



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 18, 2023 – 08:12 AM EDT

PDB ID : 1S4D  
Title : Crystal Structure Analysis of the S-adenosyl-L-methionine dependent uroporphyrinogen-III C-methyltransferase SUMT  
Authors : Vevodova, J.; Graham, R.M.; Raux, E.; Schubert, H.L.; Roper, D.I.; Brindley, A.A.; Scott, A.I.; Roessner, C.A.; Stamford, N.P.J.; Stroupe, M.E.; Getzoff, E.D.; Warren, M.J.; Wilson, K.S.  
Deposited on : 2004-01-16  
Resolution : 2.70 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (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

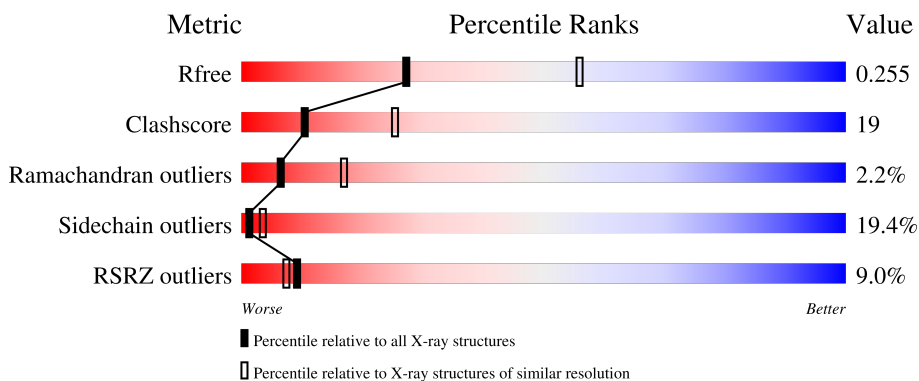
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	280	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 55%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 27%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div> <p style="margin-top: 5px;">5%      55%      27%      9% • 9%</p>
1	B	280	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 60%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 24%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="margin-top: 5px;">7%      60%      24%      9% • 6%</p>
1	D	280	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 54%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 25%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div> <p style="margin-top: 5px;">3%      54%      25%      9% • 11%</p>
1	E	280	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 60%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 24%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="margin-top: 5px;">7%      60%      24%      9% • 5%</p>
1	F	280	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 61%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div> <p style="margin-top: 5px;">5%      61%      21%      7% • 9%</p>

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Mol	Chain	Length	Quality of chain				
1	G	280	9%	63%	21%	8%	8%
1	H	280	6%	58%	25%	8%	8%
1	I	280	6%	60%	21%	10%	6%
1	J	280	7%	55%	27%	8%	10%
1	K	280	8%	60%	23%	8%	8%
1	L	280	17%	58%	22%	9%	12%
1	M	280	20%	56%	24%	8%	10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	D	2011	-	-	X	-
3	GOL	E	2001	-	-	X	-
3	GOL	G	3003	-	-	X	-
3	GOL	H	4012	-	-	X	-
3	GOL	I	4002	-	-	X	-
3	GOL	K	5001	-	-	X	-
3	GOL	K	5012	-	-	X	-

## 2 Entry composition [i](#)

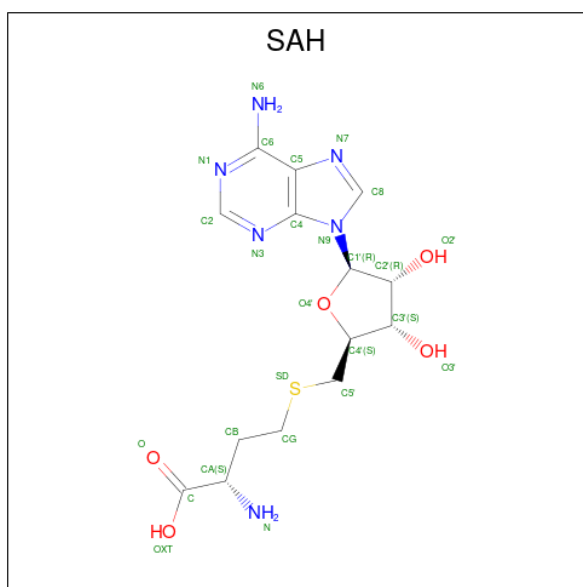
There are 4 unique types of molecules in this entry. The entry contains 23427 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Uroporphyrin-III C-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	256	Total 1878	C 1195	N 341	O 337	S 5	0	1	0
1	B	263	Total 1915	C 1213	N 348	O 349	S 5	0	1	0
1	D	248	Total 1806	C 1146	N 326	O 329	S 5	0	0	0
1	E	265	Total 1922	C 1218	N 349	O 350	S 5	0	0	0
1	F	254	Total 1852	C 1176	N 336	O 335	S 5	0	0	0
1	G	258	Total 1877	C 1186	N 345	O 341	S 5	0	0	0
1	H	259	Total 1894	C 1205	N 344	O 340	S 5	0	0	0
1	I	263	Total 1932	C 1224	N 352	O 351	S 5	0	1	0
1	J	252	Total 1840	C 1171	N 333	O 331	S 5	0	0	0
1	K	258	Total 1883	C 1197	N 342	O 339	S 5	0	1	0
1	L	247	Total 1795	C 1141	N 325	O 324	S 5	0	0	0
1	M	252	Total 1842	C 1165	N 339	O 333	S 5	0	0	0

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C<sub>14</sub>H<sub>20</sub>N<sub>6</sub>O<sub>5</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
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	D	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		
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	I	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	J	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	K	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	L	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	M	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0
3	I	1	Total C O 6 3 3	0	0
3	I	1	Total C O 6 3 3	0	0
3	J	1	Total C O 6 3 3	0	0
3	J	1	Total C O 6 3 3	0	0
3	J	1	Total C O 6 3 3	0	0
3	K	1	Total C O 6 3 3	0	0
3	K	1	Total C O 6 3 3	0	0
3	L	1	Total C O 6 3 3	0	0
3	L	1	Total C O 6 3 3	0	0
3	M	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	46	Total O 46 46	0	0
4	B	54	Total O 54 54	0	0
4	D	54	Total O 54 54	0	0
4	E	50	Total O 50 50	0	0
4	F	41	Total O 41 41	0	0
4	G	38	Total O 38 38	0	0
4	H	69	Total O 69 69	0	0

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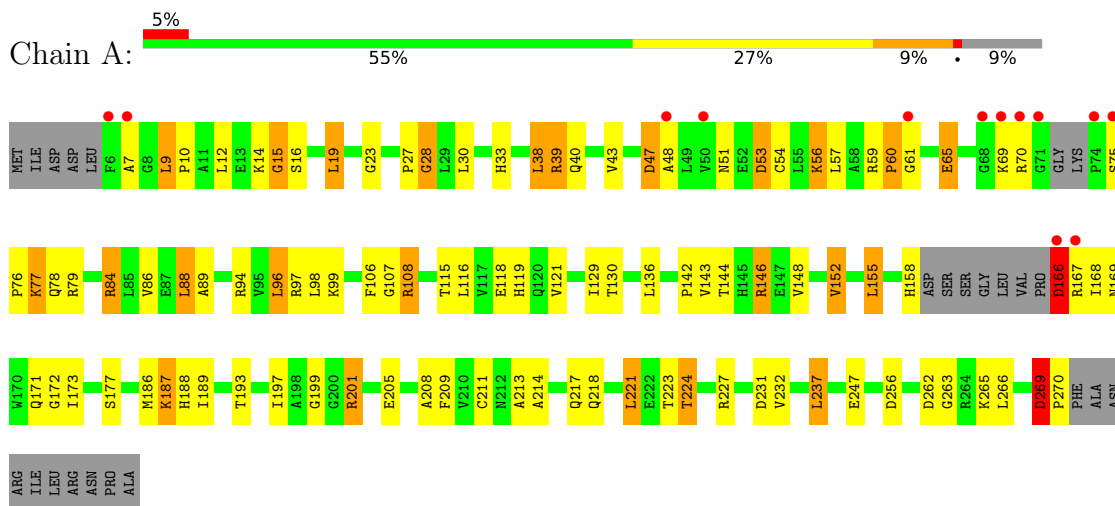
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
4	I	59	Total O 59 59	0	0
4	J	30	Total O 30 30	0	0
4	K	44	Total O 44 44	0	0
4	L	24	Total O 24 24	0	0
4	M	14	Total O 14 14	0	0

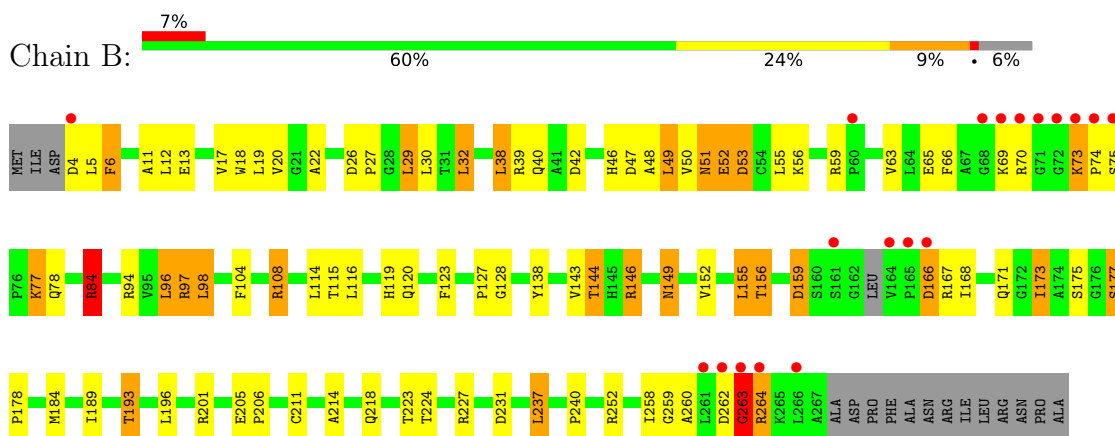
### 3 Residue-property plots [i](#)

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.

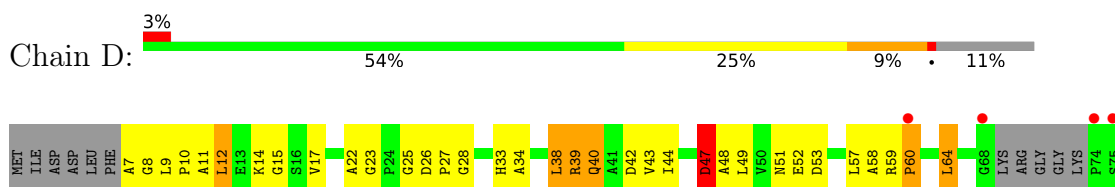
- Molecule 1: Uroporphyrin-III C-methyltransferase

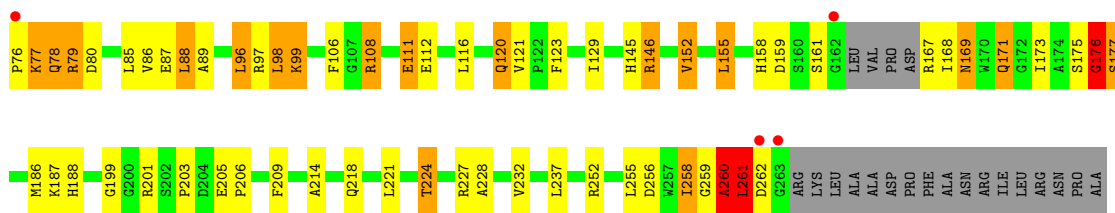


- Molecule 1: Uroporphyrin-III C-methyltransferase

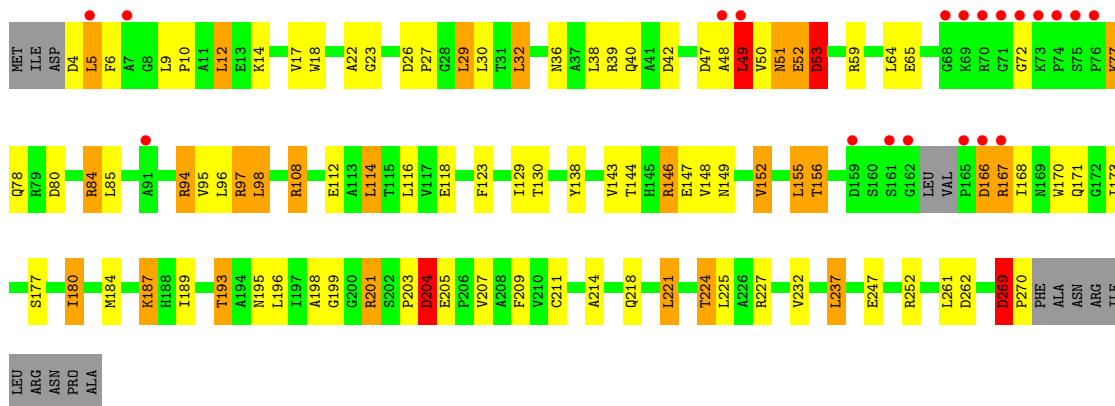


- Molecule 1: Uroporphyrin-III C-methyltransferase

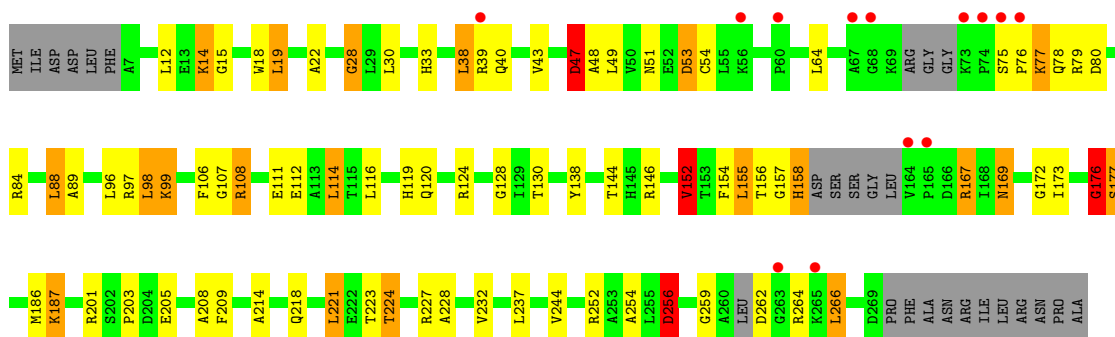




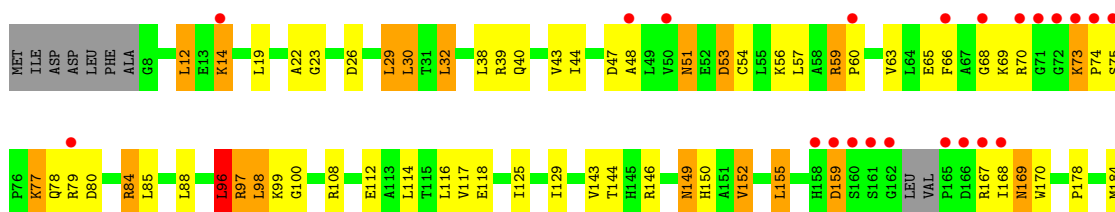
● Molecule 1: Uroporphyrin-III C-methyltransferase



● Molecule 1: Uroporphyrin-III C-methyltransferase

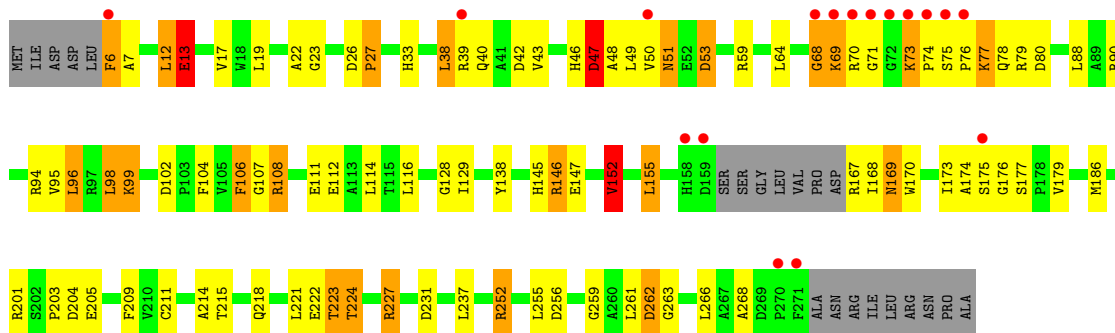


● Molecule 1: Uroporphyrin-III C-methyltransferase

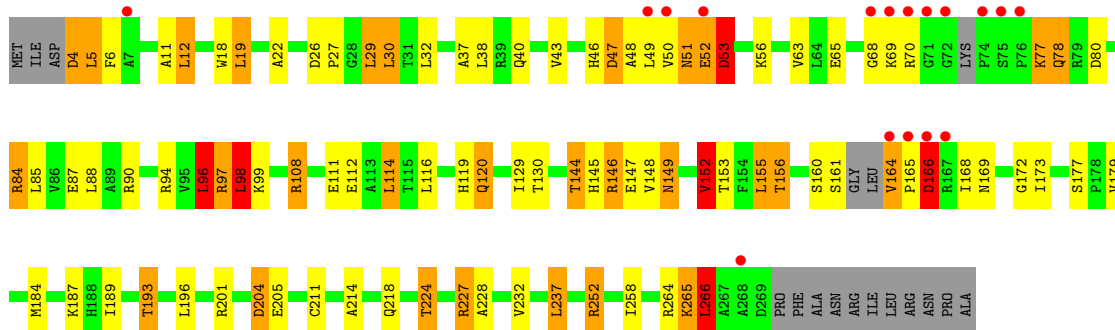




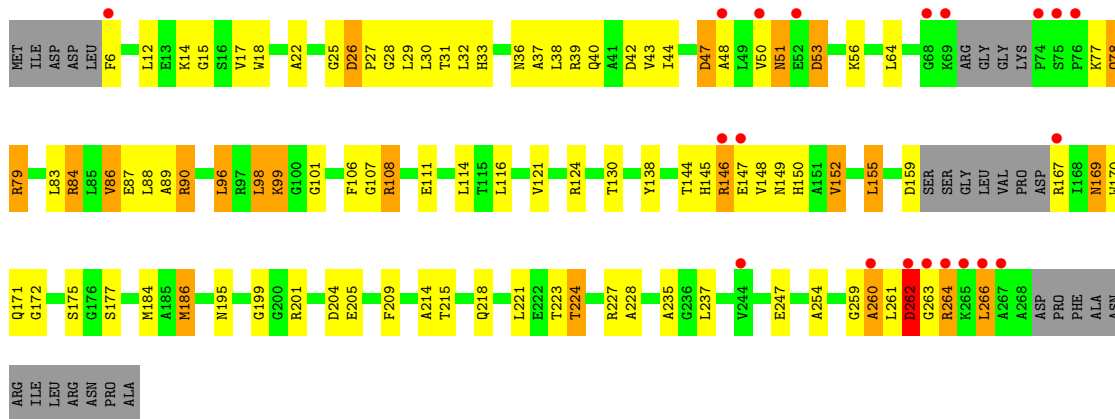
- Molecule 1: Uroporphyrin-III C-methyltransferase



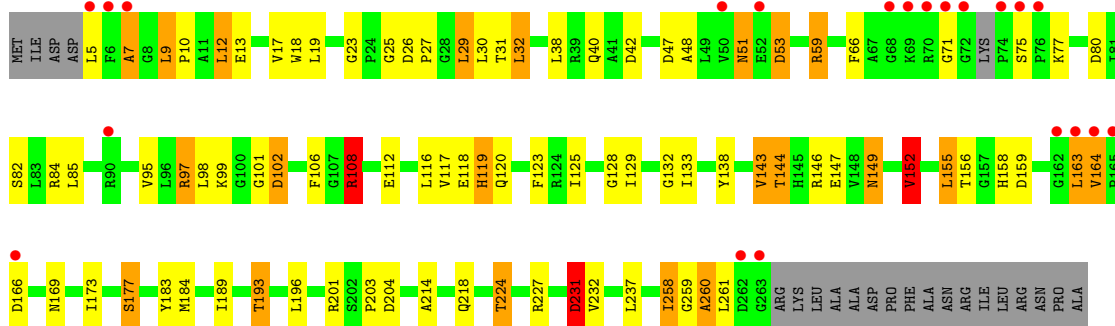
- Molecule 1: Uroporphyrin-III C-methyltransferase



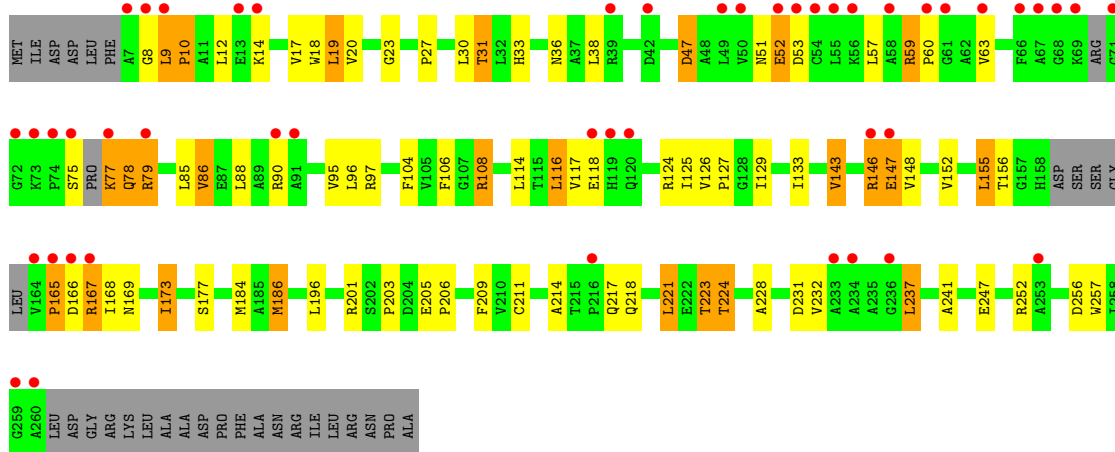
- Molecule 1: Uroporphyrin-III C-methyltransferase



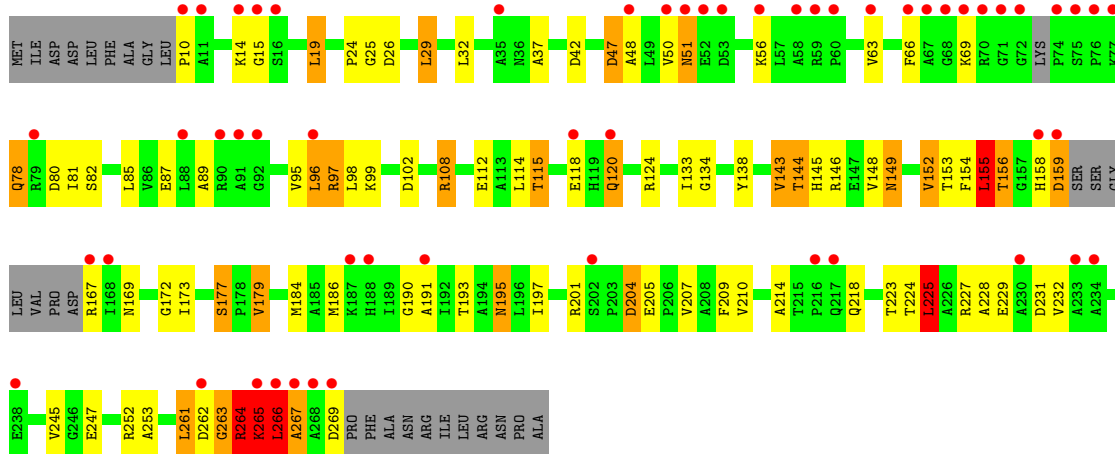
- Molecule 1: Uroporphyrin-III C-methyltransferase



• Molecule 1: Uroporphyrin-III C-methyltransferase



• Molecule 1: Uroporphyrin-III C-methyltransferase



## 4 Data and refinement statistics i

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	218.10Å 218.10Å 190.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.84 – 2.70 19.84 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.84-2.70) 100.0 (19.84-2.70)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.34 (at 2.71Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.213 , 0.260 0.211 , 0.255	Depositor DCC
$R_{free}$ test set	6099 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.4	Xtrriage
Anisotropy	0.009	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 53.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.014 for -k,-h,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	23427	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

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

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	0.67	2/1918 (0.1%)	0.95	11/2609 (0.4%)
1	B	0.62	1/1956 (0.1%)	0.96	9/2666 (0.3%)
1	D	0.64	1/1840 (0.1%)	0.92	7/2506 (0.3%)
1	E	0.56	0/1960	0.96	12/2672 (0.4%)
1	F	0.63	1/1886 (0.1%)	0.91	10/2569 (0.4%)
1	G	0.53	0/1913	0.86	5/2605 (0.2%)
1	H	0.71	1/1932 (0.1%)	0.97	15/2632 (0.6%)
1	I	0.62	0/1972	0.98	12/2683 (0.4%)
1	J	0.60	1/1875 (0.1%)	0.88	8/2554 (0.3%)
1	K	0.58	1/1924 (0.1%)	0.88	8/2621 (0.3%)
1	L	0.59	1/1828 (0.1%)	0.81	4/2490 (0.2%)
1	M	0.51	0/1876	1.00	15/2552 (0.6%)
All	All	0.61	9/22880 (0.0%)	0.93	116/31159 (0.4%)

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	A	0	3
1	B	0	3
1	D	0	5
1	E	0	4
1	F	0	5
1	H	0	2
1	I	0	1
1	J	0	4
1	K	0	4
1	L	0	2
1	M	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	39

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	79	ARG	NE-CZ	14.01	1.51	1.33
1	H	79	ARG	NE-CZ	13.53	1.50	1.33
1	F	79	ARG	NE-CZ	13.34	1.50	1.33
1	J	79	ARG	NE-CZ	13.03	1.50	1.33
1	A	79	ARG	NE-CZ	12.89	1.49	1.33

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	266	LEU	O-C-N	-21.33	88.57	122.70
1	M	263	GLY	C-N-CA	9.86	146.35	121.70
1	H	79	ARG	CD-NE-CZ	-8.97	111.04	123.60
1	M	264	ARG	C-N-CA	8.77	143.62	121.70
1	A	79	ARG	CD-NE-CZ	-8.68	111.45	123.60

There are no chirality outliers.

5 of 39 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	ASP	Peptide
1	A	28	GLY	Peptide
1	A	47	ASP	Peptide
1	B	167	ARG	Peptide
1	B	263	GLY	Peptide

## 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	1878	0	1911	86	0
1	B	1915	0	1933	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1806	0	1836	75	0
1	E	1922	0	1942	78	0
1	F	1852	0	1881	70	0
1	G	1877	0	1903	65	0
1	H	1894	0	1922	80	0
1	I	1932	0	1968	94	0
1	J	1840	0	1870	84	0
1	K	1883	0	1920	71	0
1	L	1795	0	1822	55	0
1	M	1842	0	1870	75	0
2	A	26	0	19	0	0
2	B	26	0	19	0	0
2	D	26	0	19	0	0
2	E	26	0	19	1	0
2	F	26	0	19	0	0
2	G	26	0	19	2	0
2	H	26	0	19	0	0
2	I	26	0	19	0	0
2	J	26	0	19	2	0
2	K	26	0	19	1	0
2	L	26	0	19	0	0
2	M	26	0	19	2	0
3	A	18	0	24	5	0
3	B	6	0	8	0	0
3	D	12	0	16	7	0
3	E	18	0	24	9	0
3	F	12	0	16	2	0
3	G	18	0	24	7	0
3	H	12	0	16	6	0
3	I	12	0	16	4	0
3	J	18	0	24	5	0
3	K	12	0	16	9	0
3	L	12	0	16	1	0
3	M	6	0	8	0	0
4	A	46	0	0	2	0
4	B	54	0	0	7	0
4	D	54	0	0	3	0
4	E	50	0	0	4	0
4	F	41	0	0	2	0
4	G	38	0	0	2	0
4	H	69	0	0	7	0
4	I	59	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	30	0	0	3	0
4	K	44	0	0	8	0
4	L	24	0	0	2	0
4	M	14	0	0	0	0
All	All	23427	0	23214	856	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 19.

The worst 5 of 856 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:I:160:SER:HA	1:I:166:ASP:OD2	1.41	1.20
1:J:186:MET:CE	1:J:209:PHE:HD1	1.55	1.20
1:J:186:MET:HE1	1:J:209:PHE:HD1	1.01	1.14
1:L:9:LEU:HB2	1:L:10:PRO:HD2	1.29	1.14
1:E:168:ILE:HG23	4:E:2542:HOH:O	1.46	1.12

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	250/280 (89%)	225 (90%)	18 (7%)	7 (3%)	<b>5</b> <b>11</b>
1	B	260/280 (93%)	236 (91%)	20 (8%)	4 (2%)	<b>10</b> <b>26</b>
1	D	242/280 (86%)	222 (92%)	13 (5%)	7 (3%)	<b>4</b> <b>10</b>
1	E	261/280 (93%)	239 (92%)	18 (7%)	4 (2%)	<b>10</b> <b>26</b>
1	F	246/280 (88%)	229 (93%)	12 (5%)	5 (2%)	<b>7</b> <b>19</b>
1	G	254/280 (91%)	232 (91%)	16 (6%)	6 (2%)	<b>6</b> <b>15</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	255/280 (91%)	234 (92%)	15 (6%)	6 (2%)	6	15
1	I	258/280 (92%)	239 (93%)	14 (5%)	5 (2%)	8	20
1	J	246/280 (88%)	231 (94%)	12 (5%)	3 (1%)	13	32
1	K	255/280 (91%)	229 (90%)	18 (7%)	8 (3%)	4	9
1	L	239/280 (85%)	222 (93%)	14 (6%)	3 (1%)	12	30
1	M	246/280 (88%)	225 (92%)	12 (5%)	9 (4%)	3	7
All	All	3012/3360 (90%)	2763 (92%)	182 (6%)	67 (2%)	6	17

5 of 67 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ALA
1	A	269	ASP
1	B	52	GLU
1	D	48	ALA
1	D	260	ALA

### 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	187/207 (90%)	158 (84%)	29 (16%)	2	7
1	B	190/207 (92%)	151 (80%)	39 (20%)	1	3
1	D	181/207 (87%)	145 (80%)	36 (20%)	1	3
1	E	190/207 (92%)	149 (78%)	41 (22%)	1	3
1	F	184/207 (89%)	154 (84%)	30 (16%)	2	6
1	G	186/207 (90%)	152 (82%)	34 (18%)	1	4
1	H	187/207 (90%)	155 (83%)	32 (17%)	2	5
1	I	194/207 (94%)	148 (76%)	46 (24%)	1	2
1	J	182/207 (88%)	149 (82%)	33 (18%)	1	4
1	K	188/207 (91%)	152 (81%)	36 (19%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	178/207 (86%)	140 (79%)	38 (21%)	1	3
1	M	182/207 (88%)	144 (79%)	38 (21%)	1	3
All	All	2229/2484 (90%)	1797 (81%)	432 (19%)	1	3

5 of 432 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	155	LEU
1	I	266	LEU
1	M	50	VAL
1	H	252	ARG
1	I	96	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 99 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	51	ASN
1	I	218	GLN
1	H	93	ASN
1	I	40	GLN
1	J	51	ASN

### 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](#)

38 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	A	1001	-	5,5,5	0.71	0	5,5,5	1.03	0
3	GOL	E	2001	-	5,5,5	0.66	0	5,5,5	0.62	0
3	GOL	F	3001	-	5,5,5	0.36	0	5,5,5	0.48	0
3	GOL	I	4011	-	5,5,5	0.39	0	5,5,5	0.40	0
2	SAH	A	1501	-	24,28,28	1.19	3 (12%)	25,40,40	1.56	4 (16%)
3	GOL	M	6011	-	5,5,5	0.33	0	5,5,5	0.47	0
2	SAH	G	3511	-	24,28,28	1.21	3 (12%)	25,40,40	1.79	4 (16%)
2	SAH	H	4501	-	24,28,28	1.24	3 (12%)	25,40,40	1.84	6 (24%)
3	GOL	J	5002	-	5,5,5	0.56	0	5,5,5	0.51	0
3	GOL	L	6001	-	5,5,5	0.47	0	5,5,5	0.22	0
3	GOL	A	1002	-	5,5,5	0.39	0	5,5,5	0.34	0
3	GOL	H	4012	-	5,5,5	0.41	0	5,5,5	0.63	0
3	GOL	L	6002	-	5,5,5	0.46	0	5,5,5	0.15	0
3	GOL	G	3002	-	5,5,5	0.52	0	5,5,5	0.73	0
3	GOL	G	3003	-	5,5,5	0.50	0	5,5,5	0.53	0
3	GOL	E	2003	-	5,5,5	0.48	0	5,5,5	0.45	0
3	GOL	D	2002	-	5,5,5	0.38	0	5,5,5	0.36	0
3	GOL	J	5003	-	5,5,5	0.43	0	5,5,5	0.36	0
2	SAH	B	1511	-	24,28,28	1.27	3 (12%)	25,40,40	1.78	4 (16%)
2	SAH	L	6501	-	24,28,28	1.21	3 (12%)	25,40,40	1.72	4 (16%)
3	GOL	D	2011	-	5,5,5	0.58	0	5,5,5	0.64	0
3	GOL	H	4003	-	5,5,5	0.52	0	5,5,5	0.50	0
2	SAH	M	6511	-	24,28,28	1.29	2 (8%)	25,40,40	1.66	4 (16%)
3	GOL	E	2012	-	5,5,5	0.44	0	5,5,5	0.38	0
2	SAH	E	2511	-	24,28,28	1.28	3 (12%)	25,40,40	1.89	4 (16%)
3	GOL	F	3011	-	5,5,5	0.39	0	5,5,5	0.38	0
3	GOL	A	1012	-	5,5,5	0.41	0	5,5,5	0.68	0
2	SAH	K	5511	-	24,28,28	1.22	3 (12%)	25,40,40	1.51	3 (12%)
2	SAH	I	4511	-	24,28,28	1.08	3 (12%)	25,40,40	1.97	4 (16%)
3	GOL	K	5012	-	5,5,5	0.46	0	5,5,5	0.50	0
3	GOL	B	1011	-	5,5,5	0.36	0	5,5,5	0.29	0
3	GOL	G	3012	-	5,5,5	0.39	0	5,5,5	0.26	0
3	GOL	I	4002	-	5,5,5	0.75	0	5,5,5	1.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SAH	J	5501	-	24,28,28	1.29	4 (16%)	25,40,40	1.93	6 (24%)
3	GOL	J	5011	-	5,5,5	0.41	0	5,5,5	0.45	0
2	SAH	F	3501	-	24,28,28	1.18	3 (12%)	25,40,40	1.95	6 (24%)
2	SAH	D	2501	-	24,28,28	1.11	2 (8%)	25,40,40	1.89	4 (16%)
3	GOL	K	5001	-	5,5,5	0.52	0	5,5,5	0.71	0

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
3	GOL	A	1001	-	-	2/4/4/4	-
3	GOL	E	2001	-	-	2/4/4/4	-
3	GOL	F	3001	-	-	2/4/4/4	-
3	GOL	I	4011	-	-	4/4/4/4	-
2	SAH	A	1501	-	-	2/11/31/31	0/3/3/3
3	GOL	M	6011	-	-	2/4/4/4	-
2	SAH	G	3511	-	-	2/11/31/31	0/3/3/3
2	SAH	H	4501	-	-	2/11/31/31	0/3/3/3
3	GOL	J	5002	-	-	2/4/4/4	-
3	GOL	L	6001	-	-	2/4/4/4	-
3	GOL	A	1002	-	-	3/4/4/4	-
3	GOL	H	4012	-	-	4/4/4/4	-
3	GOL	L	6002	-	-	2/4/4/4	-
3	GOL	G	3002	-	-	4/4/4/4	-
3	GOL	G	3003	-	-	4/4/4/4	-
3	GOL	E	2003	-	-	4/4/4/4	-
3	GOL	D	2002	-	-	2/4/4/4	-
3	GOL	J	5003	-	-	2/4/4/4	-
2	SAH	B	1511	-	-	0/11/31/31	0/3/3/3
2	SAH	L	6501	-	-	0/11/31/31	0/3/3/3
3	GOL	D	2011	-	-	2/4/4/4	-
3	GOL	H	4003	-	-	3/4/4/4	-
2	SAH	M	6511	-	-	0/11/31/31	0/3/3/3
3	GOL	E	2012	-	-	2/4/4/4	-
2	SAH	E	2511	-	-	2/11/31/31	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	F	3011	-	-	2/4/4/4	-
3	GOL	A	1012	-	-	4/4/4/4	-
2	SAH	K	5511	-	-	2/11/31/31	0/3/3/3
2	SAH	I	4511	-	-	2/11/31/31	0/3/3/3
3	GOL	K	5012	-	-	2/4/4/4	-
3	GOL	B	1011	-	-	4/4/4/4	-
3	GOL	G	3012	-	-	1/4/4/4	-
3	GOL	I	4002	-	-	2/4/4/4	-
2	SAH	J	5501	-	-	2/11/31/31	0/3/3/3
3	GOL	J	5011	-	-	2/4/4/4	-
2	SAH	F	3501	-	-	2/11/31/31	0/3/3/3
2	SAH	D	2501	-	-	1/11/31/31	0/3/3/3
3	GOL	K	5001	-	-	2/4/4/4	-

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1511	SAH	C2-N3	4.24	1.38	1.32
2	M	6511	SAH	C2-N3	4.24	1.38	1.32
2	L	6501	SAH	C2-N3	4.00	1.38	1.32
2	E	2511	SAH	C2-N3	3.94	1.38	1.32
2	H	4501	SAH	C2-N3	3.79	1.38	1.32

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	5501	SAH	N3-C2-N1	-6.19	119.01	128.68
2	G	3511	SAH	N3-C2-N1	-6.16	119.05	128.68
2	M	6511	SAH	N3-C2-N1	-5.88	119.49	128.68
2	L	6501	SAH	N3-C2-N1	-5.75	119.69	128.68
2	I	4511	SAH	N3-C2-N1	-5.72	119.74	128.68

There are no chirality outliers.

5 of 84 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2511	SAH	O4'-C4'-C5'-SD
2	E	2511	SAH	C3'-C4'-C5'-SD
2	G	3511	SAH	O4'-C4'-C5'-SD

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Mol	Chain	Res	Type	Atoms
2	G	3511	SAH	C3'-C4'-C5'-SD
2	K	5511	SAH	O4'-C4'-C5'-SD

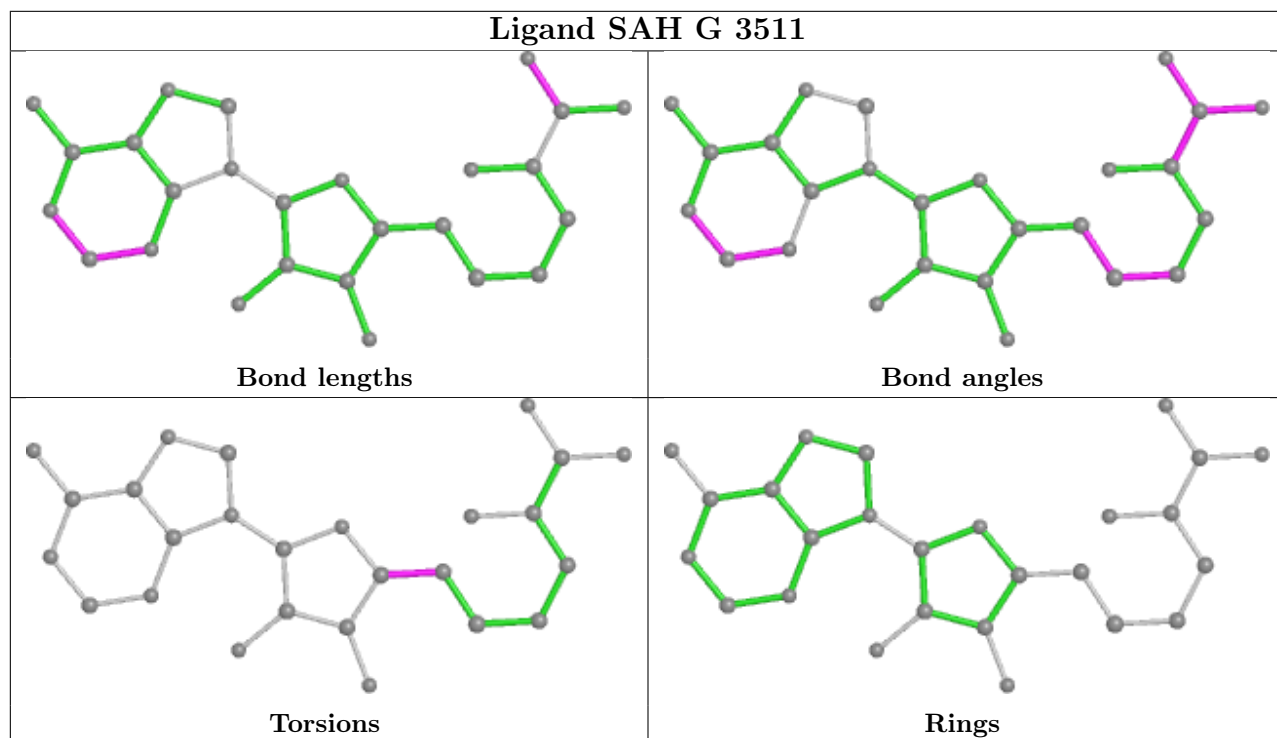
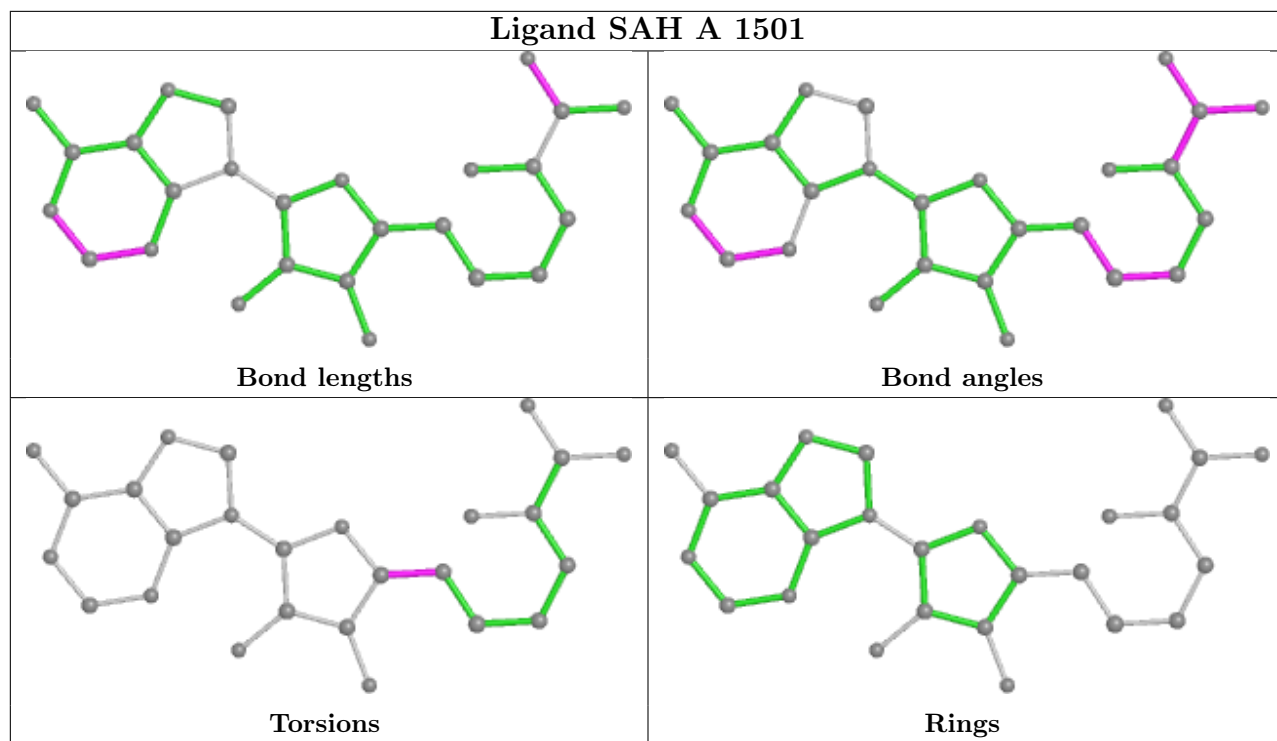
There are no ring outliers.

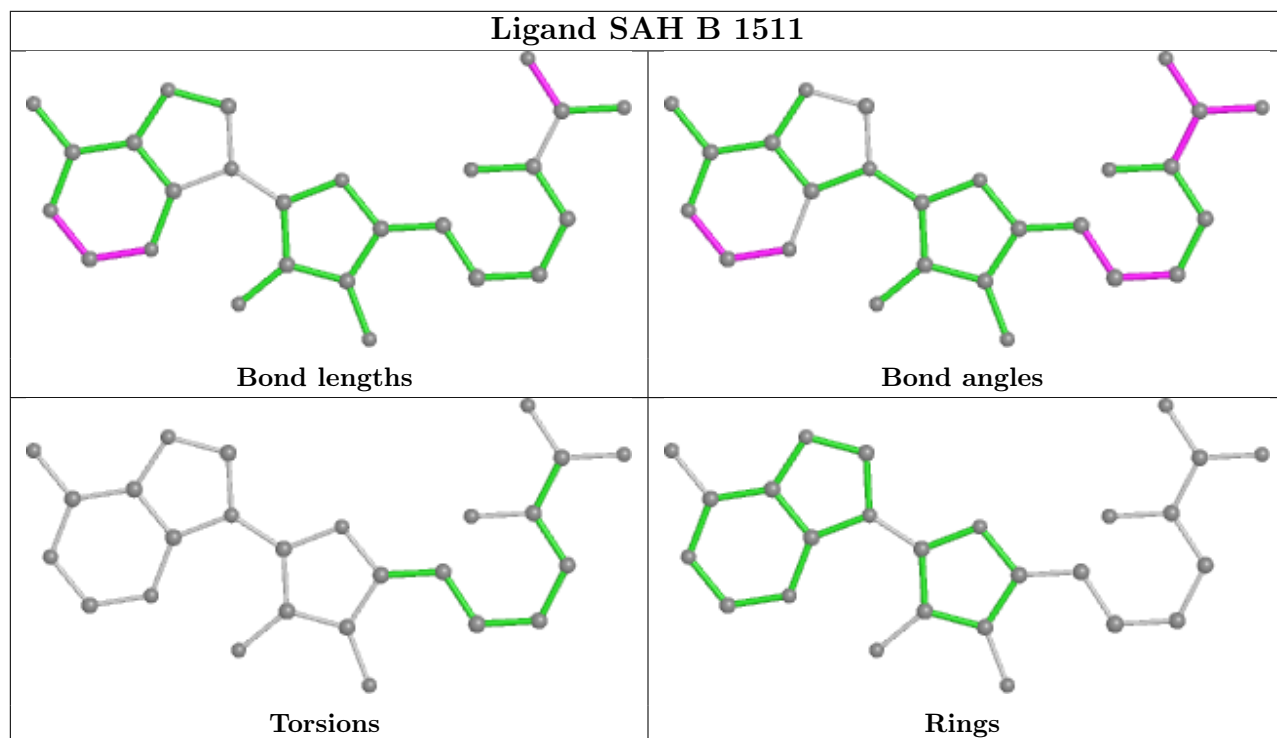
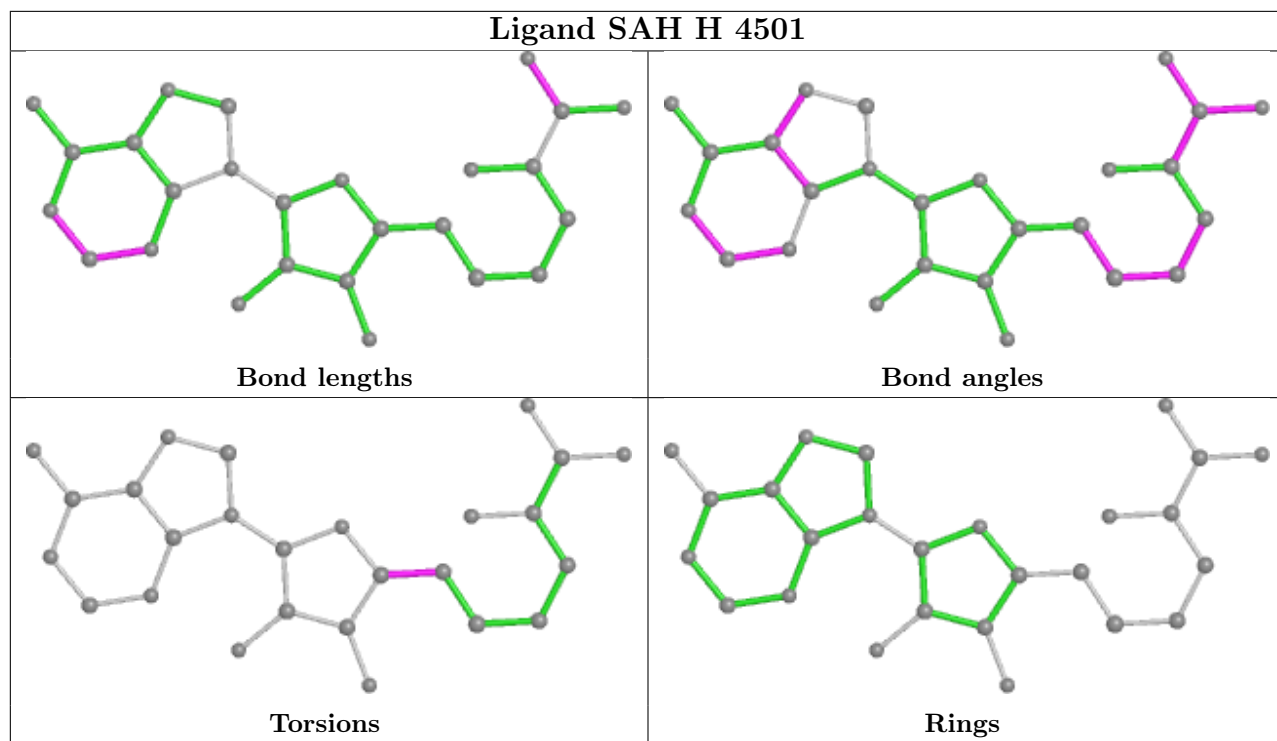
21 monomers are involved in 63 short contacts:

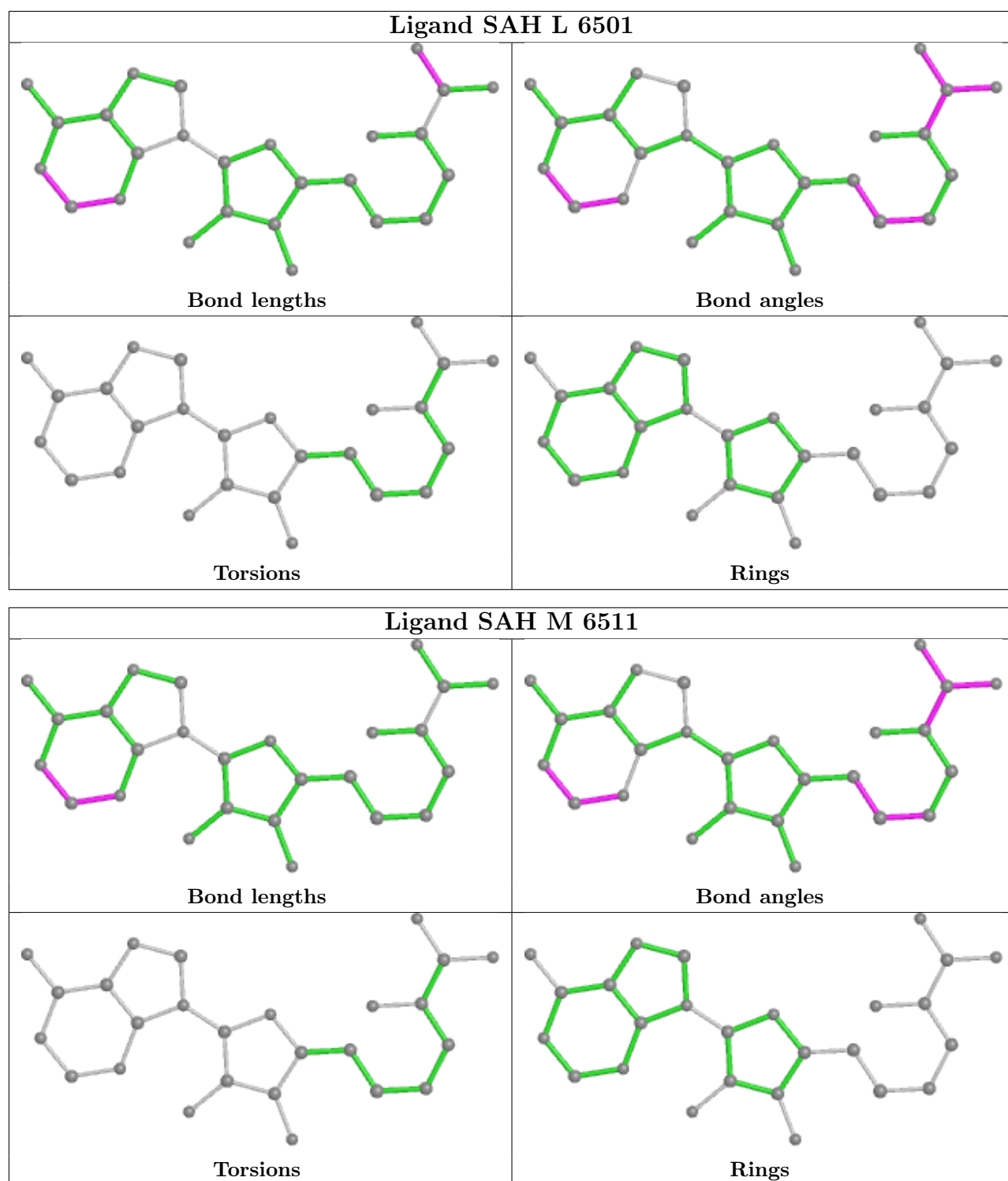
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	GOL	3	0
3	E	2001	GOL	5	0
2	G	3511	SAH	2	0
3	J	5002	GOL	2	0
3	H	4012	GOL	6	0
3	L	6002	GOL	1	0
3	G	3002	GOL	3	0
3	G	3003	GOL	4	0
3	E	2003	GOL	3	0
3	D	2011	GOL	7	0
2	M	6511	SAH	2	0
3	E	2012	GOL	1	0
2	E	2511	SAH	1	0
3	F	3011	GOL	2	0
3	A	1012	GOL	2	0
2	K	5511	SAH	1	0
3	K	5012	GOL	4	0
3	I	4002	GOL	4	0
2	J	5501	SAH	2	0
3	J	5011	GOL	3	0
3	K	5001	GOL	5	0

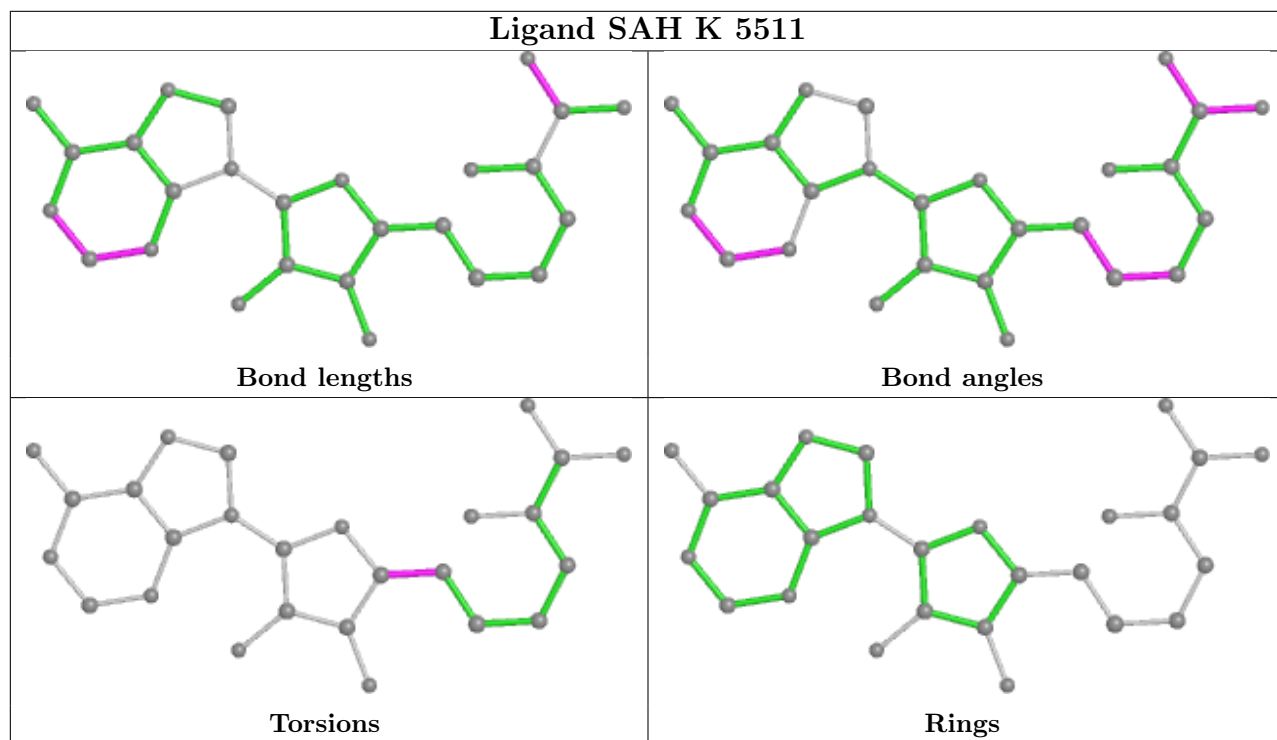
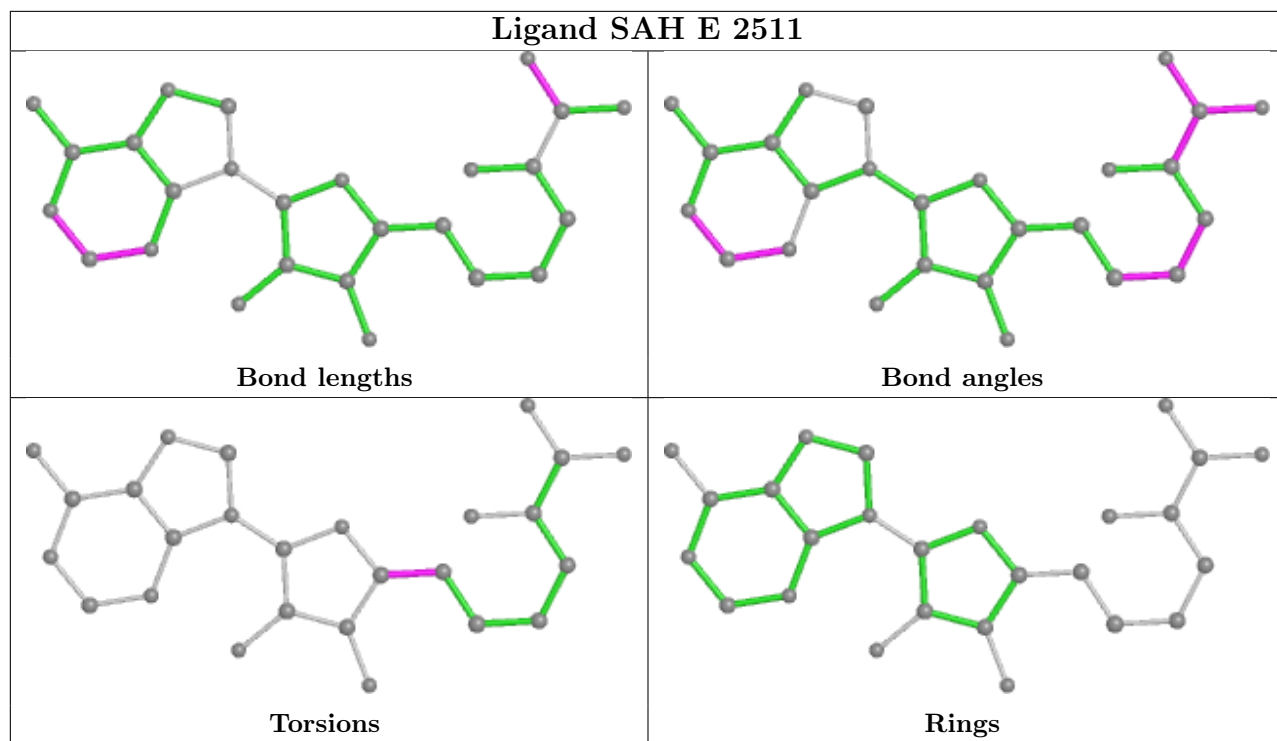
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

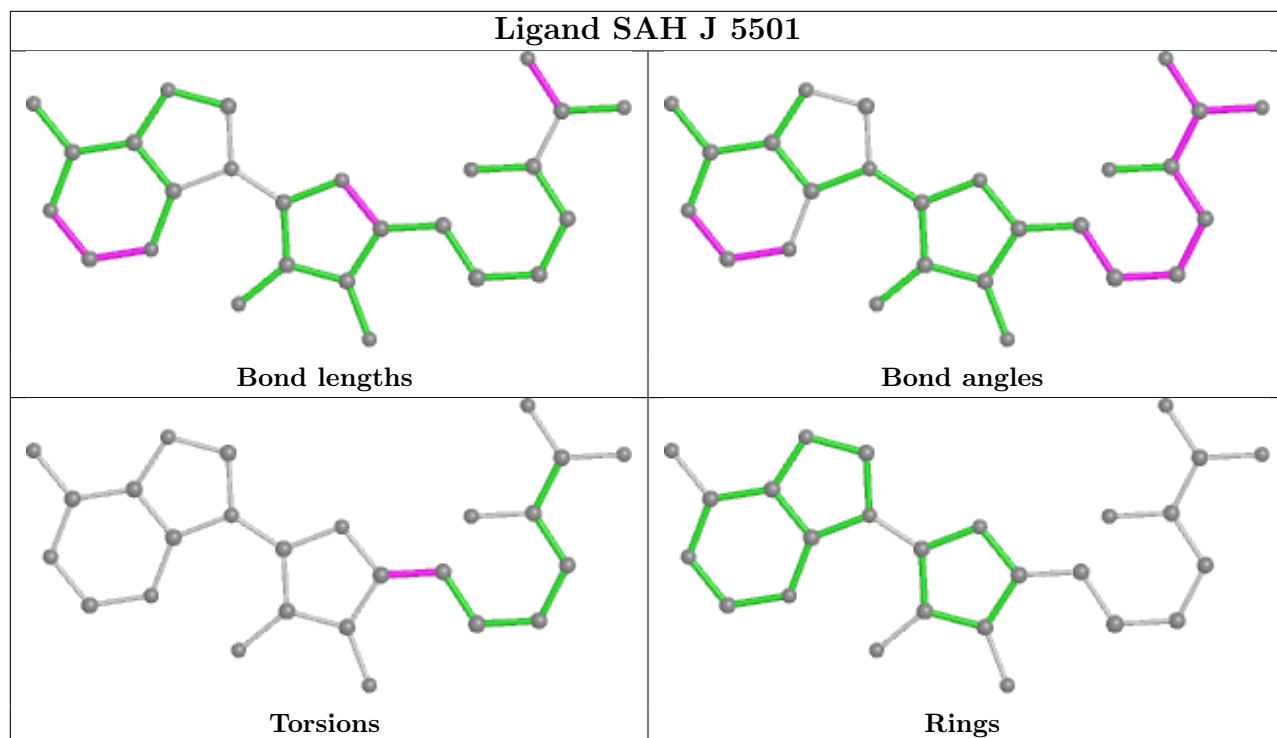
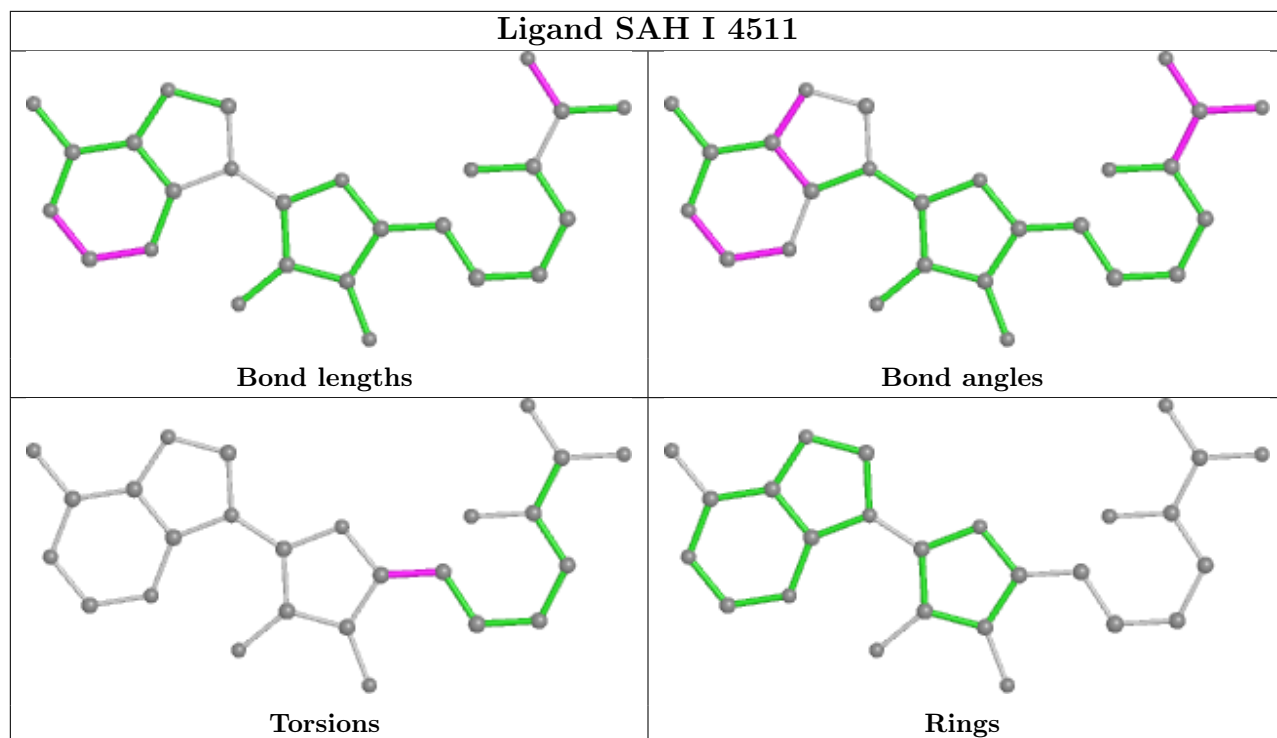


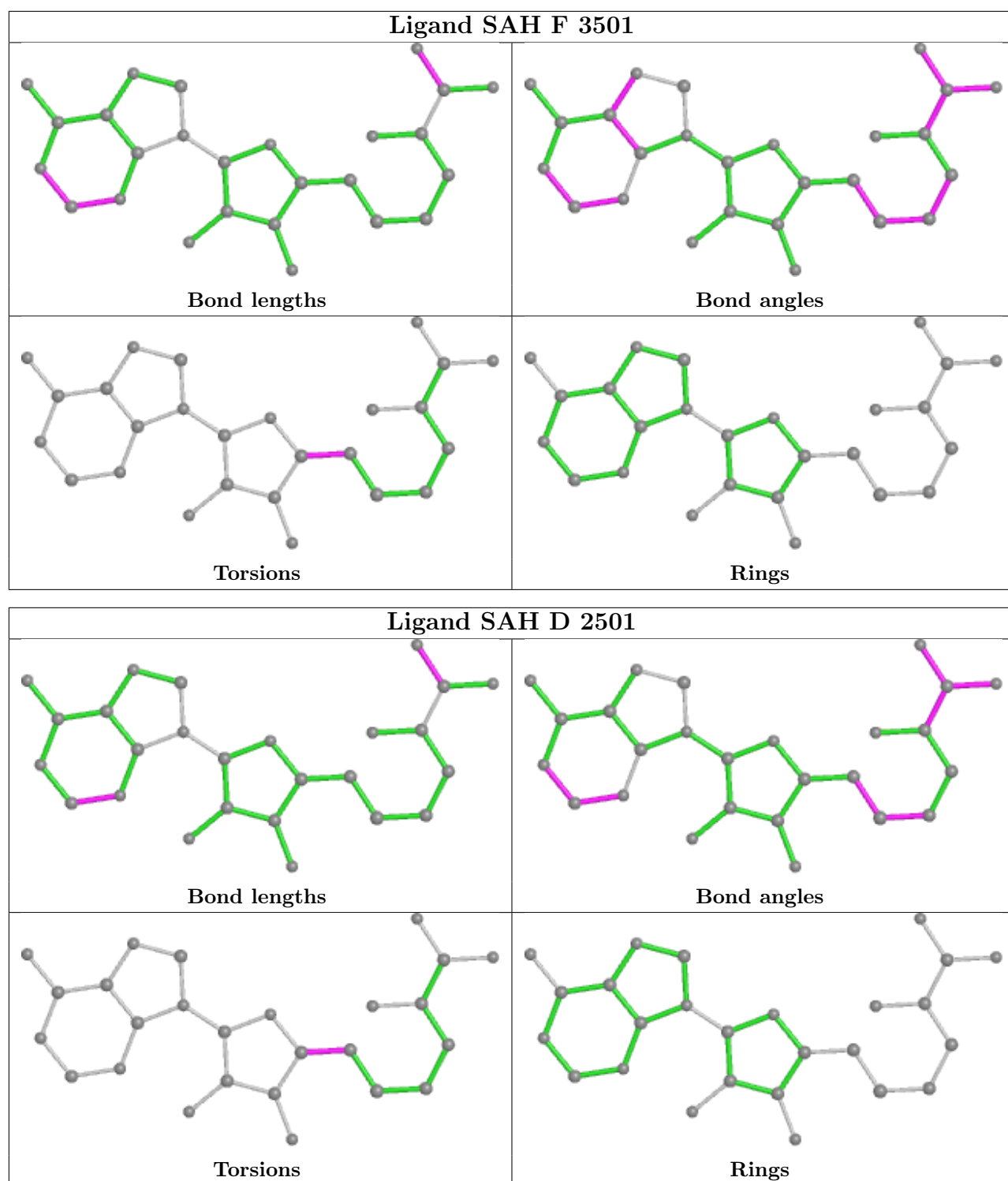












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	256/280 (91%)	-0.12	13 (5%) 28 26	16, 23, 53, 83	0
1	B	263/280 (93%)	-0.03	19 (7%) 15 13	14, 23, 56, 79	0
1	D	248/280 (88%)	-0.18	8 (3%) 47 48	15, 22, 45, 69	0
1	E	265/280 (94%)	0.00	20 (7%) 14 12	13, 23, 64, 80	0
1	F	254/280 (90%)	-0.01	13 (5%) 28 26	14, 23, 55, 63	0
1	G	258/280 (92%)	0.21	26 (10%) 7 5	14, 25, 62, 73	0
1	H	259/280 (92%)	-0.12	17 (6%) 18 16	16, 23, 53, 79	0
1	I	263/280 (93%)	-0.10	17 (6%) 18 17	12, 22, 55, 78	0
1	J	252/280 (90%)	0.07	20 (7%) 12 10	14, 24, 54, 79	0
1	K	258/280 (92%)	0.07	21 (8%) 12 10	10, 24, 69, 88	0
1	L	247/280 (88%)	0.73	47 (19%) 1 0	15, 25, 87, 92	0
1	M	252/280 (90%)	0.93	55 (21%) 0 0	16, 27, 85, 88	0
All	All	3075/3360 (91%)	0.12	276 (8%) 9 7	10, 24, 62, 92	0

The worst 5 of 276 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	71	GLY	9.3
1	M	72	GLY	7.9
1	L	49	LEU	7.7
1	L	74	PRO	7.6
1	M	50	VAL	7.5

### 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<sup>th</sup> 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.

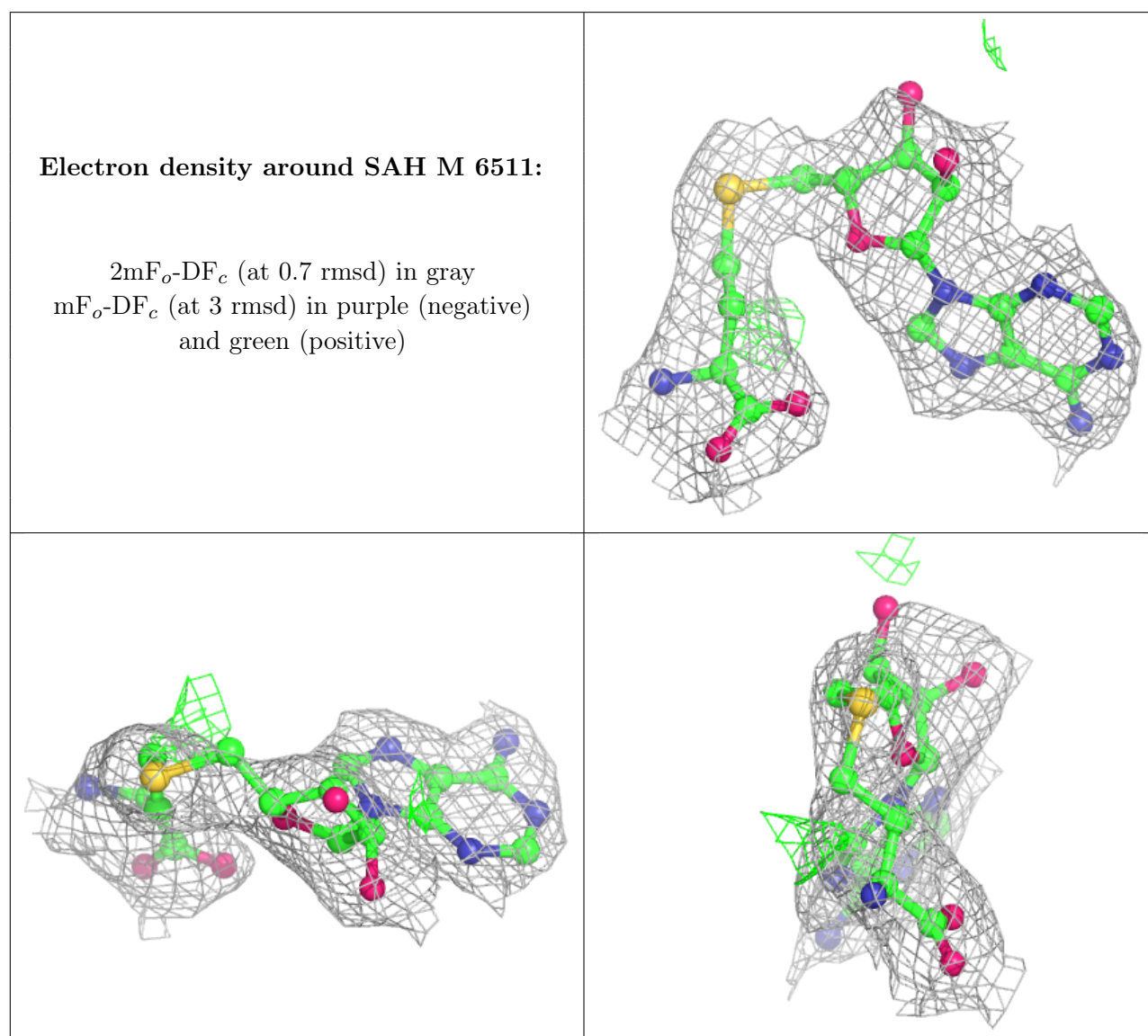
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	D	2002	6/6	0.68	0.27	77,86,87,88	0
3	GOL	A	1002	6/6	0.72	0.26	78,84,86,88	0
3	GOL	F	3001	6/6	0.72	0.26	83,90,92,93	0
3	GOL	D	2011	6/6	0.74	0.36	74,82,83,85	0
3	GOL	L	6001	6/6	0.79	0.33	105,106,106,106	0
3	GOL	I	4011	6/6	0.80	0.32	88,91,92,93	0
3	GOL	G	3012	6/6	0.80	0.28	91,93,94,96	0
3	GOL	M	6011	6/6	0.80	0.20	83,85,87,89	0
3	GOL	A	1012	6/6	0.83	0.39	71,75,76,78	0
3	GOL	H	4003	6/6	0.84	0.30	77,82,82,82	0
3	GOL	A	1001	6/6	0.84	0.31	51,57,60,61	0
3	GOL	E	2003	6/6	0.85	0.28	73,76,77,79	0
3	GOL	J	5011	6/6	0.85	0.36	95,95,97,98	0
3	GOL	F	3011	6/6	0.86	0.43	92,93,94,95	0
3	GOL	B	1011	6/6	0.87	0.22	67,77,79,79	0
3	GOL	E	2012	6/6	0.87	0.29	89,95,96,97	0
3	GOL	G	3002	6/6	0.88	0.34	78,80,81,81	0
2	SAH	M	6511	26/26	0.88	0.18	67,69,71,73	0
3	GOL	E	2001	6/6	0.88	0.29	57,63,65,67	0
3	GOL	H	4012	6/6	0.88	0.30	73,74,76,77	0
3	GOL	J	5002	6/6	0.89	0.32	66,70,70,71	0
3	GOL	L	6002	6/6	0.89	0.18	91,95,96,97	0
3	GOL	K	5001	6/6	0.89	0.34	74,77,77,77	0
3	GOL	I	4002	6/6	0.90	0.27	50,53,57,57	0
3	GOL	G	3003	6/6	0.90	0.37	73,76,77,77	0
3	GOL	K	5012	6/6	0.91	0.20	94,95,96,96	0
2	SAH	L	6501	26/26	0.92	0.24	88,96,102,102	0
3	GOL	J	5003	6/6	0.93	0.19	78,82,86,88	0
2	SAH	I	4511	26/26	0.95	0.21	52,60,64,65	0
2	SAH	J	5501	26/26	0.95	0.21	66,68,69,70	0
2	SAH	G	3511	26/26	0.95	0.23	60,69,78,78	0
2	SAH	E	2511	26/26	0.96	0.19	51,58,59,59	0

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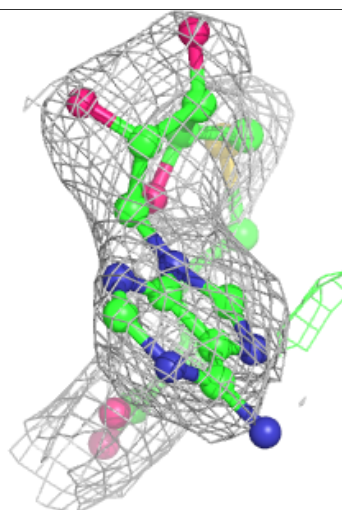
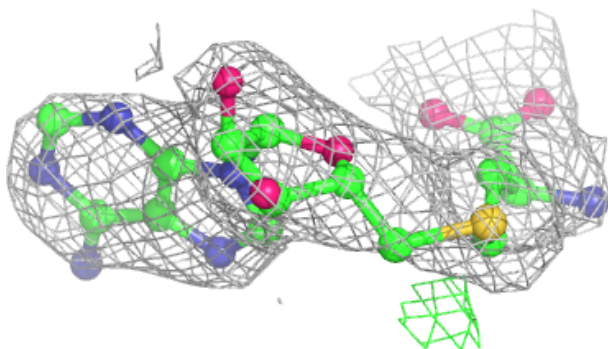
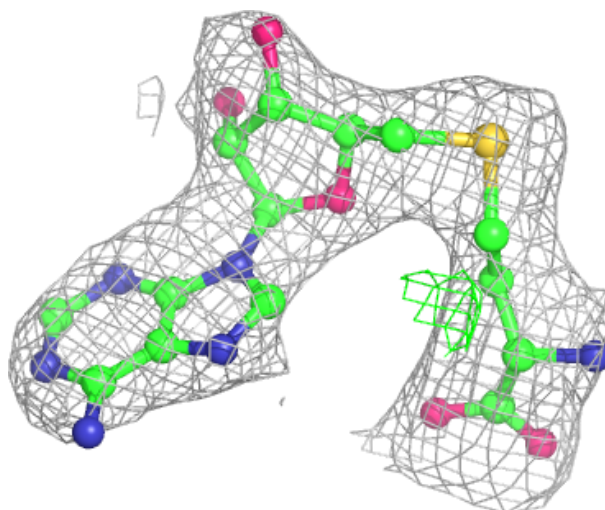
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SAH	F	3501	26/26	0.96	0.19	54,62,63,64	0
2	SAH	A	1501	26/26	0.96	0.21	46,59,67,67	0
2	SAH	H	4501	26/26	0.96	0.20	50,56,60,62	0
2	SAH	B	1511	26/26	0.96	0.18	45,49,50,51	0
2	SAH	D	2501	26/26	0.96	0.22	55,60,64,64	0
2	SAH	K	5511	26/26	0.96	0.21	56,62,64,64	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.



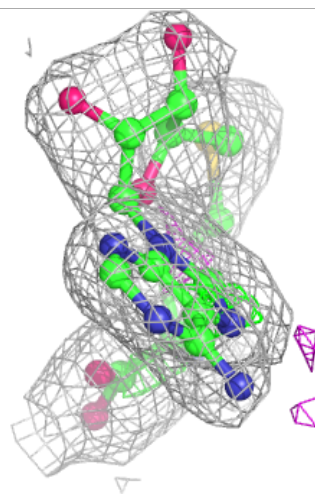
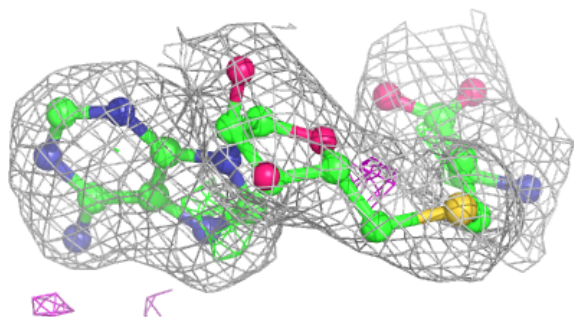
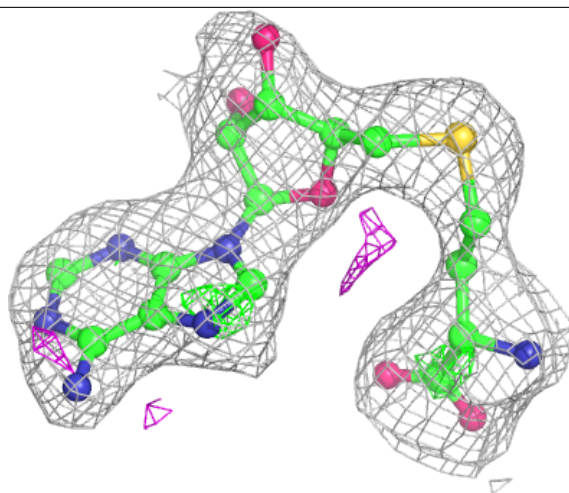
**Electron density around SAH L 6501:**

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



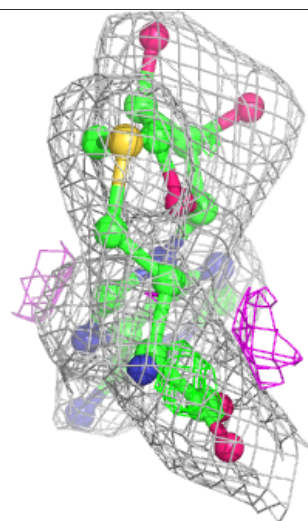
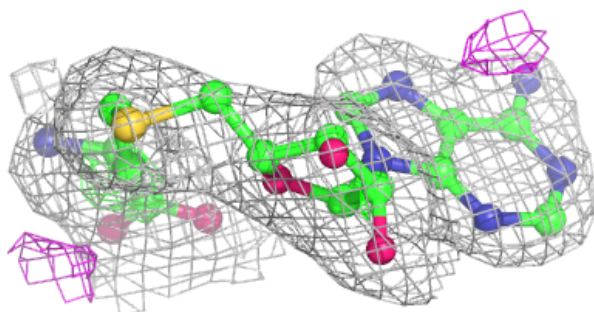
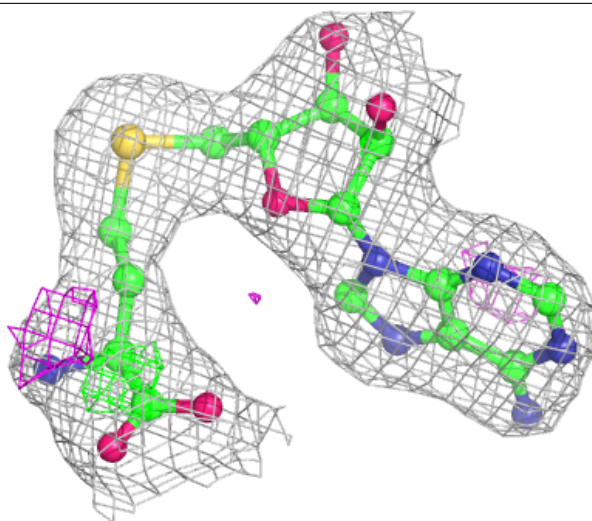
**Electron density around SAH I 4511:**

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



**Electron density around SAH J 5501:**

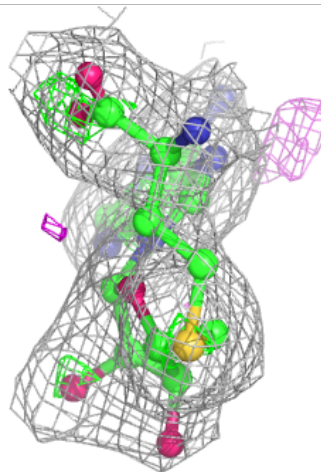
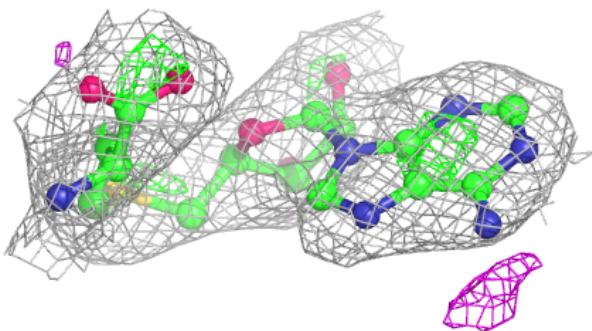
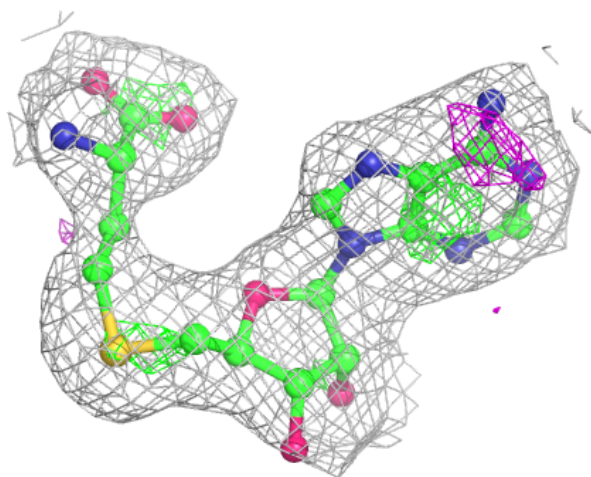
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





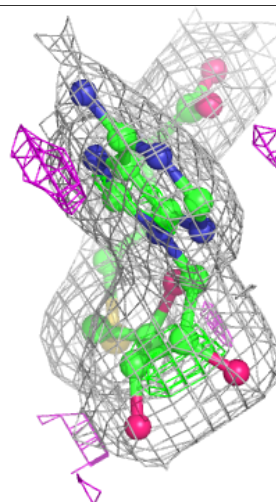
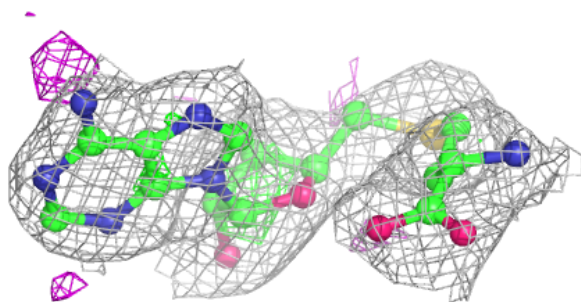
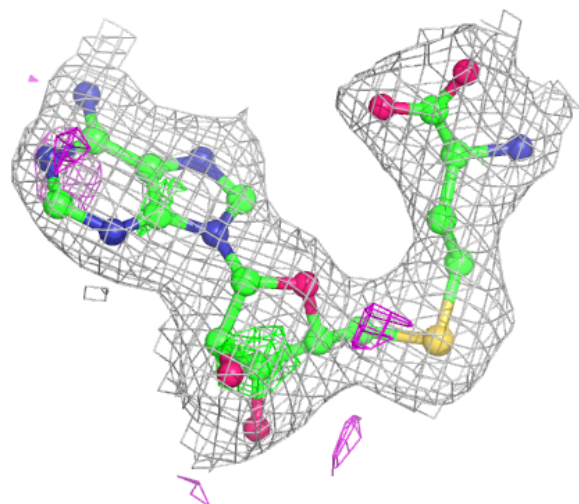
**Electron density around SAH G 3511:**

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



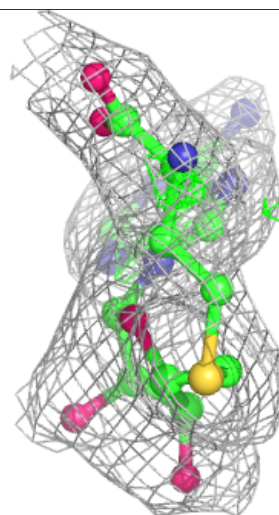
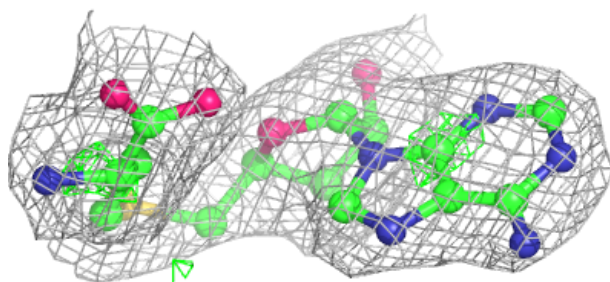
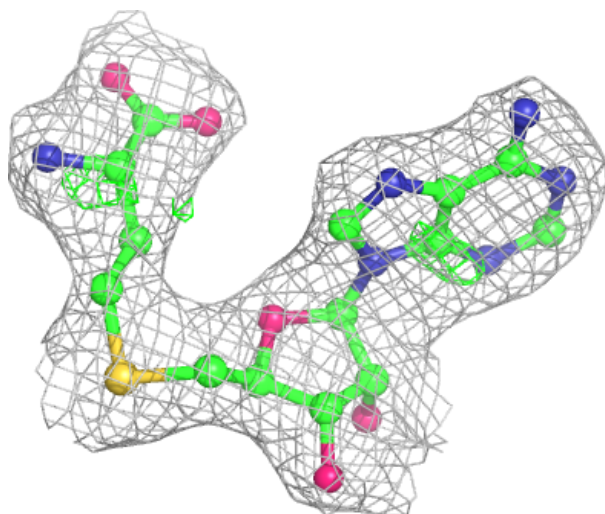
**Electron density around SAH E 2511:**

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



**Electron density around SAH F 3501:**

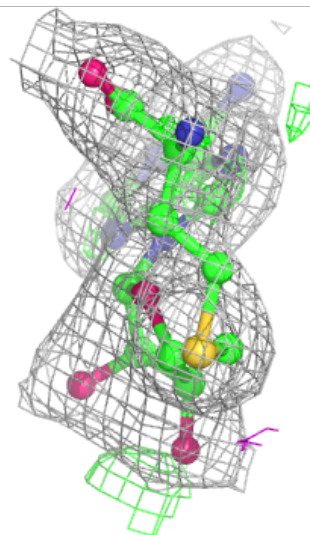
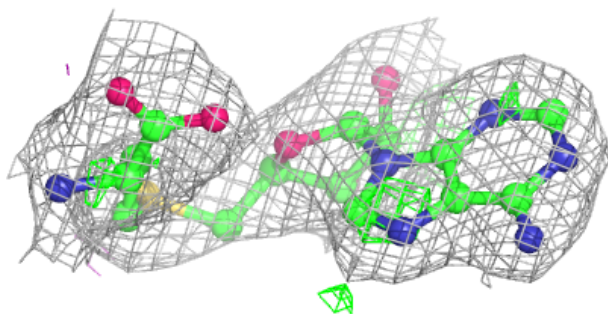
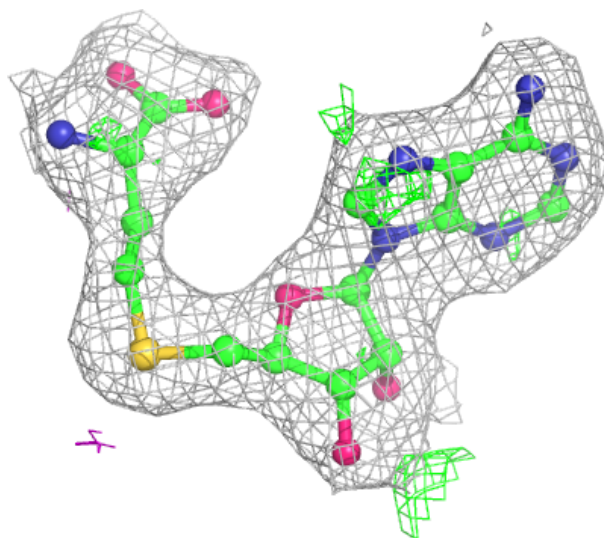
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





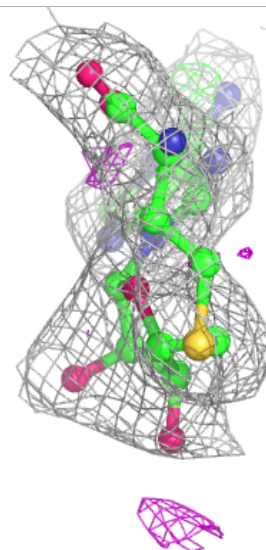
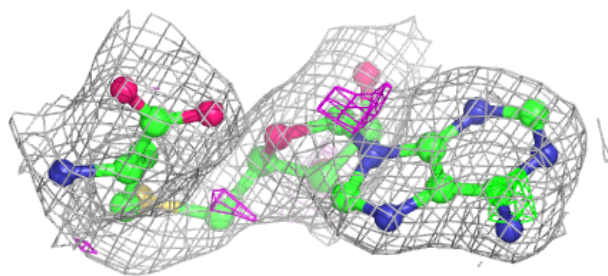
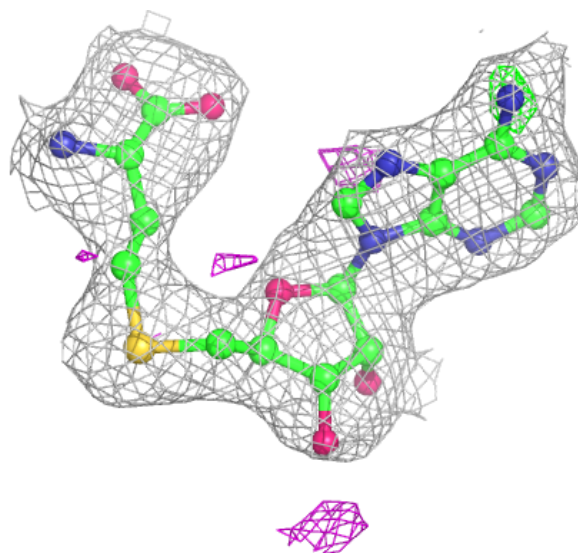
**Electron density around SAH A 1501:**

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



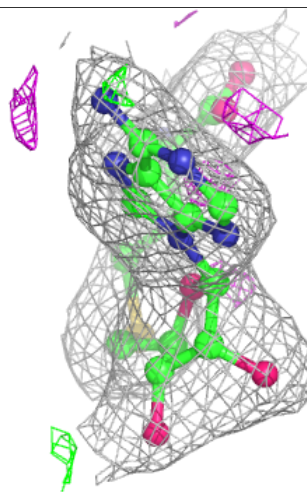
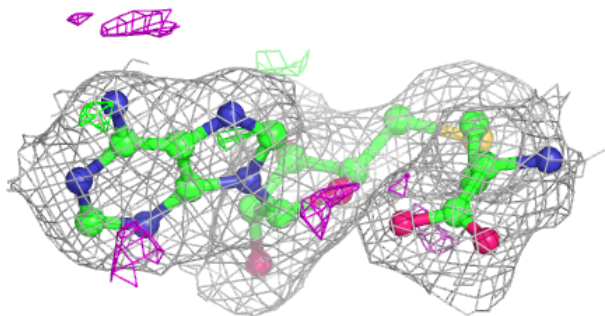
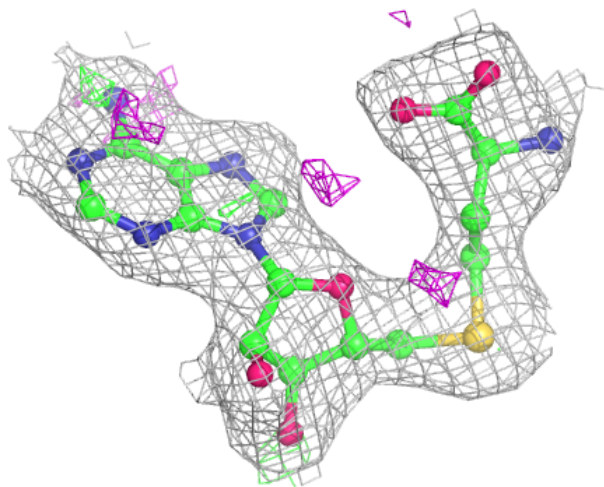
**Electron density around SAH H 4501:**

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



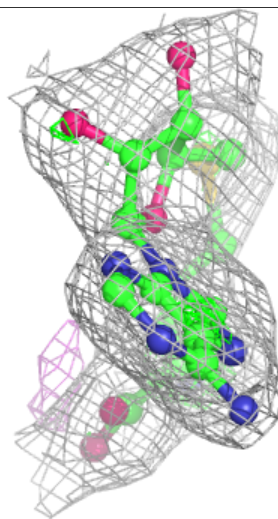
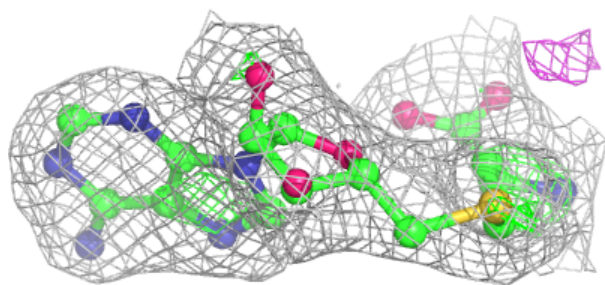
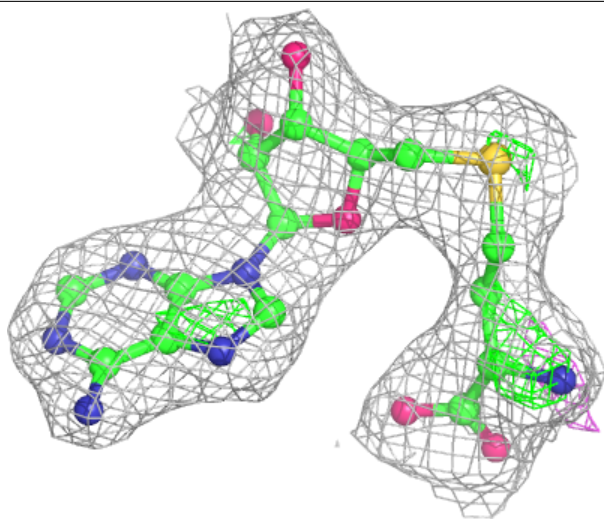
**Electron density around SAH B 1511:**

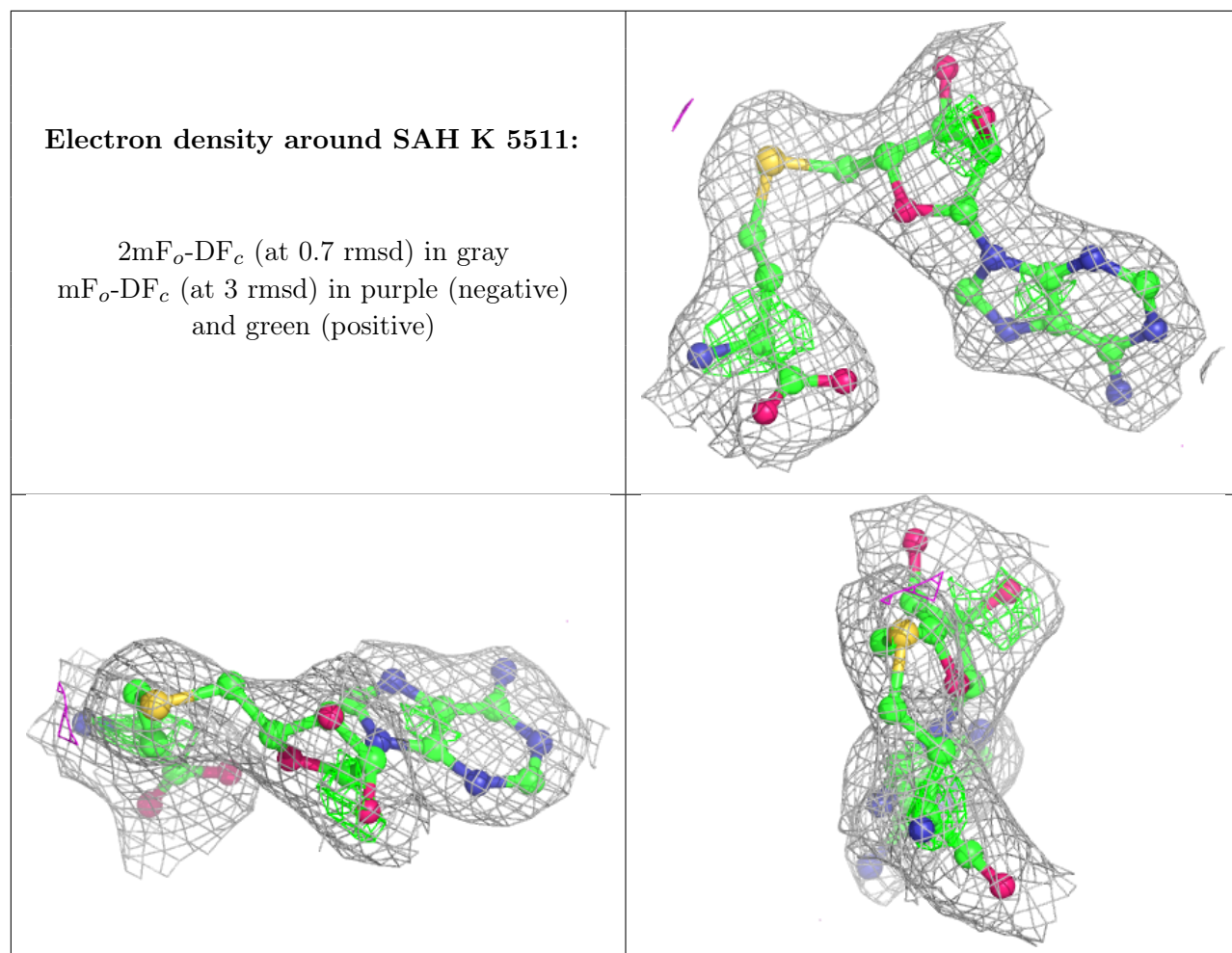
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around SAH D 2501:**

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





## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.