



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:06 PM UTC

PDB ID : 1S4D / pdb_00001s4d
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

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](#) ①) were used in the production of this report:

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

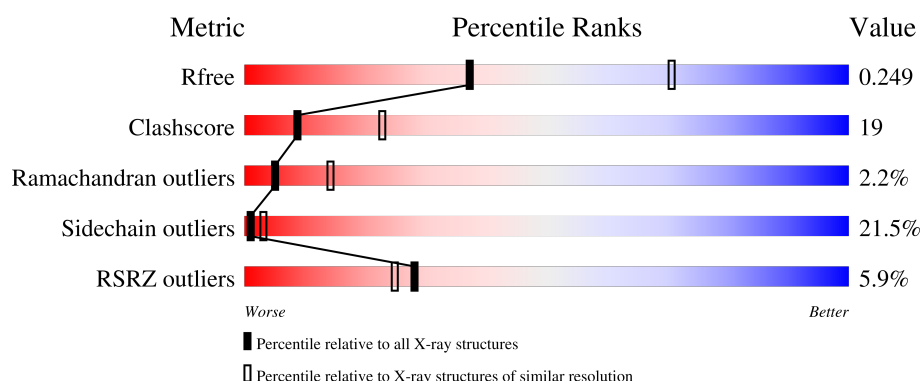
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 ≥ 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	5% 53% 29% 9% 9%
1	B	280	6% 60% 23% 10% 6%
1	D	280	0% 54% 23% 11% 11%
1	E	280	5% 60% 24% 9% 5%
1	F	280	4% 60% 23% 8% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	280	
1	H	280	
1	I	280	
1	J	280	
1	K	280	
1	L	280	
1	M	280	

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

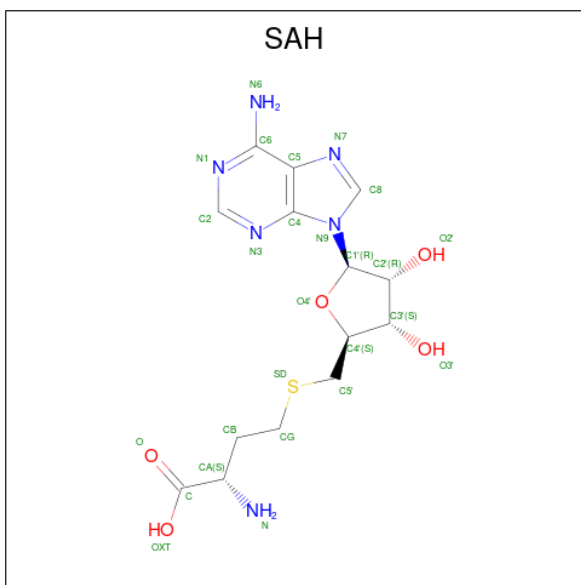
There are 4 unique types of molecules in this entry. The entry contains 23427 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



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

Continued on next page...

Continued from previous page...

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

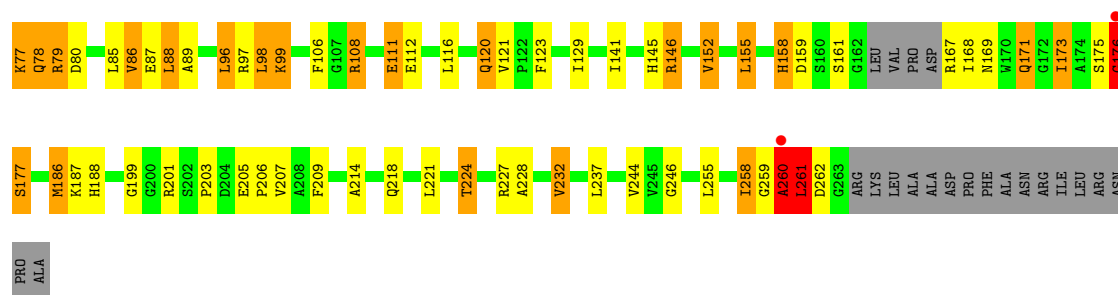
- Molecule 4 is water.

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

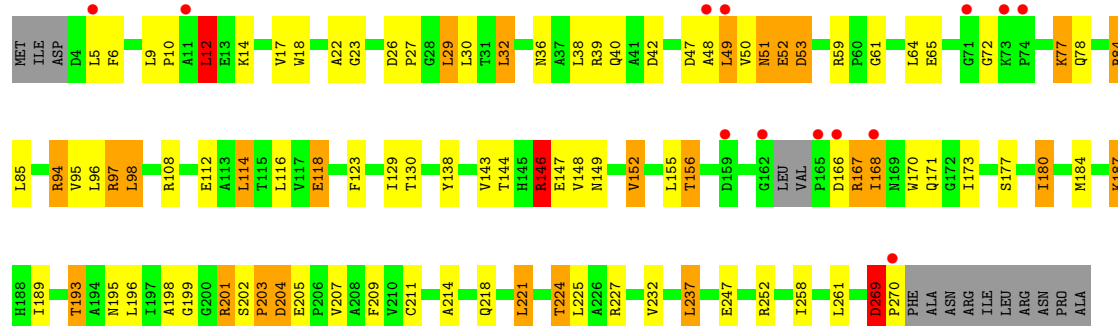
Continued on next page...

Continued from previous page...

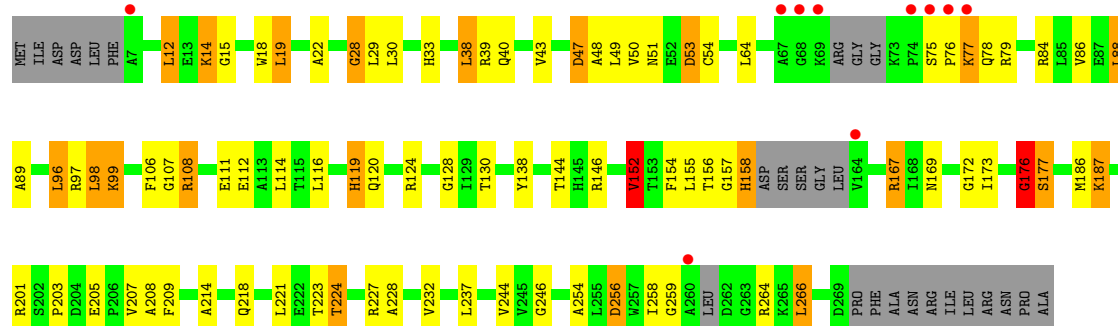
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	59	Total 59	O 59	0	0
4	J	30	Total 30	O 30	0	0
4	K	44	Total 44	O 44	0	0
4	L	24	Total 24	O 24	0	0
4	M	14	Total 14	O 14	0	0



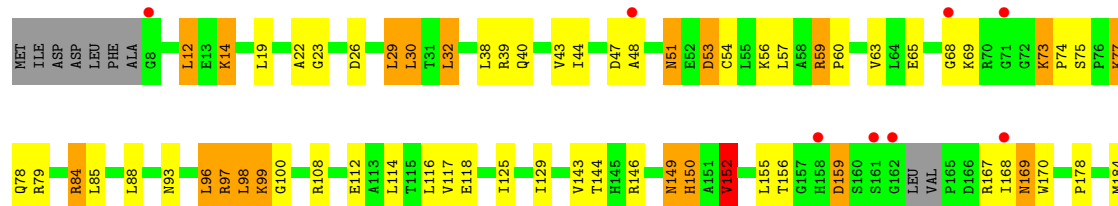
• Molecule 1: Uroporphyrin-III C-methyltransferase



• Molecule 1: Uroporphyrin-III C-methyltransferase

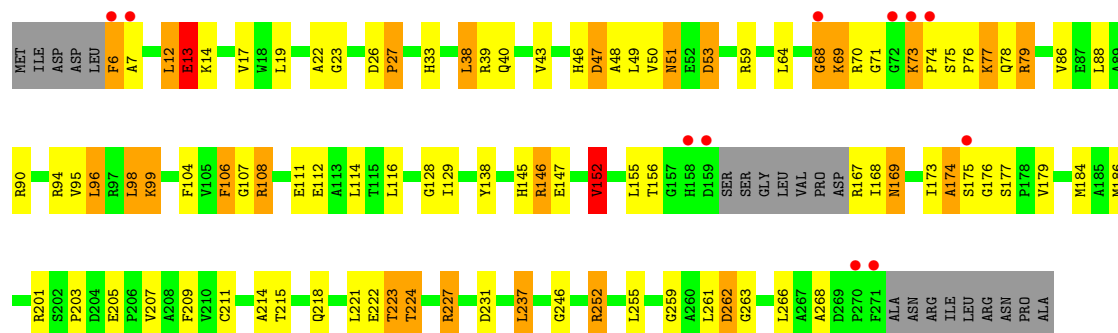


• Molecule 1: Uroporphyrin-III C-methyltransferase

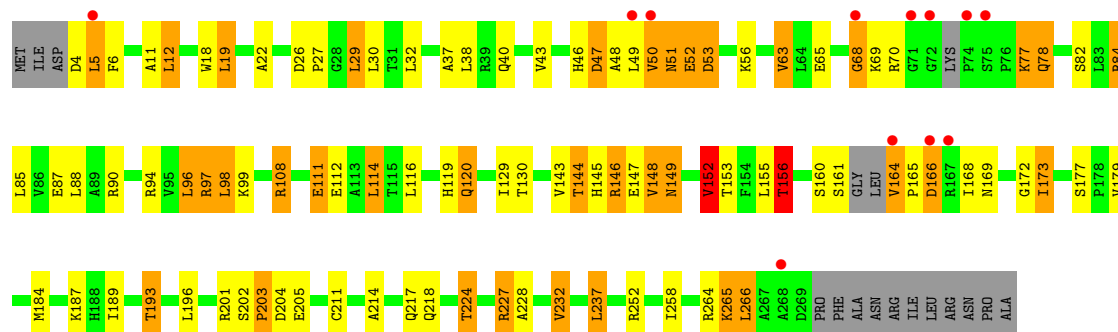




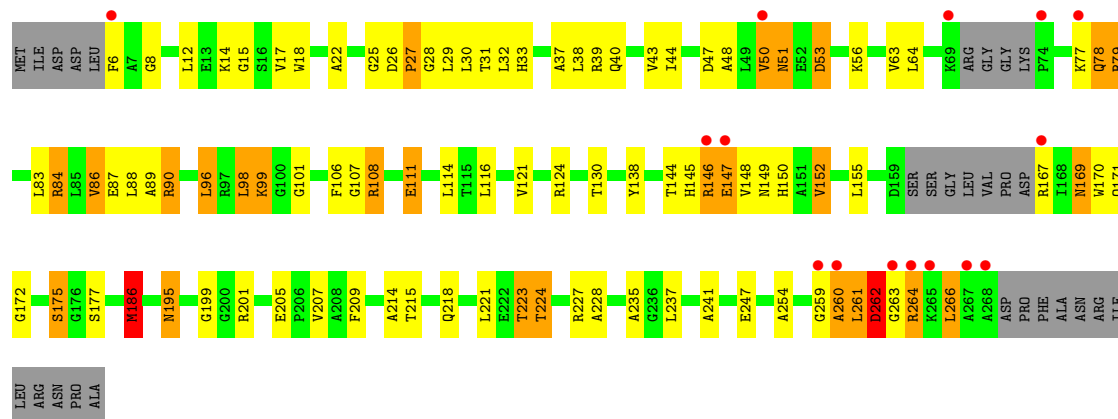
• Molecule 1: Uroporphyrin-III C-methyltransferase



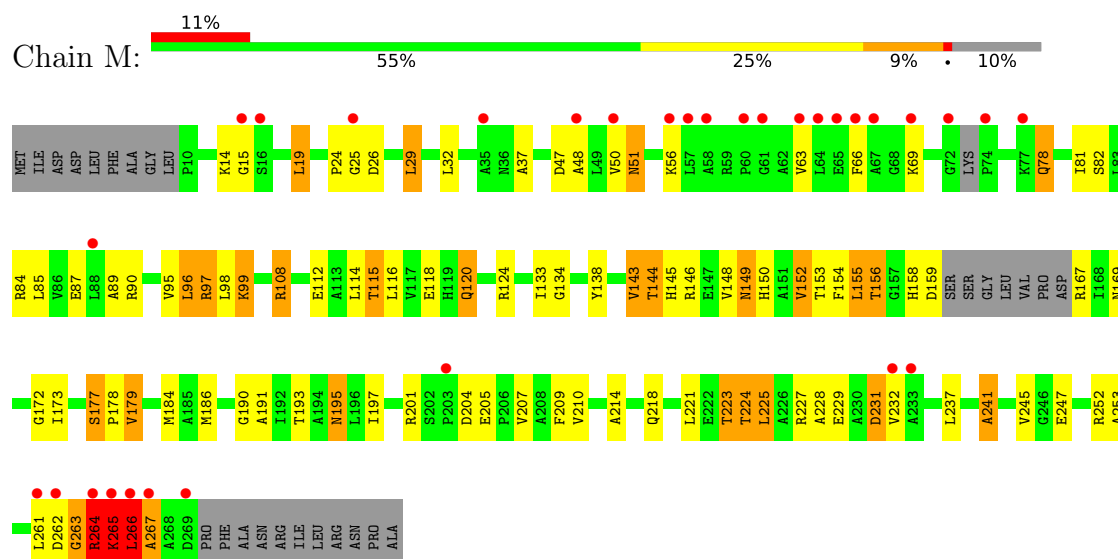
• Molecule 1: Uroporphyrin-III C-methyltransferase



• Molecule 1: Uroporphyrin-III C-methyltransferase



• Molecule 1: Uroporphyrin-III C-methyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	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) 99.7 (19.84-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.34 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.213 , 0.260 (Not available) , 0.249	Depositor DCC
R_{free} test set	6099 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	46.4	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.014 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23427	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.85	2/1918 (0.1%)	1.15	10/2609 (0.4%)
1	B	0.82	1/1956 (0.1%)	1.16	10/2666 (0.4%)
1	D	0.83	3/1840 (0.2%)	1.13	10/2506 (0.4%)
1	E	0.75	0/1960	1.13	8/2672 (0.3%)
1	F	0.82	1/1886 (0.1%)	1.11	6/2569 (0.2%)
1	G	0.72	0/1913	1.10	6/2605 (0.2%)
1	H	0.88	1/1932 (0.1%)	1.17	12/2632 (0.5%)
1	I	0.78	1/1972 (0.1%)	1.13	5/2683 (0.2%)
1	J	0.78	3/1875 (0.2%)	1.11	8/2554 (0.3%)
1	K	0.75	1/1924 (0.1%)	1.12	7/2621 (0.3%)
1	L	0.77	2/1828 (0.1%)	1.06	4/2490 (0.2%)
1	M	0.72	4/1876 (0.2%)	1.29	12/2552 (0.5%)
All	All	0.79	19/22880 (0.1%)	1.14	98/31159 (0.3%)

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

Continued on next page...

Continued from previous page...

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

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	79	ARG	NE-CZ	16.56	1.51	1.33
1	H	79	ARG	NE-CZ	15.99	1.50	1.33
1	F	79	ARG	NE-CZ	15.76	1.50	1.33
1	J	79	ARG	NE-CZ	15.40	1.50	1.33
1	A	79	ARG	NE-CZ	15.23	1.49	1.33

The worst 5 of 98 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	266	LEU	O-C-N	-25.58	88.57	122.59
1	M	263	GLY	CA-C-N	12.99	146.35	121.54
1	M	263	GLY	C-N-CA	12.99	146.35	121.54
1	M	264	ARG	CA-C-N	11.56	143.62	121.54
1	M	264	ARG	C-N-CA	11.56	143.62	121.54

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

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	85	0
1	B	1915	0	1933	79	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1806	0	1836	73	0
1	E	1922	0	1942	79	0
1	F	1852	0	1881	70	0
1	G	1877	0	1903	69	0
1	H	1894	0	1922	79	0
1	I	1932	0	1968	96	0
1	J	1840	0	1870	85	0
1	K	1883	0	1920	71	0
1	L	1795	0	1822	58	0
1	M	1842	0	1871	73	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	0	0
2	F	26	0	19	0	0
2	G	26	0	19	3	0
2	H	26	0	19	0	0
2	I	26	0	19	0	0
2	J	26	0	19	1	0
2	K	26	0	19	1	0
2	L	26	0	19	0	0
2	M	26	0	19	1	0
3	A	18	0	24	5	0
3	B	6	0	8	0	0
3	D	12	0	16	6	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	2	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

Continued on next page...

Continued from previous page...

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	23215	861	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 861 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:J:186:MET:HE1	1:J:209:PHE:CD1	1.70	1.26
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: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%)	4	9
1	B	260/280 (93%)	236 (91%)	20 (8%)	4 (2%)	8	22
1	D	242/280 (86%)	222 (92%)	13 (5%)	7 (3%)	3	9
1	E	261/280 (93%)	239 (92%)	18 (7%)	4 (2%)	8	22
1	F	246/280 (88%)	229 (93%)	12 (5%)	5 (2%)	6	16
1	G	254/280 (91%)	232 (91%)	16 (6%)	6 (2%)	4	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	255/280 (91%)	234 (92%)	15 (6%)	6 (2%)	4	12
1	I	258/280 (92%)	239 (93%)	14 (5%)	5 (2%)	6	17
1	J	246/280 (88%)	231 (94%)	12 (5%)	3 (1%)	10	27
1	K	255/280 (91%)	229 (90%)	18 (7%)	8 (3%)	3	8
1	L	239/280 (85%)	222 (93%)	14 (6%)	3 (1%)	9	25
1	M	246/280 (88%)	225 (92%)	12 (5%)	9 (4%)	2	6
All	All	3012/3360 (90%)	2763 (92%)	182 (6%)	67 (2%)	5	14

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 ⓘ

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%)	150 (80%)	37 (20%)	1	4
1	B	190/207 (92%)	147 (77%)	43 (23%)	1	3
1	D	181/207 (87%)	144 (80%)	37 (20%)	1	3
1	E	190/207 (92%)	146 (77%)	44 (23%)	1	2
1	F	184/207 (89%)	150 (82%)	34 (18%)	1	4
1	G	186/207 (90%)	151 (81%)	35 (19%)	1	4
1	H	187/207 (90%)	151 (81%)	36 (19%)	1	4
1	I	194/207 (94%)	142 (73%)	52 (27%)	0	1
1	J	182/207 (88%)	145 (80%)	37 (20%)	1	3
1	K	188/207 (91%)	149 (79%)	39 (21%)	1	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	178/207 (86%)	136 (76%)	42 (24%)	1	2
1	M	182/207 (88%)	139 (76%)	43 (24%)	1	2
All	All	2229/2484 (90%)	1750 (78%)	479 (22%)	1	3

5 of 479 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	12	LEU
1	M	63	VAL
1	I	87	GLU
1	M	29	LEU
1	M	195	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 108 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	40	GLN
1	I	169	ASN
1	M	40	GLN
1	H	51	ASN
1	H	218	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
2	SAH	D	2501	-	27,28,28	1.03	2 (7%)	36,40,40	2.17	9 (25%)
2	SAH	E	2511	-	27,28,28	1.13	4 (14%)	36,40,40	2.02	9 (25%)
3	GOL	D	2002	-	5,5,5	0.38	0	5,5,5	0.41	0
3	GOL	G	3002	-	5,5,5	0.53	0	5,5,5	0.77	0
2	SAH	K	5511	-	27,28,28	1.15	4 (14%)	36,40,40	1.93	9 (25%)
3	GOL	H	4003	-	5,5,5	0.53	0	5,5,5	0.55	0
2	SAH	L	6501	-	27,28,28	1.10	4 (14%)	36,40,40	2.02	9 (25%)
2	SAH	F	3501	-	27,28,28	1.04	4 (14%)	36,40,40	2.18	10 (27%)
3	GOL	J	5003	-	5,5,5	0.44	0	5,5,5	0.40	0
3	GOL	A	1012	-	5,5,5	0.42	0	5,5,5	0.73	0
3	GOL	D	2011	-	5,5,5	0.59	0	5,5,5	0.69	0
3	GOL	H	4012	-	5,5,5	0.42	0	5,5,5	0.67	0
3	GOL	A	1001	-	5,5,5	0.73	0	5,5,5	1.08	0
3	GOL	J	5002	-	5,5,5	0.57	0	5,5,5	0.53	0
3	GOL	M	6011	-	5,5,5	0.34	0	5,5,5	0.51	0
2	SAH	I	4511	-	27,28,28	1.00	2 (7%)	36,40,40	2.09	8 (22%)
3	GOL	G	3003	-	5,5,5	0.51	0	5,5,5	0.57	0
3	GOL	J	5011	-	5,5,5	0.42	0	5,5,5	0.48	0
3	GOL	E	2012	-	5,5,5	0.44	0	5,5,5	0.42	0
2	SAH	G	3511	-	27,28,28	1.13	4 (14%)	36,40,40	1.95	8 (22%)
3	GOL	I	4002	-	5,5,5	0.77	0	5,5,5	1.26	0
2	SAH	H	4501	-	27,28,28	1.13	4 (14%)	36,40,40	2.18	11 (30%)
2	SAH	B	1511	-	27,28,28	1.16	4 (14%)	36,40,40	2.13	10 (27%)
3	GOL	G	3012	-	5,5,5	0.39	0	5,5,5	0.30	0
3	GOL	F	3001	-	5,5,5	0.37	0	5,5,5	0.52	0
2	SAH	M	6511	-	27,28,28	1.15	2 (7%)	36,40,40	1.95	10 (27%)
2	SAH	A	1501	-	27,28,28	1.09	4 (14%)	36,40,40	1.87	9 (25%)
3	GOL	B	1011	-	5,5,5	0.37	0	5,5,5	0.32	0
3	GOL	L	6002	-	5,5,5	0.46	0	5,5,5	0.18	0
3	GOL	F	3011	-	5,5,5	0.39	0	5,5,5	0.41	0
3	GOL	K	5012	-	5,5,5	0.47	0	5,5,5	0.55	0
2	SAH	J	5501	-	27,28,28	1.17	5 (18%)	36,40,40	2.10	9 (25%)
3	GOL	E	2003	-	5,5,5	0.50	0	5,5,5	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	K	5001	-	5,5,5	0.54	0	5,5,5	0.76	0
3	GOL	L	6001	-	5,5,5	0.47	0	5,5,5	0.24	0
3	GOL	I	4011	-	5,5,5	0.39	0	5,5,5	0.43	0
3	GOL	E	2001	-	5,5,5	0.68	0	5,5,5	0.66	0
3	GOL	A	1002	-	5,5,5	0.40	0	5,5,5	0.38	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
2	SAH	D	2501	-	-	1/15/31/31	0/3/3/3
2	SAH	E	2511	-	-	2/15/31/31	0/3/3/3
3	GOL	D	2002	-	-	2/4/4/4	-
3	GOL	G	3002	-	-	4/4/4/4	-
2	SAH	K	5511	-	-	2/15/31/31	0/3/3/3
3	GOL	H	4003	-	-	2/4/4/4	-
2	SAH	L	6501	-	-	0/15/31/31	0/3/3/3
2	SAH	F	3501	-	-	2/15/31/31	0/3/3/3
3	GOL	J	5003	-	-	2/4/4/4	-
3	GOL	A	1012	-	-	3/4/4/4	-
3	GOL	D	2011	-	-	2/4/4/4	-
3	GOL	H	4012	-	-	4/4/4/4	-
3	GOL	A	1001	-	-	2/4/4/4	-
3	GOL	J	5002	-	-	2/4/4/4	-
3	GOL	M	6011	-	-	2/4/4/4	-
2	SAH	I	4511	-	-	2/15/31/31	0/3/3/3
3	GOL	G	3003	-	-	4/4/4/4	-
3	GOL	J	5011	-	-	2/4/4/4	-
3	GOL	E	2012	-	-	1/4/4/4	-
2	SAH	G	3511	-	-	2/15/31/31	0/3/3/3
3	GOL	I	4002	-	-	2/4/4/4	-
2	SAH	H	4501	-	-	2/15/31/31	0/3/3/3
2	SAH	B	1511	-	-	0/15/31/31	0/3/3/3
3	GOL	G	3012	-	-	1/4/4/4	-
3	GOL	F	3001	-	-	2/4/4/4	-
2	SAH	M	6511	-	-	0/15/31/31	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAH	A	1501	-	-	2/15/31/31	0/3/3/3
3	GOL	B	1011	-	-	4/4/4/4	-
3	GOL	L	6002	-	-	2/4/4/4	-
3	GOL	F	3011	-	-	2/4/4/4	-
3	GOL	K	5012	-	-	2/4/4/4	-
2	SAH	J	5501	-	-	2/15/31/31	0/3/3/3
3	GOL	E	2003	-	-	4/4/4/4	-
3	GOL	K	5001	-	-	2/4/4/4	-
3	GOL	L	6001	-	-	2/4/4/4	-
3	GOL	I	4011	-	-	4/4/4/4	-
3	GOL	E	2001	-	-	2/4/4/4	-
3	GOL	A	1002	-	-	3/4/4/4	-

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	6511	SAH	C2-N1	2.98	1.39	1.33
2	B	1511	SAH	C2-N3	2.82	1.38	1.33
2	M	6511	SAH	C2-N3	2.82	1.38	1.33
2	B	1511	SAH	C5-N7	-2.74	1.34	1.39
2	K	5511	SAH	C5-N7	-2.69	1.34	1.39

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	5501	SAH	N3-C2-N1	-6.32	119.01	128.58
2	G	3511	SAH	N3-C2-N1	-6.30	119.05	128.58
2	M	6511	SAH	N3-C2-N1	-6.01	119.49	128.58
2	L	6501	SAH	N3-C2-N1	-5.88	119.69	128.58
2	I	4511	SAH	N3-C2-N1	-5.84	119.74	128.58

There are no chirality outliers.

5 of 81 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
2	G	3511	SAH	C3'-C4'-C5'-SD

Continued on next page...

Continued from previous page...

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

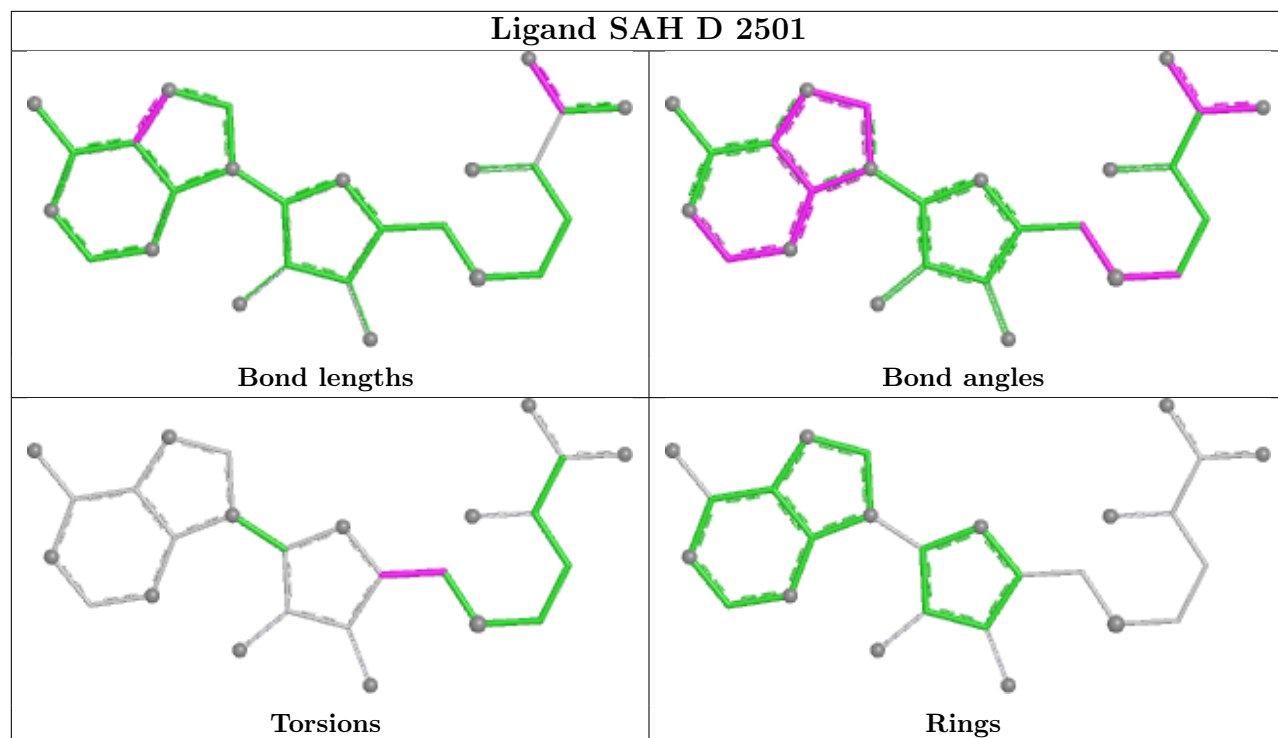
There are no ring outliers.

21 monomers are involved in 61 short contacts:

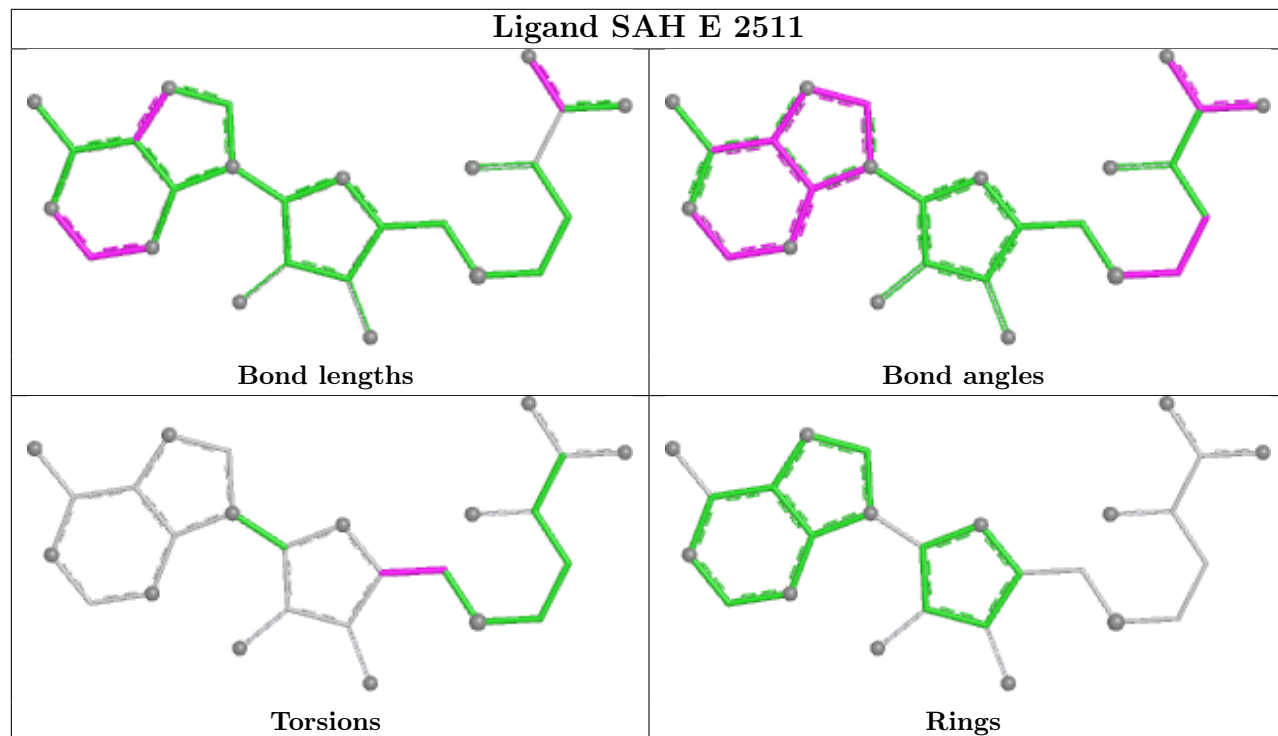
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	3002	GOL	3	0
2	K	5511	SAH	1	0
3	A	1012	GOL	2	0
3	D	2011	GOL	6	0
3	H	4012	GOL	6	0
3	A	1001	GOL	3	0
3	J	5002	GOL	2	0
3	G	3003	GOL	4	0
3	J	5011	GOL	3	0
3	E	2012	GOL	1	0
2	G	3511	SAH	3	0
3	I	4002	GOL	4	0
2	M	6511	SAH	1	0
3	L	6002	GOL	1	0
3	F	3011	GOL	2	0
3	K	5012	GOL	4	0
2	J	5501	SAH	1	0
3	E	2003	GOL	3	0
3	K	5001	GOL	5	0
3	L	6001	GOL	1	0
3	E	2001	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.

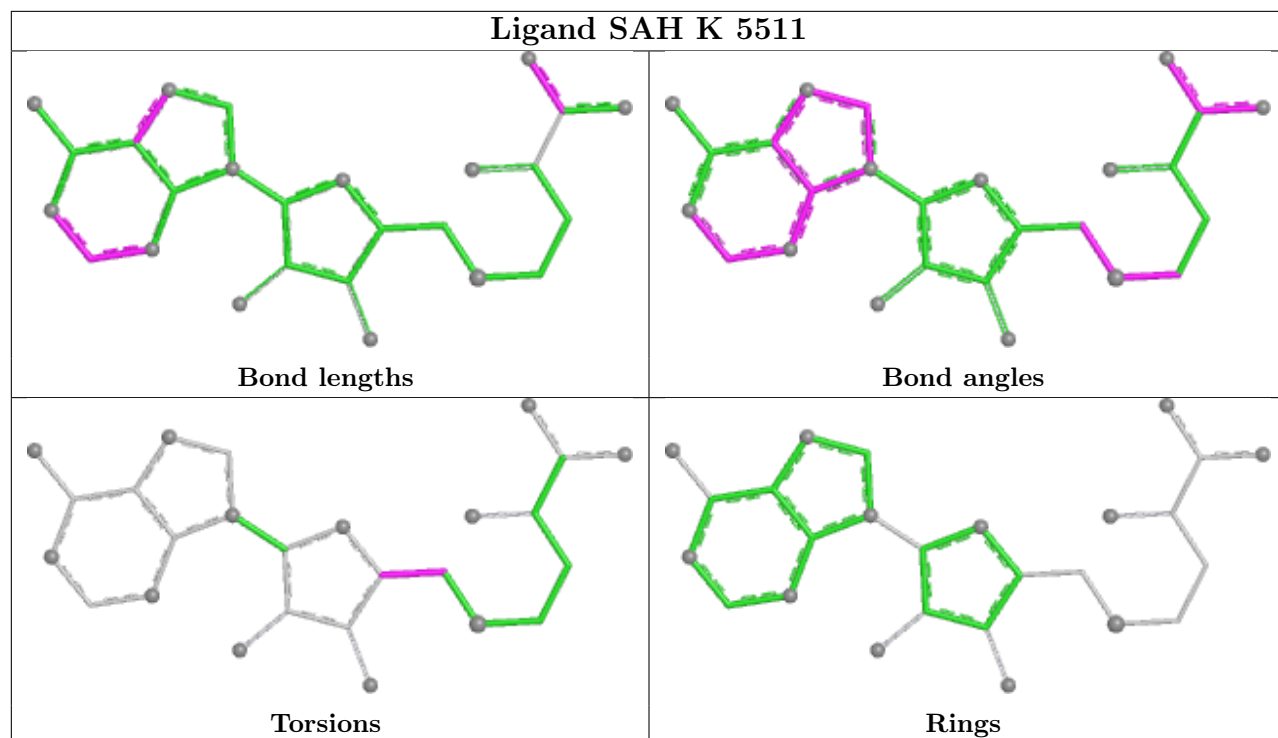
Ligand SAH D 2501



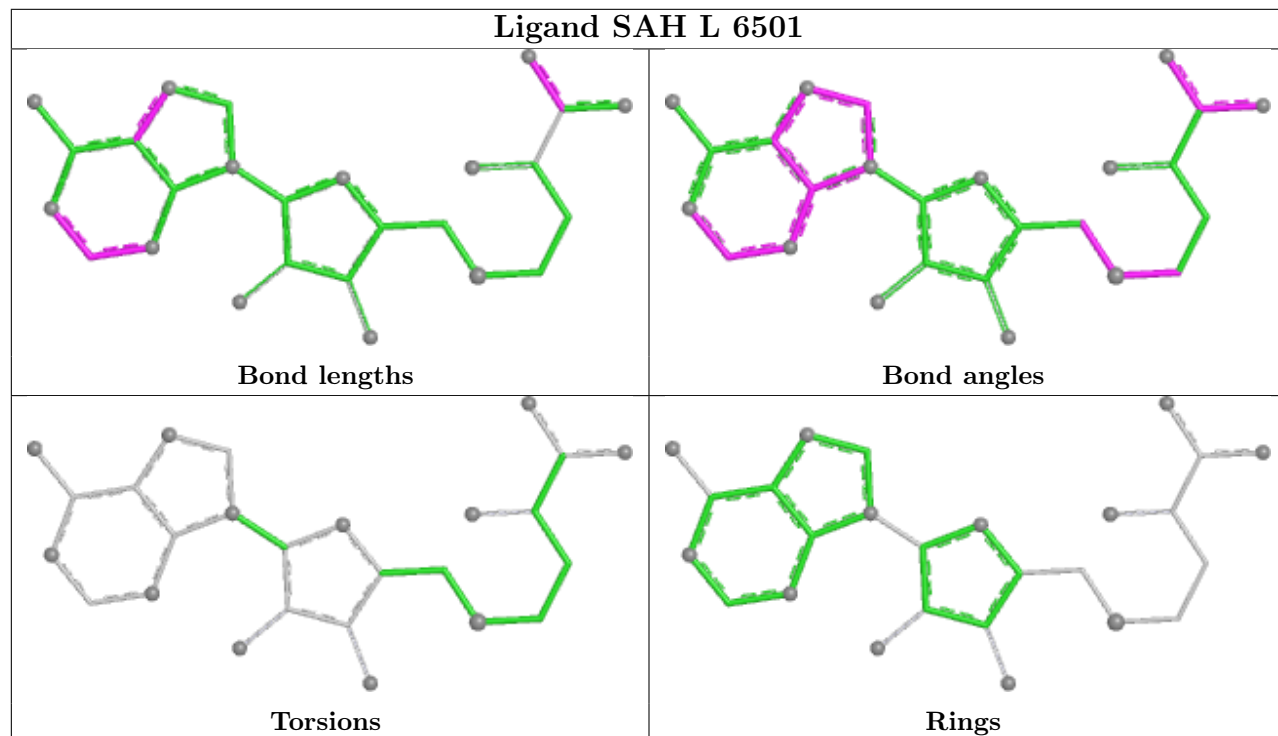
Ligand SAH E 2511

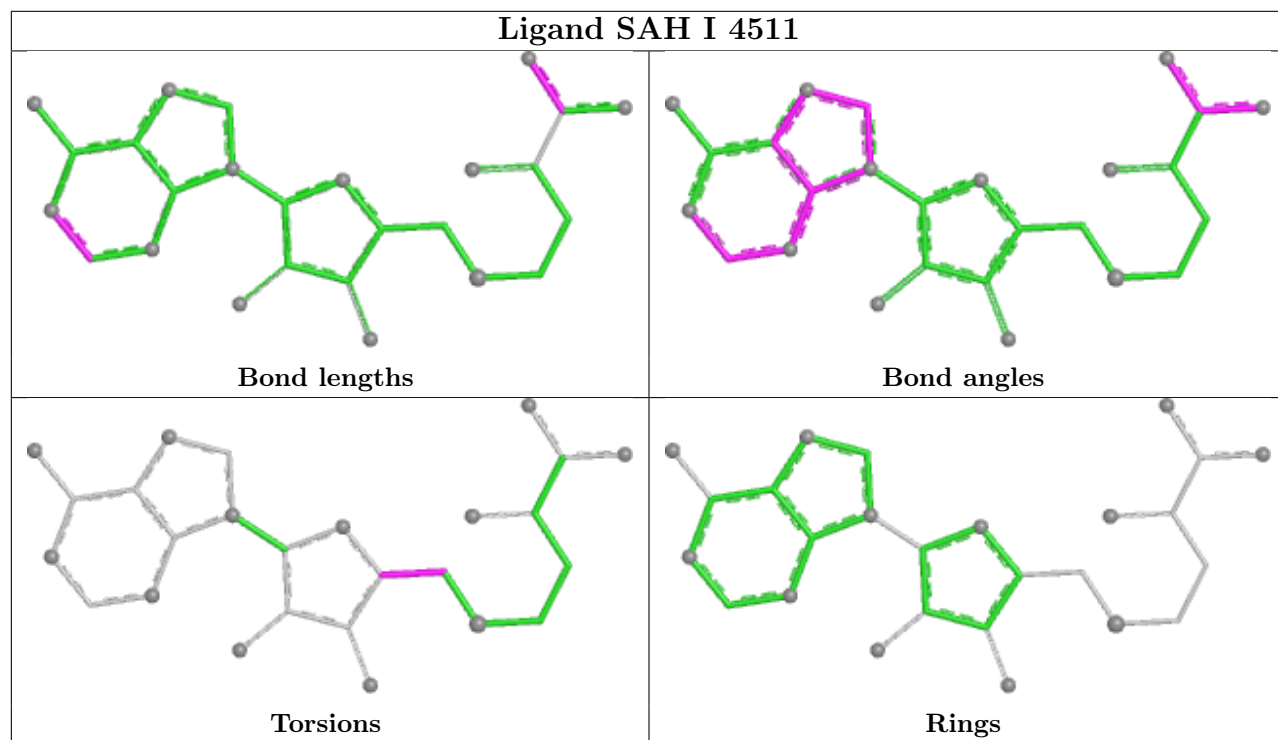
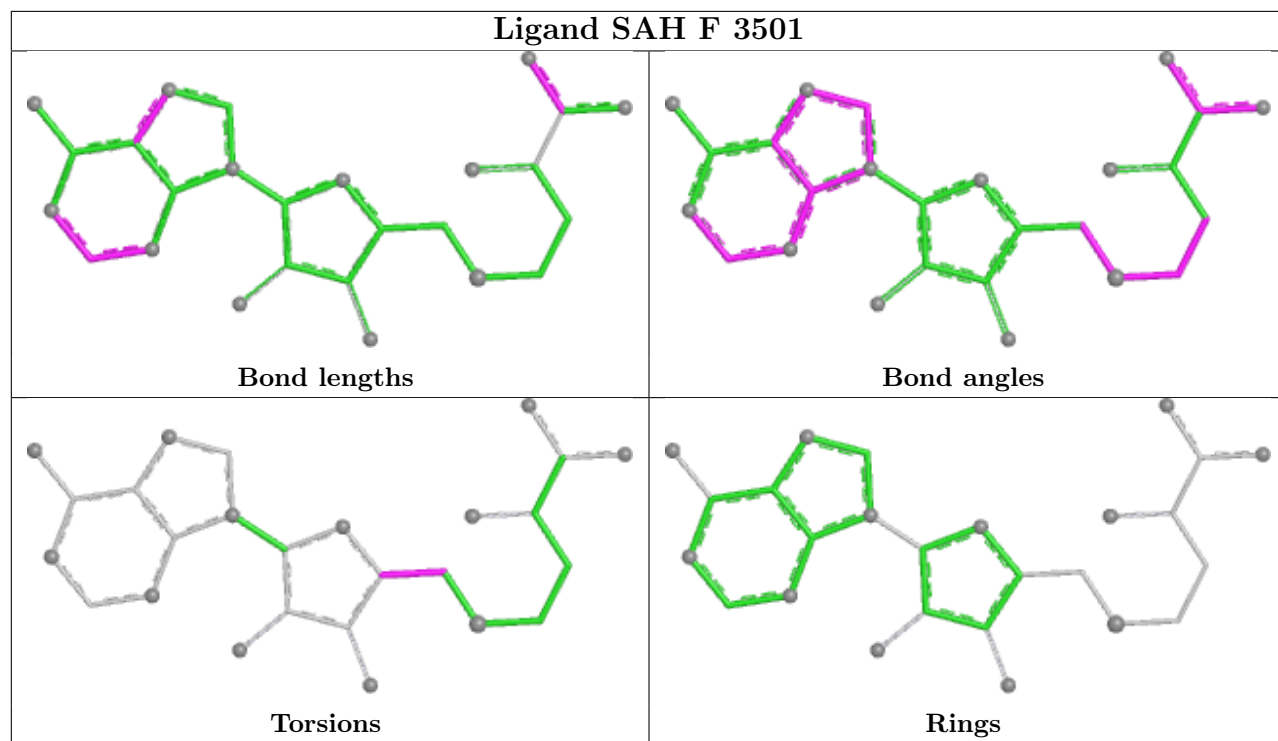


Ligand SAH K 5511

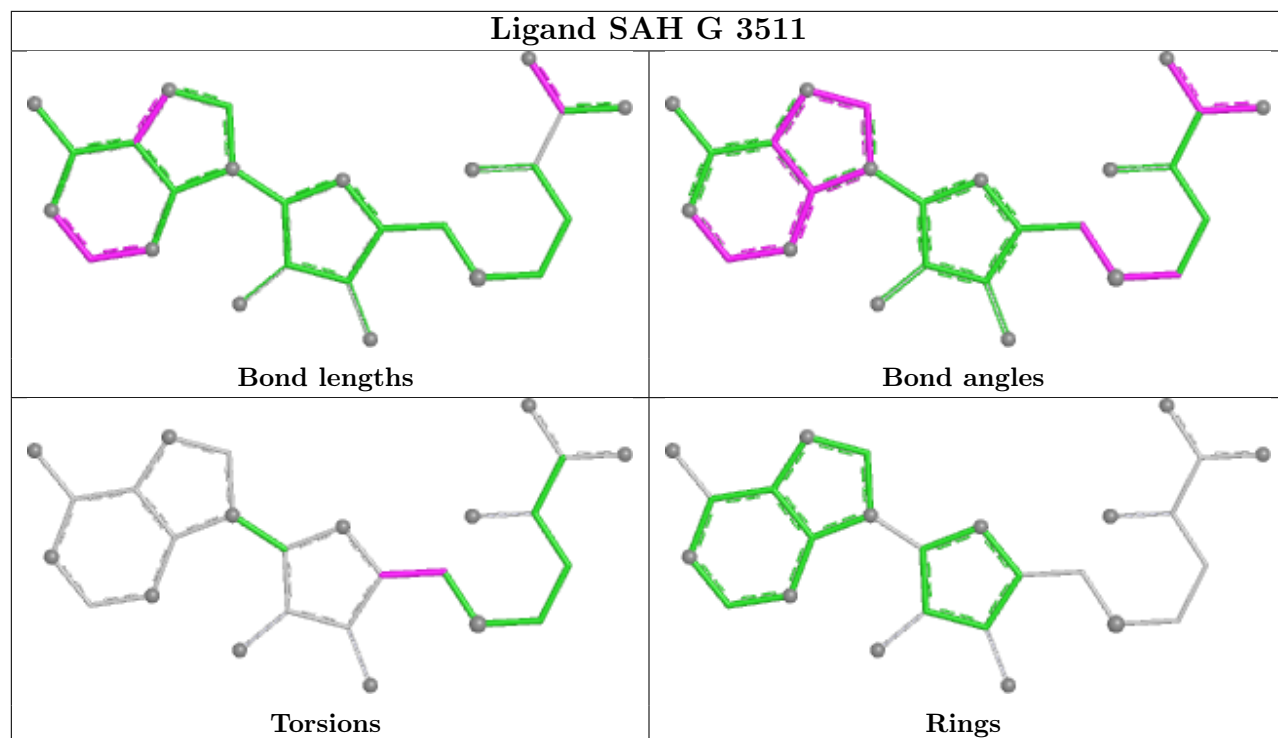


Ligand SAH L 6501

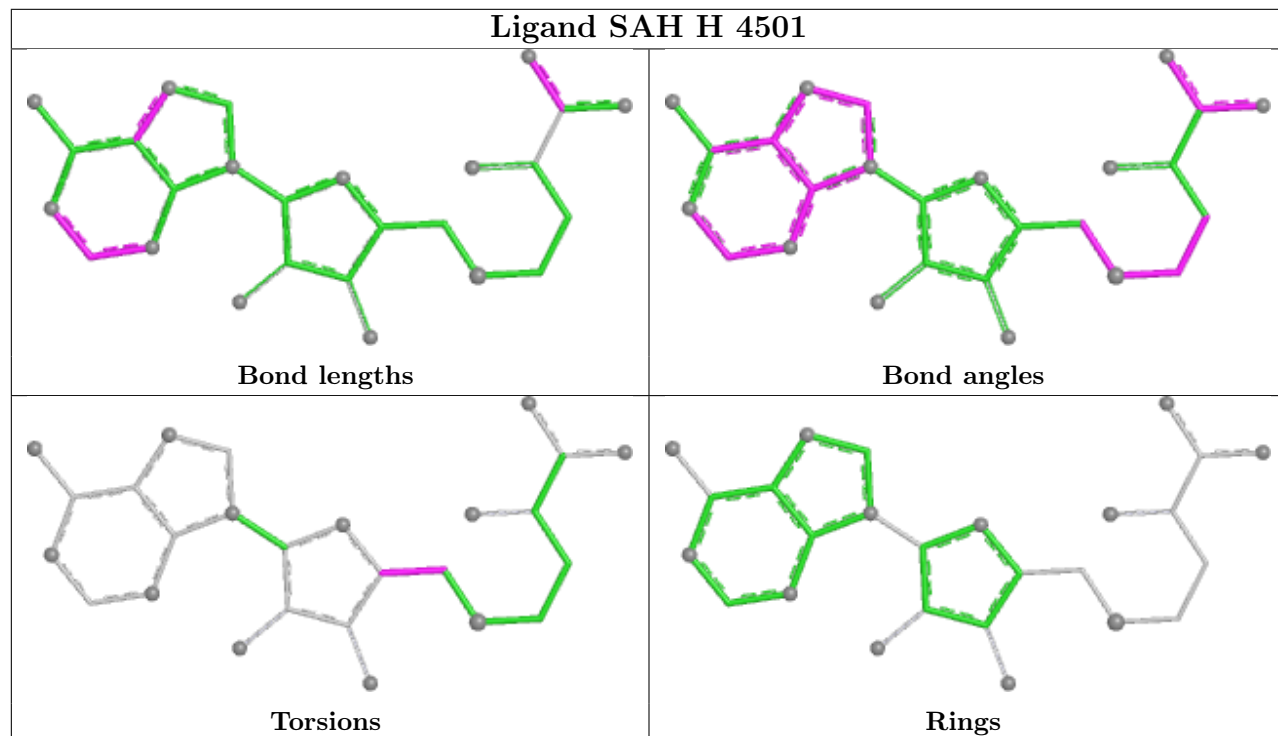


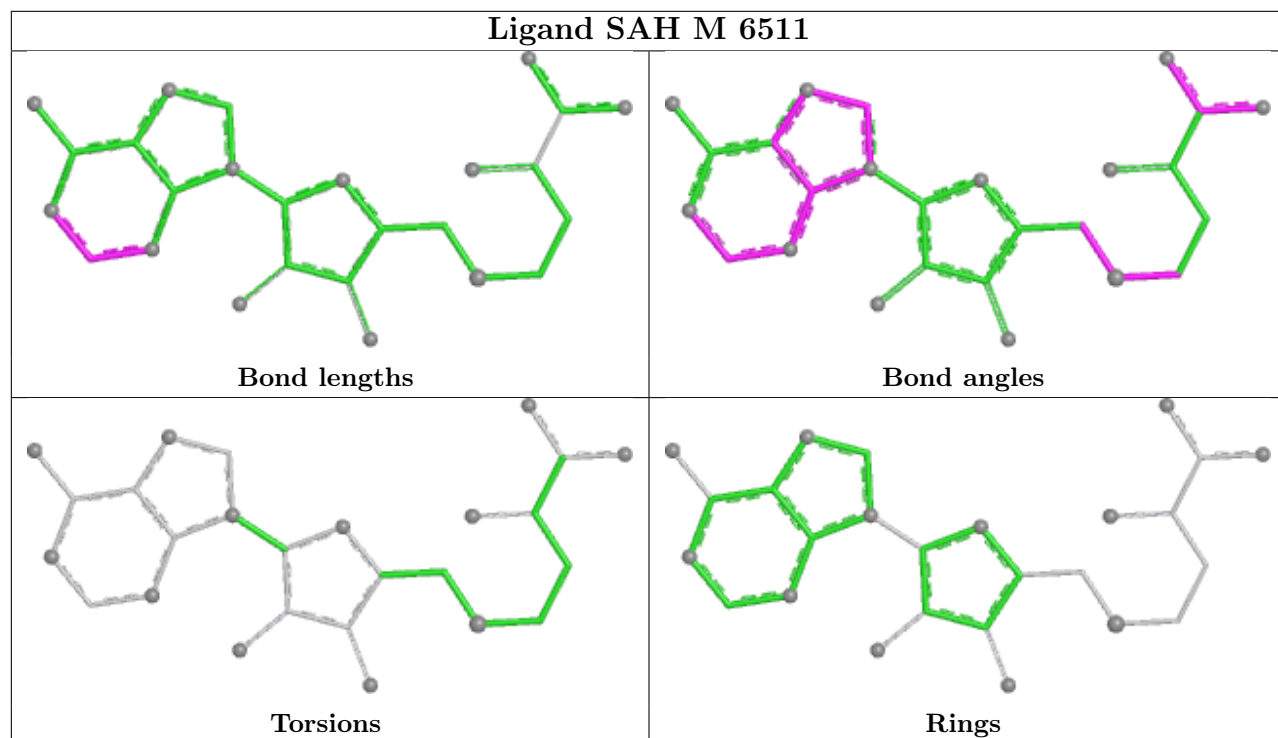
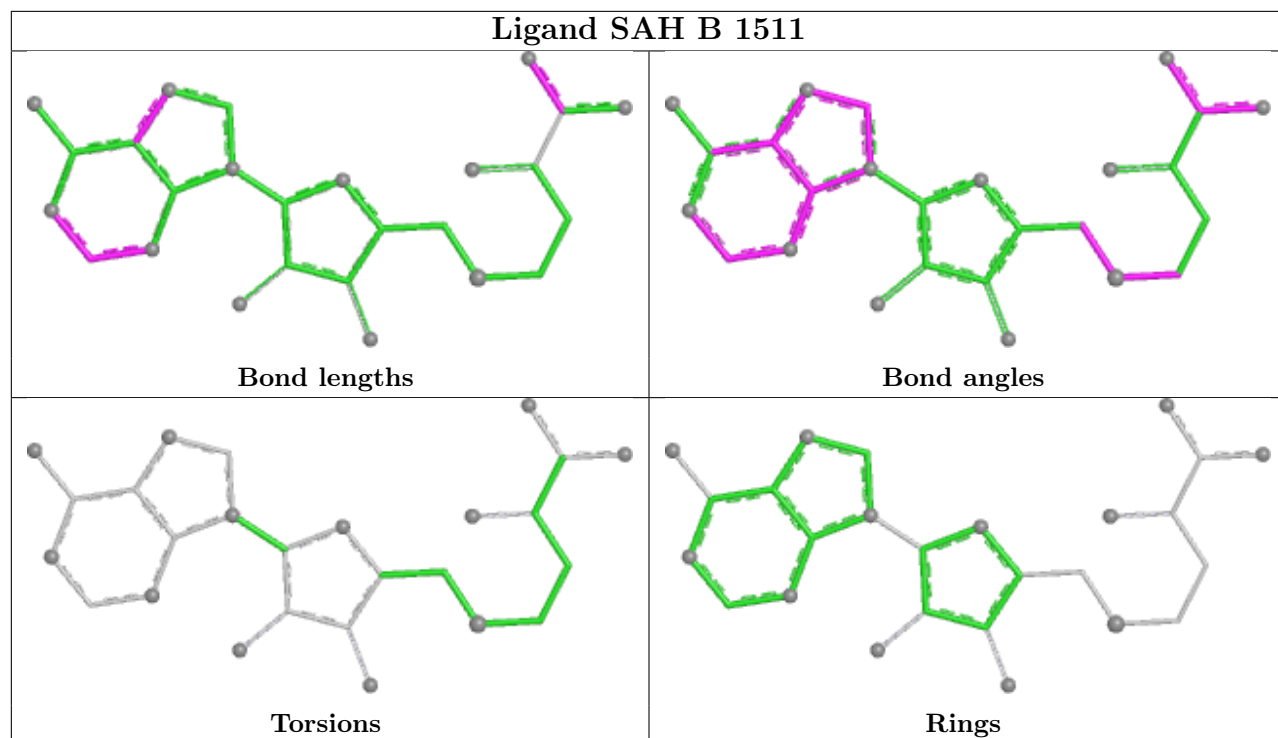


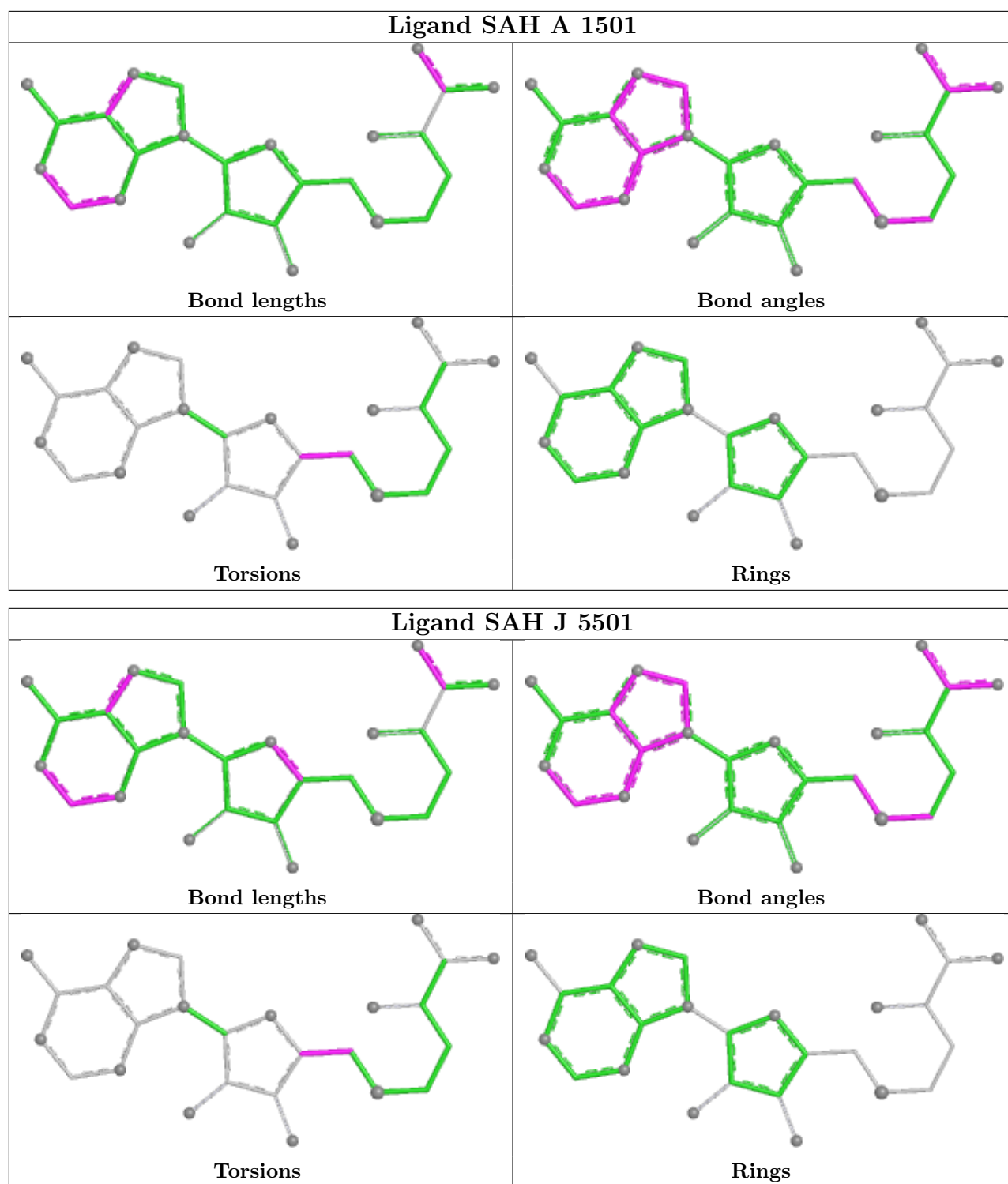
Ligand SAH G 3511



Ligand SAH H 4501







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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	256/280 (91%)	-0.06	13 (5%)	33	29	16, 23, 53, 83	1 (0%)
1	B	263/280 (93%)	-0.04	17 (6%)	25	22	14, 23, 56, 79	1 (0%)
1	D	248/280 (88%)	-0.26	4 (1%)	70	68	15, 22, 45, 69	0
1	E	265/280 (94%)	-0.05	13 (4%)	35	31	13, 23, 64, 80	0
1	F	254/280 (90%)	-0.12	10 (3%)	43	39	14, 23, 55, 63	0
1	G	258/280 (92%)	0.12	12 (4%)	36	33	14, 25, 62, 73	0
1	H	259/280 (92%)	-0.14	11 (4%)	40	37	16, 23, 53, 79	0
1	I	263/280 (93%)	-0.08	12 (4%)	37	34	12, 22, 55, 78	1 (0%)
1	J	252/280 (90%)	0.08	15 (5%)	27	24	14, 24, 54, 79	0
1	K	258/280 (92%)	0.28	16 (6%)	26	23	10, 24, 69, 88	1 (0%)
1	L	247/280 (88%)	0.63	26 (10%)	11	9	15, 25, 87, 92	0
1	M	252/280 (90%)	0.80	31 (12%)	8	7	16, 27, 85, 88	0
All	All	3075/3360 (91%)	0.09	180 (5%)	28	25	10, 24, 62, 92	4 (0%)

The worst 5 of 180 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	49	LEU	6.8
1	B	73	LYS	6.1
1	I	49	LEU	5.6
1	H	6	PHE	5.5
1	B	262	ASP	5.3

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	D	2002	6/6	0.59	0.32	77,86,87,88	0
3	GOL	M	6011	6/6	0.67	0.22	83,85,87,89	0
3	GOL	I	4011	6/6	0.69	0.38	88,91,92,93	0
3	GOL	B	1011	6/6	0.71	0.32	67,77,79,79	0
3	GOL	L	6002	6/6	0.72	0.24	91,95,96,97	0
3	GOL	H	4003	6/6	0.73	0.32	77,82,82,82	0
3	GOL	F	3001	6/6	0.73	0.31	83,90,92,93	0
3	GOL	D	2011	6/6	0.74	0.27	74,82,83,85	0
3	GOL	E	2012	6/6	0.77	0.36	89,95,96,97	0
3	GOL	A	1002	6/6	0.78	0.27	78,84,86,88	0
3	GOL	J	5011	6/6	0.79	0.29	95,95,97,98	0
3	GOL	F	3011	6/6	0.80	0.32	92,93,94,95	0
3	GOL	J	5003	6/6	0.81	0.29	78,82,86,88	0
3	GOL	A	1012	6/6	0.82	0.23	71,75,76,78	0
3	GOL	A	1001	6/6	0.82	0.21	51,57,60,61	0
3	GOL	H	4012	6/6	0.82	0.23	73,74,76,77	0
2	SAH	M	6511	26/26	0.82	0.15	67,69,71,73	0
3	GOL	K	5001	6/6	0.83	0.25	74,77,77,77	0
3	GOL	L	6001	6/6	0.83	0.26	105,106,106,106	0
3	GOL	G	3012	6/6	0.85	0.25	91,93,94,96	0
3	GOL	G	3002	6/6	0.85	0.23	78,80,81,81	0
3	GOL	J	5002	6/6	0.85	0.20	66,70,70,71	0
3	GOL	G	3003	6/6	0.86	0.22	73,76,77,77	0
3	GOL	E	2003	6/6	0.86	0.18	73,76,77,79	0
3	GOL	K	5012	6/6	0.87	0.24	94,95,96,96	0
3	GOL	E	2001	6/6	0.87	0.22	57,63,65,67	0
3	GOL	I	4002	6/6	0.88	0.18	50,53,57,57	0
2	SAH	L	6501	26/26	0.92	0.18	88,96,102,102	0
2	SAH	G	3511	26/26	0.93	0.16	60,69,78,78	0
2	SAH	A	1501	26/26	0.94	0.12	46,59,67,67	0
2	SAH	H	4501	26/26	0.94	0.12	50,56,60,62	0
2	SAH	I	4511	26/26	0.94	0.14	52,60,64,65	0

Continued on next page...

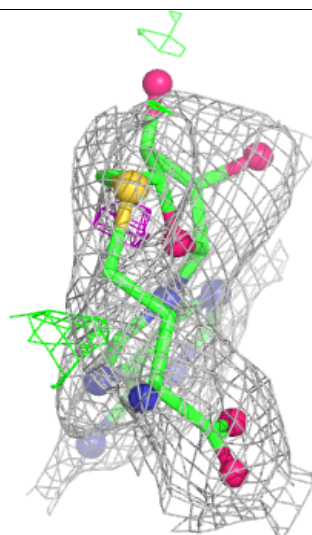
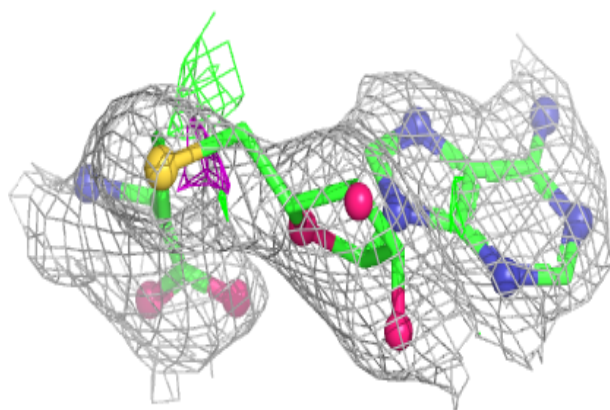
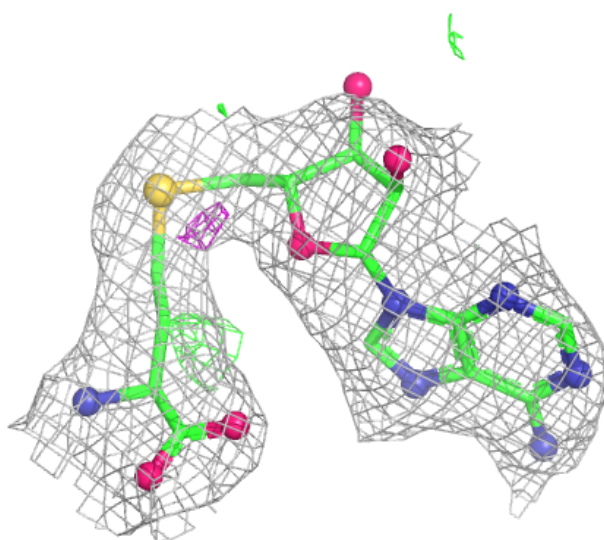
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SAH	K	5511	26/26	0.94	0.15	56,62,64,64	0
2	SAH	E	2511	26/26	0.95	0.12	51,58,59,59	0
2	SAH	F	3501	26/26	0.95	0.13	54,62,63,64	0
2	SAH	J	5501	26/26	0.95	0.14	66,68,69,70	0
2	SAH	B	1511	26/26	0.95	0.11	45,49,50,51	0
2	SAH	D	2501	26/26	0.96	0.12	55,60,64,64	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.

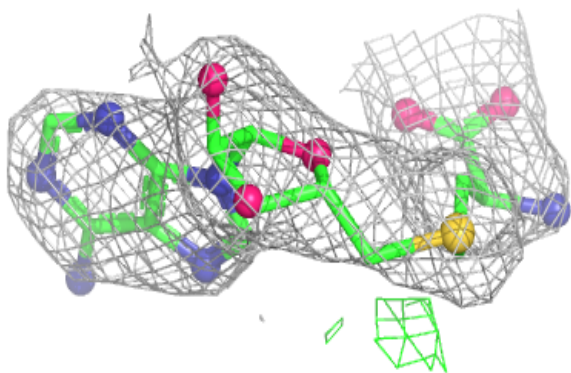
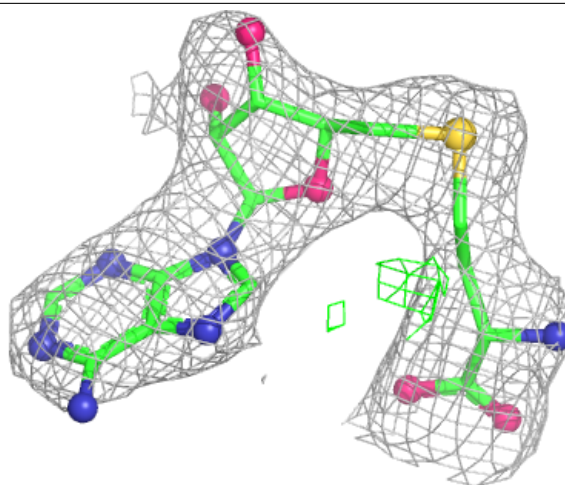
Electron density around SAH M 6511:

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



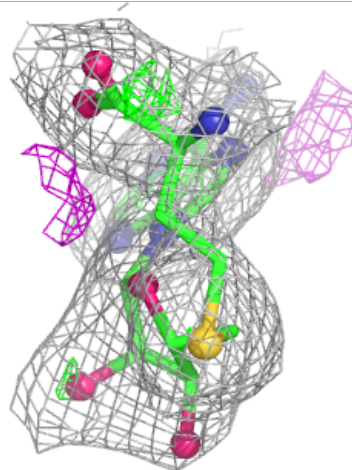
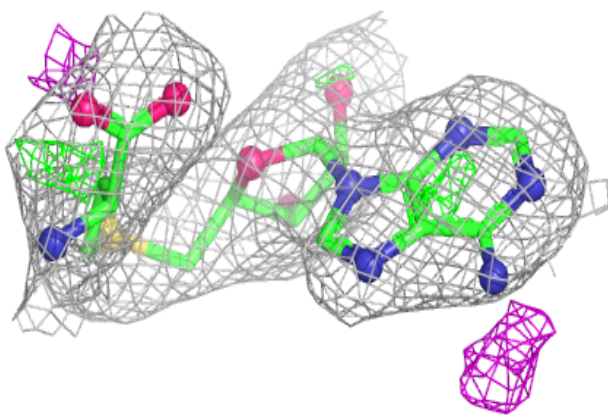
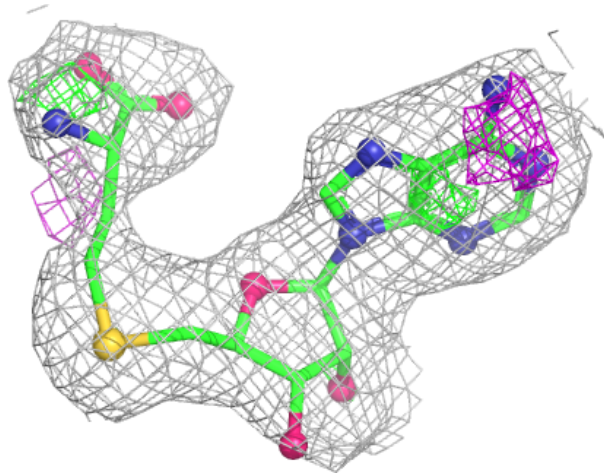
Electron density around SAH L 6501:

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



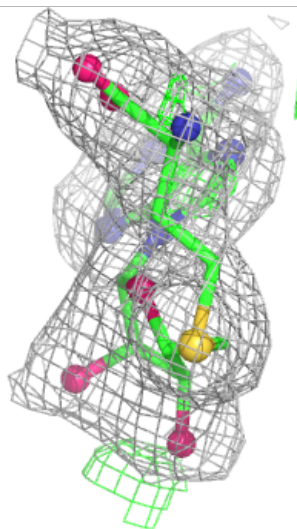
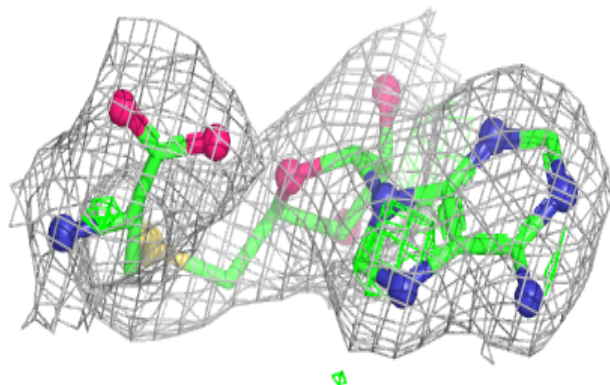
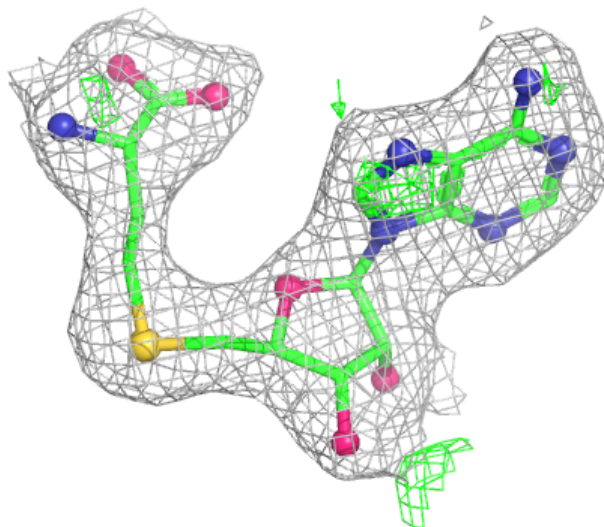
Electron density around SAH G 3511:

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



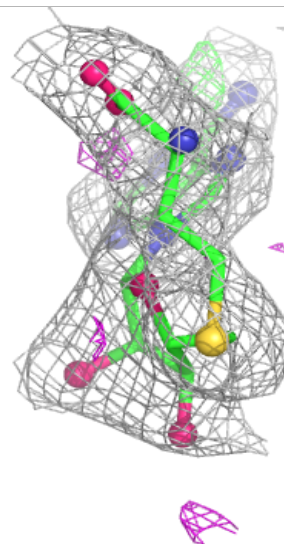
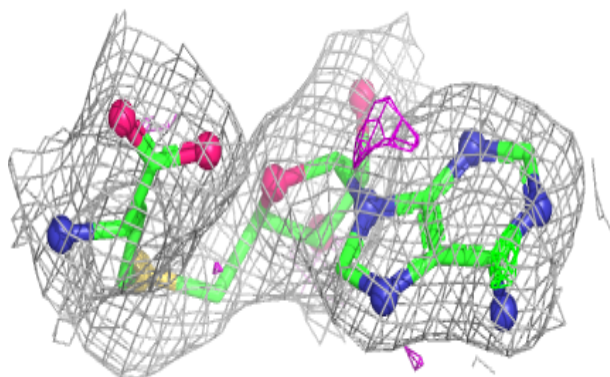
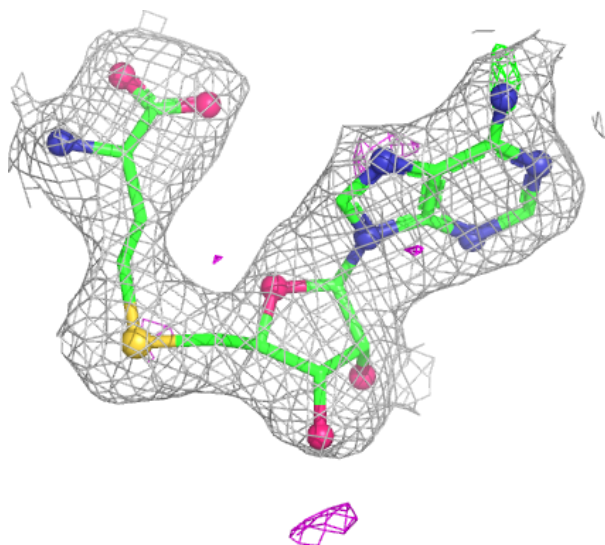
Electron density around SAH A 1501:

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



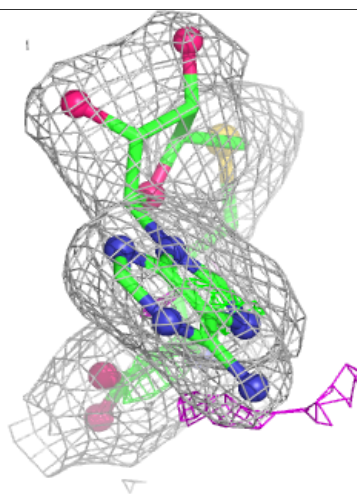
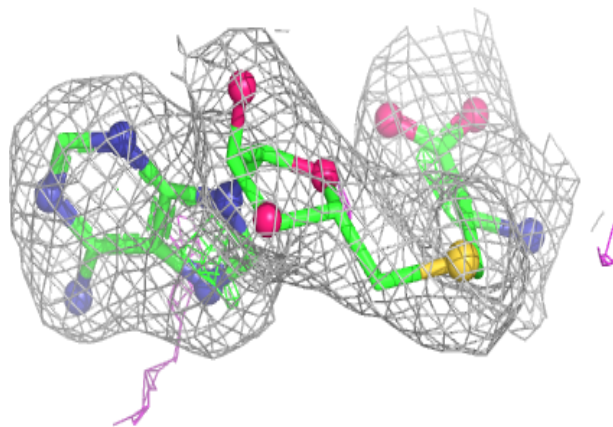
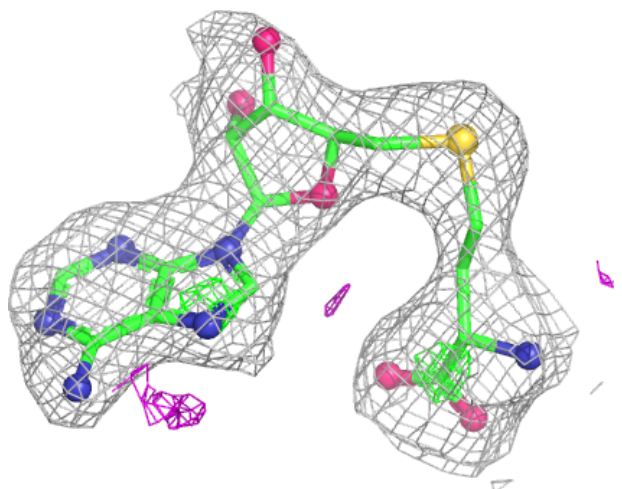
Electron density around SAH H 4501:

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



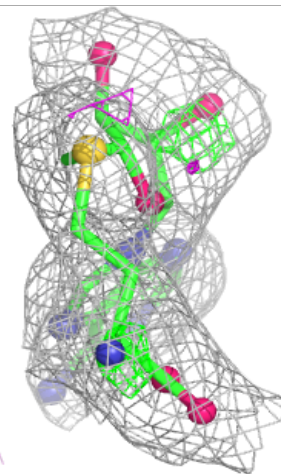
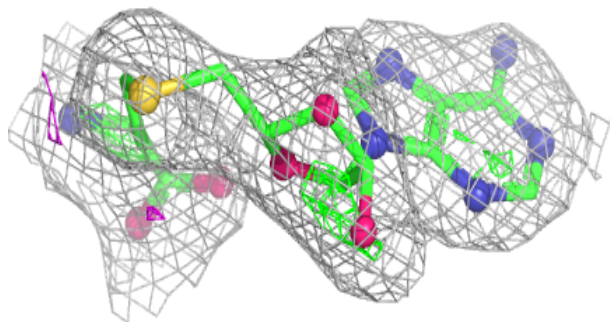
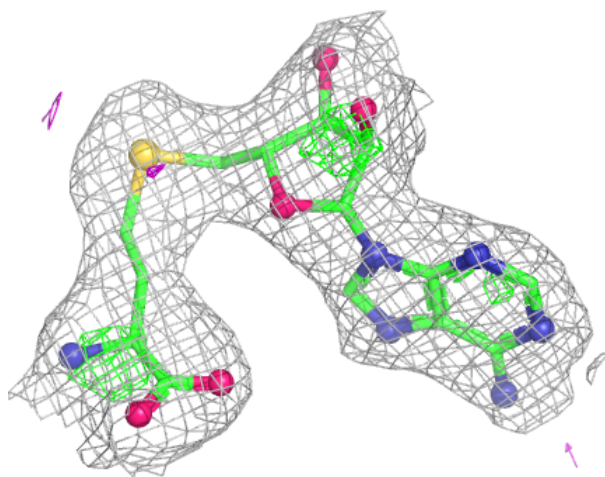
Electron density around SAH I 4511:

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



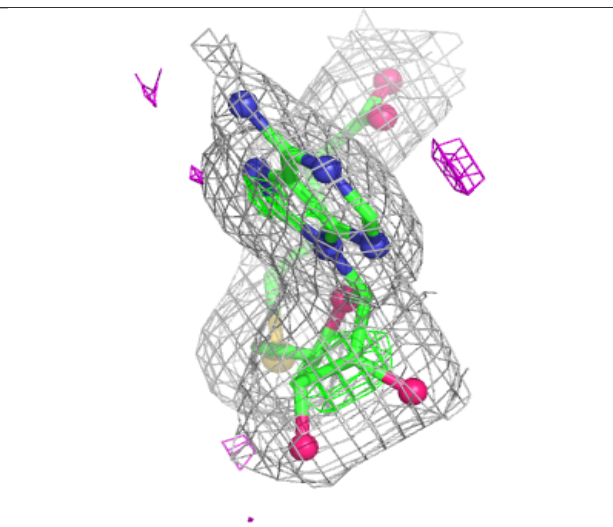
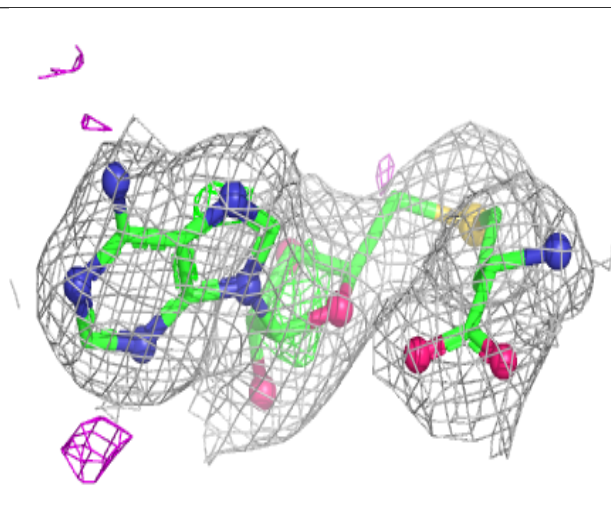
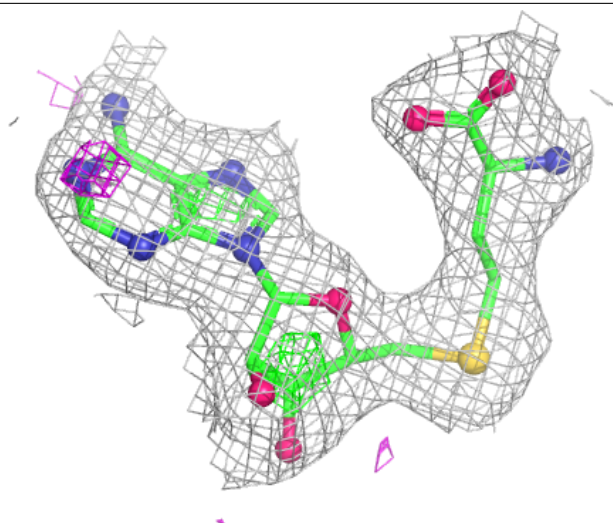
Electron density around SAH K 5511:

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



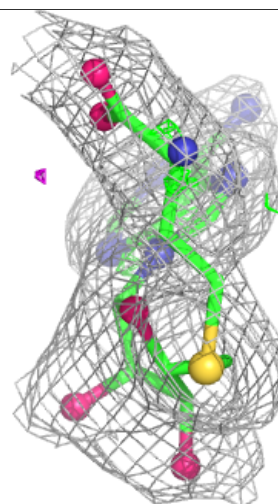
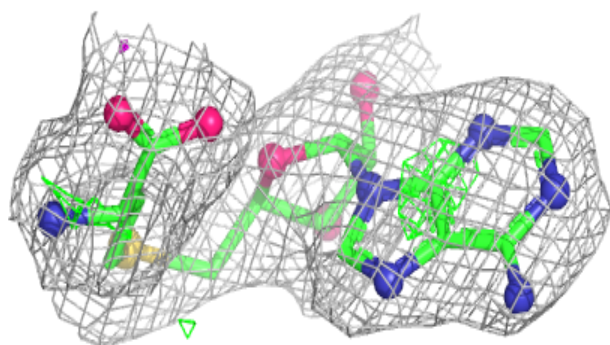
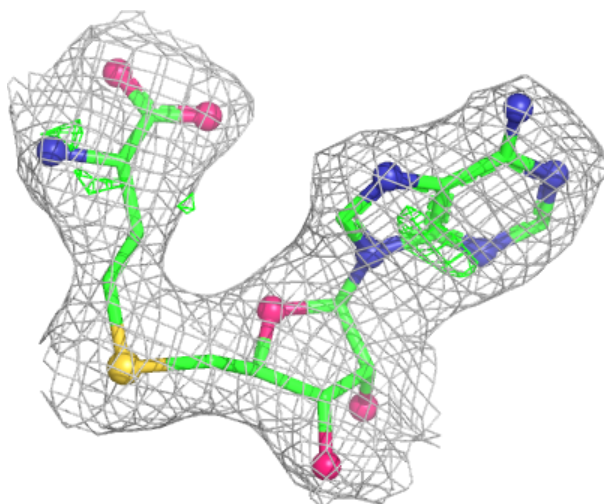
Electron density around SAH E 2511:

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



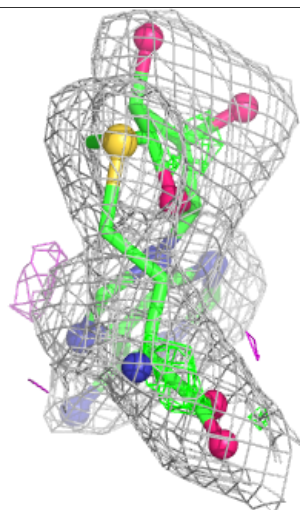
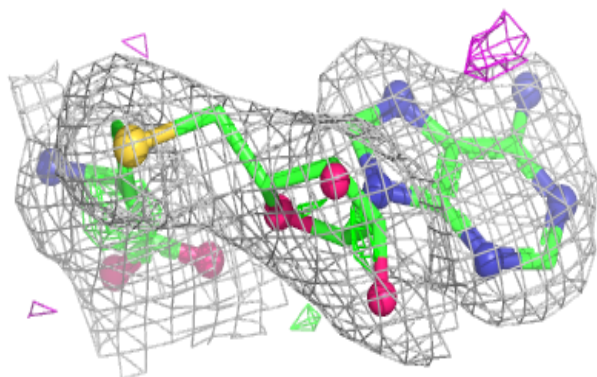
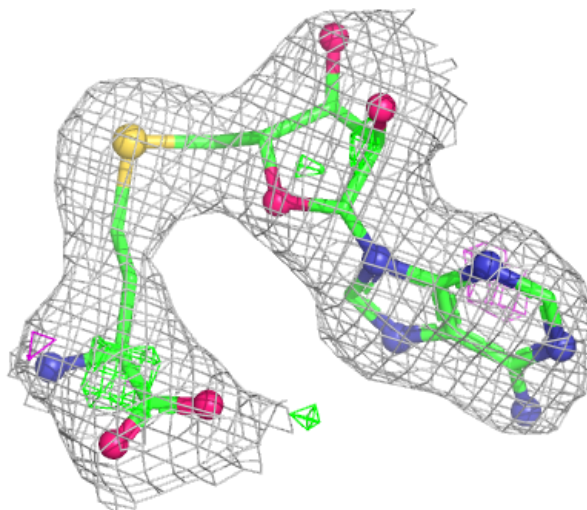
Electron density around SAH F 3501:

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



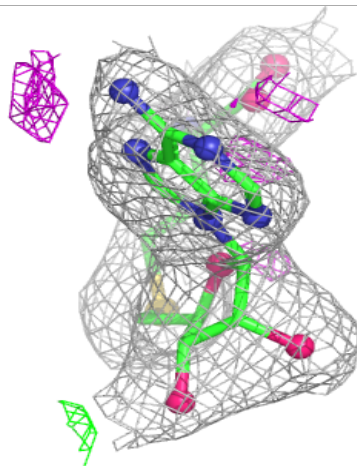
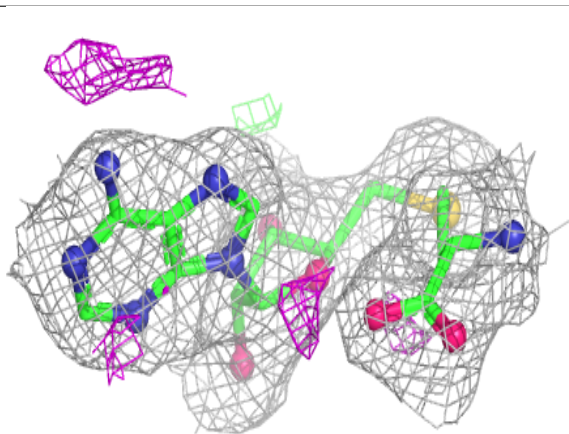
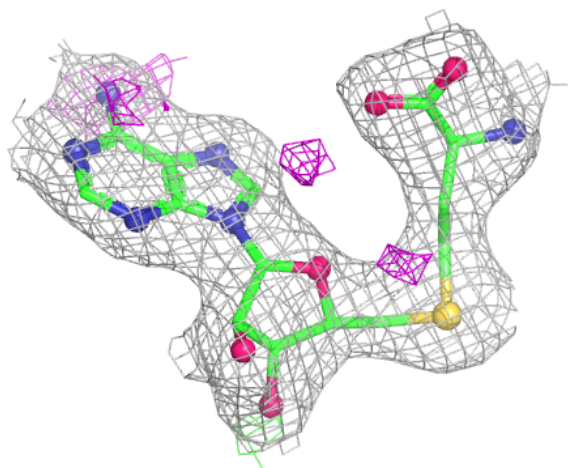
Electron density around SAH J 5501:

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



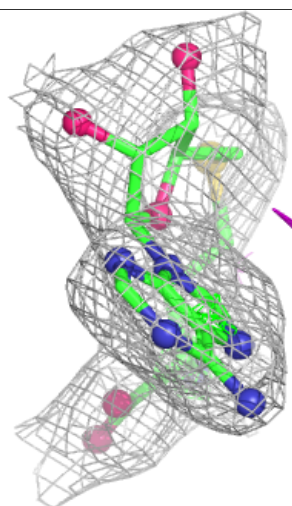
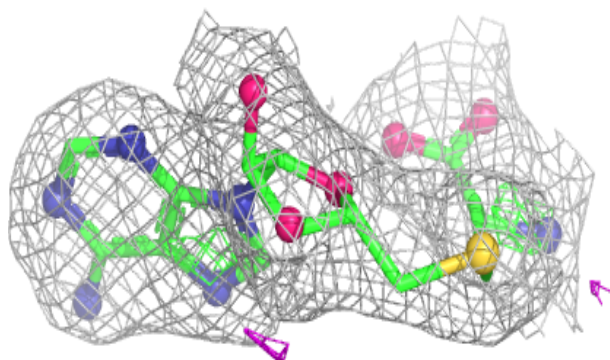
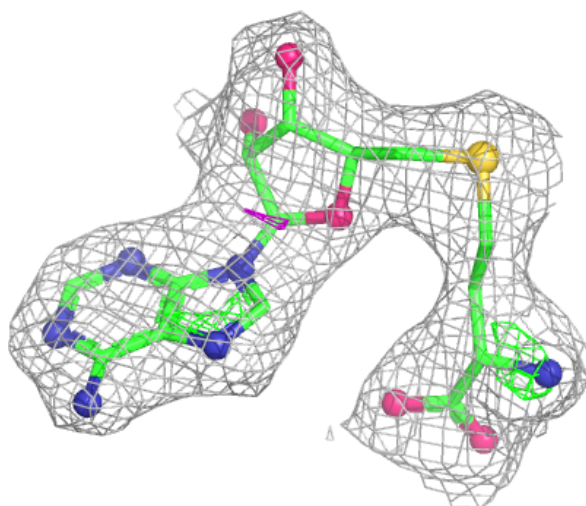
Electron density around SAH B 1511:

$2mF_o-DF_c$ (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.