Full wwPDB X-ray Structure Validation Report ⓘ

Jan 14, 2024 – 01:23 pm GMT

PDB ID	:	6RK7
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.

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:

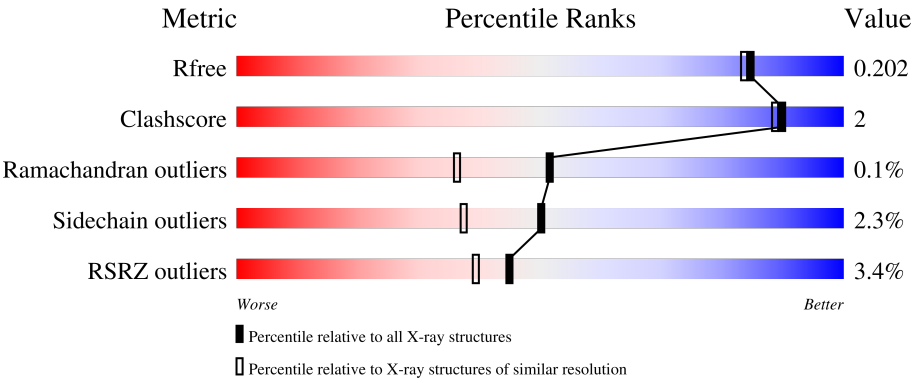
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (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 <=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	85% 12%
1	B	382	2% 89% 8%
1	E	382	% 88% 9%
1	F	382	2% 88% 9%
1	G	382	9% 88% 9%

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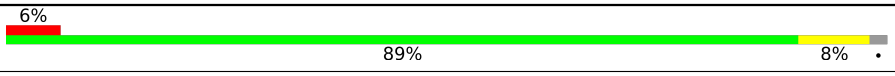
Mol	Chain	Length	Quality of chain
1	H	382	

2 Entry composition (i)

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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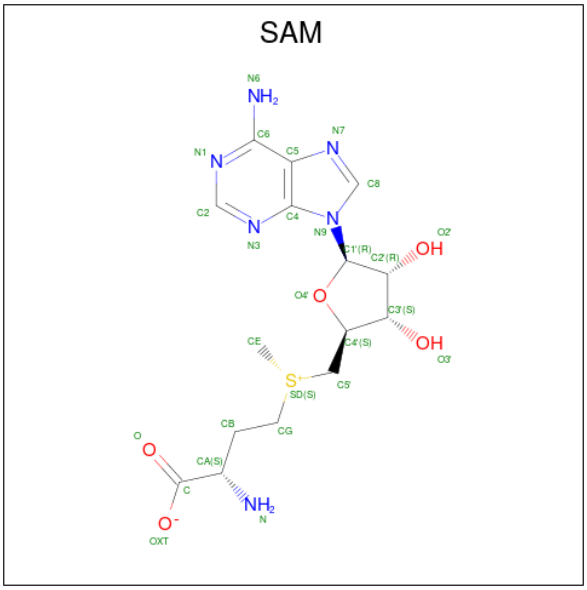
Chain	Residue	Modelled	Actual	Comment	Reference
E	382	HIS	-	expression tag	UNP B2NE58
F	377	HIS	-	expression tag	UNP B2NE58
F	378	HIS	-	expression tag	UNP B2NE58
F	379	HIS	-	expression tag	UNP B2NE58
F	380	HIS	-	expression tag	UNP B2NE58
F	381	HIS	-	expression tag	UNP B2NE58
F	382	HIS	-	expression tag	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 (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



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 (three-letter code: 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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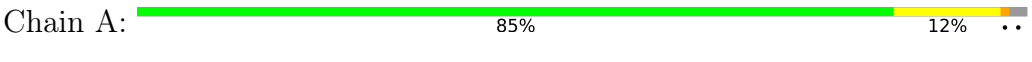
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	214	Total O 214 214	0	0
4	E	278	Total O 278 278	0	0
4	F	245	Total O 245 245	0	0
4	G	162	Total O 162 162	0	0
4	H	198	Total O 198 198	0	0

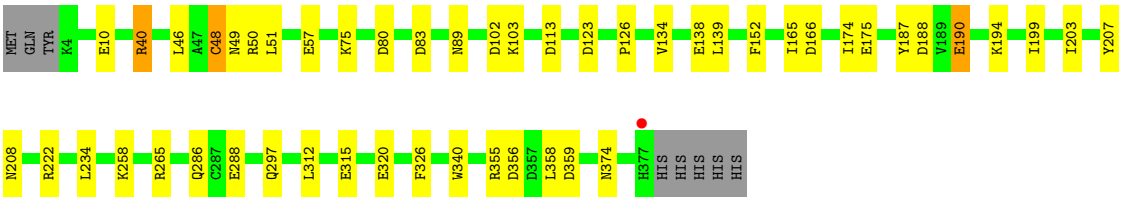
3 Residue-property plots (i)

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: Methionine adenosyltransferase

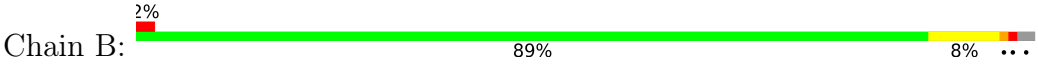
Chain A:

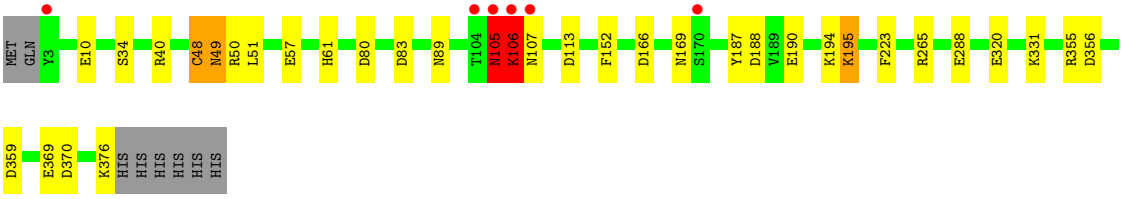




• Molecule 1: Methionine adenosyltransferase

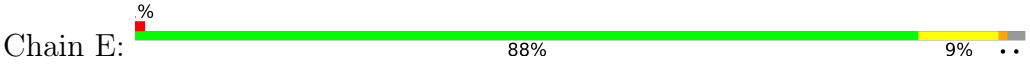
Chain B:

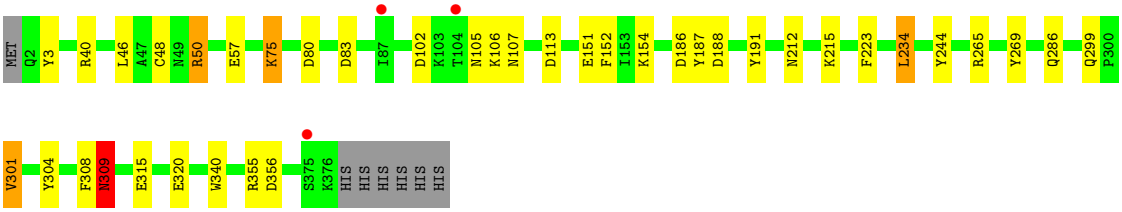




• Molecule 1: Methionine adenosyltransferase

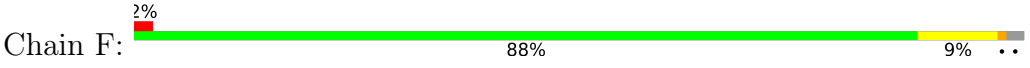
Chain E:

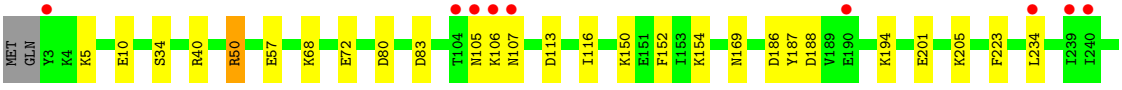


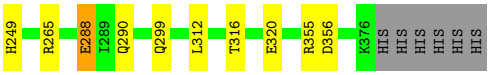


• Molecule 1: Methionine adenosyltransferase

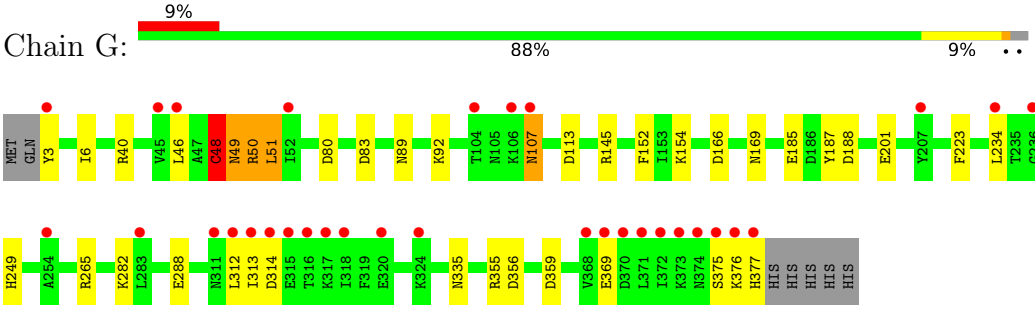
Chain F:



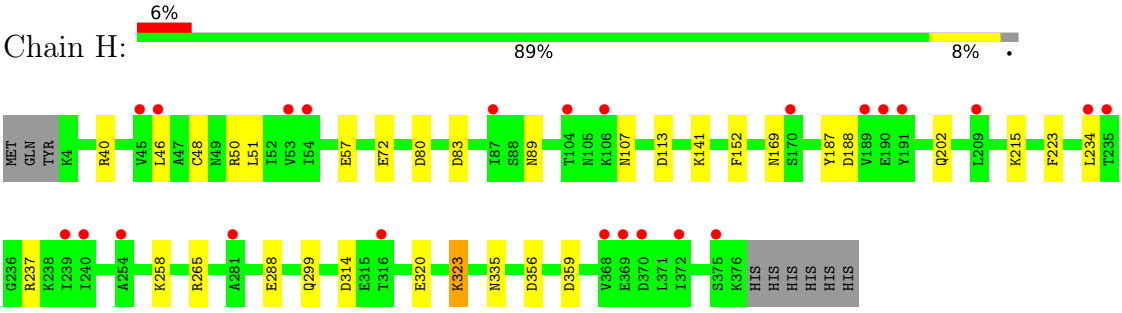




• Molecule 1: Methionine adenosyltransferase



• Molecule 1: Methionine adenosyltransferase



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (5.04%)	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)	0.33 , 40.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	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.*

[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: 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	1.22	15/3079 (0.5%)	1.24	21/4161 (0.5%)
1	B	1.11	10/3035 (0.3%)	1.09	17/4103 (0.4%)
1	E	1.17	11/3050 (0.4%)	1.12	22/4123 (0.5%)
1	F	1.14	9/3029 (0.3%)	1.07	18/4094 (0.4%)
1	G	1.04	6/3025 (0.2%)	1.06	21/4091 (0.5%)
1	H	1.05	5/3026 (0.2%)	1.05	17/4092 (0.4%)
All	All	1.12	56/18244 (0.3%)	1.11	116/24664 (0.5%)

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 (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	10	GLU	CD-OE1	9.94	1.36	1.25
1	G	48[A]	CYS	CB-SG	9.10	1.97	1.82
1	G	48[B]	CYS	CB-SG	9.10	1.97	1.82
1	F	57	GLU	CD-OE2	9.02	1.35	1.25
1	A	48[A]	CYS	CB-SG	8.94	1.97	1.82
1	A	48[B]	CYS	CB-SG	8.94	1.97	1.82
1	B	57	GLU	CD-OE1	8.33	1.34	1.25
1	E	356	ASP	CB-CG	7.72	1.68	1.51
1	F	356	ASP	CB-CG	7.61	1.67	1.51
1	B	48[A]	CYS	CB-SG	7.47	1.95	1.82
1	B	48[B]	CYS	CB-SG	7.47	1.95	1.82
1	B	288	GLU	CD-OE1	-7.30	1.17	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	48	CYS	CB-SG	7.12	1.94	1.82
1	E	286	GLN	CD-NE2	-7.11	1.15	1.32
1	E	309	ASN	CB-CG	-7.04	1.34	1.51
1	H	335[A]	ASN	CB-CG	6.99	1.67	1.51
1	H	335[B]	ASN	CB-CG	6.99	1.67	1.51
1	A	190	GLU	CG-CD	6.79	1.62	1.51
1	F	201	GLU	CD-OE1	6.02	1.32	1.25
1	E	151	GLU	CD-OE2	-5.99	1.19	1.25
1	E	315	GLU	CG-CD	5.98	1.60	1.51
1	E	191	TYR	CG-CD2	5.96	1.46	1.39
1	A	315	GLU	CD-OE1	5.94	1.32	1.25
1	G	356	ASP	CB-CG	5.90	1.64	1.51
1	H	320	GLU	CD-OE2	5.85	1.32	1.25
1	A	288	GLU	CD-OE2	-5.84	1.19	1.25
1	F	288	GLU	CD-OE1	-5.83	1.19	1.25
1	F	320	GLU	CG-CD	5.82	1.60	1.51
1	A	320	GLU	CG-CD	5.76	1.60	1.51
1	B	369	GLU	CD-OE2	5.75	1.31	1.25
1	A	10	GLU	CG-CD	5.72	1.60	1.51
1	A	75	LYS	CD-CE	-5.66	1.37	1.51
1	A	374	ASN	CG-ND2	-5.65	1.18	1.32
1	A	286	GLN	CD-OE1	-5.64	1.11	1.24
1	A	57	GLU	CD-OE1	5.64	1.31	1.25
1	G	185	GLU	CD-OE1	-5.62	1.19	1.25
1	B	34	SER	CB-OG	-5.52	1.35	1.42
1	E	340	TRP	CE3-CZ3	5.52	1.47	1.38
1	B	320	GLU	CG-CD	5.45	1.60	1.51
1	B	356	ASP	CB-CG	5.44	1.63	1.51
1	A	326	PHE	CE2-CZ	5.40	1.47	1.37
1	F	105	ASN	C-O	5.37	1.33	1.23
1	F	10	GLU	CD-OE2	5.35	1.31	1.25
1	E	57	GLU	CD-OE2	5.35	1.31	1.25
1	A	175	GLU	CG-CD	-5.34	1.44	1.51
1	E	286	GLN	CD-OE1	5.32	1.35	1.24
1	G	48[A]	CYS	C-O	5.32	1.33	1.23
1	G	48[B]	CYS	C-O	5.32	1.33	1.23
1	H	356	ASP	CB-CG	5.25	1.62	1.51
1	F	72	GLU	CG-CD	5.21	1.59	1.51
1	A	265	ARG	CZ-NH2	-5.18	1.26	1.33
1	H	57	GLU	CD-OE1	5.16	1.31	1.25
1	F	34	SER	CB-OG	-5.10	1.35	1.42
1	E	320	GLU	CG-CD	5.05	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	GLU	CD-OE2	5.03	1.31	1.25
1	B	288	GLU	CD-OE2	-5.00	1.20	1.25

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	40[A]	ARG	NE-CZ-NH1	-20.72	109.94	120.30
1	A	40[B]	ARG	NE-CZ-NH1	-20.72	109.94	120.30
1	A	265	ARG	NE-CZ-NH2	-17.89	111.36	120.30
1	B	265	ARG	NE-CZ-NH2	-16.71	111.95	120.30
1	A	40[A]	ARG	NE-CZ-NH2	13.27	126.93	120.30
1	A	40[B]	ARG	NE-CZ-NH2	13.27	126.93	120.30
1	F	265	ARG	NE-CZ-NH1	-11.66	114.47	120.30
1	E	40	ARG	NE-CZ-NH1	11.12	125.86	120.30
1	E	265	ARG	NE-CZ-NH1	-10.95	114.83	120.30
1	H	265	ARG	NE-CZ-NH1	-10.36	115.12	120.30
1	B	359	ASP	CB-CG-OD1	10.18	127.46	118.30
1	A	222	ARG	NE-CZ-NH2	-9.86	115.37	120.30
1	G	265	ARG	NE-CZ-NH1	-9.82	115.39	120.30
1	A	222	ARG	NE-CZ-NH1	9.50	125.05	120.30
1	H	80	ASP	CB-CG-OD1	9.22	126.60	118.30
1	B	80	ASP	CB-CG-OD1	8.96	126.36	118.30
1	H	356	ASP	CB-CG-OD1	8.91	126.32	118.30
1	G	80	ASP	CB-CG-OD1	8.85	126.26	118.30
1	F	80	ASP	CB-CG-OD1	8.72	126.15	118.30
1	E	80	ASP	CB-CG-OD1	8.71	126.14	118.30
1	A	80	ASP	CB-CG-OD1	8.64	126.08	118.30
1	G	356	ASP	CB-CG-OD1	8.55	126.00	118.30
1	A	166	ASP	CB-CG-OD2	-8.46	110.69	118.30
1	E	356	ASP	CB-CG-OD1	8.44	125.90	118.30
1	G	201	GLU	OE1-CD-OE2	-8.28	113.36	123.30
1	E	301	VAL	CG1-CB-CG2	8.26	124.12	110.90
1	B	356	ASP	CB-CG-OD1	8.16	125.64	118.30
1	H	40	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	F	312	LEU	CB-CG-CD2	8.00	124.59	111.00
1	F	356	ASP	CB-CG-OD1	7.93	125.44	118.30
1	G	40	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	A	355	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	G	40	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	F	40	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	G	51	LEU	CA-CB-CG	7.04	131.49	115.30
1	F	265	ARG	NE-CZ-NH2	7.02	123.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	312	LEU	CB-CG-CD1	6.99	122.89	111.00
1	H	202	GLN	CA-CB-CG	6.98	128.76	113.40
1	E	265	ARG	NE-CZ-NH2	6.98	123.79	120.30
1	F	150	LYS	CD-CE-NZ	-6.86	95.92	111.70
1	A	356	ASP	CB-CG-OD1	6.82	124.44	118.30
1	G	48[A]	CYS	CB-CA-C	6.82	124.04	110.40
1	G	48[B]	CYS	CB-CA-C	6.82	124.04	110.40
1	A	188	ASP	CB-CG-OD1	6.79	124.41	118.30
1	B	106	LYS	CB-CA-C	6.76	123.92	110.40
1	G	265	ARG	NE-CZ-NH2	6.69	123.64	120.30
1	B	113	ASP	CB-CG-OD1	6.64	124.28	118.30
1	A	265	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	F	188	ASP	CB-CG-OD1	6.50	124.15	118.30
1	F	154	LYS	CD-CE-NZ	-6.47	96.82	111.70
1	E	188	ASP	CB-CG-OD1	6.41	124.07	118.30
1	E	234	LEU	CB-CG-CD2	-6.38	100.16	111.00
1	G	188	ASP	CB-CG-OD1	6.33	124.00	118.30
1	G	50	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	E	40	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	H	80	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	A	113	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	80	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	E	301	VAL	CA-CB-CG1	6.09	120.03	110.90
1	A	315	GLU	CG-CD-OE1	6.05	130.41	118.30
1	B	188	ASP	CB-CG-OD1	6.03	123.73	118.30
1	F	186	ASP	CB-CG-OD1	5.98	123.68	118.30
1	A	358	LEU	CB-CG-CD2	-5.96	100.86	111.00
1	F	113	ASP	CB-CG-OD1	5.95	123.65	118.30
1	G	312	LEU	CA-CB-CG	5.87	128.79	115.30
1	H	188	ASP	CB-CG-OD1	5.85	123.56	118.30
1	E	102	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	E	356	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	H	113	ASP	CB-CG-OD1	5.82	123.54	118.30
1	B	265	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	B	40	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	B	370	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	H	237	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	G	314	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	F	50	ARG	NE-CZ-NH1	-5.61	117.50	120.30
1	H	323	LYS	CB-CG-CD	5.58	126.12	111.60
1	G	355	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	F	234[A]	LEU	CB-CG-CD2	-5.57	101.53	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	234[B]	LEU	CB-CG-CD2	-5.57	101.53	111.00
1	A	315	GLU	CG-CD-OE2	-5.55	107.21	118.30
1	B	355[A]	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	B	355[B]	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	H	188	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	G	359	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	B	331	LYS	CD-CE-NZ	-5.48	99.10	111.70
1	H	40	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	H	265	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	E	113	ASP	CB-CG-OD1	5.41	123.17	118.30
1	G	3	TYR	N-CA-C	5.41	125.61	111.00
1	F	50	ARG	NE-CZ-NH2	5.40	123.00	120.30
1	B	166	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	E	269	TYR	CB-CG-CD1	5.39	124.24	121.00
1	E	75	LYS	CD-CE-NZ	5.39	124.09	111.70
1	E	355[A]	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	E	355[B]	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	H	141	LYS	CG-CD-CE	5.36	127.99	111.90
1	H	359	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	A	103	LYS	CD-CE-NZ	-5.33	99.43	111.70
1	E	154	LYS	CD-CE-NZ	-5.33	99.45	111.70
1	B	359	ASP	CB-CG-OD2	-5.33	113.51	118.30
1	B	370	ASP	CB-CG-OD1	5.32	123.09	118.30
1	E	186	ASP	CB-CG-OD1	5.29	123.06	118.30
1	E	188	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	G	107	ASN	N-CA-CB	5.26	120.07	110.60
1	F	68[A]	LYS	CD-CE-NZ	-5.26	99.60	111.70
1	F	68[B]	LYS	CD-CE-NZ	-5.26	99.60	111.70
1	G	145	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	H	314	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	E	244	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	B	195	LYS	CG-CD-CE	5.18	127.45	111.90
1	G	154	LYS	CD-CE-NZ	-5.16	99.84	111.70
1	F	355	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	E	50	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	265	ARG	NH1-CZ-NH2	5.08	124.99	119.40
1	H	323	LYS	CD-CE-NZ	5.07	123.35	111.70
1	G	113	ASP	CB-CG-OD1	5.05	122.84	118.30

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 (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	2993	0	3026	22	0
1	B	2973	0	2979	11	0
1	E	2985	0	2988	9	0
1	F	2961	0	2984	10	0
1	G	2962	0	2962	9	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	4	0
All	All	19574	0	18177	65	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 (65) 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
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: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:F:116:ILE:HD11	1:F:290:GLN:CD	2.21	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: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:258[B]:LYS:NZ	4:A:507:HOH:O	2.38	0.52
1:A:208:ASN:ND2	1:E:215:LYS:HB2	2.25	0.52
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:F:194[B]:LYS:NZ	4:F:1104:HOH:O	2.43	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: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: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: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:H:215:LYS:NZ	4:H:510:HOH:O	2.48	0.45
1:A:50:ARG:HD2	1:A:83:ASP:O	2.17	0.45
1:A:138[A]:GLU:OE1	1:A:207:TYR:OH	2.29	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: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: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: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:B:105:ASN:HD22	1:B:105:ASN:C	2.22	0.41
1:H:258:LYS:NZ	4:H:509:HOH:O	2.48	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: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:E:308:PHE:O	1:E:309:ASN:HB2	2.20	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%)	29 15
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%)	41 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	378/382 (99%)	369 (98%)	9 (2%)	0	100 100
All	All	2272/2292 (99%)	2212 (97%)	57 (2%)	3 (0%)	51 36

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 (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	335/332 (101%)	332 (99%)	3 (1%)	78 75
1	B	329/332 (99%)	321 (98%)	8 (2%)	49 36
1	E	331/332 (100%)	323 (98%)	8 (2%)	49 36
1	F	329/332 (99%)	321 (98%)	8 (2%)	49 36
1	G	328/332 (99%)	318 (97%)	10 (3%)	41 27
1	H	330/332 (99%)	323 (98%)	7 (2%)	53 42
All	All	1982/1992 (100%)	1938 (98%)	44 (2%)	50 39

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	152	PHE
1	A	187	TYR
1	B	49	ASN
1	B	105	ASN
1	B	152	PHE
1	B	169	ASN
1	B	187	TYR

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Mol	Chain	Res	Type
1	B	195	LYS
1	B	223	PHE
1	B	376	LYS
1	E	75	LYS
1	E	105	ASN
1	E	152	PHE
1	E	187	TYR
1	E	223	PHE
1	E	299	GLN
1	E	301	VAL
1	E	309	ASN
1	F	106	LYS
1	F	107	ASN
1	F	152	PHE
1	F	169	ASN
1	F	187	TYR
1	F	205	LYS
1	F	223	PHE
1	F	299	GLN
1	G	51	LEU
1	G	92	LYS
1	G	107	ASN
1	G	152	PHE
1	G	169	ASN
1	G	187	TYR
1	G	223	PHE
1	G	282	LYS
1	G	335	ASN
1	G	369	GLU
1	H	107	ASN
1	H	152	PHE
1	H	169	ASN
1	H	187	TYR
1	H	223	PHE
1	H	299	GLN
1	H	323	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	89	ASN

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Mol	Chain	Res	Type
1	A	374	ASN
1	B	49	ASN
1	B	89	ASN
1	E	89	ASN
1	E	105	ASN
1	E	299	GLN
1	F	299	GLN
1	G	89	ASN
1	G	107	ASN
1	H	89	ASN
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 monosaccharides 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	401	-	24,29,29	1.24	2 (8%)	23,42,42	1.68	6 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SAM	G	402	-	24,29,29	1.27	3 (12%)	23,42,42	1.68	5 (21%)
2	SAM	H	401	-	24,29,29	1.64	6 (25%)	23,42,42	2.35	9 (39%)
2	SAM	G	401	-	24,29,29	1.35	4 (16%)	23,42,42	1.80	7 (30%)
2	SAM	H	402	-	24,29,29	1.22	2 (8%)	23,42,42	1.74	5 (21%)
2	SAM	F	402	-	24,29,29	1.43	3 (12%)	23,42,42	2.98	9 (39%)
2	SAM	B	401	-	24,29,29	1.42	3 (12%)	23,42,42	2.41	5 (21%)
2	SAM	A	402	-	24,29,29	0.99	1 (4%)	23,42,42	1.44	3 (13%)
2	SAM	A	401	-	24,29,29	1.16	3 (12%)	23,42,42	2.13	6 (26%)
2	SAM	F	401	-	24,29,29	1.70	6 (25%)	23,42,42	2.05	6 (26%)
2	SAM	E	402	-	24,29,29	1.65	4 (16%)	23,42,42	1.99	8 (34%)
2	SAM	B	402	-	24,29,29	1.10	1 (4%)	23,42,42	1.32	3 (13%)

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	401	-	-	3/12/33/33	0/3/3/3
2	SAM	G	402	-	-	0/12/33/33	0/3/3/3
2	SAM	H	401	-	-	2/12/33/33	0/3/3/3
2	SAM	G	401	-	-	2/12/33/33	0/3/3/3
2	SAM	H	402	-	-	0/12/33/33	0/3/3/3
2	SAM	F	402	-	-	3/12/33/33	0/3/3/3
2	SAM	B	401	-	-	2/12/33/33	0/3/3/3
2	SAM	A	402	-	-	1/12/33/33	0/3/3/3
2	SAM	A	401	-	-	4/12/33/33	0/3/3/3
2	SAM	F	401	-	-	1/12/33/33	0/3/3/3
2	SAM	E	402	-	-	1/12/33/33	0/3/3/3
2	SAM	B	402	-	-	0/12/33/33	0/3/3/3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	SAM	C4-N3	-4.51	1.29	1.35
2	F	402	SAM	O2'-C2'	-4.16	1.33	1.43
2	E	402	SAM	O2'-C2'	-3.92	1.33	1.43
2	G	402	SAM	C2'-C1'	3.73	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	402	SAM	C8-N7	-3.63	1.28	1.34
2	G	401	SAM	CG-CB	3.41	1.62	1.51
2	B	401	SAM	CG-CB	3.39	1.62	1.51
2	E	401	SAM	C2'-C1'	3.32	1.58	1.53
2	H	401	SAM	C2'-C1'	3.11	1.58	1.53
2	F	401	SAM	CG-CB	3.07	1.61	1.51
2	F	401	SAM	C5-C4	2.98	1.48	1.40
2	H	402	SAM	O4'-C1'	2.94	1.45	1.41
2	E	402	SAM	O4'-C1'	2.88	1.45	1.41
2	H	401	SAM	O-C	2.83	1.30	1.22
2	B	401	SAM	C2-N3	2.73	1.36	1.32
2	F	401	SAM	OXT-C	-2.69	1.21	1.30
2	H	401	SAM	C2-N3	2.68	1.36	1.32
2	H	401	SAM	O3'-C3'	2.61	1.49	1.43
2	A	401	SAM	C2-N3	2.54	1.36	1.32
2	A	401	SAM	OXT-C	-2.53	1.22	1.30
2	F	401	SAM	C2-N3	2.52	1.36	1.32
2	H	401	SAM	C5-C4	2.49	1.47	1.40
2	A	402	SAM	C2'-C1'	2.48	1.57	1.53
2	E	401	SAM	CG-CB	2.47	1.59	1.51
2	B	401	SAM	OXT-C	-2.43	1.22	1.30
2	H	401	SAM	O4'-C4'	2.41	1.50	1.45
2	F	402	SAM	O4'-C4'	-2.38	1.39	1.45
2	G	402	SAM	OXT-C	-2.38	1.22	1.30
2	F	401	SAM	O2'-C2'	2.35	1.48	1.43
2	E	402	SAM	O4'-C4'	-2.33	1.39	1.45
2	G	402	SAM	CG-CB	2.30	1.58	1.51
2	H	402	SAM	C2'-C1'	2.29	1.57	1.53
2	F	402	SAM	OXT-C	-2.28	1.23	1.30
2	G	401	SAM	C4-N3	2.23	1.38	1.35
2	G	401	SAM	O-C	2.19	1.28	1.22
2	G	401	SAM	C8-N7	2.09	1.38	1.34
2	A	401	SAM	C8-N7	2.04	1.38	1.34
2	B	402	SAM	O4'-C4'	-2.01	1.40	1.45

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	402	SAM	CG-SD-C5'	-7.06	85.41	103.40
2	F	401	SAM	CG-SD-C5'	-6.19	87.61	103.40
2	F	402	SAM	OXT-C-O	-6.16	110.11	124.09
2	A	401	SAM	CG-SD-C5'	-5.70	88.87	103.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	SAM	N6-C6-N1	5.70	130.40	118.57
2	F	402	SAM	CB-CA-C	5.63	123.72	110.30
2	F	402	SAM	CB-CA-N	-5.50	95.74	110.17
2	B	401	SAM	CG-SD-C5'	-5.43	89.56	103.40
2	G	401	SAM	CG-SD-C5'	-5.33	89.81	103.40
2	B	401	SAM	C1'-N9-C4	-5.07	117.73	126.64
2	B	401	SAM	C5-C6-N6	-4.66	113.27	120.35
2	H	401	SAM	C1'-N9-C4	-4.48	118.78	126.64
2	H	402	SAM	N3-C2-N1	-4.05	122.35	128.68
2	A	401	SAM	CB-CA-N	-3.99	99.70	110.17
2	H	401	SAM	CG-SD-C5'	-3.98	93.27	103.40
2	A	402	SAM	OXT-C-CA	3.90	126.66	113.38
2	E	402	SAM	C5-C6-N6	-3.83	114.54	120.35
2	H	401	SAM	C2-N1-C6	3.65	124.99	118.75
2	H	401	SAM	O4'-C4'-C3'	3.61	112.27	105.11
2	G	402	SAM	C1'-N9-C4	-3.61	120.31	126.64
2	B	402	SAM	CG-SD-C5'	3.59	112.55	103.40
2	H	401	SAM	N3-C2-N1	-3.56	123.12	128.68
2	A	401	SAM	C1'-N9-C4	-3.43	120.61	126.64
2	E	401	SAM	C1'-N9-C4	-3.40	120.67	126.64
2	G	402	SAM	OXT-C-O	-3.38	116.41	124.09
2	H	401	SAM	N6-C6-N1	3.38	125.59	118.57
2	E	402	SAM	OXT-C-CA	3.37	124.86	113.38
2	A	401	SAM	N3-C2-N1	-3.36	123.43	128.68
2	F	402	SAM	OXT-C-CA	3.35	124.80	113.38
2	H	402	SAM	OXT-C-CA	3.32	124.70	113.38
2	H	401	SAM	O4'-C1'-C2'	3.32	111.78	106.93
2	E	401	SAM	CG-SD-C5'	-3.19	95.27	103.40
2	E	401	SAM	C4-C5-N7	3.16	112.69	109.40
2	E	402	SAM	O4'-C1'-C2'	-3.14	102.33	106.93
2	H	402	SAM	O2'-C2'-C1'	-3.13	99.31	110.85
2	F	402	SAM	C2-N1-C6	-3.05	113.54	118.75
2	E	402	SAM	O4'-C4'-C3'	-2.96	99.26	105.11
2	F	401	SAM	C3'-C2'-C1'	2.95	105.42	100.98
2	F	401	SAM	O2'-C2'-C1'	-2.95	99.95	110.85
2	G	402	SAM	N3-C2-N1	-2.94	124.08	128.68
2	F	401	SAM	C5-C6-N6	-2.86	116.00	120.35
2	F	402	SAM	CE-SD-C5'	2.73	121.97	100.54
2	F	402	SAM	C5-C6-N6	-2.67	116.29	120.35
2	E	401	SAM	C5-C6-N6	-2.64	116.33	120.35
2	A	402	SAM	OXT-C-O	-2.58	118.22	124.09
2	A	401	SAM	O4'-C1'-C2'	2.53	110.63	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	401	SAM	CB-CA-C	2.51	116.27	110.30
2	E	401	SAM	C2'-C3'-C4'	-2.50	97.78	102.64
2	H	402	SAM	O4'-C1'-C2'	2.47	110.54	106.93
2	E	402	SAM	O-C-CA	-2.47	113.43	122.14
2	H	401	SAM	C5-C6-N6	-2.41	116.68	120.35
2	B	402	SAM	N3-C2-N1	-2.41	124.91	128.68
2	A	401	SAM	N6-C6-N1	2.41	123.57	118.57
2	G	402	SAM	O2'-C2'-C1'	-2.40	101.98	110.85
2	E	402	SAM	CB-CA-N	-2.40	103.89	110.17
2	F	402	SAM	O3'-C3'-C2'	2.39	119.55	111.82
2	E	402	SAM	N6-C6-N1	2.37	123.50	118.57
2	G	401	SAM	O4'-C4'-C3'	2.36	109.78	105.11
2	E	402	SAM	C3'-C2'-C1'	2.33	104.49	100.98
2	G	401	SAM	C3'-C2'-C1'	2.30	104.44	100.98
2	G	401	SAM	C1'-N9-C4	-2.26	122.67	126.64
2	H	402	SAM	OXT-C-O	-2.22	119.04	124.09
2	F	401	SAM	CB-CA-C	2.19	115.52	110.30
2	G	401	SAM	OXT-C-O	-2.17	119.16	124.09
2	B	402	SAM	OXT-C-O	-2.15	119.21	124.09
2	G	401	SAM	C2'-C3'-C4'	-2.14	98.48	102.64
2	B	401	SAM	OXT-C-O	-2.12	119.27	124.09
2	G	402	SAM	C5-C6-N6	-2.11	117.15	120.35
2	F	401	SAM	N6-C6-N1	2.06	122.84	118.57
2	H	401	SAM	C2'-C3'-C4'	-2.05	98.66	102.64
2	E	401	SAM	OXT-C-O	2.04	128.73	124.09
2	A	402	SAM	O-C-CA	-2.03	114.99	122.14

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	402	SAM	N-CA-CB-CG
2	F	402	SAM	C-CA-CB-CG
2	A	401	SAM	OXT-C-CA-N
2	A	401	SAM	O-C-CA-N
2	E	401	SAM	OXT-C-CA-CB
2	F	402	SAM	CA-CB-CG-SD
2	E	401	SAM	O-C-CA-CB
2	G	401	SAM	O-C-CA-CB
2	H	401	SAM	O-C-CA-CB
2	H	401	SAM	OXT-C-CA-CB
2	A	401	SAM	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
2	B	401	SAM	OXT-C-CA-CB
2	G	401	SAM	OXT-C-CA-CB
2	A	401	SAM	OXT-C-CA-CB
2	B	401	SAM	O-C-CA-CB
2	F	401	SAM	O-C-CA-CB
2	A	402	SAM	O-C-CA-N
2	E	402	SAM	O-C-CA-N
2	E	401	SAM	OXT-C-CA-N

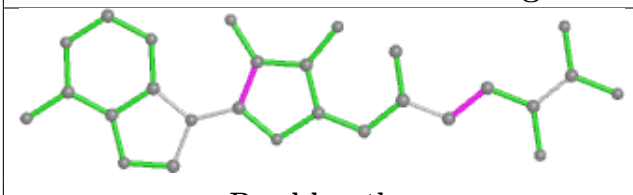
There are no ring outliers.

1 monomer is involved in 1 short contact:

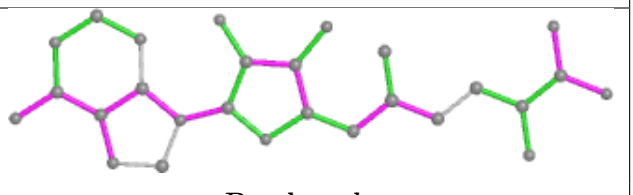
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	401	SAM	1	0

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 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.

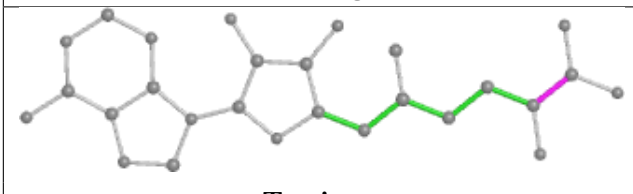
Ligand SAM E 401



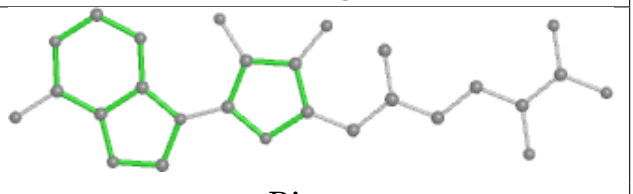
Bond lengths



Bond angles

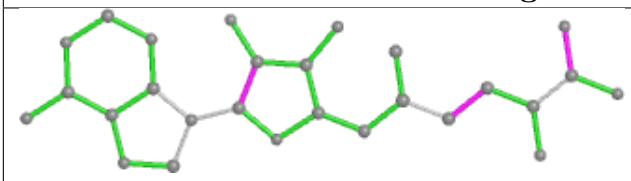


Torsions

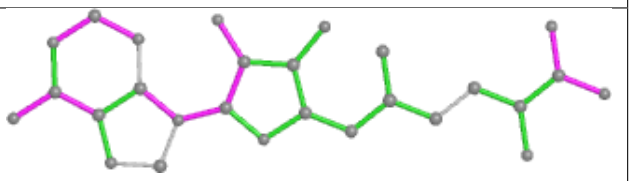


Rings

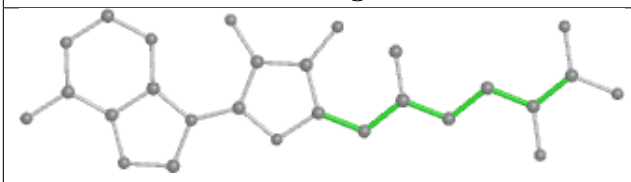
Ligand SAM G 402



Bond lengths



Bond angles



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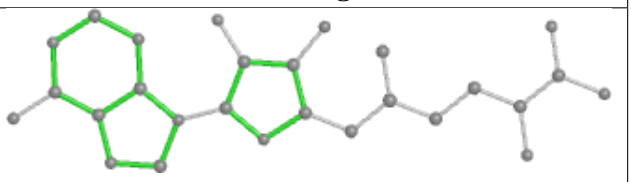
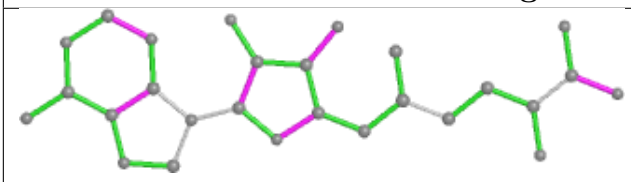
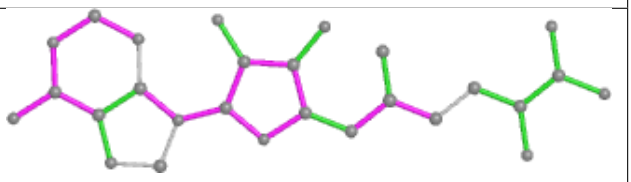


Rings

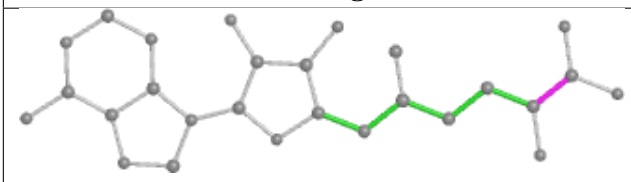
Ligand SAM H 401



Bond lengths



Bond angles



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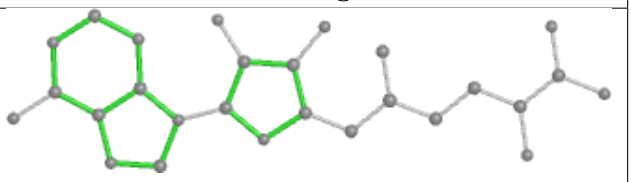
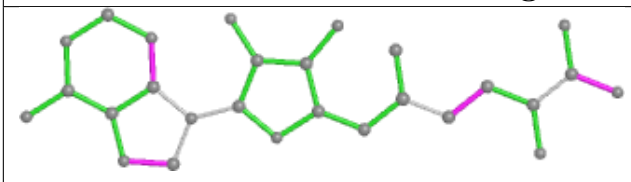
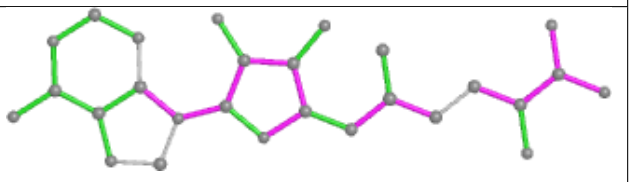


Rings

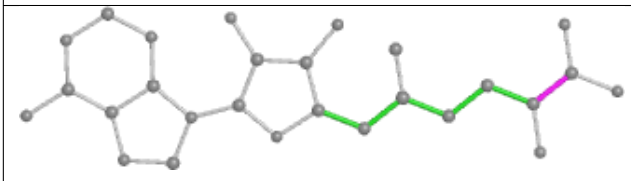
Ligand SAM G 401



Bond lengths



Bond angles



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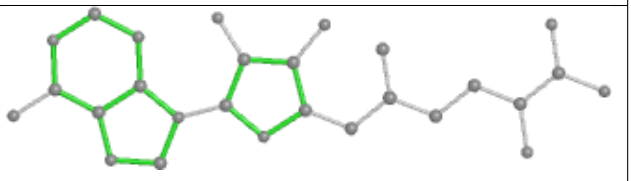
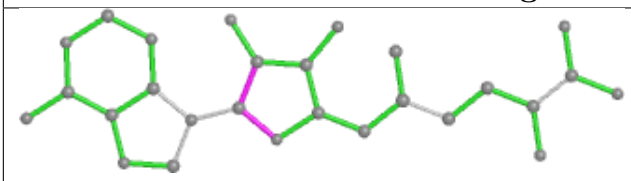
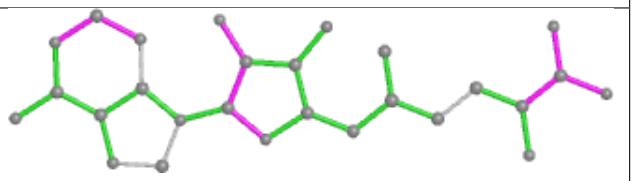


Rings

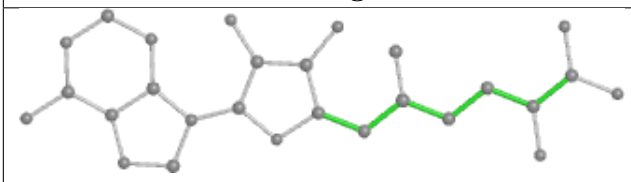
Ligand SAM H 402



Bond lengths



Bond angles



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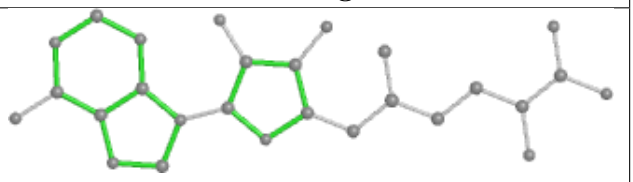
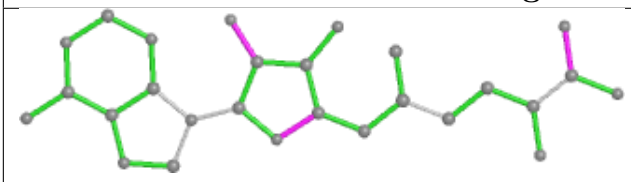
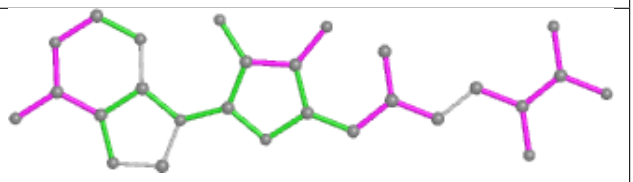


Rings

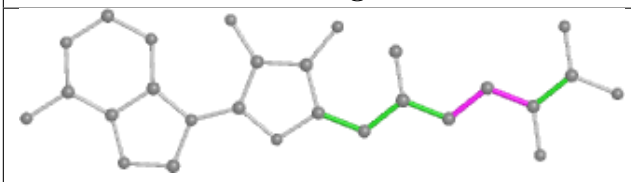
Ligand SAM F 402



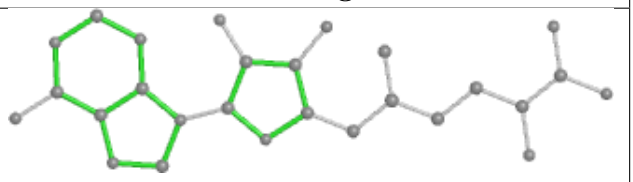
Bond lengths



Bond angles

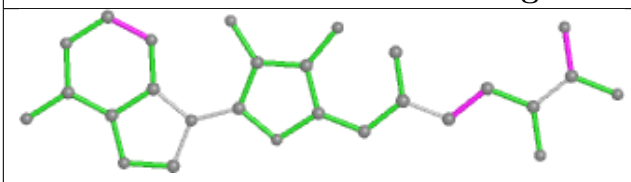


Torsions

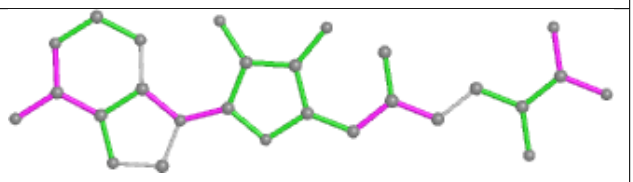


Rings

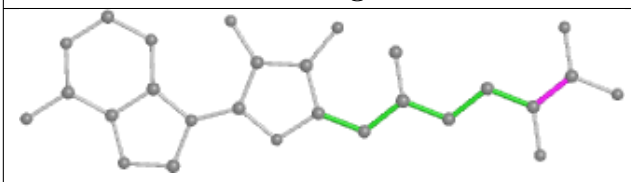
Ligand SAM B 401



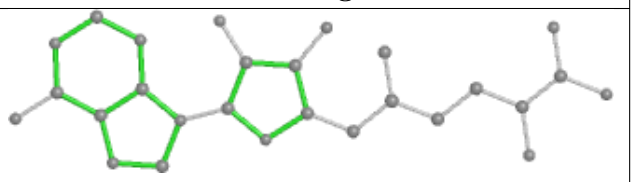
Bond lengths



Bond angles

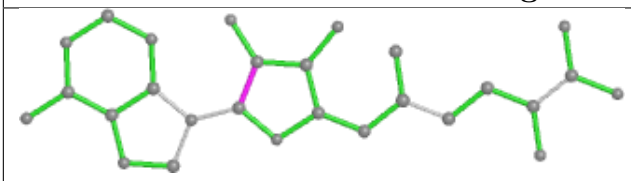


Torsions

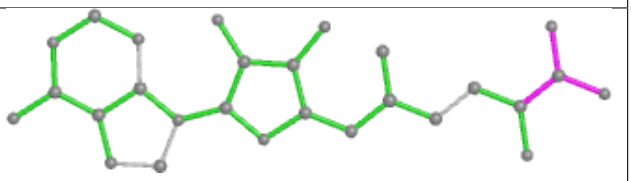


Rings

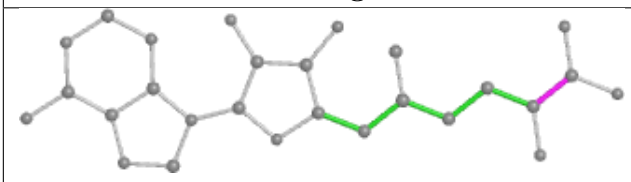
Ligand SAM A 402



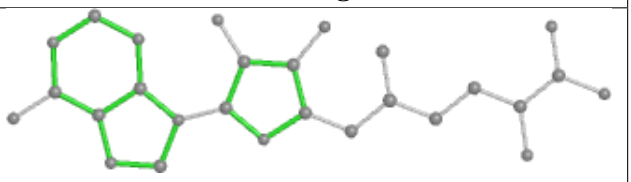
Bond lengths



Bond angles

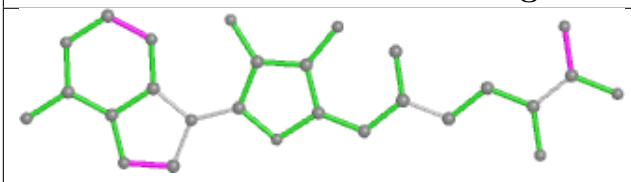


Torsions

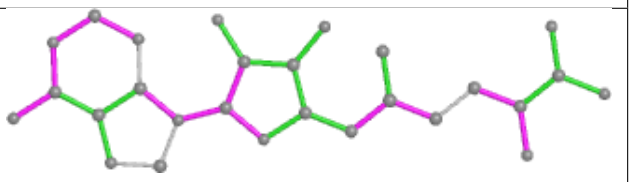


Rings

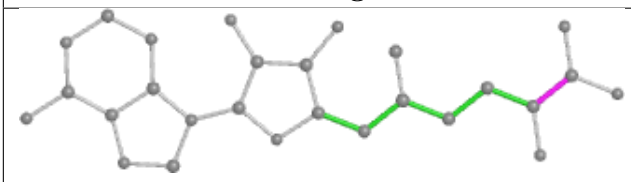
Ligand SAM A 401



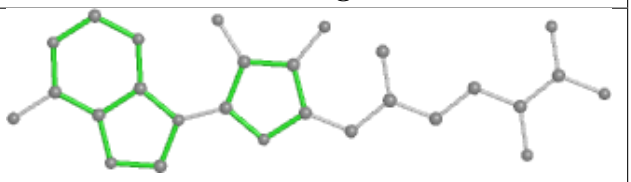
Bond lengths



Bond angles

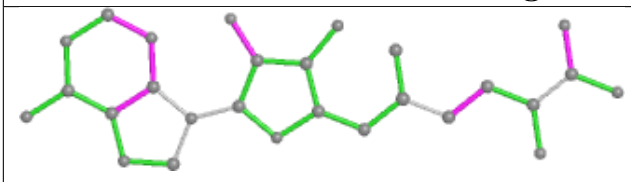


Torsions

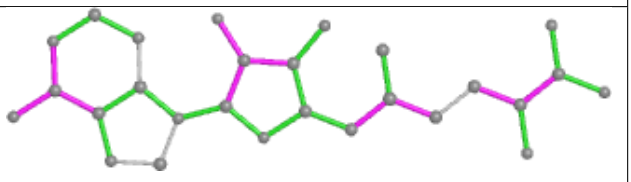


Rings

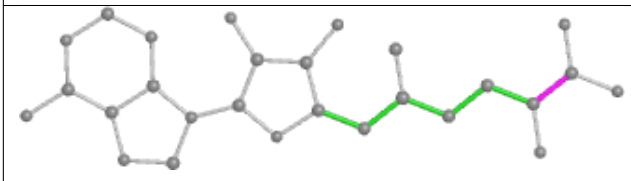
Ligand SAM F 401



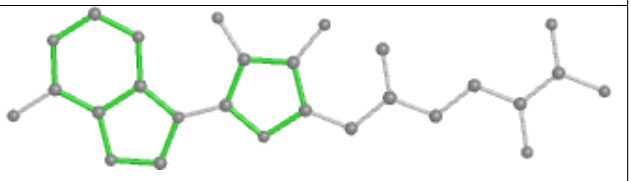
Bond lengths



Bond angles

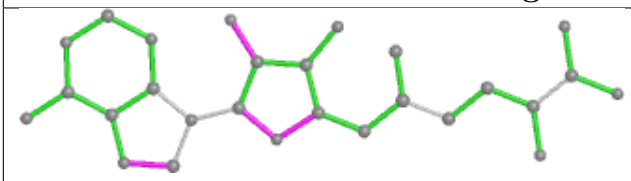


Torsions

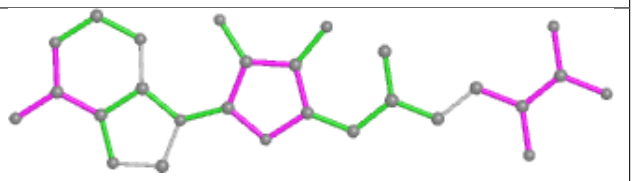


Rings

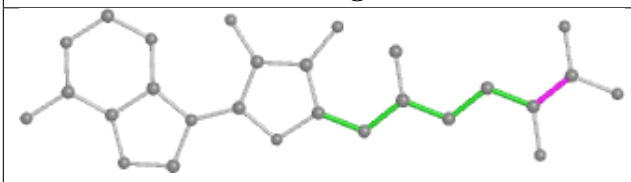
Ligand SAM E 402



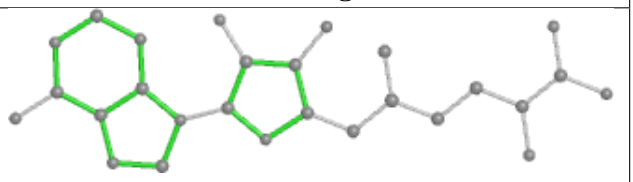
Bond lengths



Bond angles

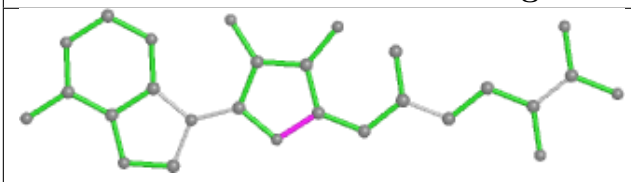


Torsions

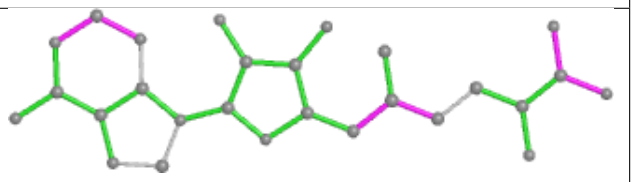


Rings

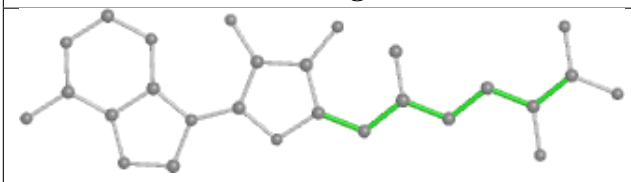
Ligand SAM B 402



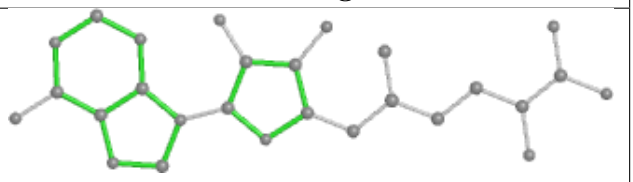
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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%)	-0.28	1 (0%) 94 92	22, 30, 44, 93	0
1	B	374/382 (97%)	-0.15	6 (1%) 72 68	26, 35, 58, 100	0
1	E	375/382 (98%)	-0.18	3 (0%) 86 84	22, 31, 52, 85	0
1	F	374/382 (97%)	-0.08	9 (2%) 59 54	24, 32, 51, 97	0
1	G	375/382 (98%)	0.39	34 (9%) 9 7	30, 43, 72, 119	0
1	H	373/382 (97%)	0.20	24 (6%) 19 15	27, 38, 62, 80	0
All	All	2245/2292 (97%)	-0.02	77 (3%) 45 39	22, 34, 59, 119	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	104	THR	6.1
1	G	377	HIS	6.0
1	G	106	LYS	5.9
1	B	170	SER	5.0
1	G	375	SER	4.7
1	F	106	LYS	4.7
1	B	104	THR	4.5
1	H	234[A]	LEU	4.3
1	F	3	TYR	4.3
1	G	368	VAL	4.2
1	G	107	ASN	4.2
1	G	369	GLU	4.2
1	G	370	ASP	3.9
1	H	170	SER	3.8
1	E	104	THR	3.8
1	F	104	THR	3.8
1	G	234	LEU	3.7
1	G	240	ILE	3.6
1	B	106	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	368	VAL	3.5
1	F	107	ASN	3.5
1	G	372	ILE	3.4
1	H	104	THR	3.4
1	H	239	ILE	3.3
1	G	371	LEU	3.2
1	H	190	GLU	3.2
1	A	377	HIS	3.2
1	G	45	VAL	3.2
1	G	374	ASN	3.2
1	B	105	ASN	3.1
1	B	3	TYR	3.1
1	G	312	LEU	3.1
1	H	53	VAL	3.1
1	G	318	ILE	3.1
1	H	372	ILE	3.0
1	G	315	GLU	3.0
1	H	281	ALA	3.0
1	G	52	ILE	2.9
1	G	3	TYR	2.9
1	H	209	LEU	2.8
1	G	254	ALA	2.8
1	F	234[A]	LEU	2.7
1	G	236	GLY	2.7
1	F	240	ILE	2.6
1	G	239	ILE	2.6
1	G	283	LEU	2.6
1	H	369	GLU	2.6
1	G	320	GLU	2.6
1	G	316	THR	2.6
1	G	207	TYR	2.5
1	H	191	TYR	2.5
1	H	240	ILE	2.4
1	E	87	ILE	2.4
1	H	46	LEU	2.4
1	B	107	ASN	2.3
1	H	316	THR	2.3
1	H	87	ILE	2.3
1	H	45	VAL	2.3
1	G	313	ILE	2.3
1	H	254	ALA	2.3
1	G	373	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	54	ILE	2.2
1	G	311	ASN	2.2
1	H	375	SER	2.2
1	F	190	GLU	2.2
1	F	105	ASN	2.1
1	G	317	LYS	2.1
1	F	239	ILE	2.1
1	H	106	LYS	2.1
1	G	314	ASP	2.0
1	H	189	VAL	2.0
1	G	46	LEU	2.0
1	E	375	SER	2.0
1	G	324	LYS	2.0
1	G	376	LYS	2.0
1	H	370	ASP	2.0
1	H	235	THR	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	0.87	0.14	35,39,55,58	0
2	SAM	F	402	27/27	0.93	0.10	28,34,55,58	0
2	SAM	B	402	27/27	0.93	0.10	31,35,50,52	0
2	SAM	H	401	27/27	0.93	0.08	37,40,47,48	0
2	SAM	A	402	27/27	0.94	0.10	25,29,42,46	0
2	SAM	G	401	27/27	0.94	0.10	28,33,42,46	0
2	SAM	E	402	27/27	0.95	0.08	26,28,33,38	0

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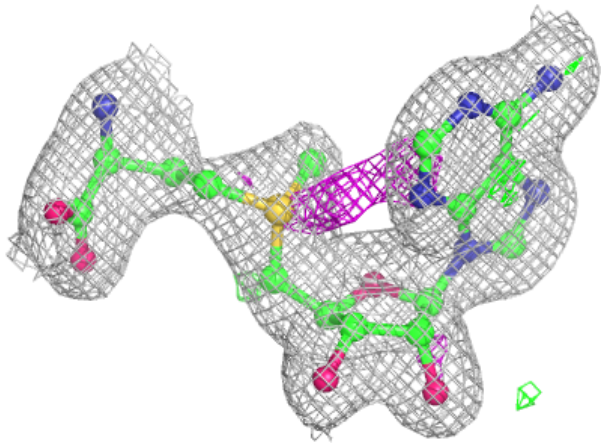
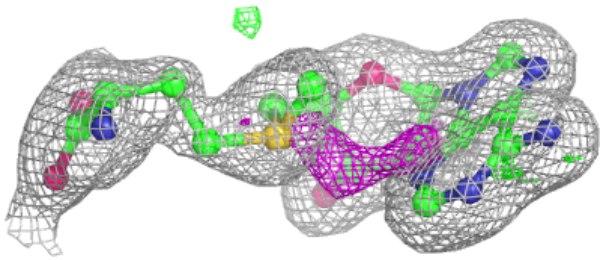
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SAM	H	402	27/27	0.95	0.07	26,29,43,45	0
2	SAM	B	401	27/27	0.96	0.10	27,31,42,43	0
2	SAM	A	401	27/27	0.96	0.08	25,29,38,42	0
2	SAM	E	401	27/27	0.96	0.08	27,29,42,45	0
2	SAM	F	401	27/27	0.98	0.08	26,27,35,37	0
3	CL	A	403	1/1	0.98	0.14	34,34,34,34	0
3	CL	H	403	1/1	0.98	0.09	39,39,39,39	0
3	CL	G	403	1/1	0.99	0.12	38,38,38,38	0
3	CL	B	403	1/1	0.99	0.07	34,34,34,34	0
3	CL	E	403	1/1	1.00	0.08	33,33,33,33	0
3	CL	F	403	1/1	1.00	0.12	31,31,31,31	0

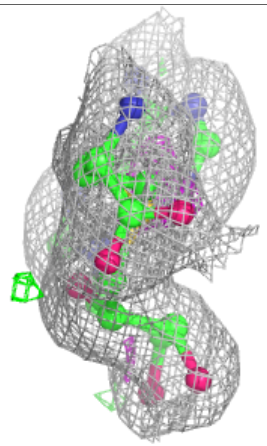
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

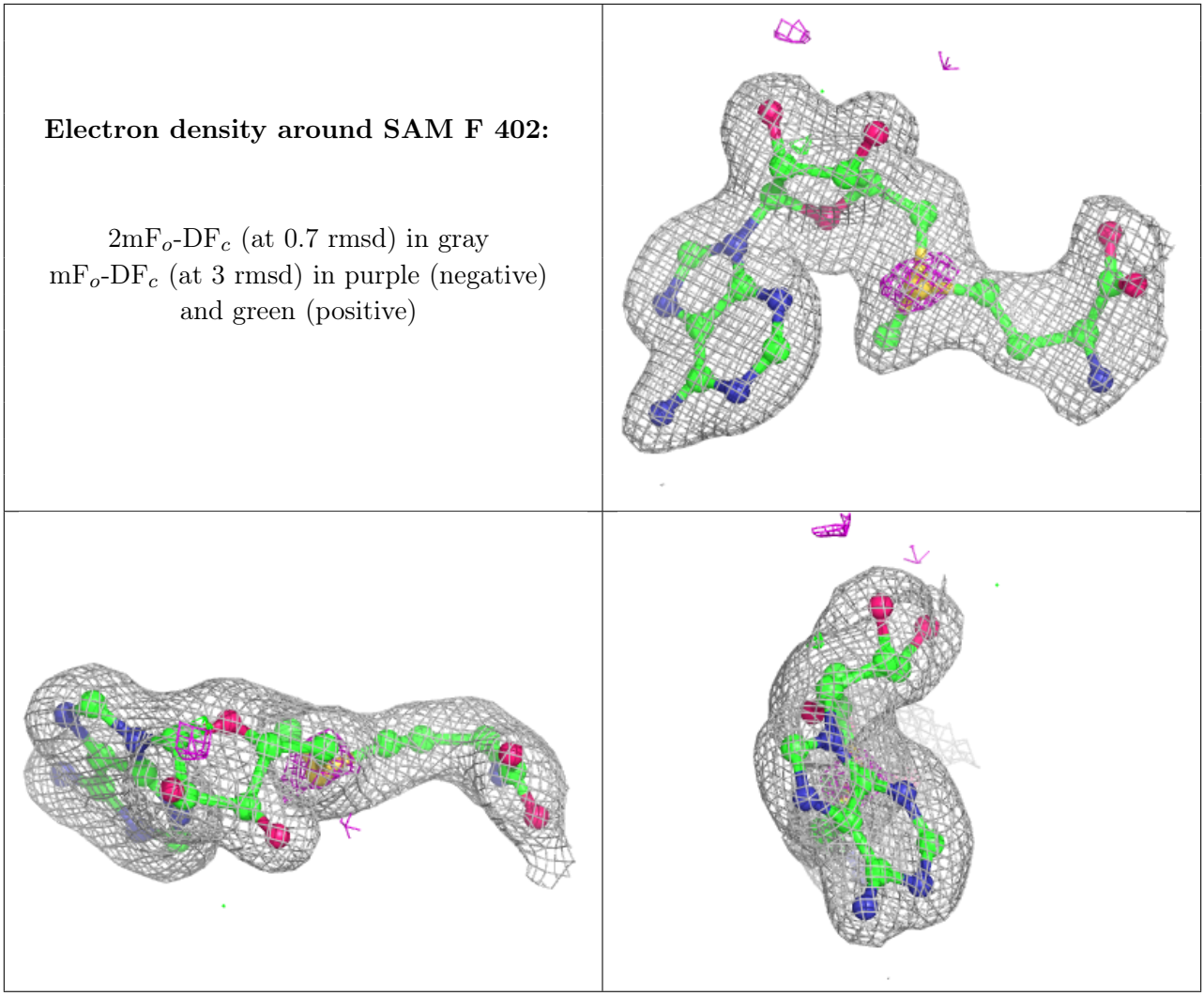






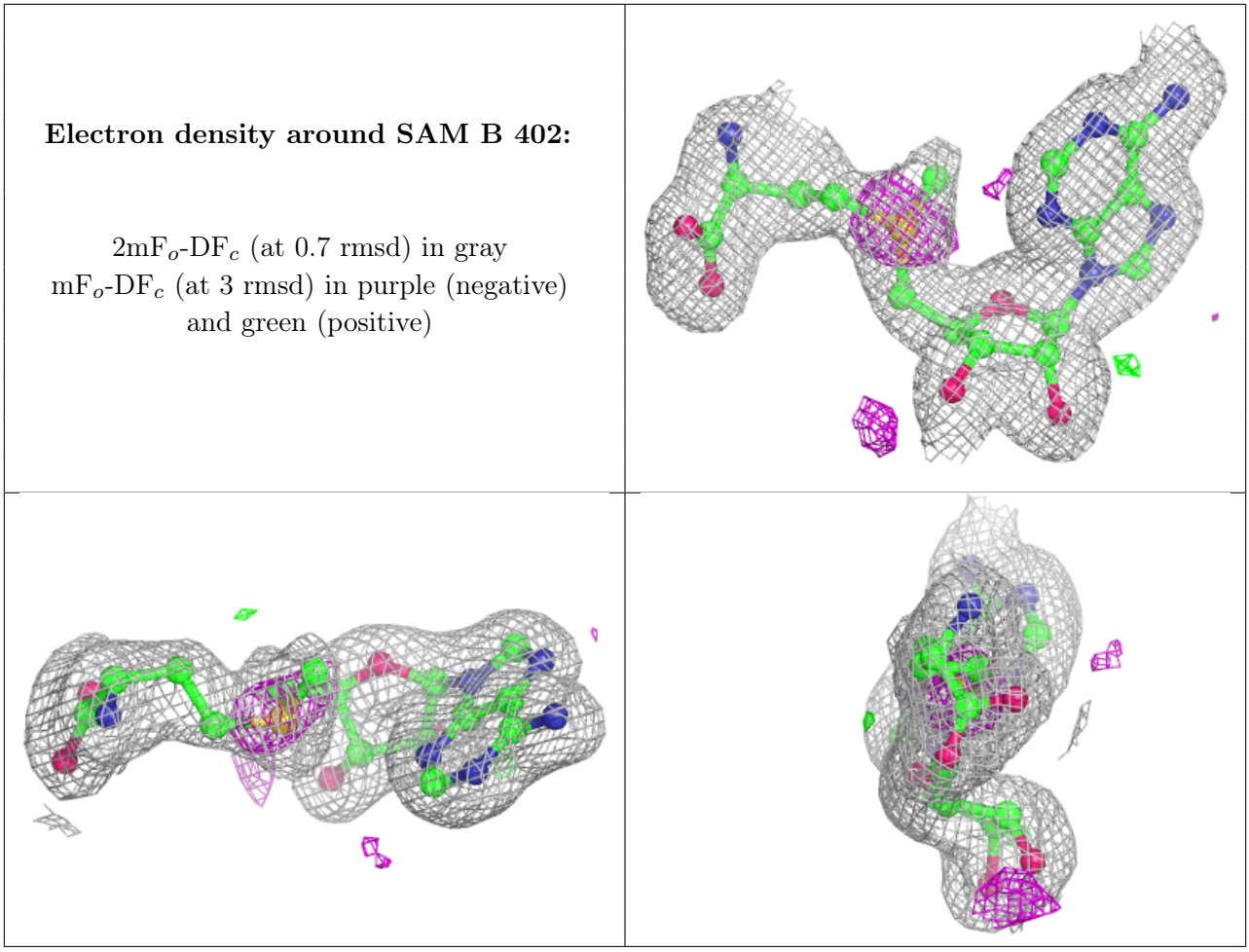
Electron density around SAM F 402:

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



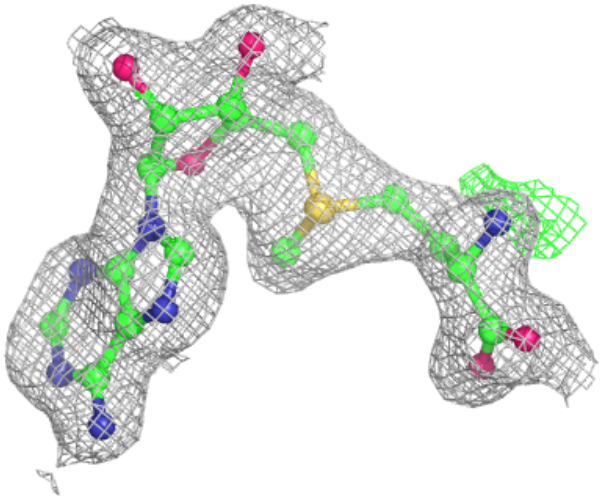
Electron density around SAM B 402:

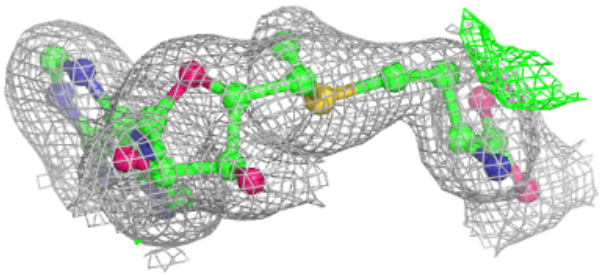
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

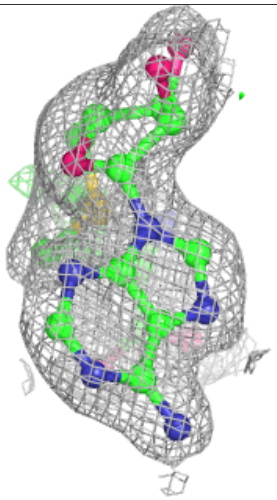


Electron density around SAM H 401:

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

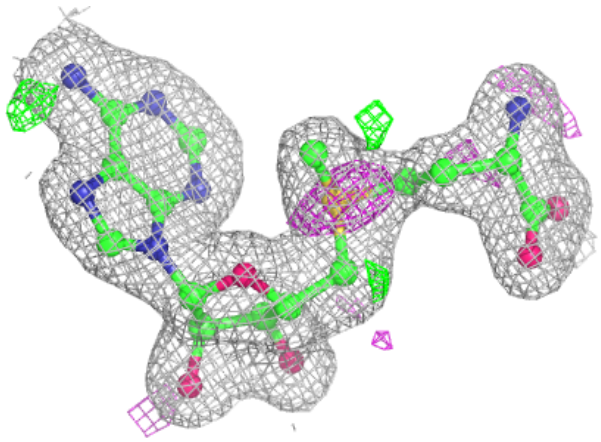


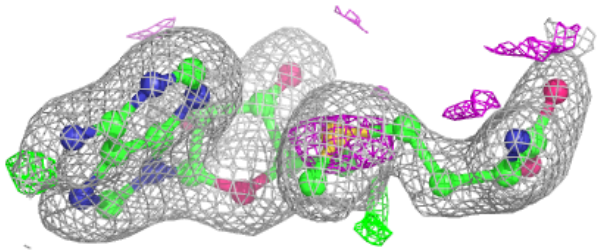


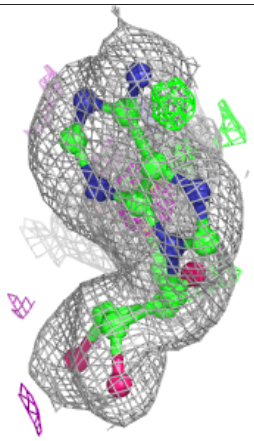


Electron density around SAM A 402:

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

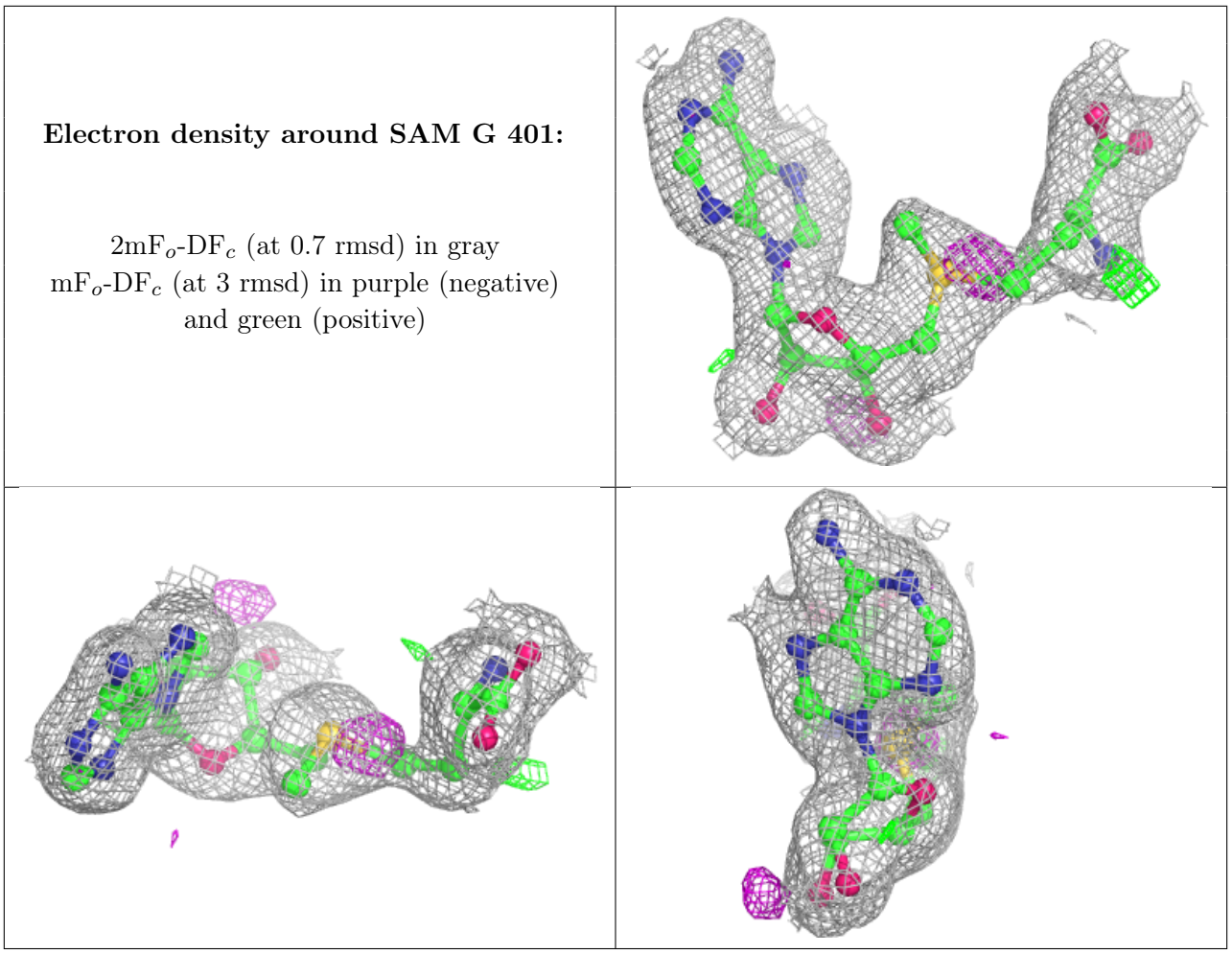






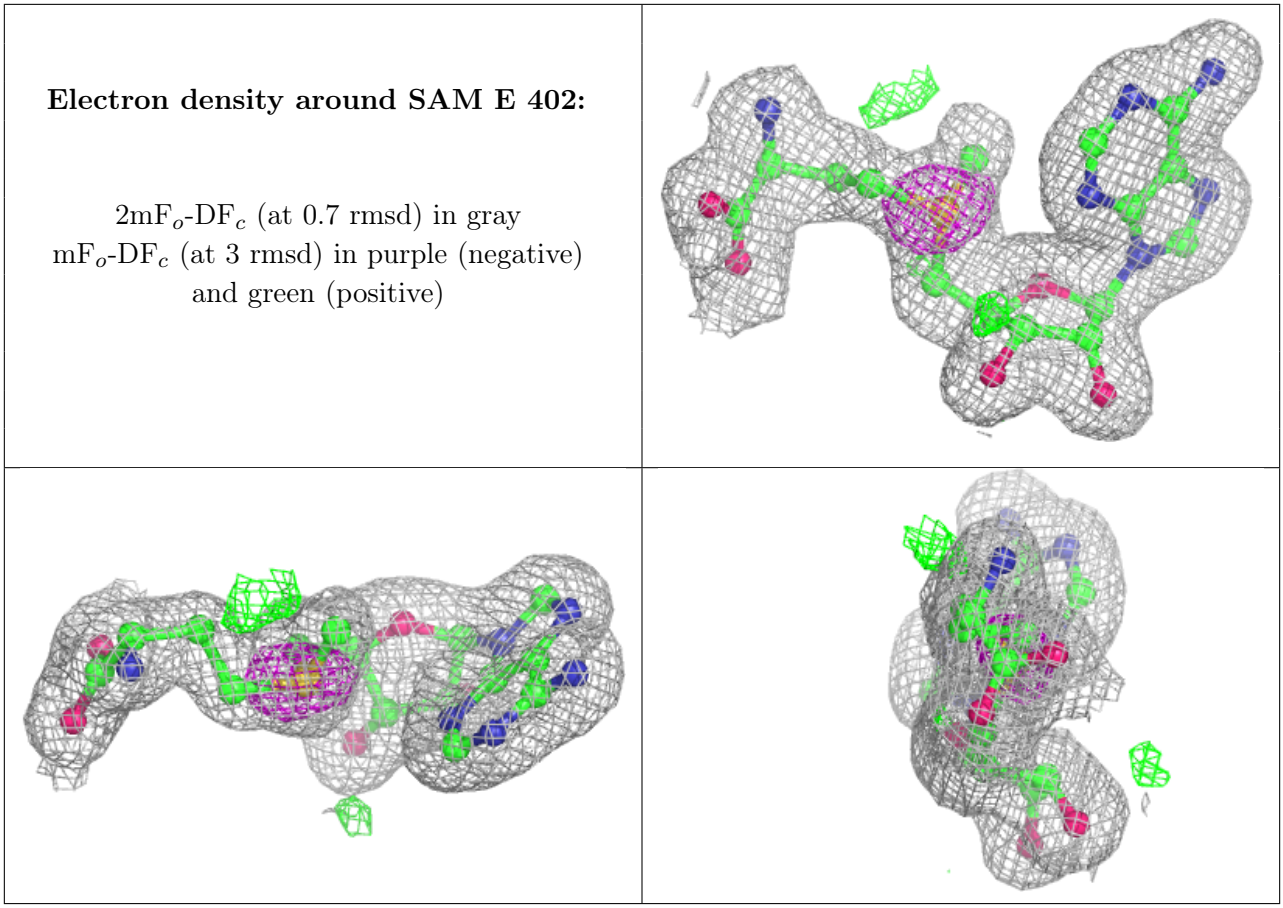
Electron density around SAM G 401:

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



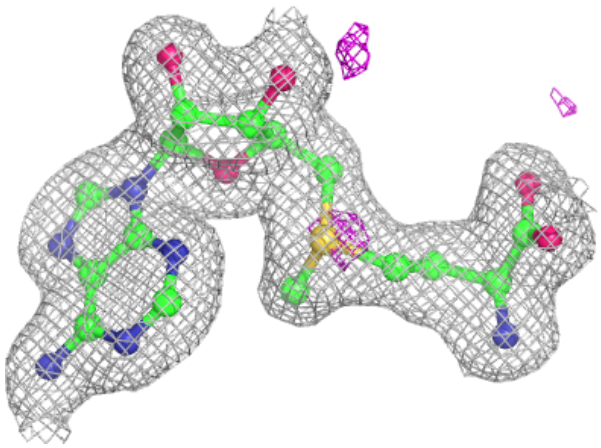
Electron density around SAM E 402:

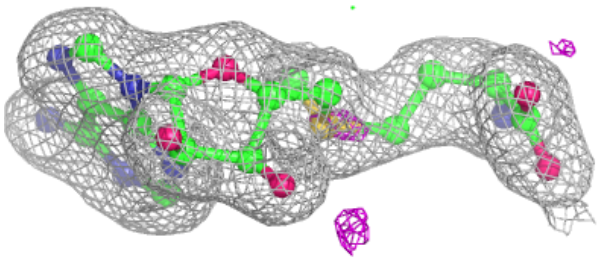
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

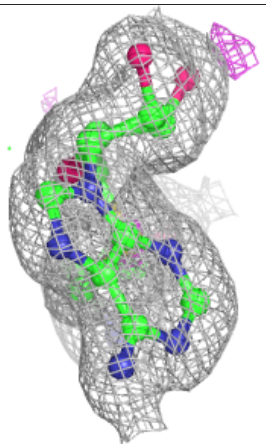


Electron density around SAM H 402:

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

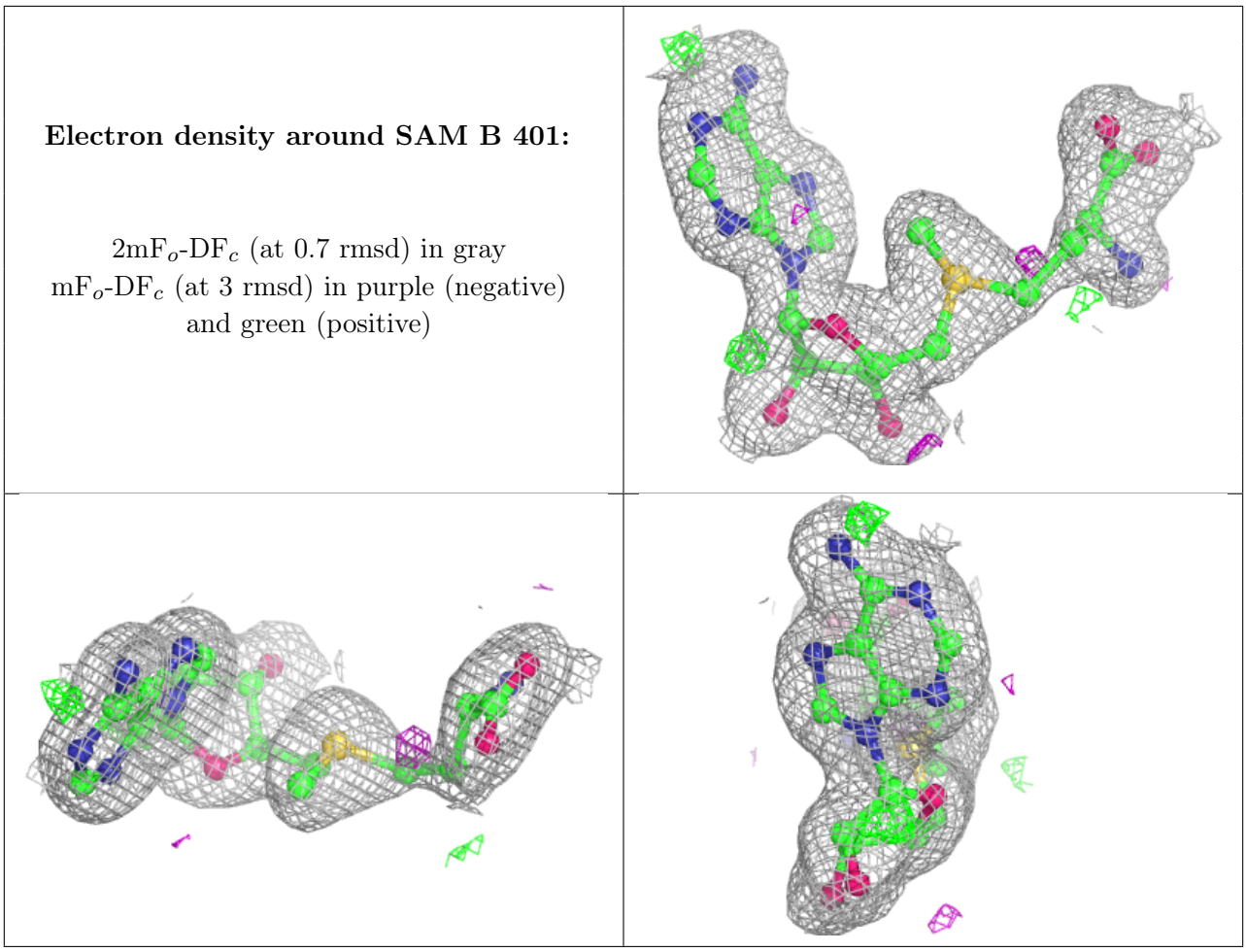






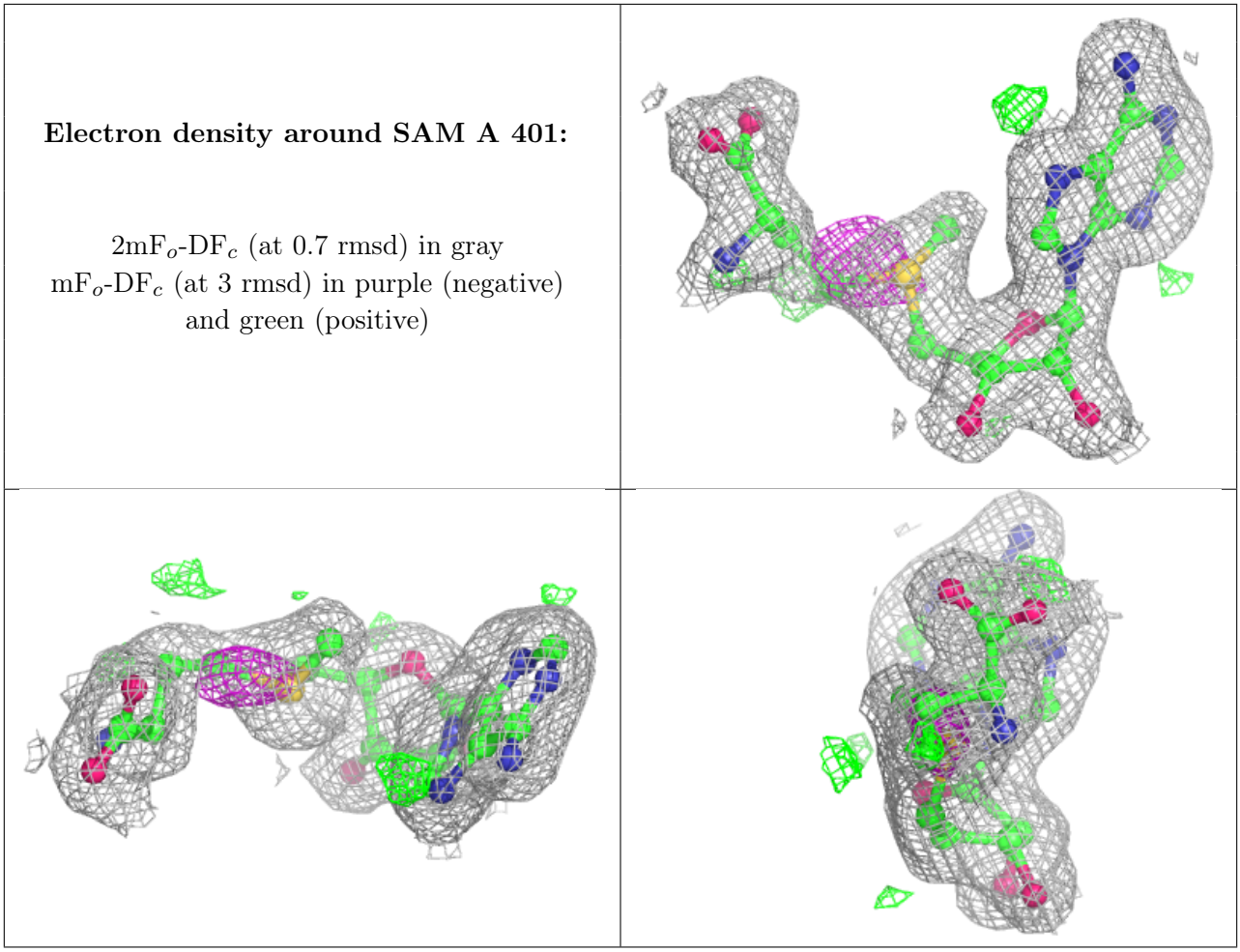
Electron density around SAM B 401:

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



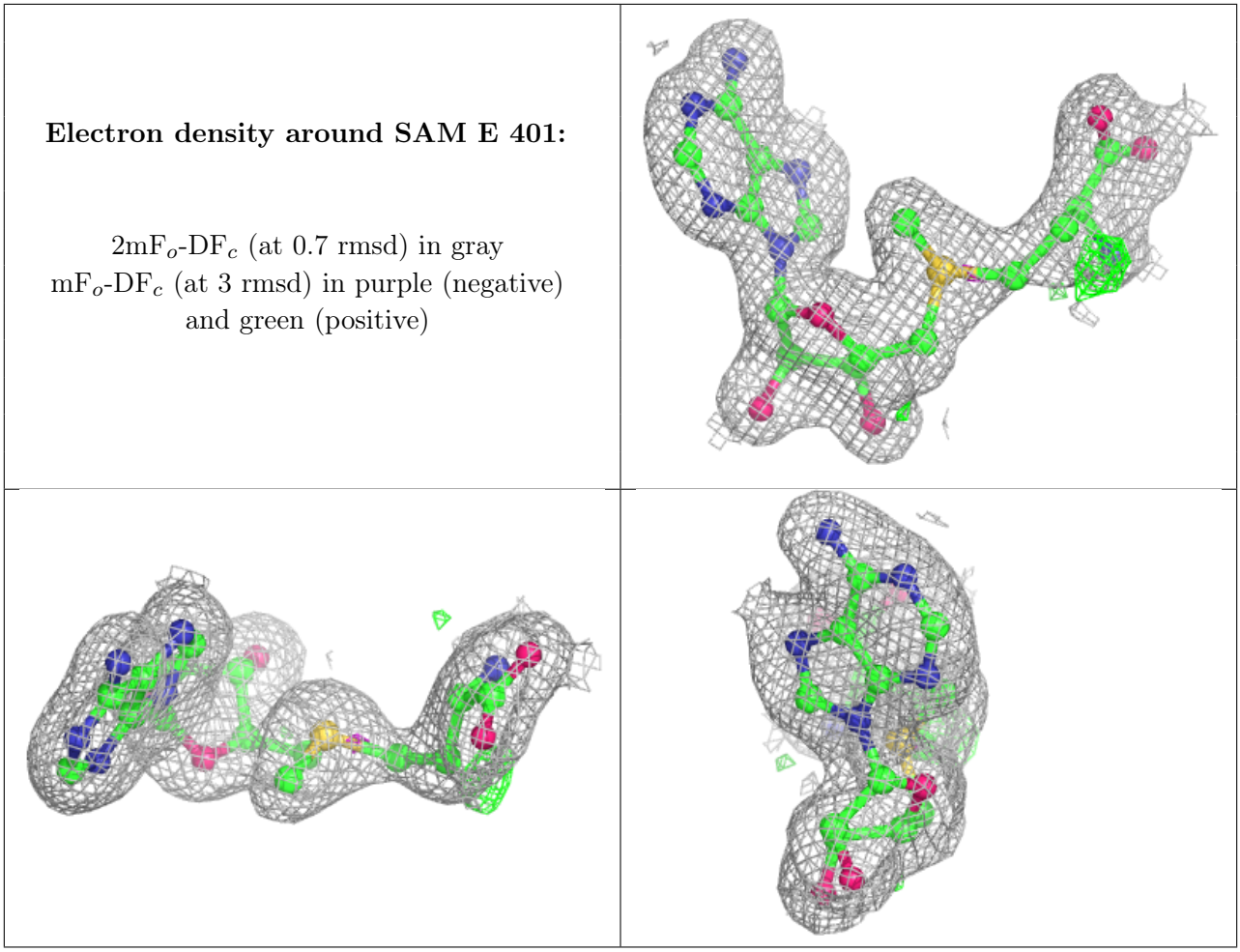
Electron density around SAM A 401:

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



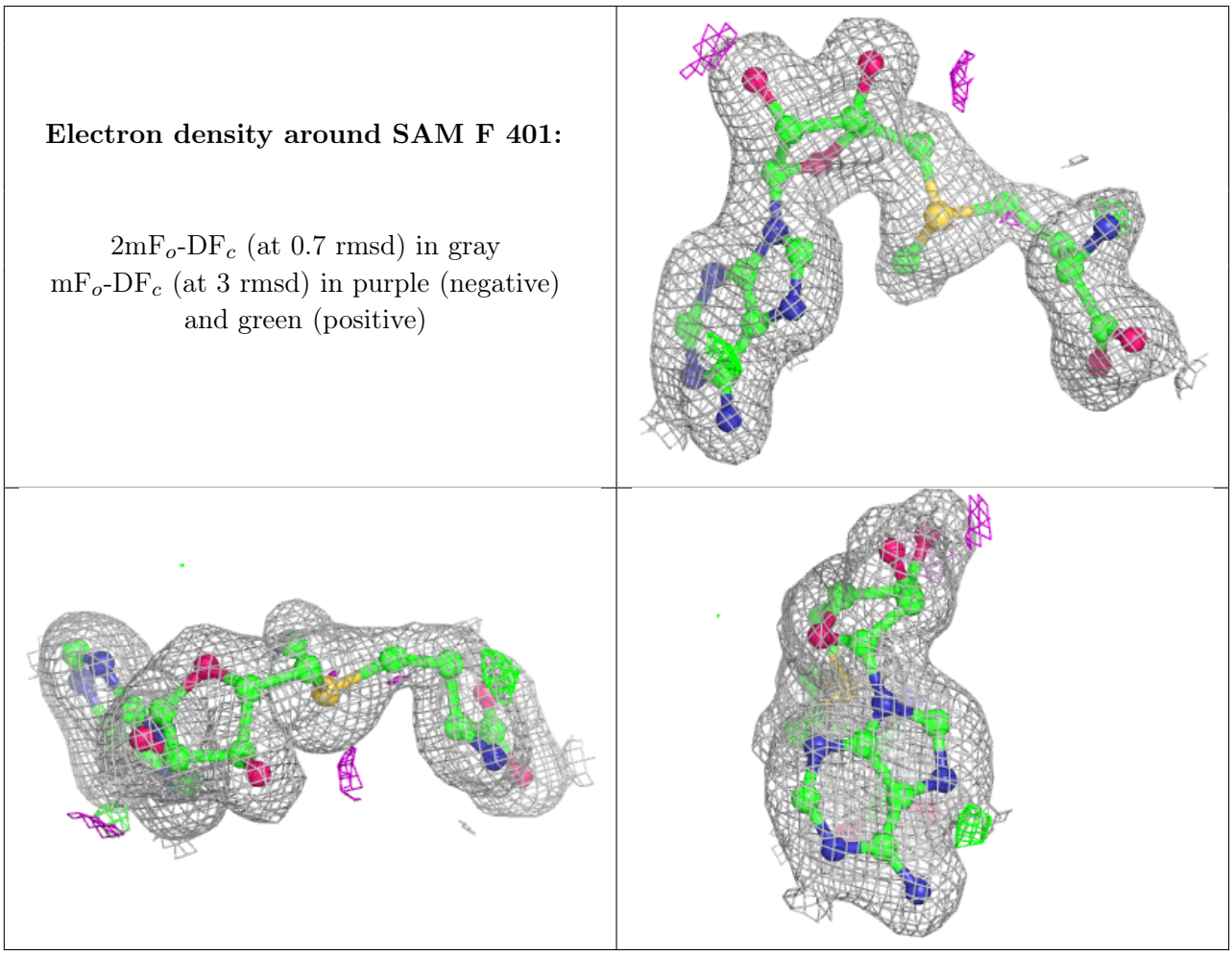
Electron density around SAM E 401:

$2mF_o$-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 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

There are no such residues in this entry.