



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:18 AM UTC

PDB ID : 5C0O / pdb_00005c0o
Title : m1A58 tRNA methyltransferase mutant - Y78A
Authors : Degut, C.; Ponchon, L.; Folly-Klan, M.; Barraud, P.; Tisne, C.
Deposited on : 2015-06-12
Resolution : 2.62 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

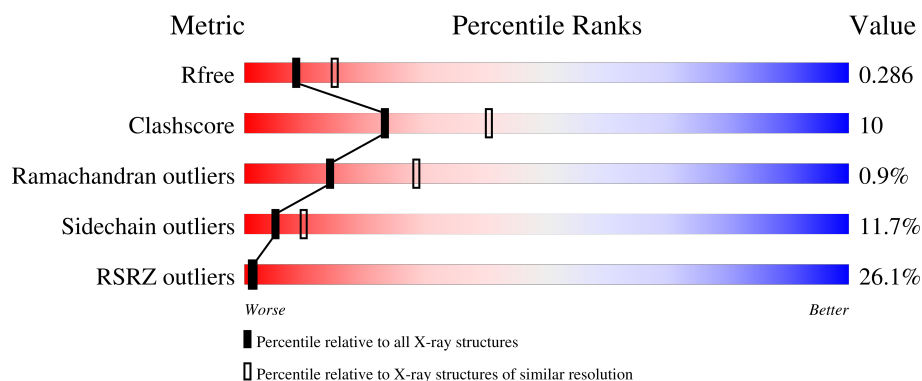
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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}	180053	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	E	255	9% 77% 16% 7%
1	F	255	40% 61% 24% 6% 9%
1	G	255	22% 69% 22% 7%
1	H	255	24% 58% 18% 7% 17%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7264 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.

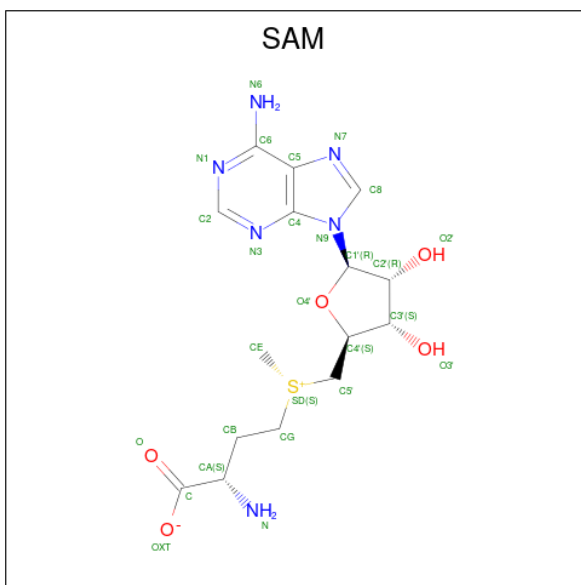
- Molecule 1 is a protein called tRNA (adenine(58)-N(1))-methyltransferase TrmI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	238	Total	C	N	O	S	0	0	0
			1823	1181	317	322	3			
1	F	232	Total	C	N	O	S	0	0	0
			1745	1134	302	306	3			
1	G	237	Total	C	N	O	S	0	0	0
			1819	1176	321	319	3			
1	H	211	Total	C	N	O	S	0	0	0
			1632	1051	293	285	3			

There are 4 discrepancies between the modelled and reference sequences:

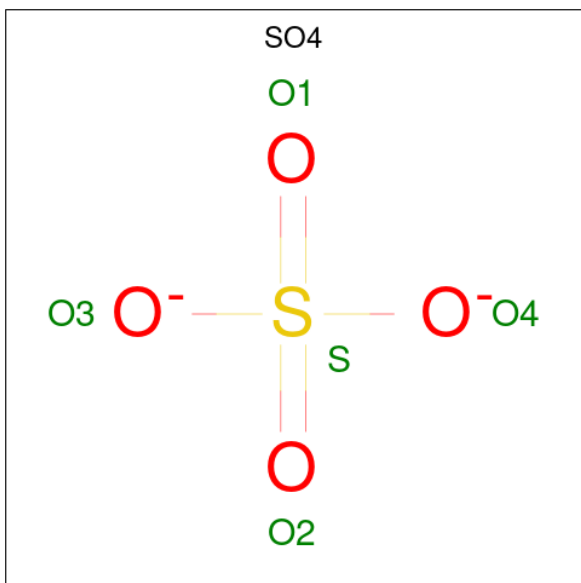
Chain	Residue	Modelled	Actual	Comment	Reference
E	78	ALA	TYR	engineered mutation	UNP Q8GBB2
F	78	ALA	TYR	engineered mutation	UNP Q8GBB2
G	78	ALA	TYR	engineered mutation	UNP Q8GBB2
H	78	ALA	TYR	engineered mutation	UNP Q8GBB2

- Molecule 2 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: C₁₅H₂₂N₆O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total 27	C 15	N 6	O 5	S 1	0	0
2	F	1	Total 27	C 15	N 6	O 5	S 1	0	0
2	G	1	Total 27	C 15	N 6	O 5	S 1	0	0
2	H	1	Total 27	C 15	N 6	O 5	S 1	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	O	S	0	0
			5	4	1		

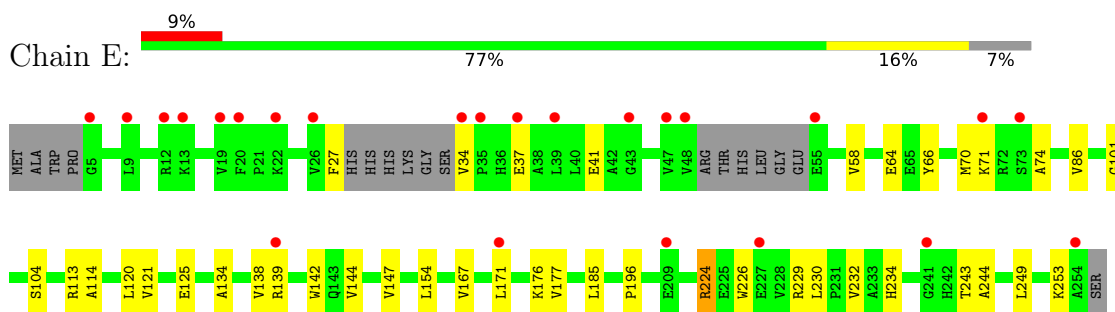
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	44	Total	O	0	0
			44	44		
4	F	27	Total	O	0	0
			27	27		
4	G	36	Total	O	0	0
			36	36		
4	H	25	Total	O	0	0
			25	25		

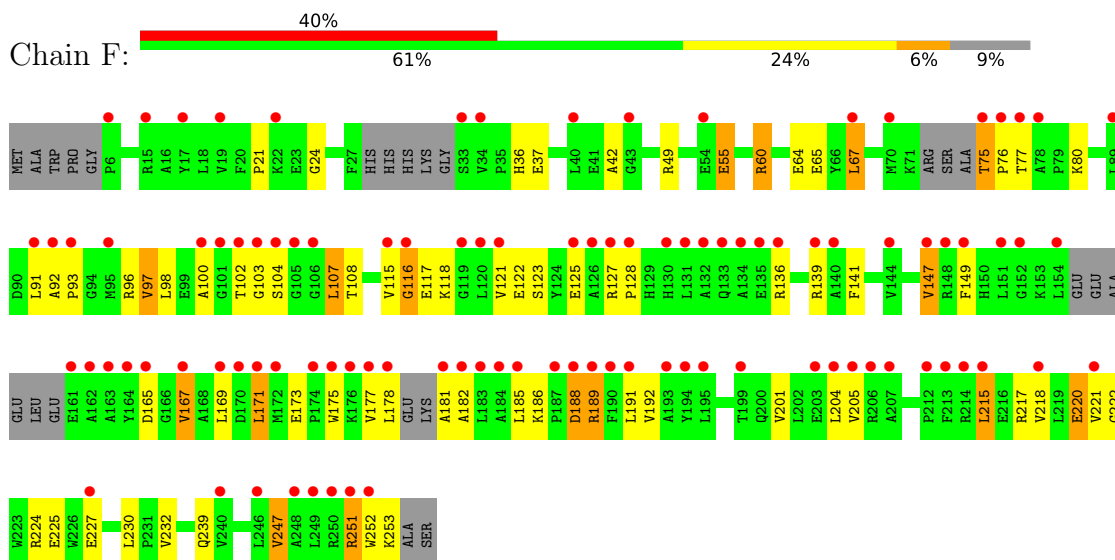
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

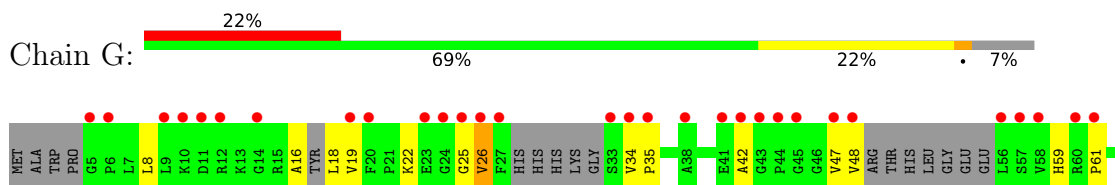
- Molecule 1: tRNA (adenine(58)-N(1))-methyltransferase TrmI

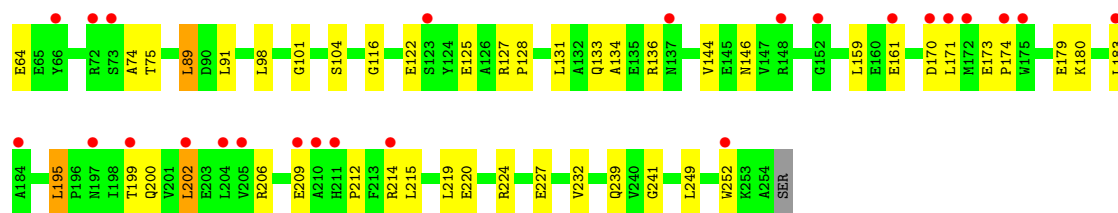


- Molecule 1: tRNA (adenine(58)-N(1))-methyltransferase TrmI

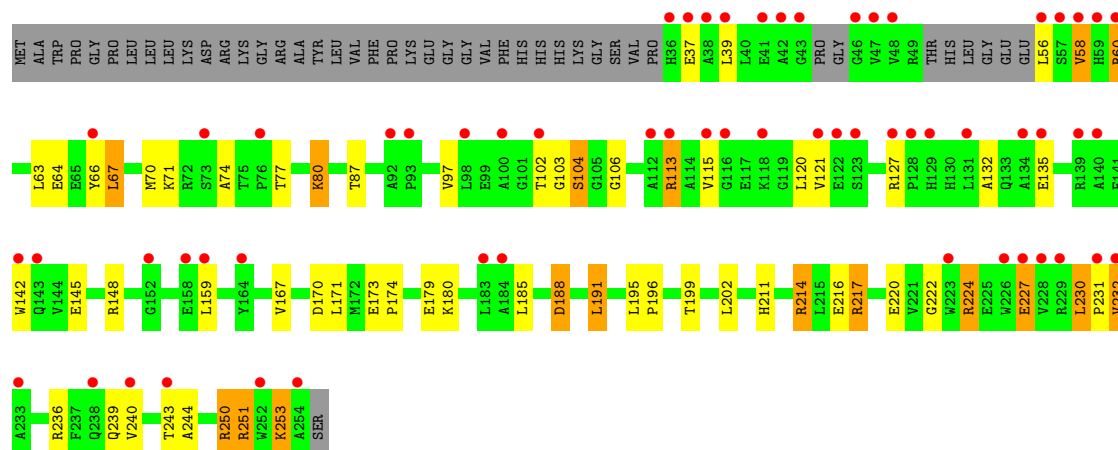


- Molecule 1: tRNA (adenine(58)-N(1))-methyltransferase TrmI





● Molecule 1: tRNA (adenine(58)-N(1))-methyltransferase TrmI



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.54Å 79.86Å 184.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.92 – 2.62 52.92 – 2.62	Depositor EDS
% Data completeness (in resolution range)	(Not available) (52.92-2.62) 99.9 (52.92-2.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.05 (at 2.48Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.235 , 0.282 0.241 , 0.286	Depositor DCC
R_{free} test set	1966 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 75.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	0.058 for k,h,-l	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	7264	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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: SAM, SO4

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	E	0.35	0/1867	0.71	1/2541 (0.0%)
1	F	0.40	0/1789	0.79	4/2442 (0.2%)
1	G	0.36	0/1862	0.73	0/2531
1	H	0.34	0/1670	0.72	0/2270
All	All	0.36	0/7188	0.74	5/9784 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	92	ALA	CA-C-N	-6.17	113.16	120.13
1	F	92	ALA	C-N-CA	-6.17	113.16	120.13
1	F	186	LYS	CA-C-N	-5.51	113.94	120.11
1	F	186	LYS	C-N-CA	-5.51	113.94	120.11
1	E	234	HIS	N-CA-C	5.41	113.08	108.22

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	E	1823	0	1808	21	0
1	F	1745	0	1687	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1819	0	1814	42	1
1	H	1632	0	1617	39	1
2	E	27	0	19	2	0
2	F	27	0	18	4	0
2	G	27	0	20	3	0
2	H	27	0	22	2	0
3	F	5	0	0	1	0
4	E	44	0	0	7	0
4	F	27	0	0	9	0
4	G	36	0	0	12	1
4	H	25	0	0	5	1
All	All	7264	0	7005	146	2

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 10.

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)
1:G:161:GLU:HG2	1:G:183:LEU:CD1	1.86	1.05
1:G:161:GLU:HG2	1:G:183:LEU:HD11	1.47	0.95
2:G:301:SAM:N	4:G:401:HOH:O	1.99	0.93
1:F:42:ALA:O	1:H:253:LYS:NZ	2.05	0.89
1:H:80:LYS:NZ	1:H:243:THR:OG1	2.06	0.89
1:G:161:GLU:CG	1:G:183:LEU:HD11	2.04	0.87
1:E:114:ALA:O	4:E:401:HOH:O	1.94	0.85
1:G:161:GLU:HG2	1:G:183:LEU:CG	2.08	0.83
1:G:25:GLY:N	4:G:404:HOH:O	2.10	0.82
1:F:218:VAL:HG22	1:F:247:VAL:HG13	1.62	0.80
1:H:148:ARG:NH1	4:H:401:HOH:O	2.05	0.79
1:G:239:GLN:O	4:G:402:HOH:O	2.03	0.76
1:H:103:GLY:HA3	2:H:301:SAM:HB1	1.66	0.76
1:G:144:VAL:O	4:G:403:HOH:O	2.05	0.75
1:F:188:ASP:OD2	1:H:60:ARG:N	2.18	0.75
1:G:18:LEU:N	4:G:405:HOH:O	2.19	0.74
1:H:87:THR:O	4:H:402:HOH:O	2.06	0.74
1:G:161:GLU:HG2	1:G:183:LEU:HG	1.68	0.73
1:G:22:LYS:O	4:G:404:HOH:O	2.05	0.72
1:F:75:THR:N	4:F:404:HOH:O	2.24	0.70
1:G:74:ALA:O	1:G:104:SER:OG	2.09	0.70
1:F:64:GLU:OE2	1:H:217:ARG:NH2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:80:LYS:NZ	1:F:221:VAL:O	2.28	0.67
1:F:93:PRO:HG2	1:H:142:TRP:HH2	1.58	0.67
1:F:116:GLY:O	1:F:118:LYS:N	2.27	0.67
1:G:161:GLU:OE2	1:G:183:LEU:HD11	1.95	0.66
1:F:181:ALA:N	4:F:405:HOH:O	2.28	0.65
1:F:182:ALA:O	4:F:401:HOH:O	2.14	0.65
1:H:66:TYR:O	1:H:70:MET:N	2.28	0.65
1:E:113:ARG:NH1	4:E:406:HOH:O	2.29	0.64
1:G:133:GLN:OE1	1:G:136:ARG:NH2	2.31	0.63
1:H:167:VAL:HG23	1:H:185:LEU:HD13	1.81	0.63
1:H:97:VAL:CG1	1:H:121:VAL:HG22	2.29	0.62
1:G:161:GLU:CD	1:G:183:LEU:HD11	2.25	0.62
1:F:222:GLY:N	1:H:222:GLY:O	2.33	0.62
1:E:74:ALA:O	1:E:104:SER:OG	2.19	0.61
1:E:253:LYS:NZ	1:G:42:ALA:O	2.28	0.61
1:F:97:VAL:HG13	1:F:121:VAL:HG22	1.84	0.59
1:F:108:THR:CG2	1:F:147:VAL:HG11	2.33	0.59
1:F:189:ARG:N	4:F:402:HOH:O	2.35	0.59
1:F:169:LEU:CD1	1:F:191:LEU:HD11	2.32	0.59
1:G:161:GLU:CG	1:G:183:LEU:CD1	2.68	0.58
1:F:251:ARG:NH2	1:F:253:LYS:O	2.37	0.57
1:E:226:TRP:NE1	1:G:220:GLU:OE1	2.33	0.57
1:G:220:GLU:OE2	1:H:224:ARG:NH2	2.37	0.57
1:G:18:LEU:N	4:G:412:HOH:O	2.37	0.57
1:F:169:LEU:HD12	1:F:191:LEU:HD11	1.87	0.56
1:G:116:GLY:O	1:G:146:ASN:ND2	2.36	0.56
1:F:167:VAL:HG23	1:F:185:LEU:HD12	1.87	0.56
1:H:37:GLU:N	4:H:405:HOH:O	2.37	0.56
1:F:115:VAL:HG21	1:F:121:VAL:HG23	1.88	0.56
1:F:169:LEU:HD23	1:F:171:LEU:HD23	1.88	0.56
1:F:165:ASP:HA	1:F:189:ARG:HG3	1.88	0.55
1:H:97:VAL:HG12	1:H:121:VAL:HG22	1.86	0.55
1:G:133:GLN:HB3	4:G:406:HOH:O	2.06	0.55
1:F:103:GLY:HA3	2:F:301:SAM:H4'	1.89	0.55
1:E:64:GLU:OE2	4:E:403:HOH:O	2.18	0.55
1:F:217:ARG:NH2	1:H:64:GLU:OE1	2.39	0.54
1:E:224:ARG:NH2	1:F:220:GLU:OE2	2.40	0.54
1:F:125:GLU:OE1	1:F:127:ARG:N	2.41	0.53
2:E:301:SAM:HA	4:E:402:HOH:O	2.08	0.53
1:F:121:VAL:HB	1:F:147:VAL:HG13	1.89	0.53
1:H:179:GLU:OE1	1:H:211:HIS:ND1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:LEU:HD23	1:E:177:VAL:HG21	1.92	0.52
1:G:215:LEU:HA	1:G:249:LEU:HD23	1.91	0.52
1:G:101:GLY:O	4:G:401:HOH:O	2.18	0.52
1:E:134:ALA:O	1:E:138:VAL:HG23	2.10	0.52
1:E:101:GLY:O	4:E:402:HOH:O	2.17	0.51
1:F:230:LEU:HD21	1:H:202:LEU:HD22	1.92	0.51
1:F:103:GLY:CA	2:F:301:SAM:H4'	2.40	0.51
1:F:227:GLU:HA	3:F:302:SO4:O4	2.12	0.50
1:H:102:THR:O	2:H:301:SAM:HA	2.12	0.49
1:G:64:GLU:N	4:G:411:HOH:O	2.36	0.49
1:H:74:ALA:O	1:H:104:SER:OG	2.31	0.48
1:F:218:VAL:HG22	1:F:247:VAL:CG1	2.39	0.48
1:G:134:ALA:N	4:G:406:HOH:O	2.45	0.48
1:H:191:LEU:C	1:H:191:LEU:HD23	2.39	0.48
1:F:102:THR:HG1	1:F:123:SER:HG	1.54	0.47
1:E:71:LYS:NZ	4:E:409:HOH:O	2.47	0.47
1:G:241:GLY:HA3	1:H:239:GLN:HG3	1.96	0.47
1:H:77:THR:OG1	1:H:170:ASP:OD2	2.32	0.47
2:F:301:SAM:HE1	4:F:404:HOH:O	2.15	0.47
1:G:8:LEU:HB2	1:G:61:PRO:HG3	1.97	0.47
1:H:188:ASP:HA	1:H:250:ARG:HD3	1.97	0.46
1:F:189:ARG:O	4:F:402:HOH:O	2.20	0.46
1:H:67:LEU:HD11	1:H:106:GLY:CA	2.46	0.46
1:G:173:GLU:N	1:G:174:PRO:HD3	2.32	0.45
1:G:212:PRO:HA	1:G:252:TRP:CE3	2.52	0.45
1:F:60:ARG:N	1:H:188:ASP:OD2	2.43	0.45
1:F:188:ASP:C	1:F:189:ARG:HD2	2.42	0.45
1:F:102:THR:H	1:F:125:GLU:CG	2.30	0.45
1:H:39:LEU:HD22	1:H:58:VAL:HG21	1.98	0.45
1:H:132:ALA:O	1:H:135:GLU:N	2.50	0.45
1:F:185:LEU:HD22	1:F:251:ARG:HG3	1.98	0.44
1:F:201:VAL:O	1:F:204:LEU:N	2.50	0.44
1:F:100:ALA:O	1:F:171:LEU:HD22	2.16	0.44
1:F:139:ARG:NE	4:F:408:HOH:O	2.49	0.44
1:E:27:PHE:O	1:E:34:VAL:N	2.50	0.44
1:F:21:PRO:HB3	1:F:36:HIS:HB3	2.00	0.44
1:G:214:ARG:HG2	1:G:252:TRP:CD1	2.52	0.44
1:G:125:GLU:HB3	1:G:131:LEU:HD13	2.00	0.44
1:G:224:ARG:NH2	4:H:408:HOH:O	2.51	0.43
1:E:125:GLU:OE1	2:E:301:SAM:H1'	2.18	0.43
1:E:167:VAL:HG23	1:E:185:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:107:LEU:HB3	2:F:301:SAM:HN1	1.82	0.43
1:F:191:LEU:HD12	1:F:192:VAL:N	2.33	0.43
1:H:230:LEU:HA	1:H:232:VAL:N	2.33	0.43
1:F:67:LEU:CD2	1:F:76:PRO:HB3	2.47	0.43
1:H:214:ARG:NE	4:H:406:HOH:O	2.47	0.43
1:E:120:LEU:HG	1:E:121:VAL:N	2.34	0.43
1:F:173:GLU:HG3	1:F:175:TRP:CZ2	2.54	0.42
1:H:115:VAL:HG21	1:H:121:VAL:HG23	2.01	0.42
1:H:171:LEU:HD12	1:H:173:GLU:H	1.85	0.42
1:E:196:PRO:HA	1:E:244:ALA:HA	2.00	0.42
1:F:49:ARG:HD2	1:F:55:GLU:HA	2.02	0.42
1:F:75:THR:N	4:F:409:HOH:O	2.52	0.42
1:F:224:ARG:HB3	1:H:220:GLU:HB2	2.01	0.42
1:F:108:THR:HG23	1:F:147:VAL:HG11	2.00	0.42
1:H:185:LEU:HD23	1:H:251:ARG:HB2	2.02	0.42
1:F:91:LEU:HB3	4:F:406:HOH:O	2.18	0.42
1:F:98:LEU:HB3	1:F:167:VAL:HG13	2.02	0.42
1:E:142:TRP:CE2	1:E:144:VAL:HB	2.55	0.42
1:E:66:TYR:O	1:E:70:MET:N	2.49	0.42
1:H:216:GLU:C	1:H:217:ARG:HG2	2.44	0.41
1:E:139:ARG:NE	4:E:411:HOH:O	2.50	0.41
1:G:26:VAL:HG13	1:G:35:PRO:HA	2.02	0.41
1:G:202:LEU:O	1:G:206:ARG:N	2.51	0.41
1:G:173:GLU:N	1:G:174:PRO:CD	2.83	0.41
1:G:26:VAL:HA	1:G:35:PRO:HA	2.03	0.41
1:H:63:LEU:HD22	1:H:113:ARG:HD3	2.02	0.41
1:G:174:PRO:HG2	1:G:195:LEU:HD21	2.03	0.41
1:E:121:VAL:HB	1:E:147:VAL:HG22	2.03	0.41
1:F:147:VAL:HB	1:F:149:PHE:CE1	2.56	0.41
1:G:89:LEU:HB3	1:G:91:LEU:HG	2.03	0.41
1:H:196:PRO:HA	1:H:244:ALA:HA	2.03	0.41
1:H:227:GLU:HG2	1:H:236:ARG:HG2	2.01	0.41
1:G:170:ASP:OD2	2:G:301:SAM:N	2.54	0.40
1:F:201:VAL:O	1:F:205:VAL:HG23	2.21	0.40
1:F:252:TRP:O	1:F:253:LYS:CB	2.69	0.40
1:G:16:ALA:O	4:G:405:HOH:O	2.22	0.40
1:G:170:ASP:HB3	2:G:301:SAM:HN2	1.85	0.40
1:F:205:VAL:HG13	1:F:215:LEU:CD1	2.52	0.40
1:H:174:PRO:HG2	1:H:195:LEU:HD21	2.04	0.40
1:E:229:ARG:O	1:E:230:LEU:C	2.65	0.40
1:F:24:GLY:N	1:F:37:GLU:OE2	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:127:ARG:HA	1:G:128:PRO:HD3	1.96	0.40

All (2) 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)
4:G:415:HOH:O	4:H:420:HOH:O[4_555]	2.07	0.13
1:G:180:LYS:NZ	1:H:179:GLU:OE2[1_565]	2.15	0.05

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	E	232/255 (91%)	218 (94%)	14 (6%)	0	100	100
1	F	222/255 (87%)	199 (90%)	16 (7%)	7 (3%)	3	4
1	G	229/255 (90%)	223 (97%)	6 (3%)	0	100	100
1	H	205/255 (80%)	195 (95%)	9 (4%)	1 (0%)	24	44
All	All	888/1020 (87%)	835 (94%)	45 (5%)	8 (1%)	14	28

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	117	GLU
1	F	128	PRO
1	F	116	GLY
1	F	141	PHE
1	F	188	ASP
1	F	177	VAL
1	F	55	GLU
1	H	231	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	179/204 (88%)	169 (94%)	10 (6%)	19	39
1	F	167/204 (82%)	144 (86%)	23 (14%)	3	6
1	G	180/204 (88%)	159 (88%)	21 (12%)	5	10
1	H	159/204 (78%)	133 (84%)	26 (16%)	2	3
All	All	685/816 (84%)	605 (88%)	80 (12%)	5	10

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	37	GLU
1	E	41	GLU
1	E	58	VAL
1	E	86	VAL
1	E	171	LEU
1	E	176	LYS
1	E	224	ARG
1	E	232	VAL
1	E	243	THR
1	E	249	LEU
1	F	60	ARG
1	F	65	GLU
1	F	67	LEU
1	F	75	THR
1	F	77	THR
1	F	96	ARG
1	F	97	VAL
1	F	104	SER
1	F	107	LEU
1	F	122	GLU
1	F	136	ARG
1	F	147	VAL
1	F	167	VAL
1	F	171	LEU

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Mol	Chain	Res	Type
1	F	178	LEU
1	F	189	ARG
1	F	215	LEU
1	F	220	GLU
1	F	225	GLU
1	F	232	VAL
1	F	239	GLN
1	F	247	VAL
1	F	251	ARG
1	G	19	VAL
1	G	26	VAL
1	G	34	VAL
1	G	47	VAL
1	G	48	VAL
1	G	59	HIS
1	G	75	THR
1	G	89	LEU
1	G	98	LEU
1	G	122	GLU
1	G	159	LEU
1	G	171	LEU
1	G	179	GLU
1	G	195	LEU
1	G	199	THR
1	G	200	GLN
1	G	202	LEU
1	G	209	GLU
1	G	219	LEU
1	G	227	GLU
1	G	232	VAL
1	H	56	LEU
1	H	58	VAL
1	H	60	ARG
1	H	67	LEU
1	H	71	LYS
1	H	80	LYS
1	H	104	SER
1	H	113	ARG
1	H	120	LEU
1	H	127	ARG
1	H	145	GLU
1	H	159	LEU

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Mol	Chain	Res	Type
1	H	180	LYS
1	H	188	ASP
1	H	191	LEU
1	H	199	THR
1	H	214	ARG
1	H	217	ARG
1	H	224	ARG
1	H	227	GLU
1	H	230	LEU
1	H	232	VAL
1	H	240	VAL
1	H	250	ARG
1	H	251	ARG
1	H	253	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	130	HIS
1	E	211	HIS
1	F	130	HIS
1	G	36	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	SAM	G	301	-	27,29,29	1.11	4 (14%)	34,42,42	2.03	9 (26%)
3	SO4	F	302	-	4,4,4	1.04	0	6,6,6	1.39	1 (16%)
2	SAM	F	301	-	27,29,29	1.08	3 (11%)	34,42,42	1.92	8 (23%)
2	SAM	H	301	-	27,29,29	1.09	4 (14%)	34,42,42	1.97	9 (26%)
2	SAM	E	301	-	27,29,29	1.11	4 (14%)	34,42,42	1.96	8 (23%)

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	SAM	G	301	-	-	3/17/33/33	0/3/3/3
2	SAM	F	301	-	-	7/17/33/33	0/3/3/3
2	SAM	H	301	-	-	8/17/33/33	0/3/3/3
2	SAM	E	301	-	-	6/17/33/33	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	SAM	C2-N1	2.65	1.38	1.33
2	G	301	SAM	C2-N3	2.62	1.38	1.33
2	F	301	SAM	C2-N3	2.62	1.38	1.33
2	E	301	SAM	C2-N1	2.55	1.38	1.33
2	G	301	SAM	C2-N1	2.53	1.38	1.33
2	E	301	SAM	C2-N3	2.52	1.38	1.33
2	H	301	SAM	C2-N1	2.42	1.38	1.33
2	H	301	SAM	C2-N3	2.40	1.38	1.33
2	E	301	SAM	OXT-C	-2.22	1.23	1.30
2	G	301	SAM	OXT-C	-2.21	1.23	1.30
2	H	301	SAM	C8-N7	2.19	1.35	1.31
2	H	301	SAM	OXT-C	-2.19	1.23	1.30
2	G	301	SAM	C8-N7	2.13	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	SAM	C8-N7	2.12	1.35	1.31
2	F	301	SAM	C8-N7	2.10	1.35	1.31

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	301	SAM	N3-C2-N1	-5.94	119.59	128.58
2	E	301	SAM	N3-C2-N1	-5.64	120.04	128.58
2	G	301	SAM	N3-C2-N1	-5.56	120.16	128.58
2	F	301	SAM	N3-C2-N1	-5.50	120.26	128.58
2	G	301	SAM	C5-C4-N3	-4.81	120.09	126.72
2	F	301	SAM	C5-C4-N3	-4.49	120.54	126.72
2	E	301	SAM	C5-C4-N3	-4.37	120.69	126.72
2	H	301	SAM	N9-C8-N7	-4.09	108.13	113.94
2	H	301	SAM	C5-C4-N3	-4.03	121.16	126.72
2	E	301	SAM	N9-C8-N7	-3.91	108.39	113.94
2	G	301	SAM	N9-C8-N7	-3.73	108.64	113.94
2	G	301	SAM	C2-N3-C4	3.55	120.49	111.83
2	F	301	SAM	N9-C8-N7	-3.53	108.92	113.94
2	H	301	SAM	C2-N3-C4	3.42	120.19	111.83
2	E	301	SAM	C2-N3-C4	3.41	120.17	111.83
2	F	301	SAM	C2-N3-C4	3.38	120.09	111.83
2	H	301	SAM	C5-N7-C8	3.36	108.72	103.45
2	G	301	SAM	C5-N7-C8	3.33	108.69	103.45
2	E	301	SAM	C5-N7-C8	3.32	108.67	103.45
2	G	301	SAM	N3-C4-N9	3.17	132.56	127.17
2	F	301	SAM	N3-C4-N9	3.15	132.52	127.17
3	F	302	SO4	O4-S-O3	3.06	125.39	108.54
2	F	301	SAM	C5-N7-C8	2.99	108.16	103.45
2	E	301	SAM	N3-C4-N9	2.91	132.12	127.17
2	G	301	SAM	OXT-C-O	-2.77	117.79	124.08
2	E	301	SAM	OXT-C-O	-2.70	117.96	124.08
2	H	301	SAM	OXT-C-O	-2.66	118.04	124.08
2	H	301	SAM	N3-C4-N9	2.55	131.51	127.17
2	G	301	SAM	C3'-C2'-C1'	2.51	106.21	101.46
2	F	301	SAM	OXT-C-O	-2.37	118.70	124.08
2	H	301	SAM	C4-C5-N7	-2.37	107.87	110.58
2	G	301	SAM	C4-C5-N7	-2.31	107.94	110.58
2	E	301	SAM	C4-C5-N7	-2.25	108.00	110.58
2	H	301	SAM	C4-N9-C8	2.11	107.95	105.74
2	F	301	SAM	C4-C5-N7	-2.01	108.28	110.58

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	301	SAM	N-CA-CB-CG
2	E	301	SAM	C-CA-CB-CG
2	E	301	SAM	O4'-C4'-C5'-SD
2	E	301	SAM	C3'-C4'-C5'-SD
2	F	301	SAM	O-C-CA-N
2	F	301	SAM	C4'-C5'-SD-CE
2	F	301	SAM	O4'-C4'-C5'-SD
2	F	301	SAM	C3'-C4'-C5'-SD
2	G	301	SAM	CA-CB-CG-SD
2	G	301	SAM	O4'-C4'-C5'-SD
2	G	301	SAM	C3'-C4'-C5'-SD
2	H	301	SAM	N-CA-CB-CG
2	H	301	SAM	CB-CG-SD-CE
2	H	301	SAM	CB-CG-SD-C5'
2	H	301	SAM	C4'-C5'-SD-CE
2	F	301	SAM	OXT-C-CA-N
2	H	301	SAM	C2'-C1'-N9-C8
2	E	301	SAM	O-C-CA-CB
2	E	301	SAM	OXT-C-CA-CB
2	H	301	SAM	C-CA-CB-CG
2	F	301	SAM	O-C-CA-CB
2	F	301	SAM	OXT-C-CA-CB
2	H	301	SAM	O4'-C1'-N9-C8
2	H	301	SAM	CA-CB-CG-SD

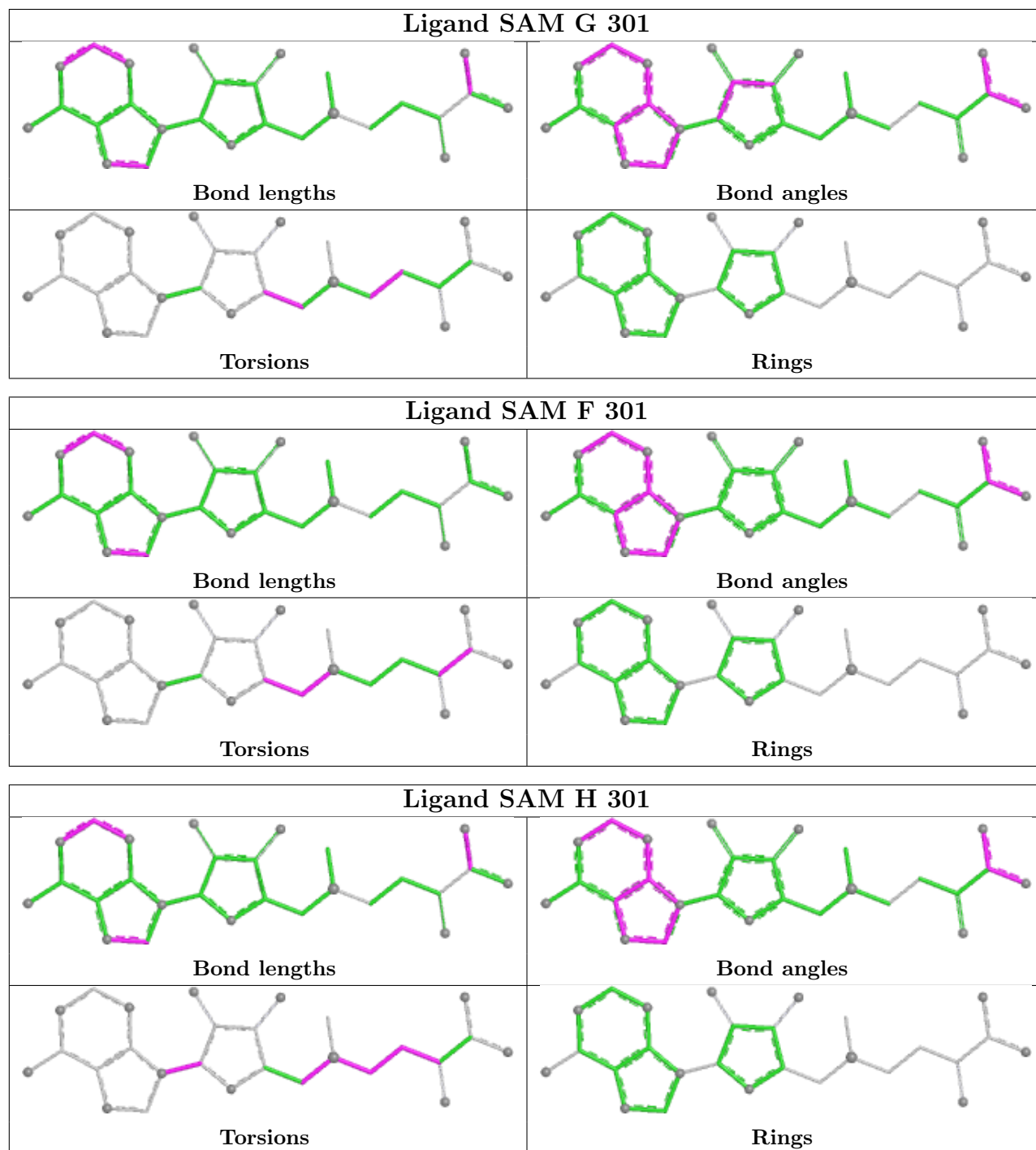
There are no ring outliers.

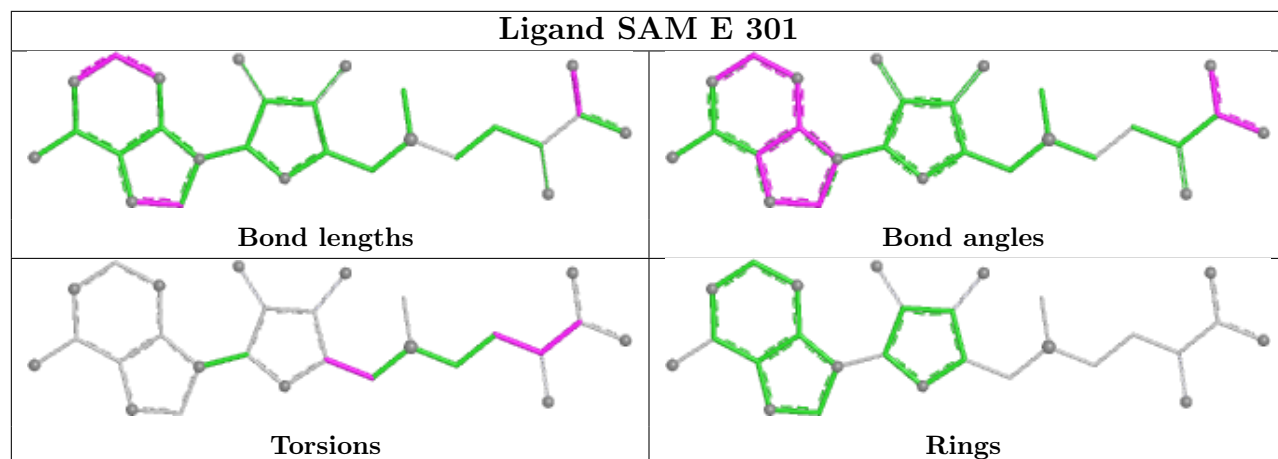
5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	301	SAM	3	0
3	F	302	SO4	1	0
2	F	301	SAM	4	0
2	H	301	SAM	2	0
2	E	301	SAM	2	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	E	238/255 (93%)	0.85	24 (10%)	12 9	12, 29, 58, 82	0
1	F	232/255 (90%)	2.04	101 (43%)	0 0	18, 50, 71, 94	0
1	G	237/255 (92%)	1.29	55 (23%)	2 1	15, 37, 67, 88	0
1	H	211/255 (82%)	1.55	60 (28%)	1 1	21, 40, 65, 80	0
All	All	918/1020 (90%)	1.42	240 (26%)	1 1	12, 40, 67, 94	0

All (240) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	250	ARG	7.6
1	F	188	ASP	7.2
1	G	34	VAL	7.0
1	F	187	PRO	5.8
1	F	147	VAL	5.5
1	F	175	TRP	5.3
1	G	35	PRO	5.0
1	F	163	ALA	4.8
1	G	56	LEU	4.8
1	F	101	GLY	4.8
1	F	15	ARG	4.6
1	E	26	VAL	4.6
1	F	149	PHE	4.6
1	F	183	LEU	4.5
1	G	5	GLY	4.5
1	F	34	VAL	4.5
1	F	126	ALA	4.4
1	F	212	PRO	4.4
1	E	34	VAL	4.4
1	G	161	GLU	4.3
1	F	172	MET	4.3

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Mol	Chain	Res	Type	RSRZ
1	F	116	GLY	4.3
1	H	59	HIS	4.3
1	F	92	ALA	4.3
1	F	75	THR	4.3
1	F	103	GLY	4.3
1	F	184	ALA	4.1
1	G	210	ALA	4.1
1	F	182	ALA	4.1
1	F	152	GLY	4.0
1	F	77	THR	4.0
1	F	40	LEU	4.0
1	F	164	TYR	4.0
1	F	115	VAL	4.0
1	F	135	GLU	4.0
1	H	93	PRO	3.9
1	E	71	LYS	3.9
1	H	58	VAL	3.9
1	H	232	VAL	3.8
1	H	46	GLY	3.8
1	F	76	PRO	3.8
1	F	205	VAL	3.8
1	F	171	LEU	3.7
1	F	78	ALA	3.7
1	H	228	VAL	3.7
1	F	169	LEU	3.7
1	F	252	TRP	3.7
1	F	134	ALA	3.6
1	G	38	ALA	3.6
1	F	174	PRO	3.5
1	H	229	ARG	3.5
1	E	48	VAL	3.5
1	F	204	LEU	3.5
1	F	93	PRO	3.5
1	F	131	LEU	3.5
1	F	132	ALA	3.4
1	E	254	ALA	3.4
1	H	73	SER	3.4
1	H	135	GLU	3.4
1	H	129	HIS	3.4
1	G	57	SER	3.3
1	F	151	LEU	3.3
1	G	174	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	H	231	PRO	3.3
1	F	193	ALA	3.3
1	F	207	ALA	3.3
1	H	43	GLY	3.2
1	F	120	LEU	3.2
1	F	119	GLY	3.2
1	H	57	SER	3.2
1	H	140	ALA	3.2
1	G	209	GLU	3.2
1	H	116	GLY	3.2
1	F	104	SER	3.2
1	G	23	GLU	3.1
1	H	60	ARG	3.1
1	F	178	LEU	3.1
1	G	14	GLY	3.1
1	H	252	TRP	3.1
1	G	12	ARG	3.1
1	G	24	GLY	3.1
1	H	139	ARG	3.1
1	F	251	ARG	3.0
1	G	44	PRO	3.0
1	G	197	ASN	3.0
1	H	243	THR	3.0
1	H	115	VAL	3.0
1	F	215	LEU	2.9
1	F	130	HIS	2.9
1	F	189	ARG	2.9
1	F	206	ARG	2.9
1	F	176	LYS	2.9
1	F	165	ASP	2.9
1	G	11	ASP	2.9
1	F	144	VAL	2.9
1	H	121	VAL	2.9
1	G	48	VAL	2.9
1	F	105	GLY	2.8
1	G	199	THR	2.8
1	H	47	VAL	2.8
1	F	154	LEU	2.8
1	H	131	LEU	2.8
1	E	37	GLU	2.8
1	G	172	MET	2.8
1	H	152	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	92	ALA	2.7
1	H	184	ALA	2.7
1	F	214	ARG	2.7
1	G	66	TYR	2.7
1	G	72	ARG	2.7
1	G	73	SER	2.7
1	F	248	ALA	2.7
1	E	5	GLY	2.7
1	H	142	TRP	2.7
1	H	227	GLU	2.6
1	H	118	LYS	2.6
1	F	100	ALA	2.6
1	F	221	VAL	2.6
1	F	191	LEU	2.6
1	G	137	ASN	2.6
1	E	20	PHE	2.6
1	H	223	TRP	2.6
1	F	218	VAL	2.6
1	G	19	VAL	2.6
1	F	95	MET	2.6
1	F	185	LEU	2.6
1	G	183	LEU	2.6
1	G	47	VAL	2.6
1	G	27	PHE	2.6
1	H	143	GLN	2.6
1	E	39	LEU	2.5
1	F	91	LEU	2.5
1	F	139	ARG	2.5
1	H	36	HIS	2.5
1	G	152	GLY	2.5
1	E	35	PRO	2.5
1	H	48	VAL	2.5
1	E	12	ARG	2.5
1	H	183	LEU	2.5
1	E	209	GLU	2.5
1	E	43	GLY	2.5
1	F	6	PRO	2.5
1	H	233	ALA	2.5
1	H	238	GLN	2.5
1	H	41	GLU	2.5
1	F	106	GLY	2.5
1	F	240	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	205	VAL	2.5
1	G	9	LEU	2.5
1	G	214	ARG	2.5
1	H	226	TRP	2.5
1	E	19	VAL	2.5
1	H	100	ALA	2.5
1	G	33	SER	2.4
1	G	252	TRP	2.4
1	E	241	GLY	2.4
1	H	66	TYR	2.4
1	F	177	VAL	2.4
1	G	26	VAL	2.4
1	G	171	LEU	2.4
1	F	33	SER	2.4
1	G	175	TRP	2.4
1	F	54	GLU	2.4
1	E	22	LYS	2.4
1	F	167	VAL	2.4
1	F	190	PHE	2.4
1	E	139	ARG	2.4
1	F	102	THR	2.4
1	G	20	PHE	2.4
1	F	43	GLY	2.4
1	F	140	ALA	2.4
1	F	249	LEU	2.3
1	H	39	LEU	2.3
1	F	161	GLU	2.3
1	F	213	PHE	2.3
1	F	67	LEU	2.3
1	F	246	LEU	2.3
1	G	184	ALA	2.3
1	H	102	THR	2.3
1	H	127	ARG	2.3
1	H	240	VAL	2.3
1	F	195	LEU	2.3
1	H	134	ALA	2.3
1	G	10	LYS	2.3
1	G	41	GLU	2.3
1	G	170	ASP	2.3
1	H	128	PRO	2.3
1	F	162	ALA	2.3
1	H	254	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	22	LYS	2.3
1	G	202	LEU	2.3
1	F	127	ARG	2.2
1	G	61	PRO	2.2
1	H	123	SER	2.2
1	F	203	GLU	2.2
1	G	25	GLY	2.2
1	H	112	ALA	2.2
1	F	125	GLU	2.2
1	H	158	GLU	2.2
1	G	148	ARG	2.2
1	E	9	LEU	2.2
1	G	45	GLY	2.2
1	H	159	LEU	2.2
1	E	227	GLU	2.2
1	F	128	PRO	2.2
1	E	13	LYS	2.2
1	H	56	LEU	2.2
1	F	70	MET	2.2
1	E	47	VAL	2.2
1	H	42	ALA	2.1
1	E	55	GLU	2.1
1	F	227	GLU	2.1
1	H	37	GLU	2.1
1	H	164	TYR	2.1
1	E	171	LEU	2.1
1	F	19	VAL	2.1
1	F	170	ASP	2.1
1	G	60	ARG	2.1
1	H	113	ARG	2.1
1	F	199	THR	2.1
1	G	6	PRO	2.1
1	F	133	GLN	2.1
1	F	89	LEU	2.1
1	F	194	TYR	2.1
1	G	43	GLY	2.1
1	F	136	ARG	2.1
1	G	42	ALA	2.1
1	G	123	SER	2.1
1	H	38	ALA	2.1
1	G	204	LEU	2.1
1	F	17	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	58	VAL	2.1
1	F	148	ARG	2.0
1	H	76	PRO	2.0
1	H	98	LEU	2.0
1	H	122	GLU	2.0
1	F	181	ALA	2.0
1	E	73	SER	2.0
1	G	211	HIS	2.0
1	F	121	VAL	2.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

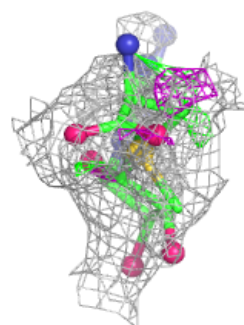
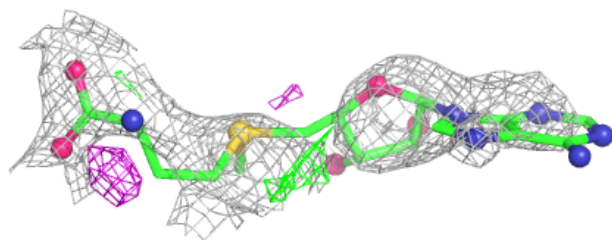
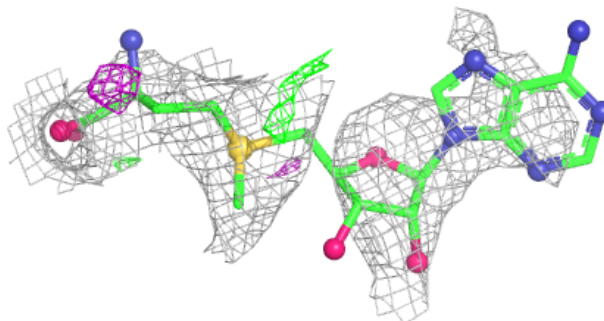
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SAM	F	301	27/27	0.64	0.23	64,91,107,108	0
3	SO4	F	302	5/5	0.80	0.26	32,40,44,83	0
2	SAM	G	301	27/27	0.84	0.15	26,37,57,62	0
2	SAM	H	301	27/27	0.88	0.14	29,41,51,59	0
2	SAM	E	301	27/27	0.93	0.11	15,26,40,54	0

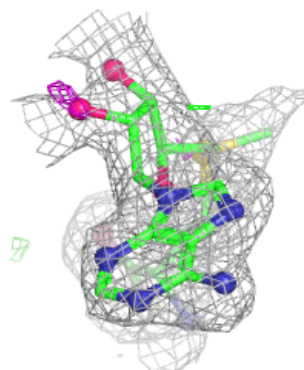
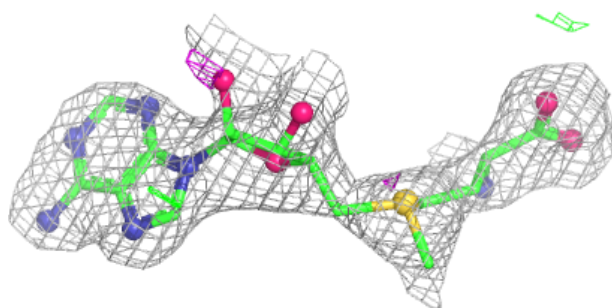
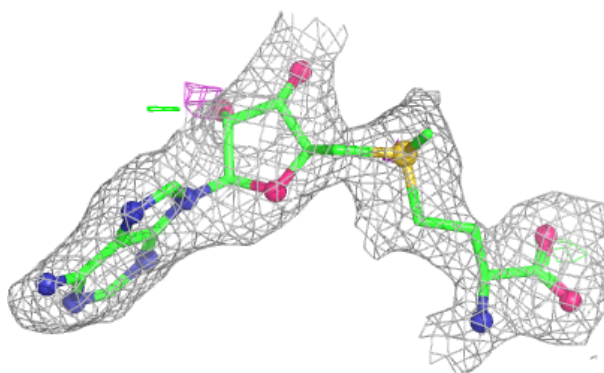
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAM 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)

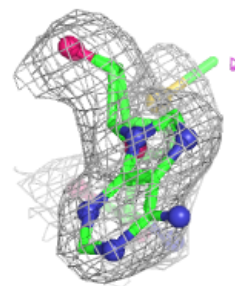
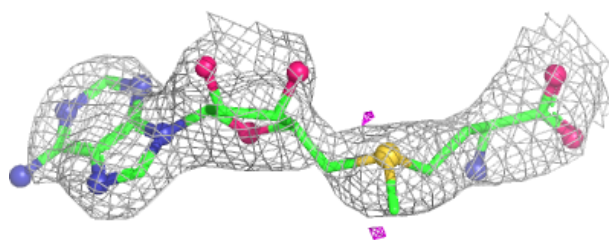
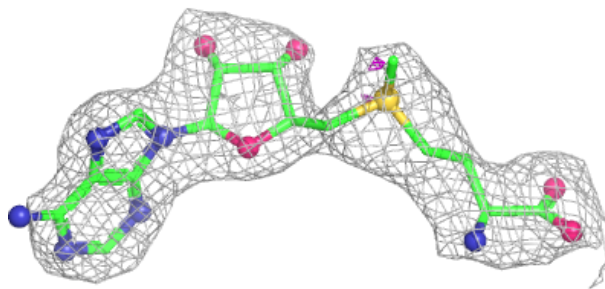
**Electron density around SAM G 301:**

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

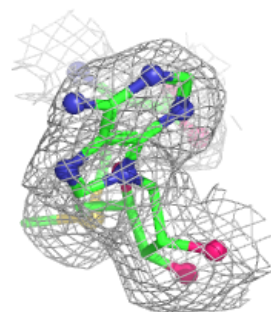
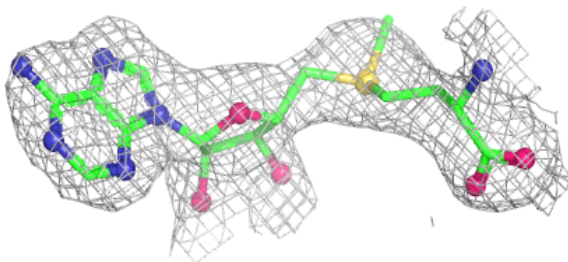
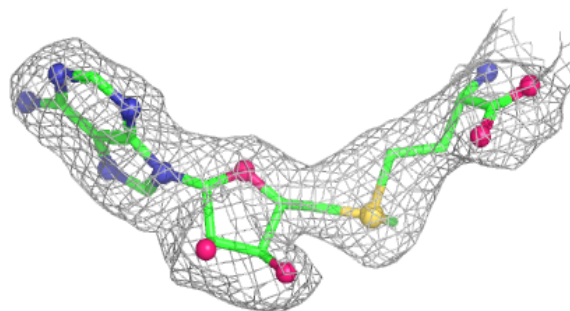


Electron density around SAM H 301:

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

**Electron density around SAM 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.