Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 10:35 AM JST

PDB ID	:	6JCL
Title	:	Crystal structure of cofactor-bound Rv0187 from MTB
Authors	:	Kim, J.; Lee, S.
Deposited on	:	2019-01-29
Resolution	:	1.64 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:

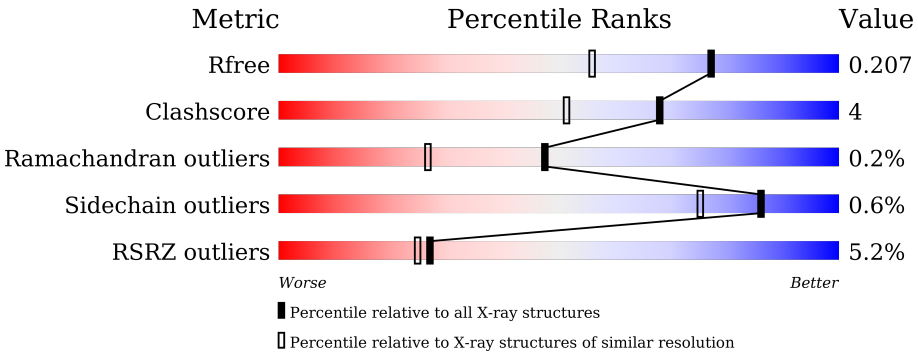
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.64 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	3122 (1.66-1.62)
Clashscore	141614	3268 (1.66-1.62)
Ramachandran outliers	138981	3215 (1.66-1.62)
Sidechain outliers	138945	3215 (1.66-1.62)
RSRZ outliers	127900	3079 (1.66-1.62)

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	235	2% 86% 6% 7%
1	B	235	2% 86% 6% 8%
1	C	235	2% 88% · 8%
1	D	235	9% 81% 10% 9%
1	E	235	2% 83% 8% · 8%
1	F	235	4% 88% · 8%

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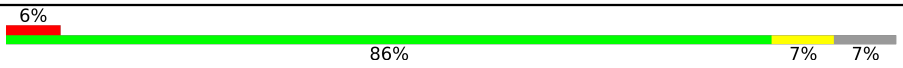
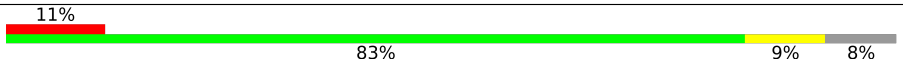
Mol	Chain	Length	Quality of chain
1	G	235	
1	H	235	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13988 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 Probable O-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	6	0
			1661	1041	307	310	3			
1	B	217	Total	C	N	O	S	0	1	0
			1607	1011	292	301	3			
1	C	216	Total	C	N	O	S	0	3	0
			1616	1016	297	300	3			
1	D	215	Total	C	N	O	S	0	1	0
			1563	988	281	291	3			
1	G	219	Total	C	N	O	S	0	2	0
			1602	1012	285	302	3			
1	H	216	Total	C	N	O	S	0	1	0
			1576	997	282	294	3			
1	E	217	Total	C	N	O	S	0	2	0
			1614	1013	293	305	3			
1	F	216	Total	C	N	O	S	0	2	0
			1585	1000	287	295	3			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	221	GLU	-	expression tag	UNP O07431
A	222	ASN	-	expression tag	UNP O07431
A	223	LEU	-	expression tag	UNP O07431
A	224	TYR	-	expression tag	UNP O07431
A	225	PHE	-	expression tag	UNP O07431
A	226	GLN	-	expression tag	UNP O07431
A	227	GLY	-	expression tag	UNP O07431
A	228	GLY	-	expression tag	UNP O07431
A	229	HIS	-	expression tag	UNP O07431
A	230	HIS	-	expression tag	UNP O07431
A	231	HIS	-	expression tag	UNP O07431
A	232	HIS	-	expression tag	UNP O07431
A	233	HIS	-	expression tag	UNP O07431

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Chain	Residue	Modelled	Actual	Comment	Reference
A	234	HIS	-	expression tag	UNP O07431
A	235	GLY	-	expression tag	UNP O07431
B	221	GLU	-	expression tag	UNP O07431
B	222	ASN	-	expression tag	UNP O07431
B	223	LEU	-	expression tag	UNP O07431
B	224	TYR	-	expression tag	UNP O07431
B	225	PHE	-	expression tag	UNP O07431
B	226	GLN	-	expression tag	UNP O07431
B	227	GLY	-	expression tag	UNP O07431
B	228	GLY	-	expression tag	UNP O07431
B	229	HIS	-	expression tag	UNP O07431
B	230	HIS	-	expression tag	UNP O07431
B	231	HIS	-	expression tag	UNP O07431
B	232	HIS	-	expression tag	UNP O07431
B	233	HIS	-	expression tag	UNP O07431
B	234	HIS	-	expression tag	UNP O07431
B	235	GLY	-	expression tag	UNP O07431
C	221	GLU	-	expression tag	UNP O07431
C	222	ASN	-	expression tag	UNP O07431
C	223	LEU	-	expression tag	UNP O07431
C	224	TYR	-	expression tag	UNP O07431
C	225	PHE	-	expression tag	UNP O07431
C	226	GLN	-	expression tag	UNP O07431
C	227	GLY	-	expression tag	UNP O07431
C	228	GLY	-	expression tag	UNP O07431
C	229	HIS	-	expression tag	UNP O07431
C	230	HIS	-	expression tag	UNP O07431
C	231	HIS	-	expression tag	UNP O07431
C	232	HIS	-	expression tag	UNP O07431
C	233	HIS	-	expression tag	UNP O07431
C	234	HIS	-	expression tag	UNP O07431
C	235	GLY	-	expression tag	UNP O07431
D	221	GLU	-	expression tag	UNP O07431
D	222	ASN	-	expression tag	UNP O07431
D	223	LEU	-	expression tag	UNP O07431
D	224	TYR	-	expression tag	UNP O07431
D	225	PHE	-	expression tag	UNP O07431
D	226	GLN	-	expression tag	UNP O07431
D	227	GLY	-	expression tag	UNP O07431
D	228	GLY	-	expression tag	UNP O07431
D	229	HIS	-	expression tag	UNP O07431
D	230	HIS	-	expression tag	UNP O07431

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Chain	Residue	Modelled	Actual	Comment	Reference
D	231	HIS	-	expression tag	UNP O07431
D	232	HIS	-	expression tag	UNP O07431
D	233	HIS	-	expression tag	UNP O07431
D	234	HIS	-	expression tag	UNP O07431
D	235	GLY	-	expression tag	UNP O07431
G	221	GLU	-	expression tag	UNP O07431
G	222	ASN	-	expression tag	UNP O07431
G	223	LEU	-	expression tag	UNP O07431
G	224	TYR	-	expression tag	UNP O07431
G	225	PHE	-	expression tag	UNP O07431
G	226	GLN	-	expression tag	UNP O07431
G	227	GLY	-	expression tag	UNP O07431
G	228	GLY	-	expression tag	UNP O07431
G	229	HIS	-	expression tag	UNP O07431
G	230	HIS	-	expression tag	UNP O07431
G	231	HIS	-	expression tag	UNP O07431
G	232	HIS	-	expression tag	UNP O07431
G	233	HIS	-	expression tag	UNP O07431
G	234	HIS	-	expression tag	UNP O07431
G	235	GLY	-	expression tag	UNP O07431
H	221	GLU	-	expression tag	UNP O07431
H	222	ASN	-	expression tag	UNP O07431
H	223	LEU	-	expression tag	UNP O07431
H	224	TYR	-	expression tag	UNP O07431
H	225	PHE	-	expression tag	UNP O07431
H	226	GLN	-	expression tag	UNP O07431
H	227	GLY	-	expression tag	UNP O07431
H	228	GLY	-	expression tag	UNP O07431
H	229	HIS	-	expression tag	UNP O07431
H	230	HIS	-	expression tag	UNP O07431
H	231	HIS	-	expression tag	UNP O07431
H	232	HIS	-	expression tag	UNP O07431
H	233	HIS	-	expression tag	UNP O07431
H	234	HIS	-	expression tag	UNP O07431
H	235	GLY	-	expression tag	UNP O07431
E	221	GLU	-	expression tag	UNP O07431
E	222	ASN	-	expression tag	UNP O07431
E	223	LEU	-	expression tag	UNP O07431
E	224	TYR	-	expression tag	UNP O07431
E	225	PHE	-	expression tag	UNP O07431
E	226	GLN	-	expression tag	UNP O07431
E	227	GLY	-	expression tag	UNP O07431

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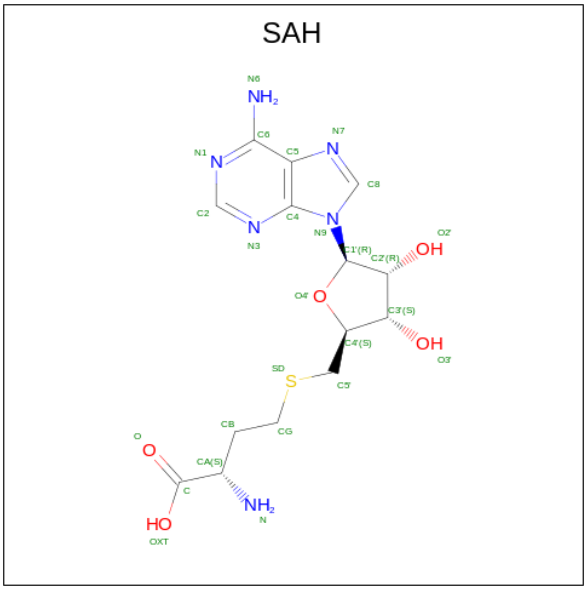
Chain	Residue	Modelled	Actual	Comment	Reference
E	228	GLY	-	expression tag	UNP O07431
E	229	HIS	-	expression tag	UNP O07431
E	230	HIS	-	expression tag	UNP O07431
E	231	HIS	-	expression tag	UNP O07431
E	232	HIS	-	expression tag	UNP O07431
E	233	HIS	-	expression tag	UNP O07431
E	234	HIS	-	expression tag	UNP O07431
E	235	GLY	-	expression tag	UNP O07431
F	221	GLU	-	expression tag	UNP O07431
F	222	ASN	-	expression tag	UNP O07431
F	223	LEU	-	expression tag	UNP O07431
F	224	TYR	-	expression tag	UNP O07431
F	225	PHE	-	expression tag	UNP O07431
F	226	GLN	-	expression tag	UNP O07431
F	227	GLY	-	expression tag	UNP O07431
F	228	GLY	-	expression tag	UNP O07431
F	229	HIS	-	expression tag	UNP O07431
F	230	HIS	-	expression tag	UNP O07431
F	231	HIS	-	expression tag	UNP O07431
F	232	HIS	-	expression tag	UNP O07431
F	233	HIS	-	expression tag	UNP O07431
F	234	HIS	-	expression tag	UNP O07431
F	235	GLY	-	expression tag	UNP O07431

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).

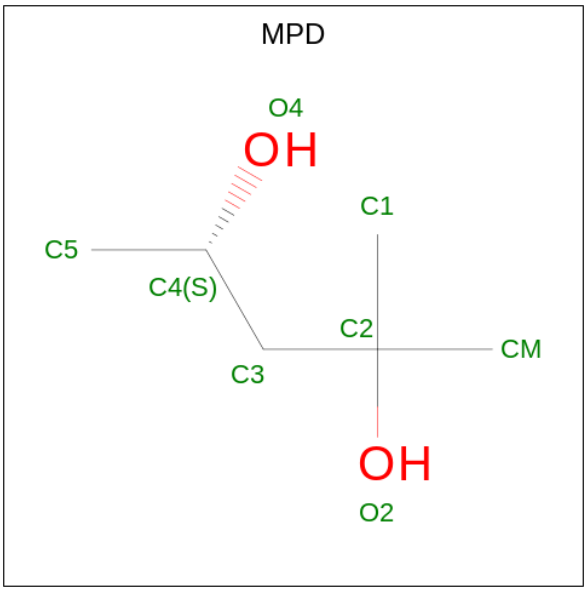


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	G	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	H	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	E	1	Total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

- Molecule 3 is STRONTIUM ION (three-letter code: SR) (formula: Sr) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Sr	0	0
			3	3		
3	B	2	Total	Sr	0	0
			2	2		
3	D	2	Total	Sr	0	0
			2	2		
3	G	3	Total	Sr	0	0
			3	3		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0
4	C	1	Total C O 8 6 2	0	0
4	D	1	Total C O 8 6 2	0	0
4	G	1	Total C O 8 6 2	0	0
4	H	1	Total C O 8 6 2	0	0
4	E	1	Total C O 8 6 2	0	0
4	F	1	Total C O 8 6 2	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Na 1 1	0	0

- Molecule 6 is water.

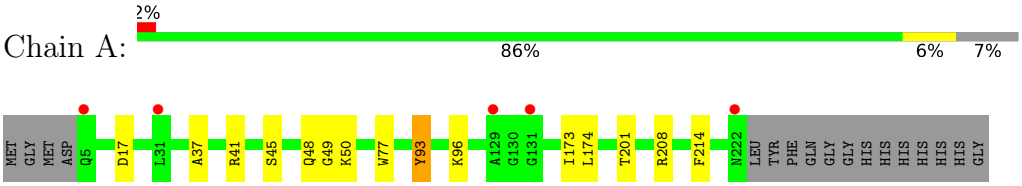
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	145	Total O 145 145	0	0
6	B	137	Total O 137 137	0	0
6	C	126	Total O 126 126	0	0
6	D	84	Total O 84 84	0	0
6	G	81	Total O 81 81	0	0
6	H	73	Total O 73 73	0	0
6	E	136	Total O 136 136	0	0
6	F	91	Total O 91 91	0	0

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.

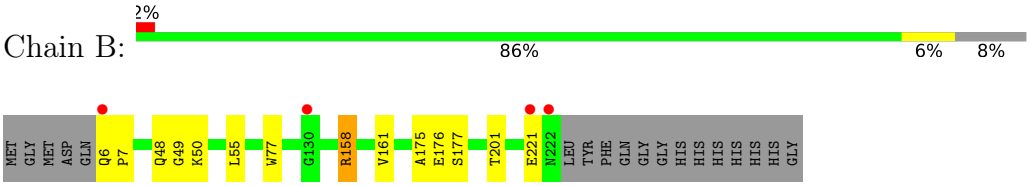
• Molecule 1: Probable O-methyltransferase

Chain A:



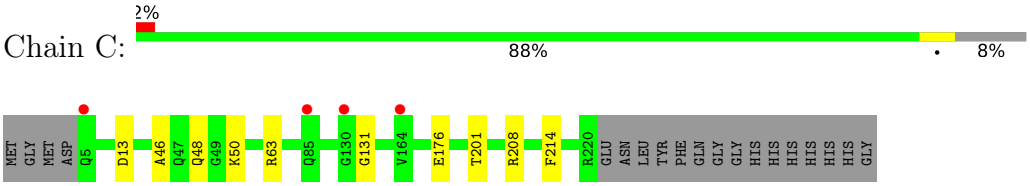
• Molecule 1: Probable O-methyltransferase

Chain B:



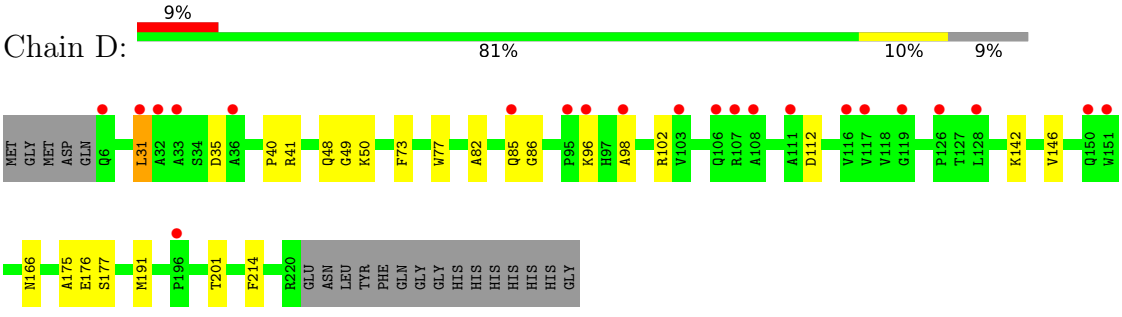
• Molecule 1: Probable O-methyltransferase

Chain C:



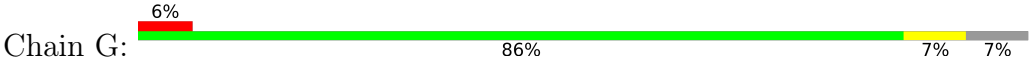
• Molecule 1: Probable O-methyltransferase

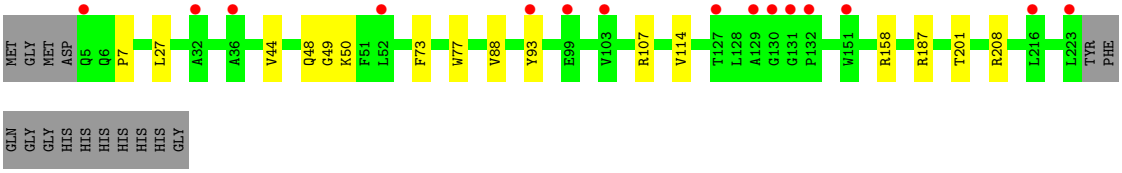
Chain D:



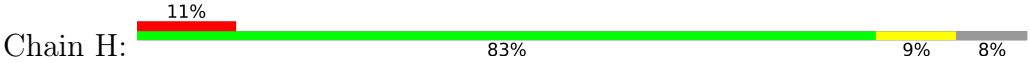
• Molecule 1: Probable O-methyltransferase

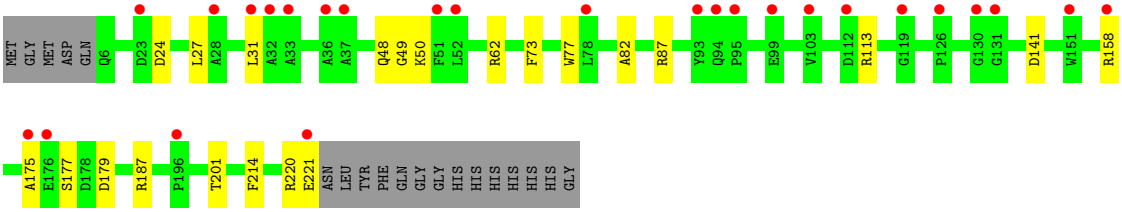
Chain G:



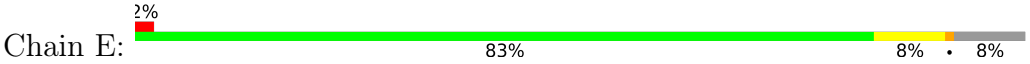


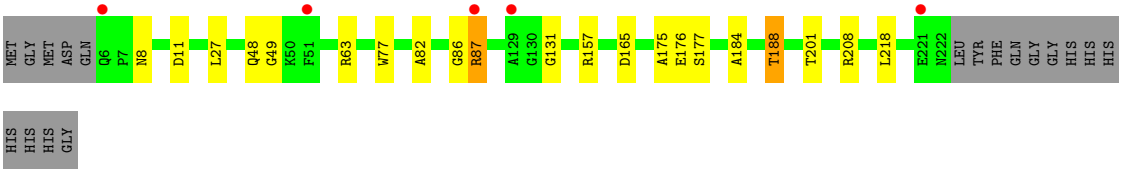
• Molecule 1: Probable O-methyltransferase



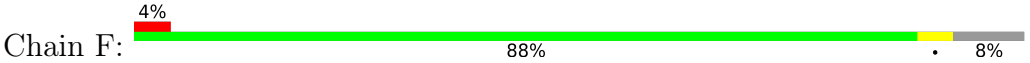


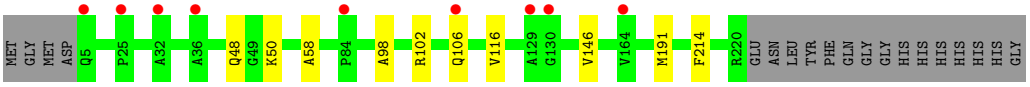
• Molecule 1: Probable O-methyltransferase





• Molecule 1: Probable O-methyltransferase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	75.30Å 75.92Å 329.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.23 – 1.64 36.23 – 1.64	Depositor EDS
% Data completeness (in resolution range)	98.6 (36.23-1.64) 98.6 (36.23-1.64)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 1.64Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.181 , 0.207 0.181 , 0.207	Depositor DCC
R_{free} test set	11295 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	21.3	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.045 for k,h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	13988	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% 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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.41	0/1687	0.56	0/2297
1	B	0.40	0/1633	0.56	0/2226
1	C	0.39	0/1642	0.57	0/2237
1	D	0.38	1/1589 (0.1%)	0.53	1/2171 (0.0%)
1	E	0.37	0/1640	0.65	3/2237 (0.1%)
1	F	0.34	0/1611	0.53	0/2199
1	G	0.33	0/1629	0.49	0/2226
1	H	0.36	0/1603	0.55	0/2190
All	All	0.37	1/13034 (0.0%)	0.56	4/17783 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	85	GLN	CB-CG	-5.66	1.37	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	87	ARG	CA-CB-CG	-9.15	93.26	113.40
1	E	87	ARG	CB-CG-CD	7.89	132.12	111.60
1	E	87	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	D	85	GLN	CA-CB-CG	-5.34	101.66	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1661	0	1668	14	0
1	B	1607	0	1616	12	0
1	C	1616	0	1626	13	0
1	D	1563	0	1563	17	0
1	E	1614	0	1612	15	0
1	F	1585	0	1584	9	0
1	G	1602	0	1580	13	0
1	H	1576	0	1568	15	0
2	A	26	0	19	1	0
2	B	26	0	19	0	0
2	C	26	0	19	0	0
2	D	26	0	19	0	0
2	E	26	0	19	0	0
2	F	26	0	19	0	0
2	G	26	0	19	2	0
2	H	26	0	19	0	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
3	D	2	0	0	0	0
3	G	3	0	0	0	0
4	A	8	0	14	3	0
4	B	16	0	28	1	0
4	C	8	0	14	2	0
4	D	8	0	14	2	0
4	E	8	0	14	3	0
4	F	8	0	14	2	0
4	G	8	0	14	2	0
4	H	8	0	14	3	0
5	B	1	0	0	0	0
6	A	145	0	0	2	0
6	B	137	0	0	0	0
6	C	126	0	0	4	0
6	D	84	0	0	2	0
6	E	136	0	0	1	0
6	F	91	0	0	0	0
6	G	81	0	0	1	0
6	H	73	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13988	0	13095	99	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 4.

All (99) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ASP:OD2	1:A:208[A]:ARG:NH1	2.11	0.83
1:G:48:GLN:HG2	4:G:303:MPD:H53	1.61	0.83
1:E:48:GLN:HG2	4:E:302:MPD:H4	1.68	0.75
1:H:158:ARG:NH2	1:H:220:ARG:O	2.25	0.69
1:E:208:ARG:NH1	6:E:401:HOH:O	2.21	0.68
1:A:208[A]:ARG:NH2	6:A:401:HOH:O	2.26	0.67
1:F:102[B]:ARG:NH2	1:F:116:VAL:H	1.93	0.67
1:D:146:VAL:HG22	1:D:191:MET:HE2	1.77	0.65
1:A:208[B]:ARG:NH2	6:A:403:HOH:O	2.31	0.63
1:B:48:GLN:HG2	4:B:303:MPD:H4	1.80	0.63
1:B:158:ARG:HH21	1:B:221[B]:GLU:HA	1.63	0.62
1:H:48:GLN:HB3	4:H:302:MPD:HM1	1.82	0.61
1:D:175:ALA:O	1:D:177:SER:N	2.33	0.61
1:H:158:ARG:NH2	1:H:221:GLU:OE1	2.24	0.61
1:B:158:ARG:HH21	1:B:221[A]:GLU:HA	1.65	0.61
1:C:48:GLN:HG2	4:C:302:MPD:H4	1.83	0.60
1:D:102[A]:ARG:NH1	6:D:401:HOH:O	2.24	0.60
1:C:63:ARG:HD2	1:C:131:GLY:HA2	1.84	0.60
1:A:173:ILE:HG13	1:A:174:LEU:HD13	1.85	0.58
1:D:82:ALA:HB1	1:D:86:GLY:HA3	1.84	0.58
1:G:187:ARG:NH1	6:G:401:HOH:O	2.30	0.58
1:D:48:GLN:HG2	4:D:303:MPD:H4	1.85	0.57
1:E:86:GLY:O	1:E:87:ARG:HG2	2.05	0.56
1:G:7:PRO:HG3	1:H:175:ALA:HB2	1.86	0.56
1:E:175:ALA:O	1:E:177:SER:N	2.36	0.56
1:A:201:THR:HB	1:B:50:LYS:HG2	1.88	0.56
1:E:63:ARG:NH1	1:E:131:GLY:O	2.39	0.56
1:E:201:THR:HB	1:F:50:LYS:HG2	1.89	0.55
1:G:50:LYS:HG2	1:H:201:THR:HB	1.88	0.55
1:G:201:THR:HB	1:H:50:LYS:HG2	1.89	0.54
1:A:50:LYS:HG2	1:B:201:THR:HB	1.88	0.54
1:A:45:SER:HA	1:A:208[B]:ARG:HH11	1.72	0.54
1:C:50:LYS:HG2	1:D:201:THR:HB	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:88:VAL:HB	1:G:114:VAL:HG22	1.90	0.53
4:H:302:MPD:O4	4:H:302:MPD:O2	2.19	0.53
1:C:201:THR:HB	1:D:50:LYS:HG2	1.93	0.51
4:E:302:MPD:O4	4:E:302:MPD:HM1	2.10	0.51
1:F:48:GLN:HG2	4:F:302:MPD:H4	1.92	0.51
1:C:208[A]:ARG:HG2	6:C:401:HOH:O	2.10	0.51
1:G:27:LEU:HD13	1:G:73[A]:PHE:CZ	2.46	0.51
1:E:184:ALA:O	1:E:188:THR:HG23	2.11	0.51
1:H:214:PHE:CE1	4:H:302:MPD:H53	2.45	0.50
1:A:214:PHE:CE1	4:A:303:MPD:H53	2.47	0.50
1:A:48:GLN:HG2	4:A:303:MPD:H4	1.93	0.49
1:H:49:GLY:HA3	1:H:77:TRP:CD1	2.47	0.49
1:E:49:GLY:HA3	1:E:77:TRP:CD1	2.47	0.49
1:C:13:ASP:HB3	1:C:208[A]:ARG:HG3	1.94	0.49
1:G:49:GLY:HA3	1:G:77:TRP:CD1	2.48	0.49
1:E:82:ALA:HB1	1:E:86:GLY:HA3	1.94	0.49
1:F:146:VAL:HA	1:F:191:MET:HE2	1.95	0.48
1:D:49:GLY:HA3	1:D:77:TRP:CD1	2.50	0.47
1:H:62:ARG:NH2	1:H:82:ALA:O	2.48	0.47
1:B:158:ARG:NH2	1:B:221[B]:GLU:OE1	2.49	0.46
1:D:112:ASP:OD1	1:D:112:ASP:N	2.46	0.46
1:D:31:LEU:HD21	1:D:41:ARG:HH21	1.79	0.46
1:A:214:PHE:HB3	4:A:303:MPD:H13	1.96	0.46
1:E:165:ASP:OD1	4:E:302:MPD:HM2	2.16	0.46
1:B:175:ALA:O	1:B:177:SER:N	2.50	0.45
1:E:157:ARG:HH11	1:E:157:ARG:HG3	1.80	0.45
1:E:218:LEU:HD21	1:F:58:ALA:HB2	1.97	0.45
1:B:55:LEU:HD21	1:B:161:VAL:HG11	1.99	0.45
1:C:214:PHE:HB3	4:C:302:MPD:H13	1.99	0.45
1:A:37:ALA:HB1	1:A:96:LYS:HE2	1.98	0.45
1:C:208[B]:ARG:HG3	6:C:403:HOH:O	2.17	0.44
1:C:208[A]:ARG:NH1	6:C:403:HOH:O	2.48	0.44
1:D:98:ALA:O	1:D:102[A]:ARG:HG3	2.17	0.44
1:B:49:GLY:HA3	1:B:77:TRP:CD1	2.52	0.44
1:G:27:LEU:HD23	1:G:27:LEU:HA	1.79	0.44
1:H:87:ARG:HA	1:H:113:ARG:O	2.18	0.44
1:F:146:VAL:HG22	1:F:191:MET:CE	2.47	0.43
1:G:93:TYR:HB2	2:G:301:SAH:C4	2.48	0.43
1:E:86:GLY:C	1:E:87:ARG:HG2	2.38	0.43
1:D:31:LEU:HB2	1:D:73:PHE:HZ	1.83	0.43
1:D:40:PRO:HD3	1:H:187:ARG:NH1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:ASP:OD2	1:D:41:ARG:NH2	2.52	0.43
1:D:214:PHE:HB3	4:D:303:MPD:H13	2.02	0.42
1:E:8:ASN:ND2	1:E:11:ASP:OD2	2.53	0.42
1:G:48:GLN:HB3	4:G:303:MPD:H31	2.00	0.42
1:A:93:TYR:CE1	2:A:301:SAH:C8	3.03	0.42
1:F:98:ALA:O	1:F:102[B]:ARG:HG3	2.19	0.42
1:A:41:ARG:HD3	1:C:176:GLU:OE1	2.20	0.42
1:D:142:LYS:HE3	1:D:166:ASN:HB2	2.01	0.42
1:C:208[A]:ARG:NH1	6:C:401:HOH:O	2.52	0.42
1:G:44:VAL:HG13	2:G:301:SAH:OXT	2.20	0.42
1:B:6:GLN:HB3	1:B:7:PRO:HD3	2.01	0.41
1:H:31:LEU:HA	1:H:73[A]:PHE:HZ	1.85	0.41
1:F:146:VAL:HG22	1:F:191:MET:HE2	2.01	0.41
1:C:13:ASP:CB	1:C:208[A]:ARG:HG3	2.50	0.41
1:D:96:LYS:HG2	6:D:471:HOH:O	2.19	0.41
1:E:27:LEU:HD23	1:E:27:LEU:HA	1.87	0.41
1:H:24:ASP:CG	1:H:27:LEU:HD12	2.41	0.41
1:G:107:ARG:HD2	1:G:107:ARG:O	2.20	0.41
1:A:49:GLY:HA3	1:A:77:TRP:CD1	2.56	0.40
1:H:141:ASP:OD1	1:H:141:ASP:N	2.53	0.40
1:C:46:ALA:H	1:C:208[B]:ARG:NH1	2.19	0.40
1:H:177:SER:O	1:H:179:ASP:N	2.55	0.40
1:F:214:PHE:CE1	4:F:302:MPD:H53	2.57	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	222/235 (94%)	215 (97%)	7 (3%)	0	100	100
1	B	216/235 (92%)	208 (96%)	7 (3%)	1 (0%)	29	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	217/235 (92%)	210 (97%)	7 (3%)	0	100 100
1	D	214/235 (91%)	208 (97%)	5 (2%)	1 (0%)	29 11
1	E	217/235 (92%)	209 (96%)	7 (3%)	1 (0%)	29 11
1	F	216/235 (92%)	209 (97%)	7 (3%)	0	100 100
1	G	219/235 (93%)	212 (97%)	7 (3%)	0	100 100
1	H	215/235 (92%)	208 (97%)	7 (3%)	0	100 100
All	All	1736/1880 (92%)	1679 (97%)	54 (3%)	3 (0%)	47 26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	176	GLU
1	E	176	GLU
1	B	176	GLU

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	164/173 (95%)	163 (99%)	1 (1%)	86 75
1	B	158/173 (91%)	157 (99%)	1 (1%)	86 75
1	C	158/173 (91%)	158 (100%)	0	100 100
1	D	151/173 (87%)	150 (99%)	1 (1%)	84 71
1	E	159/173 (92%)	158 (99%)	1 (1%)	86 75
1	F	153/173 (88%)	152 (99%)	1 (1%)	84 71
1	G	154/173 (89%)	151 (98%)	3 (2%)	57 32
1	H	152/173 (88%)	152 (100%)	0	100 100
All	All	1249/1384 (90%)	1241 (99%)	8 (1%)	86 75

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	TYR
1	B	158	ARG
1	D	31	LEU
1	G	158	ARG
1	G	208[A]	ARG
1	G	208[B]	ARG
1	E	188	THR
1	F	106	GLN

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 11 are monoatomic - leaving 17 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	SAH	H	301	-	24,28,28	1.19	2 (8%)	25,40,40	1.77	5 (20%)
4	MPD	A	303	-	7,7,7	0.24	0	9,10,10	0.52	0
2	SAH	D	301	-	24,28,28	1.15	2 (8%)	25,40,40	1.70	6 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SAH	G	301	-	24,28,28	1.20	3 (12%)	25,40,40	1.60	4 (16%)
4	MPD	E	302	-	7,7,7	0.43	0	9,10,10	1.43	1 (11%)
4	MPD	G	303	-	7,7,7	0.31	0	9,10,10	0.45	0
4	MPD	F	302	-	7,7,7	0.27	0	9,10,10	0.43	0
4	MPD	H	302	-	7,7,7	0.23	0	9,10,10	0.86	0
2	SAH	F	301	-	24,28,28	1.15	3 (12%)	25,40,40	1.60	3 (12%)
4	MPD	D	303	-	7,7,7	0.30	0	9,10,10	0.57	0
4	MPD	B	304	-	7,7,7	0.24	0	9,10,10	0.35	0
2	SAH	B	301	-	24,28,28	1.17	3 (12%)	25,40,40	1.60	5 (20%)
4	MPD	C	302	-	7,7,7	0.32	0	9,10,10	0.61	0
2	SAH	E	301	-	24,28,28	1.23	3 (12%)	25,40,40	1.64	3 (12%)
4	MPD	B	303	-	7,7,7	0.34	0	9,10,10	0.80	0
2	SAH	C	301	-	24,28,28	1.20	3 (12%)	25,40,40	1.69	5 (20%)
2	SAH	A	301	-	24,28,28	1.21	3 (12%)	25,40,40	1.48	3 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAH	H	301	-	-	2/11/31/31	0/3/3/3
4	MPD	A	303	-	-	3/5/5/5	-
2	SAH	D	301	-	-	0/11/31/31	0/3/3/3
2	SAH	G	301	-	-	2/11/31/31	0/3/3/3
4	MPD	E	302	-	-	3/5/5/5	-
4	MPD	G	303	-	-	1/5/5/5	-
4	MPD	F	302	-	-	2/5/5/5	-
4	MPD	H	302	-	-	1/5/5/5	-
2	SAH	F	301	-	-	2/11/31/31	0/3/3/3
4	MPD	D	303	-	-	3/5/5/5	-
4	MPD	B	304	-	-	1/5/5/5	-
2	SAH	B	301	-	-	2/11/31/31	0/3/3/3
4	MPD	C	302	-	-	3/5/5/5	-
2	SAH	E	301	-	-	2/11/31/31	0/3/3/3
4	MPD	B	303	-	-	3/5/5/5	-
2	SAH	C	301	-	-	1/11/31/31	0/3/3/3
2	SAH	A	301	-	-	2/11/31/31	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	SAH	C2-N3	4.26	1.39	1.32
2	E	301	SAH	C2-N3	4.16	1.38	1.32
2	G	301	SAH	C2-N3	3.96	1.38	1.32
2	F	301	SAH	C2-N3	3.91	1.38	1.32
2	A	301	SAH	C2-N3	3.86	1.38	1.32
2	D	301	SAH	C2-N3	3.79	1.38	1.32
2	B	301	SAH	C2-N3	3.74	1.38	1.32
2	H	301	SAH	C2-N3	3.47	1.37	1.32
2	A	301	SAH	C2-N1	2.84	1.39	1.33
2	G	301	SAH	C2-N1	2.63	1.38	1.33
2	H	301	SAH	C2-N1	2.44	1.38	1.33
2	B	301	SAH	C2-N1	2.40	1.38	1.33
2	E	301	SAH	C2-N1	2.40	1.38	1.33
2	A	301	SAH	OXT-C	-2.34	1.22	1.30
2	D	301	SAH	C2-N1	2.29	1.38	1.33
2	E	301	SAH	OXT-C	-2.23	1.23	1.30
2	G	301	SAH	OXT-C	-2.23	1.23	1.30
2	F	301	SAH	C2-N1	2.16	1.37	1.33
2	C	301	SAH	C2-N1	2.13	1.37	1.33
2	C	301	SAH	OXT-C	-2.10	1.23	1.30
2	F	301	SAH	OXT-C	-2.02	1.23	1.30
2	B	301	SAH	OXT-C	-2.02	1.24	1.30

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	301	SAH	N3-C2-N1	-6.33	118.78	128.68
2	E	301	SAH	N3-C2-N1	-5.86	119.52	128.68
2	F	301	SAH	N3-C2-N1	-5.82	119.58	128.68
2	G	301	SAH	N3-C2-N1	-5.72	119.74	128.68
2	D	301	SAH	N3-C2-N1	-5.71	119.75	128.68
2	C	301	SAH	N3-C2-N1	-5.64	119.87	128.68
2	A	301	SAH	N3-C2-N1	-5.06	120.78	128.68
2	B	301	SAH	N3-C2-N1	-4.83	121.14	128.68
4	E	302	MPD	CM-C2-C1	-3.70	102.86	110.57
2	D	301	SAH	C5'-SD-CG	-2.64	94.33	102.27
2	H	301	SAH	C5'-SD-CG	-2.59	94.50	102.27
2	D	301	SAH	OXT-C-CA	2.56	122.10	113.38
2	B	301	SAH	OXT-C-O	-2.48	118.47	124.09
2	H	301	SAH	CB-CG-SD	-2.42	107.87	113.31
2	G	301	SAH	OXT-C-O	-2.42	118.59	124.09
2	H	301	SAH	OXT-C-O	-2.39	118.66	124.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	301	SAH	O4'-C1'-C2'	-2.38	103.45	106.93
2	C	301	SAH	C1'-N9-C4	-2.34	122.54	126.64
2	B	301	SAH	C5'-SD-CG	-2.33	95.28	102.27
2	A	301	SAH	O4'-C1'-C2'	-2.33	103.53	106.93
2	B	301	SAH	OXT-C-CA	2.32	121.28	113.38
2	D	301	SAH	OXT-C-O	-2.29	118.89	124.09
2	D	301	SAH	C1'-N9-C4	-2.24	122.71	126.64
2	F	301	SAH	C5'-SD-CG	-2.18	95.72	102.27
2	G	301	SAH	OXT-C-CA	2.16	120.74	113.38
2	H	301	SAH	OXT-C-CA	2.12	120.60	113.38
2	E	301	SAH	C5'-SD-CG	-2.11	95.92	102.27
2	E	301	SAH	C1'-N9-C4	-2.10	122.95	126.64
2	C	301	SAH	CB-CG-SD	-2.10	108.60	113.31
2	C	301	SAH	O4'-C4'-C5'	-2.08	103.49	108.83
2	A	301	SAH	OXT-C-O	-2.07	119.39	124.09
2	D	301	SAH	CB-CG-SD	-2.06	108.69	113.31
2	F	301	SAH	OXT-C-O	-2.06	119.42	124.09
2	B	301	SAH	C1'-N9-C4	-2.05	123.05	126.64
2	C	301	SAH	O4'-C1'-C2'	-2.05	103.94	106.93

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	302	MPD	O2-C2-C3-C4
4	E	302	MPD	O2-C2-C3-C4
4	E	302	MPD	CM-C2-C3-C4
2	A	301	SAH	O-C-CA-N
2	G	301	SAH	O-C-CA-N
2	E	301	SAH	O-C-CA-N
2	F	301	SAH	O-C-CA-N
4	A	303	MPD	O2-C2-C3-C4
4	B	303	MPD	O2-C2-C3-C4
4	D	303	MPD	O2-C2-C3-C4
4	F	302	MPD	O2-C2-C3-C4
4	B	304	MPD	C2-C3-C4-C5
4	G	303	MPD	C2-C3-C4-C5
2	B	301	SAH	OXT-C-CA-N
2	H	301	SAH	OXT-C-CA-N
4	A	303	MPD	C1-C2-C3-C4
4	A	303	MPD	CM-C2-C3-C4
4	B	303	MPD	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
4	B	303	MPD	CM-C2-C3-C4
4	C	302	MPD	C1-C2-C3-C4
4	C	302	MPD	CM-C2-C3-C4
4	D	303	MPD	C1-C2-C3-C4
4	D	303	MPD	CM-C2-C3-C4
4	E	302	MPD	C1-C2-C3-C4
4	F	302	MPD	C1-C2-C3-C4
2	C	301	SAH	OXT-C-CA-N
2	B	301	SAH	O-C-CA-N
2	H	301	SAH	O-C-CA-N
2	A	301	SAH	OXT-C-CA-N
2	G	301	SAH	OXT-C-CA-N
2	E	301	SAH	OXT-C-CA-N
2	F	301	SAH	OXT-C-CA-N
4	H	302	MPD	O2-C2-C3-C4

There are no ring outliers.

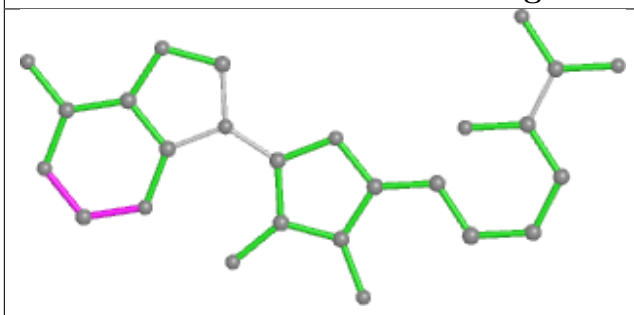
10 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	303	MPD	3	0
2	G	301	SAH	2	0
4	E	302	MPD	3	0
4	G	303	MPD	2	0
4	F	302	MPD	2	0
4	H	302	MPD	3	0
4	D	303	MPD	2	0
4	C	302	MPD	2	0
4	B	303	MPD	1	0
2	A	301	SAH	1	0

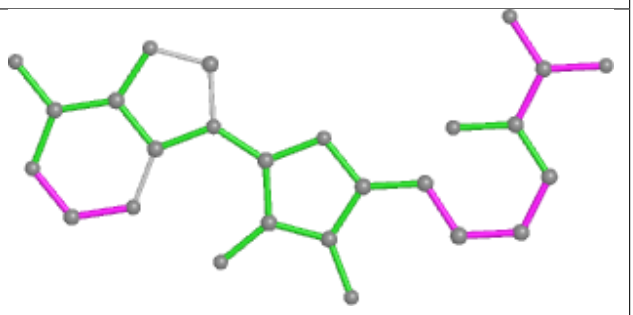
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

equivalents in the CSD to analyse the geometry.

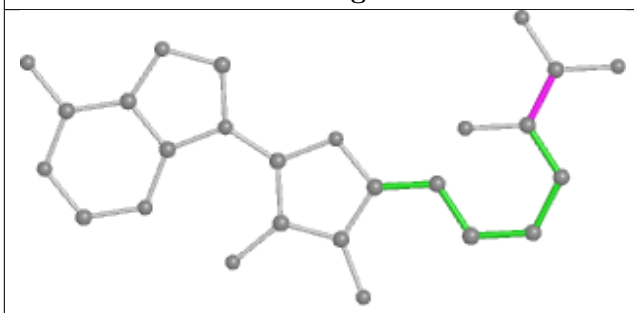
Ligand SAH H 301



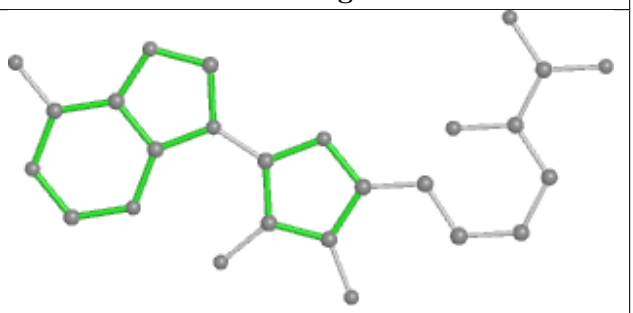
Bond lengths



Bond angles

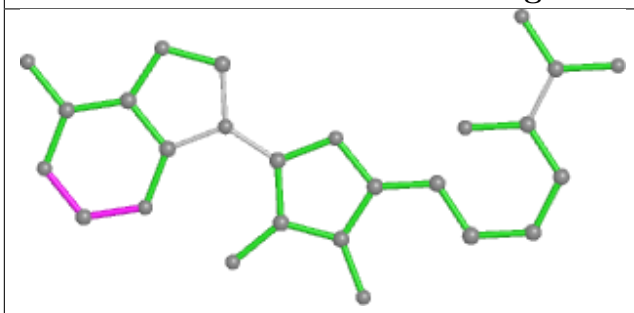


Torsions

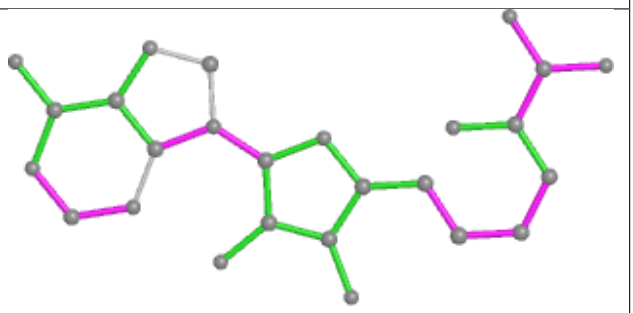


Rings

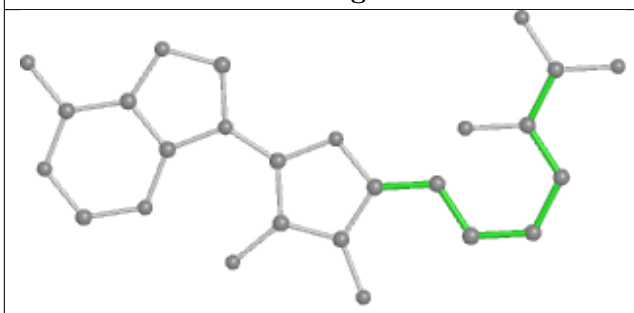
Ligand SAH D 301



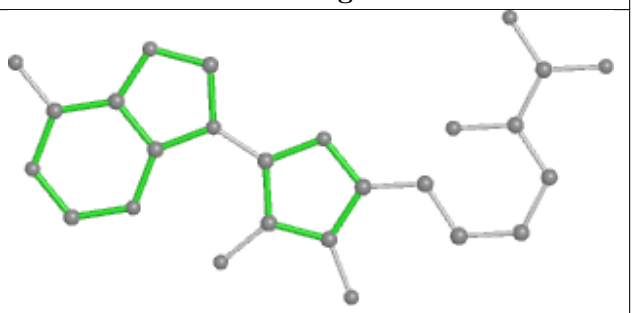
Bond lengths



Bond angles

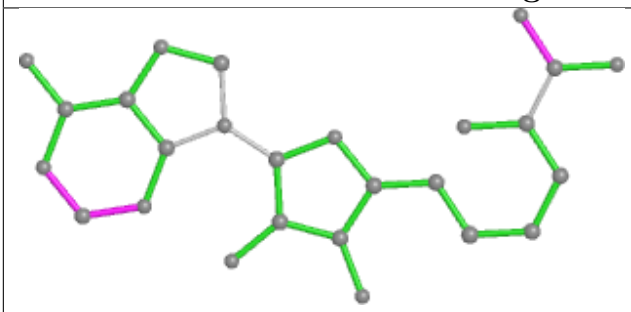


Torsions

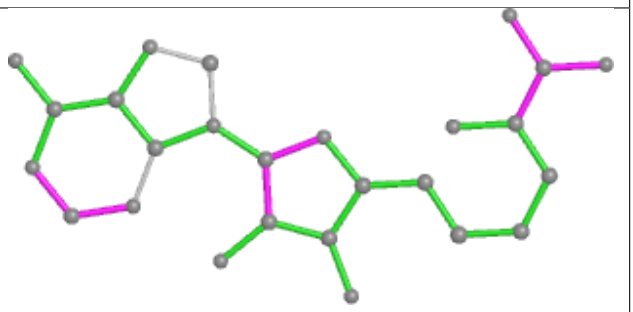


Rings

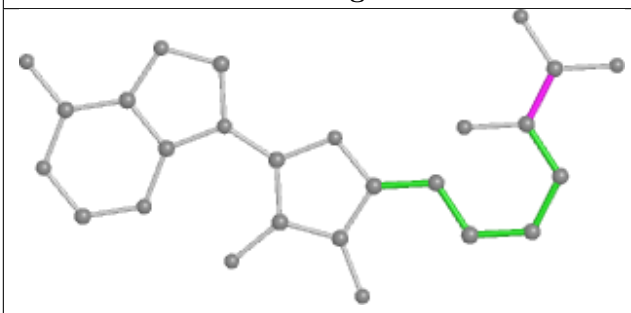
Ligand SAH G 301



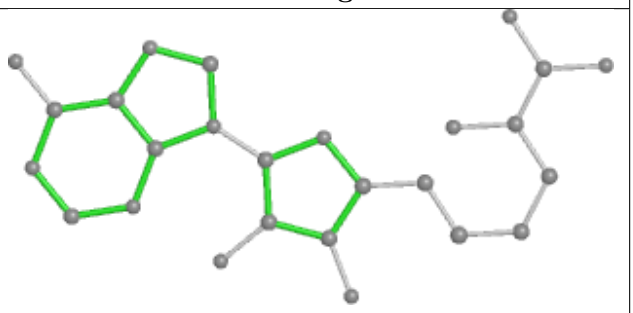
Bond lengths



Bond angles

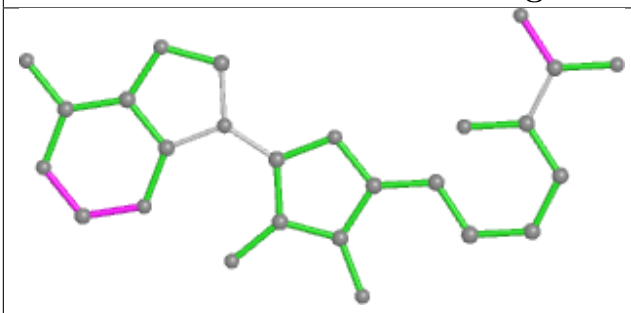


Torsions

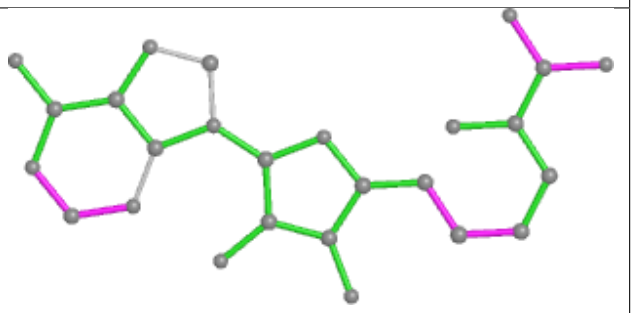


Rings

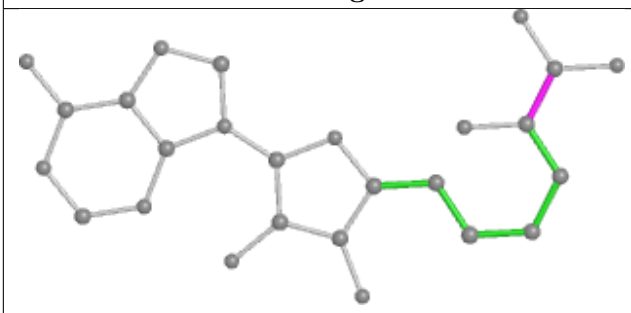
Ligand SAH F 301



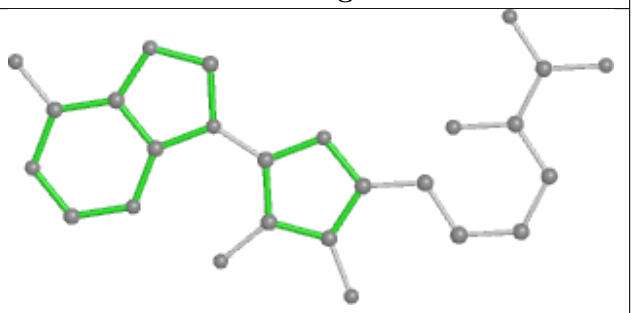
Bond lengths



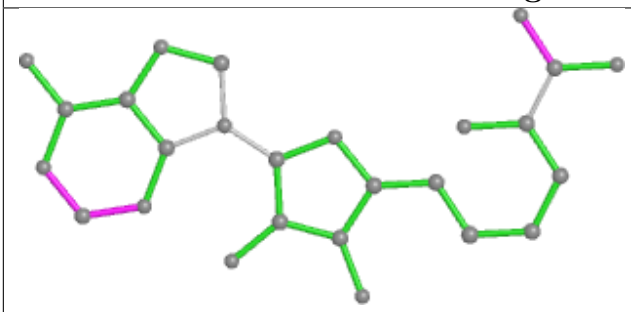
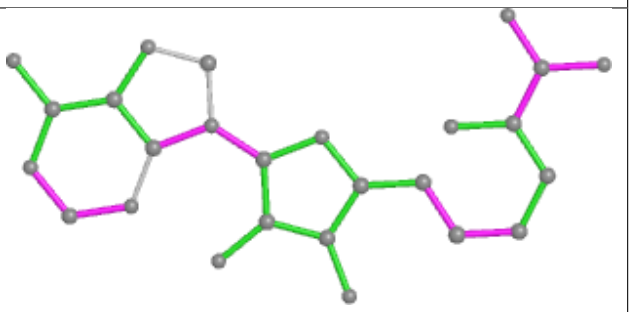
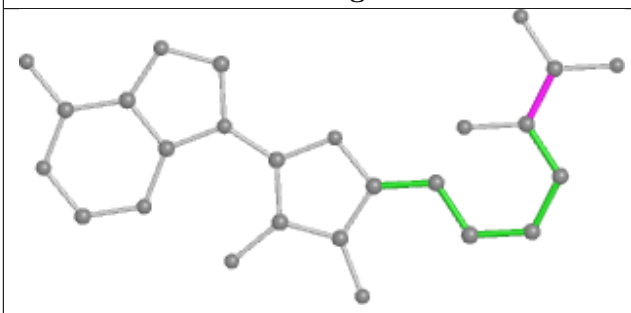
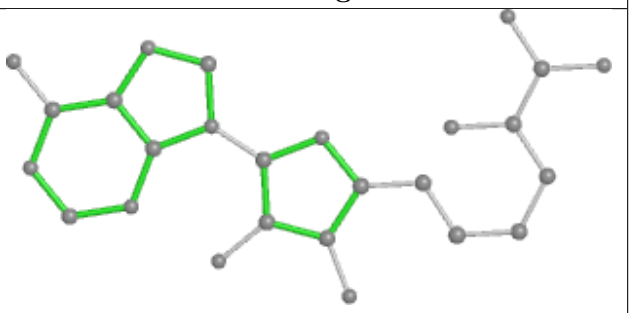
Bond angles

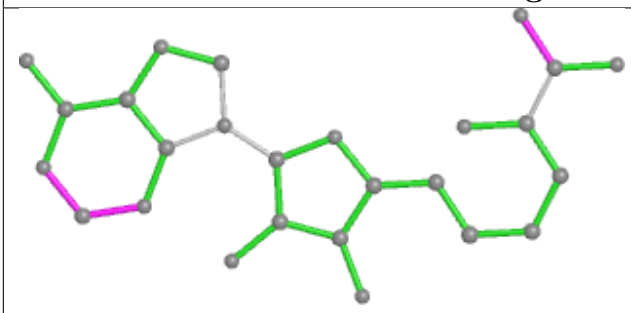
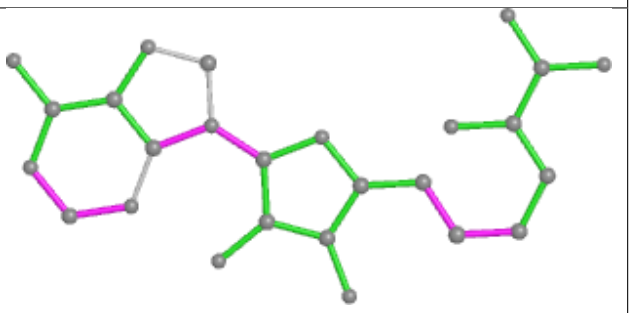
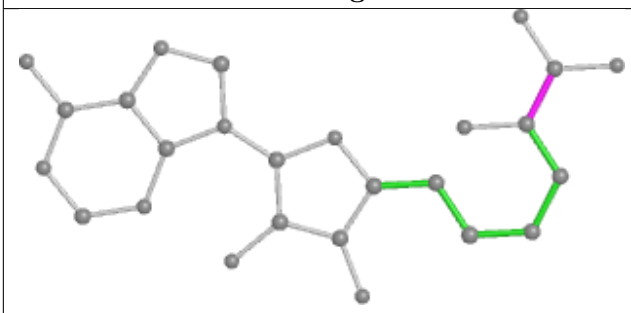
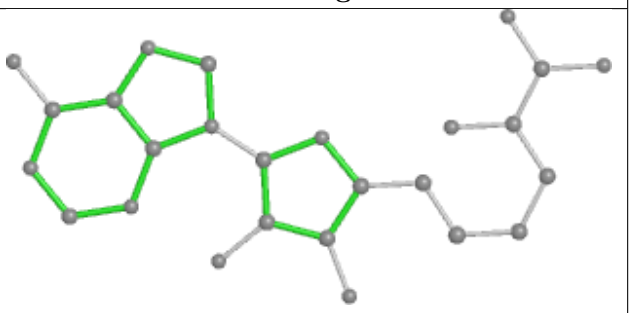


Torsions

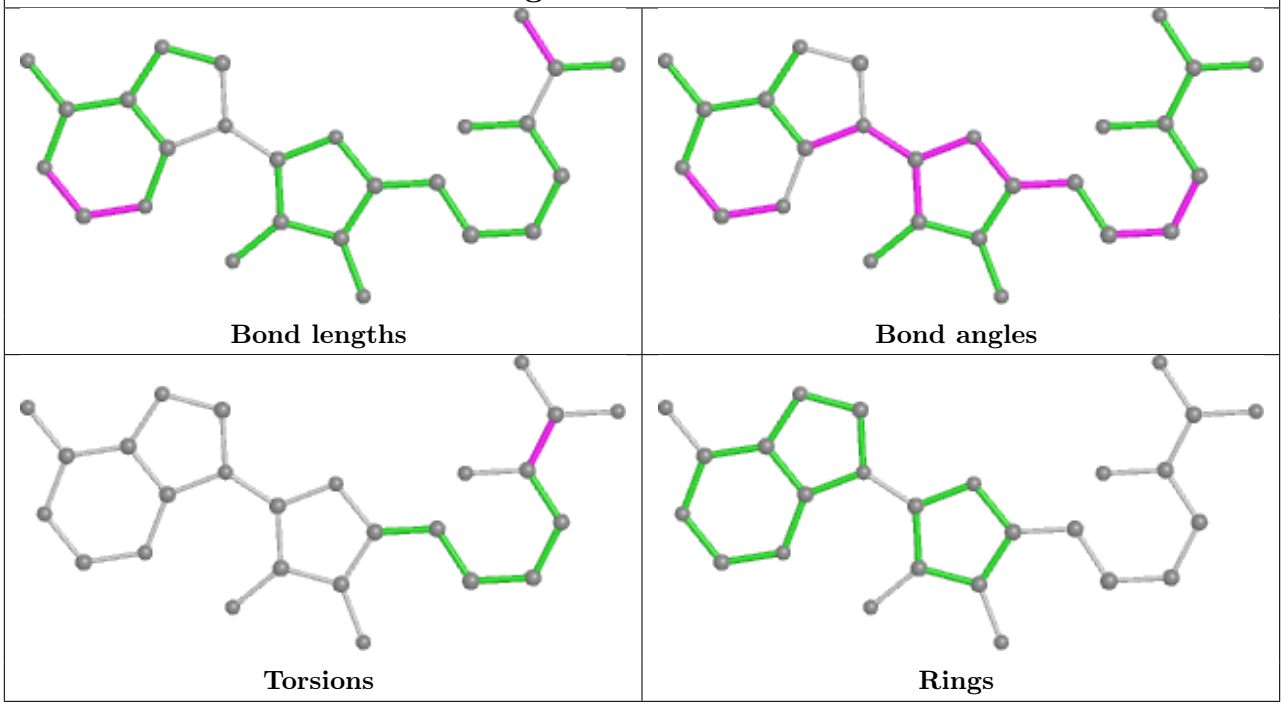


Rings

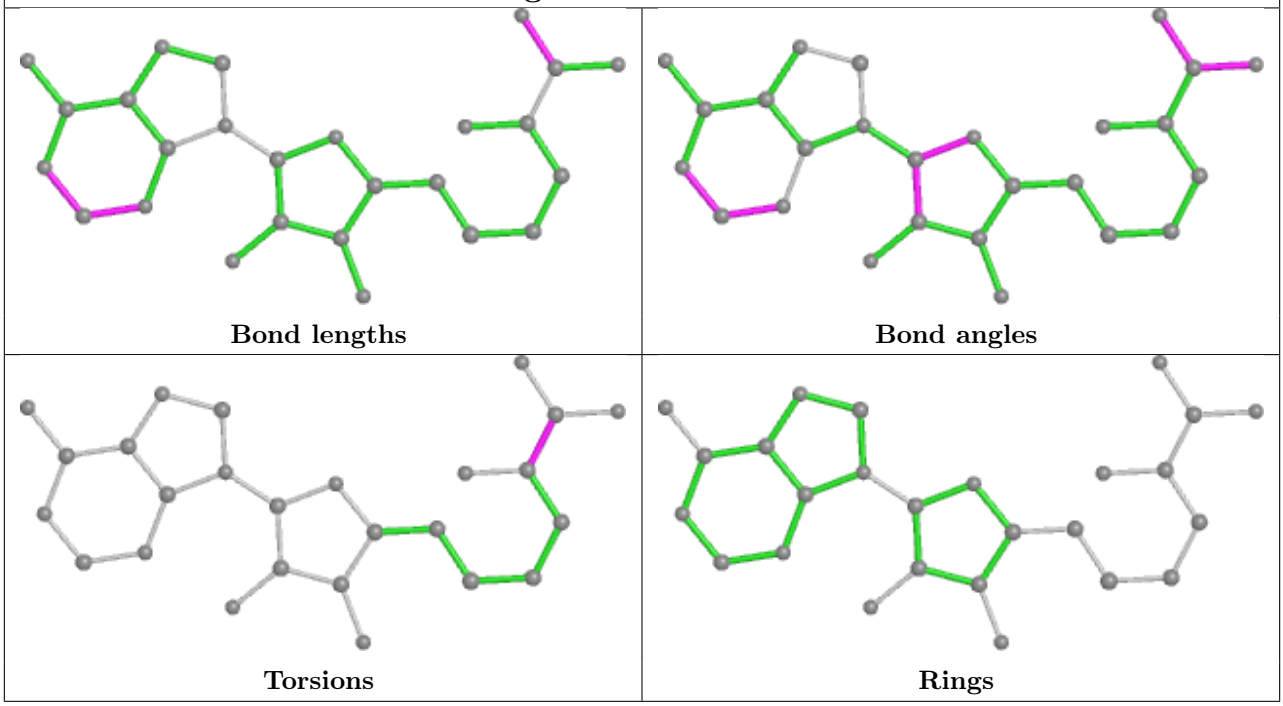
Ligand SAH B 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SAH E 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SAH C 301



Ligand SAH A 301



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	218/235 (92%)	-0.13	5 (2%) 60 60	14, 23, 43, 59	0
1	B	217/235 (92%)	-0.14	4 (1%) 68 69	15, 24, 46, 68	0
1	C	216/235 (91%)	-0.15	4 (1%) 66 67	16, 25, 46, 67	0
1	D	215/235 (91%)	0.36	22 (10%) 6 5	20, 42, 64, 74	0
1	E	217/235 (92%)	-0.03	5 (2%) 60 60	17, 29, 52, 77	0
1	F	216/235 (91%)	0.19	9 (4%) 36 33	18, 35, 55, 79	0
1	G	219/235 (93%)	0.39	15 (6%) 17 15	25, 44, 61, 85	0
1	H	216/235 (91%)	0.56	26 (12%) 4 3	26, 46, 66, 90	0
All	All	1734/1880 (92%)	0.13	90 (5%) 27 25	14, 33, 58, 90	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	129	ALA	9.0
1	F	130	GLY	7.2
1	G	130	GLY	6.7
1	G	223	LEU	6.3
1	F	129	ALA	5.6
1	H	130	GLY	5.1
1	B	130	GLY	5.0
1	H	93	TYR	4.8
1	G	129	ALA	4.6
1	H	95	PRO	4.6
1	F	5	GLN	4.6
1	D	151	TRP	4.0
1	H	131	GLY	3.9
1	D	111	ALA	3.7
1	C	85	GLN	3.7
1	H	196	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	5	GLN	3.5
1	H	119	GLY	3.5
1	H	221	GLU	3.3
1	H	31	LEU	3.3
1	F	36	ALA	3.3
1	B	222	ASN	3.3
1	A	5	GLN	3.3
1	D	85	GLN	3.3
1	H	23	ASP	3.2
1	H	103	VAL	3.2
1	D	106	GLN	3.1
1	D	32	ALA	3.1
1	F	84	PRO	2.9
1	E	221	GLU	2.9
1	G	5	GLN	2.9
1	H	99	GLU	2.8
1	E	6	GLN	2.8
1	F	106	GLN	2.8
1	A	129	ALA	2.8
1	G	99	GLU	2.8
1	H	126	PRO	2.8
1	D	36	ALA	2.7
1	D	98	ALA	2.7
1	D	108	ALA	2.6
1	H	36	ALA	2.6
1	H	33	ALA	2.6
1	C	164	VAL	2.6
1	G	36	ALA	2.6
1	D	107	ARG	2.6
1	F	32	ALA	2.6
1	H	151	TRP	2.5
1	D	103	VAL	2.5
1	D	31	LEU	2.5
1	H	32	ALA	2.5
1	B	6	GLN	2.5
1	C	130	GLY	2.5
1	D	95	PRO	2.4
1	D	128	LEU	2.4
1	H	78	LEU	2.4
1	G	103	VAL	2.4
1	D	196	PRO	2.4
1	H	52	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	158	ARG	2.3
1	G	127	THR	2.3
1	A	222	ASN	2.3
1	D	150	GLN	2.3
1	G	216	LEU	2.3
1	H	176	GLU	2.3
1	D	96	LYS	2.3
1	D	6	GLN	2.2
1	F	25	PRO	2.2
1	D	116	VAL	2.2
1	G	131	GLY	2.2
1	E	87	ARG	2.2
1	G	132	PRO	2.2
1	G	32	ALA	2.2
1	G	151	TRP	2.2
1	H	94	GLN	2.2
1	G	93	TYR	2.2
1	H	51	PHE	2.2
1	A	31[A]	LEU	2.2
1	D	117	VAL	2.1
1	F	164	VAL	2.1
1	D	126	PRO	2.1
1	H	37	ALA	2.1
1	G	52	LEU	2.1
1	H	28	ALA	2.1
1	B	221[A]	GLU	2.1
1	D	33	ALA	2.1
1	H	175	ALA	2.1
1	H	112	ASP	2.1
1	A	131	GLY	2.0
1	E	51	PHE	2.0
1	D	119	GLY	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)

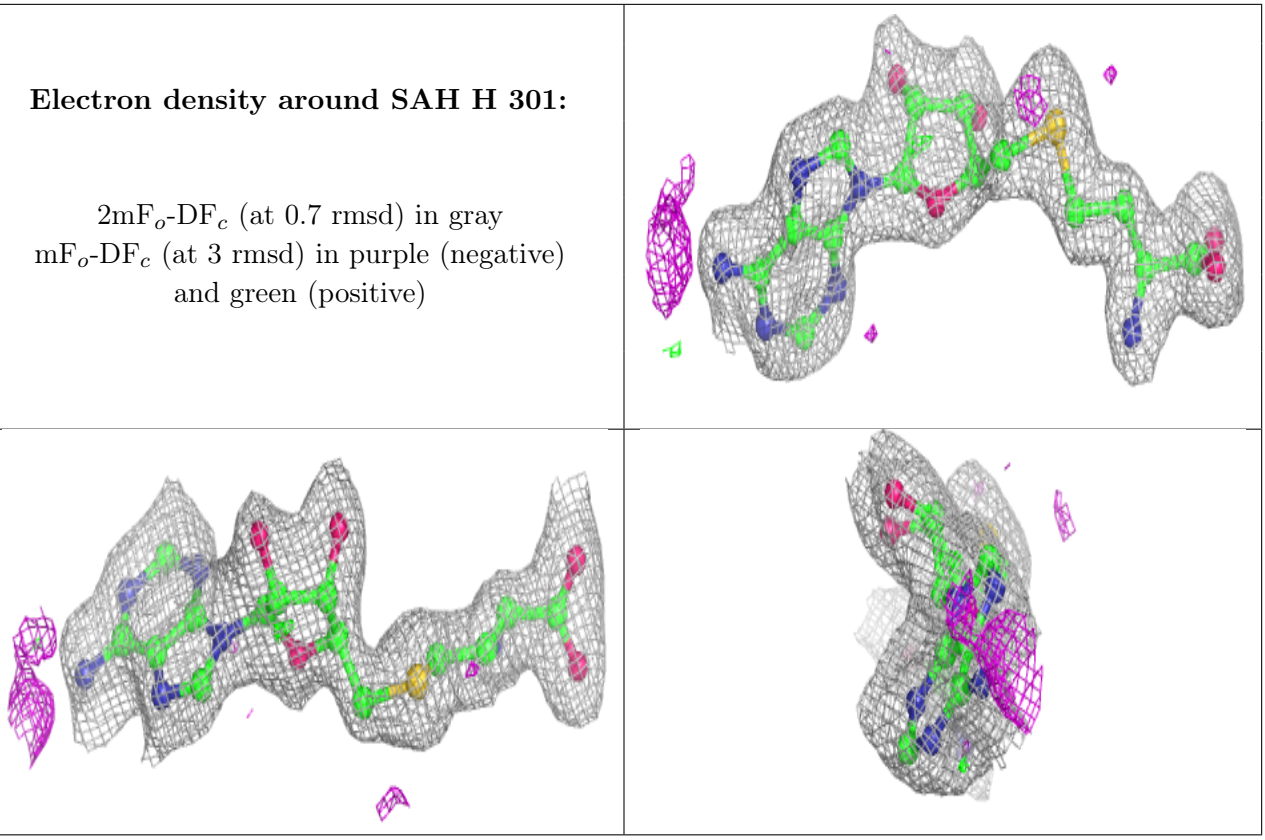
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	MPD	A	303	8/8	0.89	0.15	24,27,33,35	0
4	MPD	B	304	8/8	0.91	0.11	42,48,52,54	0
4	MPD	H	302	8/8	0.92	0.20	42,49,52,53	0
4	MPD	E	302	8/8	0.92	0.16	16,25,36,36	0
4	MPD	F	302	8/8	0.92	0.15	30,35,38,43	0
4	MPD	G	303	8/8	0.93	0.12	30,45,50,51	0
4	MPD	C	302	8/8	0.93	0.15	24,29,32,37	0
4	MPD	D	303	8/8	0.94	0.18	32,35,38,41	0
4	MPD	B	303	8/8	0.95	0.14	21,26,33,37	0
2	SAH	H	301	26/26	0.95	0.09	38,44,47,54	0
2	SAH	D	301	26/26	0.96	0.07	37,44,48,51	0
2	SAH	G	301	26/26	0.96	0.09	34,37,41,43	0
2	SAH	F	301	26/26	0.97	0.09	27,31,35,37	0
5	NA	B	305	1/1	0.97	0.06	33,33,33,33	0
2	SAH	B	301	26/26	0.98	0.07	18,21,24,26	0
2	SAH	C	301	26/26	0.98	0.09	15,18,21,23	0
2	SAH	E	301	26/26	0.98	0.08	18,23,27,30	0
2	SAH	A	301	26/26	0.98	0.09	15,19,23,23	0
3	SR	G	304	1/1	0.98	0.06	23,23,23,23	1
3	SR	D	304	1/1	0.99	0.06	34,34,34,34	1
3	SR	A	304	1/1	0.99	0.08	16,16,16,16	1
3	SR	A	302	1/1	1.00	0.08	18,18,18,18	1
3	SR	G	302	1/1	1.00	0.07	32,32,32,32	1
3	SR	A	305	1/1	1.00	0.08	18,18,18,18	1
3	SR	G	305	1/1	1.00	0.06	28,28,28,28	1
3	SR	B	302	1/1	1.00	0.07	18,18,18,18	1
3	SR	B	306	1/1	1.00	0.10	19,19,19,19	1
3	SR	D	302	1/1	1.00	0.08	33,33,33,33	1

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

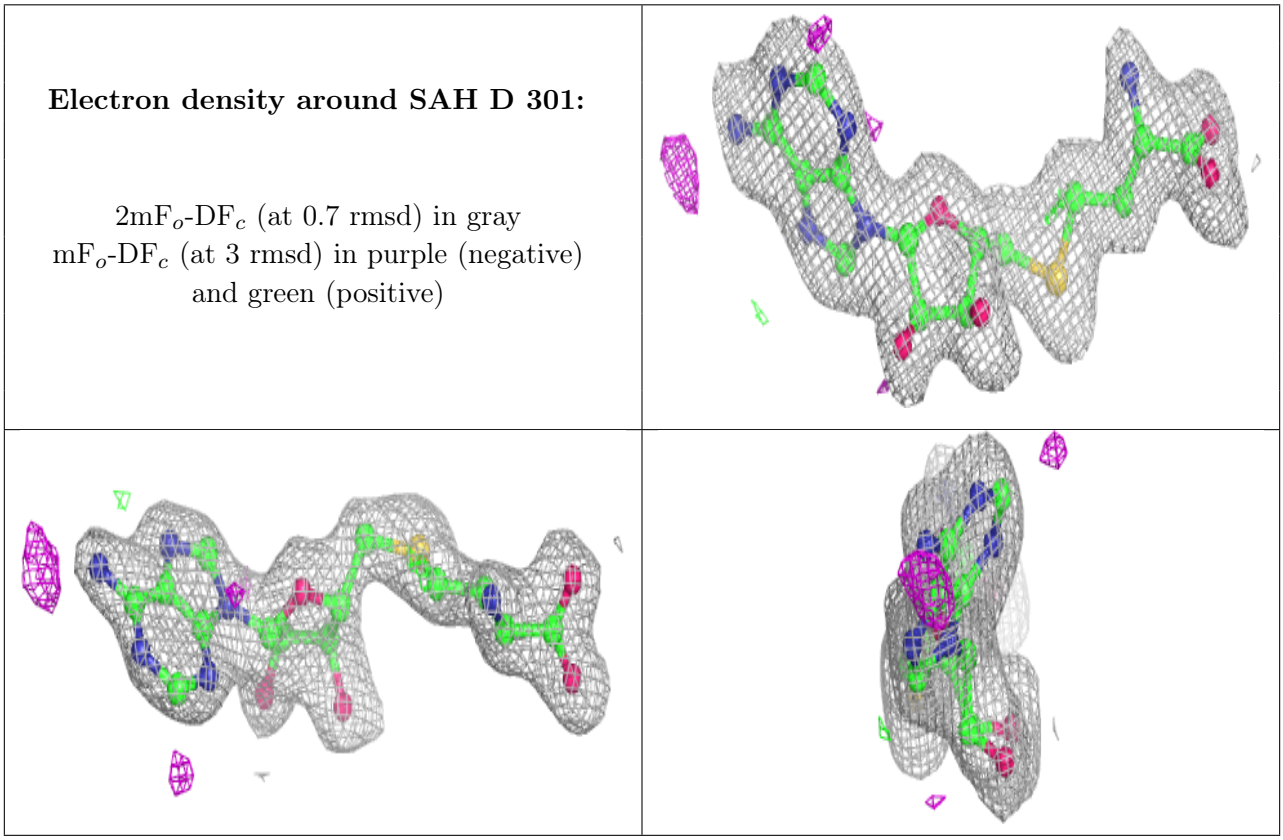
Electron density around SAH H 301:

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



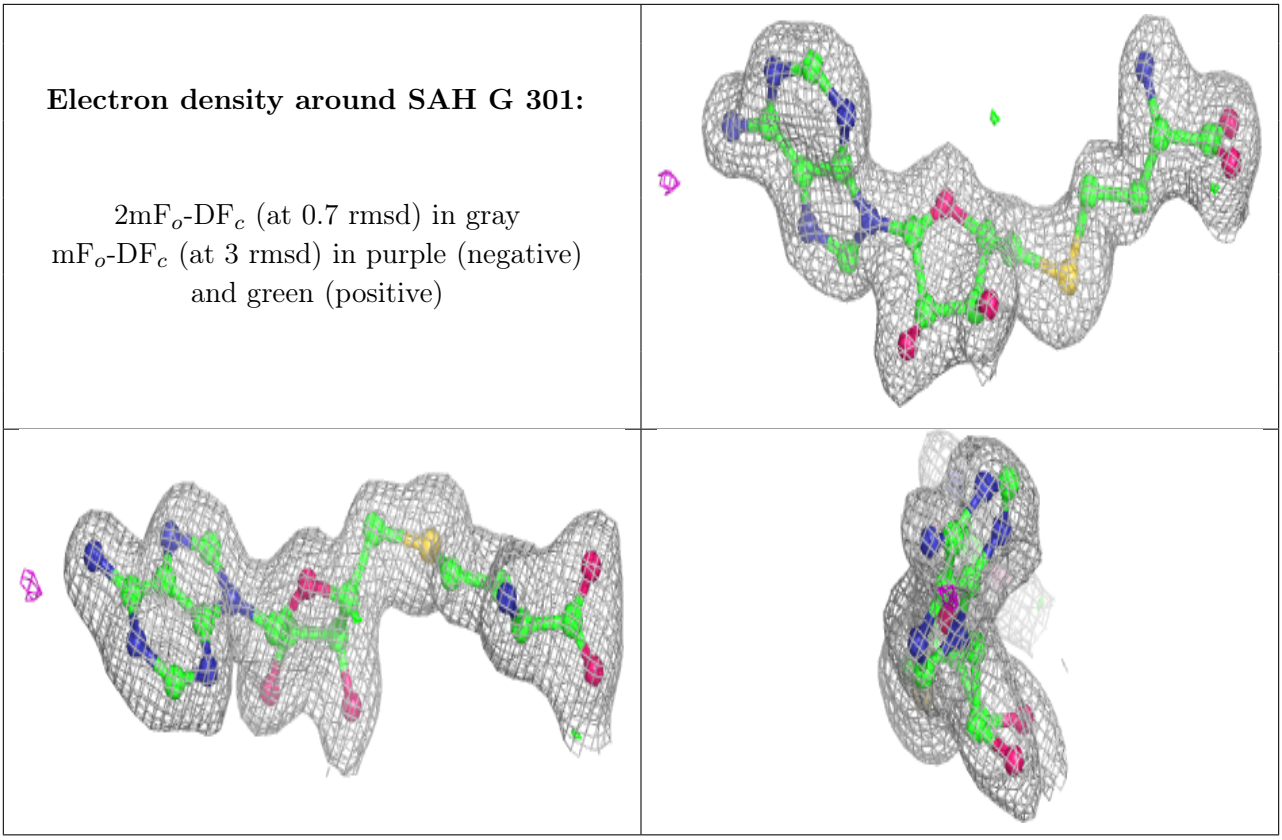
Electron density around SAH D 301:

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



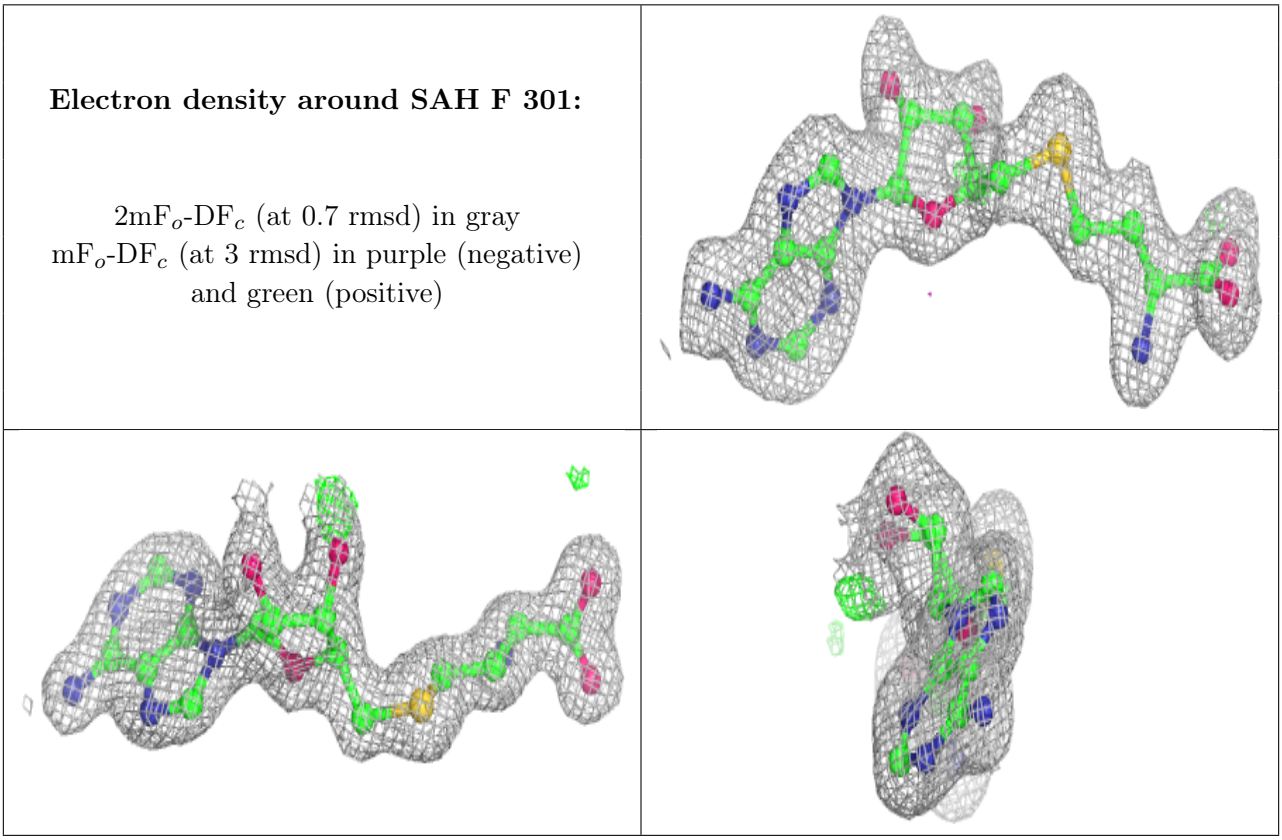
Electron density around SAH G 301:

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



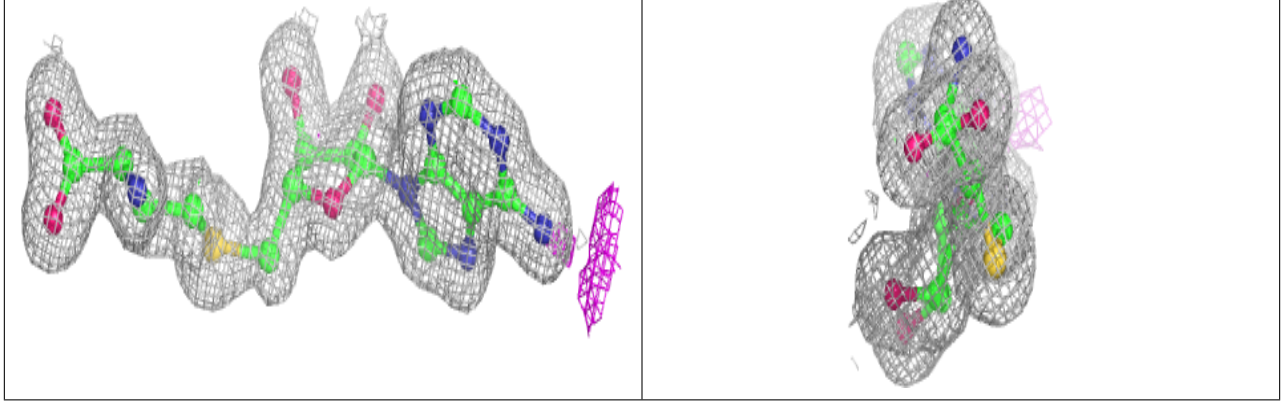
Electron density around SAH F 301:

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



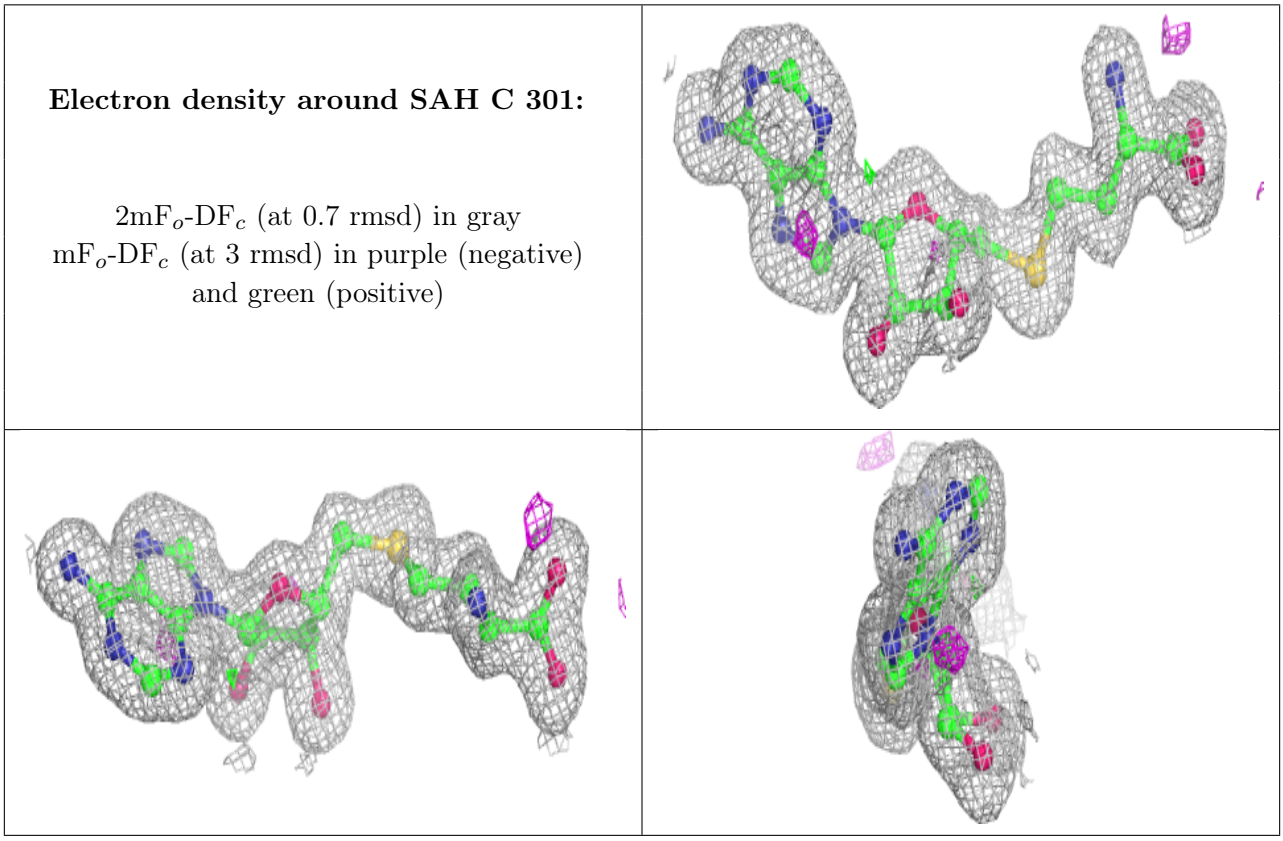
Electron density around SAH B 301:

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



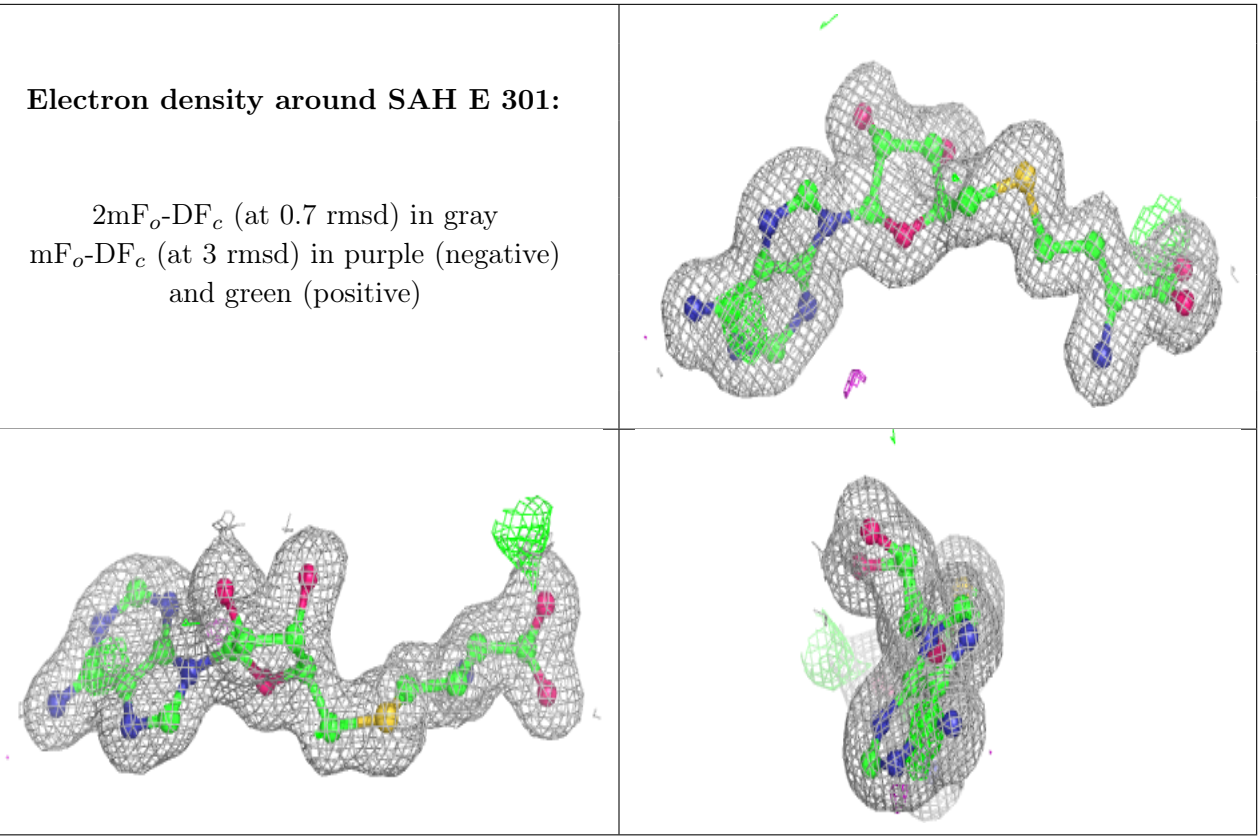
Electron density around SAH C 301:

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



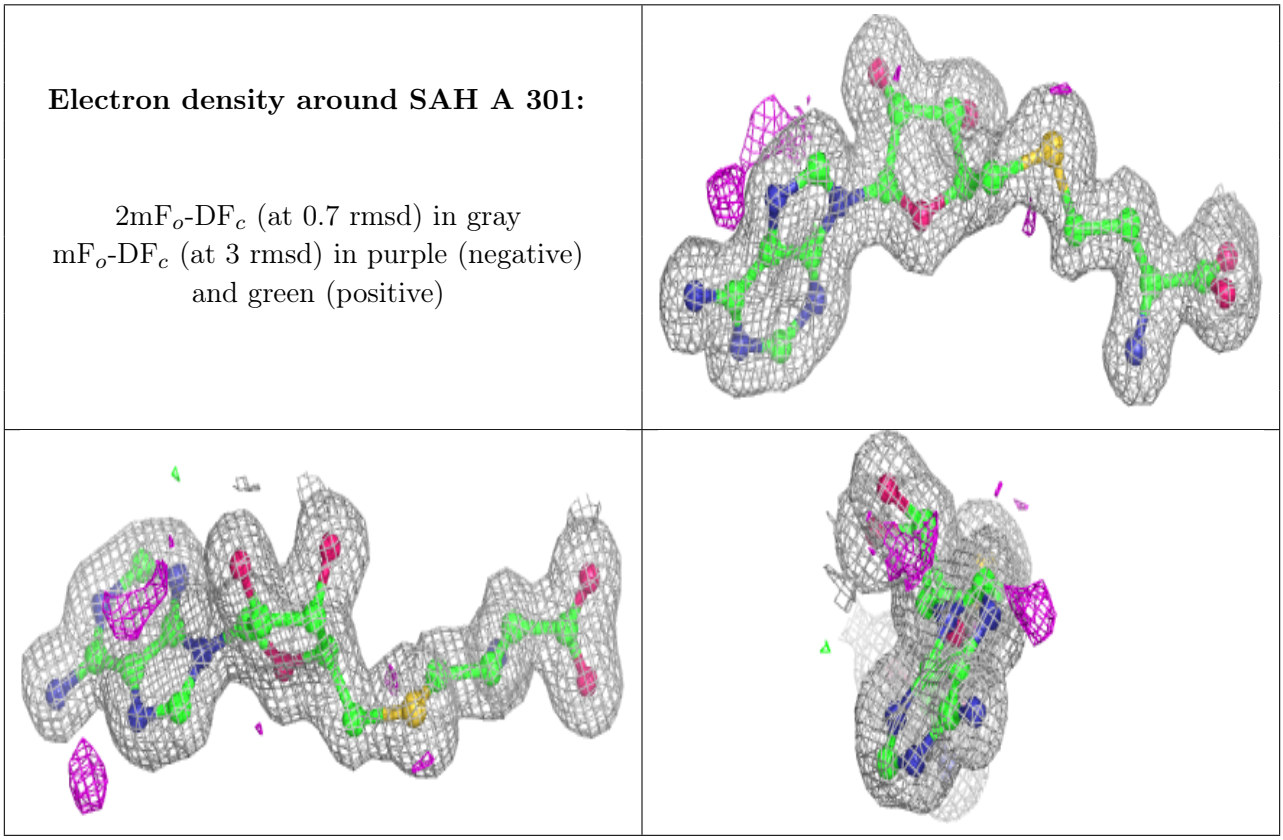
Electron density around SAH E 301:

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



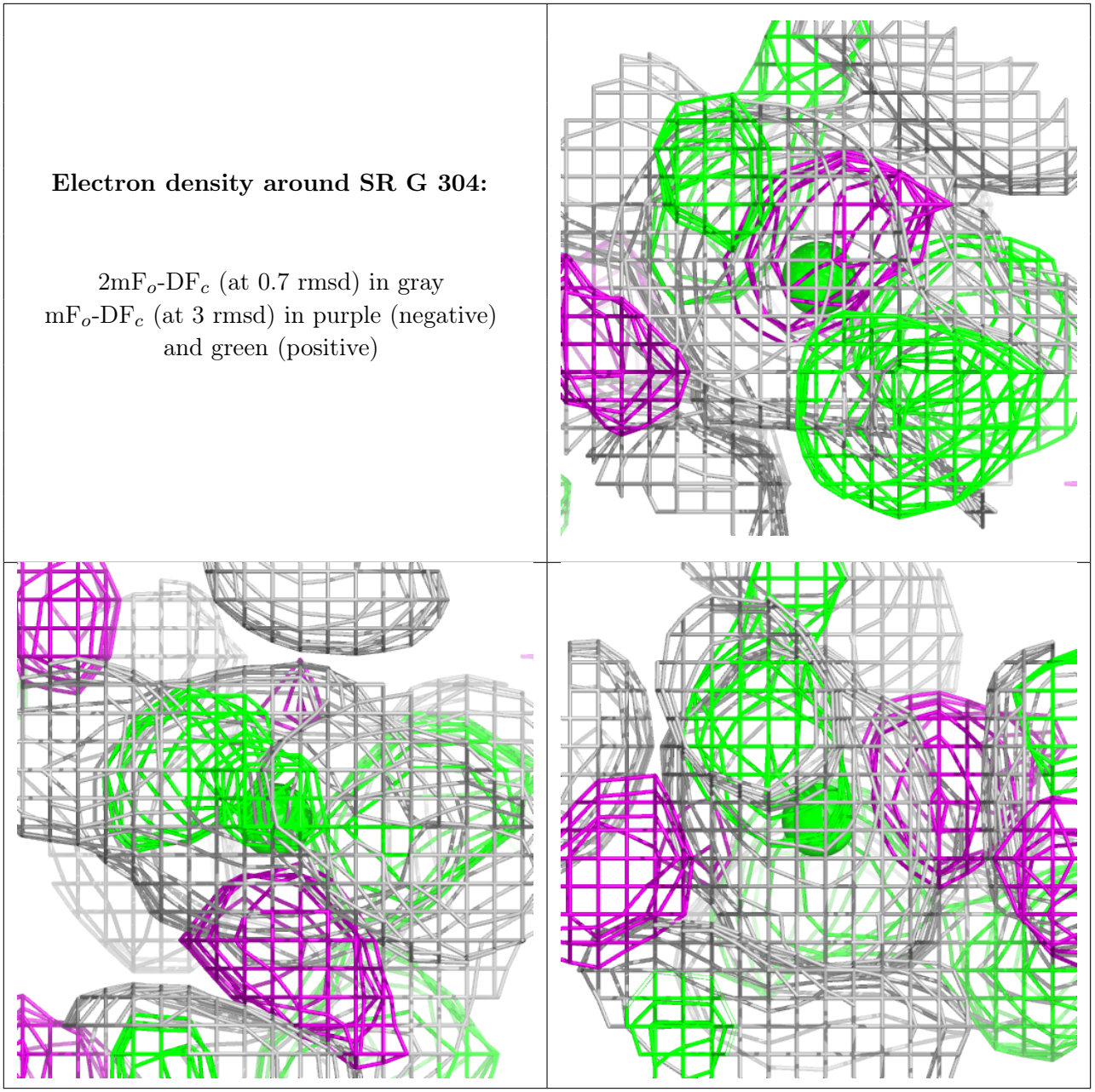
Electron density around SAH A 301:

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



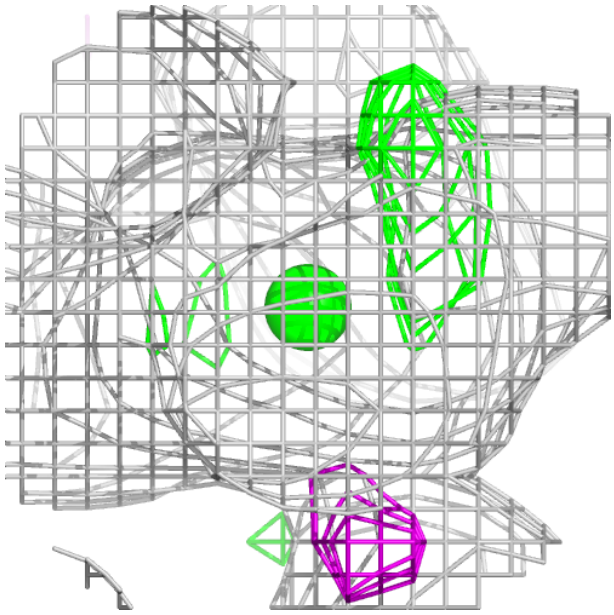
Electron density around SR G 304:

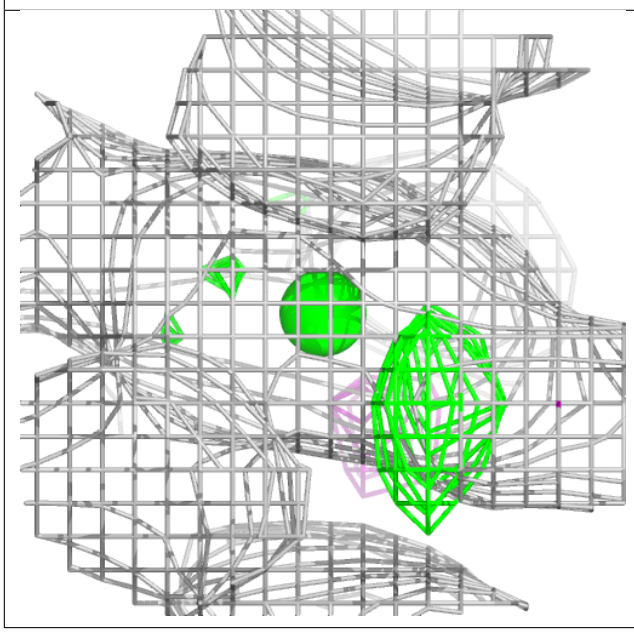
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

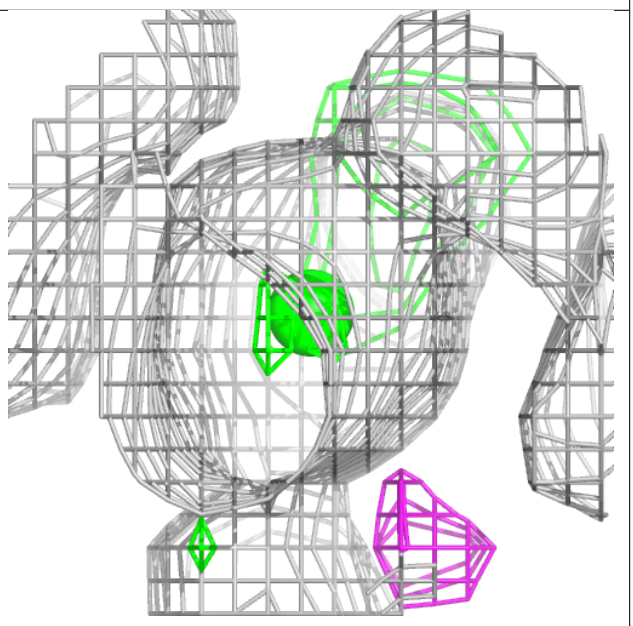


Electron density around SR D 304:

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

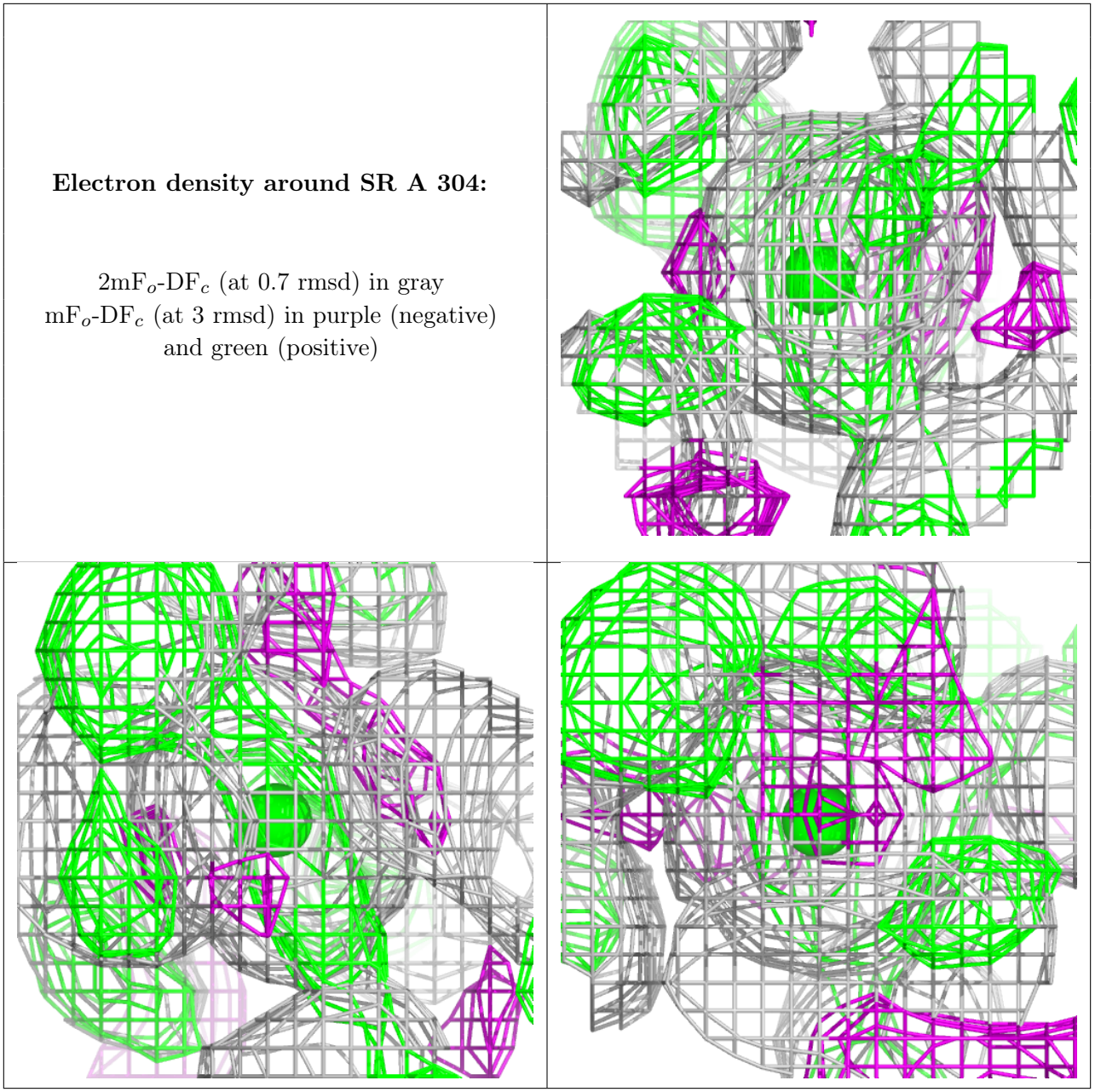






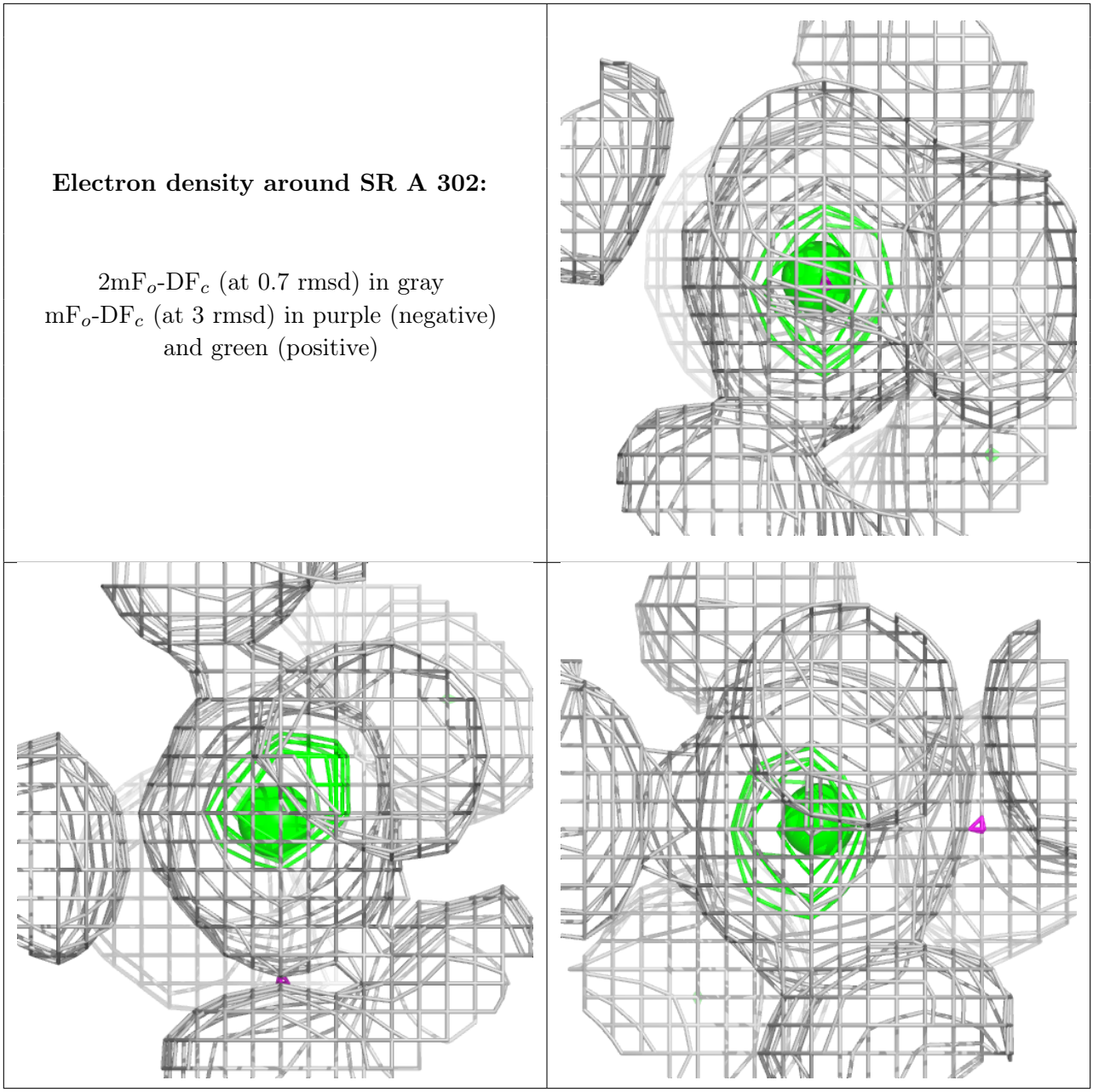
Electron density around SR A 304:

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



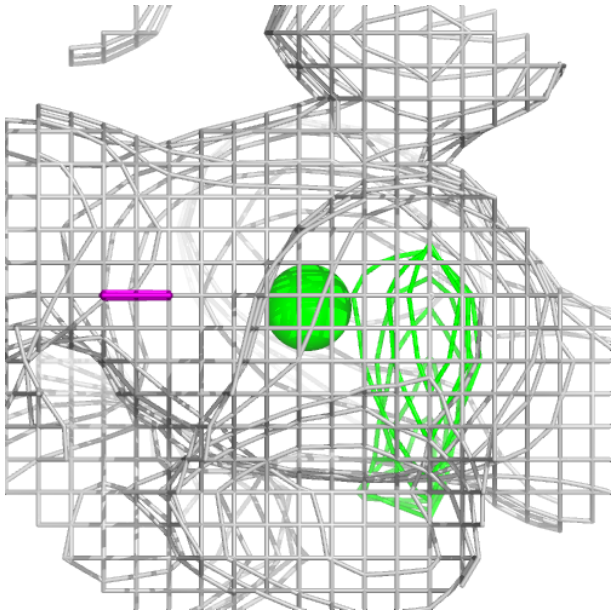
Electron density around SR A 302:

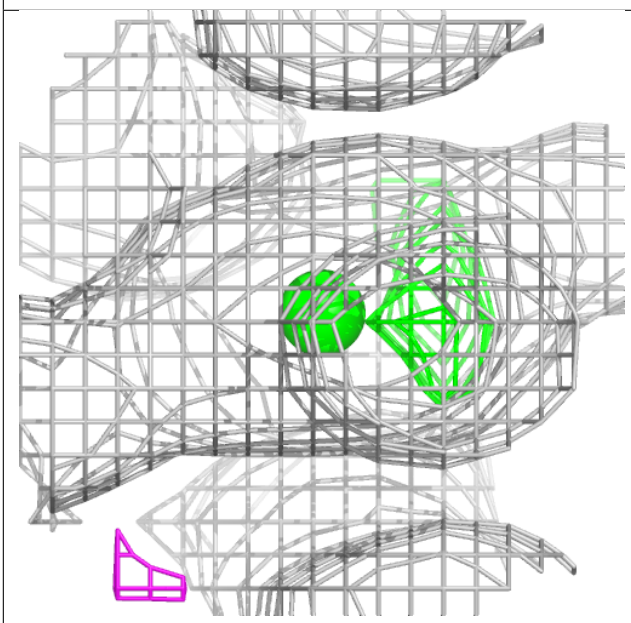
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

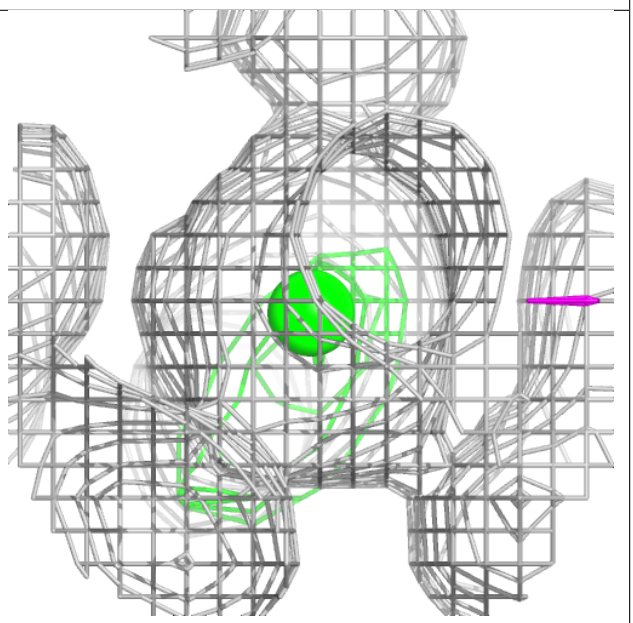


Electron density around SR G 302:

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

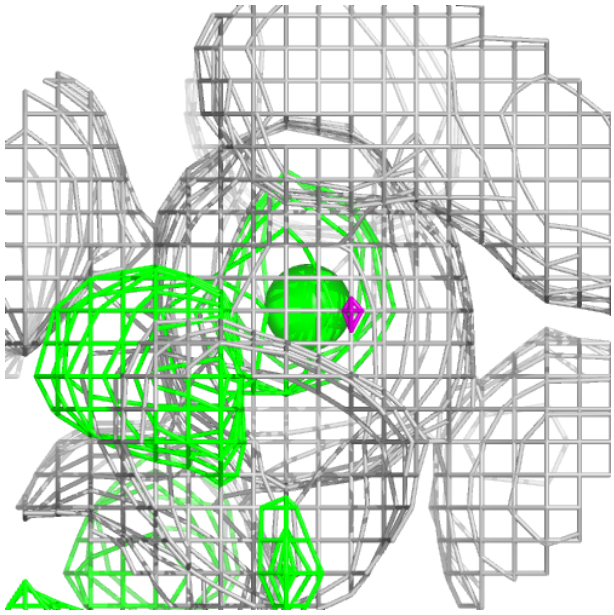


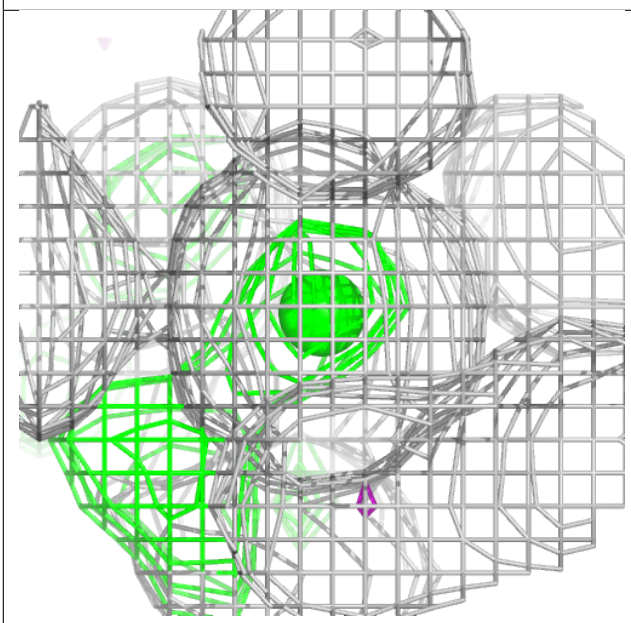


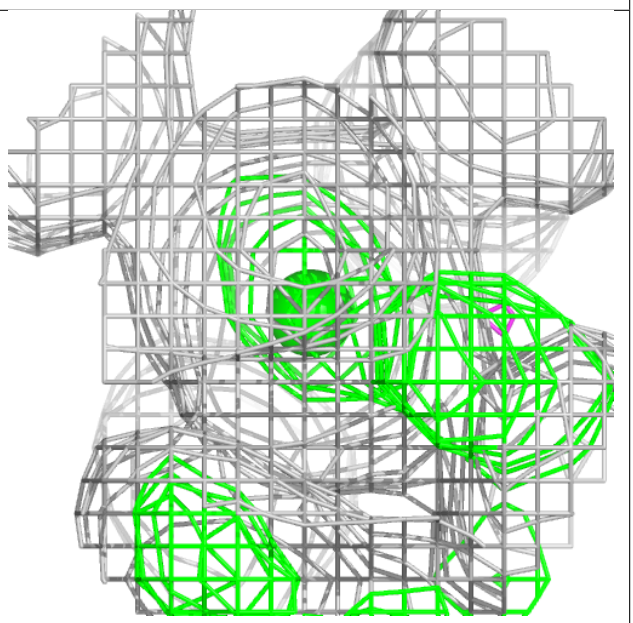


Electron density around SR A 305:

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

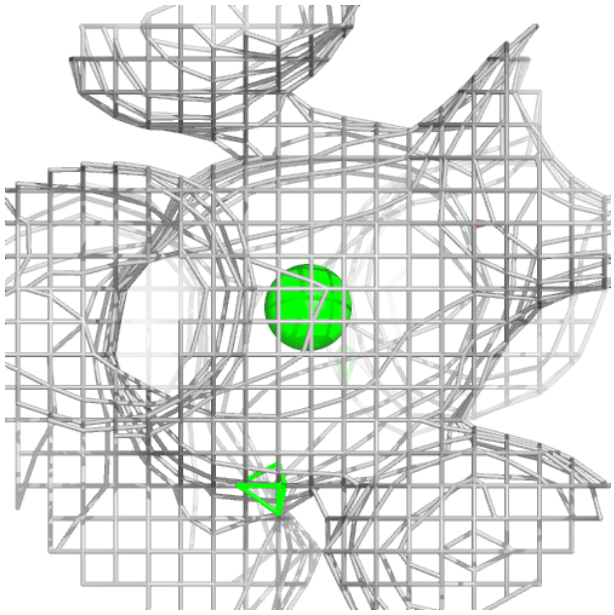


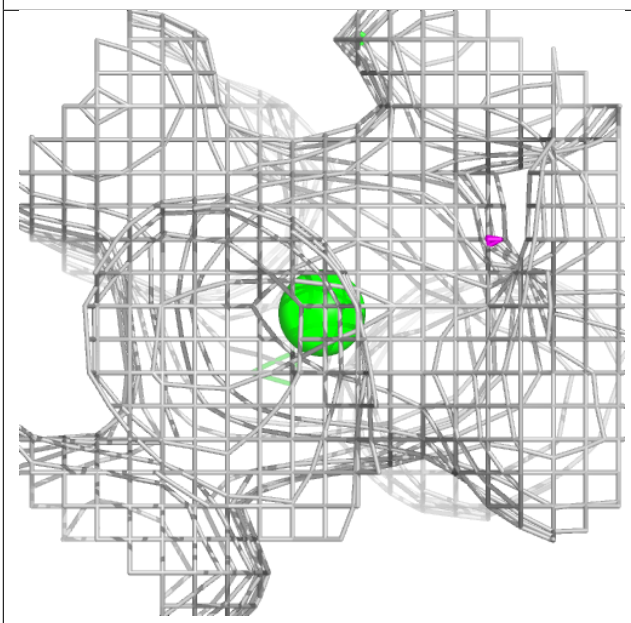


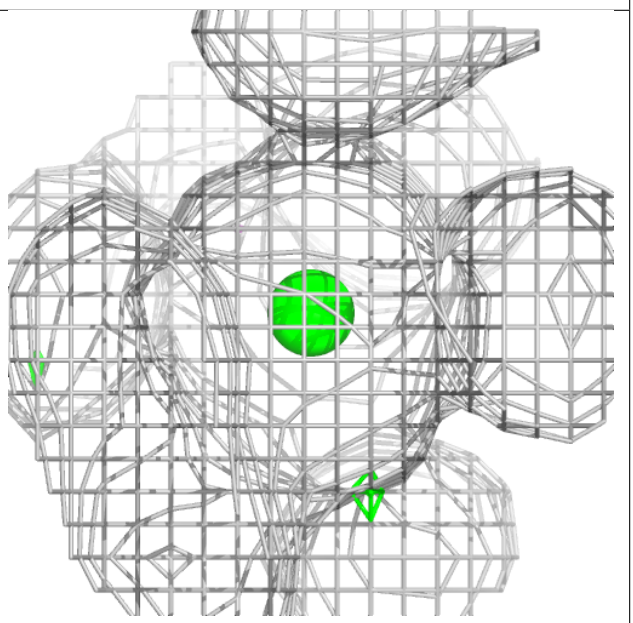


Electron density around SR G 305:

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

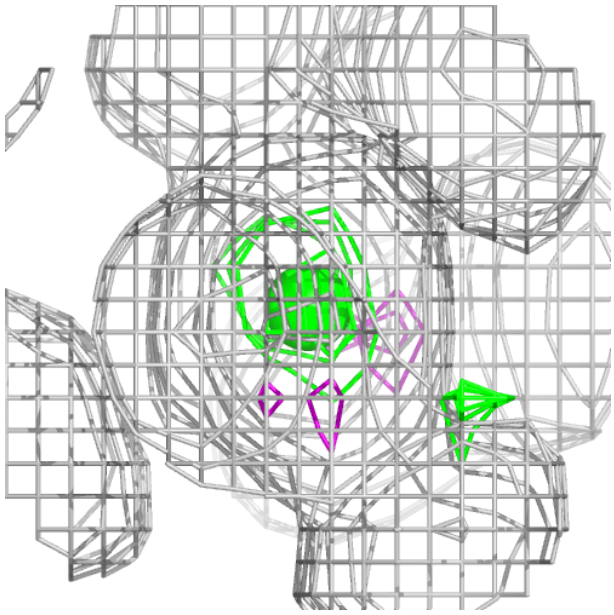


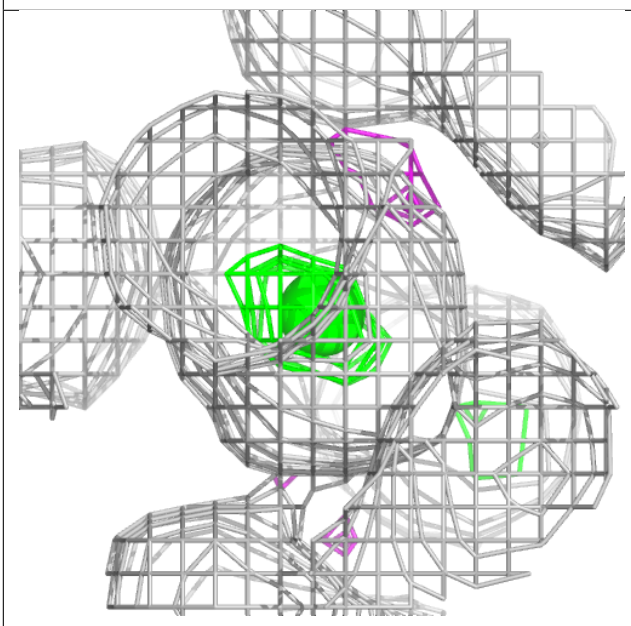


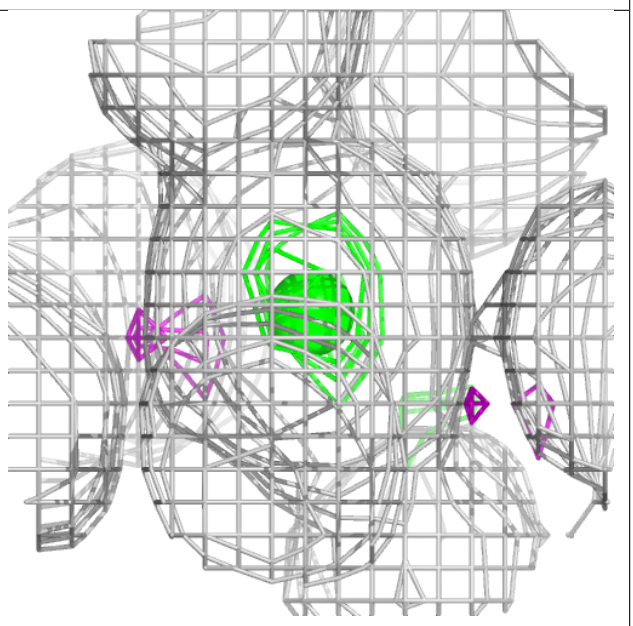


Electron density around SR B 302:

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

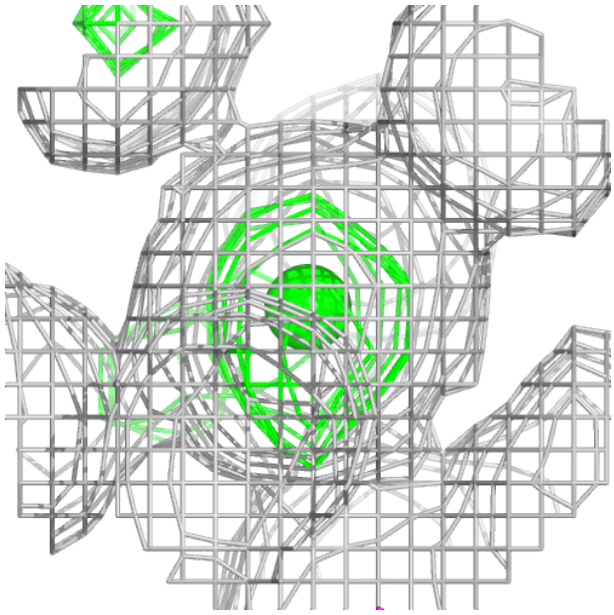


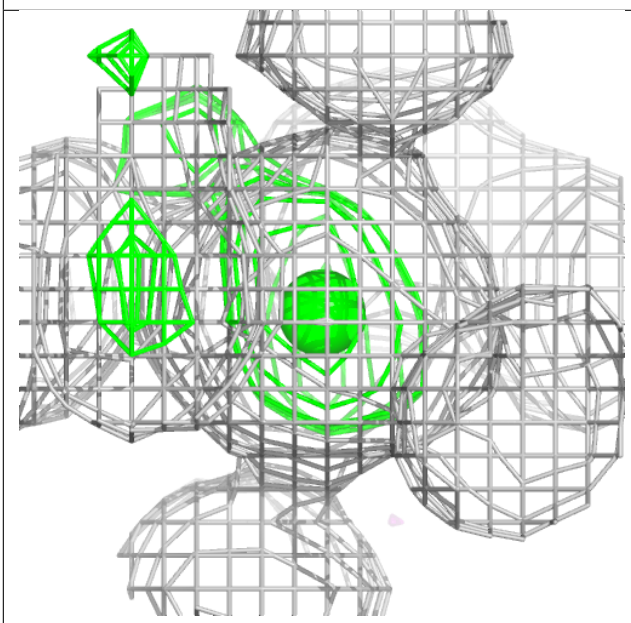


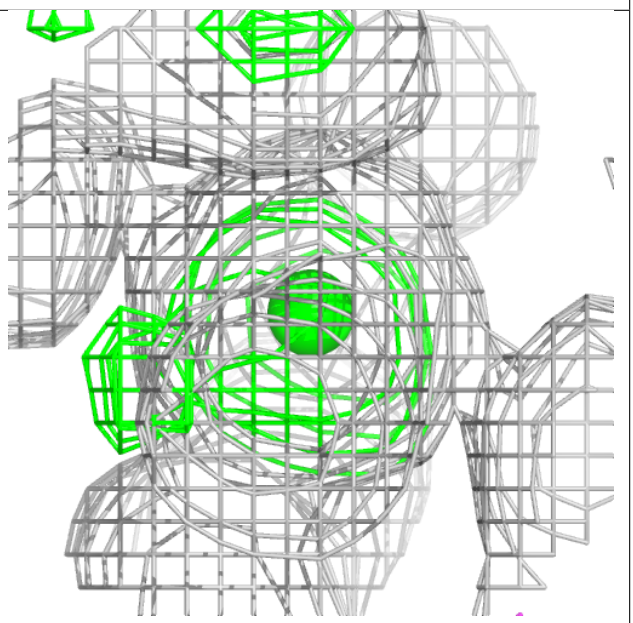


Electron density around SR B 306:

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

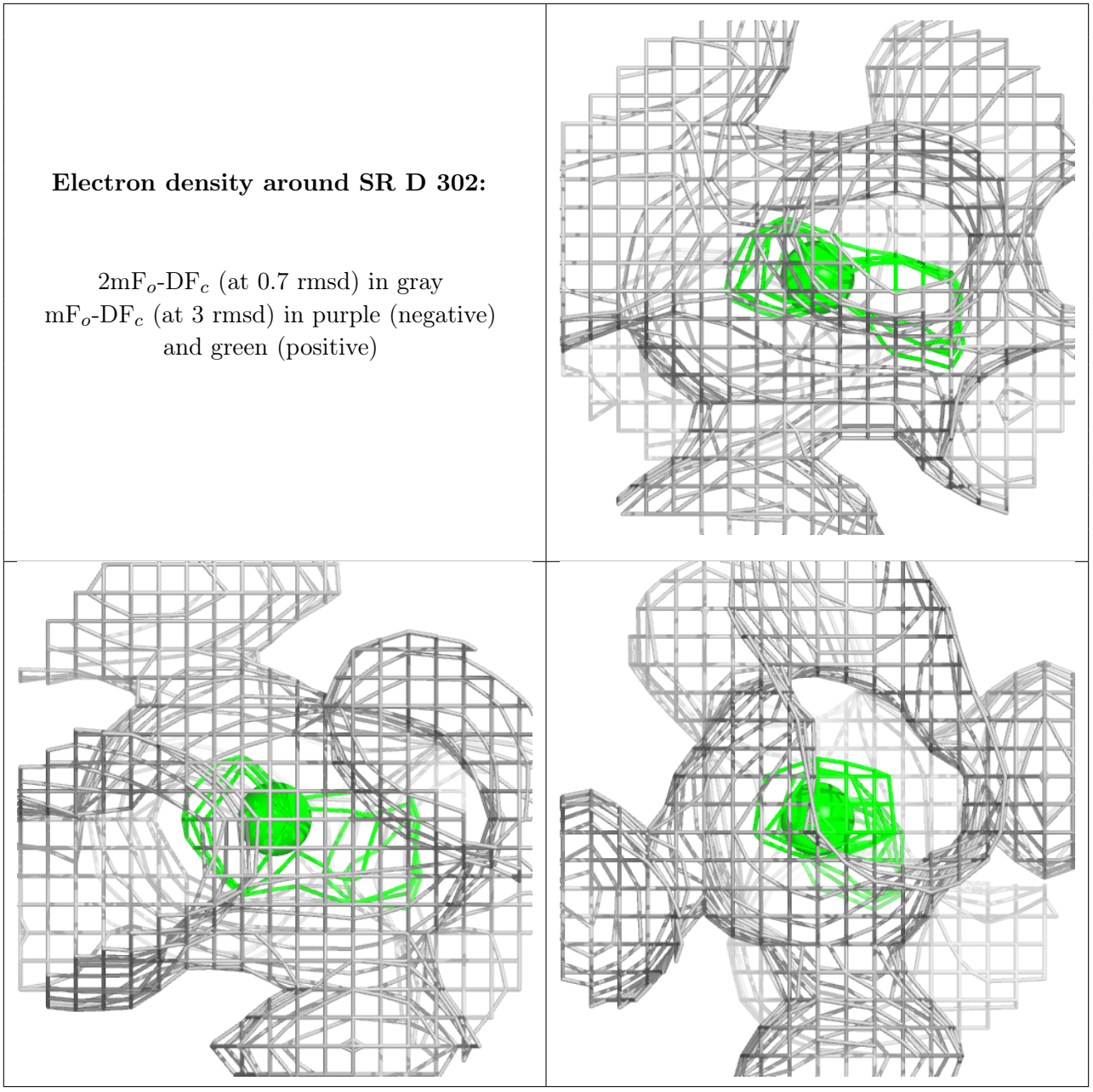






Electron density around SR D 302:

$2mF_o$-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.