



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:37 PM UTC

PDB ID : 6RK7 / pdb_00006rk7
Title : Inter-dimeric interface controls function and stability of S-methionine adenosyltransferase from *U. urealiticum*
Authors : Shahar, A.; Zarivach, R.; Bershtein, S.; Kleiner, D.; Shmulevich, F.
Deposited on : 2019-04-30
Resolution : 1.80 Å(reported)

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

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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:

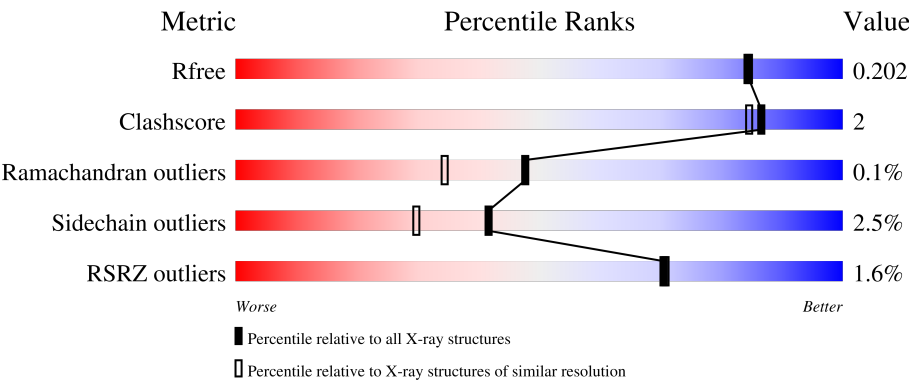
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	382	86%12%..
1	B	382	2% 91%6%..
1	E	382	% 91%6%..
1	F	382	% 90%7%. .
1	G	382	3% 88%9%..

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Mol	Chain	Length	Quality of chain
1	H	382	% 90% 7% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19574 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 Methionine adenosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	11	0
			2993	1904	502	575	12			
1	B	374	Total	C	N	O	S	0	6	0
			2973	1888	500	573	12			
1	E	375	Total	C	N	O	S	0	7	0
			2985	1893	503	578	11			
1	F	374	Total	C	N	O	S	0	5	0
			2961	1885	495	570	11			
1	G	375	Total	C	N	O	S	0	3	0
			2962	1881	498	571	12			
1	H	373	Total	C	N	O	S	0	7	0
			2953	1878	493	570	12			

There are 36 discrepancies between the modelled and reference sequences:

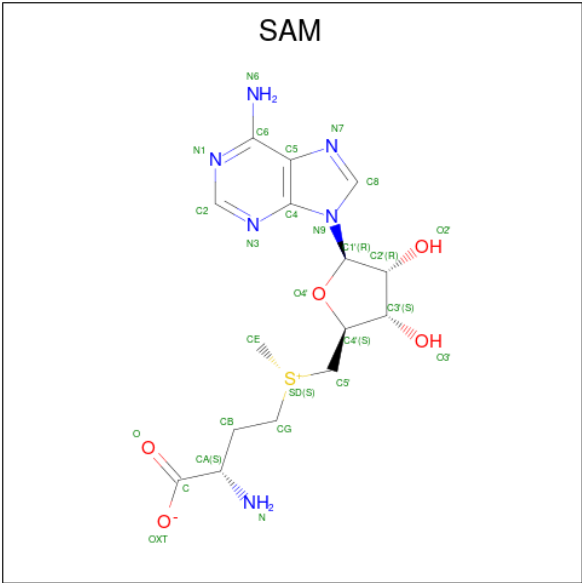
Chain	Residue	Modelled	Actual	Comment	Reference
A	377	HIS	-	expression tag	UNP B2NE58
A	378	HIS	-	expression tag	UNP B2NE58
A	379	HIS	-	expression tag	UNP B2NE58
A	380	HIS	-	expression tag	UNP B2NE58
A	381	HIS	-	expression tag	UNP B2NE58
A	382	HIS	-	expression tag	UNP B2NE58
B	377	HIS	-	expression tag	UNP B2NE58
B	378	HIS	-	expression tag	UNP B2NE58
B	379	HIS	-	expression tag	UNP B2NE58
B	380	HIS	-	expression tag	UNP B2NE58
B	381	HIS	-	expression tag	UNP B2NE58
B	382	HIS	-	expression tag	UNP B2NE58
E	377	HIS	-	expression tag	UNP B2NE58
E	378	HIS	-	expression tag	UNP B2NE58
E	379	HIS	-	expression tag	UNP B2NE58
E	380	HIS	-	expression tag	UNP B2NE58
E	381	HIS	-	expression tag	UNP B2NE58

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Chain	Residue	Modelled	Actual	Comment	Reference
E	382	HIS	-	expression tag	UNP B2NE58
F	377	HIS	-	expression tag	UNP B2NE58
F	378	HIS	-	expression tag	UNP B2NE58
F	379	HIS	-	expression tag	UNP B2NE58
F	380	HIS	-	expression tag	UNP B2NE58
F	381	HIS	-	expression tag	UNP B2NE58
F	382	HIS	-	expression tag	UNP B2NE58
G	377	HIS	-	expression tag	UNP B2NE58
G	378	HIS	-	expression tag	UNP B2NE58
G	379	HIS	-	expression tag	UNP B2NE58
G	380	HIS	-	expression tag	UNP B2NE58
G	381	HIS	-	expression tag	UNP B2NE58
G	382	HIS	-	expression tag	UNP B2NE58
H	377	HIS	-	expression tag	UNP B2NE58
H	378	HIS	-	expression tag	UNP B2NE58
H	379	HIS	-	expression tag	UNP B2NE58
H	380	HIS	-	expression tag	UNP B2NE58
H	381	HIS	-	expression tag	UNP B2NE58
H	382	HIS	-	expression tag	UNP B2NE58

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



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

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	E	1	Total	Cl	0	0
			1	1		
3	F	1	Total	Cl	0	0
			1	1		
3	G	1	Total	Cl	0	0
			1	1		
3	H	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

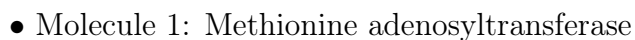
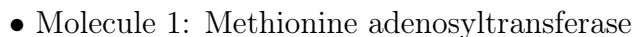
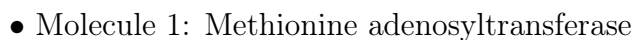
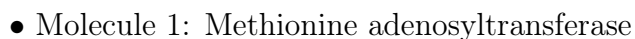
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	320	Total	O	0	0
			320	320		

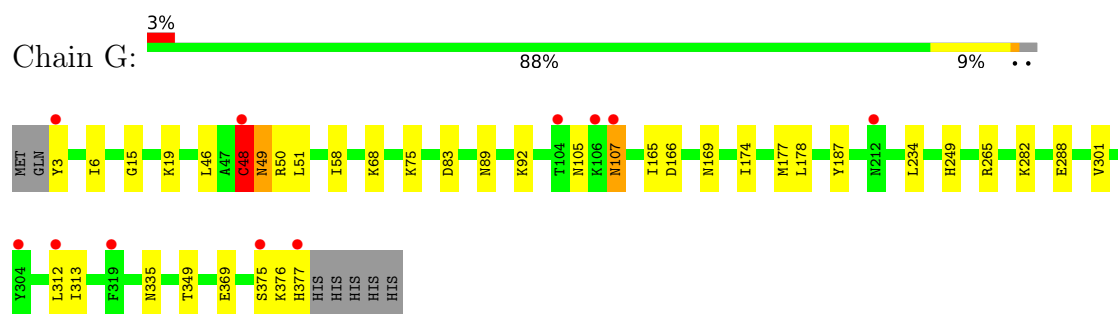
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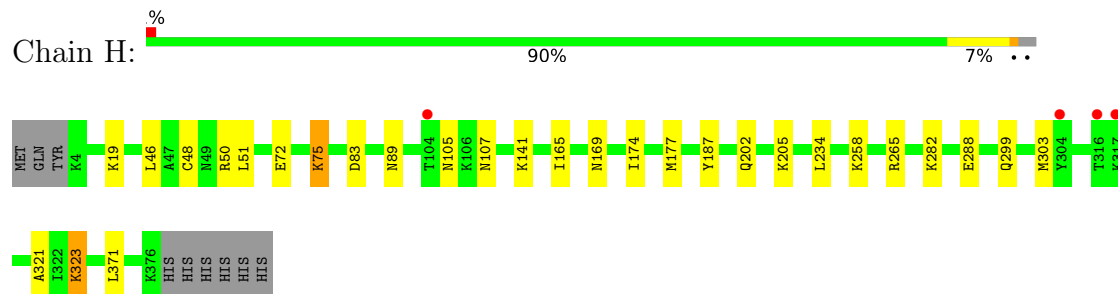
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	214	Total 214	O 214	0	0
4	E	278	Total 278	O 278	0	0
4	F	245	Total 245	O 245	0	0
4	G	162	Total 162	O 162	0	0
4	H	198	Total 198	O 198	0	0

- Molecule 1: Methionine adenosyltransferase





- Molecule 1: Methionine adenosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	114.00Å 106.14Å 234.38Å 90.00° 96.86° 90.00°	Depositor
Resolution (Å)	48.66 – 1.80 48.66 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.66-1.80) 99.8 (48.66-1.80)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.169 , 0.194 0.178 , 0.202	Depositor DCC
R_{free} test set	12863 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	19574	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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: CL, 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	1.43	16/3079 (0.5%)	1.14	6/4161 (0.1%)
1	B	1.31	4/3035 (0.1%)	1.10	3/4103 (0.1%)
1	E	1.42	7/3050 (0.2%)	1.16	10/4123 (0.2%)
1	F	1.37	12/3029 (0.4%)	1.10	2/4094 (0.0%)
1	G	1.26	9/3025 (0.3%)	1.07	7/4091 (0.2%)
1	H	1.25	6/3026 (0.2%)	1.09	4/4092 (0.1%)
All	All	1.34	54/18244 (0.3%)	1.11	32/24664 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	2

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	286	GLN	CD-NE2	-8.65	1.15	1.33
1	F	75	LYS	C-O	-8.12	1.16	1.24
1	F	105	ASN	C-O	8.12	1.33	1.23
1	B	75	LYS	C-O	-7.91	1.17	1.24
1	G	75	LYS	C-O	-7.82	1.17	1.24
1	G	48[A]	CYS	C-O	7.50	1.33	1.23
1	G	48[B]	CYS	C-O	7.50	1.33	1.23
1	A	374	ASN	CG-ND2	-6.92	1.18	1.33
1	E	309	ASN	CB-CG	-6.87	1.34	1.52
1	A	356	ASP	C-O	-6.44	1.15	1.24
1	H	371	LEU	CA-C	6.40	1.61	1.52
1	E	286	GLN	CD-OE1	6.37	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	356	ASP	CB-CG	6.37	1.68	1.52
1	F	300	PRO	C-O	-6.36	1.16	1.23
1	A	286	GLN	CD-OE1	-6.32	1.11	1.23
1	G	58	ILE	C-O	6.31	1.30	1.24
1	F	356	ASP	CB-CG	6.28	1.67	1.52
1	B	106	LYS	N-CA	-6.22	1.38	1.46
1	H	75	LYS	C-O	-6.20	1.18	1.24
1	G	48[A]	CYS	C-N	-6.06	1.25	1.33
1	G	48[B]	CYS	C-N	-6.06	1.25	1.33
1	A	171	THR	CA-C	6.02	1.59	1.52
1	B	10	GLU	CD-OE1	5.91	1.36	1.25
1	A	104	THR	N-CA	5.79	1.53	1.46
1	F	290	GLN	CD-NE2	5.71	1.45	1.33
1	H	105	ASN	C-O	5.69	1.30	1.23
1	A	69	THR	N-CA	5.64	1.53	1.46
1	F	86	ILE	C-O	-5.55	1.18	1.24
1	E	108	LEU	C-O	-5.52	1.16	1.23
1	A	265	ARG	CZ-NH2	-5.49	1.26	1.33
1	A	102	ASP	C-N	-5.47	1.26	1.33
1	H	321	ALA	CA-C	5.47	1.59	1.52
1	F	213	PHE	N-CA	-5.46	1.38	1.45
1	A	102	ASP	C-O	-5.42	1.16	1.23
1	A	244	TYR	N-CA	-5.42	1.40	1.46
1	A	338	ASN	CG-ND2	-5.39	1.22	1.33
1	F	75	LYS	N-CA	5.39	1.51	1.46
1	F	57	GLU	CD-OE2	5.38	1.35	1.25
1	E	75	LYS	C-O	-5.35	1.19	1.24
1	G	15	GLY	N-CA	5.31	1.51	1.45
1	B	171	THR	CA-C	5.31	1.59	1.52
1	A	37	GLN	CD-OE1	5.27	1.33	1.23
1	G	105	ASN	C-O	5.22	1.30	1.24
1	F	53	VAL	C-O	5.20	1.29	1.24
1	A	49	ASN	CA-CB	5.18	1.62	1.53
1	A	75	LYS	CD-CE	-5.11	1.37	1.52
1	A	75	LYS	C-O	-5.11	1.19	1.24
1	H	202	GLN	CA-C	5.09	1.59	1.52
1	F	223	PHE	CA-CB	5.09	1.58	1.53
1	A	49	ASN	CG-OD1	-5.08	1.13	1.23
1	G	349	THR	CA-C	5.06	1.58	1.52
1	E	185	GLU	C-O	-5.04	1.18	1.24
1	H	303	MET	SD-CE	-5.03	1.67	1.79
1	F	212	ASN	C-O	-5.02	1.17	1.24

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	103	LYS	CA-C-O	-9.53	110.34	122.63
1	A	265	ARG	NE-CZ-NH2	-8.72	111.36	119.20
1	B	265	ARG	NE-CZ-NH2	-8.06	111.95	119.20
1	E	103	LYS	CB-CA-C	-7.49	100.88	112.12
1	H	202	GLN	CA-CB-CG	7.33	128.76	114.10
1	H	141	LYS	CG-CD-CE	7.25	127.99	111.30
1	F	265	ARG	NE-CZ-NH1	-7.03	114.47	121.50
1	B	195	LYS	CG-CD-CE	7.02	127.45	111.30
1	B	106	LYS	CB-CA-C	6.78	123.92	110.42
1	A	376	LYS	N-CA-C	6.67	119.97	109.96
1	E	265	ARG	NE-CZ-NH1	-6.67	114.83	121.50
1	G	107	ASN	N-CA-CB	6.62	120.07	110.47
1	H	323	LYS	CB-CG-CD	6.44	126.12	111.30
1	H	265	ARG	NE-CZ-NH1	-6.38	115.12	121.50
1	G	265	ARG	NE-CZ-NH1	-6.11	115.39	121.50
1	E	301	VAL	CG1-CB-CG2	6.05	124.12	110.80
1	E	103	LYS	N-CA-C	-5.77	100.96	109.62
1	A	169	ASN	CA-CB-CG	-5.74	106.86	112.60
1	E	301	VAL	CA-CB-CG1	5.67	120.03	110.40
1	A	141	LYS	CG-CD-CE	5.61	124.21	111.30
1	G	48[A]	CYS	CA-C-N	5.30	131.66	121.54
1	G	48[A]	CYS	C-N-CA	5.30	131.66	121.54
1	G	48[B]	CYS	CA-C-N	5.30	131.66	121.54
1	G	48[B]	CYS	C-N-CA	5.30	131.66	121.54
1	A	315	GLU	CG-CD-OE1	5.22	130.41	118.40
1	G	3	TYR	N-CA-C	5.22	125.61	111.00
1	A	110	GLY	N-CA-C	-5.20	105.09	112.37
1	E	268	SER	N-CA-CB	5.15	117.69	110.12
1	F	265	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	E	265	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	E	331	LYS	CG-CD-CE	-5.10	99.57	111.30
1	E	234	LEU	CD1-CG-CD2	-5.02	99.76	110.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	48[A]	CYS	Mainchain
1	G	48[B]	CYS	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2993	0	3026	24	0
1	B	2973	0	2979	14	0
1	E	2985	0	2988	11	0
1	F	2961	0	2984	11	0
1	G	2962	0	2963	11	0
1	H	2953	0	2976	11	0
2	A	54	0	44	0	0
2	B	54	0	44	0	0
2	E	54	0	43	0	0
2	F	54	0	43	1	0
2	G	54	0	44	0	0
2	H	54	0	44	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	320	0	0	5	0
4	B	214	0	0	1	0
4	E	278	0	0	2	0
4	F	245	0	0	2	0
4	G	162	0	0	0	0
4	H	198	0	0	3	0
All	All	19574	0	18178	75	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 2.

All (75) 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:B:105:ASN:ND2	1:B:106:LYS:O	1.66	1.28
1:H:46:LEU:HD12	1:H:234[B]:LEU:HD21	1.35	1.09
1:G:48[B]:CYS:SG	1:H:89:ASN:ND2	2.30	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ASN:ND2	1:B:48[B]:CYS:SG	2.43	0.92
1:G:89:ASN:ND2	1:H:48[B]:CYS:SG	2.43	0.91
1:A:48[B]:CYS:SG	1:B:89:ASN:ND2	2.45	0.89
1:A:359[A]:ASP:OD1	4:A:501:HOH:O	2.03	0.75
1:H:48[B]:CYS:SG	1:H:51:LEU:HB3	2.31	0.70
1:A:340:TRP:HZ3	4:A:689:HOH:O	1.74	0.70
1:G:313:ILE:CD1	1:G:375:SER:OG	2.43	0.67
1:H:288:GLU:OE1	4:H:501:HOH:O	2.13	0.67
1:A:40[A]:ARG:NH1	1:A:102:ASP:OD1	2.26	0.65
1:F:116:ILE:HD11	1:F:290:GLN:CD	2.21	0.65
1:A:48[B]:CYS:SG	1:A:51:LEU:HB3	2.37	0.65
1:A:340:TRP:CZ3	4:A:689:HOH:O	2.51	0.60
1:B:48[B]:CYS:SG	1:B:51:LEU:HB3	2.42	0.60
1:E:46:LEU:HD12	1:E:234:LEU:HD21	1.85	0.59
1:F:116:ILE:HD11	1:F:290:GLN:CG	2.33	0.57
1:F:116:ILE:HD11	1:F:290:GLN:HG3	1.85	0.57
1:A:258[B]:LYS:NZ	4:A:507:HOH:O	2.38	0.56
1:G:376:LYS:O	1:G:377:HIS:ND1	2.35	0.53
1:A:297[B]:GLN:OE1	4:A:502:HOH:O	2.18	0.53
1:H:72:GLU:OE2	4:H:502:HOH:O	2.18	0.53
1:A:208:ASN:ND2	1:E:215:LYS:HB2	2.25	0.52
1:F:194[B]:LYS:NZ	4:F:1104:HOH:O	2.43	0.51
1:G:46:LEU:HD12	1:G:234:LEU:HD21	1.93	0.51
1:B:106:LYS:O	1:B:107:ASN:HB2	2.12	0.50
1:A:165:ILE:HD13	1:A:174:ILE:HA	1.93	0.50
1:B:190:GLU:O	1:B:194:LYS:HD3	2.14	0.48
1:A:138[A]:GLU:OE1	1:A:207:TYR:OH	2.29	0.48
1:A:199:ILE:O	1:A:203:ILE:HD12	2.14	0.47
1:A:134:VAL:O	1:A:138[B]:GLU:HG2	2.14	0.47
1:B:61:HIS:CE1	4:B:520:HOH:O	2.67	0.47
1:E:106:LYS:O	1:E:107:ASN:CB	2.61	0.46
1:B:105:ASN:HD22	1:B:105:ASN:C	2.22	0.46
1:E:3:TYR:CD2	1:F:316:THR:HG22	2.50	0.46
1:H:46:LEU:HD12	1:H:234[B]:LEU:CD2	2.25	0.46
1:H:258:LYS:NZ	4:H:509:HOH:O	2.48	0.46
1:G:6:ILE:HD13	1:G:166:ASP:HA	1.97	0.46
1:A:190:GLU:O	1:A:194[B]:LYS:HE2	2.16	0.46
1:G:174:ILE:HD13	1:G:177:MET:HE3	1.98	0.45
1:A:50:ARG:HD2	1:A:83:ASP:O	2.17	0.45
1:E:215:LYS:HE3	4:E:594:HOH:O	2.16	0.45
2:F:401:SAM:HB2	4:F:1303:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:ARG:HD2	1:E:83:ASP:O	2.17	0.44
1:F:116:ILE:CD1	1:F:290:GLN:OE1	2.65	0.44
1:F:174:ILE:HD13	1:F:177:MET:HE3	1.99	0.44
1:H:50:ARG:HD2	1:H:83:ASP:O	2.17	0.44
1:E:304:TYR:CE1	1:F:5:LYS:HG3	2.52	0.44
1:B:50:ARG:HD2	1:B:83:ASP:O	2.18	0.44
1:F:50:ARG:HD2	1:F:83:ASP:O	2.18	0.44
1:H:174:ILE:HD13	1:H:177:MET:HE3	2.00	0.43
1:A:40[A]:ARG:HH12	1:A:102:ASP:CG	2.20	0.43
1:B:174:ILE:HD13	1:B:177:MET:HE3	2.00	0.43
1:G:50:ARG:HD2	1:G:83:ASP:O	2.19	0.43
1:B:49:ASN:HD22	1:B:49:ASN:HA	1.46	0.42
1:E:174:ILE:HD13	1:E:177:MET:HE3	2.00	0.42
1:F:249:HIS:ND1	1:F:288:GLU:OE2	2.37	0.42
1:G:249:HIS:ND1	1:G:288:GLU:OE2	2.34	0.42
1:A:126:PRO:HB3	4:E:632:HOH:O	2.19	0.42
1:A:174:ILE:HD13	1:A:177:MET:HE3	2.00	0.41
1:G:178:LEU:C	1:G:178:LEU:HD23	2.45	0.41
1:A:139:LEU:HD23	1:A:203:ILE:HD13	2.01	0.41
1:A:46:LEU:HD12	1:A:234[B]:LEU:HD21	2.01	0.41
1:B:178:LEU:C	1:B:178:LEU:HD23	2.46	0.41
1:A:123:ASP:O	1:E:212:ASN:HB3	2.21	0.41
1:B:106:LYS:HA	1:B:106:LYS:HD3	1.83	0.41
1:B:105:ASN:C	1:B:106:LYS:O	2.63	0.40
1:E:308:PHE:O	1:E:309:ASN:HB2	2.20	0.40
1:E:178:LEU:C	1:E:178:LEU:HD23	2.46	0.40
1:F:194[B]:LYS:HA	1:F:194[B]:LYS:HD3	1.74	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	383/382 (100%)	373 (97%)	10 (3%)	0	100	100
1	B	378/382 (99%)	367 (97%)	9 (2%)	2 (0%)	24	14
1	E	380/382 (100%)	369 (97%)	11 (3%)	0	100	100
1	F	377/382 (99%)	368 (98%)	9 (2%)	0	100	100
1	G	376/382 (98%)	366 (97%)	9 (2%)	1 (0%)	36	25
1	H	378/382 (99%)	369 (98%)	9 (2%)	0	100	100
All	All	2272/2292 (99%)	2212 (97%)	57 (2%)	3 (0%)	48	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	49	ASN
1	B	106	LYS
1	B	105	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	335/332 (101%)	330 (98%)	5 (2%)	57	49
1	B	329/332 (99%)	322 (98%)	7 (2%)	47	36
1	E	331/332 (100%)	325 (98%)	6 (2%)	51	43
1	F	329/332 (99%)	322 (98%)	7 (2%)	47	36
1	G	328/332 (99%)	315 (96%)	13 (4%)	28	15
1	H	330/332 (99%)	320 (97%)	10 (3%)	36	24
All	All	1982/1992 (100%)	1934 (98%)	48 (2%)	42	31

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LYS
1	A	187	TYR

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Mol	Chain	Res	Type
1	A	203	ILE
1	A	282	LYS
1	A	376	LYS
1	B	19	LYS
1	B	105	ASN
1	B	165	ILE
1	B	169	ASN
1	B	187	TYR
1	B	195	LYS
1	B	376	LYS
1	E	19	LYS
1	E	75	LYS
1	E	187	TYR
1	E	299	GLN
1	E	301	VAL
1	E	309	ASN
1	F	19	LYS
1	F	106	LYS
1	F	107	ASN
1	F	169	ASN
1	F	187	TYR
1	F	205	LYS
1	F	299	GLN
1	G	19	LYS
1	G	51	LEU
1	G	68	LYS
1	G	92	LYS
1	G	107	ASN
1	G	165	ILE
1	G	169	ASN
1	G	187	TYR
1	G	282	LYS
1	G	301	VAL
1	G	312	LEU
1	G	335	ASN
1	G	369	GLU
1	H	19	LYS
1	H	75	LYS
1	H	107	ASN
1	H	165	ILE
1	H	169	ASN
1	H	187	TYR

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Mol	Chain	Res	Type
1	H	205	LYS
1	H	282	LYS
1	H	299	GLN
1	H	323	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	89	ASN
1	A	208	ASN
1	A	286	GLN
1	A	374	ASN
1	B	49	ASN
1	B	89	ASN
1	B	114	GLN
1	B	193	ASN
1	B	286	GLN
1	B	309	ASN
1	E	89	ASN
1	E	93	GLN
1	E	105	ASN
1	E	299	GLN
1	F	93	GLN
1	F	202	GLN
1	F	286	GLN
1	F	297	GLN
1	F	299	GLN
1	G	89	ASN
1	G	93	GLN
1	G	107	ASN
1	G	286	GLN
1	H	37	GLN
1	H	89	ASN
1	H	93	GLN
1	H	286	GLN
1	H	297	GLN
1	H	299	GLN
1	H	374	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

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	E	402	-	27,29,29	1.46	3 (11%)	34,42,42	2.00	11 (32%)
2	SAM	F	401	-	27,29,29	1.92	7 (25%)	34,42,42	2.05	11 (32%)
2	SAM	B	401	-	27,29,29	1.59	5 (18%)	34,42,42	2.21	12 (35%)
2	SAM	G	401	-	27,29,29	1.70	6 (22%)	34,42,42	1.79	8 (23%)
2	SAM	G	402	-	27,29,29	1.33	3 (11%)	34,42,42	2.48	10 (29%)
2	SAM	A	401	-	27,29,29	1.28	3 (11%)	34,42,42	1.99	10 (29%)
2	SAM	A	402	-	27,29,29	1.36	3 (11%)	34,42,42	1.64	4 (11%)
2	SAM	H	402	-	27,29,29	1.27	2 (7%)	34,42,42	2.33	11 (32%)
2	SAM	B	402	-	27,29,29	1.42	5 (18%)	34,42,42	1.99	10 (29%)
2	SAM	F	402	-	27,29,29	1.72	6 (22%)	34,42,42	2.77	13 (38%)
2	SAM	H	401	-	27,29,29	1.76	7 (25%)	34,42,42	2.32	17 (50%)
2	SAM	E	401	-	27,29,29	1.49	4 (14%)	34,42,42	1.78	10 (29%)

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	E	402	-	-	2/17/33/33	0/3/3/3
2	SAM	F	401	-	-	5/17/33/33	0/3/3/3
2	SAM	B	401	-	-	4/17/33/33	0/3/3/3
2	SAM	G	401	-	-	4/17/33/33	0/3/3/3
2	SAM	G	402	-	-	0/17/33/33	0/3/3/3
2	SAM	A	401	-	-	5/17/33/33	0/3/3/3
2	SAM	A	402	-	-	1/17/33/33	0/3/3/3
2	SAM	H	402	-	-	1/17/33/33	0/3/3/3
2	SAM	B	402	-	-	0/17/33/33	0/3/3/3
2	SAM	F	402	-	-	3/17/33/33	0/3/3/3
2	SAM	H	401	-	-	4/17/33/33	0/3/3/3
2	SAM	E	401	-	-	5/17/33/33	0/3/3/3

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	SAM	C5-C4	5.46	1.48	1.39
2	F	402	SAM	C4-N9	-5.11	1.27	1.37
2	H	401	SAM	C5-C4	4.72	1.47	1.39
2	F	401	SAM	C4-N9	-4.64	1.28	1.37
2	G	401	SAM	C4-N9	-4.30	1.28	1.37
2	E	401	SAM	C4-N9	-4.19	1.29	1.37
2	F	402	SAM	O2'-C2'	-3.95	1.33	1.43
2	E	402	SAM	O2'-C2'	-3.72	1.33	1.43
2	G	401	SAM	C8-N7	3.51	1.38	1.31
2	A	401	SAM	C8-N7	3.46	1.38	1.31
2	G	401	SAM	CG-CB	3.37	1.62	1.51
2	E	402	SAM	C5-C6	3.35	1.50	1.41
2	B	401	SAM	CG-CB	3.34	1.62	1.51
2	B	401	SAM	C5-C6	3.23	1.50	1.41
2	B	402	SAM	C5-N7	-3.21	1.33	1.39
2	A	402	SAM	C8-N9	-3.20	1.32	1.37
2	B	402	SAM	C4-N9	-3.06	1.31	1.37
2	F	401	SAM	CG-CB	3.04	1.61	1.51
2	G	402	SAM	C8-N9	-3.03	1.32	1.37
2	H	401	SAM	O-C	2.93	1.30	1.22
2	B	401	SAM	C8-N9	-2.90	1.32	1.37
2	B	402	SAM	C8-N9	-2.88	1.32	1.37
2	E	401	SAM	C5-C6	2.87	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	SAM	OXT-C	-2.80	1.21	1.30
2	A	402	SAM	C4-N9	-2.79	1.31	1.37
2	H	401	SAM	C5-N7	-2.74	1.34	1.39
2	B	401	SAM	C5-N7	-2.67	1.34	1.39
2	F	401	SAM	C4-N3	-2.67	1.29	1.34
2	A	401	SAM	OXT-C	-2.63	1.22	1.30
2	F	402	SAM	C6-N6	-2.62	1.27	1.34
2	A	401	SAM	C5-C6	2.62	1.48	1.41
2	H	401	SAM	C4-N9	-2.55	1.32	1.37
2	B	401	SAM	OXT-C	-2.53	1.22	1.30
2	H	401	SAM	O3'-C3'	2.49	1.49	1.43
2	E	401	SAM	C6-N1	-2.49	1.28	1.35
2	G	401	SAM	C5-C4	2.48	1.43	1.39
2	G	402	SAM	OXT-C	-2.47	1.22	1.30
2	E	401	SAM	CG-CB	2.45	1.59	1.51
2	H	401	SAM	O4'-C4'	2.43	1.50	1.45
2	F	401	SAM	C8-N9	2.39	1.41	1.37
2	F	402	SAM	O4'-C4'	-2.39	1.39	1.45
2	F	402	SAM	OXT-C	-2.37	1.23	1.30
2	F	402	SAM	C8-N7	2.37	1.36	1.31
2	E	402	SAM	O4'-C4'	-2.34	1.39	1.45
2	A	402	SAM	C5-N7	2.31	1.43	1.39
2	G	401	SAM	C4-N3	2.31	1.38	1.34
2	G	402	SAM	CG-CB	2.29	1.58	1.51
2	G	401	SAM	O-C	2.26	1.28	1.22
2	F	401	SAM	O2'-C2'	2.24	1.48	1.43
2	H	402	SAM	C5-C4	2.20	1.43	1.39
2	H	401	SAM	C5-C6	2.10	1.46	1.41
2	H	402	SAM	C2-N1	2.04	1.37	1.33
2	B	402	SAM	O4'-C4'	-2.02	1.40	1.45
2	B	402	SAM	C5-C6	2.02	1.46	1.41

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	402	SAM	C4-N9-C8	8.57	114.73	105.74
2	F	402	SAM	CG-SD-C5'	-7.37	85.41	103.43
2	F	401	SAM	CG-SD-C5'	-6.47	87.61	103.43
2	F	402	SAM	OXT-C-O	-6.16	110.11	124.08
2	A	401	SAM	CG-SD-C5'	-5.96	88.87	103.43
2	B	401	SAM	CG-SD-C5'	-5.67	89.56	103.43
2	H	402	SAM	C4-N9-C8	5.64	111.67	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	401	SAM	CG-SD-C5'	-5.57	89.81	103.43
2	F	402	SAM	CB-CA-N	-5.52	95.74	110.12
2	B	401	SAM	N6-C6-N1	5.40	130.40	118.38
2	B	402	SAM	C5-C4-N3	-5.39	119.30	126.72
2	A	402	SAM	C4-N9-C8	5.23	111.23	105.74
2	F	402	SAM	CB-CA-C	5.01	123.72	110.45
2	G	402	SAM	N9-C8-N7	-4.97	106.89	113.94
2	E	402	SAM	C4-N9-C8	4.76	110.74	105.74
2	B	402	SAM	N3-C4-N9	4.55	134.90	127.17
2	F	402	SAM	C5-C4-N3	-4.46	120.57	126.72
2	G	402	SAM	C5-C4-N9	-4.40	101.01	105.81
2	H	402	SAM	O4'-C1'-N9	-4.34	99.75	108.09
2	H	401	SAM	N3-C4-N9	4.28	134.45	127.17
2	F	402	SAM	C4-N9-C8	4.20	110.15	105.74
2	H	401	SAM	CG-SD-C5'	-4.16	93.27	103.43
2	H	402	SAM	N3-C2-N1	-4.12	122.35	128.58
2	H	402	SAM	N3-C4-N9	4.10	134.13	127.17
2	B	401	SAM	C5-C6-N6	-4.04	113.27	123.29
2	G	402	SAM	N3-C4-N9	4.02	134.01	127.17
2	A	401	SAM	CB-CA-N	-4.00	99.70	110.12
2	H	402	SAM	C5-C4-N3	-4.00	121.22	126.72
2	F	401	SAM	C5-C4-N3	-3.98	121.24	126.72
2	H	401	SAM	C2-N1-C6	3.81	124.99	118.73
2	B	401	SAM	C4-N9-C1'	-3.81	117.73	126.63
2	E	402	SAM	N3-C4-N9	3.77	133.57	127.17
2	G	401	SAM	C4-N9-C8	3.75	109.67	105.74
2	B	402	SAM	CG-SD-C5'	3.73	112.55	103.43
2	E	401	SAM	N3-C4-N9	3.70	133.46	127.17
2	H	401	SAM	N3-C2-N1	-3.61	123.12	128.58
2	H	402	SAM	C4'-O4'-C1'	-3.61	101.50	109.47
2	B	402	SAM	C4-N9-C8	3.58	109.50	105.74
2	H	401	SAM	O4'-C4'-C3'	3.58	112.27	105.15
2	F	402	SAM	N3-C4-N9	3.57	133.24	127.17
2	E	402	SAM	C5-C6-N6	-3.53	114.54	123.29
2	H	402	SAM	N9-C8-N7	-3.43	109.07	113.94
2	A	401	SAM	N3-C2-N1	-3.40	123.43	128.58
2	G	402	SAM	OXT-C-O	-3.38	116.41	124.08
2	B	402	SAM	C2-N3-C4	3.38	120.08	111.83
2	H	401	SAM	C4-N9-C1'	-3.36	118.78	126.63
2	E	401	SAM	CG-SD-C5'	-3.34	95.27	103.43
2	H	401	SAM	C5-C4-N3	-3.33	122.14	126.72
2	B	401	SAM	C1'-N9-C8	3.29	134.40	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	SAM	C5-C4-N3	-3.26	122.22	126.72
2	H	401	SAM	N6-C6-N1	3.24	125.59	118.38
2	E	402	SAM	N9-C8-N7	-3.21	109.39	113.94
2	F	402	SAM	C2-N1-C6	-3.16	113.54	118.73
2	H	402	SAM	O2'-C2'-C1'	-3.14	99.31	110.10
2	B	401	SAM	C5-C4-N3	-3.11	122.43	126.72
2	E	401	SAM	C4-N9-C8	3.01	108.90	105.74
2	A	402	SAM	N3-C4-N9	3.00	132.26	127.17
2	G	402	SAM	N3-C2-N1	-2.97	124.08	128.58
2	F	402	SAM	C2-N3-C4	2.97	119.09	111.83
2	E	402	SAM	O4'-C4'-C3'	-2.97	99.26	105.15
2	F	401	SAM	O2'-C2'-C1'	-2.95	99.95	110.10
2	H	402	SAM	C2-N3-C4	2.95	119.03	111.83
2	H	401	SAM	C4'-O4'-C1'	-2.94	102.96	109.47
2	F	401	SAM	C5-C6-N6	-2.94	116.00	123.29
2	G	401	SAM	N9-C8-N7	-2.93	109.77	113.94
2	H	401	SAM	C4-N9-C8	2.88	108.76	105.74
2	A	401	SAM	C5-C4-N3	-2.83	122.82	126.72
2	F	402	SAM	C5-C6-N6	-2.82	116.29	123.29
2	F	401	SAM	N3-C4-N9	2.81	131.94	127.17
2	E	401	SAM	C5-C6-N6	-2.81	116.33	123.29
2	E	402	SAM	C5-C4-N3	-2.81	122.85	126.72
2	B	402	SAM	N9-C8-N7	-2.79	109.98	113.94
2	B	402	SAM	C4-C5-N7	-2.73	107.45	110.58
2	F	402	SAM	CE-SD-C5'	2.73	121.97	100.54
2	G	402	SAM	C4-N9-C1'	-2.70	120.31	126.63
2	A	401	SAM	C4-N9-C8	2.70	108.57	105.74
2	A	402	SAM	C5-C4-N3	-2.70	123.00	126.72
2	G	401	SAM	C5-C4-N3	-2.69	123.01	126.72
2	H	401	SAM	C5-C6-N6	-2.67	116.68	123.29
2	A	402	SAM	OXT-C-O	-2.58	118.22	124.08
2	A	401	SAM	C4-N9-C1'	-2.58	120.61	126.63
2	B	401	SAM	C2'-C1'-N9	-2.56	106.95	113.30
2	E	401	SAM	C4-N9-C1'	-2.55	120.67	126.63
2	E	402	SAM	C5-C4-N9	-2.52	103.07	105.81
2	E	401	SAM	C2'-C3'-C4'	-2.50	97.78	102.61
2	E	401	SAM	C5-N7-C8	-2.48	99.55	103.45
2	G	402	SAM	C5-C6-N6	-2.48	117.15	123.29
2	B	401	SAM	N9-C8-N7	-2.47	110.43	113.94
2	F	402	SAM	C5-C6-N1	2.45	123.72	117.51
2	F	401	SAM	C4-C5-N7	-2.43	107.80	110.58
2	B	402	SAM	N3-C2-N1	-2.43	124.91	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	401	SAM	C1'-N9-C8	2.42	132.47	127.09
2	F	401	SAM	C6-C5-N7	2.42	136.75	132.09
2	F	401	SAM	C4-N9-C8	2.42	108.27	105.74
2	F	402	SAM	O3'-C3'-C2'	2.41	119.55	111.82
2	H	401	SAM	O4'-C1'-C2'	2.41	111.78	106.62
2	E	402	SAM	CB-CA-N	-2.39	103.89	110.12
2	E	402	SAM	C2-N3-C4	2.37	117.63	111.83
2	G	402	SAM	O2'-C2'-C1'	-2.36	101.98	110.10
2	A	401	SAM	C5-C6-N6	-2.36	117.45	123.29
2	A	401	SAM	N6-C6-N1	2.33	123.57	118.38
2	G	401	SAM	O4'-C4'-C3'	2.33	109.78	105.15
2	A	401	SAM	C2-N3-C4	2.32	117.51	111.83
2	H	401	SAM	C5-C4-N9	-2.31	103.29	105.81
2	E	402	SAM	N6-C6-N1	2.30	123.50	118.38
2	E	401	SAM	C6-C5-C4	-2.28	114.07	117.18
2	B	402	SAM	C5-N7-C8	2.27	107.01	103.45
2	B	401	SAM	C4-C5-N7	-2.25	108.01	110.58
2	B	401	SAM	C6-C5-C4	2.25	120.25	117.18
2	H	402	SAM	OXT-C-O	-2.22	119.04	124.08
2	G	401	SAM	CB-CA-C	2.20	116.27	110.45
2	H	401	SAM	C2-N3-C4	2.19	117.17	111.83
2	G	401	SAM	OXT-C-O	-2.17	119.16	124.08
2	F	401	SAM	C2-N3-C4	2.17	117.13	111.83
2	H	401	SAM	O4'-C1'-N9	2.15	112.22	108.09
2	B	402	SAM	OXT-C-O	-2.15	119.21	124.08
2	G	401	SAM	C2'-C3'-C4'	-2.14	98.48	102.61
2	B	401	SAM	OXT-C-O	-2.12	119.27	124.08
2	F	401	SAM	C3'-C2'-C1'	2.09	105.42	101.46
2	A	401	SAM	N3-C4-N9	2.09	130.71	127.17
2	E	401	SAM	OXT-C-O	2.05	128.73	124.08
2	H	401	SAM	C2'-C3'-C4'	-2.05	98.66	102.61
2	B	401	SAM	C4-N9-C8	2.03	107.87	105.74
2	H	402	SAM	C6-C5-N7	2.02	135.98	132.09
2	G	402	SAM	C6-C5-C4	-2.02	114.42	117.18
2	F	401	SAM	N6-C6-N1	2.01	122.84	118.38
2	E	402	SAM	O4'-C1'-C2'	-2.00	102.33	106.62

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	402	SAM	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	F	402	SAM	C-CA-CB-CG
2	A	401	SAM	OXT-C-CA-N
2	F	401	SAM	C2'-C1'-N9-C8
2	E	401	SAM	OXT-C-CA-CB
2	H	401	SAM	O-C-CA-CB
2	A	401	SAM	C2'-C1'-N9-C8
2	E	401	SAM	C2'-C1'-N9-C8
2	G	401	SAM	C2'-C1'-N9-C8
2	H	401	SAM	C2'-C1'-N9-C8
2	F	402	SAM	CA-CB-CG-SD
2	B	401	SAM	C2'-C1'-N9-C8
2	G	401	SAM	O-C-CA-CB
2	H	401	SAM	OXT-C-CA-CB
2	A	401	SAM	O-C-CA-CB
2	B	401	SAM	OXT-C-CA-CB
2	E	401	SAM	O-C-CA-CB
2	G	401	SAM	OXT-C-CA-CB
2	F	401	SAM	O-C-CA-CB
2	E	402	SAM	O-C-CA-N
2	B	401	SAM	O-C-CA-CB
2	A	401	SAM	OXT-C-CA-CB
2	A	401	SAM	O4'-C1'-N9-C8
2	F	401	SAM	O4'-C1'-N9-C8
2	E	401	SAM	O4'-C1'-N9-C8
2	G	401	SAM	O4'-C1'-N9-C8
2	H	401	SAM	O4'-C1'-N9-C8
2	E	402	SAM	O4'-C1'-N9-C8
2	F	401	SAM	CA-CB-CG-SD
2	F	401	SAM	OXT-C-CA-CB
2	H	402	SAM	O4'-C1'-N9-C8
2	A	402	SAM	O-C-CA-N
2	B	401	SAM	O-C-CA-N
2	E	401	SAM	OXT-C-CA-N

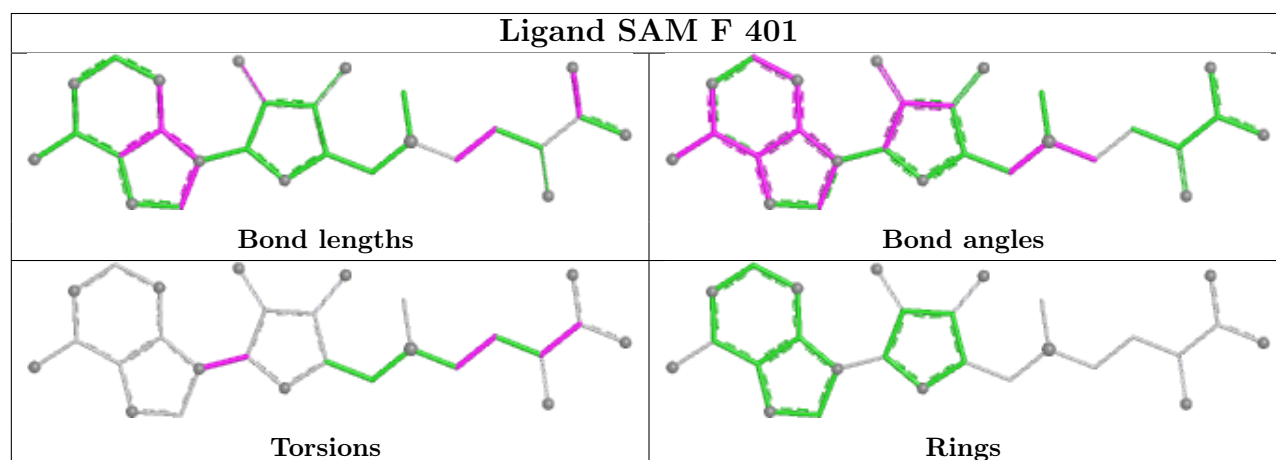
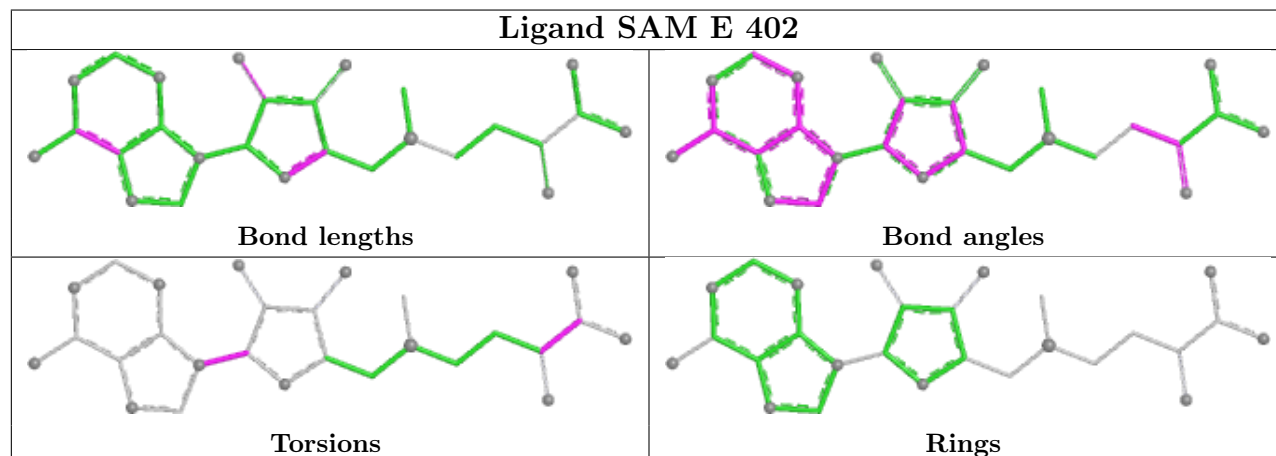
There are no ring outliers.

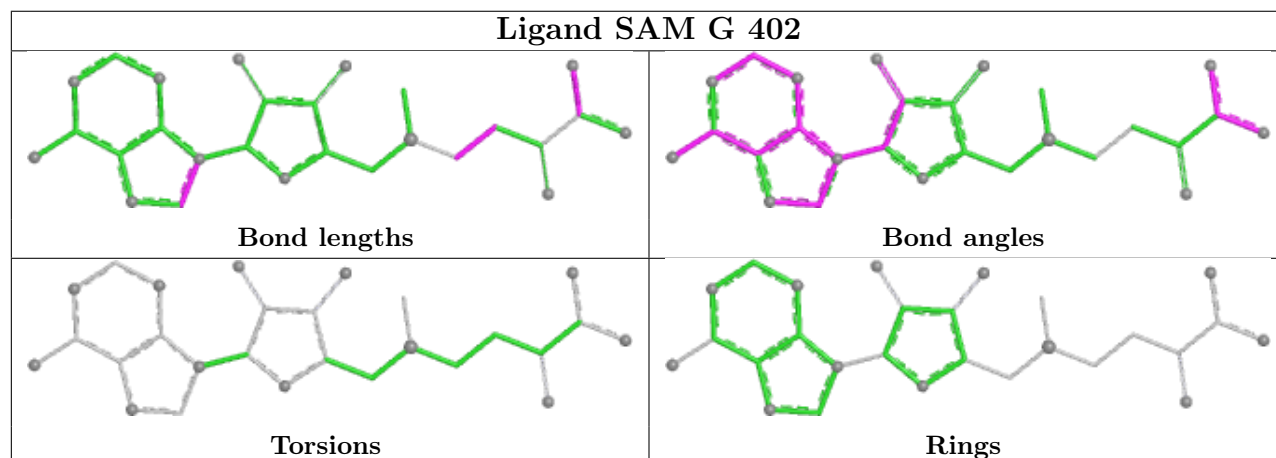
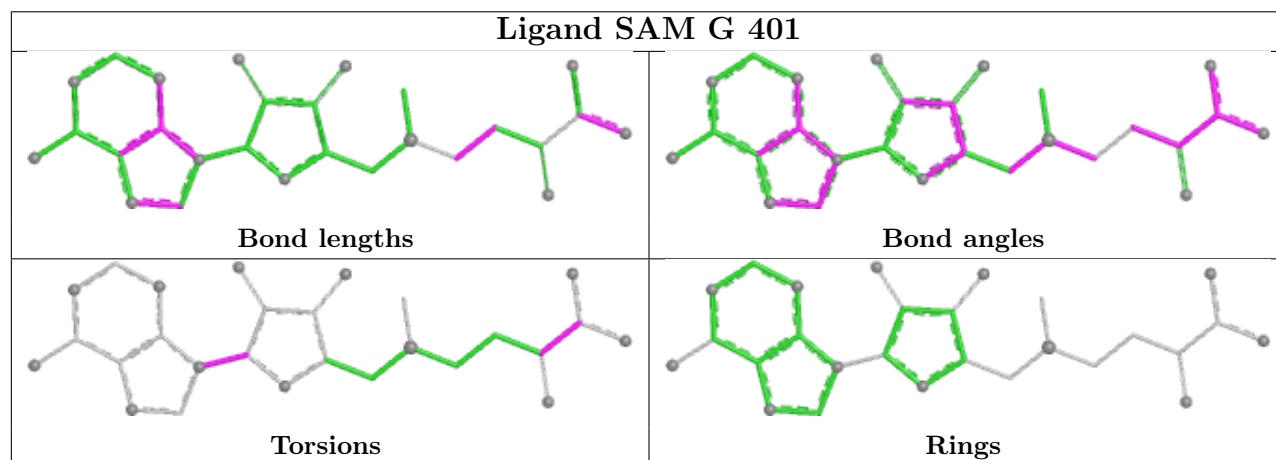
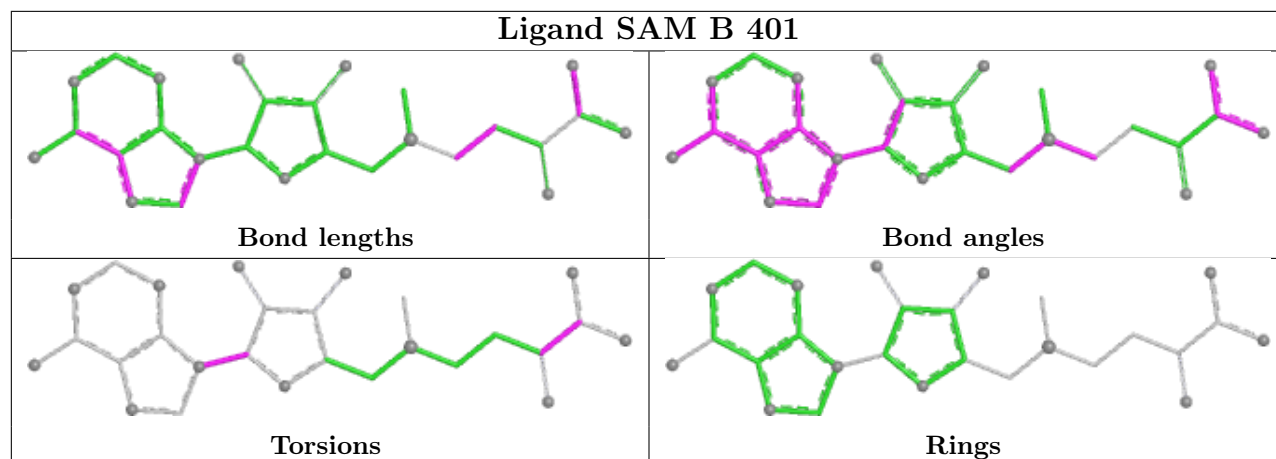
1 monomer is involved in 1 short contact:

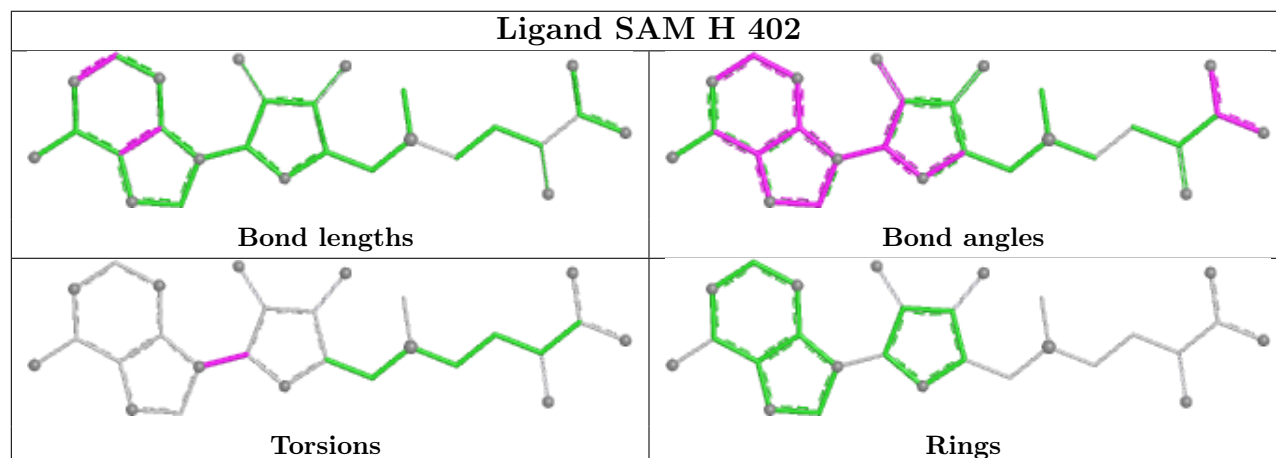
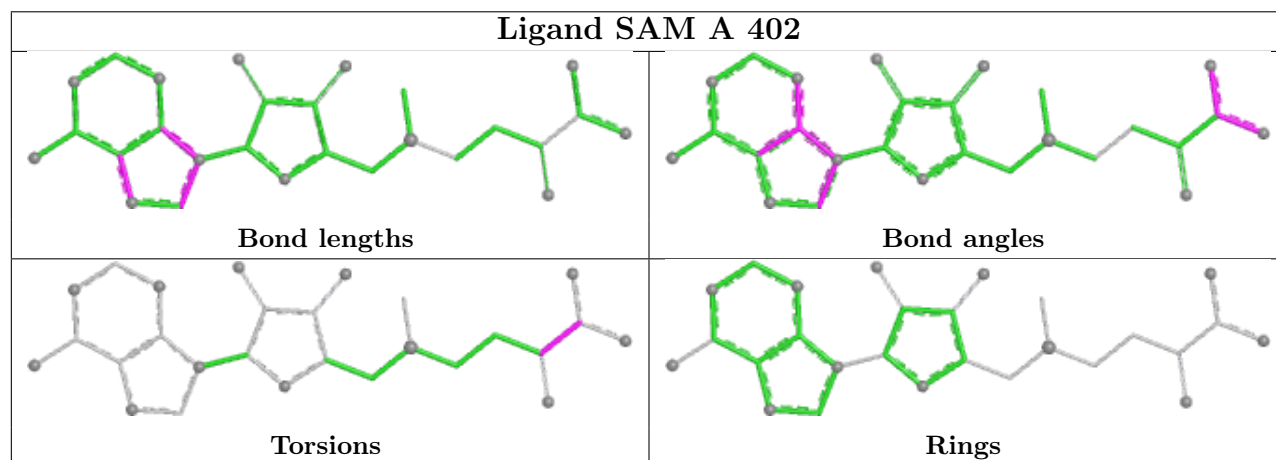
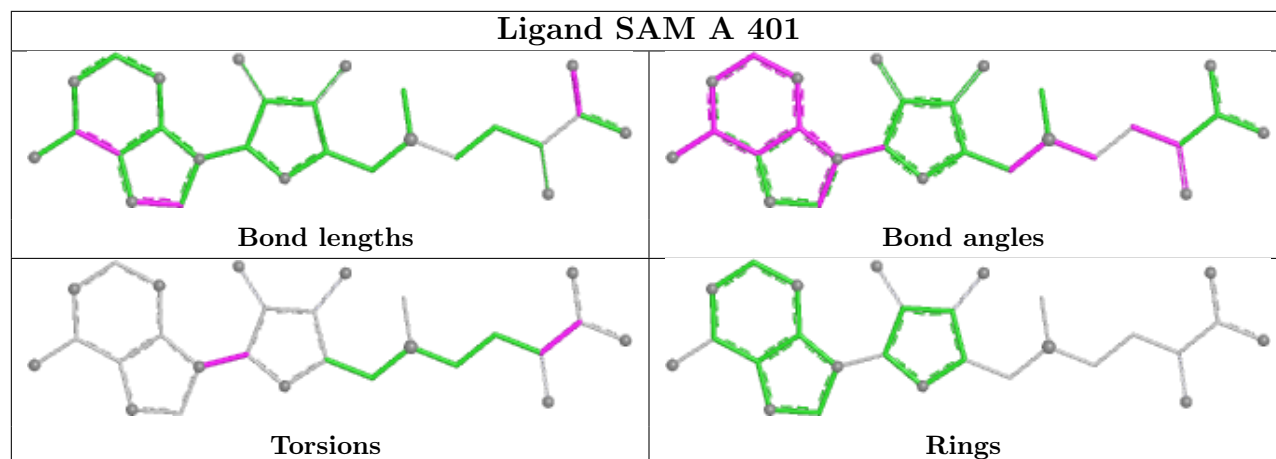
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	401	SAM	1	0

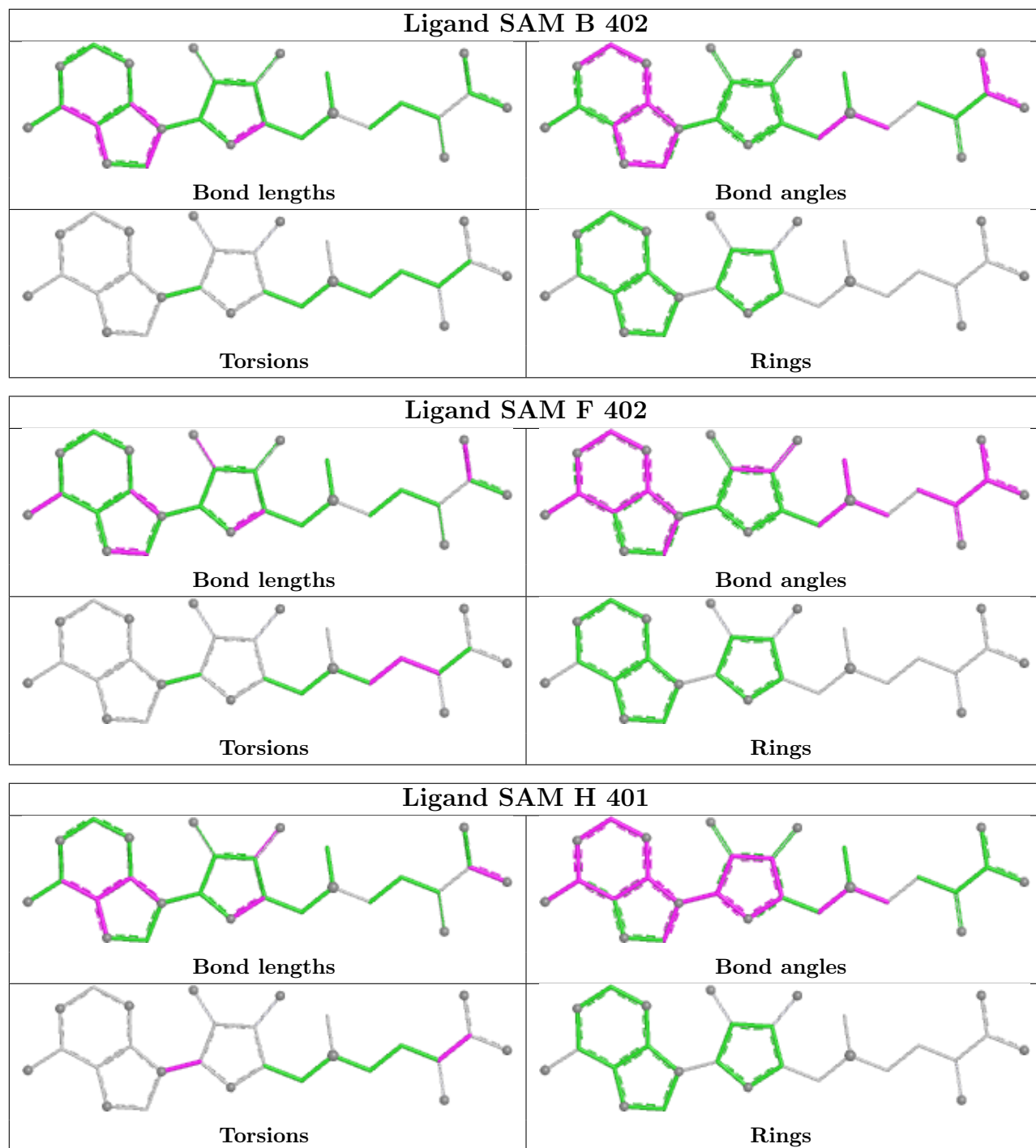
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

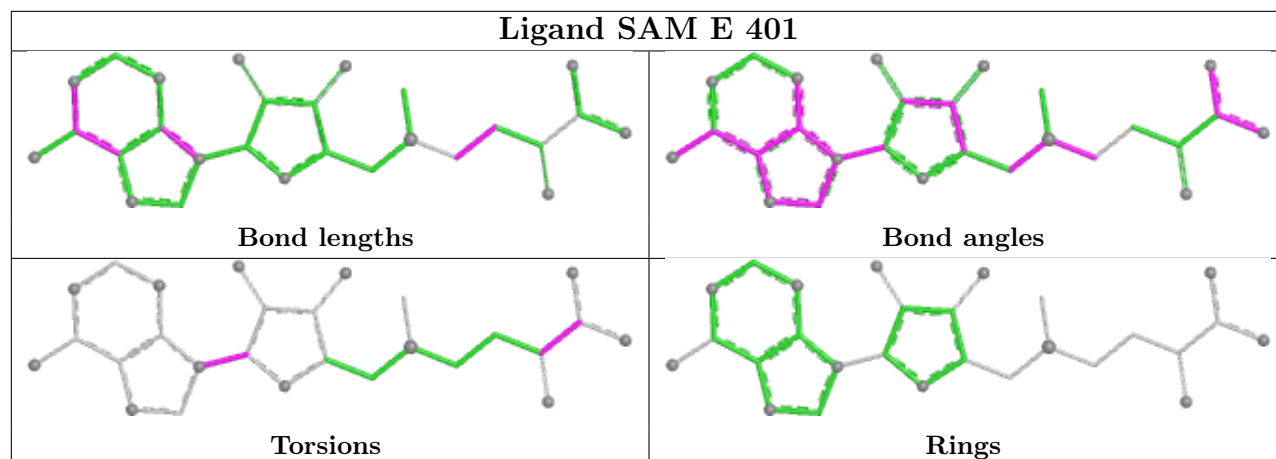
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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	374/382 (97%)	-0.29	1 (0%) 90 90	15, 30, 44, 93	11 (2%)
1	B	374/382 (97%)	0.00	9 (2%) 59 60	17, 35, 58, 100	6 (1%)
1	E	375/382 (98%)	-0.22	5 (1%) 75 75	14, 31, 52, 85	7 (1%)
1	F	374/382 (97%)	-0.12	5 (1%) 75 75	15, 32, 51, 97	5 (1%)
1	G	375/382 (98%)	0.31	11 (2%) 53 53	24, 42, 72, 119	3 (0%)
1	H	373/382 (97%)	0.07	4 (1%) 78 78	19, 38, 62, 80	7 (1%)
All	All	2245/2292 (97%)	-0.04	35 (1%) 70 71	14, 34, 59, 119	39 (1%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	TYR	5.6
1	E	104	THR	4.3
1	G	3	TYR	4.0
1	F	3	TYR	3.9
1	G	377	HIS	3.6
1	A	377	HIS	3.6
1	G	104	THR	3.6
1	G	375	SER	3.2
1	B	170	SER	3.2
1	F	106	LYS	3.0
1	G	304	TYR	3.0
1	F	116	ILE	2.9
1	F	105	ASN	2.9
1	B	104	THR	2.9
1	F	104	THR	2.8
1	H	317	LYS	2.8
1	B	173	LEU	2.7
1	G	319	PHE	2.6
1	B	171	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	106	LYS	2.4
1	B	169	ASN	2.3
1	G	107	ASN	2.3
1	E	105	ASN	2.2
1	E	48	CYS	2.2
1	B	312	LEU	2.1
1	G	312	LEU	2.1
1	B	304	TYR	2.1
1	E	304	TYR	2.1
1	H	104	THR	2.1
1	G	212	ASN	2.1
1	G	48[A]	CYS	2.1
1	G	106	LYS	2.0
1	H	316	THR	2.0
1	B	106	LYS	2.0
1	H	304	TYR	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	G	402	27/27	0.92	0.10	35,39,55,58	0
2	SAM	A	402	27/27	0.95	0.07	25,29,42,46	0
2	SAM	F	402	27/27	0.95	0.08	28,34,55,58	0
2	SAM	G	401	27/27	0.95	0.08	28,33,42,46	0
2	SAM	A	401	27/27	0.95	0.08	25,29,38,42	0
2	SAM	B	402	27/27	0.96	0.07	31,35,50,52	0
2	SAM	E	401	27/27	0.96	0.07	27,29,42,45	0

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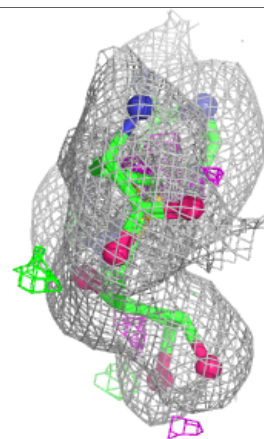
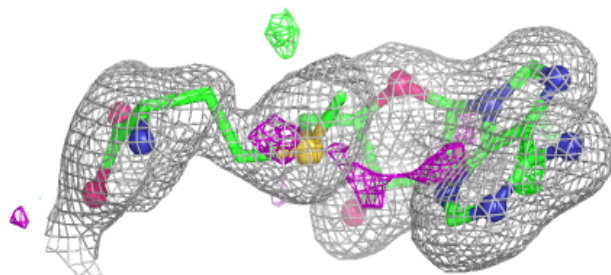
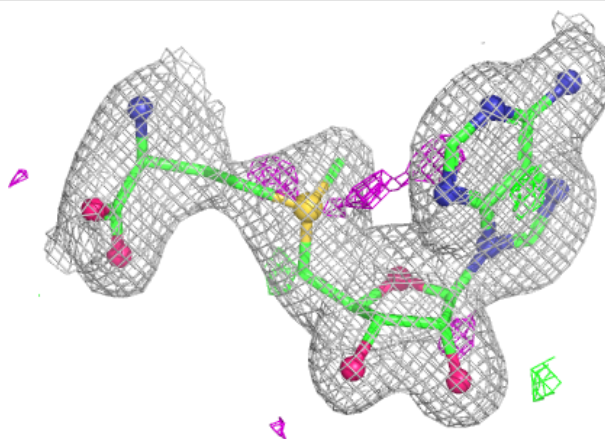
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SAM	E	402	27/27	0.96	0.06	26,28,33,38	0
2	SAM	H	401	27/27	0.96	0.07	37,40,47,48	0
2	SAM	B	401	27/27	0.97	0.06	27,31,42,43	0
2	SAM	F	401	27/27	0.97	0.06	26,27,35,37	0
2	SAM	H	402	27/27	0.97	0.06	26,29,43,45	0
3	CL	A	403	1/1	0.99	0.04	34,34,34,34	0
3	CL	B	403	1/1	0.99	0.09	34,34,34,34	0
3	CL	E	403	1/1	0.99	0.08	33,33,33,33	0
3	CL	F	403	1/1	0.99	0.03	31,31,31,31	0
3	CL	G	403	1/1	0.99	0.04	38,38,38,38	0
3	CL	H	403	1/1	0.99	0.11	39,39,39,39	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.

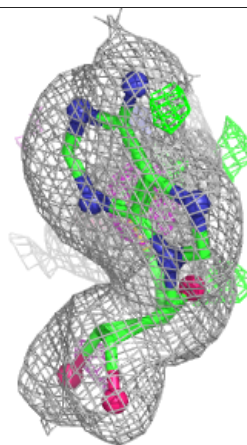
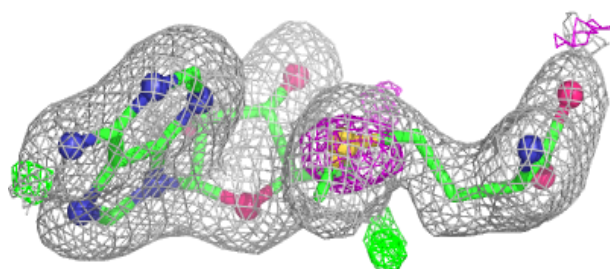
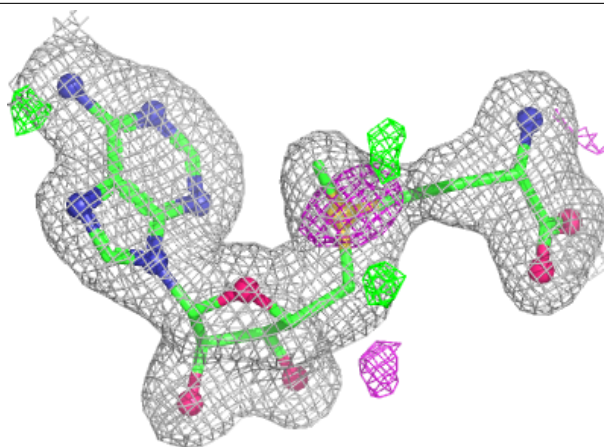
Electron density around SAM G 402:

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



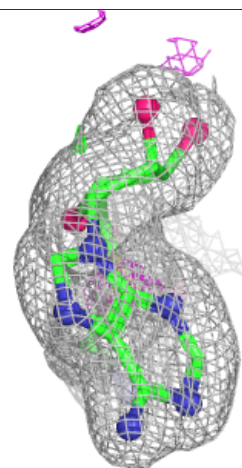
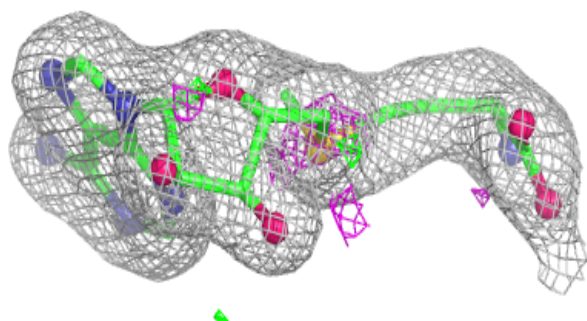
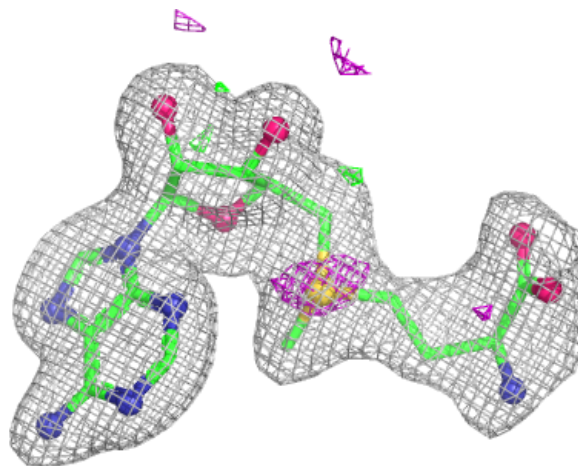
Electron density around SAM A 402:

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



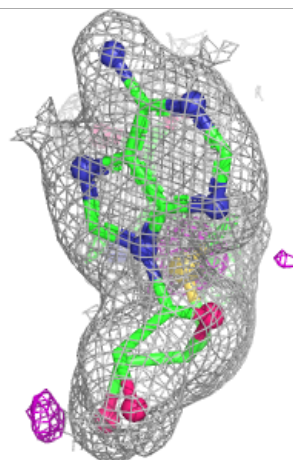
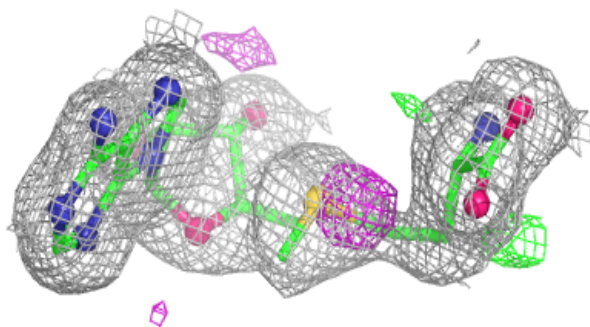
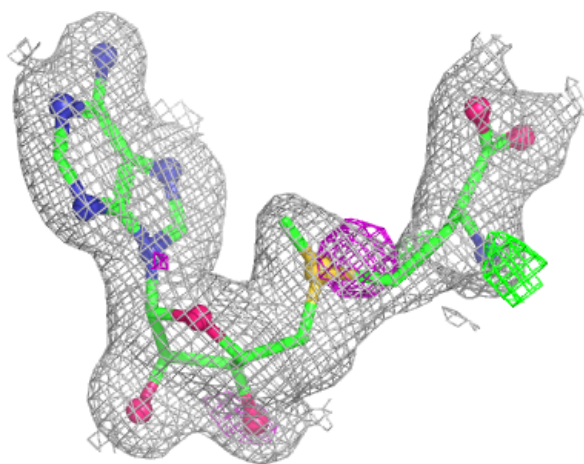
Electron density around SAM F 402:

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



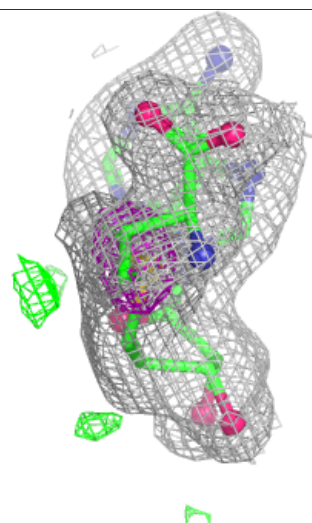
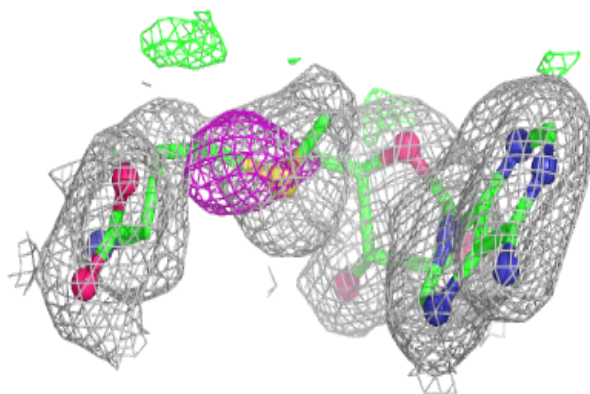
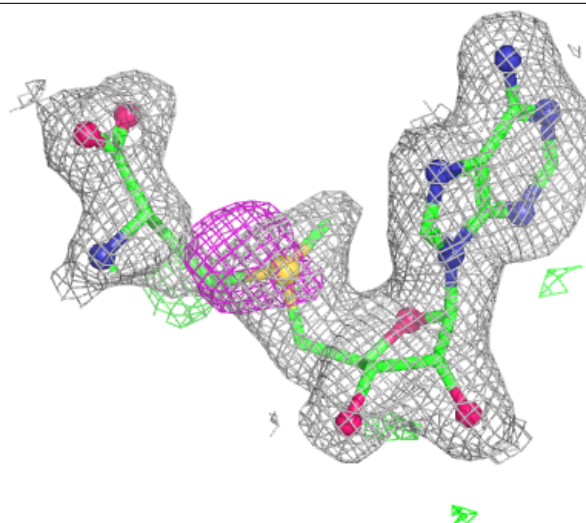
Electron density around SAM G 401:

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



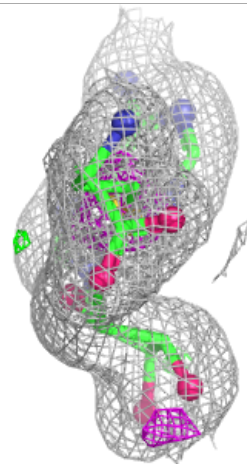
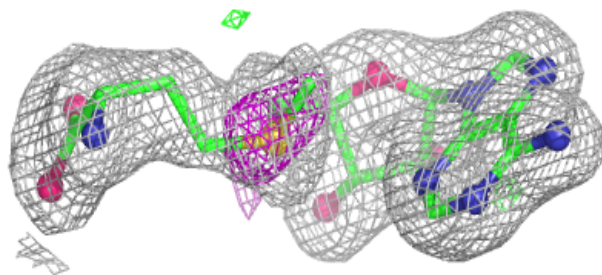
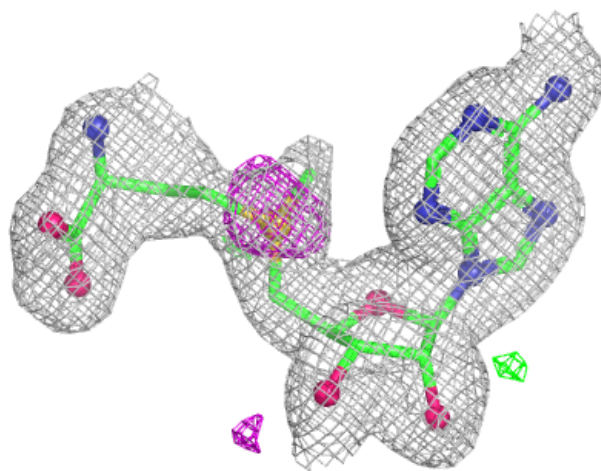
Electron density around SAM A 401:

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



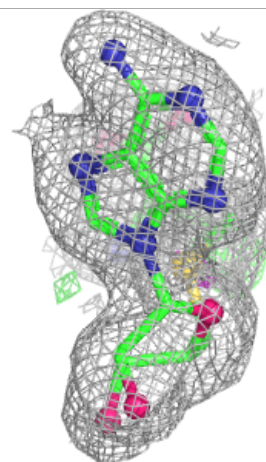
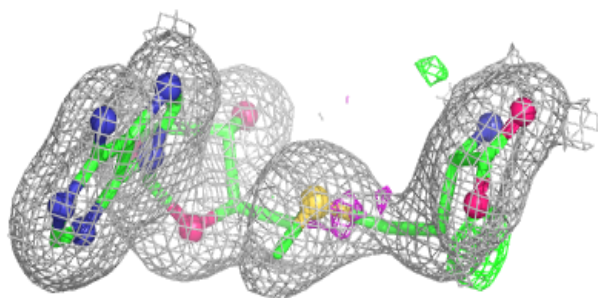
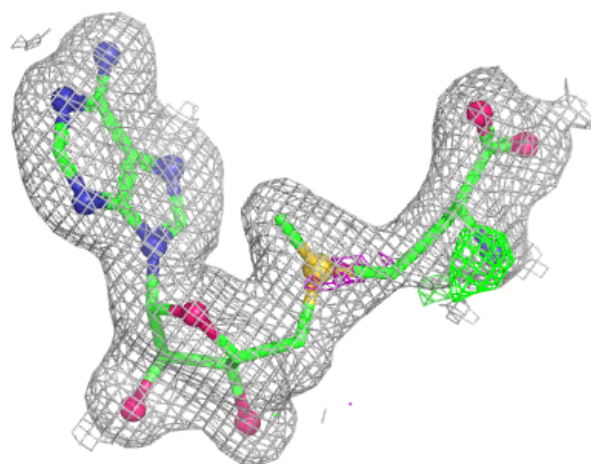
Electron density around SAM B 402:

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



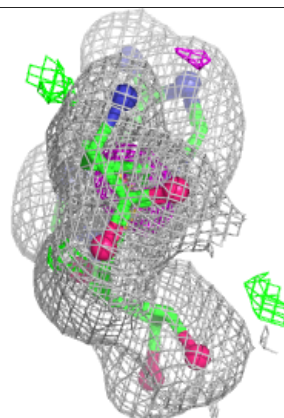
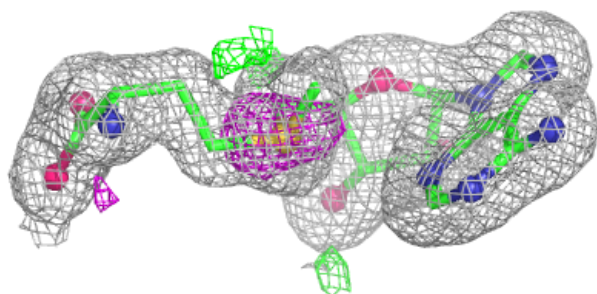
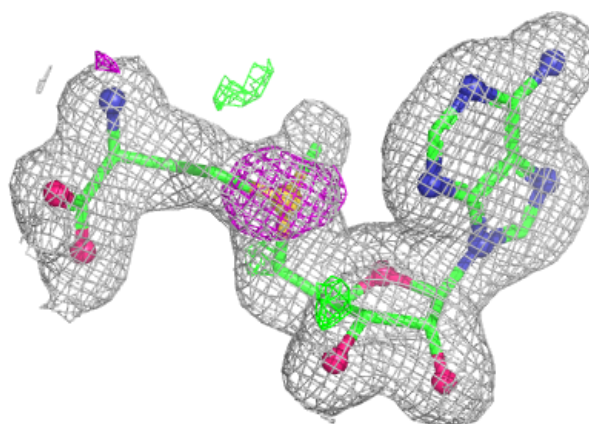
Electron density around SAM E 401:

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



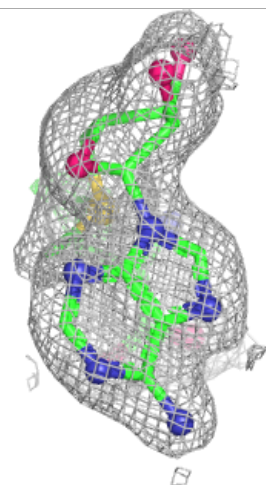
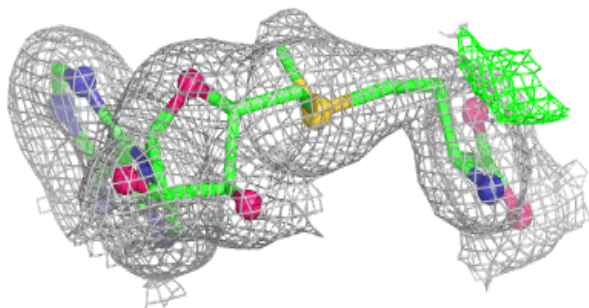
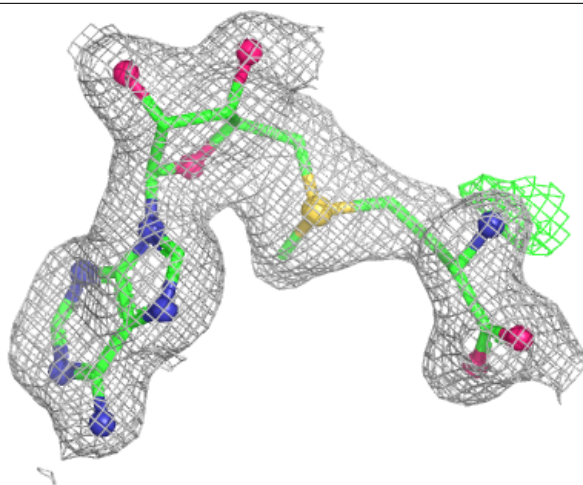
Electron density around SAM E 402:

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



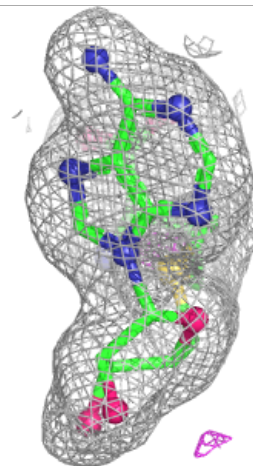
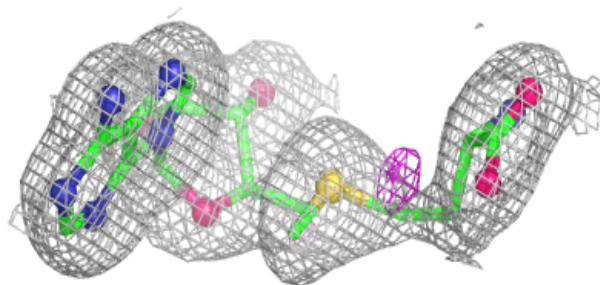
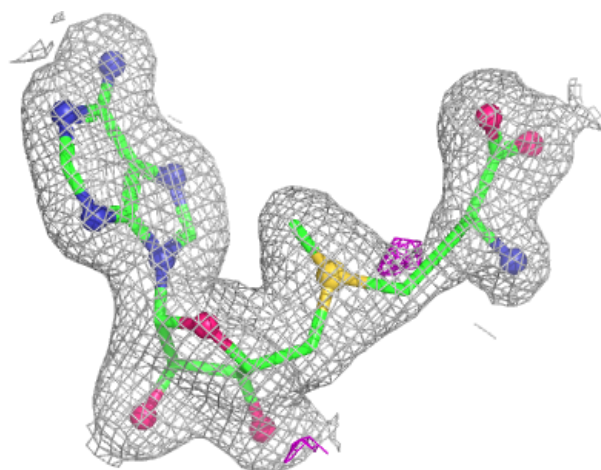
Electron density around SAM H 401:

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



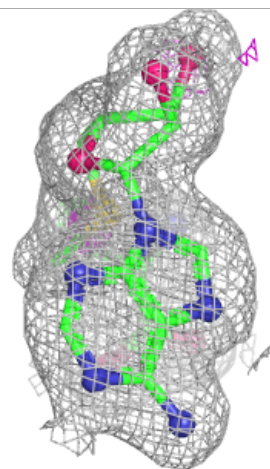
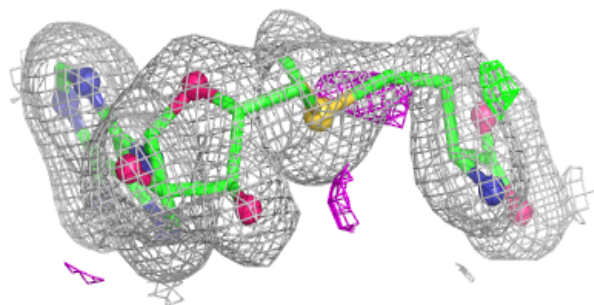
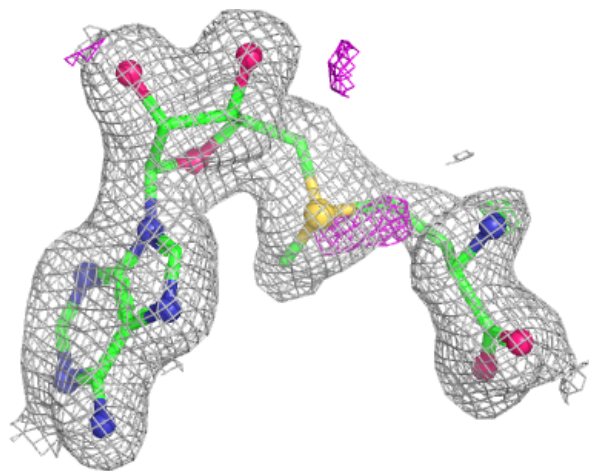
Electron density around SAM B 401:

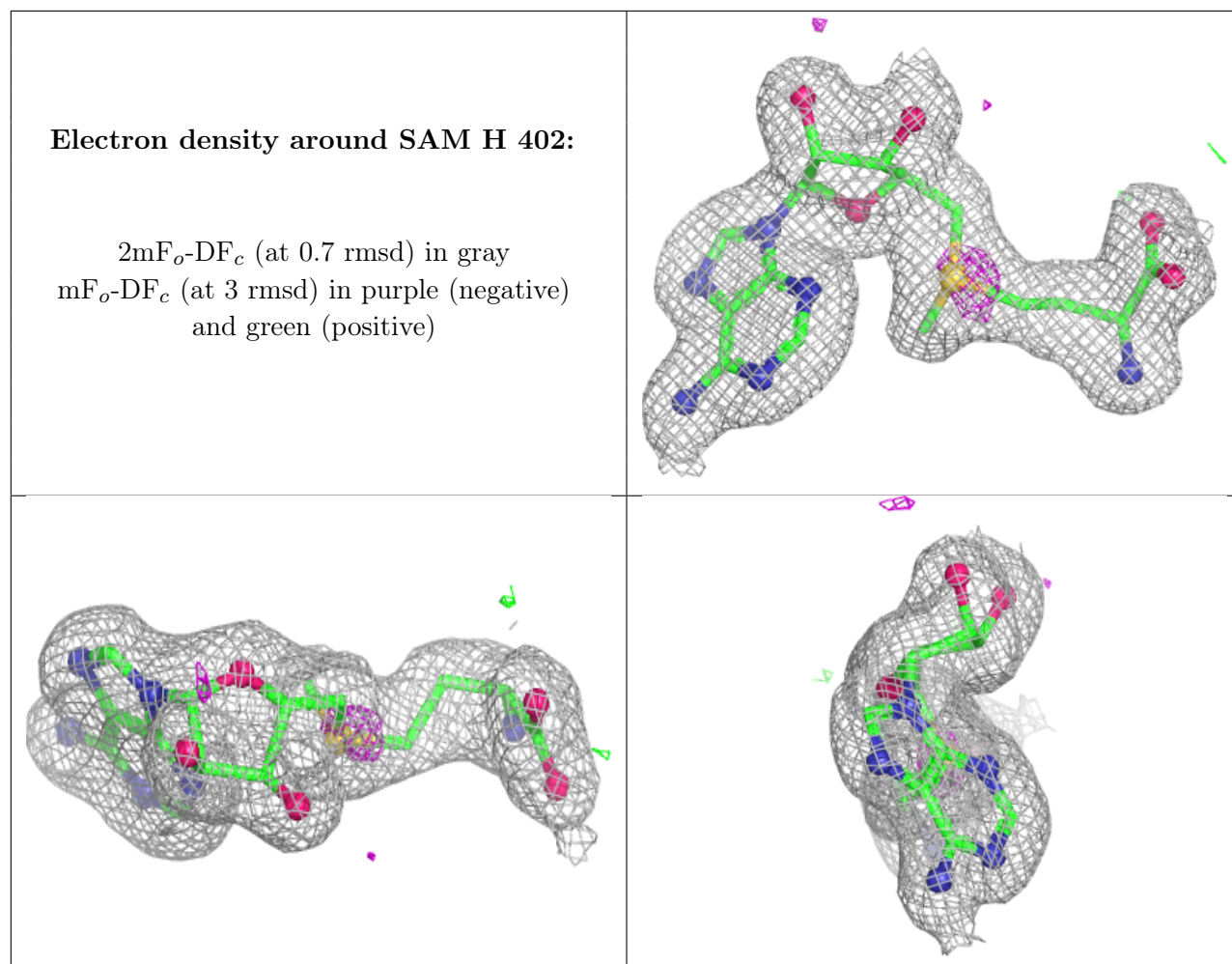
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SAM F 401:

$2mF_o-DF_c$ (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.