



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 10:35 am BST

PDB ID : 5GIP
Title : Crystal structure of box C/D RNP with 13 nt guide regions and 11 nt substrates
Authors : Yang, Z.; Lin, J.; Ye, K.
Deposited on : 2016-06-24
Resolution : 3.13 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

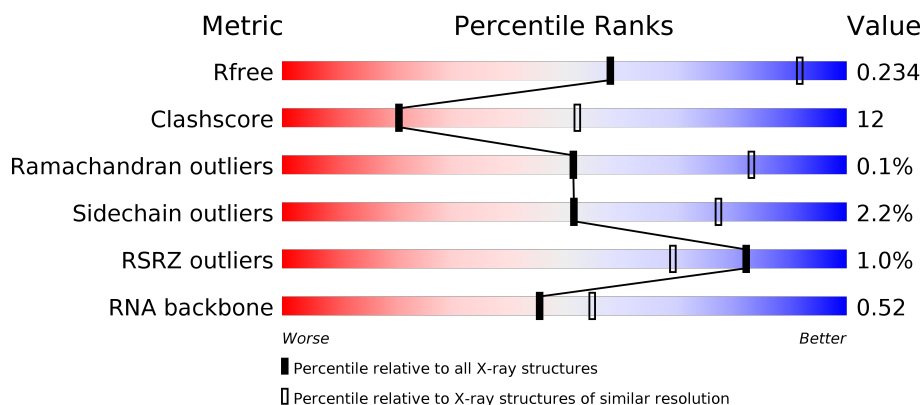
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.13 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	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)
RNA backbone	3102	1134 (3.44-2.80)

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 style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 74%, green 22%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 74% 22% .. </div> </div>
1	B	388	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 73%, green 22%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 73% 22% .. </div> </div>
1	K	388	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 73%, green 22%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 73% 22% .. </div> </div>
1	L	388	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 72%, green 24%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 72% 24% .. </div> </div>

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Mol	Chain	Length	Quality of chain
2	C	130	
2	D	130	
2	M	130	
2	N	130	
3	E	232	
3	F	232	
3	O	232	
3	P	232	
4	G	41	
4	H	41	
4	Q	41	
4	R	41	
5	I	11	
5	J	11	
5	S	11	
5	T	11	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SAH	O	301	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26608 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 C/D box methylation guide ribonucleoprotein complex aNOP56 subunit.

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

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A0E3MJI1
A	2	VAL	-	expression tag	UNP A0A0E3MJI1
A	3	LYS	-	expression tag	UNP A0A0E3MJI1
A	381	HIS	-	expression tag	UNP A0A0E3MJI1
A	382	HIS	-	expression tag	UNP A0A0E3MJI1
A	383	HIS	-	expression tag	UNP A0A0E3MJI1
A	384	HIS	-	expression tag	UNP A0A0E3MJI1
A	385	HIS	-	expression tag	UNP A0A0E3MJI1
A	386	HIS	-	expression tag	UNP A0A0E3MJI1
A	387	HIS	-	expression tag	UNP A0A0E3MJI1
A	388	HIS	-	expression tag	UNP A0A0E3MJI1
B	1	MET	-	initiating methionine	UNP A0A0E3MJI1
B	2	VAL	-	expression tag	UNP A0A0E3MJI1
B	3	LYS	-	expression tag	UNP A0A0E3MJI1
B	381	HIS	-	expression tag	UNP A0A0E3MJI1
B	382	HIS	-	expression tag	UNP A0A0E3MJI1
B	383	HIS	-	expression tag	UNP A0A0E3MJI1
B	384	HIS	-	expression tag	UNP A0A0E3MJI1
B	385	HIS	-	expression tag	UNP A0A0E3MJI1
B	386	HIS	-	expression tag	UNP A0A0E3MJI1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	387	HIS	-	expression tag	UNP A0A0E3MJI1
B	388	HIS	-	expression tag	UNP A0A0E3MJI1
K	1	MET	-	initiating methionine	UNP A0A0E3MJI1
K	2	VAL	-	expression tag	UNP A0A0E3MJI1
K	3	LYS	-	expression tag	UNP A0A0E3MJI1
K	381	HIS	-	expression tag	UNP A0A0E3MJI1
K	382	HIS	-	expression tag	UNP A0A0E3MJI1
K	383	HIS	-	expression tag	UNP A0A0E3MJI1
K	384	HIS	-	expression tag	UNP A0A0E3MJI1
K	385	HIS	-	expression tag	UNP A0A0E3MJI1
K	386	HIS	-	expression tag	UNP A0A0E3MJI1
K	387	HIS	-	expression tag	UNP A0A0E3MJI1
K	388	HIS	-	expression tag	UNP A0A0E3MJI1
L	1	MET	-	initiating methionine	UNP A0A0E3MJI1
L	2	VAL	-	expression tag	UNP A0A0E3MJI1
L	3	LYS	-	expression tag	UNP A0A0E3MJI1
L	381	HIS	-	expression tag	UNP A0A0E3MJI1
L	382	HIS	-	expression tag	UNP A0A0E3MJI1
L	383	HIS	-	expression tag	UNP A0A0E3MJI1
L	384	HIS	-	expression tag	UNP A0A0E3MJI1
L	385	HIS	-	expression tag	UNP A0A0E3MJI1
L	386	HIS	-	expression tag	UNP A0A0E3MJI1
L	387	HIS	-	expression tag	UNP A0A0E3MJI1
L	388	HIS	-	expression tag	UNP A0A0E3MJI1

- 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	M	122	Total	C	N	O	S	0	0	0
			927	588	156	181	2			
2	N	122	Total	C	N	O	S	0	0	0
			927	588	156	181	2			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	initiating methionine	UNP A0A0E3JZF7
C	2	ASP	-	expression tag	UNP A0A0E3JZF7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	3	ALA	-	expression tag	UNP A0A0E3JZF7
C	4	MET	-	expression tag	UNP A0A0E3JZF7
C	5	SER	-	expression tag	UNP A0A0E3JZF7
D	1	MET	-	initiating methionine	UNP A0A0E3JZF7
D	2	ASP	-	expression tag	UNP A0A0E3JZF7
D	3	ALA	-	expression tag	UNP A0A0E3JZF7
D	4	MET	-	expression tag	UNP A0A0E3JZF7
D	5	SER	-	expression tag	UNP A0A0E3JZF7
M	1	MET	-	initiating methionine	UNP A0A0E3JZF7
M	2	ASP	-	expression tag	UNP A0A0E3JZF7
M	3	ALA	-	expression tag	UNP A0A0E3JZF7
M	4	MET	-	expression tag	UNP A0A0E3JZF7
M	5	SER	-	expression tag	UNP A0A0E3JZF7
N	1	MET	-	initiating methionine	UNP A0A0E3JZF7
N	2	ASP	-	expression tag	UNP A0A0E3JZF7
N	3	ALA	-	expression tag	UNP A0A0E3JZF7
N	4	MET	-	expression tag	UNP A0A0E3JZF7
N	5	SER	-	expression tag	UNP A0A0E3JZF7

- 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	O	227	Total	C	N	O	S	0	0	0
			1829	1175	309	341	4			
3	P	227	Total	C	N	O	S	0	0	0
			1829	1175	309	341	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	MET	-	initiating methionine	UNP A0A0E3JUC9
E	2	ALA	-	expression tag	UNP A0A0E3JUC9
F	1	MET	-	initiating methionine	UNP A0A0E3JUC9
F	2	ALA	-	expression tag	UNP A0A0E3JUC9
O	1	MET	-	initiating methionine	UNP A0A0E3JUC9
O	2	ALA	-	expression tag	UNP A0A0E3JUC9
P	1	MET	-	initiating methionine	UNP A0A0E3JUC9
P	2	ALA	-	expression tag	UNP A0A0E3JUC9

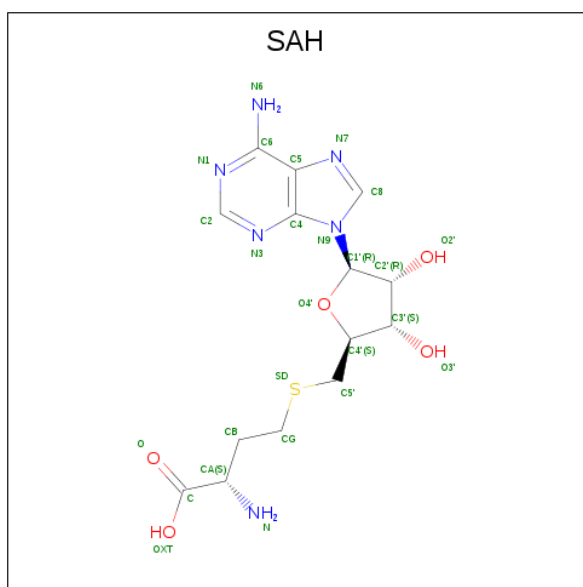
- Molecule 4 is a RNA chain called C/D RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	31	Total	C	N	O	P	0	0	0
			662	296	118	217	31			
4	H	30	Total	C	N	O	P	0	0	0
			642	287	116	209	30			
4	Q	31	Total	C	N	O	P	0	0	0
			662	296	118	217	31			
4	R	29	Total	C	N	O	P	0	0	0
			622	278	113	202	29			

- Molecule 5 is a RNA chain called substrate.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	11	Total	C	N	O	P	0	0	0
			230	104	39	77	10			
5	J	11	Total	C	N	O	P	0	0	0
			230	104	39	77	10			
5	S	11	Total	C	N	O	P	0	0	0
			230	104	39	77	10			
5	T	11	Total	C	N	O	P	0	0	0
			230	104	39	77	10			

- Molecule 6 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).

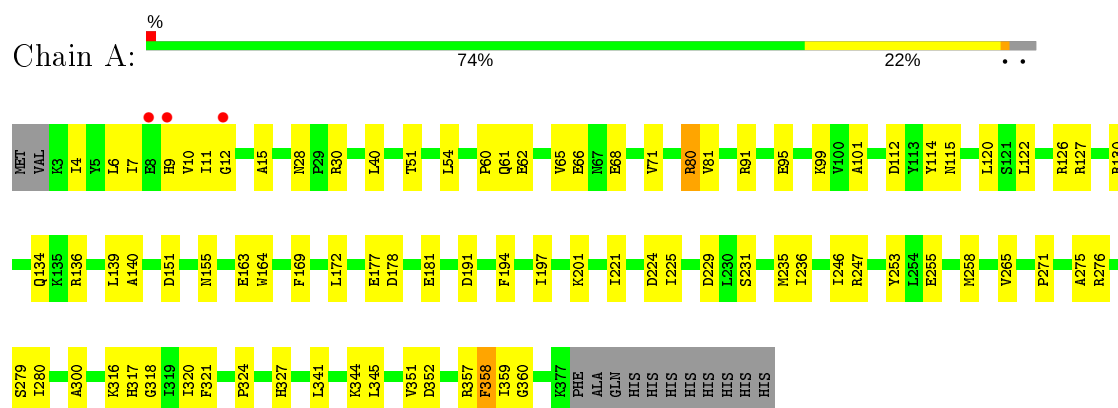


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	E	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
6	F	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
6	O	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
6	P	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

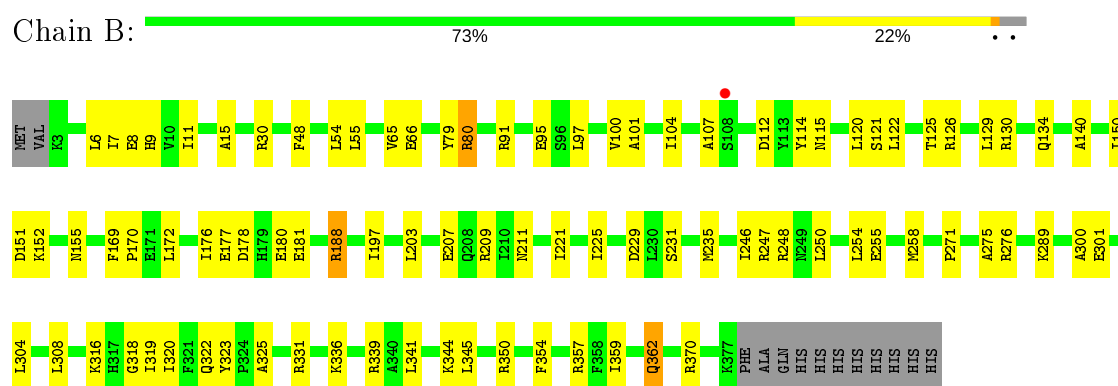
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

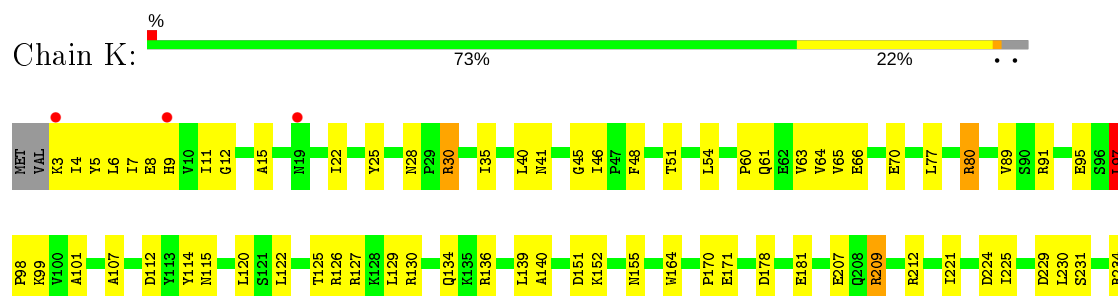
- Molecule 1: C/D box methylation guide ribonucleoprotein complex aNOP56 subunit



- Molecule 1: C/D box methylation guide ribonucleoprotein complex aNOP56 subunit

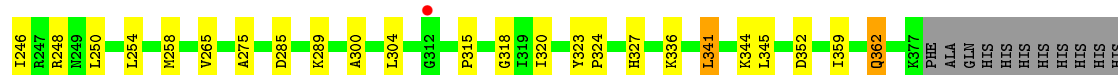
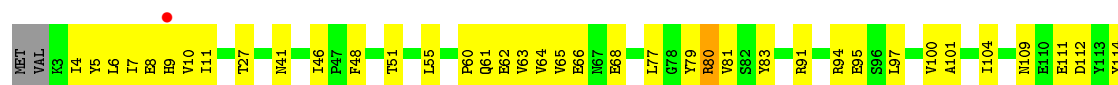
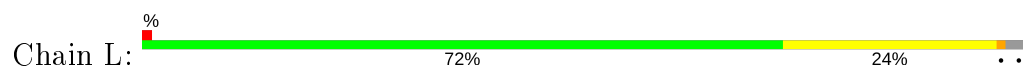


- Molecule 1: C/D box methylation guide ribonucleoprotein complex aNOP56 subunit





- Molecule 1: C/D box methylation guide ribonucleoprotein complex aNOP56 subunit



- Molecule 2: 50S ribosomal protein L7Ae



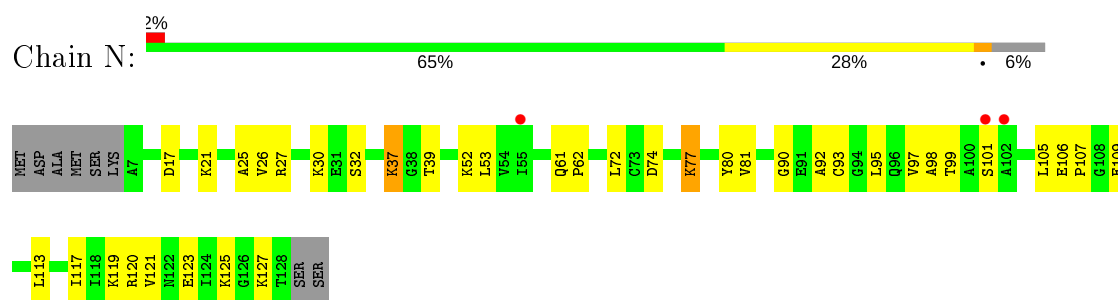
- Molecule 2: 50S ribosomal protein L7Ae



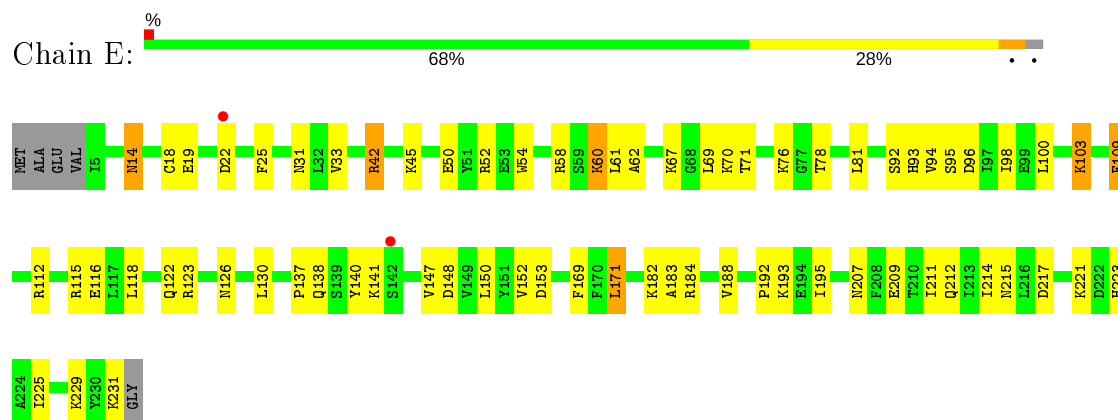
- Molecule 2: 50S ribosomal protein L7Ae



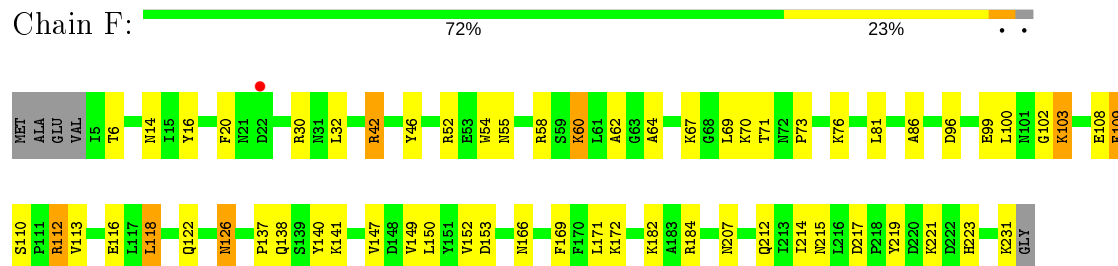
- Molecule 2: 50S ribosomal protein L7Ae



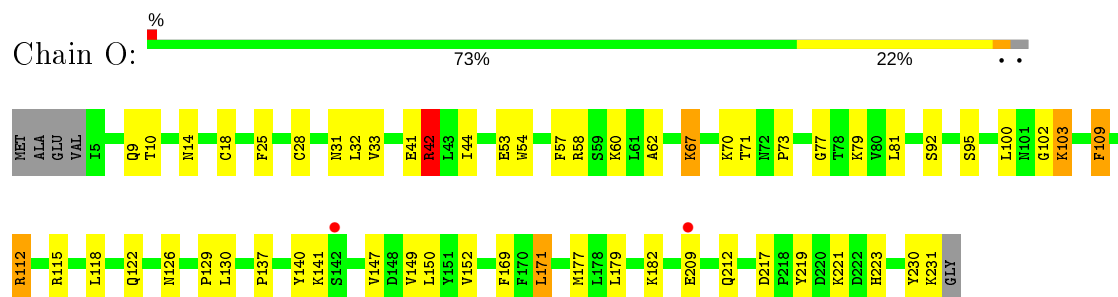
- Molecule 3: Fibrillarin-like rRNA/tRNA 2'-O-methyltransferase



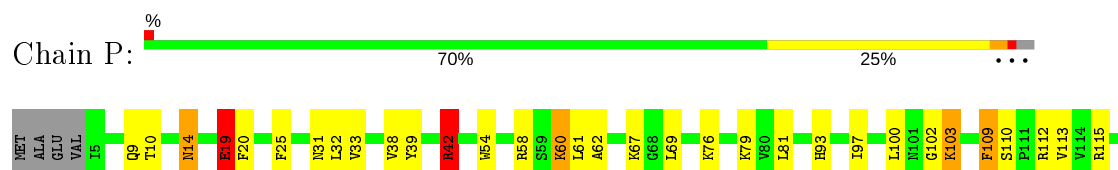
- Molecule 3: Fibrillarin-like rRNA/tRNA 2'-O-methyltransferase

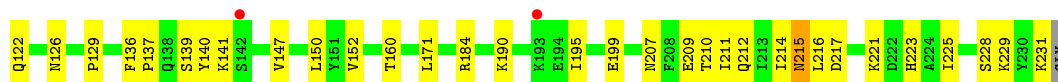


- Molecule 3: Fibrillarin-like rRNA/tRNA 2'-O-methyltransferase



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

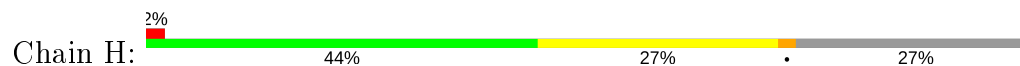




- Molecule 4: C/D RNA



- Molecule 4: C/D RNA



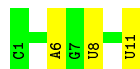
- Molecule 4: C/D RNA



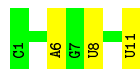
- Molecule 4: C/D RNA



- Molecule 5: substrate



- Molecule 5: substrate



- Molecule 5: substrate





- Molecule 5: substrate



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	97.92Å 97.72Å 128.79Å 108.98° 104.42° 89.86°	Depositor
Resolution (Å)	24.86 – 3.13 24.86 – 3.13	Depositor EDS
% Data completeness (in resolution range)	96.9 (24.86-3.13) 96.9 (24.86-3.13)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.22 (at 3.11Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.178 , 0.234 0.178 , 0.234	Depositor DCC
R_{free} test set	2002 reflections (2.69%)	wwPDB-VP
Wilson B-factor (Å ²)	68.3	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26608	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% 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	0.61	3/3043 (0.1%)	0.69	0/4106
1	B	0.72	13/3043 (0.4%)	0.66	0/4106
1	K	0.65	7/3043 (0.2%)	0.66	1/4106 (0.0%)
1	L	0.65	6/3043 (0.2%)	0.64	0/4106
2	C	0.51	1/936 (0.1%)	0.63	0/1260
2	D	0.56	1/936 (0.1%)	0.64	0/1260
2	M	0.52	0/936	0.65	0/1260
2	N	0.53	1/936 (0.1%)	0.63	0/1260
3	E	0.86	12/1863 (0.6%)	0.69	0/2521
3	F	0.78	8/1863 (0.4%)	0.69	1/2521 (0.0%)
3	O	0.65	5/1863 (0.3%)	0.70	0/2521
3	P	0.79	11/1863 (0.6%)	0.71	1/2521 (0.0%)
4	G	0.70	0/740	1.20	1/1151 (0.1%)
4	H	0.73	0/718	1.21	2/1117 (0.2%)
4	Q	0.67	1/740 (0.1%)	1.22	1/1151 (0.1%)
4	R	0.65	0/696	1.23	2/1083 (0.2%)
5	I	0.69	0/256	1.24	3/397 (0.8%)
5	J	0.74	0/256	1.25	1/397 (0.3%)
5	S	0.76	0/256	1.53	6/397 (1.5%)
5	T	0.83	0/256	1.33	3/397 (0.8%)
All	All	0.68	69/27286 (0.3%)	0.79	22/37638 (0.1%)

The worst 5 of 69 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	42	ARG	CZ-NH2	-9.99	1.20	1.33
3	E	42	ARG	NE-CZ	-9.88	1.20	1.33
1	B	188	ARG	NE-CZ	-9.82	1.20	1.33
3	E	42	ARG	CZ-NH1	-9.44	1.20	1.33
1	L	80	ARG	NE-CZ	-9.25	1.21	1.33

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	11	U	C2-N1-C1'	9.63	129.26	117.70
5	S	11	U	C6-N1-C1'	-7.65	110.48	121.20
5	S	11	U	N1-C2-O2	7.22	127.86	122.80
5	T	11	U	N3-C4-O4	-7.19	114.37	119.40
5	S	11	U	O4'-C1'-N1	6.90	113.72	108.20

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	2993	0	3055	83	0
1	B	2993	0	3055	85	0
1	K	2993	0	3055	95	0
1	L	2993	0	3055	98	0
2	C	927	0	981	33	0
2	D	927	0	981	31	0
2	M	927	0	981	26	0
2	N	927	0	981	28	0
3	E	1829	0	1862	54	0
3	F	1829	0	1862	54	0
3	O	1829	0	1862	56	0
3	P	1829	0	1862	57	0
4	G	662	0	333	6	0
4	H	642	0	323	4	0
4	Q	662	0	333	7	0
4	R	622	0	312	9	0
5	I	230	0	119	2	0
5	J	230	0	119	2	0
5	S	230	0	119	2	0
5	T	230	0	119	2	0
6	E	26	0	19	2	0
6	F	26	0	19	7	0
6	O	26	0	19	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	P	26	0	19	7	0
All	All	26608	0	25445	640	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 12.

The worst 5 of 640 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)
3:P:54:TRP:CH2	3:P:61:LEU:HD12	1.90	1.06
1:K:139:LEU:HD11	1:L:225:ILE:CD1	1.94	0.97
1:K:139:LEU:CD1	1:L:225:ILE:HD11	1.95	0.96
1:K:139:LEU:HD11	1:L:225:ILE:HD11	0.99	0.96
1:B:130:ARG:HH12	1:B:134:GLN:HE21	1.15	0.95

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%)	361 (97%)	12 (3%)	0	100	100
1	B	373/388 (96%)	361 (97%)	12 (3%)	0	100	100
1	K	373/388 (96%)	361 (97%)	12 (3%)	0	100	100
1	L	373/388 (96%)	362 (97%)	11 (3%)	0	100	100
2	C	120/130 (92%)	117 (98%)	3 (2%)	0	100	100
2	D	120/130 (92%)	117 (98%)	3 (2%)	0	100	100
2	M	120/130 (92%)	117 (98%)	3 (2%)	0	100	100
2	N	120/130 (92%)	117 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	225/232 (97%)	205 (91%)	19 (8%)	1 (0%)	34	68
3	F	225/232 (97%)	208 (92%)	17 (8%)	0	100	100
3	O	225/232 (97%)	207 (92%)	17 (8%)	1 (0%)	34	68
3	P	225/232 (97%)	208 (92%)	16 (7%)	1 (0%)	34	68
All	All	2872/3000 (96%)	2741 (95%)	128 (4%)	3 (0%)	51	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	P	14	ASN
3	E	14	ASN
3	O	14	ASN

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%)	314 (99%)	4 (1%)	69	86
1	B	318/330 (96%)	312 (98%)	6 (2%)	57	80
1	K	318/330 (96%)	311 (98%)	7 (2%)	52	77
1	L	318/330 (96%)	314 (99%)	4 (1%)	69	86
2	C	100/107 (94%)	99 (99%)	1 (1%)	76	89
2	D	100/107 (94%)	99 (99%)	1 (1%)	76	89
2	M	100/107 (94%)	99 (99%)	1 (1%)	76	89
2	N	100/107 (94%)	99 (99%)	1 (1%)	76	89
3	E	202/205 (98%)	196 (97%)	6 (3%)	41	70
3	F	202/205 (98%)	195 (96%)	7 (4%)	36	67
3	O	202/205 (98%)	193 (96%)	9 (4%)	27	59
3	P	202/205 (98%)	194 (96%)	8 (4%)	31	64
All	All	2480/2568 (97%)	2425 (98%)	55 (2%)	52	77

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	171	LEU
1	K	260	GLU
3	P	103	LYS
1	K	61	GLN
1	K	97	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	9	HIS
1	K	362	GLN
3	P	31	ASN
1	K	155	ASN
1	L	9	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	G	30/41 (73%)	5 (16%)	0
4	H	29/41 (70%)	6 (20%)	0
4	Q	30/41 (73%)	6 (20%)	0
4	R	28/41 (68%)	6 (21%)	1 (3%)
5	I	10/11 (90%)	0	0
5	J	10/11 (90%)	0	0
5	S	10/11 (90%)	0	0
5	T	10/11 (90%)	0	0
All	All	157/208 (75%)	23 (14%)	1 (0%)

5 of 23 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	G	17	G
4	G	19	A
4	G	30	C
4	G	32	G
4	G	34	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	R	17	G

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](#)

4 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	E	301	-	21,28,28	1.26	2 (9%)	20,40,40	1.49	3 (15%)
6	SAH	O	301	-	21,28,28	1.24	2 (9%)	20,40,40	1.80	2 (10%)
6	SAH	F	301	-	21,28,28	1.17	2 (9%)	20,40,40	1.57	2 (10%)
6	SAH	P	301	-	21,28,28	1.30	3 (14%)	20,40,40	1.64	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	E	301	-	-	2/7/31/31	0/3/3/3
6	SAH	O	301	-	-	3/7/31/31	0/3/3/3
6	SAH	F	301	-	-	3/7/31/31	0/3/3/3
6	SAH	P	301	-	-	1/7/31/31	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)
6	E	301	SAH	C2-N3	4.02	1.38	1.32
6	O	301	SAH	C2-N3	3.87	1.38	1.32
6	P	301	SAH	C2-N3	3.65	1.38	1.32
6	F	301	SAH	C2-N3	3.47	1.37	1.32
6	E	301	SAH	C2-N1	2.61	1.38	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	P	301	SAH	N3-C2-N1	-5.79	119.62	128.68
6	O	301	SAH	N3-C2-N1	-5.79	119.63	128.68
6	F	301	SAH	N3-C2-N1	-5.48	120.11	128.68
6	E	301	SAH	N3-C2-N1	-5.03	120.82	128.68
6	O	301	SAH	C5'-SD-CG	-2.90	93.58	102.27

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	O	301	SAH	N-CA-CB-CG
6	O	301	SAH	C-CA-CB-CG
6	F	301	SAH	N-CA-CB-CG
6	F	301	SAH	C-CA-CB-CG
6	P	301	SAH	N-CA-CB-CG

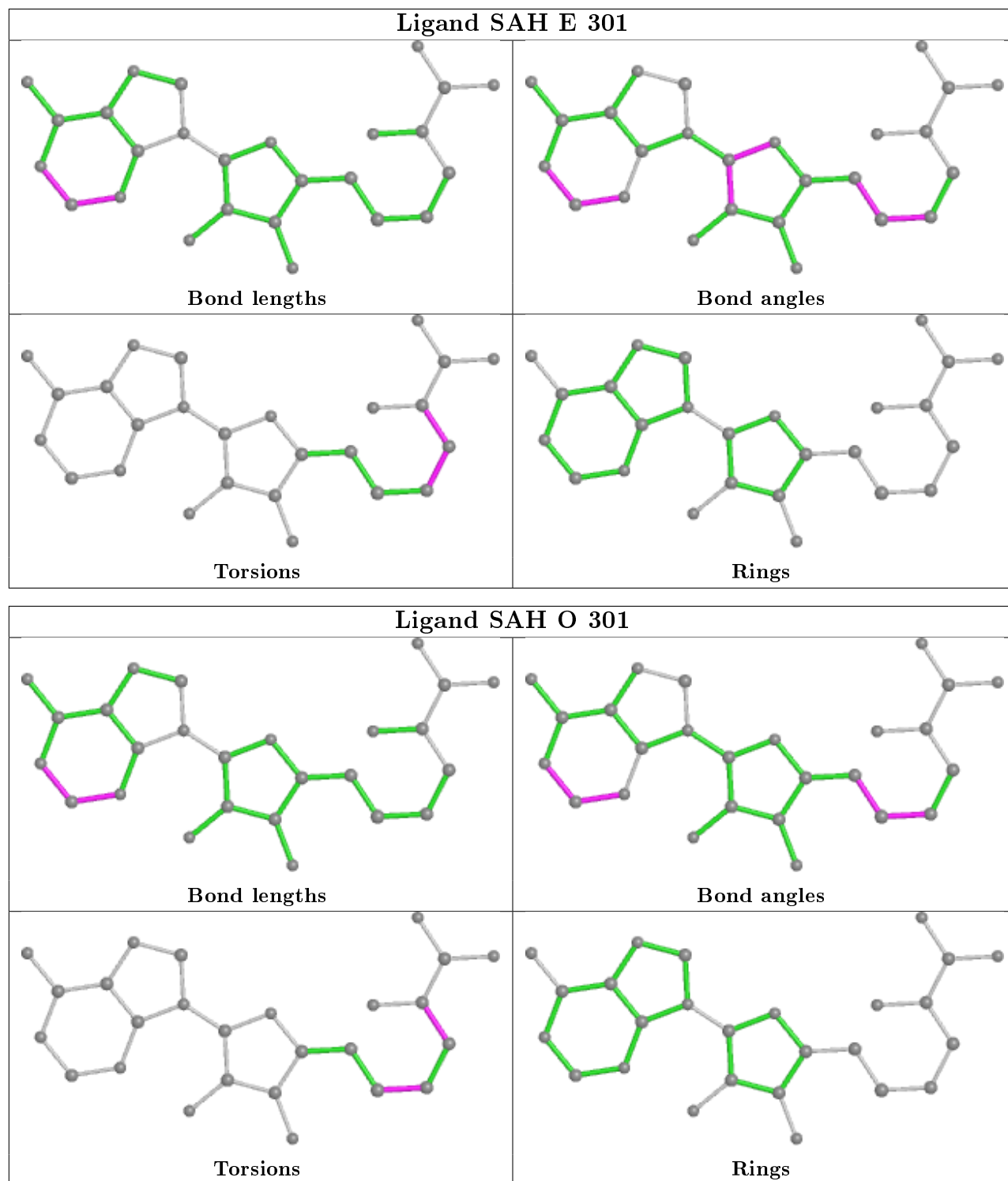
There are no ring outliers.

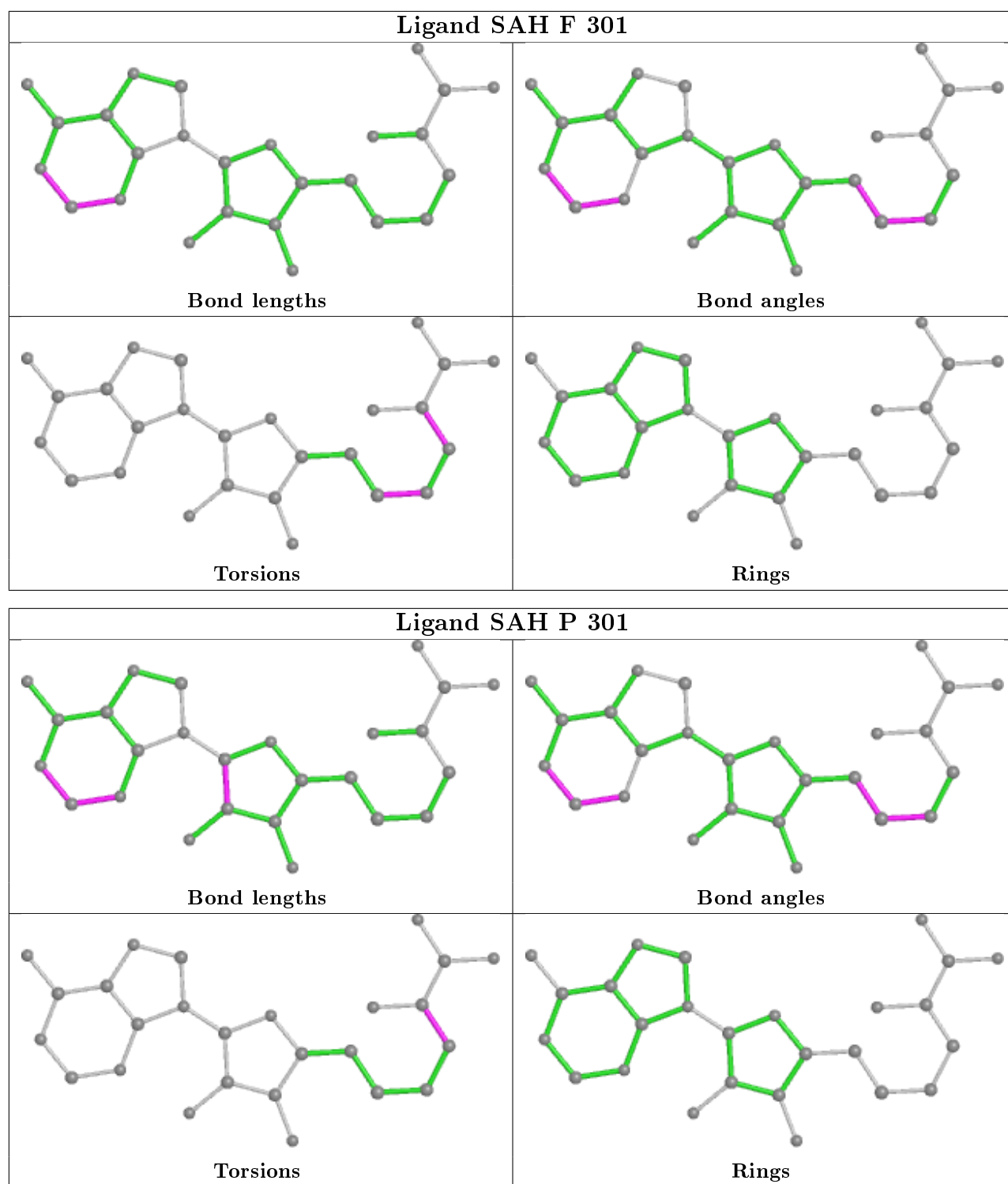
4 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	301	SAH	2	0
6	O	301	SAH	12	0
6	F	301	SAH	7	0
6	P	301	SAH	7	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 ⓘ

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%)	-0.31	3 (0%) 86 74	31, 58, 89, 122	0
1	B	375/388 (96%)	-0.31	1 (0%) 94 89	32, 59, 97, 119	0
1	K	375/388 (96%)	-0.28	5 (1%) 77 60	37, 66, 100, 128	0
1	L	375/388 (96%)	-0.27	2 (0%) 91 82	38, 67, 93, 106	0
2	C	122/130 (93%)	-0.25	1 (0%) 86 74	53, 82, 104, 113	0
2	D	122/130 (93%)	-0.23	2 (1%) 72 52	46, 73, 93, 103	0
2	M	122/130 (93%)	-0.17	2 (1%) 72 52	53, 74, 101, 122	0
2	N	122/130 (93%)	-0.07	3 (2%) 57 35	53, 76, 105, 112	0
3	E	227/232 (97%)	-0.25	2 (0%) 84 71	44, 64, 85, 92	0
3	F	227/232 (97%)	-0.21	1 (0%) 92 85	40, 64, 88, 103	0
3	O	227/232 (97%)	-0.22	2 (0%) 84 71	47, 67, 85, 101	0
3	P	227/232 (97%)	-0.29	2 (0%) 84 71	42, 57, 78, 106	0
4	G	31/41 (75%)	-0.20	0 100 100	37, 56, 102, 123	0
4	H	30/41 (73%)	-0.24	1 (3%) 46 25	32, 61, 92, 114	0
4	Q	31/41 (75%)	-0.05	3 (9%) 7 3	38, 63, 102, 121	0
4	R	29/41 (70%)	-0.25	0 100 100	41, 57, 86, 113	0
5	I	11/11 (100%)	-0.41	0 100 100	39, 43, 53, 53	0
5	J	11/11 (100%)	-0.51	0 100 100	34, 41, 48, 49	0
5	S	11/11 (100%)	-0.40	0 100 100	39, 45, 49, 59	0
5	T	11/11 (100%)	-0.32	0 100 100	41, 46, 50, 57	0
All	All	3061/3208 (95%)	-0.26	30 (0%) 82 69	31, 65, 96, 128	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	96	GLN	3.9
3	P	142	SER	3.4
4	H	37	C	3.2
2	M	109	GLU	3.1
3	E	142	SER	2.6

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](#)

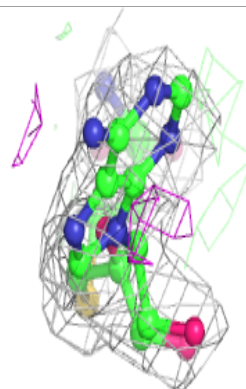
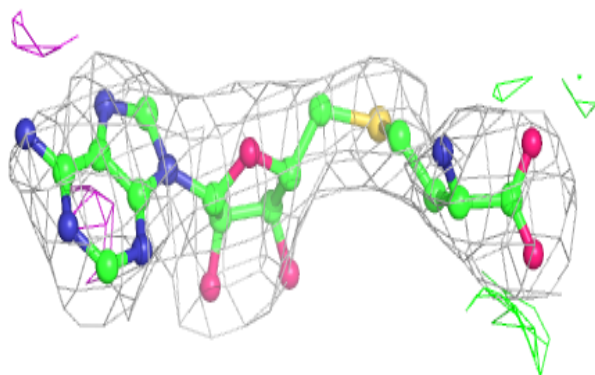
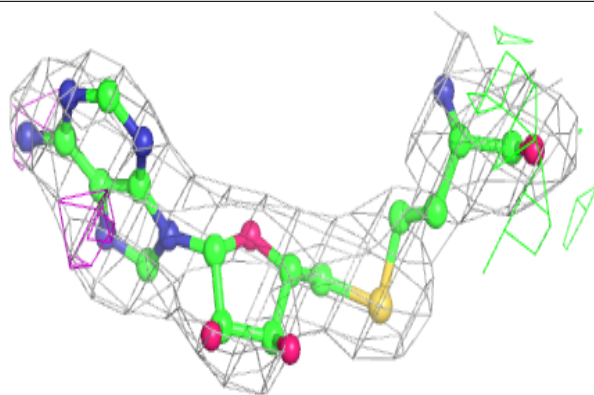
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	O	301	26/26	0.91	0.20	50,58,66,69	0
6	SAH	F	301	26/26	0.93	0.20	43,52,69,74	0
6	SAH	P	301	26/26	0.93	0.18	42,52,64,68	0
6	SAH	E	301	26/26	0.95	0.18	50,54,69,71	0

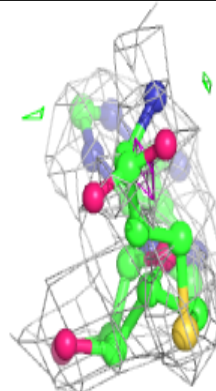
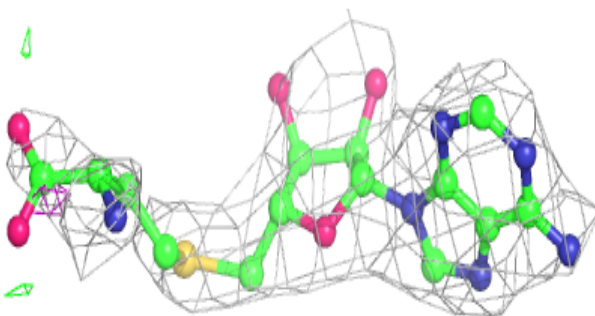
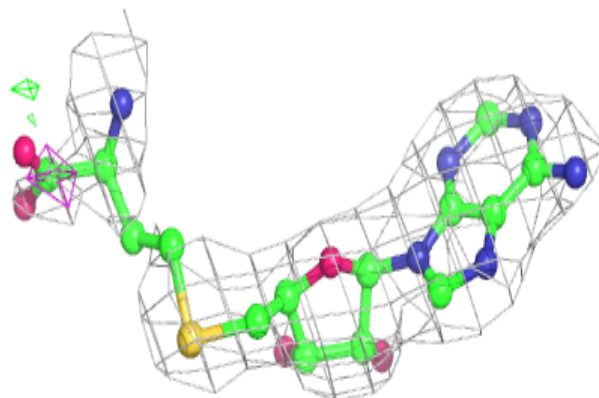
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAH O 301:

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

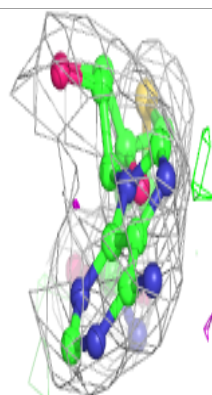
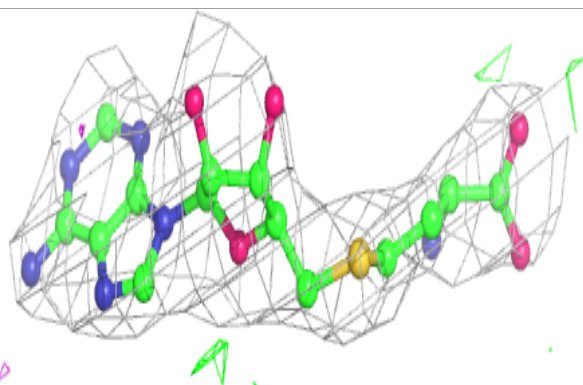
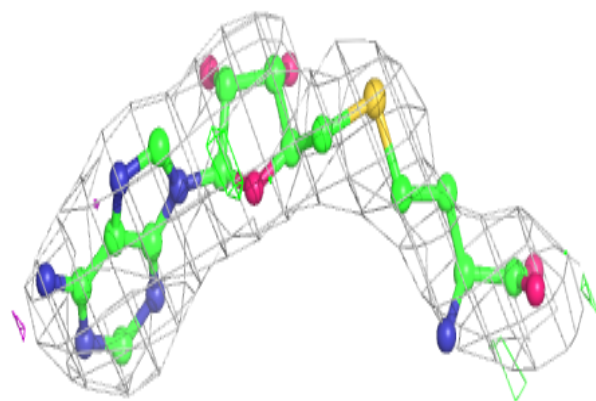
**Electron density around SAH F 301:**

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

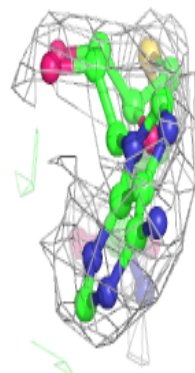
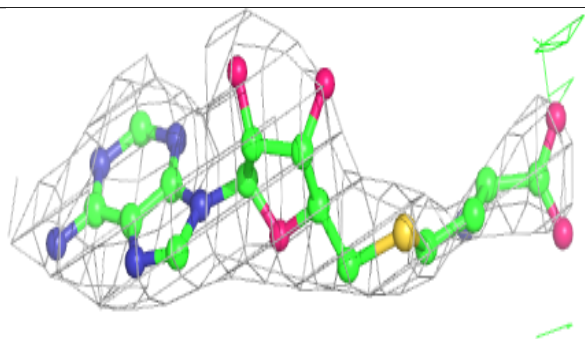
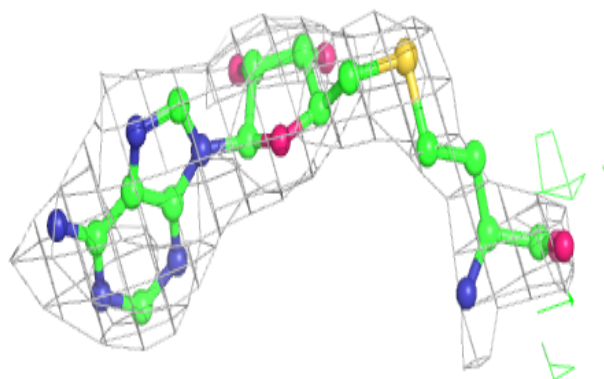


Electron density around SAH P 301:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.