



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 01:29 am BST

PDB ID : 3PLA
Title : Crystal structure of a catalytically active substrate-bound box C/D RNP from *Sulfolobus solfataricus*
Authors : Lin, J.; Lai, S.; Jia, R.; Xu, A.; Zhang, L.; Lu, J.; Ye, K.
Deposited on : 2010-11-15
Resolution : 3.15 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 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

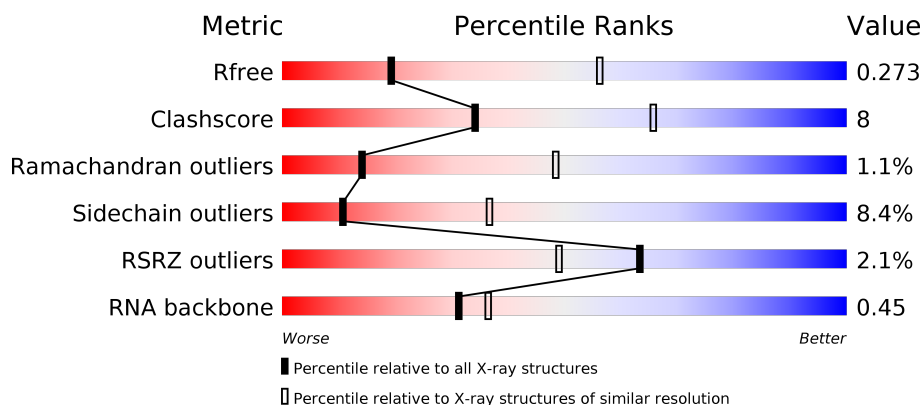
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)
RNA backbone	3102	1073 (3.50-2.82)

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 ≥ 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	388	<div> <div>0%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>• •</div> </div> </div>
1	B	388	<div> <div></div> <div> <div>78%</div> <div>16%</div> <div>• •</div> </div> </div>
1	K	388	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>• •</div> </div> </div>
2	C	130	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>19%</div> <div>• 6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	D	130	<div><div></div><div>68%24%6%</div></div>
2	L	130	<div><div>9%</div><div>68%23%6%</div></div>
3	E	232	<div><div></div><div>65%28%. .</div></div>
3	F	232	<div><div>2%</div><div>67%26%. . .</div></div>
3	M	232	<div><div>4%</div><div>66%27%. .</div></div>
4	G	40	<div><div>3%</div><div>43%35%10%13%</div></div>
4	H	40	<div><div>3%</div><div>45%20%10%5%20%</div></div>
4	N	40	<div><div>8%</div><div>50%20%8%23%</div></div>
5	I	10	<div><div></div><div>40%50%10%</div></div>
5	J	10	<div><div></div><div>70%20%10%</div></div>
5	O	10	<div><div></div><div>50%40%10%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20046 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 Pre mRNA splicing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	0	0
			2993	1902	528	558	5			
1	B	375	Total	C	N	O	S	0	0	0
			2993	1902	528	558	5			
1	K	375	Total	C	N	O	S	0	0	0
			2993	1902	528	558	5			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	MET	ENGINEERED MUTATION	UNP Q97ZH3
A	381	HIS	-	EXPRESSION TAG	UNP Q97ZH3
A	382	HIS	-	EXPRESSION TAG	UNP Q97ZH3
A	383	HIS	-	EXPRESSION TAG	UNP Q97ZH3
A	384	HIS	-	EXPRESSION TAG	UNP Q97ZH3
A	385	HIS	-	EXPRESSION TAG	UNP Q97ZH3
A	386	HIS	-	EXPRESSION TAG	UNP Q97ZH3
A	387	HIS	-	EXPRESSION TAG	UNP Q97ZH3
A	388	HIS	-	EXPRESSION TAG	UNP Q97ZH3
B	2	VAL	MET	ENGINEERED MUTATION	UNP Q97ZH3
B	381	HIS	-	EXPRESSION TAG	UNP Q97ZH3
B	382	HIS	-	EXPRESSION TAG	UNP Q97ZH3
B	383	HIS	-	EXPRESSION TAG	UNP Q97ZH3
B	384	HIS	-	EXPRESSION TAG	UNP Q97ZH3
B	385	HIS	-	EXPRESSION TAG	UNP Q97ZH3
B	386	HIS	-	EXPRESSION TAG	UNP Q97ZH3
B	387	HIS	-	EXPRESSION TAG	UNP Q97ZH3
B	388	HIS	-	EXPRESSION TAG	UNP Q97ZH3
K	2	VAL	MET	ENGINEERED MUTATION	UNP Q97ZH3
K	381	HIS	-	EXPRESSION TAG	UNP Q97ZH3
K	382	HIS	-	EXPRESSION TAG	UNP Q97ZH3
K	383	HIS	-	EXPRESSION TAG	UNP Q97ZH3
K	384	HIS	-	EXPRESSION TAG	UNP Q97ZH3

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Chain	Residue	Modelled	Actual	Comment	Reference
K	385	HIS	-	EXPRESSION TAG	UNP Q97ZH3
K	386	HIS	-	EXPRESSION TAG	UNP Q97ZH3
K	387	HIS	-	EXPRESSION TAG	UNP Q97ZH3
K	388	HIS	-	EXPRESSION TAG	UNP Q97ZH3

- Molecule 2 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	122	Total	C	N	O	S	0	0	0
			927	588	156	181	2			
2	D	122	Total	C	N	O	S	0	0	0
			927	588	156	181	2			
2	L	122	Total	C	N	O	S	0	0	0
			927	588	156	181	2			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	ASP	ASN	ENGINEERED MUTATION	UNP D0KRE2
D	2	ASP	ASN	ENGINEERED MUTATION	UNP D0KRE2
L	2	ASP	ASN	ENGINEERED MUTATION	UNP D0KRE2

- Molecule 3 is a protein called Fibrillarin-like rRNA/tRNA 2'-O-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	227	Total	C	N	O	S	0	0	0
			1829	1175	309	341	4			
3	F	227	Total	C	N	O	S	0	0	0
			1829	1175	309	341	4			
3	M	227	Total	C	N	O	S	0	0	0
			1829	1175	309	341	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	2	ALA	SER	ENGINEERED MUTATION	UNP P58032
F	2	ALA	SER	ENGINEERED MUTATION	UNP P58032
M	2	ALA	SER	ENGINEERED MUTATION	UNP P58032

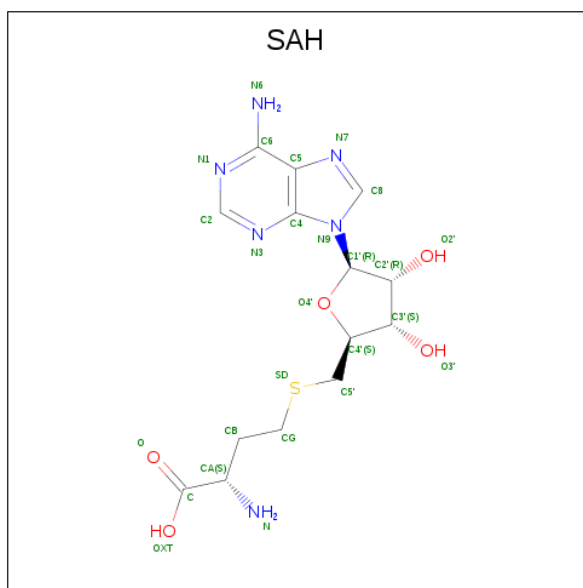
- Molecule 4 is a RNA chain called C/D guide RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	35	Total	C	N	O	P	0	0	0
			753	336	138	244	35			
4	H	32	Total	C	N	O	P	0	0	0
			679	304	120	223	32			
4	N	31	Total	C	N	O	P	0	0	0
			659	295	116	217	31			

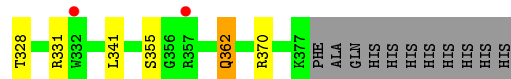
- Molecule 5 is a RNA chain called RNA (5'-R(*CP*CP*AP*UP*GP*AP*GP*UP*GP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	10	Total	C	N	O	P	0	0	0
			210	95	37	69	9			
5	J	10	Total	C	N	O	P	0	0	0
			210	95	37	69	9			
5	O	10	Total	C	N	O	P	0	0	0
			210	95	37	69	9			

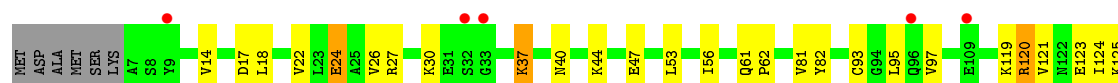
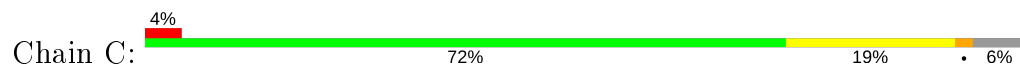
- Molecule 6 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C₁₄H₂₀N₆O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	E	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
6	F	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
6	M	1	Total	C	N	O	S	0	0
			26	14	6	5	1		



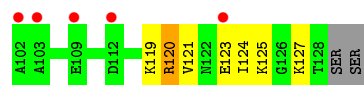
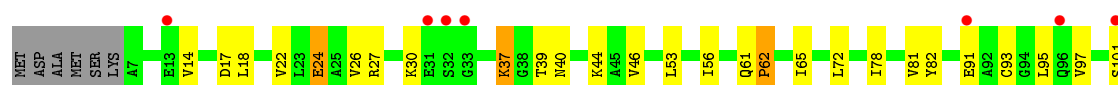
- Molecule 2: 50S ribosomal protein L7Ae



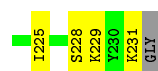
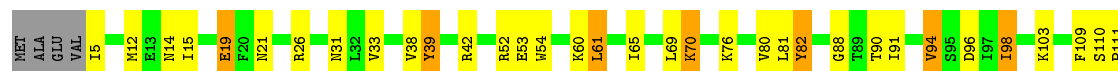
- Molecule 2: 50S ribosomal protein L7Ae



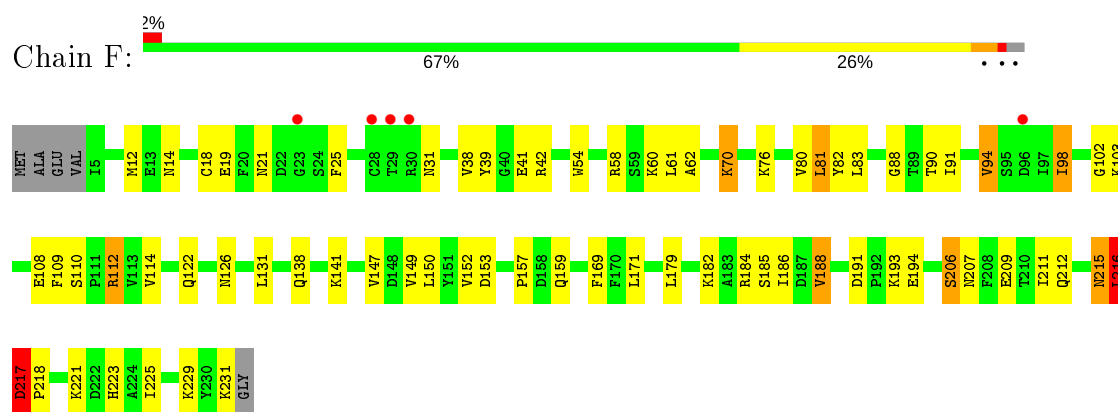
- Molecule 2: 50S ribosomal protein L7Ae



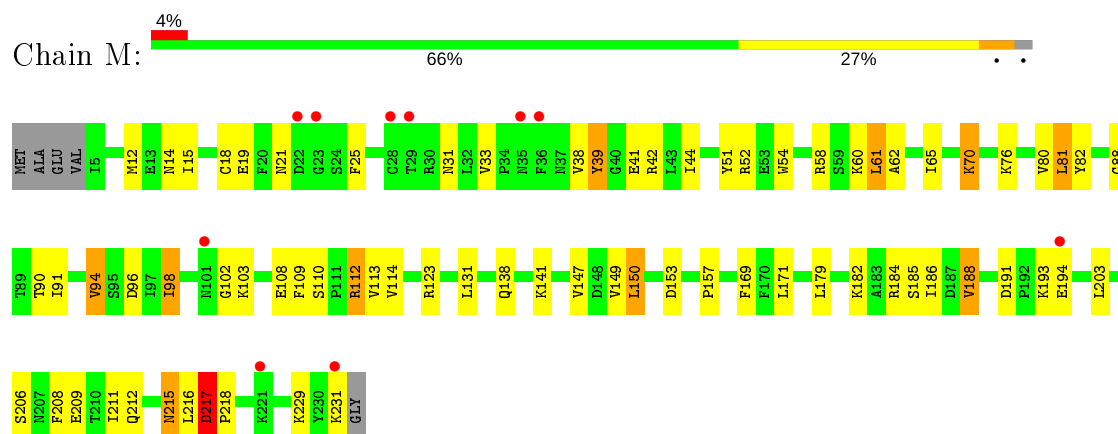
- Molecule 3: Fibrillarin-like rRNA/tRNA 2'-O-methyltransferase



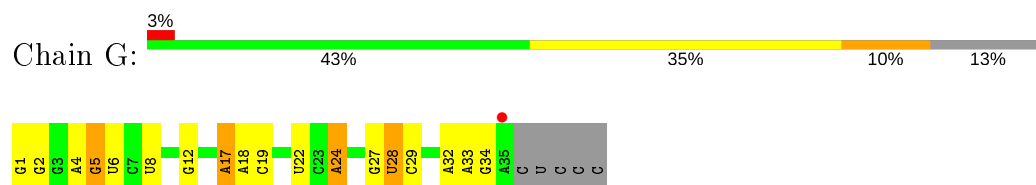
- Molecule 3: Fibrillarin-like rRNA/tRNA 2'-O-methyltransferase



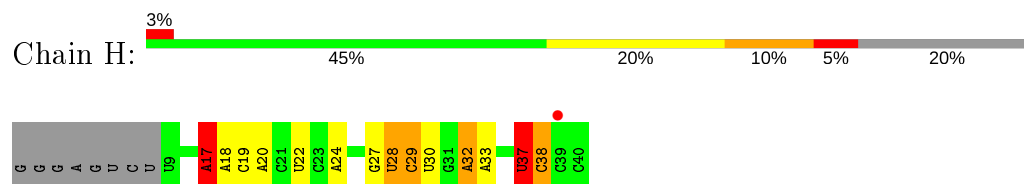
- Molecule 3: Fibrillarin-like rRNA/tRNA 2'-O-methyltransferase



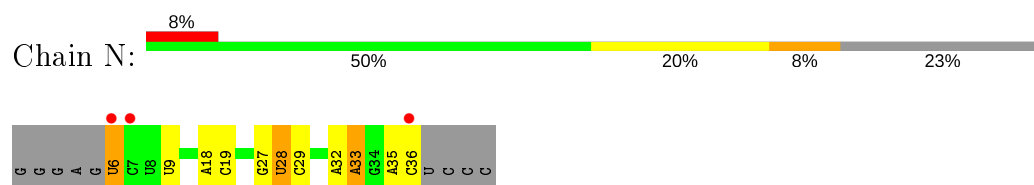
- Molecule 4: C/D guide RNA



- Molecule 4: C/D guide RNA

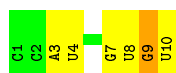


- Molecule 4: C/D guide RNA



- Molecule 5: RNA (5'-R(*CP*CP*AP*UP*GP*AP*GP*UP*GP*U)-3')

Chain I:  40% 50% 10%



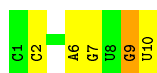
- Molecule 5: RNA (5'-R(*CP*CP*AP*UP*GP*AP*GP*UP*GP*U)-3')

Chain J:  70% 20% 10%



- Molecule 5: RNA (5'-R(*CP*CP*AP*UP*GP*AP*GP*UP*GP*U)-3')

Chain O:  50% 40% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	241.20 Å 241.20 Å 145.41 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 3.15 19.91 – 3.15	Depositor EDS
% Data completeness (in resolution range)	95.1 (19.91-3.15) 95.1 (19.91-3.15)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 3.15 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.248 , 0.278 0.243 , 0.273	Depositor DCC
R_{free} test set	3540 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	78.6	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	20046	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% 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: 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	0.44	0/3043	0.58	0/4106
1	B	0.44	0/3043	0.59	0/4106
1	K	0.38	0/3043	0.53	0/4106
2	C	0.40	0/936	0.60	0/1260
2	D	0.47	0/936	0.62	1/1260 (0.1%)
2	L	0.35	0/936	0.56	0/1260
3	E	0.48	0/1863	0.68	2/2521 (0.1%)
3	F	0.45	0/1863	0.62	2/2521 (0.1%)
3	M	0.38	0/1863	0.57	0/2521
4	G	0.89	0/843	1.59	14/1313 (1.1%)
4	H	0.94	1/758 (0.1%)	1.57	15/1178 (1.3%)
4	N	1.53	8/736 (1.1%)	1.41	10/1144 (0.9%)
5	I	1.03	0/234	1.74	7/363 (1.9%)
5	J	0.86	0/234	1.55	2/363 (0.6%)
5	O	0.71	0/234	1.38	2/363 (0.6%)
All	All	0.57	9/20565 (0.0%)	0.83	55/28385 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	C	0	1
2	D	0	1
2	L	0	1
3	E	0	1
3	F	0	1
3	M	0	1
All	All	0	7

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	33	A	N9-C8	19.43	1.53	1.37
4	N	33	A	N3-C4	16.18	1.44	1.34
4	N	33	A	C8-N7	11.92	1.39	1.31
4	N	33	A	C6-N1	11.64	1.43	1.35
4	N	33	A	C5-C4	11.03	1.46	1.38

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	9	G	C3'-C2'-C1'	-11.29	92.47	101.50
4	H	28	U	O3'-P-O5'	-10.84	83.41	104.00
4	G	1	G	O3'-P-O5'	-9.99	85.02	104.00
5	O	9	G	C3'-C2'-C1'	-9.44	93.94	101.50
4	G	1	G	OP1-P-O3'	-9.04	85.32	105.20

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	355	SER	Peptide
2	C	61	GLN	Peptide
2	D	61	GLN	Peptide
3	E	217	ASP	Peptide
3	F	217	ASP	Peptide

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	2993	0	3055	48	0
1	B	2993	0	3055	50	0
1	K	2993	0	3055	44	0
2	C	927	0	981	20	0
2	D	927	0	981	23	0
2	L	927	0	981	24	0
3	E	1829	0	1862	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1829	0	1862	40	0
3	M	1829	0	1862	39	0
4	G	753	0	377	5	0
4	H	679	0	345	5	0
4	N	659	0	333	1	0
5	I	210	0	109	1	0
5	J	210	0	109	1	0
5	O	210	0	109	2	0
6	E	26	0	19	0	0
6	F	26	0	19	0	0
6	M	26	0	19	0	0
All	All	20046	0	19133	327	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 8.

The worst 5 of 327 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)
2:D:30:LYS:HE2	2:D:93:CYS:HA	1.22	1.19
2:L:30:LYS:HE2	2:L:93:CYS:HA	1.29	1.12
2:C:30:LYS:HE2	2:C:93:CYS:HA	1.36	1.05
1:A:11:ILE:HD11	1:A:101:ALA:HA	1.42	1.01
1:K:11:ILE:HD11	1:K:101:ALA:HA	1.50	0.94

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	373/388 (96%)	354 (95%)	14 (4%)	5 (1%)	12 44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	373/388 (96%)	350 (94%)	21 (6%)	2 (0%)	29	65
1	K	373/388 (96%)	356 (95%)	16 (4%)	1 (0%)	41	73
2	C	120/130 (92%)	111 (92%)	7 (6%)	2 (2%)	9	38
2	D	120/130 (92%)	112 (93%)	6 (5%)	2 (2%)	9	38
2	L	120/130 (92%)	112 (93%)	7 (6%)	1 (1%)	19	55
3	E	225/232 (97%)	206 (92%)	16 (7%)	3 (1%)	12	44
3	F	225/232 (97%)	204 (91%)	17 (8%)	4 (2%)	8	37
3	M	225/232 (97%)	202 (90%)	19 (8%)	4 (2%)	8	37
All	All	2154/2250 (96%)	2007 (93%)	123 (6%)	24 (1%)	14	48

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	355	SER
2	C	62	PRO
2	D	62	PRO
3	E	206	SER
3	E	218	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	318/330 (96%)	294 (92%)	24 (8%)	13	42
1	B	318/330 (96%)	292 (92%)	26 (8%)	11	38
1	K	318/330 (96%)	294 (92%)	24 (8%)	13	42
2	C	100/107 (94%)	94 (94%)	6 (6%)	19	51
2	D	100/107 (94%)	94 (94%)	6 (6%)	19	51
2	L	100/107 (94%)	94 (94%)	6 (6%)	19	51
3	E	202/205 (98%)	182 (90%)	20 (10%)	8	28
3	F	202/205 (98%)	180 (89%)	22 (11%)	6	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	M	202/205 (98%)	179 (89%)	23 (11%)	5	23
All	All	1860/1926 (97%)	1703 (92%)	157 (8%)	11	37

5 of 157 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	94	VAL
3	F	61	LEU
3	M	109	PHE
3	E	103	LYS
3	E	193	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
3	E	122	GLN
3	F	31	ASN
3	M	122	GLN
3	E	212	GLN
3	E	223	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	G	34/40 (85%)	8 (23%)	1 (2%)
4	H	31/40 (77%)	6 (19%)	1 (3%)
4	N	31/40 (77%)	7 (22%)	1 (3%)
5	I	9/10 (90%)	2 (22%)	1 (11%)
5	J	9/10 (90%)	1 (11%)	1 (11%)
5	O	9/10 (90%)	2 (22%)	1 (11%)
All	All	123/150 (82%)	26 (21%)	6 (4%)

5 of 26 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	G	5	G
4	G	6	U
4	G	17	A
4	G	18	A
4	G	28	U

5 of 6 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	I	9	G
5	O	9	G
5	J	9	G
4	H	32	A
4	N	6	U

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](#)

3 ligands are 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	$\# Z > 2$
6	SAH	F	301	-	21,28,28	1.03	1 (4%)	20,40,40	1.35	3 (15%)
6	SAH	E	301	-	21,28,28	1.01	1 (4%)	20,40,40	1.51	3 (15%)
6	SAH	M	301	-	21,28,28	1.03	1 (4%)	20,40,40	1.32	2 (10%)

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
6	SAH	F	301	-	-	3/7/31/31	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SAH	E	301	-	-	2/7/31/31	0/3/3/3
6	SAH	M	301	-	-	3/7/31/31	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	301	SAH	C5-C4	2.66	1.48	1.40
6	E	301	SAH	C5-C4	2.47	1.47	1.40
6	M	301	SAH	C5-C4	2.46	1.47	1.40

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	301	SAH	N3-C2-N1	-4.15	122.20	128.68
6	M	301	SAH	N3-C2-N1	-3.46	123.28	128.68
6	F	301	SAH	N3-C2-N1	-3.43	123.32	128.68
6	M	301	SAH	C4-C5-N7	-2.77	106.51	109.40
6	E	301	SAH	C4'-C5'-SD	-2.27	105.62	113.78

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

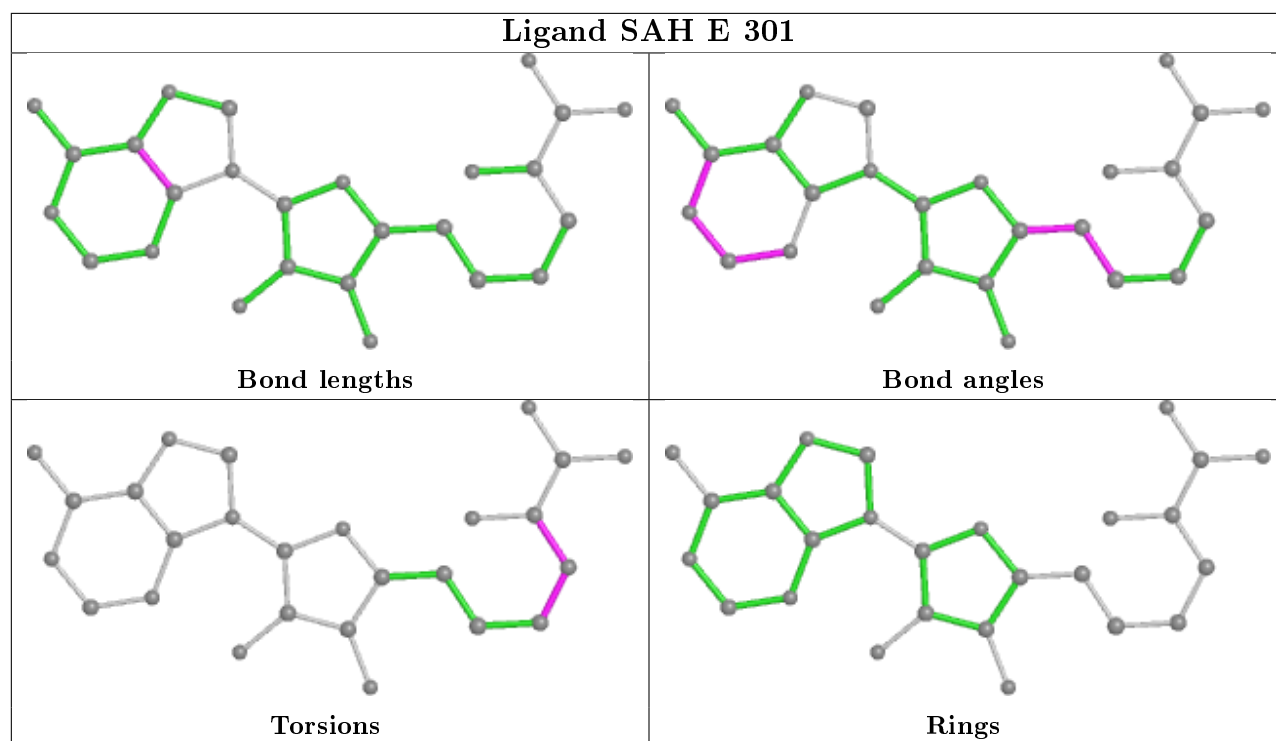
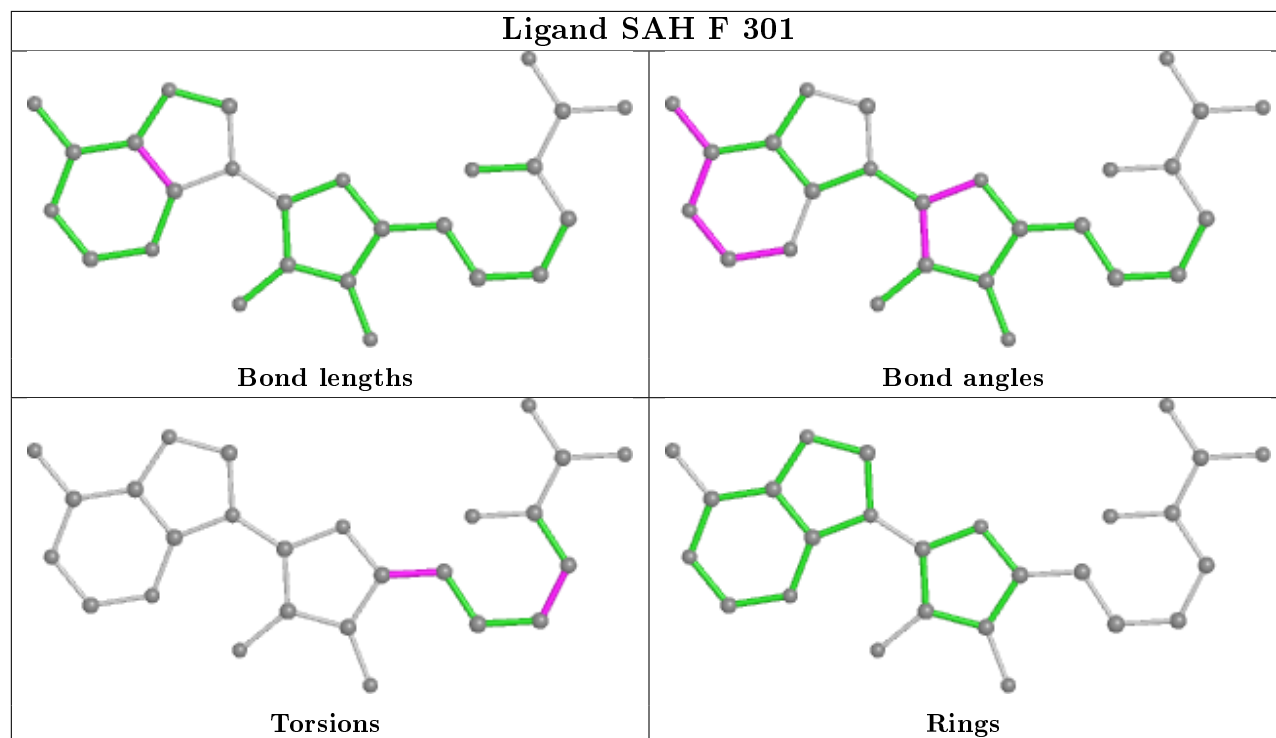
Mol	Chain	Res	Type	Atoms
6	F	301	SAH	CA-CB-CG-SD
6	E	301	SAH	CA-CB-CG-SD
6	M	301	SAH	CA-CB-CG-SD
6	F	301	SAH	C3'-C4'-C5'-SD
6	F	301	SAH	O4'-C4'-C5'-SD

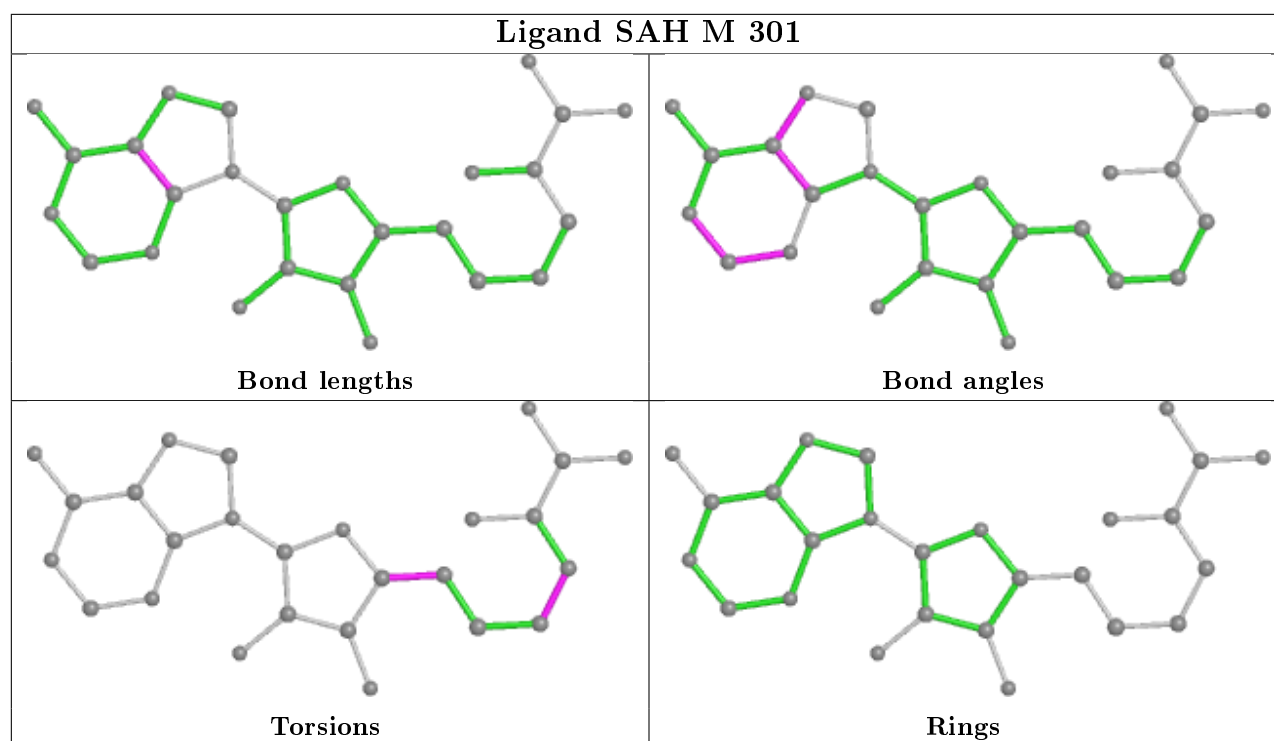
There are no ring outliers.

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	375/388 (96%)	-0.23	3 (0%) 86 78	45, 79, 111, 127	0
1	B	375/388 (96%)	-0.35	0 100 100	45, 70, 109, 123	0
1	K	375/388 (96%)	0.04	9 (2%) 59 43	70, 98, 145, 157	0
2	C	122/130 (93%)	0.15	5 (4%) 37 22	79, 105, 127, 134	0
2	D	122/130 (93%)	-0.23	0 100 100	50, 72, 92, 107	0
2	L	122/130 (93%)	0.46	12 (9%) 7 4	104, 130, 145, 152	0
3	E	227/232 (97%)	-0.27	0 100 100	50, 66, 91, 101	0
3	F	227/232 (97%)	-0.14	5 (2%) 62 47	57, 75, 99, 107	0
3	M	227/232 (97%)	0.25	10 (4%) 34 20	98, 115, 128, 134	0
4	G	35/40 (87%)	-0.08	1 (2%) 51 35	46, 61, 121, 137	0
4	H	32/40 (80%)	-0.10	1 (3%) 49 32	51, 73, 99, 113	0
4	N	31/40 (77%)	0.41	3 (9%) 7 4	82, 114, 142, 161	0
5	I	10/10 (100%)	-0.35	0 100 100	46, 55, 59, 60	0
5	J	10/10 (100%)	-0.31	0 100 100	57, 64, 69, 74	0
5	O	10/10 (100%)	-0.02	0 100 100	84, 93, 103, 103	0
All	All	2300/2400 (95%)	-0.08	49 (2%) 63 49	45, 86, 134, 161	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	112	ASP	3.7
1	K	332	TRP	3.6
3	M	29	THR	3.5
2	L	96	GLN	3.2
3	F	29	THR	3.1

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 carbohydrates in this entry.

6.4 Ligands [i](#)

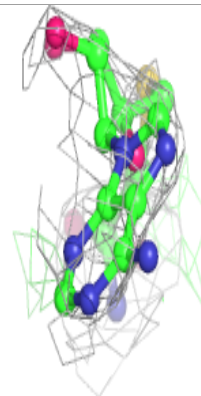
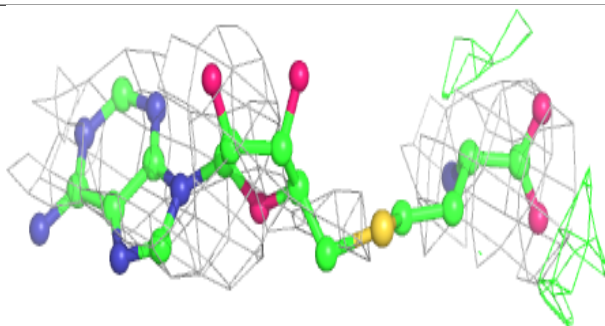
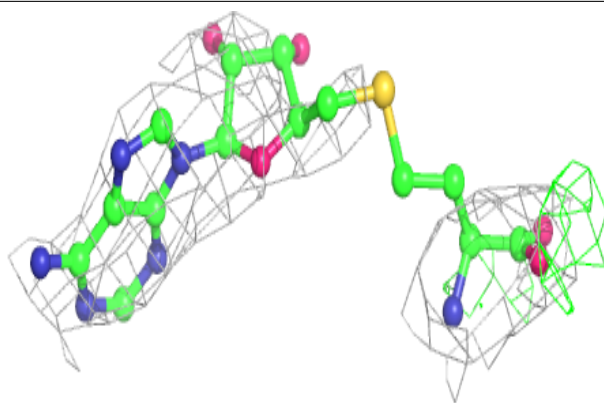
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	SAH	M	301	26/26	0.73	0.40	122,125,128,128	0
6	SAH	E	301	26/26	0.88	0.25	69,78,80,80	0
6	SAH	F	301	26/26	0.90	0.25	74,76,77,78	0

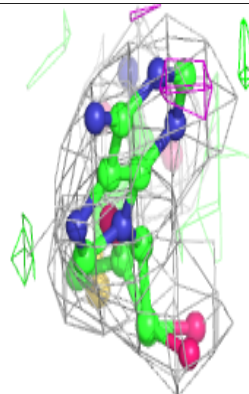
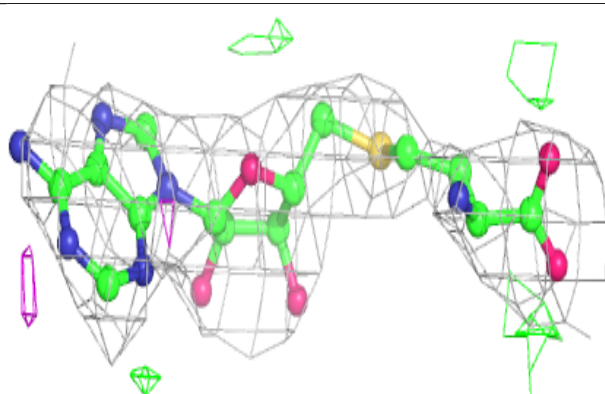
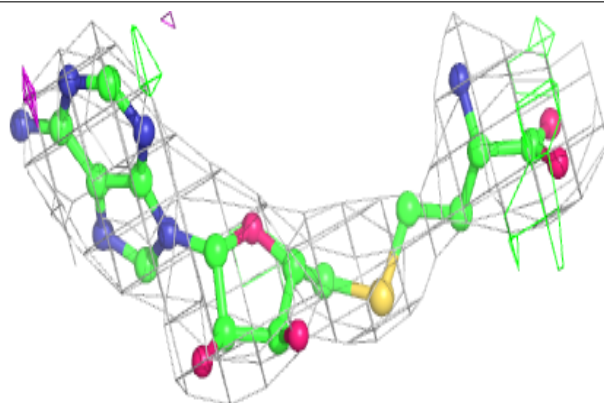
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAH M 301:

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

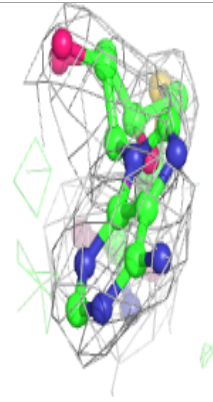
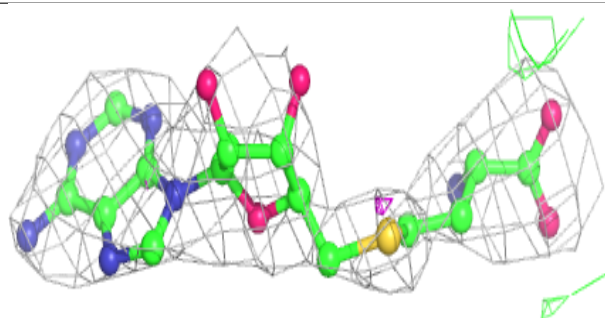
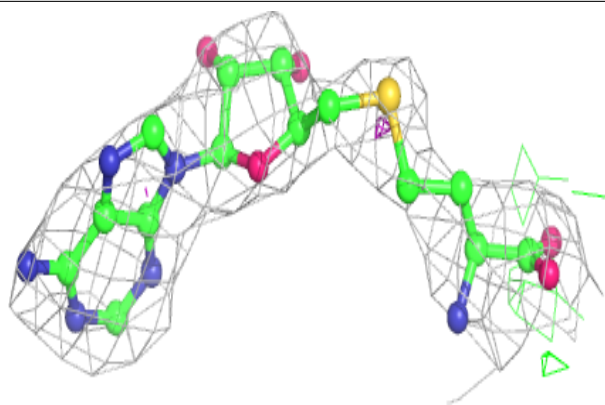
**Electron density around SAH E 301:**

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



Electron density around SAH F 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.