



Full wwPDB EM Validation Report ⓘ

Oct 26, 2025 – 02:22 PM JST

PDB ID : 8XYX / pdb_00008xyx
EMDB ID : EMD-38782
Title : Cryo-EM structure of SAM-bound Tetrahymena DNA methyltransferase complex MTA1c (D209A)
Authors : Xu, Q.; Shi, Z.B.
Deposited on : 2024-01-20
Resolution : 2.80 Å(reported)
Based on initial model : .

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

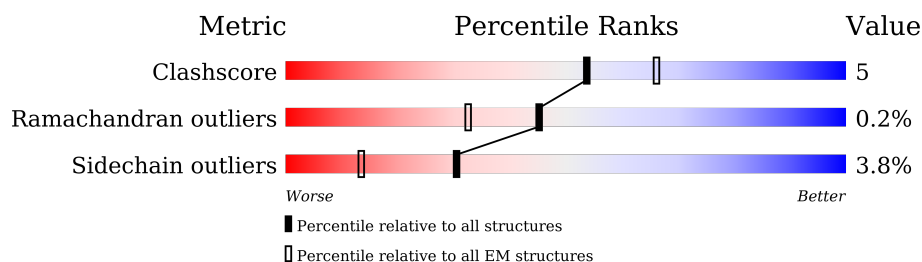
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	378	
2	B	357	
3	C	364	
4	D	146	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5292 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 MT-a70 family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	223	Total	C	N	O	S	0	0
			1814	1157	318	329	10		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q22GC0
A	-4	PRO	-	expression tag	UNP Q22GC0
A	-3	GLU	-	expression tag	UNP Q22GC0
A	-2	PHE	-	expression tag	UNP Q22GC0
A	-1	LYS	-	expression tag	UNP Q22GC0
A	0	LEU	-	expression tag	UNP Q22GC0
A	209	ALA	ASP	engineered mutation	UNP Q22GC0

- Molecule 2 is a protein called Methyltransferase MT, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	260	Total	C	N	O	S	0	0
			2149	1378	353	409	9		

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP Q22XT1
B	-3	PRO	-	expression tag	UNP Q22XT1
B	-2	GLY	-	expression tag	UNP Q22XT1
B	-1	ARG	-	expression tag	UNP Q22XT1
B	0	PRO	-	expression tag	UNP Q22XT1
B	325	TRP	-	expression tag	UNP Q22XT1
B	326	SER	-	expression tag	UNP Q22XT1
B	327	HIS	-	expression tag	UNP Q22XT1
B	328	PRO	-	expression tag	UNP Q22XT1
B	329	GLN	-	expression tag	UNP Q22XT1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	330	PHE	-	expression tag	UNP Q22XT1
B	331	GLU	-	expression tag	UNP Q22XT1
B	332	LYS	-	expression tag	UNP Q22XT1
B	333	GLY	-	expression tag	UNP Q22XT1
B	334	GLY	-	expression tag	UNP Q22XT1
B	335	GLY	-	expression tag	UNP Q22XT1
B	336	SER	-	expression tag	UNP Q22XT1
B	337	GLY	-	expression tag	UNP Q22XT1
B	338	GLY	-	expression tag	UNP Q22XT1
B	339	GLY	-	expression tag	UNP Q22XT1
B	340	SER	-	expression tag	UNP Q22XT1
B	341	GLY	-	expression tag	UNP Q22XT1
B	342	GLY	-	expression tag	UNP Q22XT1
B	343	GLY	-	expression tag	UNP Q22XT1
B	344	SER	-	expression tag	UNP Q22XT1
B	345	TRP	-	expression tag	UNP Q22XT1
B	346	SER	-	expression tag	UNP Q22XT1
B	347	HIS	-	expression tag	UNP Q22XT1
B	348	PRO	-	expression tag	UNP Q22XT1
B	349	GLN	-	expression tag	UNP Q22XT1
B	350	PHE	-	expression tag	UNP Q22XT1
B	351	GLU	-	expression tag	UNP Q22XT1
B	352	LYS	-	expression tag	UNP Q22XT1

- Molecule 3 is a protein called Myb-like DNA-binding domain protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	31	Total	C	N	O	0	0
			260	166	44	50		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP Q22VV9
C	-2	PRO	-	expression tag	UNP Q22VV9
C	-1	GLY	-	expression tag	UNP Q22VV9
C	0	ARG	-	expression tag	UNP Q22VV9
C	1	PRO	-	expression tag	UNP Q22VV9

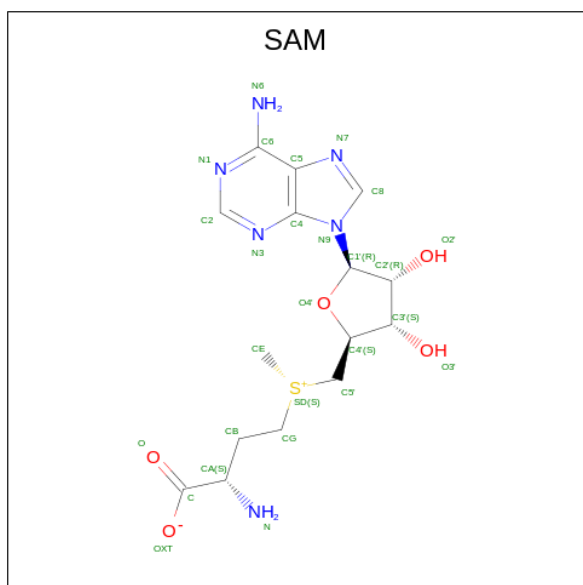
- Molecule 4 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	127	Total	C	N	O	S	0	0
			1042	661	175	202	4		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	GLY	-	expression tag	UNP I7M8B9
D	-2	PRO	-	expression tag	UNP I7M8B9
D	-1	GLU	-	expression tag	UNP I7M8B9
D	0	PHE	-	expression tag	UNP I7M8B9

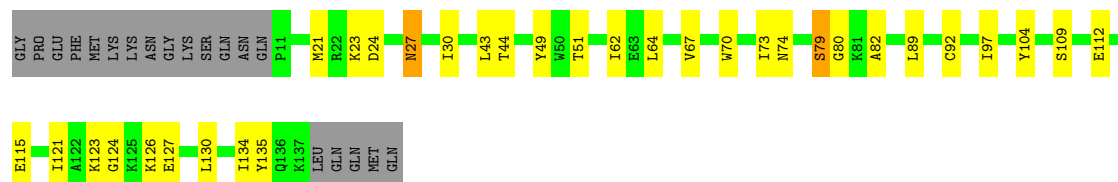
- Molecule 5 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: $C_{15}H_{22}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



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

SER	GLU	GLU	ASP	ASP	ILE	GLU	GLU	ASP	GLN	GLU	GLU	ASP	GLU	LEU	VAL	VAL	ASN	GLU	GLU	GLU	ILE	PHE	GLU	GLU	ASP	ASP	ASP	ASP	GLU	ASN	GLN	ASP	SER	SER	GLU	ASP	ASP	ASP	ASP	ASP	ASP	GLU
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Chain D: 64% 21% 13%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	479074	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

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: 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	0.13	0/1851	0.31	0/2489
2	B	0.14	0/2192	0.35	0/2941
3	C	0.08	0/262	0.21	0/353
4	D	0.13	0/1059	0.38	0/1417
All	All	0.14	0/5364	0.34	0/7200

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1814	0	1814	23	0
2	B	2149	0	2149	19	0
3	C	260	0	267	4	0
4	D	1042	0	1039	18	0
5	A	27	0	22	1	0
All	All	5292	0	5291	53	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 5.

All (53) 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)
4:D:112:GLU:HA	4:D:115:GLU:HG2	1.78	0.66
1:A:198:HIS:NE2	4:D:24:ASP:OD2	2.29	0.65
2:B:96:ILE:HG12	2:B:305:LEU:HD12	1.78	0.64
4:D:124:GLY:HA3	4:D:130:LEU:HD13	1.82	0.62
2:B:321:TYR:HB3	2:B:324:GLU:HG3	1.83	0.61
4:D:74:ASN:ND2	4:D:82:ALA:O	2.34	0.60
2:B:56:ARG:NH1	2:B:209:GLU:OE2	2.35	0.59
1:A:192:ILE:HD11	1:A:243:LEU:HD12	1.84	0.58
2:B:128:ILE:HG12	2:B:240:ARG:HG3	1.86	0.57
1:A:294:TYR:HB2	2:B:154:GLU:HG3	1.88	0.56
3:C:167:LEU:HD22	4:D:89:LEU:HD11	1.86	0.56
1:A:317:LYS:NZ	2:B:227:SER:OG	2.39	0.54
1:A:297:HIS:NE2	2:B:154:GLU:OE2	2.41	0.53
2:B:162:SER:OG	2:B:265:GLN:OE1	2.26	0.52
1:A:325:PHE:O	2:B:218:GLN:NE2	2.43	0.51
1:A:158:PHE:HD2	4:D:134:ILE:HD13	1.75	0.51
2:B:133:SER:HB2	2:B:237:LEU:HG	1.93	0.51
4:D:79:SER:OG	4:D:80:GLY:N	2.44	0.51
1:A:332:SER:O	5:A:401:SAM:N	2.44	0.50
1:A:154:LYS:HG3	3:C:167:LEU:HD21	1.94	0.49
1:A:146:ILE:HD11	3:C:170:LEU:HD22	1.95	0.49
4:D:49:TYR:HD2	4:D:51:THR:HG22	1.78	0.48
4:D:70:TRP:HA	4:D:73:ILE:HD12	1.96	0.47
2:B:103:SER:HB3	2:B:106:GLN:HG2	1.95	0.47
1:A:231:SER:HB3	1:A:234:LYS:HB2	1.95	0.47
1:A:329:ARG:HH12	1:A:335:PRO:HA	1.79	0.47
2:B:80:SER:HB3	2:B:116:LYS:HB3	1.97	0.47
1:A:210:PRO:HB3	1:A:235:ILE:HD13	1.97	0.47
1:A:159:LYS:HB2	1:A:159:LYS:HE2	1.68	0.46
2:B:102:LEU:HD21	2:B:137:ILE:HD13	1.97	0.46
1:A:361:LEU:HD21	1:A:372:LEU:HD21	1.96	0.46
4:D:23:LYS:HB2	4:D:23:LYS:HE3	1.73	0.46
1:A:149:ARG:HD2	1:A:149:ARG:HA	1.65	0.45
1:A:170:SER:HB3	4:D:43:LEU:HG	1.99	0.45
1:A:213:GLN:HA	1:A:229:SER:HB3	2.00	0.44
1:A:192:ILE:HD12	1:A:202:MET:HE2	1.99	0.43
2:B:111:ILE:HD11	2:B:141:ILE:HG13	2.01	0.43
1:A:178:PRO:HG2	4:D:30:ILE:HG21	1.99	0.43
1:A:246:ASP:OD1	1:A:309:ASP:N	2.52	0.43
2:B:284:GLU:HG2	2:B:302:MET:HE1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:21:MET:HE3	4:D:21:MET:HB3	1.93	0.42
2:B:223:ASN:HB3	2:B:230:ARG:HD2	2.01	0.42
2:B:305:LEU:HD23	2:B:305:LEU:HA	1.79	0.42
4:D:27:ASN:OD1	4:D:27:ASN:N	2.53	0.42
1:A:331:GLN:O	1:A:333:GLN:N	2.53	0.41
4:D:123:LYS:HA	4:D:126:LYS:HG2	2.02	0.41
4:D:62:ILE:HD12	4:D:67:VAL:HG22	2.03	0.41
4:D:127:GLU:OE1	4:D:135:TYR:OH	2.24	0.41
2:B:304:GLU:HG2	2:B:312:GLN:HG2	2.03	0.41
3:C:179:ARG:HE	3:C:179:ARG:HB3	1.76	0.41
1:A:137:LYS:HB2	1:A:138:GLY:H	1.64	0.40
2:B:79:ILE:HD11	2:B:322:GLU:HB2	2.02	0.40
4:D:121:ILE:HD12	4:D:121:ILE:HA	1.88	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 PDB entries followed by that with respect to all EM entries.

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	219/378 (58%)	204 (93%)	15 (7%)	0	100	100
2	B	256/357 (72%)	244 (95%)	12 (5%)	0	100	100
3	C	29/364 (8%)	27 (93%)	2 (7%)	0	100	100
4	D	125/146 (86%)	112 (90%)	12 (10%)	1 (1%)	16	44
All	All	629/1245 (50%)	587 (93%)	41 (6%)	1 (0%)	45	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	79	SER

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 PDB entries followed by that with respect to all EM entries.

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	197/336 (59%)	195 (99%)	2 (1%)	73	91
2	B	241/324 (74%)	230 (95%)	11 (5%)	23	55
3	C	29/335 (9%)	27 (93%)	2 (7%)	13	37
4	D	113/130 (87%)	106 (94%)	7 (6%)	15	43
All	All	580/1125 (52%)	558 (96%)	22 (4%)	30	62

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	LYS
1	A	340	GLN
2	B	57	SER
2	B	91	VAL
2	B	111	ILE
2	B	120	SER
2	B	162	SER
2	B	167	LEU
2	B	198	SER
2	B	214	ASN
2	B	262	ILE
2	B	269	ASN
2	B	295	GLU
3	C	162	THR
3	C	167	LEU
4	D	27	ASN
4	D	44	THR
4	D	64	LEU
4	D	92	CYS
4	D	97	ILE
4	D	104	TYR
4	D	109	SER

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

Mol	Chain	Res	Type
1	A	236	GLN
1	A	350	ASN
2	B	204	GLN
2	B	208	GLN
4	D	20	ASN
4	D	128	ASN
4	D	136	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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	SAM	A	401	-	24,29,29	0.68	0	23,42,42	1.07	3 (13%)

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
5	SAM	A	401	-	-	9/12/33/33	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	401	SAM	CG-SD-C5'	-2.30	97.53	103.40
5	A	401	SAM	C5-C6-N6	2.24	123.76	120.35
5	A	401	SAM	O4'-C1'-C2'	-2.23	103.66	106.93

There are no chirality outliers.

All (9) torsion outliers are listed below:

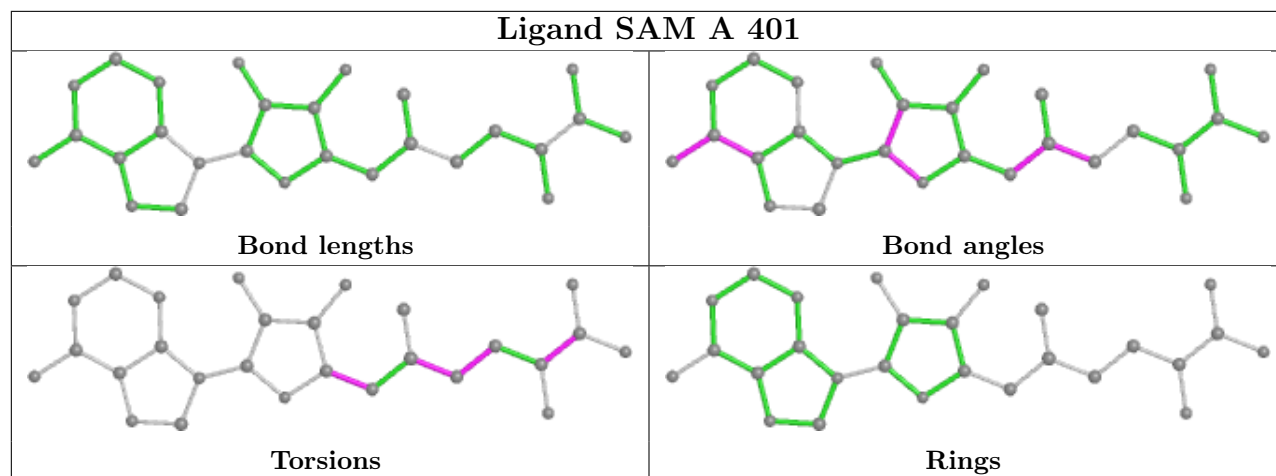
Mol	Chain	Res	Type	Atoms
5	A	401	SAM	CB-CG-SD-CE
5	A	401	SAM	CB-CG-SD-C5'
5	A	401	SAM	OXT-C-CA-N
5	A	401	SAM	O-C-CA-CB
5	A	401	SAM	OXT-C-CA-CB
5	A	401	SAM	O-C-CA-N
5	A	401	SAM	O4'-C4'-C5'-SD
5	A	401	SAM	CA-CB-CG-SD
5	A	401	SAM	C3'-C4'-C5'-SD

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	401	SAM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.