Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2020 – 12:25 am BST

PDB ID	:	3G8A
Title	:	T. thermophilus 16S rRNA G527 methyltransferase in complex with AdoHcy in space group P61
Authors	:	Demirci, H.; Gregory, S.T.; Belardinelli, R.; Gualerzi, C.; Dahlberg, A.E.; Jogl, G.
Deposited on	:	2009-02-11
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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.
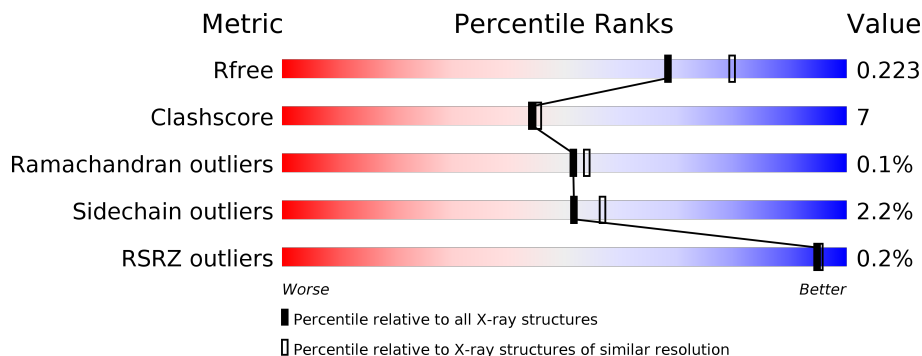
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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.

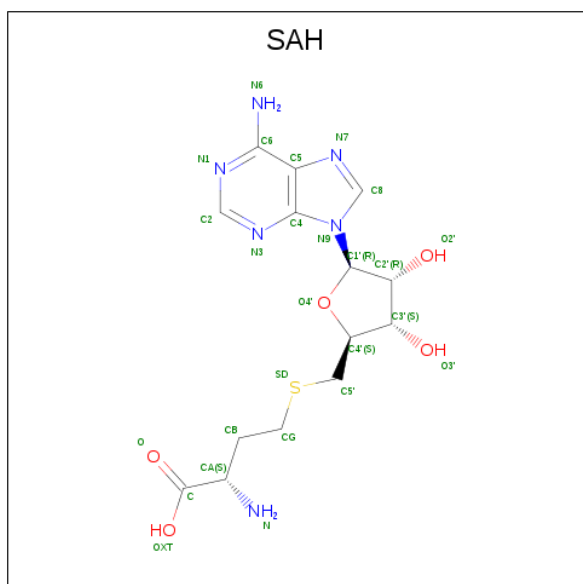| Mol	Chain	Length	Quality of chain
1	A	249	80%　　14%　・5%
1	B	249	81%　　14%　・
1	C	249	82%　　13%　・
1	D	249	81%　　15%　・
1	E	249	80%　　14%　・・
1	F	249	85%　　11%　・

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12573 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 Ribosomal RNA small subunit methyltransferase G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	236	Total	C	N	O	S	0	3	0
			1821	1176	331	310	4			
1	B	239	Total	C	N	O	S	0	3	0
			1849	1193	337	315	4			
1	C	238	Total	C	N	O	S	0	5	0
			1850	1195	335	316	4			
1	D	239	Total	C	N	O	S	0	5	0
			1855	1198	336	317	4			
1	E	239	Total	C	N	O	S	0	5	0
			1858	1198	339	317	4			
1	F	239	Total	C	N	O	S	0	2	0
			1837	1186	333	314	4			

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	B	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	C	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	D	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	E	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	F	1	Total 26	C 14	N 6	O 5	S 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	214	Total 214	O 214	0	0
3	B	238	Total 238	O 238	0	0
3	C	211	Total 211	O 211	0	0
3	D	233	Total 233	O 233	0	0
3	E	210	Total 210	O 210	0	0
3	F	241	Total 241	O 241	0	0

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: Ribosomal RNA small subunit methyltransferase G
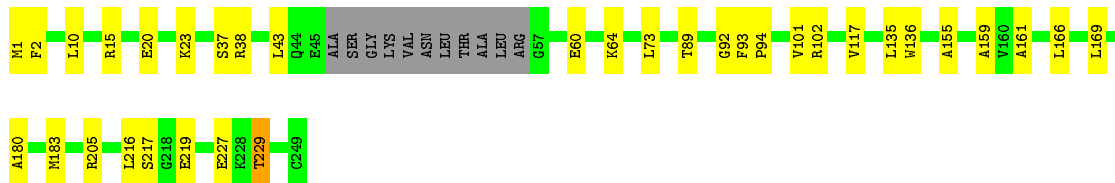
Chain A:
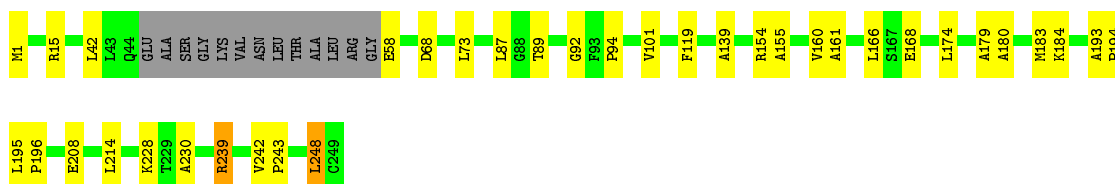
- Molecule 1: Ribosomal RNA small subunit methyltransferase G

Chain B:

- Molecule 1: Ribosomal RNA small subunit methyltransferase G

Chain C:

- Molecule 1: Ribosomal RNA small subunit methyltransferase G

Chain D:

A159 V160 A161 P162 L166 A179 M183 A193 P194 R205 R245 C249

• Molecule 1: Ribosomal RNA small subunit methyltransferase G

Chain E:

80%   14%

M1 L19 K30 A46 SER GLY LYS VAL ASN LEU THR ALA LEU ARG G57 E60 K64 L73 L87 G88 T89 G90 A91 G92 L96 K99 I100 V101 L107 K116 V117 R133 W136 A139 R154 V160 A161 P162 L166 L169 L174

A179 A180 E189 E190 P196 P197 G203 G204 R205 L214 P215 L216 T229 P234 C249

• Molecule 1: Ribosomal RNA small subunit methyltransferase G

Chain F:

85%   11%

M1 K5 R15 K23 K30 E34 A46 SER GLY LYS VAL ASN LEU THR ALA LEU ARG G57 H65 L73 L87 G88 T89 G92 F93 P94 K99 I100 V101 R102 L107 R114 V117 W136 A139 A155 A180 M183 E189

A193 P194 E200 T229 R239 C249
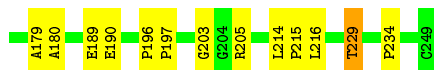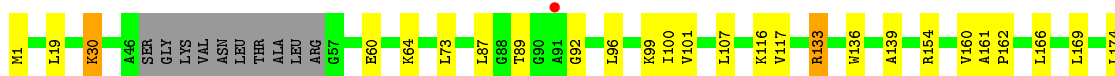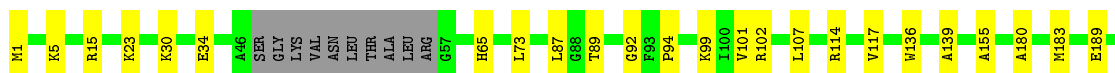
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	134.85Å 134.85Å 167.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.14 – 2.10 24.15 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.8 (24.14-2.10) 98.9 (24.15-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.69 (at 2.10Å)	Xtriage
Refinement program	PHENIX, REFMAC	Depositor
R, R_{free}	0.174 , 0.229 0.169 , 0.223	Depositor DCC
R_{free} test set	4940 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	31.4	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.3	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.477 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	12573	wwPDB-VP
Average B, all atoms (Å^2)	38.0	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 33.26 % 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 8.2292e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.35	0/1847	0.61	1/2505 (0.0%)
1	B	0.34	0/1875	0.60	1/2540 (0.0%)
1	C	0.33	0/1876	0.59	2/2545 (0.1%)
1	D	0.36	0/1881	0.63	2/2552 (0.1%)
1	E	0.32	0/1884	0.59	1/2554 (0.0%)
1	F	0.33	0/1863	0.57	1/2525 (0.0%)
All	All	0.34	0/11226	0.60	8/15221 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	144	ARG	CG-CD-NE	-7.12	96.86	111.80
1	A	1	MET	CB-CA-C	-5.89	98.62	110.40
1	F	1	MET	CB-CA-C	-5.63	99.14	110.40
1	D	1	MET	CB-CA-C	-5.51	99.37	110.40
1	B	1	MET	CB-CA-C	-5.41	99.59	110.40
1	C	2	PHE	CB-CG-CD2	-5.37	117.04	120.80
1	C	1	MET	CB-CA-C	-5.28	99.84	110.40
1	E	1	MET	CB-CA-C	-5.21	99.99	110.40

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	1821	0	1921	32	0
1	B	1849	0	1948	19	0
1	C	1850	0	1951	33	0
1	D	1855	0	1956	28	0
1	E	1858	0	1957	29	0
1	F	1837	0	1934	21	0
2	A	26	0	19	0	0
2	B	26	0	19	0	0
2	C	26	0	19	0	0
2	D	26	0	19	1	0
2	E	26	0	19	0	0
2	F	26	0	19	1	0
3	A	214	0	0	3	0
3	B	238	0	0	4	0
3	C	211	0	0	5	0
3	D	233	0	0	1	0
3	E	210	0	0	8	0
3	F	241	0	0	6	0
All	All	12573	0	11781	152	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 7.

All (152) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:LEU:HD12	1:A:248:LEU:H	1.15	1.09
1:B:99:LYS:HB2	1:B:107[B]:LEU:HD12	1.40	1.03
1:C:205:ARG:HH22	1:D:23:LYS:NZ	1.64	0.96
1:F:239:ARG:HH11	1:F:239:ARG:HG2	1.28	0.96
1:A:42:LEU:HD23	1:A:119:PHE:CE1	2.13	0.84
1:E:64:LYS:HE2	1:E:216:LEU:HB2	1.58	0.83
1:A:42:LEU:HD23	1:A:119:PHE:CZ	2.15	0.82
1:A:248:LEU:CD1	1:A:248:LEU:H	1.91	0.81
1:C:205:ARG:HH22	1:D:23:LYS:HZ1	1.29	0.77
1:C:64:LYS:HE2	1:C:216:LEU:HB2	1.66	0.77
1:E:73[A]:LEU:HD11	1:E:101:VAL:HG21	1.67	0.76
1:C:23:LYS:NZ	1:D:205:ARG:HH22	1.87	0.73
1:C:23:LYS:HZ1	1:D:205:ARG:HH22	1.37	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ARG:HG2	1:A:239:ARG:HH11	1.55	0.70
1:A:73:LEU:HD11	1:A:101:VAL:HG21	1.73	0.70
1:E:189:GLU:CD	1:E:189:GLU:H	1.96	0.70
1:C:73[A]:LEU:HD11	1:C:101:VAL:HG21	1.75	0.69
1:E:160[B]:VAL:HA	3:E:333:HOH:O	1.92	0.68
1:A:239:ARG:HG2	1:A:239:ARG:NH1	2.09	0.68
1:E:60:GLU:O	1:E:64:LYS:HG2	1.94	0.67
1:C:23:LYS:NZ	1:D:205:ARG:NH2	2.43	0.66
1:C:205:ARG:HH22	1:D:23:LYS:HZ2	1.45	0.64
1:A:248:LEU:HD12	1:A:248:LEU:N	2.00	0.64
1:E:160[B]:VAL:HB	1:E:166:LEU:HD21	1.80	0.64
1:A:168:GLU:OE1	1:A:248:LEU:HD11	1.97	0.63
1:B:99:LYS:HB2	1:B:107[B]:LEU:CD1	2.25	0.62
1:C:161[B]:ALA:HB3	1:C:166:LEU:HD12	1.81	0.62
1:B:9:GLY:N	3:B:481:HOH:O	2.19	0.61
1:F:239:ARG:NH1	1:F:239:ARG:HG2	2.06	0.61
1:A:94:PRO:HG3	1:A:183:MET:SD	2.41	0.61
1:D:13:ARG:NH2	3:D:474:HOH:O	2.30	0.61
1:A:73:LEU:HD11	1:A:101:VAL:CG2	2.31	0.60
1:E:196:PRO:HB2	1:E:197:PRO:HD3	1.82	0.60
1:F:73[A]:LEU:HD11	1:F:101[A]:VAL:HG21	1.83	0.60
1:A:42:LEU:CD2	1:A:119:PHE:CZ	2.84	0.59
1:F:89:THR:O	2:F:303:SAH:HA	2.03	0.59
1:F:200:GLU:HB2	3:F:539:HOH:O	2.03	0.57
1:B:87:LEU:HD11	1:B:139:ALA:HB2	1.87	0.57
1:A:239:ARG:HH11	1:A:239:ARG:CG	2.18	0.56
1:A:42:LEU:CD2	1:A:119:PHE:CE1	2.88	0.56
1:C:15:ARG:NH2	3:C:339:HOH:O	2.34	0.55
1:A:58:GLU:N	3:A:361:HOH:O	2.38	0.55
1:D:57:GLY:O	1:D:61:VAL:HG23	2.07	0.55
1:E:160[B]:VAL:HG22	3:E:333:HOH:O	2.07	0.55
1:C:161[B]:ALA:HB3	1:C:166:LEU:CD1	2.36	0.55
1:D:73[B]:LEU:HD23	1:D:102:ARG:NH2	2.22	0.55
1:E:73[A]:LEU:HD11	1:E:101:VAL:CG2	2.34	0.55
1:C:23:LYS:HZ1	1:D:205:ARG:NH2	2.02	0.54
1:C:73[A]:LEU:HD11	1:C:101:VAL:CG2	2.38	0.53
1:B:193:ALA:HB3	1:B:194:PRO:HD3	1.91	0.53
1:F:239:ARG:CG	1:F:239:ARG:HH11	2.10	0.53
1:D:120:VAL:HG12	1:D:134:ALA:HB2	1.91	0.52
1:E:96:LEU:O	1:E:100:ILE:HG13	2.10	0.52
1:F:73[B]:LEU:HD23	1:F:102:ARG:NH2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:LEU:HD11	1:E:180:ALA:HB2	1.92	0.52
1:B:94:PRO:HG3	1:B:183:MET:SD	2.50	0.51
1:F:65:HIS:CG	3:F:441:HOH:O	2.64	0.51
1:E:133:ARG:NH1	3:E:393:HOH:O	2.44	0.51
1:D:160[B]:VAL:HB	1:D:166:LEU:HD21	1.93	0.51
1:C:23:LYS:HZ2	1:D:205:ARG:NH2	2.10	0.50
1:E:133:ARG:NE	3:E:362:HOH:O	2.31	0.50
1:F:34:GLU:HG2	3:F:335:HOH:O	2.10	0.50
1:C:159[A]:ALA:HB3	3:C:341:HOH:O	2.12	0.50
1:E:160[B]:VAL:HG13	3:E:333:HOH:O	2.11	0.49
1:C:161[B]:ALA:O	1:C:166:LEU:HD13	2.12	0.49
1:D:6:HIS:ND1	1:D:9:GLY:N	2.61	0.49
1:B:6:HIS:C	3:B:481:HOH:O	2.51	0.48
1:E:161[A]:ALA:HA	1:E:162:PRO:HD3	1.52	0.48
1:E:19:LEU:HD12	3:E:405:HOH:O	2.12	0.48
1:C:43:LEU:HD11	1:C:93:PHE:HZ	1.78	0.48
1:F:193:ALA:HB3	1:F:194:PRO:HD3	1.95	0.48
1:C:135:LEU:HD12	1:C:136:TRP:N	2.29	0.47
1:D:115:LYS:HE3	1:D:115:LYS:HB3	1.51	0.47
1:B:117:VAL:HG21	1:B:136:TRP:HA	1.96	0.47
1:E:189:GLU:HG3	3:E:375:HOH:O	2.14	0.47
1:A:68:ASP:OD1	1:A:214:LEU:HD21	2.15	0.47
1:D:89:THR:OG1	1:D:92:GLY:HA2	2.14	0.47
1:E:87:LEU:HD11	1:E:139:ALA:HB2	1.97	0.46
1:A:228:LYS:HE2	1:A:230:ALA:O	2.15	0.46
1:C:117:VAL:HG21	1:C:136:TRP:HA	1.96	0.46
1:E:189:GLU:HG3	3:E:416:HOH:O	2.14	0.46
1:E:116:LYS:HD3	1:E:116:LYS:HA	1.68	0.46
1:A:193:ALA:HB3	1:A:194:PRO:HD3	1.98	0.46
1:D:89:THR:O	2:D:303:SAH:HA	2.15	0.46
1:F:117:VAL:HG21	1:F:136:TRP:HA	1.97	0.46
1:C:60:GLU:HG2	3:C:377:HOH:O	2.16	0.46
1:C:73[B]:LEU:HD23	1:C:102:ARG:NH2	2.31	0.46
1:F:99:LYS:HB2	1:F:107:LEU:HD22	1.98	0.46
1:C:20:GLU:HG3	3:C:468:HOH:O	2.15	0.45
1:C:64:LYS:HA	1:C:64:LYS:HD3	1.59	0.45
1:D:117:VAL:HG21	1:D:136:TRP:HA	1.97	0.45
1:E:203:GLY:O	1:E:229:THR:HG22	2.15	0.45
1:C:94:PRO:HG3	1:C:183:MET:SD	2.57	0.45
1:F:94:PRO:HG3	1:F:183:MET:SD	2.57	0.45
1:F:87:LEU:HD11	1:F:139:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161[B]:ALA:O	1:A:184:LYS:NZ	2.37	0.45
1:D:193:ALA:HB3	1:D:194:PRO:HD3	1.99	0.45
1:E:89:THR:OG1	1:E:92:GLY:HA2	2.17	0.44
1:A:174:LEU:HD11	1:A:180:ALA:HB2	1.98	0.44
1:A:160[B]:VAL:HB	1:A:166:LEU:HD21	1.99	0.44
1:B:149:ARG:HG2	1:B:150:GLU:HG3	1.99	0.44
1:D:43:LEU:HD11	1:D:93:PHE:HZ	1.82	0.44
1:A:208:GLU:OE2	1:B:74:ARG:NH2	2.38	0.44
1:B:114:ARG:NH2	3:B:399:HOH:O	2.49	0.44
1:C:64:LYS:HE2	1:C:216:LEU:HD12	1.99	0.44
1:B:73[B]:LEU:HD23	1:B:102:ARG:NH2	2.33	0.44
1:F:114:ARG:NH2	3:F:386:HOH:O	2.49	0.44
1:D:58:GLU:CD	1:D:58:GLU:H	2.20	0.44
1:D:87:LEU:HD11	1:D:139:ALA:HB2	1.98	0.44
1:D:154:ARG:HA	1:D:179:ALA:O	2.18	0.43
1:C:89:THR:OG1	1:C:92:GLY:HA2	2.17	0.43
1:A:242:VAL:N	1:A:243:PRO:CD	2.81	0.43
1:A:15:ARG:HD3	3:A:478:HOH:O	2.18	0.43
1:E:214:LEU:HA	1:E:215:PRO:HD3	1.86	0.43
1:F:239:ARG:CG	1:F:239:ARG:NH1	2.74	0.43
1:F:15:ARG:NH1	3:F:423:HOH:O	2.51	0.43
1:A:154:ARG:HA	1:A:179:ALA:O	2.19	0.43
1:B:155:ALA:O	1:B:180:ALA:HA	2.18	0.43
1:C:155:ALA:O	1:C:180:ALA:HA	2.19	0.43
1:F:30:LYS:HE3	3:F:512:HOH:O	2.19	0.43
1:B:15:ARG:HD2	3:B:484:HOH:O	2.19	0.42
1:E:99:LYS:HB2	1:E:107:LEU:HD22	2.01	0.42
1:C:205:ARG:NE	1:C:229:THR:OG1	2.35	0.42
1:A:87:LEU:HD11	1:A:139:ALA:HB2	2.00	0.42
1:B:96:LEU:HB2	1:B:97:PRO:HD3	2.02	0.42
1:E:30:LYS:HB3	1:E:30:LYS:NZ	2.34	0.42
1:D:94:PRO:HG3	1:D:183:MET:SD	2.59	0.42
1:A:248:LEU:N	1:A:248:LEU:CD1	2.69	0.42
1:E:117:VAL:HG21	1:E:136:TRP:HA	2.01	0.42
1:D:61:VAL:O	1:D:64:LYS:HB3	2.19	0.42
1:C:217:SER:HB2	1:C:219:GLU:OE2	2.19	0.42
1:A:168:GLU:OE1	1:A:248:LEU:HD21	2.20	0.42
1:F:89:THR:OG1	1:F:92:GLY:HA2	2.20	0.42
1:A:195:LEU:N	1:A:196:PRO:CD	2.83	0.41
1:E:205:ARG:HB2	1:E:205:ARG:HE	1.59	0.41
1:C:10:LEU:HG	1:C:37:SER:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:THR:OG1	1:A:92:GLY:HA2	2.21	0.41
1:C:161[A]:ALA:O	1:C:166:LEU:HD13	2.19	0.41
1:B:90:GLY:O	1:B:116:LYS:HB3	2.21	0.41
1:B:96:LEU:HD23	1:B:96:LEU:HA	1.88	0.41
1:F:5:LYS:HE3	1:F:5:LYS:HB2	1.91	0.41
1:A:155:ALA:O	1:A:180:ALA:HA	2.21	0.41
1:B:89:THR:OG1	1:B:92:GLY:HA2	2.21	0.41
1:E:154:ARG:HA	1:E:179:ALA:O	2.20	0.41
1:B:45:GLU:HG2	1:B:46:ALA:N	2.33	0.41
1:D:135:LEU:HD23	1:D:135:LEU:C	2.42	0.40
1:D:161[A]:ALA:HA	1:D:162:PRO:HD3	1.69	0.40
1:F:155:ALA:O	1:F:180:ALA:HA	2.22	0.40
1:E:190:GLU:CD	1:E:190:GLU:H	2.24	0.40
1:A:160[A]:VAL:HG22	3:A:459:HOH:O	2.20	0.40
1:C:38:ARG:NH2	3:C:372:HOH:O	2.54	0.40
1:C:205:ARG:NH2	1:D:23:LYS:NZ	2.48	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	234/249 (94%)	229 (98%)	5 (2%)	0	100	100
1	B	237/249 (95%)	233 (98%)	4 (2%)	0	100	100
1	C	238/249 (96%)	235 (99%)	3 (1%)	0	100	100
1	D	239/249 (96%)	233 (98%)	5 (2%)	1 (0%)	34	32
1	E	239/249 (96%)	234 (98%)	5 (2%)	0	100	100
1	F	236/249 (95%)	232 (98%)	4 (2%)	0	100	100
All	All	1423/1494 (95%)	1396 (98%)	26 (2%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	7	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	184/192 (96%)	182 (99%)	2 (1%)	73	79
1	B	187/192 (97%)	179 (96%)	8 (4%)	29	29
1	C	187/192 (97%)	184 (98%)	3 (2%)	62	69
1	D	187/192 (97%)	184 (98%)	3 (2%)	62	69
1	E	187/192 (97%)	182 (97%)	5 (3%)	44	48
1	F	186/192 (97%)	183 (98%)	3 (2%)	62	69
All	All	1118/1152 (97%)	1094 (98%)	24 (2%)	52	59

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	239	ARG
1	A	248	LEU
1	B	44	GLN
1	B	45	GLU
1	B	79	GLN
1	B	169	LEU
1	B	189	GLU
1	B	195	LEU
1	B	200	GLU
1	B	229	THR
1	C	169	LEU
1	C	227	GLU
1	C	229	THR
1	D	45	GLU
1	D	144	ARG
1	D	245	ARG

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Mol	Chain	Res	Type
1	E	30	LYS
1	E	133	ARG
1	E	169	LEU
1	E	229	THR
1	E	234	PRO
1	F	23	LYS
1	F	189	GLU
1	F	239	ARG

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

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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	$\#|Z| > 2$
1	HIC	B	3	1	8,11,12	1.60	2 (25%)	6,14,16	1.63	1 (16%)
1	HIC	D	3	1	8,11,12	1.55	2 (25%)	6,14,16	1.75	2 (33%)
1	HIC	E	3	1	8,11,12	1.72	2 (25%)	6,14,16	1.68	1 (16%)
1	HIC	C	3	1	8,11,12	1.56	2 (25%)	6,14,16	1.60	1 (16%)
1	HIC	A	3	1	8,11,12	1.60	2 (25%)	6,14,16	1.53	1 (16%)
1	HIC	F	3	1	8,11,12	1.60	2 (25%)	6,14,16	1.73	1 (16%)

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
1	HIC	B	3	1	-	0/5/6/8	0/1/1/1
1	HIC	D	3	1	-	0/5/6/8	0/1/1/1
1	HIC	E	3	1	-	1/5/6/8	0/1/1/1
1	HIC	C	3	1	-	0/5/6/8	0/1/1/1
1	HIC	A	3	1	-	1/5/6/8	0/1/1/1
1	HIC	F	3	1	-	0/5/6/8	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	3	HIC	CD2-NE2	-3.93	1.32	1.38
1	F	3	HIC	CD2-NE2	-3.66	1.32	1.38
1	B	3	HIC	CD2-NE2	-3.62	1.32	1.38
1	A	3	HIC	CD2-NE2	-3.58	1.32	1.38
1	C	3	HIC	CD2-NE2	-3.54	1.32	1.38
1	D	3	HIC	CD2-NE2	-3.51	1.33	1.38
1	E	3	HIC	CD2-CG	-2.46	1.32	1.36
1	F	3	HIC	CD2-CG	-2.21	1.32	1.36
1	A	3	HIC	CD2-CG	-2.20	1.32	1.36
1	B	3	HIC	CD2-CG	-2.17	1.33	1.36
1	D	3	HIC	CD2-CG	-2.11	1.33	1.36
1	C	3	HIC	CD2-CG	-2.08	1.33	1.36

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	3	HIC	CZ-NE2-CD2	-3.06	115.70	126.31
1	D	3	HIC	CZ-NE2-CD2	-2.88	116.31	126.31
1	B	3	HIC	CZ-NE2-CD2	-2.87	116.34	126.31
1	A	3	HIC	CZ-NE2-CD2	-2.67	117.04	126.31
1	E	3	HIC	CZ-NE2-CD2	-2.66	117.09	126.31
1	C	3	HIC	CZ-NE2-CD2	-2.62	117.22	126.31
1	D	3	HIC	CB-CG-CD2	-2.13	123.55	127.95

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	3	HIC	O-C-CA-CB
1	A	3	HIC	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	#$|Z| > 2$
2	SAH	C	303	-	21,28,28	1.16	2 (9%)	20,40,40	1.66	2 (10%)
2	SAH	F	303	-	21,28,28	1.17	2 (9%)	20,40,40	1.76	2 (10%)
2	SAH	E	303	-	21,28,28	1.23	2 (9%)	20,40,40	1.70	3 (15%)
2	SAH	D	303	-	21,28,28	1.20	2 (9%)	20,40,40	1.63	2 (10%)
2	SAH	B	303	-	21,28,28	1.17	2 (9%)	20,40,40	1.71	2 (10%)
2	SAH	A	303	-	21,28,28	1.19	2 (9%)	20,40,40	1.67	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.
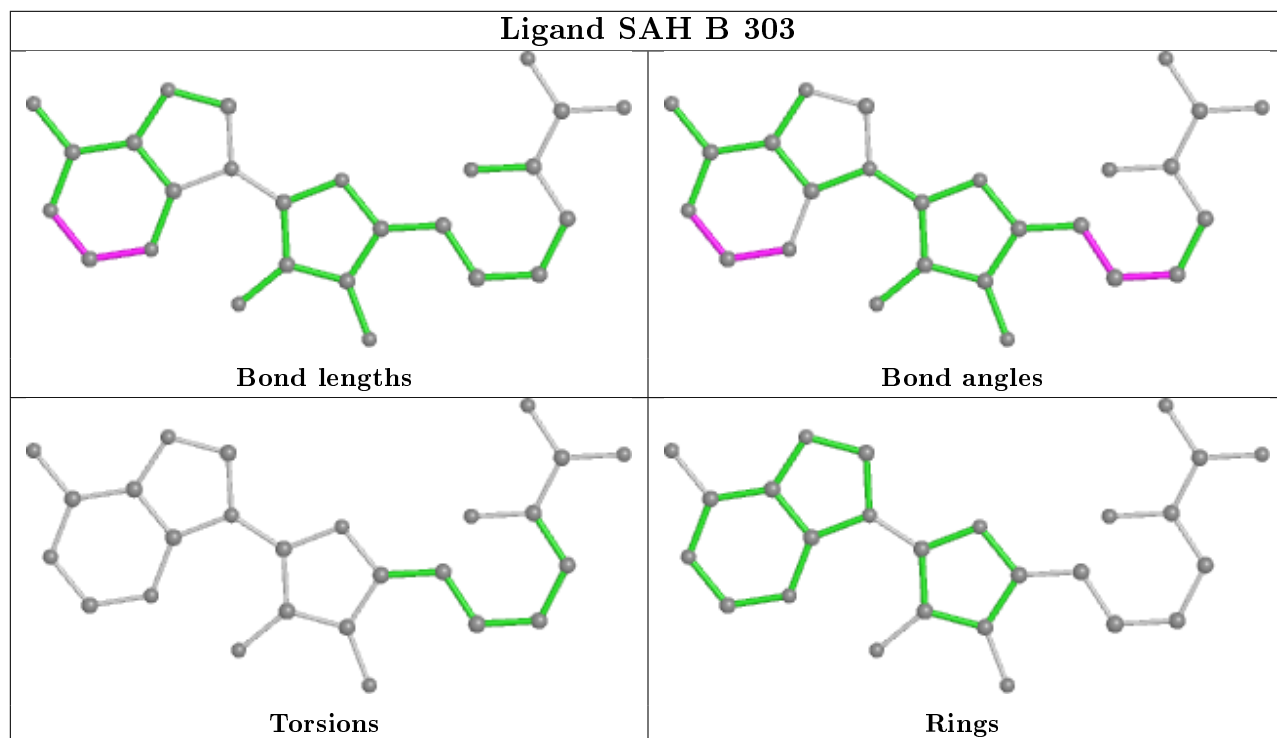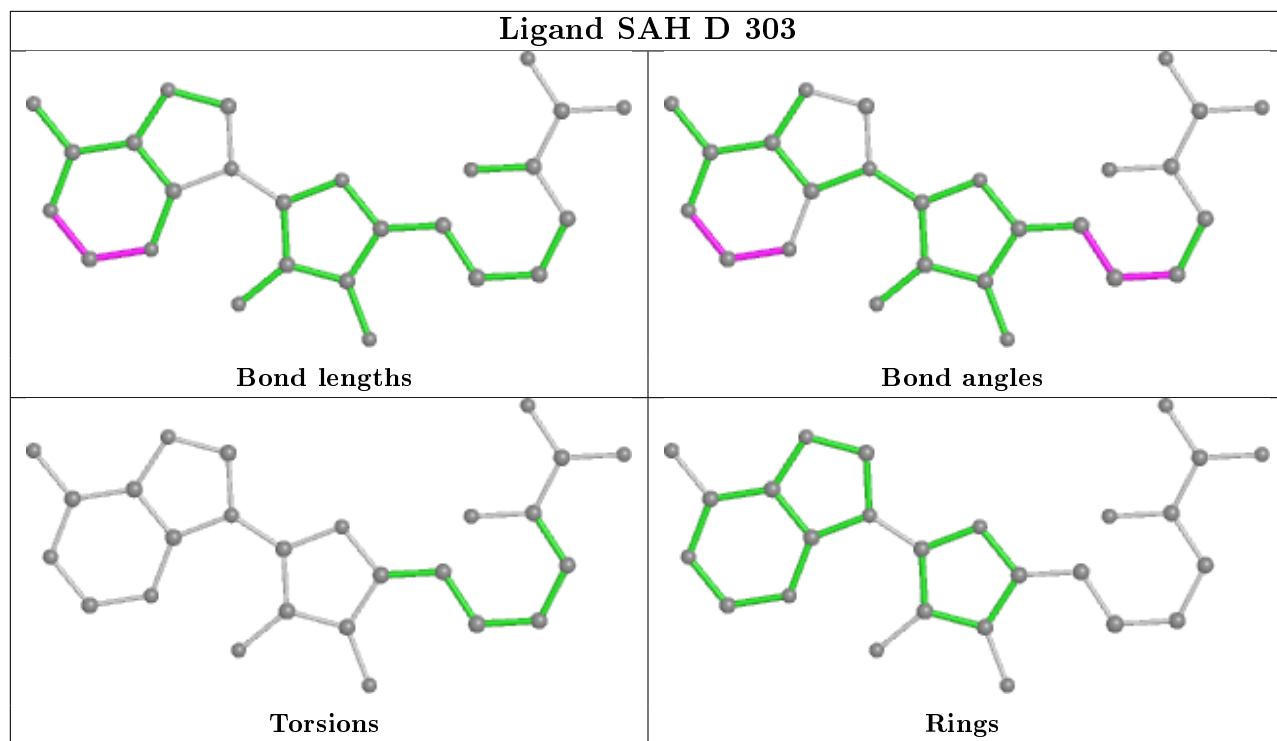
Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAH	C	303	-	-	0/7/31/31	0/3/3/3
2	SAH	F	303	-	-	0/7/31/31	0/3/3/3
2	SAH	E	303	-	-	0/7/31/31	0/3/3/3
2	SAH	D	303	-	-	0/7/31/31	0/3/3/3
2	SAH	B	303	-	-	0/7/31/31	0/3/3/3
2	SAH	A	303	-	-	0/7/31/31	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	303	SAH	C2-N3	4.22	1.38	1.32
2	D	303	SAH	C2-N3	4.08	1.38	1.32
2	A	303	SAH	C2-N3	4.05	1.38	1.32
2	C	303	SAH	C2-N3	3.94	1.38	1.32
2	F	303	SAH	C2-N3	3.92	1.38	1.32
2	B	303	SAH	C2-N3	3.92	1.38	1.32
2	E	303	SAH	C2-N1	2.50	1.38	1.33
2	B	303	SAH	C2-N1	2.49	1.38	1.33
2	D	303	SAH	C2-N1	2.48	1.38	1.33
2	A	303	SAH	C2-N1	2.45	1.38	1.33
2	F	303	SAH	C2-N1	2.43	1.38	1.33
2	C	303	SAH	C2-N1	2.42	1.38	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	303	SAH	N3-C2-N1	-5.35	120.31	128.68
2	D	303	SAH	N3-C2-N1	-5.21	120.54	128.68
2	F	303	SAH	N3-C2-N1	-5.13	120.67	128.68
2	A	303	SAH	N3-C2-N1	-5.11	120.70	128.68
2	B	303	SAH	N3-C2-N1	-5.07	120.75	128.68
2	E	303	SAH	N3-C2-N1	-4.83	121.13	128.68
2	B	303	SAH	C5'-SD-CG	-4.29	89.39	102.27
2	F	303	SAH	C5'-SD-CG	-4.19	89.70	102.27
2	D	303	SAH	C5'-SD-CG	-3.65	91.30	102.27
2	A	303	SAH	C5'-SD-CG	-3.57	91.56	102.27
2	E	303	SAH	C5'-SD-CG	-3.56	91.57	102.27
2	C	303	SAH	C5'-SD-CG	-3.52	91.72	102.27
2	E	303	SAH	C3'-C2'-C1'	2.14	104.20	100.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

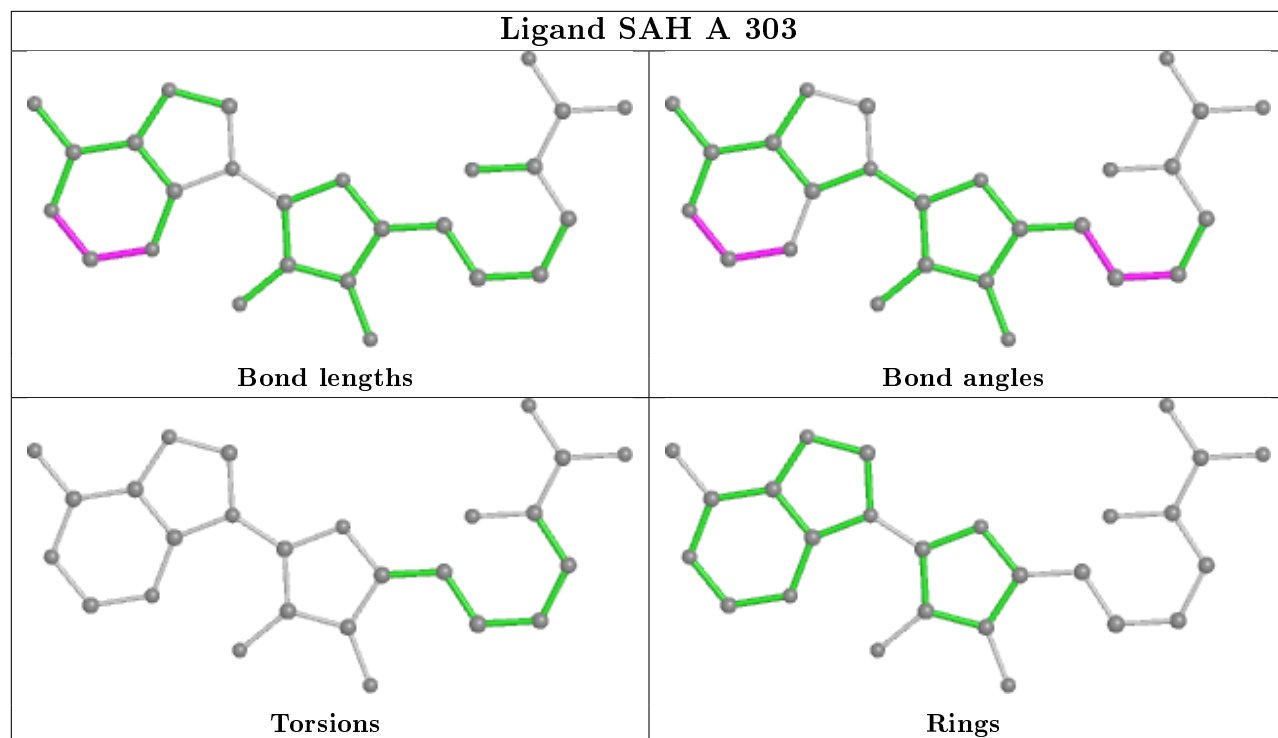| Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	303	SAH	1	0
2	D	303	SAH	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand SAH C 303

Bond lengths

Bond angles

Torsions

Rings

Ligand SAH F 303

Bond lengths

Bond angles

Torsions

Rings

Ligand SAH E 303

Bond lengths

Bond angles

Torsions

Rings

Ligand SAH D 303

Bond lengths

Bond angles

Torsions

Rings

Ligand SAH B 303

Bond lengths

Bond angles

Torsions

Rings

Ligand SAH A 303
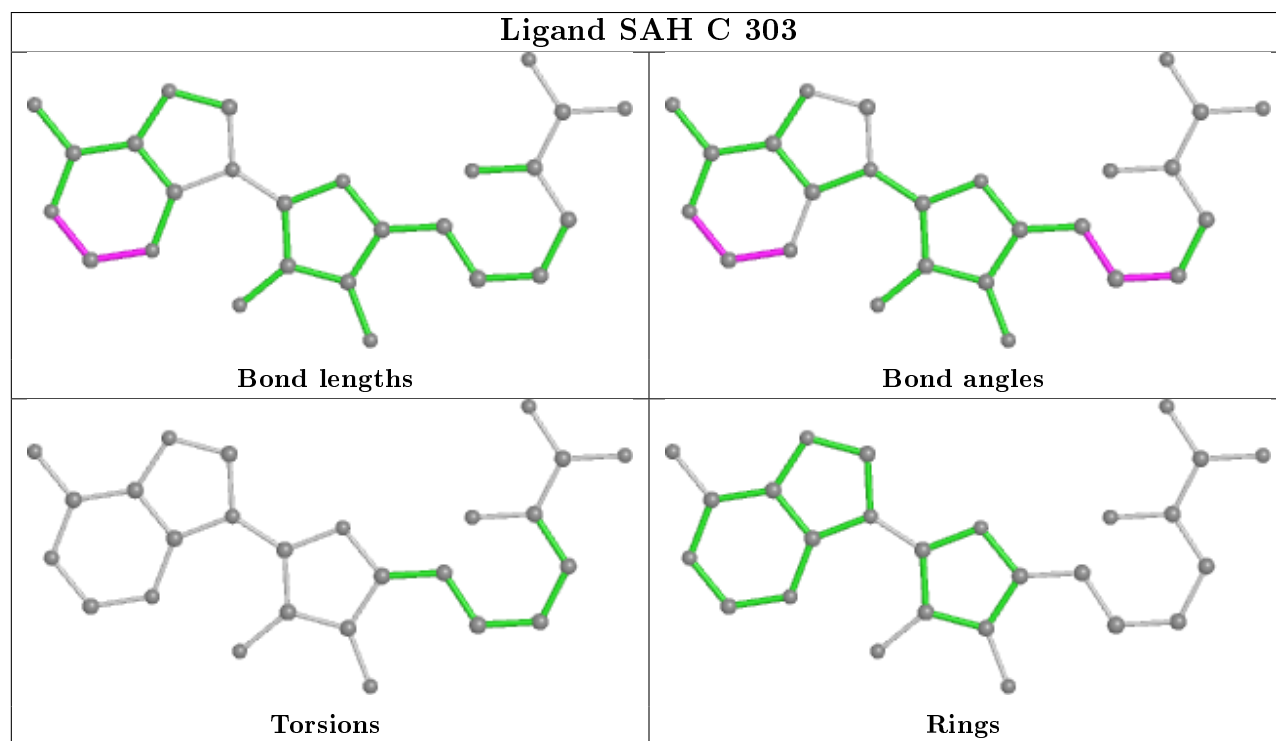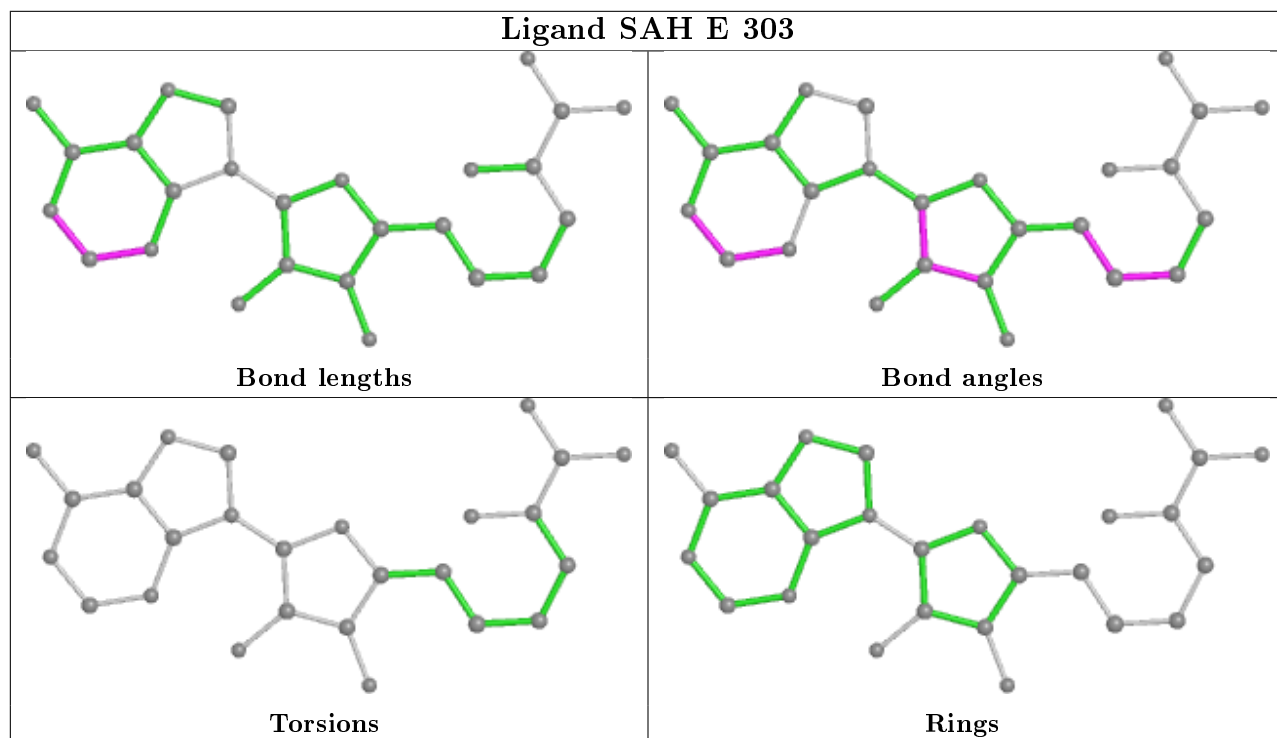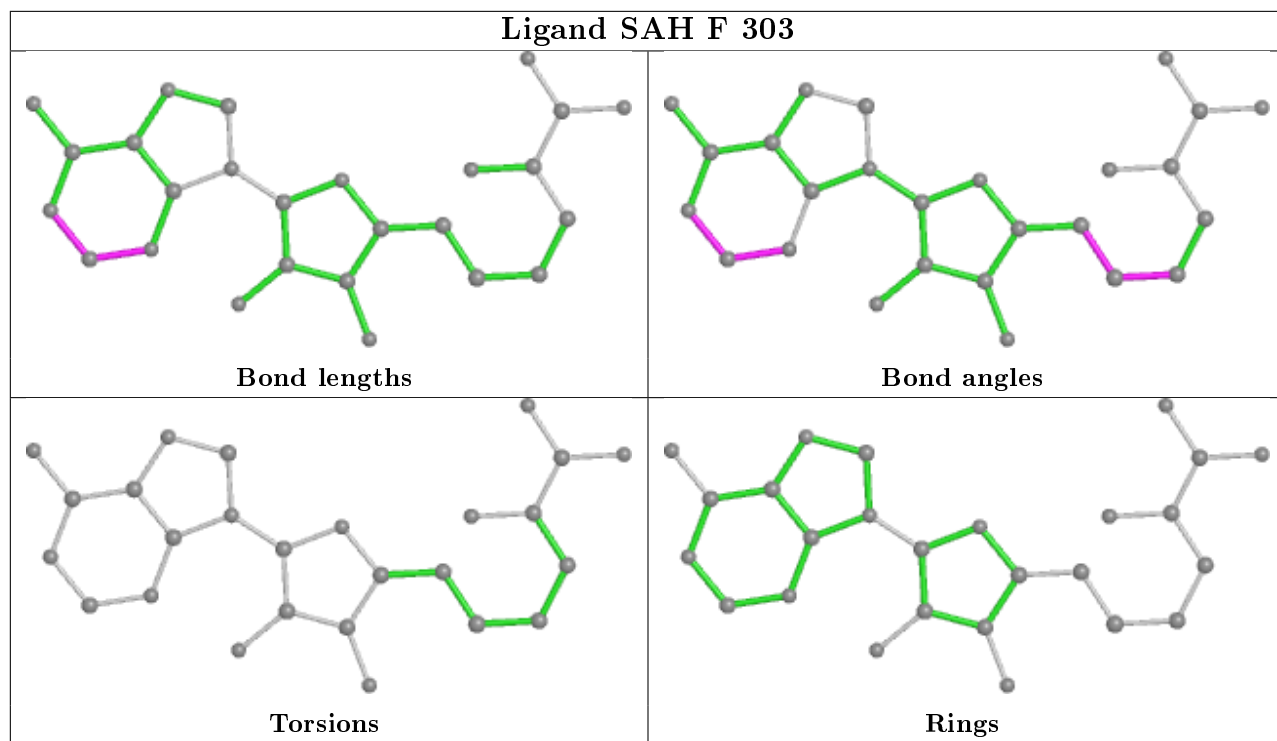
5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	235/249 (94%)	-0.78	0	100	100	21, 34, 60, 88	0
1	B	238/249 (95%)	-0.82	0	100	100	20, 33, 56, 82	0
1	C	237/249 (95%)	-0.79	0	100	100	19, 33, 58, 85	0
1	D	238/249 (95%)	-0.78	1 (0%)	92	93	21, 33, 60, 81	0
1	E	238/249 (95%)	-0.75	1 (0%)	92	93	20, 35, 65, 89	0
1	F	238/249 (95%)	-0.80	1 (0%)	92	93	20, 33, 57, 74	0
All	All	1424/1494 (95%)	-0.79	3 (0%)	95	95	19, 34, 59, 89	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	91	ALA	2.2
1	F	229	THR	2.1
1	D	159[A]	ALA	2.0

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

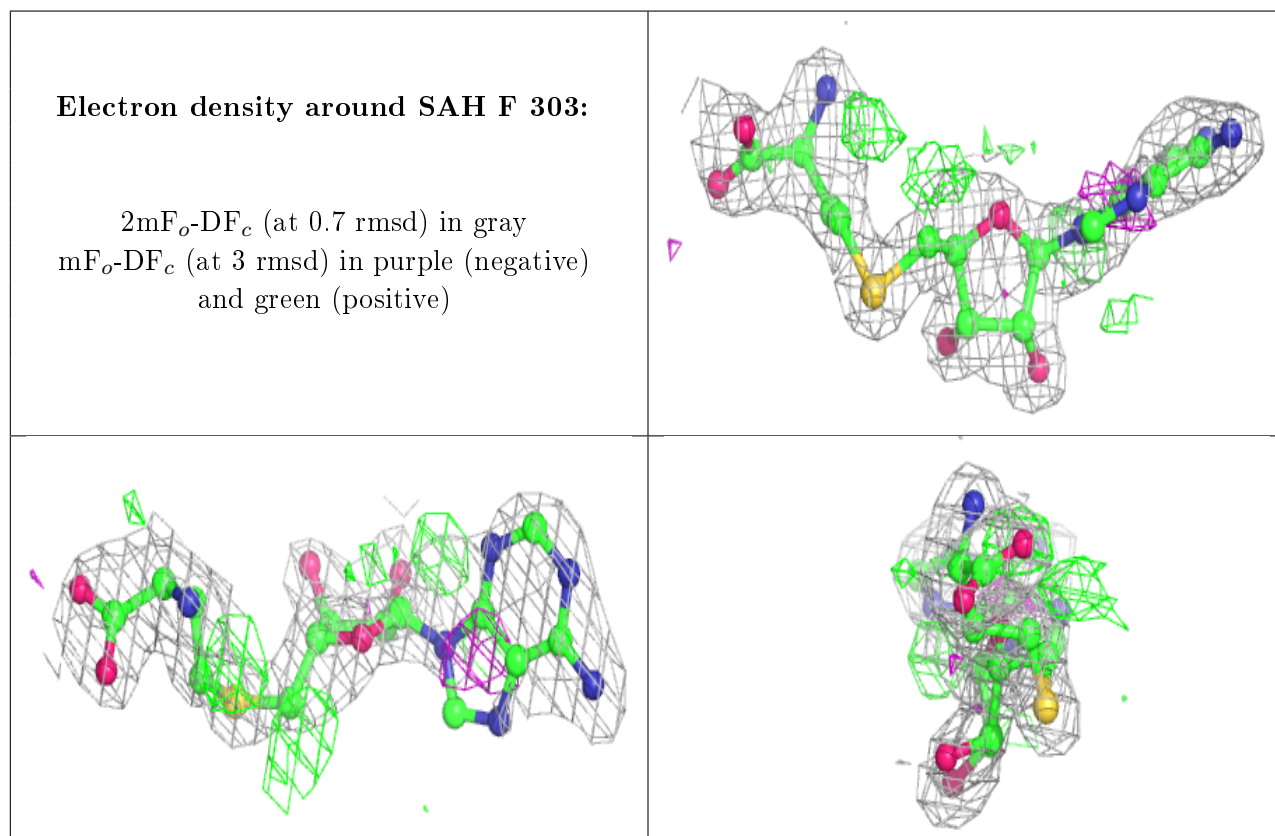| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
1	HIC	D	3	11/12	0.94	0.11	42,49,52,55	0
1	HIC	F	3	11/12	0.95	0.09	29,36,40,41	0
1	HIC	C	3	11/12	0.96	0.09	42,49,53,55	0
1	HIC	B	3	11/12	0.96	0.07	23,38,44,47	0
1	HIC	A	3	11/12	0.98	0.07	35,44,49,51	0
1	HIC	E	3	11/12	0.98	0.07	40,43,54,57	0

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(Å^2)	Q<0.9
2	SAH	F	303	26/26	0.76	0.21	38,50,70,70	26
2	SAH	B	303	26/26	0.79	0.17	37,56,70,74	26
2	SAH	E	303	26/26	0.85	0.14	39,49,56,77	26
2	SAH	A	303	26/26	0.86	0.13	33,47,58,63	26
2	SAH	D	303	26/26	0.87	0.13	33,42,54,62	26
2	SAH	C	303	26/26	0.88	0.11	32,45,51,76	26

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.
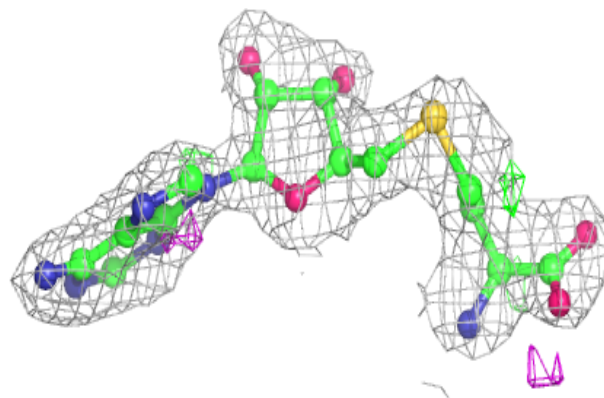
Electron density around SAH F 303:

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

Electron density around SAH B 303:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
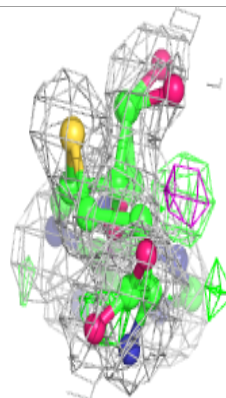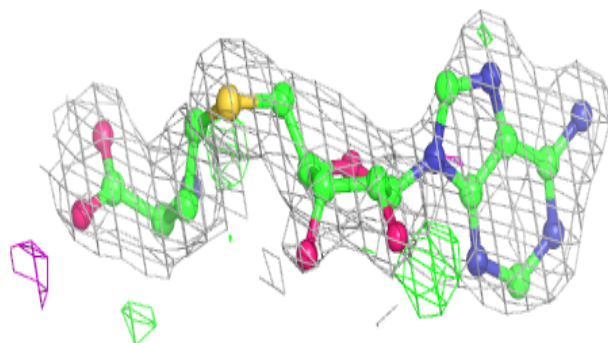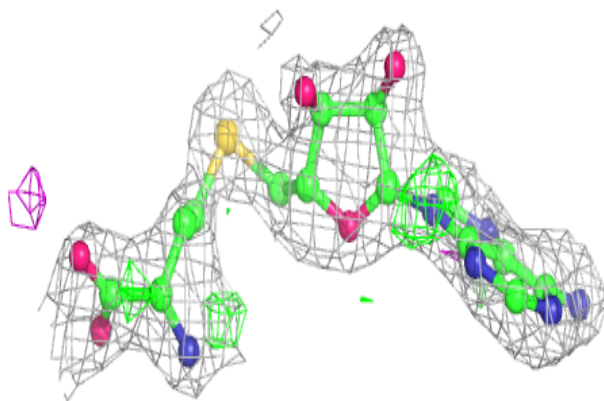
Electron density around SAH E 303:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
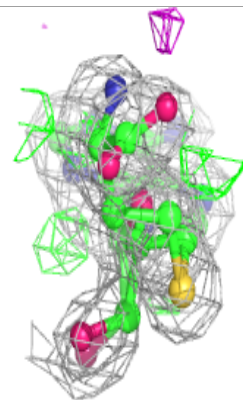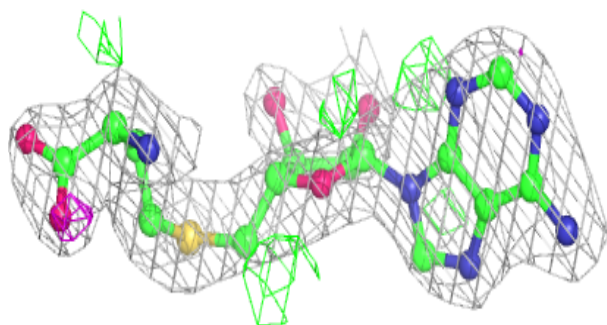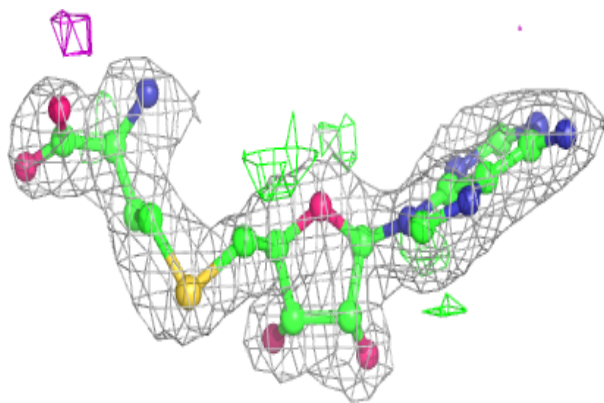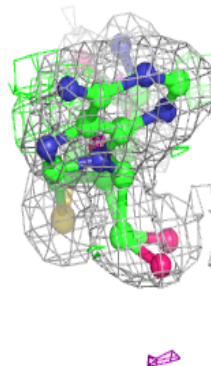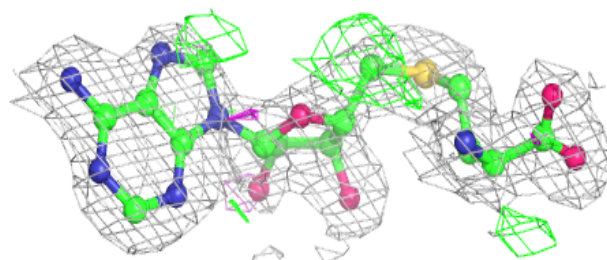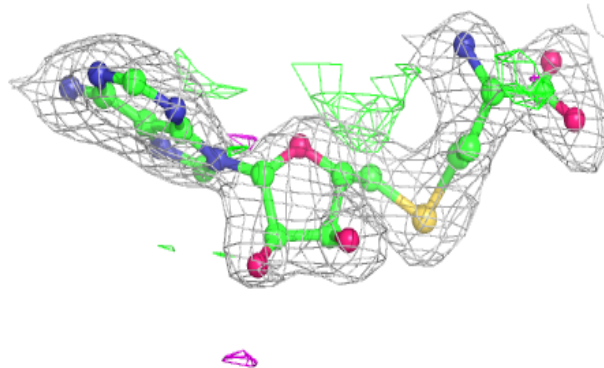$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
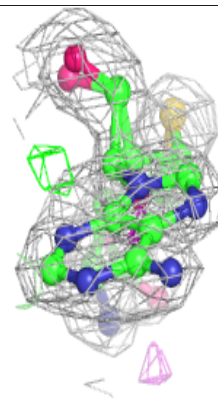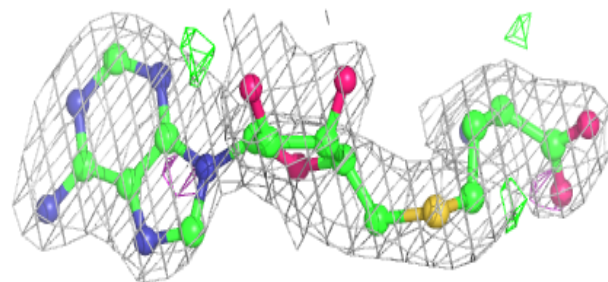
Electron density around SAH A 303:

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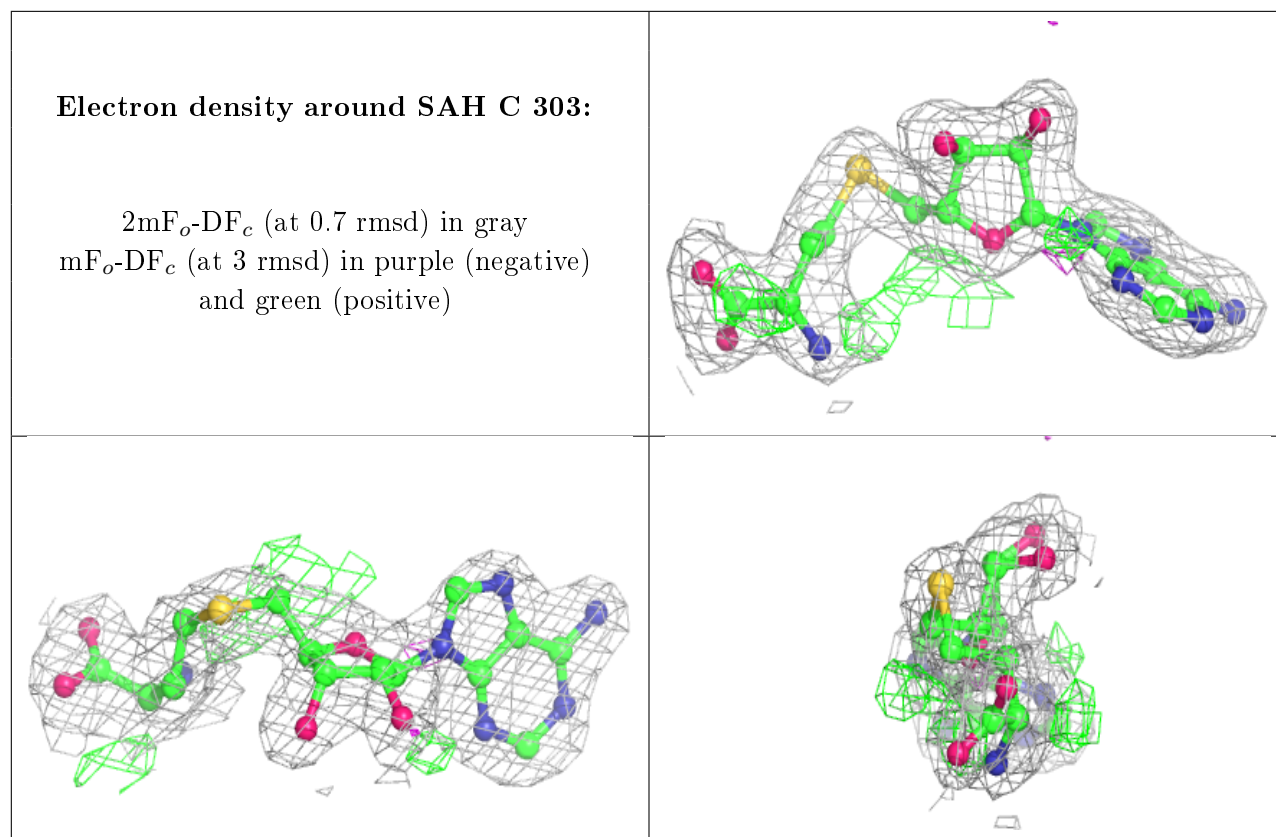mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around SAH D 303:

$2mF_o$-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 C 303:

$2mF_o$-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 ⓘ

There are no such residues in this entry.