY:N	2.38	0.56
1:A:1413:ARG:O	1:A:1553:ARG:HD2	2.05	0.56
1:A:1259:ASP:HA	1:A:1293:MET:HE3	1.89	0.55
1:A:1023:LYS:HE2	1:A:1052:ALA:HB2	1.87	0.54
1:A:472:LEU:H	1:A:603:ALA:HB1	1.73	0.54
1:A:526:PRO:O	1:A:527:ASP:HB2	2.09	0.53
1:A:1139:LEU:HD21	1:A:1163:ILE:HG22	1.89	0.53
1:A:595:GLY:HA3	1:A:1504:HIS:CE1	2.44	0.53
1:A:380:ALA:HB1	1:A:462:LYS:HB3	1.90	0.53
1:A:955:LYS:H	1:A:955:LYS:NZ	2.07	0.53
1:A:1330:PHE:H	1:A:1356:ASN:HD21	1.57	0.52
1:A:1005:CYS:HB2	1:A:1017:ILE:HA	1.90	0.52
1:A:1371:ARG:NH2	1:A:1522:ASP:OD1	2.44	0.51
1:A:774:SER:O	1:A:776:PRO:HD3	2.10	0.51
1:A:386:MET:HG3	1:A:459:ILE:HD13	1.93	0.50
1:A:1171:GLU:O	1:A:1191:THR:HA	2.10	0.50
1:A:1306:GLN:HB3	1:A:1333:PRO:HB3	1.93	0.50
1:A:410:MET:HG2	1:A:491:GLU:HB2	1.93	0.50
1:A:535:ASN:O	1:A:539:THR:HB	2.12	0.50
1:A:1040:THR:CG2	1:A:1366:ARG:HH22	2.24	0.50
1:A:580:PRO:HD2	1:A:583:LEU:HD12	1.94	0.49
1:A:1407:HIS:HD2	1:A:1409:GLN:HE21	1.60	0.49
1:A:1143:ARG:HG2	1:A:1167:LEU:HD11	1.94	0.49
1:A:1449:LEU:HD21	1:A:1455:ALA:HB2	1.94	0.49
1:A:730:ASN:HD21	1:A:732:ASP:HB2	1.77	0.49
1:A:770:PRO:HB3	1:A:778:TYR:CE1	2.47	0.49
1:A:908:GLN:HA	1:A:911:MET:HE3	1.94	0.49
1:A:1374:MET:HE1	1:A:1525:PHE:CZ	2.45	0.49
1:A:886:THR:OG1	1:A:887:GLN:HA	2.13	0.49
1:A:705:ASP:O	1:A:1235:MET:HB2	2.12	0.48
1:A:567:VAL:HG13	1:A:581:ILE:HG23	1.95	0.48
1:A:793:MET:HB3	1:A:828:LEU:HD12	1.95	0.48
1:A:1030:THR:HG22	1:A:1032:ARG:H	1.78	0.48
1:A:966:ASP:HB2	1:A:967:PRO:HD2	1.96	0.47
1:A:1275:VAL:HG22	1:A:1283:LEU:HD22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:HIS:CE1	1:A:462:LYS:HB2	2.50	0.47
1:A:735:SER:HA	1:A:793:MET:HE1	1.95	0.47
1:A:1027:PRO:O	1:A:1030:THR:HB	2.14	0.47
1:A:1370:VAL:O	1:A:1374:MET:HG2	2.15	0.47
1:A:1254:PHE:HD2	1:A:1268:LEU:HD12	1.80	0.46
1:A:1002:GLU:HB2	1:A:1020:ARG:HB3	1.98	0.46
1:A:783:THR:CG2	1:A:897:CYS:HB2	2.45	0.46
1:A:1302:LEU:O	1:A:1314:ARG:HA	2.16	0.46
1:A:1274:PHE:HA	1:A:1277:TYR:CD1	2.51	0.46
1:A:522:LEU:HB3	1:A:581:ILE:HG13	1.97	0.46
1:A:639:ILE:HD11	1:A:1238:PHE:HB3	1.97	0.45
1:A:1462:PHE:O	1:A:1475:LEU:HB3	2.16	0.45
1:A:1302:LEU:HD12	1:A:1317:ILE:HD13	1.98	0.45
1:A:357:PRO:HB2	1:A:366:LEU:HD22	1.98	0.45
1:A:1275:VAL:HG11	1:A:1346:VAL:HG22	1.99	0.45
1:A:1440:ARG:NH2	1:A:1513:ALA:HA	2.31	0.45
1:A:1403:LEU:HD12	1:A:1557:ARG:HD3	1.99	0.45
1:A:414:THR:HG22	1:A:415:SER:H	1.82	0.45
1:A:472:LEU:H	1:A:603:ALA:CB	2.29	0.45
1:A:1030:THR:C	1:A:1032:ARG:H	2.23	0.45
1:A:392:LEU:HB3	1:A:411:HIS:CE1	2.52	0.45
1:A:978:ARG:NH2	1:A:1507:ASN:OD1	2.50	0.45
1:A:1266:PHE:HB3	1:A:1320:ALA:HB3	1.98	0.45
1:A:434:GLU:C	1:A:436:ASN:H	2.24	0.45
1:A:780:ALA:HB2	1:A:799:TRP:CE3	2.51	0.45
1:A:533:LEU:HD22	1:A:537:ILE:HD12	1.98	0.44
1:A:513:TYR:CE2	1:A:517:ILE:HD11	2.52	0.44
1:A:737:LEU:HB2	1:A:753:VAL:HG12	1.99	0.44
1:A:914:VAL:HA	1:A:930:ILE:HG22	2.00	0.44
1:A:472:LEU:HD21	1:A:512:ILE:HG12	2.00	0.44
1:A:1464:ASP:HA	1:A:1482:ALA:HB1	1.98	0.44
1:A:1439:TRP:HB3	1:A:1516:TYR:HB2	2.00	0.44
1:A:1426:ALA:O	1:A:1430:HIS:HD2	2.01	0.44
1:A:1360:LEU:CB	1:A:1361:SER:HB2	2.47	0.43
1:A:811:THR:HG21	1:A:1284:LYS:HB3	2.01	0.43
1:A:446:LYS:NZ	1:A:454:SER:O	2.46	0.43
1:A:726:LYS:HA	1:A:770:PRO:HA	2.00	0.43
1:A:1048:SER:OG	1:A:1050:GLU:HB2	2.18	0.43
1:A:371:LEU:HD11	1:A:424:HIS:CD2	2.52	0.43
1:A:776:PRO:O	1:A:777:LEU:HB2	2.19	0.43
1:A:526:PRO:O	1:A:527:ASP:CB	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1246:PHE:HA	1:A:1249:SER:HB3	2.02	0.42
1:A:1330:PHE:H	1:A:1356:ASN:ND2	2.17	0.42
1:A:802:ALA:HA	1:A:817:LEU:HD12	2.00	0.42
1:A:708:ALA:HB2	1:A:1235:MET:HE3	2.02	0.42
1:A:964:LYS:O	1:A:965:LYS:HB2	2.20	0.42
1:A:980:TYR:HA	1:A:981:SER:HA	1.73	0.42
1:A:723:GLN:N	1:A:724:GLY:HA3	2.34	0.42
1:A:1293:MET:HE2	1:A:1295:TYR:CD1	2.55	0.42
1:A:1143:ARG:HB2	1:A:1221:GLU:HG3	2.01	0.42
1:A:1394:GLU:HG3	1:A:1395:PRO:HD2	2.02	0.41
1:A:413:PHE:HD2	1:A:416:PHE:HB3	1.85	0.41
1:A:1360:LEU:HD22	1:A:1360:LEU:HA	1.89	0.41
1:A:594:ALA:HB1	1:A:1492:ARG:HH21	1.85	0.41
1:A:635:PHE:HD1	1:A:1243:TYR:CD2	2.39	0.41
1:A:1223:LEU:CB	1:A:1263:PRO:HG3	2.50	0.41
1:A:410:MET:HE3	1:A:491:GLU:HB3	2.03	0.41
1:A:1144:THR:HA	1:A:1222:MET:O	2.20	0.41
1:A:588:ARG:O	1:A:592:HIS:HD2	2.03	0.41
1:A:1076:GLN:HE22	1:A:1080:GLN:HG3	1.84	0.41
1:A:1173:TRP:CD1	1:A:1175:PRO:HD2	2.56	0.41
1:A:1151:CYS:HB3	1:A:1577:GLN:HG2	2.03	0.41
1:A:1418:LYS:HD2	1:A:1532:PRO:HD2	2.03	0.41
1:A:414:THR:HG21	1:A:453:PRO:O	2.21	0.41
1:A:631:PHE:HE1	1:A:1246:PHE:CE2	2.38	0.40
1:A:381:VAL:O	1:A:461:GLY:HA2	2.22	0.40
1:A:664:GLN:O	1:A:692:ARG:HG3	2.21	0.40
1:A:897:CYS:HB3	1:A:900:CYS:HB2	2.04	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	1113/1330 (84%)	991 (89%)	94 (8%)	28 (2%)	4	21

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	465	GLY
1	A	573	ALA
1	A	772	ASP
1	A	777	LEU
1	A	896	PHE
1	A	965	LYS
1	A	1230	GLN
1	A	1233	SER
1	A	1361	SER
1	A	430	THR
1	A	476	ASP
1	A	732	ASP
1	A	1037	SER
1	A	408	SER
1	A	730	ASN
1	A	850	GLY
1	A	1229	CYS
1	A	1513	ALA
1	A	480	LYS
1	A	603	ALA
1	A	921	VAL
1	A	1038	TYR
1	A	379	ASP
1	A	776	PRO
1	A	922	ASP
1	A	1362	SER
1	A	1410	PRO
1	A	409	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	1000/1162 (86%)	861 (86%)	139 (14%)	3 15

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	358	LYS
1	A	372	LYS
1	A	375	GLN
1	A	385	GLN
1	A	386	MET
1	A	405	TYR
1	A	406	GLU
1	A	408	SER
1	A	410	MET
1	A	414	THR
1	A	421	SER
1	A	428	VAL
1	A	429	ASP
1	A	448	ILE
1	A	451	GLU
1	A	459	ILE
1	A	476	ASP
1	A	479	GLU
1	A	481	VAL
1	A	500	GLU
1	A	507	LEU
1	A	515	SER
1	A	529	VAL
1	A	533	LEU
1	A	537	ILE
1	A	539	THR
1	A	548	VAL
1	A	549	ASN
1	A	566	GLN
1	A	581	ILE
1	A	590	LEU
1	A	602	ARG
1	A	623	THR
1	A	639	ILE
1	A	654	ARG
1	A	656	CYS
1	A	666	GLU
1	A	693	ARG

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Mol	Chain	Res	Type
1	A	697	LEU
1	A	707	GLU
1	A	710	ASP
1	A	714	GLU
1	A	719	LYS
1	A	723	GLN
1	A	725	LYS
1	A	728	LYS
1	A	729	GLN
1	A	739	GLN
1	A	743	ILE
1	A	749	TYR
1	A	755	ILE
1	A	758	GLU
1	A	759	MET
1	A	760	LEU
1	A	772	ASP
1	A	775	LYS
1	A	779	LEU
1	A	783	THR
1	A	792	GLN
1	A	817	LEU
1	A	826	MET
1	A	844	GLU
1	A	845	ASN
1	A	865	LYS
1	A	876	GLU
1	A	882	SER
1	A	890	GLU
1	A	892	ASN
1	A	900	CYS
1	A	908	GLN
1	A	915	LEU
1	A	917	GLN
1	A	918	ILE
1	A	920	GLU
1	A	936	VAL
1	A	943	VAL
1	A	948	GLU
1	A	951	THR
1	A	953	ASN
1	A	955	LYS

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Mol	Chain	Res	Type
1	A	981	SER
1	A	989	LEU
1	A	990	ASP
1	A	1008	LYS
1	A	1012	VAL
1	A	1021	LEU
1	A	1028	GLU
1	A	1040	THR
1	A	1042	ILE
1	A	1050	GLU
1	A	1055	ASN
1	A	1066	GLU
1	A	1069	GLU
1	A	1094	SER
1	A	1095	LYS
1	A	1100	GLU
1	A	1142	LEU
1	A	1196	VAL
1	A	1197	LEU
1	A	1198	LEU
1	A	1199	LYS
1	A	1207	THR
1	A	1209	SER
1	A	1223	LEU
1	A	1229	CYS
1	A	1232	PHE
1	A	1237	ARG
1	A	1241	ARG
1	A	1270	ASN
1	A	1271	VAL
1	A	1272	ARG
1	A	1275	VAL
1	A	1289	CYS
1	A	1309	VAL
1	A	1312	THR
1	A	1317	ILE
1	A	1332	GLU
1	A	1354	VAL
1	A	1360	LEU
1	A	1361	SER
1	A	1412	LEU
1	A	1416	ILE

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Mol	Chain	Res	Type
1	A	1446	GLN
1	A	1451	ASP
1	A	1453	VAL
1	A	1457	LYS
1	A	1458	LEU
1	A	1459	GLN
1	A	1461	THR
1	A	1478	VAL
1	A	1480	SER
1	A	1490	GLU
1	A	1508	ARG
1	A	1528	THR
1	A	1537	LYS
1	A	1541	VAL
1	A	1549	VAL
1	A	1576	ARG
1	A	1601	SER

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	376	HIS
1	A	385	GLN
1	A	468	ASN
1	A	469	GLN
1	A	535	ASN
1	A	600	GLN
1	A	696	ASN
1	A	723	GLN
1	A	730	ASN
1	A	798	HIS
1	A	832	HIS
1	A	892	ASN
1	A	917	GLN
1	A	933	ASN
1	A	953	ASN
1	A	1035	ASN
1	A	1060	GLN
1	A	1076	GLN
1	A	1105	HIS
1	A	1159	HIS

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Mol	Chain	Res	Type
1	A	1212	GLN
1	A	1239	ASN
1	A	1273	ASN
1	A	1386	ASN
1	A	1392	ASN
1	A	1402	GLN
1	A	1409	GLN
1	A	1430	HIS
1	A	1446	GLN
1	A	1509	HIS
1	A	1543	HIS
1	A	1570	ASN

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	SAM	A	1	-	27,29,29	1.04	2 (7%)	34,42,42	2.29	10 (29%)

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	SAM	A	1	-	-	4/17/33/33	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	SAM	C5-C4	2.10	1.42	1.39
3	A	1	SAM	OXT-C	-2.01	1.24	1.30

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	SAM	O3'-C3'-C4'	-4.92	96.94	111.08
3	A	1	SAM	C5-C4-N3	-4.83	120.07	126.72
3	A	1	SAM	N3-C2-N1	-4.11	122.36	128.58
3	A	1	SAM	C5-N7-C8	4.02	109.77	103.45
3	A	1	SAM	CG-SD-C5'	3.87	112.90	103.43
3	A	1	SAM	C4-C5-N7	-3.84	106.19	110.58
3	A	1	SAM	N3-C4-N9	3.80	133.63	127.17
3	A	1	SAM	C2-N3-C4	3.45	120.25	111.83
3	A	1	SAM	O2'-C2'-C3'	2.95	121.29	111.82
3	A	1	SAM	N9-C8-N7	-2.83	109.92	113.94

There are no chirality outliers.

All (4) torsion outliers are listed below:

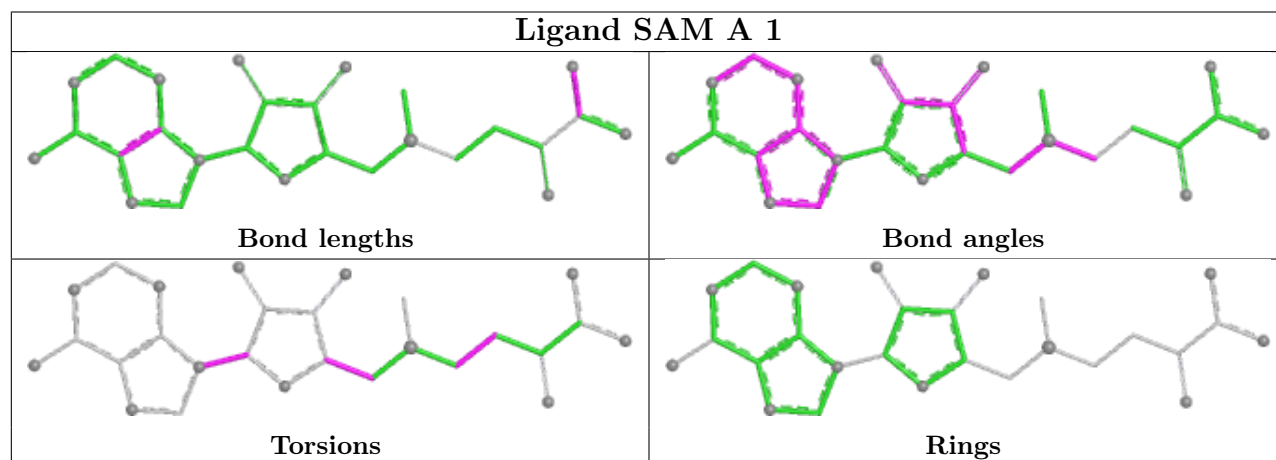
Mol	Chain	Res	Type	Atoms
3	A	1	SAM	CA-CB-CG-SD
3	A	1	SAM	C2'-C1'-N9-C8
3	A	1	SAM	O4'-C4'-C5'-SD
3	A	1	SAM	C3'-C4'-C5'-SD

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, 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	1135/1330 (85%)	0.01	35 (3%)	51 30	13, 52, 100, 127	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1608	ALA	5.8
1	A	690	LEU	5.2
1	A	408	SER	5.1
1	A	851	GLY	4.1
1	A	1607	SER	3.3
1	A	731	LYS	3.2
1	A	378	GLU	3.1
1	A	357	PRO	3.0
1	A	390	GLU	3.0
1	A	886	THR	3.0
1	A	547	ASN	2.9
1	A	1022	TYR	2.8
1	A	393	SER	2.8
1	A	376	HIS	2.7
1	A	923	GLY	2.6
1	A	981	SER	2.5
1	A	478	GLY	2.5
1	A	749	TYR	2.5
1	A	1452	GLY	2.4
1	A	618	PRO	2.4
1	A	1606	ALA	2.3
1	A	1450	GLY	2.3
1	A	689	CYS	2.3
1	A	710	ASP	2.3
1	A	688	ALA	2.2
1	A	379	ASP	2.2
1	A	640	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	666	GLU	2.1
1	A	602	ARG	2.1
1	A	377	PRO	2.1
1	A	480	LYS	2.1
1	A	918	ILE	2.1
1	A	604	THR	2.1
1	A	473	SER	2.0
1	A	695	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](#)

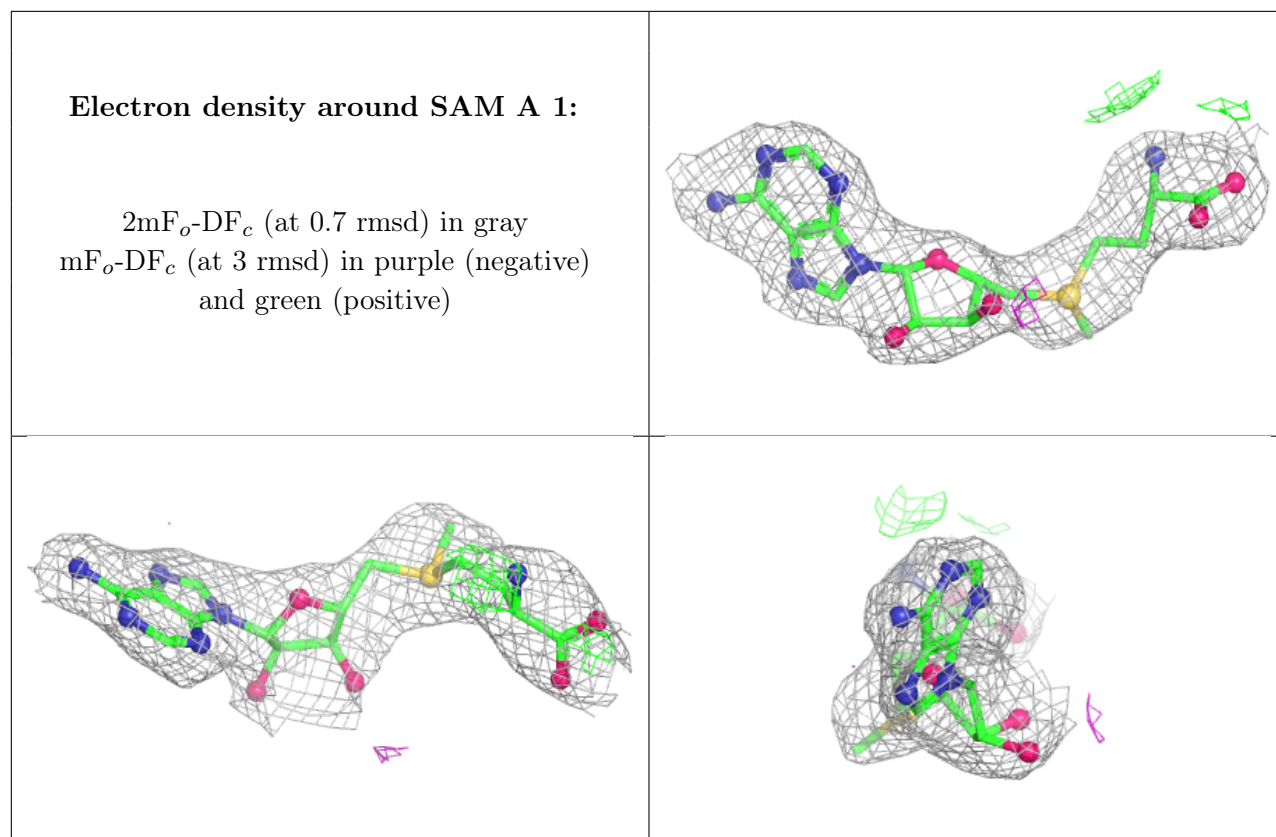
There are no oligosaccharides in this entry.

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	SAM	A	1	27/27	0.96	0.08	42,43,50,51	0
2	ZN	A	2002	1/1	0.99	0.02	58,58,58,58	0
2	ZN	A	2004	1/1	1.00	0.01	47,47,47,47	0
2	ZN	A	2005	1/1	1.00	0.01	33,33,33,33	0
2	ZN	A	2001	1/1	1.00	0.02	55,55,55,55	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.