



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 15, 2026 – 01:32 AM UTC

PDB ID : 5CD1 / pdb_00005cd1
Title : Structure of an asymmetric tetramer of human tRNA m1A58 methyltransferase in a complex with SAH and tRNA3Lys
Authors : Finer-Moore, J.; Czudnochowski, N.; O'Connell III, J.D.; Wang, A.L.; Stroud, R.M.
Deposited on : 2015-07-02
Resolution : 3.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

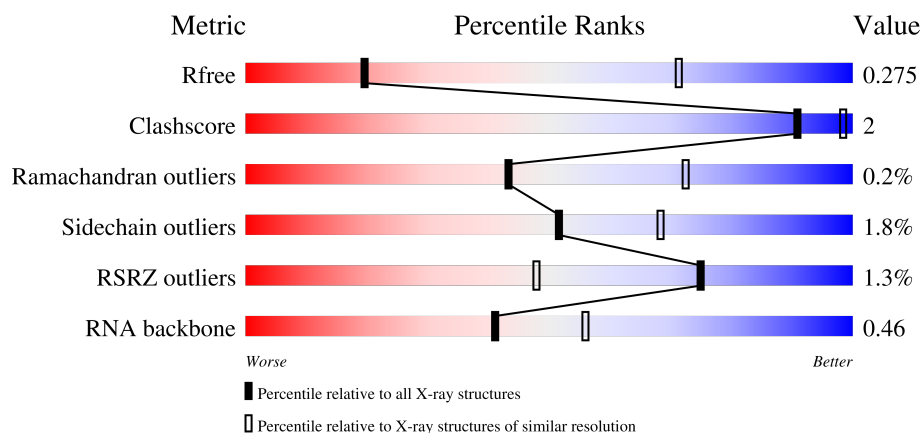
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)
RNA backbone	3983	1014 (4.14-3.06)

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	289	 2% 91% 7%
1	D	289	 % 92% 5%
2	B	497	 % 62% 35%

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Mol	Chain	Length	Quality of chain
2	E	497	<div><div>%</div><div><div></div><div>69%</div><div></div><div>26%</div></div><div></div></div>
3	M	77	<div><div>3%</div><div><div></div><div>74%</div><div></div><div>19%</div></div><div><div></div><div></div></div></div>
3	N	77	<div><div>4%</div><div><div></div><div>70%</div><div></div><div>25%</div></div><div><div></div><div></div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24065 atoms, of which 11174 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 tRNA (adenine(58)-N(1))-methyltransferase catalytic subunit TRMT61A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	281	Total	C	H	N	O	S	0	0	0
			4268	1354	2121	386	397	10			
1	D	281	Total	C	H	N	O	S	0	0	0
			4275	1355	2126	388	396	10			

- Molecule 2 is a protein called tRNA (adenine(58)-N(1))-methyltransferase non-catalytic subunit TRM6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	321	Total	C	H	N	O	S	0	0	0
			4941	1599	2452	426	450	14			
2	E	367	Total	C	H	N	O	S	0	0	0
			5673	1815	2821	497	526	14			

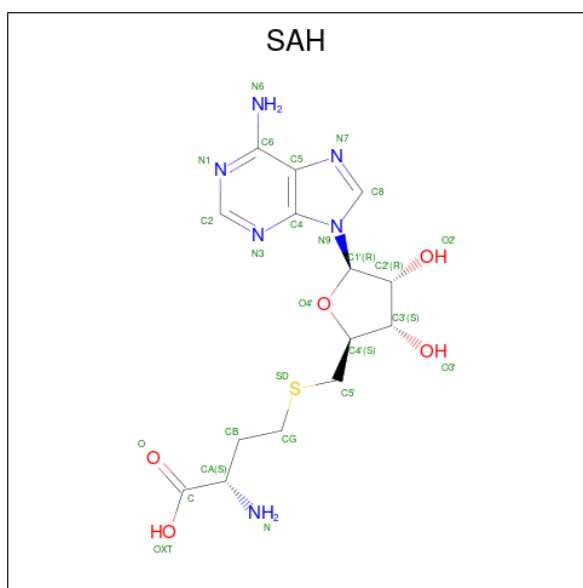
- Molecule 3 is a RNA chain called tRNA3Lys.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	M	74	Total	C	H	N	O	P	0	0	0
			2378	704	798	282	520	74			
3	N	76	Total	C	H	N	O	P	0	0	0
			2438	722	818	286	536	76			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	74	C	-	insertion	GB 339572
M	75	C	-	insertion	GB 339572
M	76	A	-	insertion	GB 339572
N	74	C	-	insertion	GB 339572
N	75	C	-	insertion	GB 339572
N	76	A	-	insertion	GB 339572

- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	S	0	0
			45	14	19	6	5	1		
4	D	1	Total	C	H	N	O	S	0	0
			45	14	19	6	5	1		

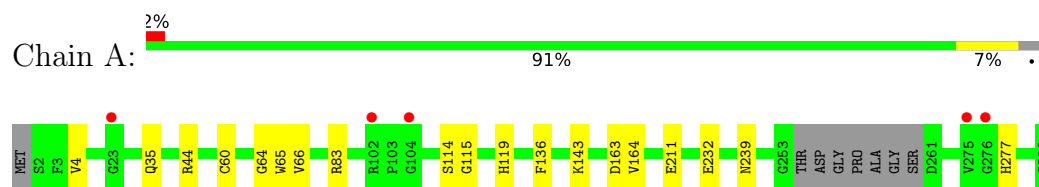
- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	1	Total	Na	0	0
			1	1		
5	N	1	Total	Na	0	0
			1	1		

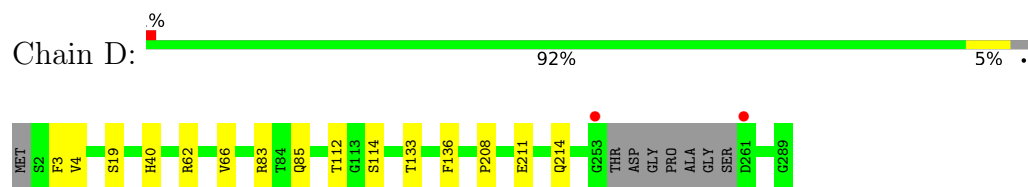
3 Residue-property plots [i](#)

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.

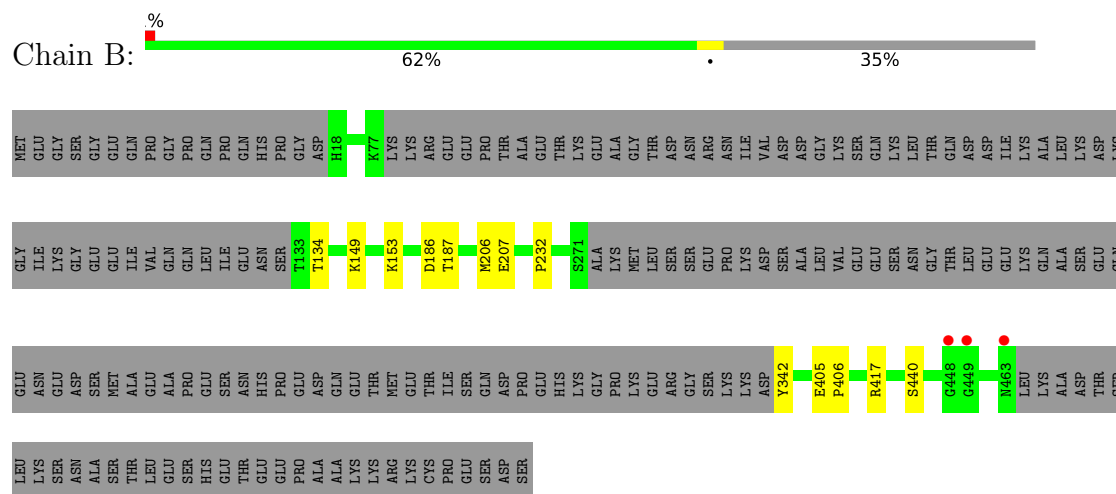
- Molecule 1: tRNA (adenine(58)-N(1))-methyltransferase catalytic subunit TRMT61A



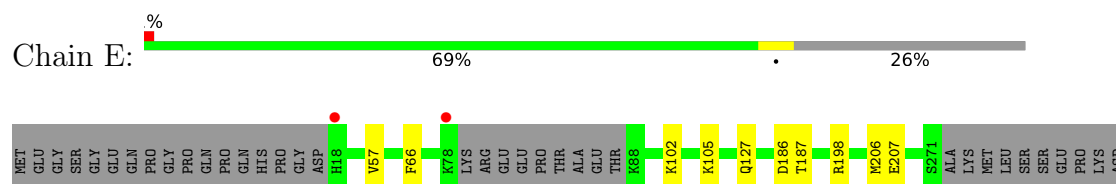
- Molecule 1: tRNA (adenine(58)-N(1))-methyltransferase catalytic subunit TRMT61A

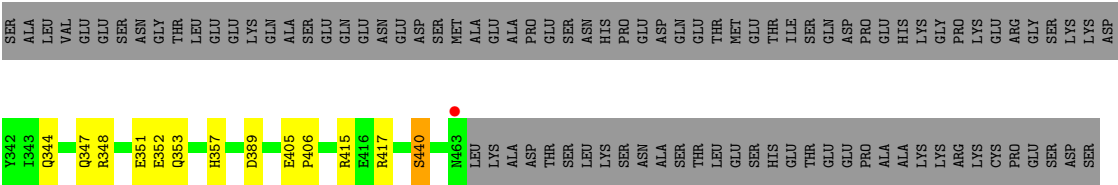


- Molecule 2: tRNA (adenine(58)-N(1))-methyltransferase non-catalytic subunit TRM6

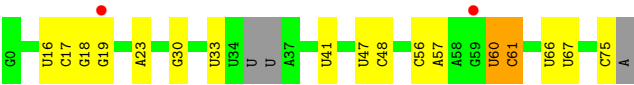
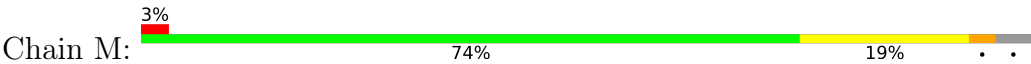


- Molecule 2: tRNA (adenine(58)-N(1))-methyltransferase non-catalytic subunit TRM6





● Molecule 3: tRNA3Lys



● Molecule 3: tRNA3Lys



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
4	SAH	D	301	-	-	2/15/31/31	0/3/3/3
4	SAH	A	301	-	-	2/15/31/31	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	301	SAH	C2-N3	2.54	1.38	1.33
4	A	301	SAH	C2-N3	2.48	1.38	1.33
4	D	301	SAH	C2-N1	2.44	1.38	1.33
4	A	301	SAH	C2-N1	2.43	1.38	1.33
4	A	301	SAH	OXT-C	-2.20	1.23	1.30

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	301	SAH	N3-C2-N1	-5.52	120.22	128.58
4	A	301	SAH	N3-C2-N1	-5.50	120.25	128.58
4	D	301	SAH	C5-C4-N3	-4.91	119.96	126.72
4	A	301	SAH	C5-C4-N3	-4.68	120.28	126.72
4	A	301	SAH	C5'-SD-CG	-4.28	89.55	102.26

There are no chirality outliers.

All (4) torsion outliers are listed below:

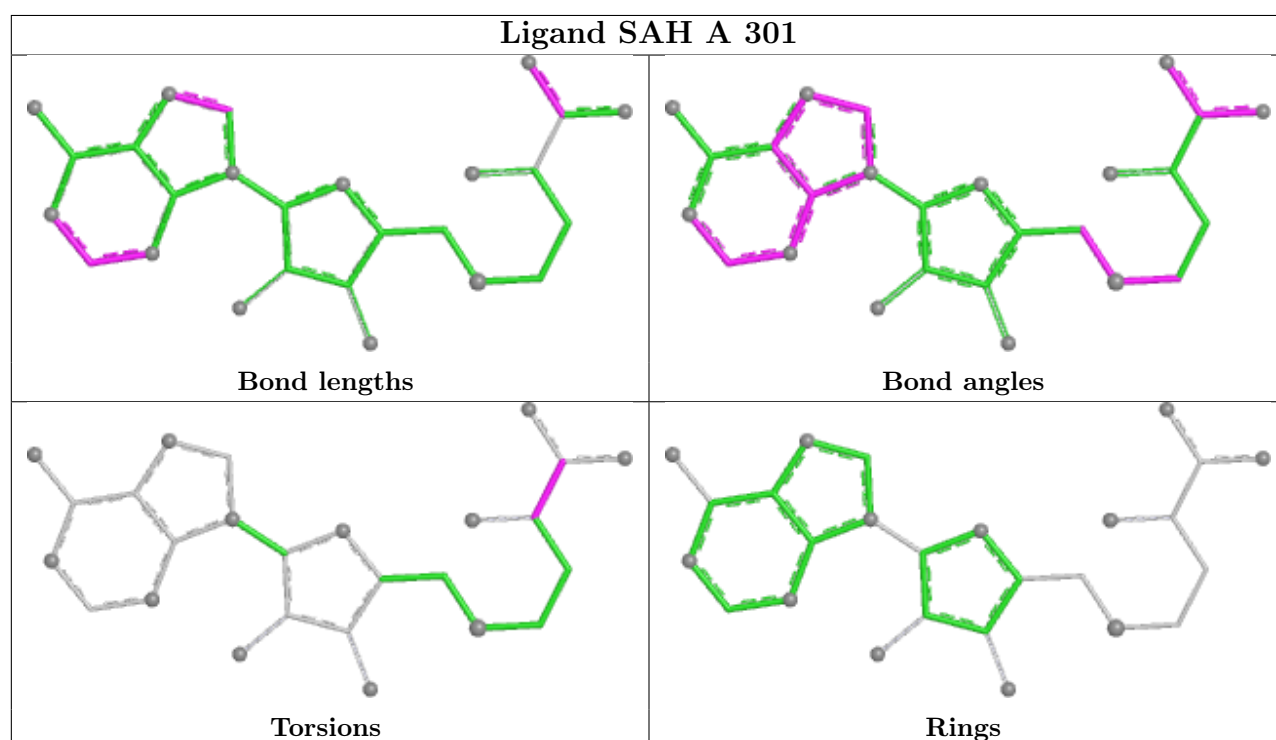
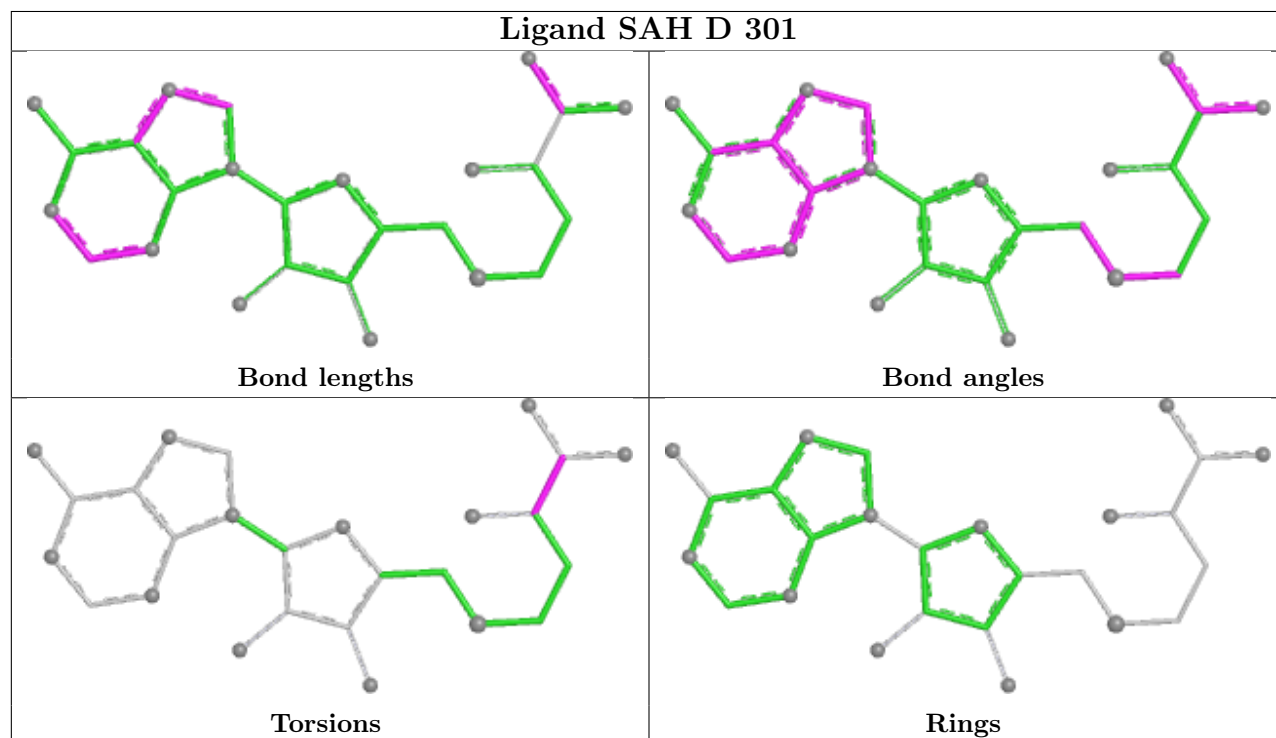
Mol	Chain	Res	Type	Atoms
4	A	301	SAH	OXT-C-CA-N
4	D	301	SAH	OXT-C-CA-N
4	A	301	SAH	O-C-CA-N
4	D	301	SAH	O-C-CA-N

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.

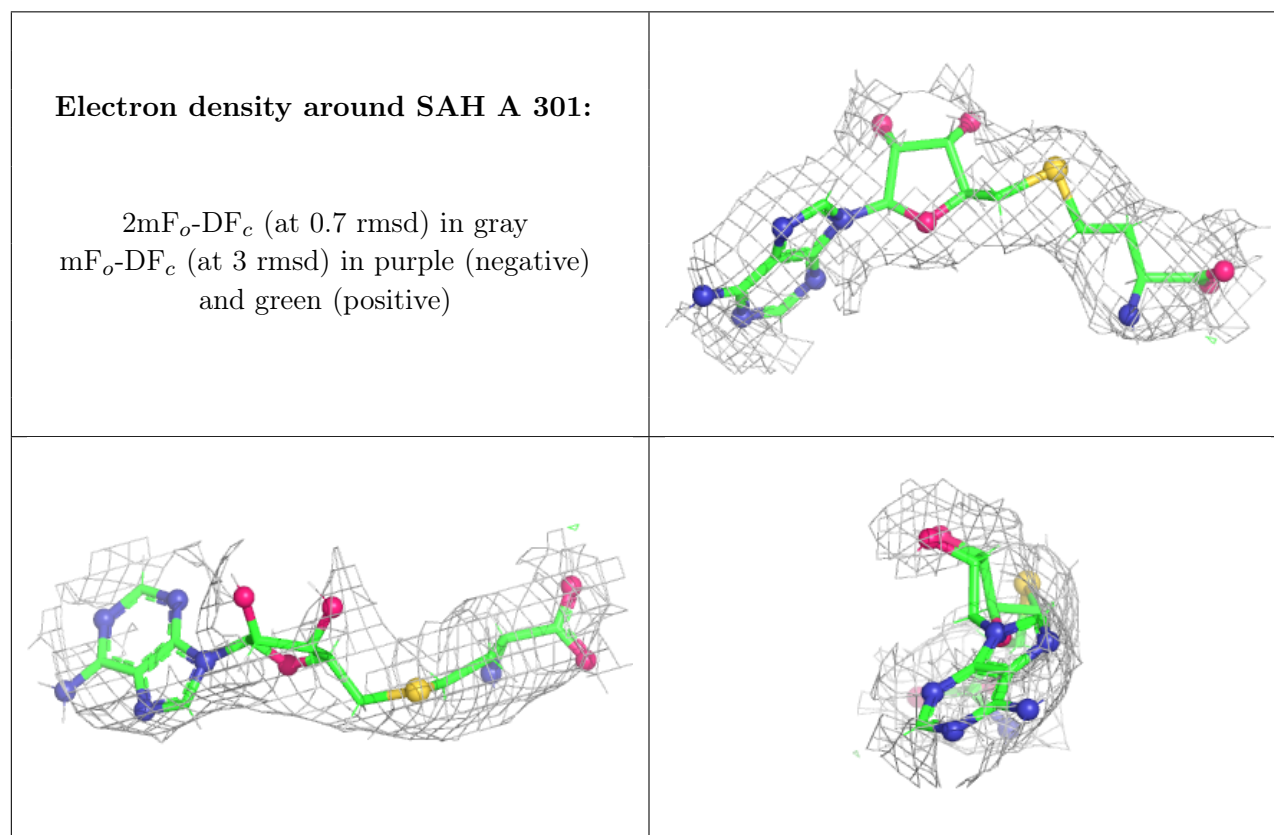


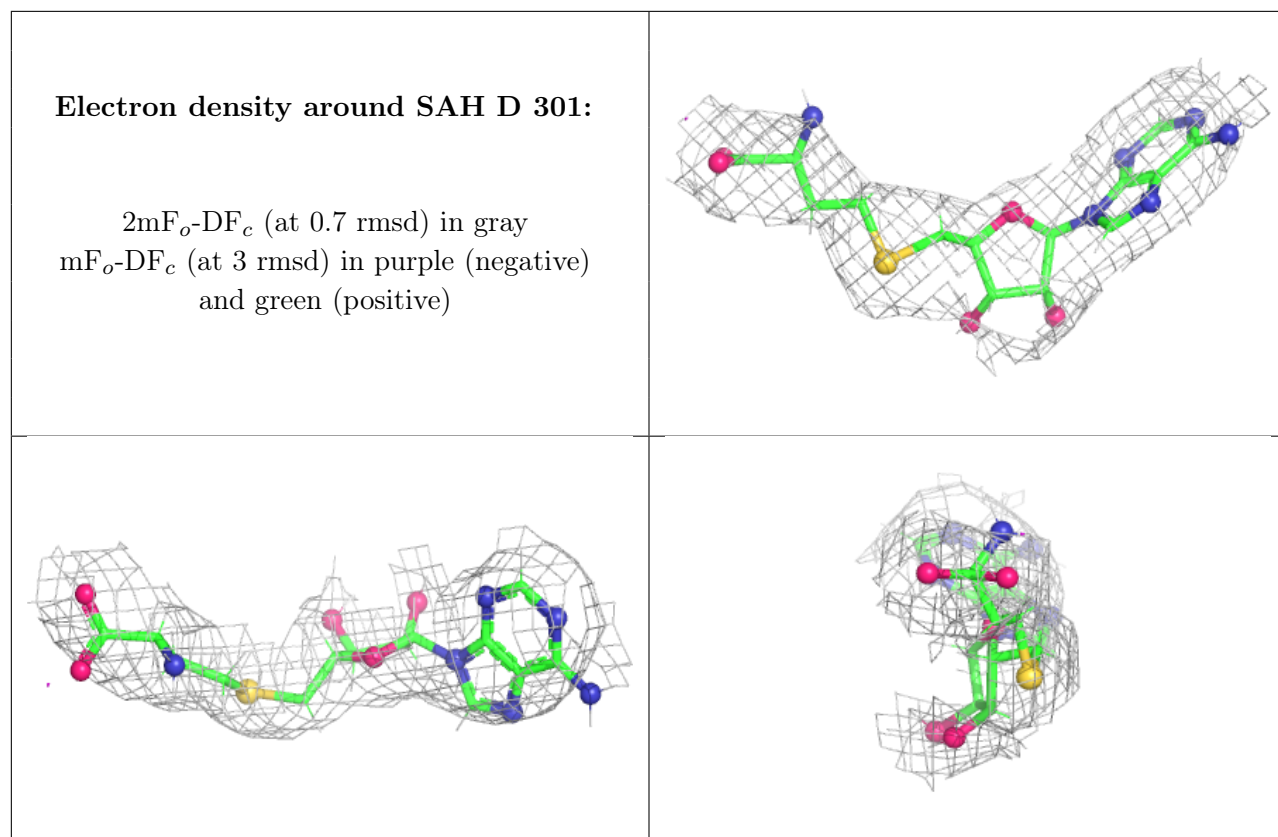
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
5	NA	N	101	1/1	0.69	0.20	69,69,69,69	0
5	NA	M	101	1/1	0.89	0.15	50,50,50,50	0
4	SAH	A	301	26/26	0.90	0.08	63,100,120,131	0
4	SAH	D	301	26/26	0.91	0.11	65,105,137,145	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.