Full wwPDB X-ray Structure Validation Report (i)

Sep 18, 2023 – 08:16 PM EDT

PDB ID	:	5CD1
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 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 (i) 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 (i)) were used in the production of this report:

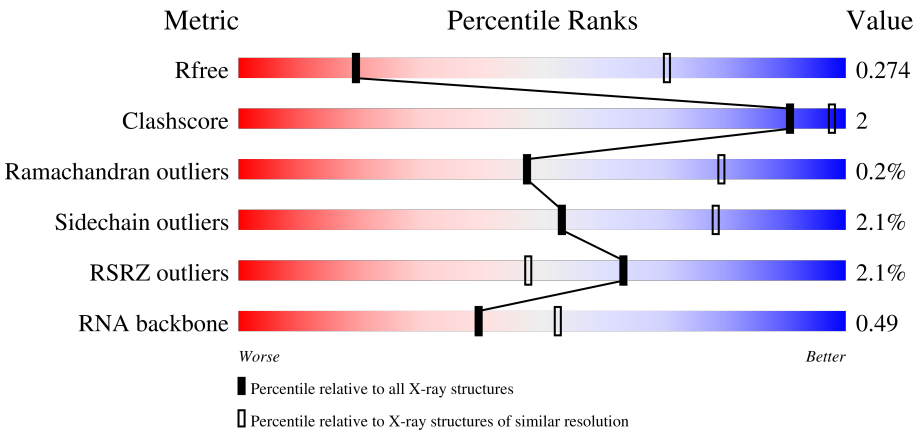
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)
RNA backbone	3102	1017 (4.20-3.00)

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 <=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	91% 6% •
1	D	289	% 92% 5% •
2	B	497	3% 61% • 35%

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Mol	Chain	Length	Quality of chain
2	E	497	%, 69%, 5%, 26%
3	M	77	4%, 73%, 21%
3	N	77	3%, 70%, 23%, 5%

2 Entry composition (i)

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
			Total	C	H	N	O	S			
1	A	281	4268	1354	2121	386	397	10	0	0	0
1	D	281	4275	1355	2126	388	396	10	0	0	0

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

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

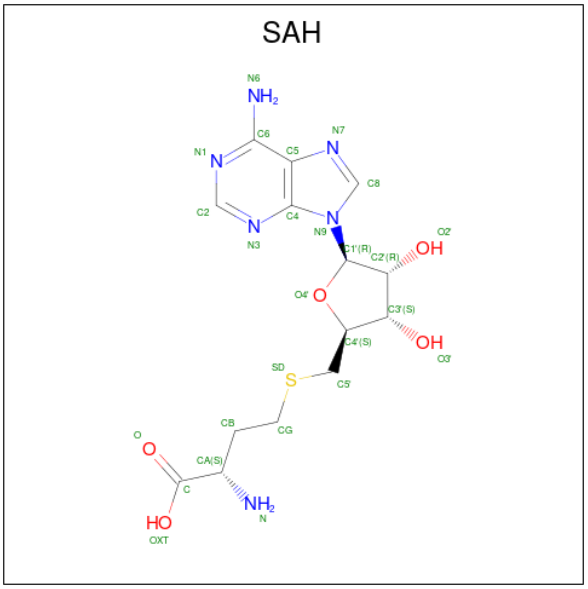
- Molecule 3 is a RNA chain called tRNA3Lys.

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

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



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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

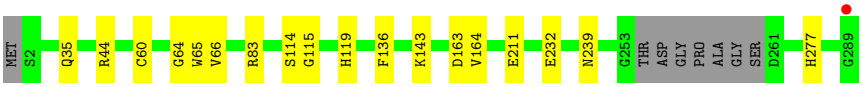
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
5	M	1	1	1	0	0
			Total	Na		
5	N	1	1	1	0	0

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.

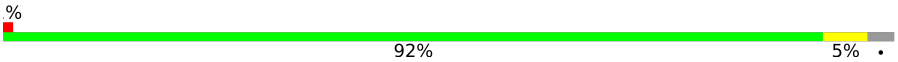
• Molecule 1: tRNA (adenine(58)-N(1))-methyltransferase catalytic subunit TRMT61A

Chain A:



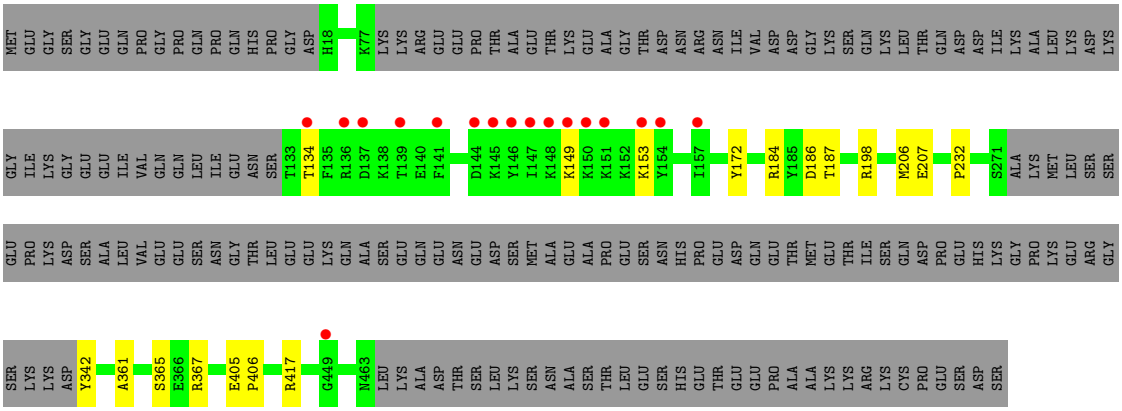
• Molecule 1: tRNA (adenine(58)-N(1))-methyltransferase catalytic subunit TRMT61A

Chain D:



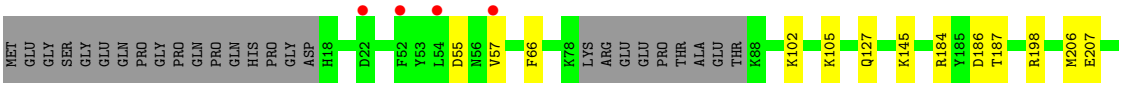
• Molecule 2: tRNA (adenine(58)-N(1))-methyltransferase non-catalytic subunit TRM6

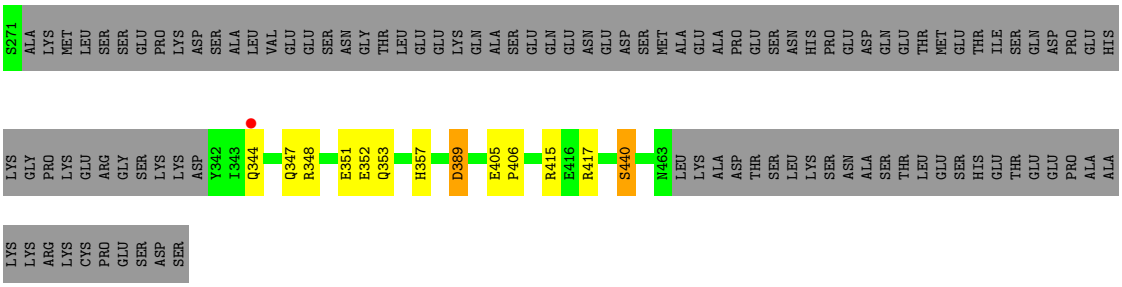
Chain B:



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

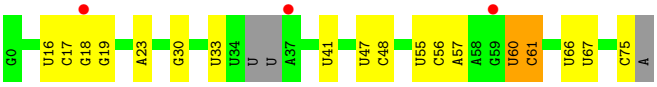
Chain E:





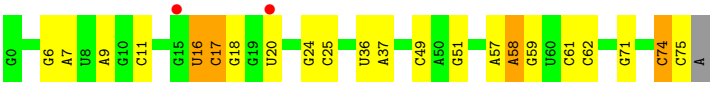
- Molecule 3: tRNA3Lys

Chain M:



- Molecule 3: tRNA3Lys

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	128.24Å 137.44Å 157.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.39 – 3.60 59.39 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (59.39-3.60) 87.0 (59.39-3.60)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.44 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.232 , 0.273 0.233 , 0.274	Depositor DCC
R_{free} test set	1640 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	84.5	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 50.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	24065	wwPDB-VP
Average B, all atoms (Å^2)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: SAH, NA

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	0.25	0/2200	0.50	0/2995
1	D	0.25	0/2202	0.52	0/2997
2	B	0.25	0/2543	0.50	2/3437 (0.1%)
2	E	0.25	0/2906	0.50	1/3921 (0.0%)
3	M	0.25	0/1764	0.85	0/2746
3	N	0.27	0/1809	0.96	3/2818 (0.1%)
All	All	0.25	0/13424	0.65	6/18914 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	N	74	C	C6-N1-C2	-10.07	116.27	120.30
3	N	74	C	N3-C2-O2	-7.39	116.73	121.90
3	N	74	C	N1-C2-O2	5.99	122.50	118.90
2	E	184	ARG	NE-CZ-NH1	5.50	123.05	120.30
2	B	184	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	B	367	ARG	NE-CZ-NH1	5.28	122.94	120.30

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	2147	2121	2108	10	0
1	D	2149	2126	2113	8	0
2	B	2489	2452	2445	4	0
2	E	2852	2821	2814	12	0
3	M	1580	798	800	6	0
3	N	1620	818	819	12	0
4	A	26	19	19	0	0
4	D	26	19	19	0	0
5	M	1	0	0	0	0
5	N	1	0	0	0	0
All	All	12891	11174	11137	41	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 2.

All (41) 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:83:ARG:NH2	1:A:114:SER:O	2.22	0.73
1:A:211:GLU:OE2	1:D:214:GLN:NE2	2.26	0.68
1:D:62:ARG:NH2	3:N:71:G:OP1	2.29	0.66
1:D:83:ARG:NH2	1:D:114:SER:O	2.31	0.63
1:A:115:GLY:O	1:A:119:HIS:ND1	2.33	0.61
3:M:19:G:OP2	3:M:19:G:N2	2.38	0.57
1:D:3:PHE:O	2:E:198:ARG:NH1	2.38	0.57
2:E:348:ARG:O	2:E:352:GLU:N	2.40	0.54
2:B:186:ASP:OD1	2:B:187:THR:N	2.44	0.50
2:B:361:ALA:O	2:B:365:SER:OG	2.24	0.49
1:A:211:GLU:OE2	2:E:440:SER:OG	2.32	0.48
3:M:60:U:O2'	3:M:61:C:OP2	2.24	0.47
1:A:65:TRP:N	3:M:16:U:O4	2.44	0.47
1:D:40:HIS:CE1	3:N:16:U:C5	3.02	0.47
2:E:353:GLN:O	2:E:357:HIS:N	2.48	0.47
1:A:60:CYS:N	1:A:64:GLY:O	2.47	0.46
2:E:389:ASP:OD1	2:E:417:ARG:NH2	2.49	0.46
2:E:102:LYS:O	2:E:105:LYS:NZ	2.44	0.46
3:N:6:G:O6	3:N:7:A:N6	2.48	0.46
2:E:186:ASP:OD1	2:E:187:THR:N	2.51	0.44
3:N:58:A:N6	3:N:61:C:C2	2.86	0.43
1:A:163:ASP:OD1	1:A:164:VAL:N	2.52	0.43
2:E:347:GLN:O	2:E:351:GLU:N	2.49	0.43
1:D:208:PRO:HG2	3:N:57:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ARG:HD3	1:A:143:LYS:HG2	2.01	0.43
3:M:30:G:N2	3:M:41:U:O2	2.52	0.43
2:E:145:LYS:NZ	3:M:55:U:O4	2.42	0.42
1:A:35:GLN:OE1	1:A:44:ARG:NH1	2.53	0.42
2:E:405:GLU:N	2:E:406:PRO:CD	2.82	0.42
3:N:7:A:C6	3:N:49:C:N4	2.88	0.42
3:M:66:U:C4	3:M:67:U:C4	3.09	0.41
2:E:415:ARG:NH2	3:N:17:C:O3'	2.53	0.41
3:N:58:A:C5	3:N:61:C:C4	3.09	0.41
2:B:153:LYS:NZ	3:N:51:G:OP2	2.43	0.41
2:B:405:GLU:N	2:B:406:PRO:CD	2.84	0.41
1:A:232:GLU:OE1	1:A:277:HIS:ND1	2.54	0.41
3:N:24:G:C6	3:N:25:C:C4	3.09	0.41
1:D:85:GLN:CB	3:N:57:A:C2	3.04	0.41
2:E:57:VAL:HG23	2:E:66:PHE:CE2	2.56	0.41
3:N:16:U:O2	3:N:16:U:C2'	2.70	0.40
1:D:112:THR:OG1	1:D:133:THR:OG1	2.25	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	277/289 (96%)	257 (93%)	20 (7%)	0	100 100
1	D	277/289 (96%)	260 (94%)	17 (6%)	0	100 100
2	B	315/497 (63%)	298 (95%)	15 (5%)	2 (1%)	25 64
2	E	361/497 (73%)	333 (92%)	28 (8%)	0	100 100
All	All	1230/1572 (78%)	1148 (93%)	80 (6%)	2 (0%)	47 79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	417	ARG
2	B	232	PRO

5.3.2 Protein sidechains (i)

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	231/238 (97%)	228 (99%)	3 (1%)	69	86
1	D	231/238 (97%)	227 (98%)	4 (2%)	60	82
2	B	257/428 (60%)	250 (97%)	7 (3%)	44	73
2	E	297/428 (69%)	290 (98%)	7 (2%)	49	75
All	All	1016/1332 (76%)	995 (98%)	21 (2%)	53	78

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	VAL
1	A	136	PHE
1	A	239	ASN
2	B	134	THR
2	B	149	LYS
2	B	172	TYR
2	B	198	ARG
2	B	206	MET
2	B	207	GLU
2	B	342	TYR
1	D	19	SER
1	D	39	ARG
1	D	66	VAL
1	D	136	PHE
2	E	55	ASP
2	E	127	GLN
2	E	206	MET
2	E	207	GLU
2	E	344	GLN
2	E	389	ASP

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Mol	Chain	Res	Type
2	E	440	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	M	72/77 (93%)	11 (15%)	0
3	N	75/77 (97%)	12 (16%)	1 (1%)
All	All	147/154 (95%)	23 (15%)	1 (0%)

All (23) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	M	17	C
3	M	18	G
3	M	23	A
3	M	33	U
3	M	47	U
3	M	48	C
3	M	56	C
3	M	57	A
3	M	60	U
3	M	61	C
3	M	75	C
3	N	9	A
3	N	11	C
3	N	16	U
3	N	17	C
3	N	18	G
3	N	20	U
3	N	36	U
3	N	37	A
3	N	58	A
3	N	59	G
3	N	62	C
3	N	75	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	N	74	C

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
4	SAH	A	301	-	24,28,28	1.17	3 (12%)	25,40,40	1.71	5 (20%)
4	SAH	D	301	-	24,28,28	1.17	3 (12%)	25,40,40	1.74	5 (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
4	SAH	A	301	-	-	3/11/31/31	0/3/3/3
4	SAH	D	301	-	-	3/11/31/31	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	301	SAH	C2-N3	3.93	1.38	1.32
4	A	301	SAH	C2-N3	3.87	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	301	SAH	C2-N1	2.35	1.38	1.33
4	A	301	SAH	C2-N1	2.34	1.38	1.33
4	A	301	SAH	OXT-C	-2.11	1.23	1.30
4	D	301	SAH	OXT-C	-2.11	1.23	1.30

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	301	SAH	N3-C2-N1	-5.41	120.22	128.68
4	A	301	SAH	N3-C2-N1	-5.39	120.25	128.68
4	A	301	SAH	C5'-SD-CG	-4.24	89.55	102.27
4	D	301	SAH	C5'-SD-CG	-4.12	89.91	102.27
4	D	301	SAH	C3'-C2'-C1'	2.81	105.21	100.98
4	A	301	SAH	OXT-C-O	-2.52	118.37	124.09
4	D	301	SAH	OXT-C-O	-2.50	118.42	124.09
4	A	301	SAH	C3'-C2'-C1'	2.23	104.34	100.98
4	D	301	SAH	OXT-C-CA	2.11	120.57	113.38
4	A	301	SAH	OXT-C-CA	2.10	120.53	113.38

There are no chirality outliers.

All (6) 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
4	A	301	SAH	N-CA-CB-CG
4	D	301	SAH	N-CA-CB-CG

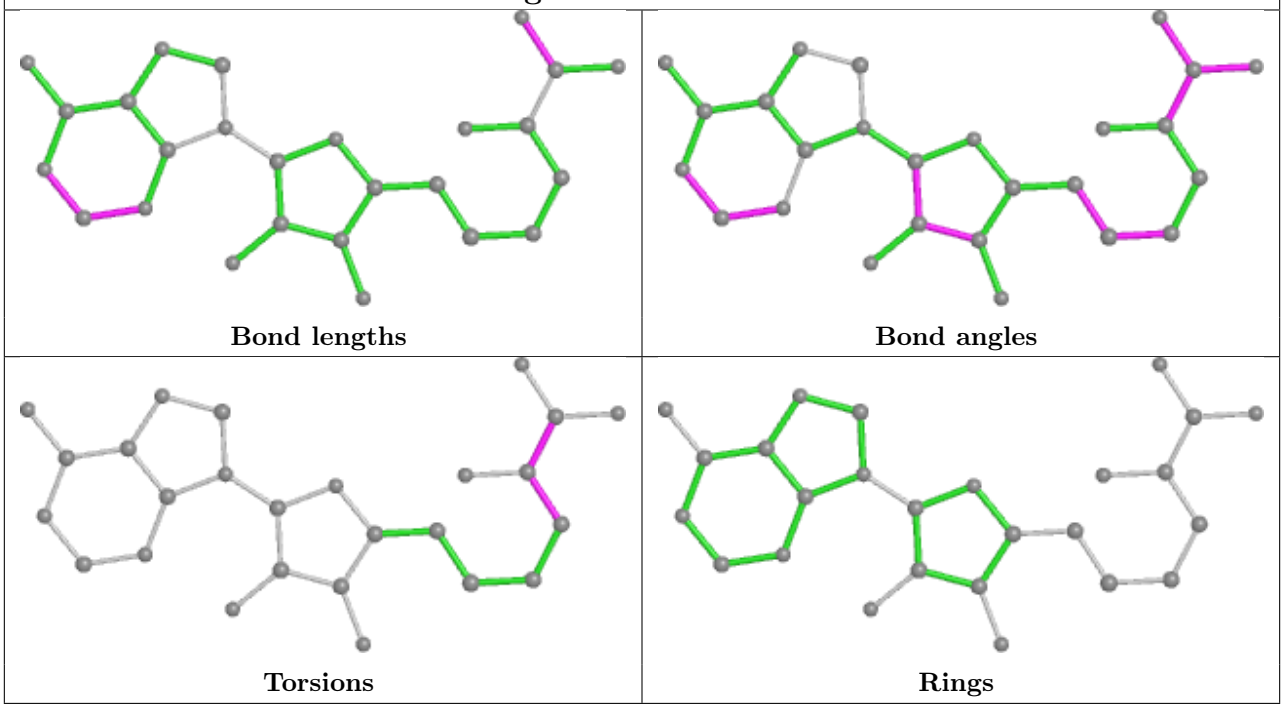
There are no ring outliers.

No monomer is involved in short contacts.

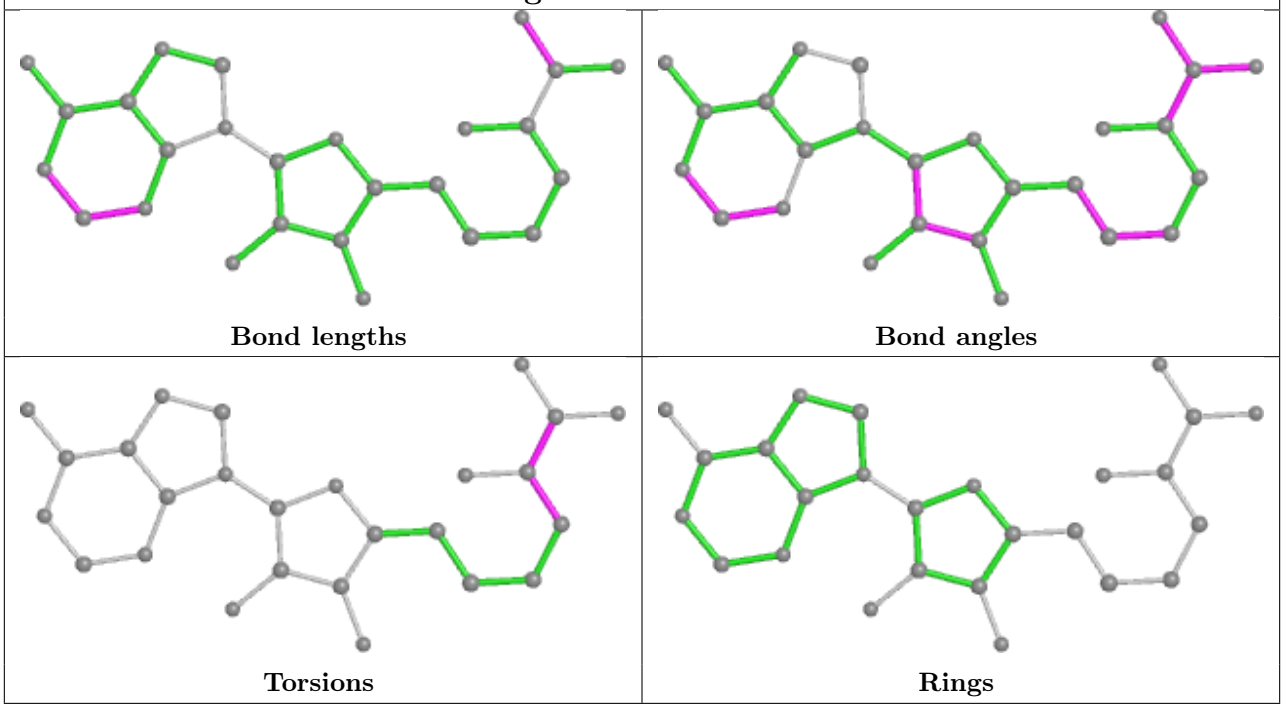
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand SAH A 301



Ligand SAH D 301



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	281/289 (97%)	-0.28	1 (0%)	92	86	68, 101, 129, 157	0
1	D	281/289 (97%)	-0.12	2 (0%)	87	78	57, 91, 128, 162	0
2	B	321/497 (64%)	0.09	17 (5%)	26	16	56, 96, 193, 220	0
2	E	367/497 (73%)	-0.09	5 (1%)	75	61	60, 101, 154, 196	0
3	M	74/77 (96%)	0.09	3 (4%)	37	24	87, 117, 181, 205	0
3	N	76/77 (98%)	-0.09	2 (2%)	56	40	86, 117, 178, 191	0
All	All	1400/1726 (81%)	-0.08	30 (2%)	63	48	56, 99, 162, 220	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	289	GLY	7.0
2	B	146	TYR	5.7
2	B	137	ASP	5.6
2	B	154	TYR	4.5
2	B	148	LYS	4.0
2	B	147	ILE	4.0
2	B	136	ARG	3.7
2	B	150	LYS	3.7
2	B	144	ASP	3.6
2	B	153	LYS	3.5
2	E	54	LEU	3.2
2	B	134	THR	3.1
1	D	62	ARG	3.0
2	E	52	PHE	3.0
2	E	344	GLN	2.9
2	B	149	LYS	2.9
3	M	37	A	2.8
2	B	145	LYS	2.6
3	M	18	G	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	139	THR	2.5
1	D	35	GLN	2.4
2	E	22	ASP	2.4
3	M	59	G	2.3
2	E	57	VAL	2.3
2	B	449	GLY	2.3
2	B	151	LYS	2.2
3	N	15	G	2.2
2	B	141	PHE	2.1
3	N	20	U	2.1
2	B	157	ILE	2.1

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 monosaccharides in this entry.

6.4 Ligands (i)

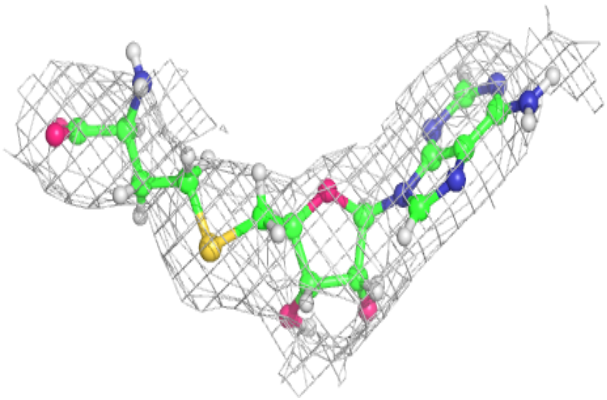
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

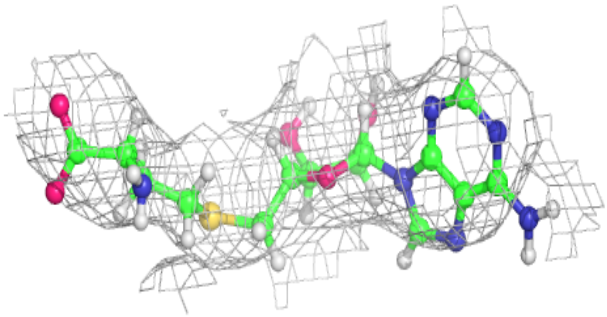
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NA	N	101	1/1	0.88	0.36	69,69,69,69	0
4	SAH	D	301	26/26	0.91	0.28	65,105,137,145	0
5	NA	M	101	1/1	0.93	0.08	50,50,50,50	0
4	SAH	A	301	26/26	0.93	0.17	63,100,120,131	0

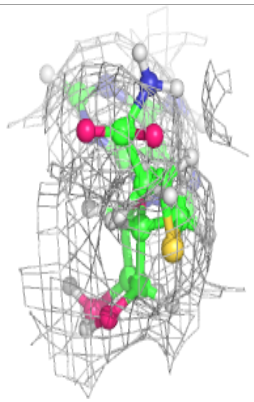
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SAH D 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

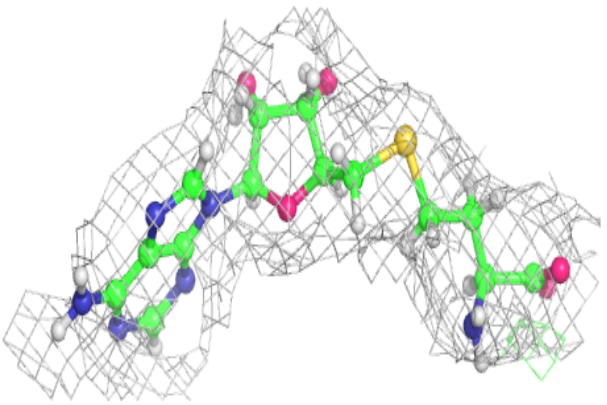


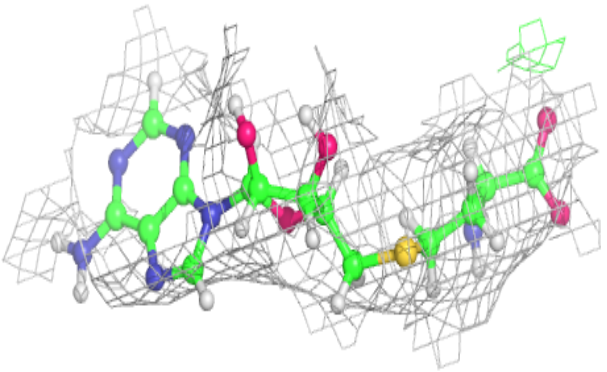


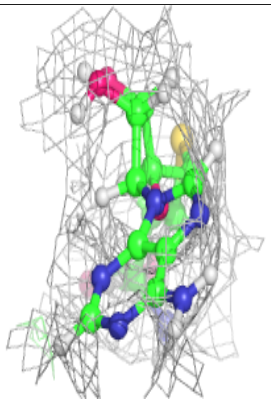


Electron density around SAH A 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.