



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 21, 2021 – 12:08 PM EDT

PDB ID : 7LTR
Title : Structure of the heteromeric complex between the alpha-N-methyltransferase (SonM) and a truncated construct of the RiPP precursor (SonA) (with SAM)
Authors : Miller, F.S.; Crone, K.K.; Jensen, M.R.; Shaw, S.; Harcombe, W.R.; Elias, M.; Freeman, M.F.
Deposited on : 2021-02-19
Resolution : 1.75 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

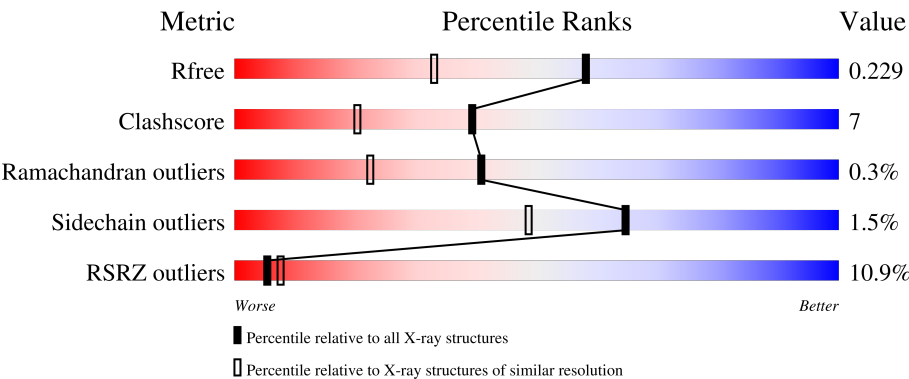
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

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 1.75 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.



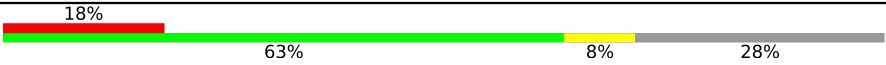


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	263	<div><div>12%</div><div>86%</div><div>13%</div><div>.</div></div>
1	C	263	<div><div>11%</div><div>85%</div><div>15%</div></div>
1	H	263	<div><div>8%</div><div>89%</div><div>11%</div></div>
1	J	263	<div><div>8%</div><div>81%</div><div>17%</div><div>.</div></div>
2	B	71	<div><div>11%</div><div>65%</div><div>7%</div><div>28%</div></div>

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Mol	Chain	Length	Quality of chain
2	D	71	
2	I	71	
2	K	71	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10919 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.

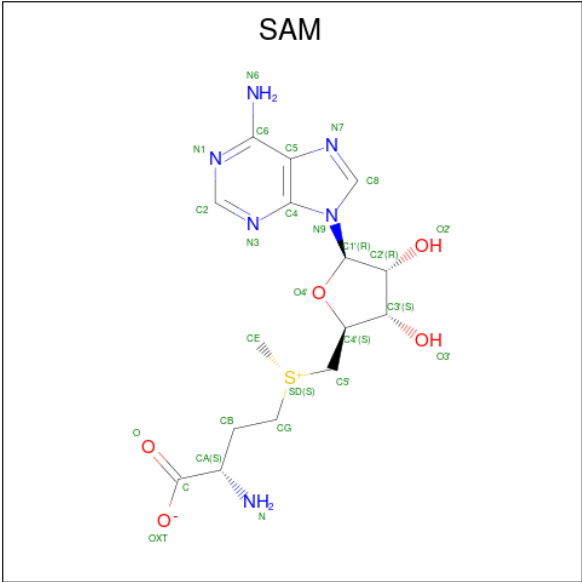
- Molecule 1 is a protein called TP-methylase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	6	0
			2064	1324	356	374	10			
1	C	262	Total	C	N	O	S	0	5	0
			2066	1324	357	375	10			
1	H	262	Total	C	N	O	S	0	3	0
			2053	1316	353	375	9			
1	J	262	Total	C	N	O	S	0	4	0
			2058	1319	354	375	10			

- Molecule 2 is a protein called LigA domain-containing protein.

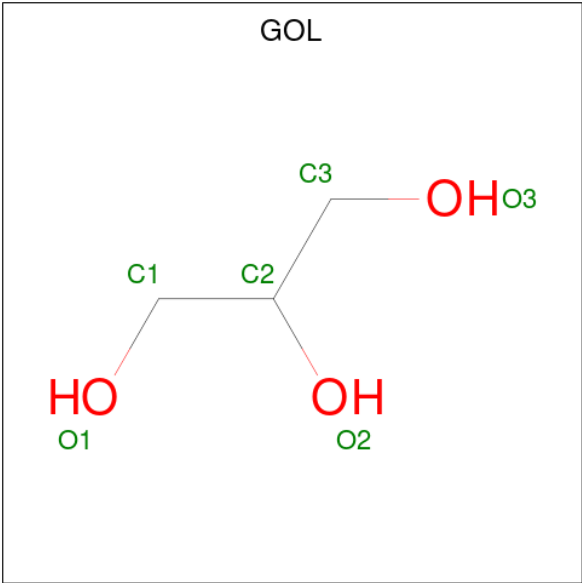
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	51	Total	C	N	O	S	0	0	0
			398	246	66	82	4			
2	D	51	Total	C	N	O	S	0	0	0
			400	247	66	83	4			
2	I	52	Total	C	N	O	S	0	1	0
			410	253	68	85	4			
2	K	51	Total	C	N	O	S	0	0	0
			400	247	66	83	4			

- Molecule 3 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: C₁₅H₂₂N₆O₅S) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		

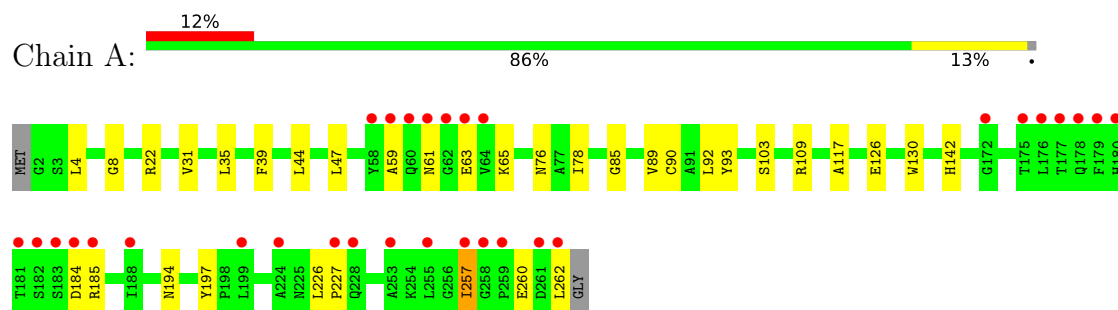
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	167	Total	O	0	0
			167	167		
5	B	33	Total	O	0	0
			33	33		
5	C	201	Total	O	0	0
			201	201		
5	D	38	Total	O	0	0
			38	38		
5	H	250	Total	O	0	0
			250	250		
5	I	41	Total	O	0	0
			41	41		
5	J	226	Total	O	0	0
			226	226		
5	K	36	Total	O	0	0
			36	36		

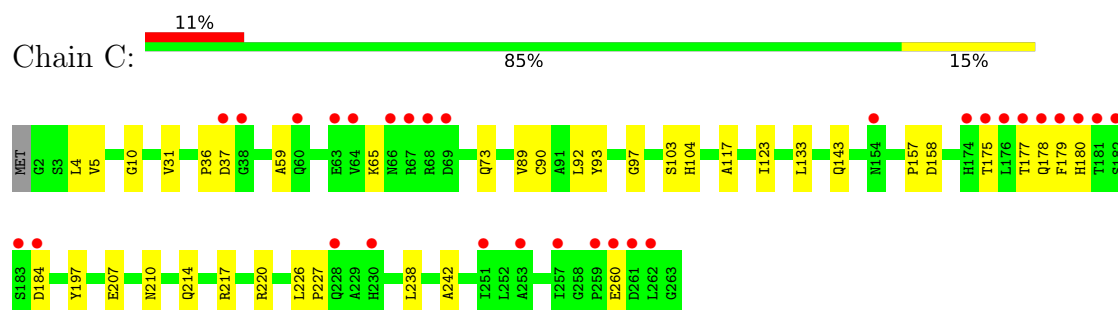
3 Residue-property plots [i](#)

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.

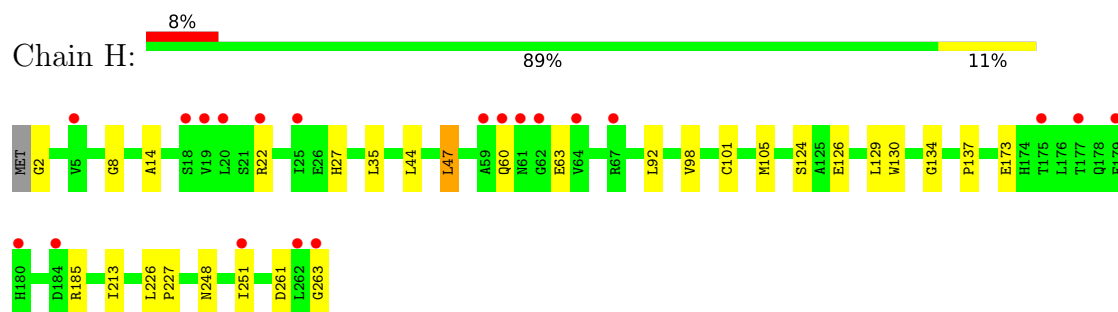
- Molecule 1: TP-methylase family protein



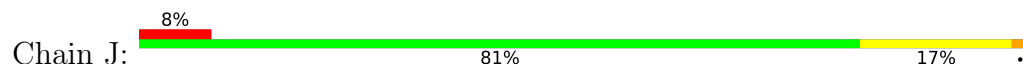
- Molecule 1: TP-methylase family protein

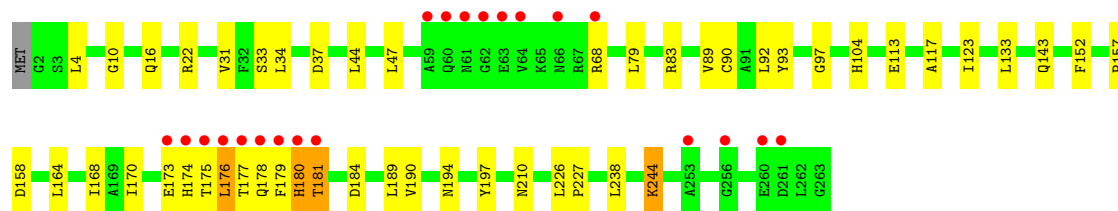


- Molecule 1: TP-methylase family protein



- Molecule 1: TP-methylase family protein

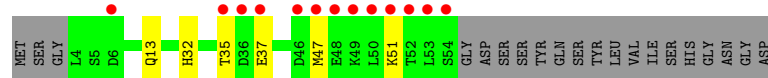




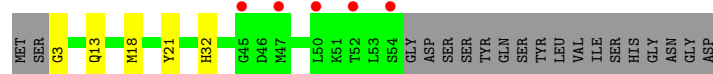
• Molecule 2: LigA domain-containing protein



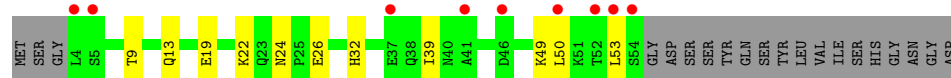
• Molecule 2: LigA domain-containing protein



• Molecule 2: LigA domain-containing protein



• Molecule 2: LigA domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.24Å 112.86Å 85.87Å 90.00° 97.82° 90.00°	Depositor
Resolution (Å)	56.43 – 1.75 56.43 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.3 (56.43-1.75) 98.3 (56.43-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0266	Depositor
R, R_{free}	0.187 , 0.219 0.197 , 0.229	Depositor DCC
R_{free} test set	6742 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10919	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.04 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4192e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SAM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.62	0/2133	0.65	0/2904
1	C	0.61	0/2132	0.66	0/2901
1	H	0.61	0/2113	0.65	0/2876
1	J	0.61	0/2121	0.67	0/2887
2	B	0.63	0/402	0.64	0/539
2	D	0.63	0/404	0.65	0/542
2	I	0.65	0/417	0.68	0/559
2	K	0.63	0/404	0.62	0/542
All	All	0.62	0/10126	0.65	0/13750

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2064	0	2071	26	0
1	C	2066	0	2067	30	0
1	H	2053	0	2050	27	0
1	J	2058	0	2056	42	0
2	B	398	0	384	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	400	0	386	7	0
2	I	410	0	397	8	0
2	K	400	0	386	8	0
3	A	27	0	22	1	0
3	H	27	0	22	0	0
4	A	12	0	16	0	0
4	H	12	0	16	3	0
5	A	167	0	0	4	0
5	B	33	0	0	0	0
5	C	201	0	0	2	0
5	D	38	0	0	3	0
5	H	250	0	0	3	1
5	I	41	0	0	2	0
5	J	226	0	0	7	1
5	K	36	0	0	6	0
All	All	10919	0	9873	146	1

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 7.

All (146) 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:I:18:MET:HG2	5:J:447:HOH:O	1.35	1.24
1:C:103[B]:SER:OG	5:C:301:HOH:O	1.78	1.01
2:B:26:GLU:OE1	2:B:30:ARG:NH1	2.03	0.91
1:A:257:ILE:HD11	1:A:262:LEU:HD21	1.55	0.87
1:C:93:TYR:OH	1:C:210[A]:ASN:OD1	1.94	0.86
1:J:177:THR:HG23	1:J:179:PHE:H	1.40	0.84
1:J:93:TYR:OH	1:J:210[A]:ASN:OD1	1.96	0.84
2:K:22:LYS:HE2	5:K:133:HOH:O	1.76	0.83
2:I:18:MET:CE	5:J:447:HOH:O	2.26	0.82
1:C:133:LEU:HD23	1:C:238:LEU:HD22	1.63	0.81
1:C:178:GLN:NE2	1:C:178:GLN:HA	1.96	0.80
2:K:19:GLU:OE1	5:K:101:HOH:O	1.98	0.80
1:J:176:LEU:O	1:J:176:LEU:HD12	1.84	0.77
1:C:133:LEU:CD2	1:C:238:LEU:HD22	2.15	0.75
1:A:103[B]:SER:OG	5:A:401:HOH:O	2.04	0.74
1:C:143:GLN:HE22	1:C:158:ASP:H	1.36	0.72
1:H:248:ASN:OD1	1:H:251:ILE:HD13	1.90	0.72
1:J:181:THR:HG23	1:J:184:ASP:H	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:143:GLN:HE22	1:J:158:ASP:H	1.39	0.71
2:I:18:MET:CG	5:J:447:HOH:O	2.10	0.70
2:I:3:GLY:N	5:I:101:HOH:O	2.24	0.69
1:J:83:ARG:HD3	1:J:113:GLU:OE1	1.93	0.68
1:J:181:THR:CG2	1:J:184:ASP:H	2.07	0.68
1:H:98:VAL:HG21	4:H:303:GOL:H11	1.76	0.68
1:H:251:ILE:CD1	5:H:442:HOH:O	2.43	0.67
1:J:180:HIS:HB3	1:J:184:ASP:HB2	1.77	0.66
1:C:59:ALA:HB2	1:C:65:LYS:HB3	1.75	0.66
1:J:97:GLY:O	1:J:104:HIS:HE1	1.79	0.66
2:I:18:MET:SD	5:J:447:HOH:O	2.52	0.65
1:C:143:GLN:NE2	1:C:158:ASP:H	1.95	0.64
1:H:263:GLY:O	1:J:152:PHE:HB3	1.97	0.64
1:A:257:ILE:HG22	1:C:177:THR:CG2	2.28	0.63
1:J:133:LEU:HD23	1:J:238:LEU:HD22	1.80	0.63
1:J:181:THR:HG22	1:J:184:ASP:CG	2.20	0.63
1:J:143:GLN:NE2	1:J:158:ASP:H	1.97	0.62
1:H:134:GLY:HA2	5:H:444:HOH:O	2.01	0.60
1:C:65:LYS:NZ	1:C:73:GLN:HE22	2.00	0.60
1:J:178:GLN:OE1	1:J:178:GLN:N	2.31	0.60
1:J:133:LEU:HD23	1:J:238:LEU:CD2	2.33	0.59
1:C:133:LEU:HD23	1:C:238:LEU:CD2	2.31	0.59
2:K:49:LYS:O	2:K:53:LEU:HG	2.02	0.59
1:J:133:LEU:CD2	1:J:238:LEU:HD22	2.32	0.59
2:D:51:LYS:HA	2:D:51:LYS:HE2	1.85	0.59
1:J:244:LYS:HD3	5:J:404:HOH:O	2.03	0.58
2:K:22:LYS:CE	5:K:133:HOH:O	2.42	0.58
1:C:178:GLN:HA	1:C:178:GLN:HE21	1.68	0.58
2:D:35:THR:HG22	2:D:37:GLU:H	1.68	0.58
1:A:257:ILE:CD1	1:A:262:LEU:HD21	2.31	0.57
1:C:220[A]:ARG:NH2	5:C:302:HOH:O	2.38	0.57
1:C:65:LYS:HZ1	1:C:73:GLN:HE22	1.52	0.57
1:H:126:GLU:OE2	1:H:130:TRP:HZ2	1.88	0.56
1:C:97:GLY:O	1:C:104:HIS:HE1	1.89	0.56
1:H:22[A]:ARG:HG3	1:H:47:LEU:HD11	1.88	0.56
1:A:226:LEU:N	1:A:227:PRO:CD	2.69	0.56
1:J:180:HIS:HB3	1:J:184:ASP:CB	2.35	0.56
1:J:22[B]:ARG:HG3	1:J:47:LEU:HD21	1.86	0.56
1:H:2:GLY:N	5:H:401:HOH:O	2.38	0.55
1:A:185:ARG:NH2	5:A:404:HOH:O	2.40	0.55
1:A:8:GLY:HA2	1:A:92:LEU:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:177:THR:HG23	1:J:179:PHE:N	2.18	0.54
2:B:26:GLU:CD	2:B:30:ARG:HH12	2.09	0.54
1:H:261:ASP:O	1:J:174:HIS:NE2	2.35	0.54
2:B:26:GLU:CD	2:B:30:ARG:NH1	2.60	0.54
1:C:90[A]:CYS:SG	1:C:92:LEU:HD21	2.47	0.54
1:A:78:ILE:HD13	1:A:90[B]:CYS:SG	2.47	0.54
1:H:213:ILE:C	1:H:213:ILE:HD12	2.28	0.53
2:K:32:HIS:HD2	5:K:127:HOH:O	1.91	0.53
1:C:214:GLN:HB2	2:D:47:MET:HE3	1.91	0.53
1:J:16:GLN:HG3	5:J:501:HOH:O	2.08	0.53
1:J:181:THR:HG22	1:J:184:ASP:CB	2.39	0.53
1:A:78:ILE:CD1	1:A:90[B]:CYS:SG	2.96	0.52
1:J:79:LEU:O	1:J:83:ARG:HG3	2.09	0.52
1:H:124:SER:HB3	4:H:303:GOL:H12	1.92	0.52
1:C:226:LEU:N	1:C:227:PRO:CD	2.72	0.52
1:A:78:ILE:HG12	1:A:90[B]:CYS:SG	2.50	0.52
1:J:143:GLN:HE22	1:J:157:PRO:HA	1.76	0.51
2:K:9:THR:O	2:K:13:GLN:HG2	2.10	0.51
1:A:22[B]:ARG:HG3	1:A:47:LEU:HD11	1.94	0.50
1:C:4:LEU:O	1:C:117:ALA:HA	2.12	0.50
1:H:130:TRP:CD1	1:H:137:PRO:HG3	2.47	0.50
1:A:194:ASN:HA	1:A:197:TYR:O	2.12	0.49
1:A:257:ILE:CG2	1:C:177:THR:CG2	2.90	0.49
1:H:35:LEU:HD11	1:H:44:LEU:HD22	1.94	0.49
1:C:180:HIS:O	1:C:184:ASP:HB2	2.13	0.49
1:J:164:LEU:HD21	1:J:238:LEU:HD13	1.93	0.49
1:H:14:ALA:HB1	2:I:13[A]:GLN:HG3	1.93	0.48
1:A:184:ASP:OD2	1:A:185:ARG:NH1	2.45	0.48
1:J:226:LEU:N	1:J:227:PRO:CD	2.77	0.48
1:H:261:ASP:HB3	1:J:174:HIS:CE1	2.49	0.48
1:H:248:ASN:CG	1:H:251:ILE:HD13	2.32	0.47
1:H:27:HIS:HD2	5:K:102:HOH:O	1.97	0.47
1:J:92:LEU:HD22	1:J:92:LEU:N	2.29	0.47
2:B:49:LYS:O	2:B:52:THR:HB	2.14	0.47
1:A:76[B]:ASN:OD1	1:A:109:ARG:NH1	2.47	0.47
2:D:51:LYS:HA	2:D:51:LYS:CE	2.44	0.47
1:J:179:PHE:O	1:J:181:THR:N	2.48	0.47
2:I:32:HIS:HD2	5:I:135:HOH:O	1.97	0.47
1:H:8:GLY:HA2	1:H:92:LEU:O	2.15	0.46
1:H:60:GLN:O	1:H:63:GLU:HG2	2.16	0.46
1:C:207:GLU:HB2	1:C:217:ARG:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:170:ILE:O	1:J:173:GLU:HB2	2.15	0.45
1:C:226:LEU:N	1:C:227:PRO:HD3	2.32	0.45
2:D:13:GLN:NE2	5:D:101:HOH:O	2.31	0.45
2:B:26:GLU:CG	2:B:30:ARG:NH1	2.80	0.45
1:H:226:LEU:N	1:H:227:PRO:CD	2.79	0.45
1:J:33:SER:HB3	1:J:44:LEU:CD2	2.47	0.45
1:A:85:GLY:HA2	5:K:109:HOH:O	2.16	0.45
1:A:226:LEU:N	1:A:227:PRO:HD3	2.31	0.45
1:H:251:ILE:N	1:H:251:ILE:HD12	2.32	0.44
1:J:174:HIS:O	1:J:177:THR:HG22	2.18	0.44
1:C:10:GLY:HA2	1:C:123:ILE:O	2.18	0.44
1:C:31:VAL:HA	1:C:89:VAL:O	2.17	0.44
1:J:90[A]:CYS:SG	1:J:92:LEU:HD21	2.58	0.44
2:D:13:GLN:NE2	5:D:103:HOH:O	2.37	0.44
1:J:4:LEU:O	1:J:117:ALA:HA	2.19	0.43
5:A:490:HOH:O	2:B:51:LYS:HD2	2.18	0.43
1:H:101:CYS:O	1:H:105:MET:HG3	2.19	0.43
1:H:129:LEU:C	1:H:129:LEU:HD23	2.39	0.43
1:H:226:LEU:HB3	1:H:227:PRO:HD3	2.00	0.43
1:A:22[A]:ARG:HG3	1:A:47:LEU:HD11	2.01	0.43
2:K:26:GLU:HG3	2:K:39:ILE:HG21	1.99	0.43
1:H:213:ILE:HG22	2:I:21:TYR:CZ	2.54	0.42
1:J:10:GLY:HA2	1:J:123:ILE:O	2.19	0.42
1:A:59:ALA:HB2	1:A:65:LYS:HB3	2.01	0.42
1:J:16:GLN:NE2	5:J:305:HOH:O	2.47	0.42
2:K:50:LEU:HD23	2:K:50:LEU:HA	1.94	0.42
2:D:32:HIS:HD2	5:D:125:HOH:O	2.02	0.42
1:A:39:PHE:CE2	2:B:51:LYS:HD3	2.55	0.42
1:C:143:GLN:HE22	1:C:157:PRO:HA	1.85	0.41
1:H:124:SER:CB	4:H:303:GOL:H12	2.50	0.41
1:A:35:LEU:HD11	1:A:44:LEU:HD22	2.01	0.41
1:A:126:GLU:HG2	1:A:130:TRP:NE1	2.34	0.41
1:A:142:HIS:HD2	5:A:426:HOH:O	2.03	0.41
1:C:260:GLU:CD	1:C:260:GLU:H	2.24	0.41
1:C:197:TYR:CD1	1:C:242:ALA:HB2	2.55	0.40
1:J:34:LEU:HD12	1:J:34:LEU:HA	1.91	0.40
1:C:92:LEU:HD22	1:C:92:LEU:N	2.36	0.40
1:J:31:VAL:HA	1:J:89:VAL:O	2.21	0.40
1:A:4:LEU:O	1:A:117:ALA:HA	2.20	0.40
1:A:93:TYR:OH	3:A:301:SAM:HG2	2.21	0.40
1:J:194:ASN:HA	1:J:197:TYR:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:VAL:HA	1:A:89:VAL:O	2.22	0.40
1:C:5:VAL:O	1:C:89:VAL:HA	2.21	0.40
1:H:213:ILE:C	1:H:213:ILE:CD1	2.89	0.40
1:J:168:ILE:HD11	1:J:189:LEU:CD2	2.51	0.40
1:J:181:THR:HG22	1:J:184:ASP:HB2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:650:HOH:O	5:J:521:HOH:O[2_646]	2.08	0.12

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	265/263 (101%)	257 (97%)	7 (3%)	1 (0%)	34	17
1	C	265/263 (101%)	254 (96%)	10 (4%)	1 (0%)	34	17
1	H	263/263 (100%)	258 (98%)	5 (2%)	0	100	100
1	J	264/263 (100%)	257 (97%)	5 (2%)	2 (1%)	19	6
2	B	49/71 (69%)	49 (100%)	0	0	100	100
2	D	49/71 (69%)	48 (98%)	1 (2%)	0	100	100
2	I	51/71 (72%)	51 (100%)	0	0	100	100
2	K	49/71 (69%)	49 (100%)	0	0	100	100
All	All	1255/1336 (94%)	1223 (98%)	28 (2%)	4 (0%)	41	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	J	180	HIS
1	C	36	PRO
1	J	181	THR

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	224/219 (102%)	221 (99%)	3 (1%)	69	54
1	C	223/219 (102%)	220 (99%)	3 (1%)	69	54
1	H	221/219 (101%)	218 (99%)	3 (1%)	67	52
1	J	222/219 (101%)	216 (97%)	6 (3%)	44	22
2	B	43/60 (72%)	43 (100%)	0	100	100
2	D	44/60 (73%)	44 (100%)	0	100	100
2	I	45/60 (75%)	45 (100%)	0	100	100
2	K	44/60 (73%)	43 (98%)	1 (2%)	50	28
All	All	1066/1116 (96%)	1050 (98%)	16 (2%)	65	49

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	GLU
1	A	257	ILE
1	A	260	GLU
1	C	37	ASP
1	C	175	THR
1	C	179	PHE
1	H	47	LEU
1	H	173	GLU
1	H	185	ARG
1	J	37	ASP
1	J	68	ARG
1	J	175	THR

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Mol	Chain	Res	Type
1	J	176	LEU
1	J	190	VAL
1	J	244	LYS
2	K	24	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	56	GLN
1	A	60	GLN
1	A	210	ASN
1	C	55	GLN
1	C	56	GLN
1	C	73	GLN
1	C	104	HIS
1	C	143	GLN
1	C	167	GLN
1	C	178	GLN
1	H	27	HIS
1	H	167	GLN
1	H	210	ASN
2	I	32	HIS
1	J	27	HIS
1	J	61	ASN
1	J	104	HIS
1	J	143	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

6 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$
4	GOL	H	302	-	5,5,5	0.08	0	5,5,5	0.26	0
3	SAM	H	301	-	21,29,29	0.61	0	18,42,42	0.85	1 (5%)
4	GOL	A	302	-	5,5,5	0.09	0	5,5,5	0.25	0
4	GOL	H	303	-	5,5,5	0.08	0	5,5,5	0.25	0
3	SAM	A	301	-	21,29,29	0.62	0	18,42,42	0.84	1 (5%)
4	GOL	A	303	-	5,5,5	0.09	0	5,5,5	0.29	0

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	GOL	H	302	-	-	0/4/4/4	-
3	SAM	H	301	-	-	1/8/33/33	0/3/3/3
4	GOL	A	302	-	-	0/4/4/4	-
4	GOL	H	303	-	-	2/4/4/4	-
3	SAM	A	301	-	-	1/8/33/33	0/3/3/3
4	GOL	A	303	-	-	4/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	301	SAM	C5-C6-N6	2.29	123.84	120.35
3	A	301	SAM	C5-C6-N6	2.24	123.76	120.35

There are no chirality outliers.

All (8) torsion outliers are listed below:

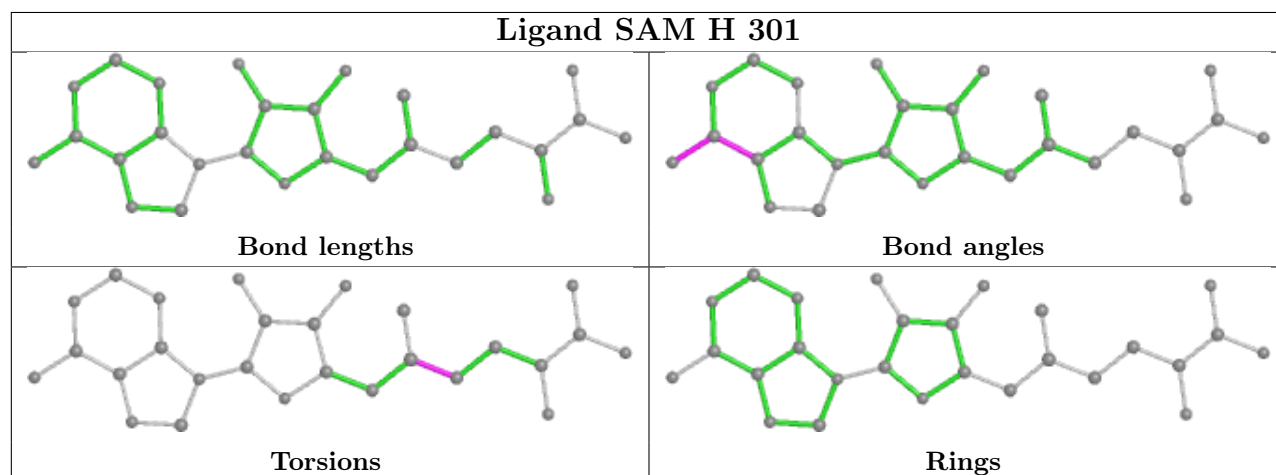
Mol	Chain	Res	Type	Atoms
4	A	303	GOL	O1-C1-C2-C3
4	H	303	GOL	O1-C1-C2-O2
4	H	303	GOL	O1-C1-C2-C3
4	A	303	GOL	C1-C2-C3-O3
4	A	303	GOL	O1-C1-C2-O2
4	A	303	GOL	O2-C2-C3-O3
3	A	301	SAM	CB-CG-SD-C5'
3	H	301	SAM	CB-CG-SD-C5'

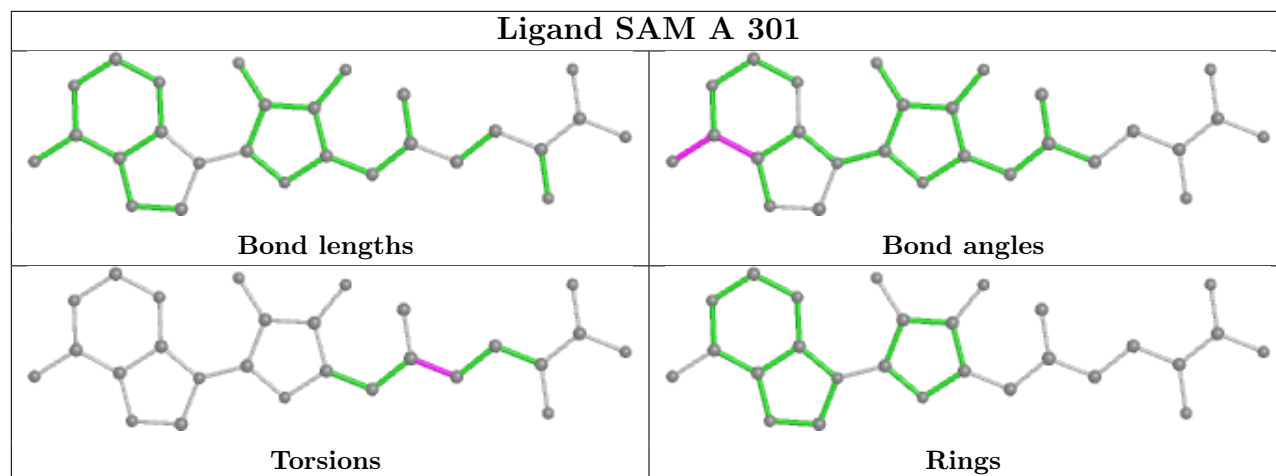
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	303	GOL	3	0
3	A	301	SAM	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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	261/263 (99%)	0.86	31 (11%) 4 6	20, 31, 50, 78	4 (1%)
1	C	262/263 (99%)	0.82	30 (11%) 4 6	20, 30, 55, 77	5 (1%)
1	H	262/263 (99%)	0.70	20 (7%) 13 18	18, 25, 42, 64	3 (1%)
1	J	262/263 (99%)	0.99	21 (8%) 12 16	18, 26, 50, 105	1 (0%)
2	B	51/71 (71%)	0.83	8 (15%) 2 3	21, 30, 57, 60	0
2	D	51/71 (71%)	1.25	13 (25%) 0 0	21, 30, 68, 74	0
2	I	52/71 (73%)	0.75	5 (9%) 8 10	19, 27, 51, 67	0
2	K	51/71 (71%)	1.01	9 (17%) 1 2	20, 29, 55, 72	2 (3%)
All	All	1252/1336 (93%)	0.86	137 (10%) 5 7	18, 28, 53, 105	15 (1%)

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	176	LEU	13.0
1	J	179	PHE	10.4
1	J	177	THR	9.7
1	C	179	PHE	9.0
1	C	175	THR	8.7
1	J	178	GLN	8.1
1	H	262	LEU	8.0
1	J	175	THR	7.9
1	A	179	PHE	7.6
1	A	62	GLY	7.2
1	C	178	GLN	7.1
1	J	62	GLY	6.6
2	D	52	THR	6.6
1	C	64	VAL	6.5
1	C	177	THR	6.2
1	A	61	ASN	6.2

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Mol	Chain	Res	Type	RSRZ
2	D	37	GLU	5.8
1	J	180	HIS	5.7
1	A	184	ASP	5.5
1	J	64	VAL	5.2
1	H	64	VAL	5.0
1	H	263	GLY	5.0
1	J	181	THR	4.8
1	A	60	GLN	4.8
1	J	174	HIS	4.6
1	H	60	GLN	4.5
1	A	258	GLY	4.5
1	A	262	LEU	4.5
2	D	48	GLU	4.4
1	A	253	ALA	4.3
2	K	52	THR	4.3
1	J	68	ARG	4.3
1	C	176	LEU	4.2
2	B	53	LEU	4.1
1	A	257	ILE	4.1
2	D	46	ASP	4.1
1	A	180	HIS	4.0
1	A	59	ALA	4.0
1	C	174	HIS	4.0
1	C	60	GLN	4.0
1	A	259	PRO	4.0
1	A	181	THR	4.0
2	D	50	LEU	3.9
1	A	176	LEU	3.9
2	D	49	LYS	3.9
1	A	177	THR	3.8
1	H	179	PHE	3.8
2	D	54	SER	3.7
1	C	181	THR	3.7
1	A	224	ALA	3.7
1	H	184	ASP	3.7
1	H	59	ALA	3.6
1	C	260	GLU	3.5
1	C	66	ASN	3.4
1	A	182	SER	3.4
1	H	62	GLY	3.4
2	B	52	THR	3.4
1	C	262	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
2	K	53	LEU	3.4
1	C	68	ARG	3.3
2	I	54	SER	3.3
1	A	255	LEU	3.3
2	B	48	GLU	3.3
2	D	53	LEU	3.3
1	J	66	ASN	3.3
2	D	47	MET	3.2
1	A	228	GLN	3.2
2	K	54	SER	3.2
1	C	228	GLN	3.2
1	A	185	ARG	3.1
1	H	177	THR	3.1
2	K	37	GLU	3.0
1	J	59	ALA	3.0
1	A	175	THR	3.0
1	C	37	ASP	3.0
1	C	259	PRO	3.0
1	J	253	ALA	3.0
1	H	5	VAL	2.9
1	C	253	ALA	2.9
1	J	63	GLU	2.9
1	A	63	GLU	2.9
1	C	182	SER	2.9
2	I	50	LEU	2.8
1	A	172	GLY	2.8
1	C	230	HIS	2.8
1	H	61	ASN	2.8
1	C	261	ASP	2.8
1	J	61	ASN	2.8
1	A	261	ASP	2.7
2	I	47	MET	2.7
1	H	180	HIS	2.7
2	B	47	MET	2.7
2	B	37	GLU	2.7
1	A	58	TYR	2.6
1	C	180	HIS	2.6
1	A	178	GLN	2.6
2	K	50	LEU	2.6
1	J	261	ASP	2.6
1	C	184	ASP	2.5
1	J	173	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	60	GLN	2.5
1	C	67	ARG	2.4
1	C	183	SER	2.4
1	A	64	VAL	2.4
1	A	183	SER	2.4
2	D	35	THR	2.4
1	H	19	VAL	2.4
1	J	256	GLY	2.4
1	A	199	LEU	2.3
1	H	18[A]	SER	2.3
1	A	227	PRO	2.3
1	C	63	GLU	2.3
2	B	33	GLY	2.3
2	K	46	ASP	2.3
2	I	52	THR	2.2
2	K	41	ALA	2.2
1	C	257	ILE	2.2
1	H	175	THR	2.2
2	K	5	SER	2.2
1	C	251	ILE	2.2
2	I	45	GLY	2.2
1	H	251	ILE	2.1
1	J	260	GLU	2.1
1	C	69	ASP	2.1
2	B	50	LEU	2.1
1	C	154	ASN	2.1
1	H	67	ARG	2.1
2	B	45	GLY	2.1
1	H	22[A]	ARG	2.1
2	D	51	LYS	2.1
2	D	6	ASP	2.1
2	D	36	ASP	2.1
2	K	4	LEU	2.0
1	A	188	ILE	2.0
1	H	25	ILE	2.0
1	C	38	GLY	2.0
1	H	20	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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](#)

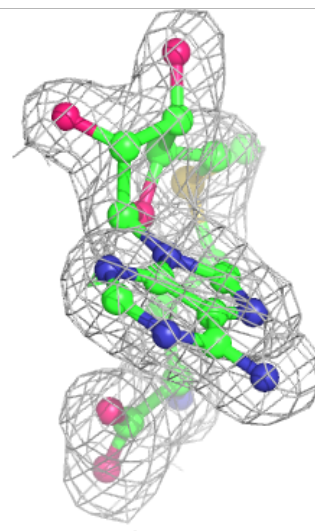
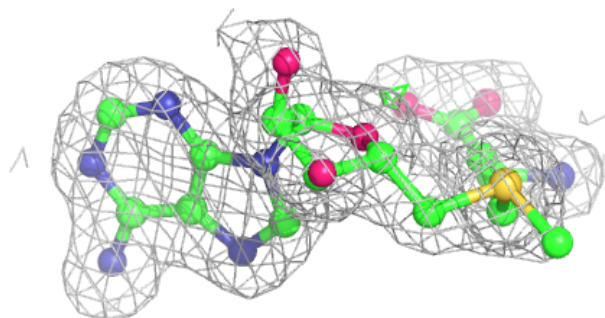
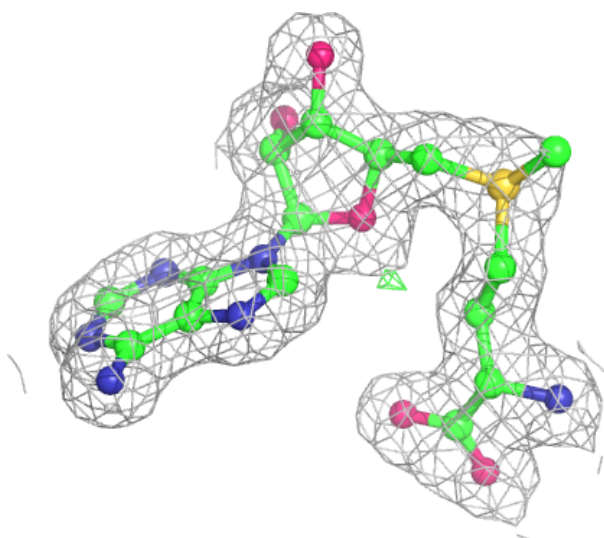
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	A	303	6/6	0.78	0.23	38,43,48,49	0
4	GOL	H	303	6/6	0.80	0.24	30,38,40,41	0
4	GOL	A	302	6/6	0.86	0.18	41,48,50,54	0
4	GOL	H	302	6/6	0.90	0.12	34,40,42,43	0
3	SAM	A	301	27/27	0.91	0.11	28,31,36,42	0
3	SAM	H	301	27/27	0.94	0.11	24,26,30,34	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.

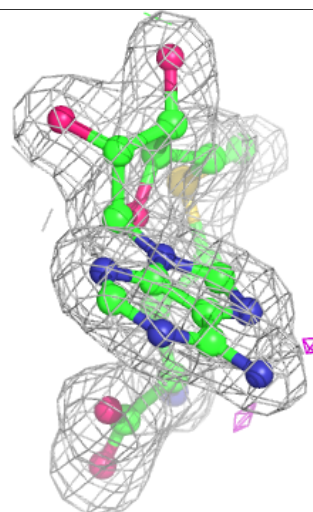
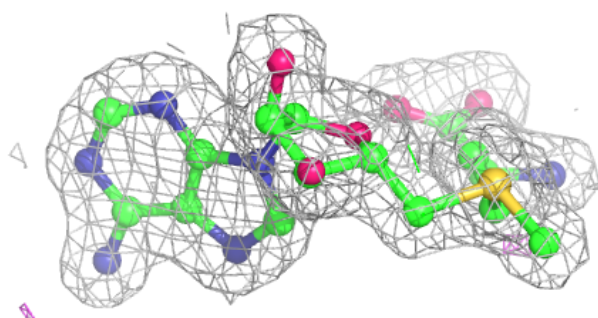
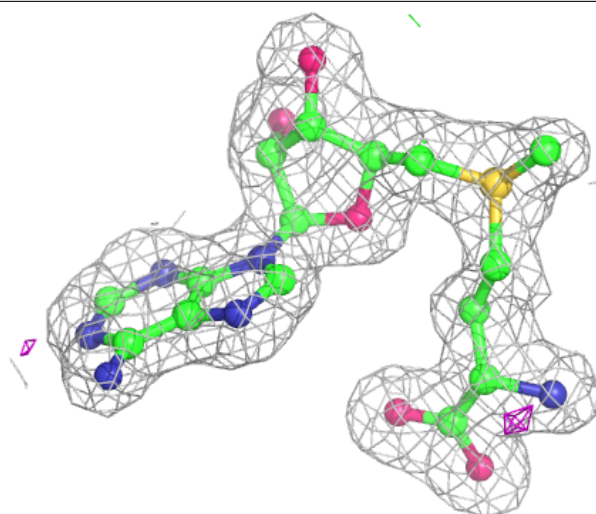
Electron density around SAM A 301:

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



Electron density around SAM H 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.