Full wwPDB X-ray Structure Validation Report ⓘ

Nov 11, 2023 – 06:06 pm GMT

PDB ID	:	8BIH
Title	:	O-Methyltransferase Plu4890 in complex with SAH and AQ-284b
Authors	:	Huber, E.M.; Groll, M.
Deposited on	:	2022-11-02
Resolution	:	2.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

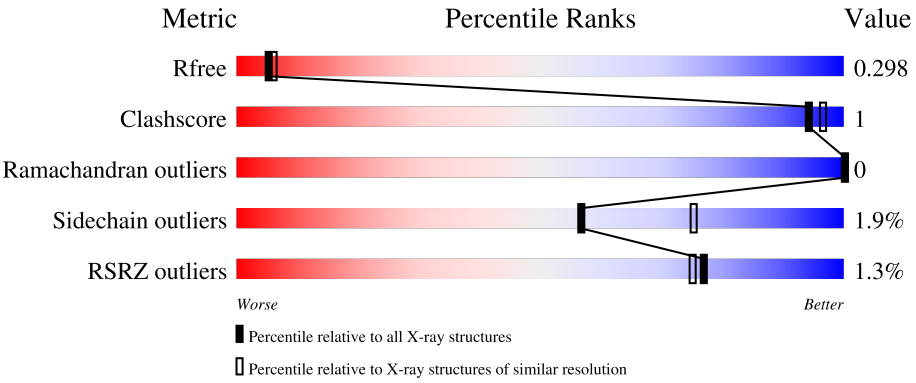
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	319	96% ·
1	B	319	2% 95% 5%
1	C	319	2% 96% ·
1	D	319	% 96% ·
1	E	319	% 95% 5%

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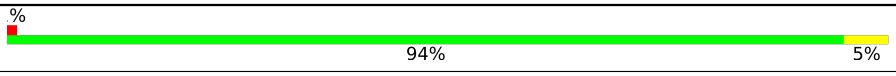
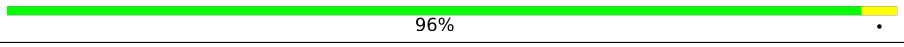
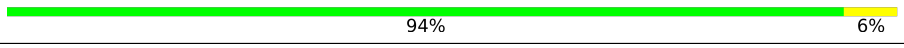
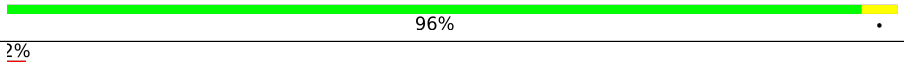
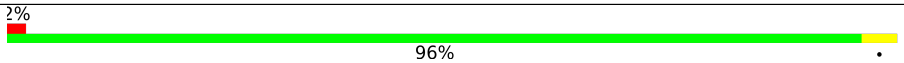
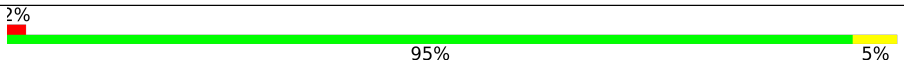
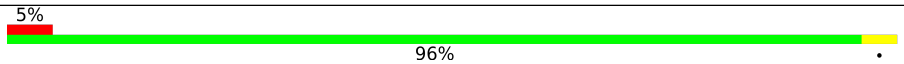
Mol	Chain	Length	Quality of chain
1	F	319	
1	G	319	
1	H	319	
1	I	319	
1	J	319	
1	K	319	
1	L	319	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 31601 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 Methyltransferase Plu4890.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2574	1650	425	487	12			
1	B	319	Total	C	N	O	S	0	0	0
			2574	1650	425	487	12			
1	C	319	Total	C	N	O	S	0	0	0
			2574	1650	425	487	12			
1	D	319	Total	C	N	O	S	0	0	0
			2574	1650	425	487	12			
1	E	319	Total	C	N	O	S	0	0	0
			2574	1650	425	487	12			
1	F	319	Total	C	N	O	S	0	0	0
			2574	1650	425	487	12			
1	G	319	Total	C	N	O	S	0	0	0
			2574	1650	425	487	12			
1	H	319	Total	C	N	O	S	0	0	0
			2574	1650	425	487	12			
1	I	319	Total	C	N	O	S	0	0	0
			2574	1650	425	487	12			
1	J	319	Total	C	N	O	S	0	0	0
			2574	1650	425	487	12			
1	K	319	Total	C	N	O	S	0	0	0
			2574	1650	425	487	12			
1	L	319	Total	C	N	O	S	0	1	0
			2585	1656	429	488	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP A0A6L9JR93
B	0	SER	-	expression tag	UNP A0A6L9JR93
C	0	SER	-	expression tag	UNP A0A6L9JR93
D	0	SER	-	expression tag	UNP A0A6L9JR93
E	0	SER	-	expression tag	UNP A0A6L9JR93

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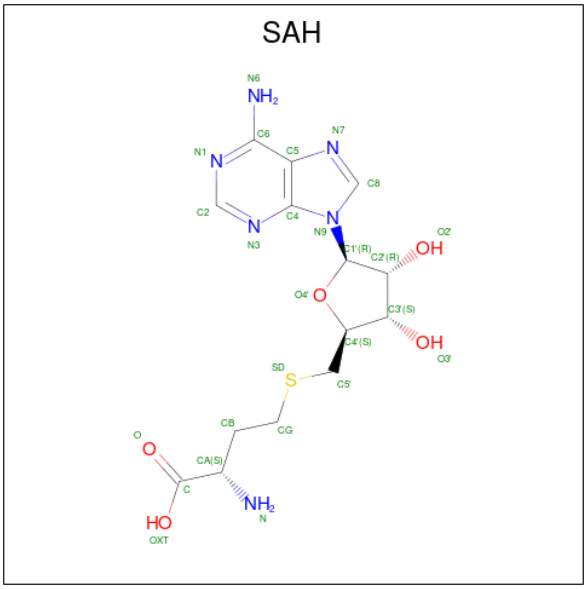
Chain	Residue	Modelled	Actual	Comment	Reference
F	0	SER	-	expression tag	UNP A0A6L9JR93
G	0	SER	-	expression tag	UNP A0A6L9JR93
H	0	SER	-	expression tag	UNP A0A6L9JR93
I	0	SER	-	expression tag	UNP A0A6L9JR93
J	0	SER	-	expression tag	UNP A0A6L9JR93
K	0	SER	-	expression tag	UNP A0A6L9JR93
L	0	SER	-	expression tag	UNP A0A6L9JR93

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



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	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		

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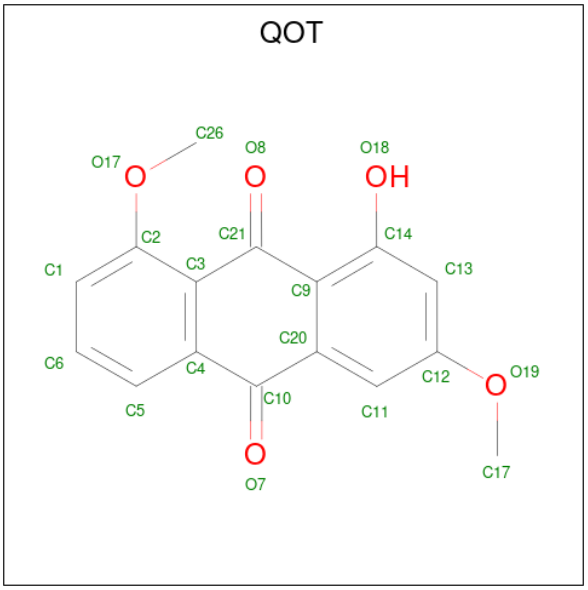
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total C N O S 26 14 6 5 1	0	0
2	I	1	Total C N O S 26 14 6 5 1	0	0
2	J	1	Total C N O S 26 14 6 5 1	0	0
2	K	1	Total C N O S 26 14 6 5 1	0	0
2	L	1	Total C N O S 26 14 6 5 1	0	0

- Molecule 3 is 3,8-dimethoxy-1-oxidanyl-anthracene-9,10-dione (three-letter code: QOT) (formula: $C_{16}H_{12}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 21 16 5	0	0
3	B	1	Total C O 21 16 5	0	0
3	C	1	Total C O 21 16 5	0	0
3	D	1	Total C O 21 16 5	0	0
3	E	1	Total C O 21 16 5	0	0
3	F	1	Total C O 21 16 5	0	0

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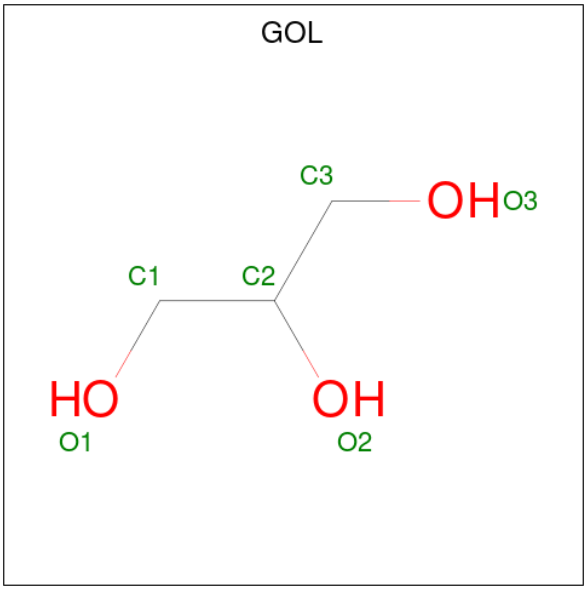
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total C O 21 16 5	0	0
3	H	1	Total C O 21 16 5	0	0
3	I	1	Total C O 21 16 5	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	C	3	Total Cl 3 3	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total Na 1 1	0	0
6	K	1	Total Na 1 1	0	0

- Molecule 7 is water.

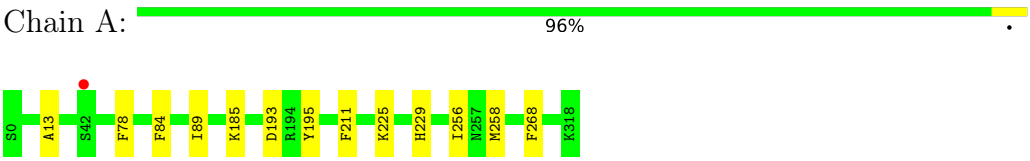
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	20	Total O 20 20	0	0
7	B	9	Total O 9 9	0	0
7	C	12	Total O 12 12	0	0
7	D	27	Total O 27 27	0	0
7	E	14	Total O 14 14	0	0
7	F	11	Total O 11 11	0	0
7	G	15	Total O 15 15	0	0
7	H	15	Total O 15 15	0	0
7	I	24	Total O 24 24	0	0
7	J	16	Total O 16 16	0	0
7	K	12	Total O 12 12	0	0
7	L	8	Total O 8 8	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.

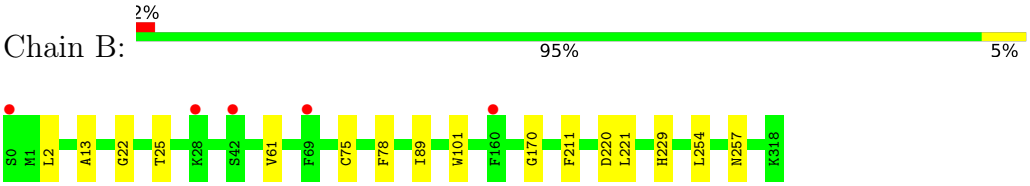
• Molecule 1: Methyltransferase Plu4890

Chain A:



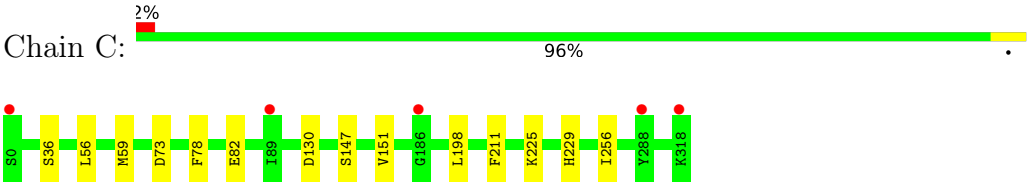
• Molecule 1: Methyltransferase Plu4890

Chain B:



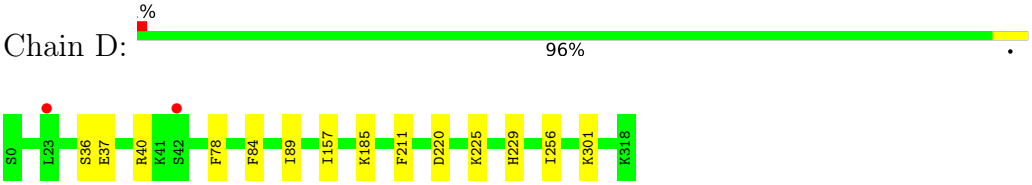
• Molecule 1: Methyltransferase Plu4890

Chain C:



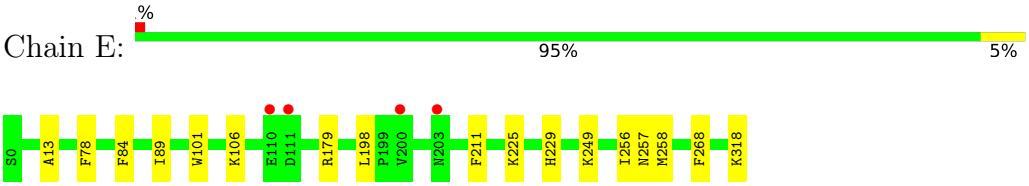
• Molecule 1: Methyltransferase Plu4890

Chain D:



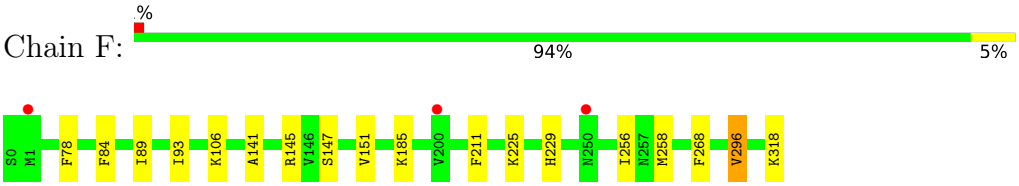
• Molecule 1: Methyltransferase Plu4890

Chain E:



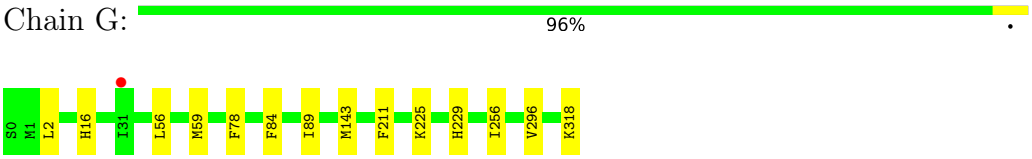
• Molecule 1: Methyltransferase Plu4890

Chain F:



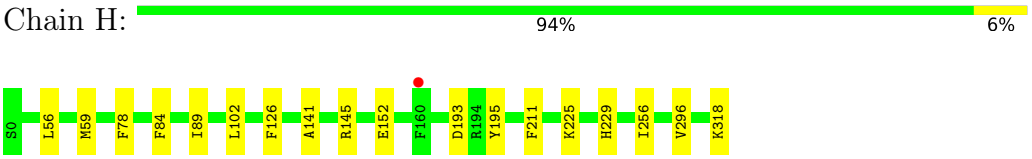
• Molecule 1: Methyltransferase Plu4890

Chain G:



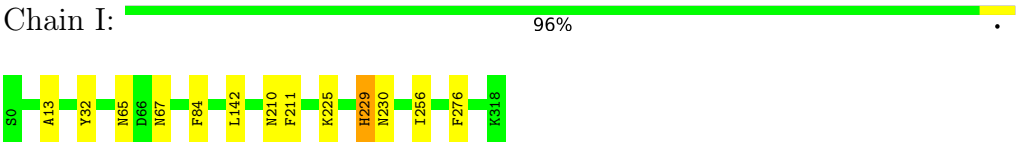
• Molecule 1: Methyltransferase Plu4890

Chain H:



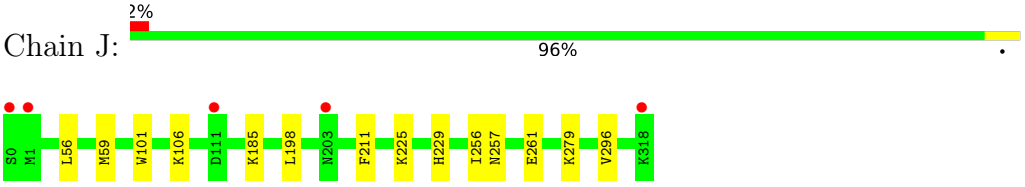
• Molecule 1: Methyltransferase Plu4890

Chain I:



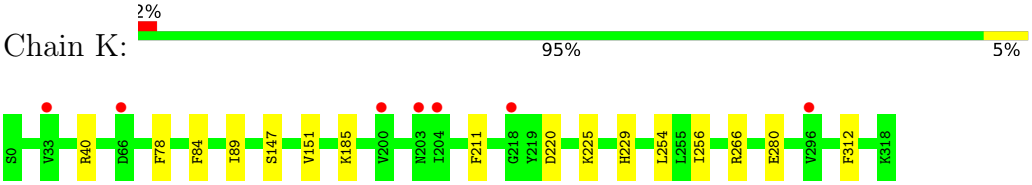
• Molecule 1: Methyltransferase Plu4890

Chain J:



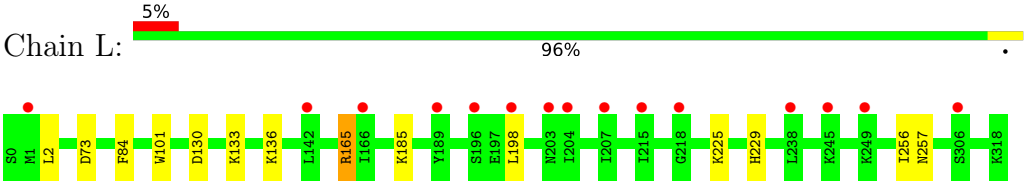
• Molecule 1: Methyltransferase Plu4890

Chain K:



• Molecule 1: Methyltransferase Plu4890

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	91.00Å 91.13Å 150.41Å 89.96° 106.18° 119.97°	Depositor
Resolution (Å)	30.00 – 2.40 48.67 – 2.40	Depositor EDS
% Data completeness (in resolution range)	92.4 (30.00-2.40) 92.5 (48.67-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.267 , 0.296 0.271 , 0.298	Depositor DCC
R_{free} test set	7166 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	41.6	Xtriage
Anisotropy	0.666	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 19.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.139 for k,-h-k,h+l 0.139 for -h-k,h,h+k+l 0.047 for h,-h-k,-h-l 0.038 for k,h,-h-k-l 0.044 for -h-k,k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	31601	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.20% 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: SAH, CL, GOL, QOT, NA

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	0.66	0/2628	0.70	0/3538
1	B	0.66	0/2628	0.69	0/3538
1	C	0.67	0/2628	0.69	0/3538
1	D	0.66	0/2628	0.69	0/3538
1	E	0.66	0/2628	0.69	0/3538
1	F	0.67	0/2628	0.69	0/3538
1	G	0.66	0/2628	0.69	0/3538
1	H	0.66	0/2628	0.69	0/3538
1	I	0.66	0/2628	0.69	0/3538
1	J	0.67	0/2628	0.69	0/3538
1	K	0.66	0/2628	0.69	0/3538
1	L	0.66	0/2639	0.69	0/3552
All	All	0.66	0/31547	0.69	0/42470

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2574	0	2531	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2574	0	2531	8	0
1	C	2574	0	2531	6	0
1	D	2574	0	2531	5	0
1	E	2574	0	2531	8	0
1	F	2574	0	2531	7	0
1	G	2574	0	2531	7	0
1	H	2574	0	2531	9	0
1	I	2574	0	2531	7	0
1	J	2574	0	2531	4	0
1	K	2574	0	2530	5	0
1	L	2585	0	2543	18	0
2	A	26	0	19	0	0
2	B	26	0	19	1	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	0	0
2	H	26	0	19	1	0
2	I	26	0	19	1	0
2	J	26	0	19	0	0
2	K	26	0	19	0	0
2	L	26	0	19	0	0
3	A	21	0	0	0	0
3	B	21	0	0	0	0
3	C	21	0	0	1	0
3	D	21	0	0	0	0
3	E	21	0	0	0	0
3	F	21	0	0	0	0
3	G	21	0	0	1	0
3	H	21	0	0	1	0
3	I	21	0	0	3	0
4	A	1	0	0	1	0
4	C	3	0	0	0	0
5	C	6	0	8	0	0
5	D	6	0	8	0	0
6	H	1	0	0	0	0
6	K	1	0	0	0	0
7	A	20	0	0	0	0
7	B	9	0	0	0	0
7	C	12	0	0	0	0
7	D	27	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	14	0	0	1	0
7	F	11	0	0	0	0
7	G	15	0	0	0	0
7	H	15	0	0	0	0
7	I	24	0	0	0	0
7	J	16	0	0	0	0
7	K	12	0	0	0	0
7	L	8	0	0	0	0
All	All	31601	0	30627	83	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 1.

All (83) 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:L:165[A]:ARG:HH21	1:L:165[A]:ARG:HG3	1.11	1.15
1:L:165[B]:ARG:HH21	1:L:165[B]:ARG:HG2	1.07	1.12
1:L:165[A]:ARG:HH21	1:L:165[A]:ARG:CG	1.70	1.03
1:L:165[B]:ARG:HH21	1:L:165[B]:ARG:CG	1.75	0.98
1:L:165[B]:ARG:HG2	1:L:165[B]:ARG:NH2	1.90	0.80
1:L:165[A]:ARG:HG3	1:L:165[A]:ARG:NH2	1.91	0.75
1:L:165[A]:ARG:NH2	1:L:165[A]:ARG:HB2	2.02	0.74
1:C:225:LYS:HA	1:C:256:ILE:O	1.93	0.69
1:L:165[A]:ARG:HH21	1:L:165[A]:ARG:CB	2.06	0.69
1:L:165[A]:ARG:CG	1:L:165[A]:ARG:NH2	2.41	0.68
1:L:165[A]:ARG:NH2	1:L:165[A]:ARG:CB	2.59	0.66
1:A:225:LYS:HA	1:A:256:ILE:O	1.97	0.63
1:L:165[B]:ARG:NH2	1:L:165[B]:ARG:HB3	2.15	0.61
1:L:165[B]:ARG:CG	1:L:165[B]:ARG:NH2	2.44	0.60
1:F:78:PHE:CE1	1:F:89:ILE:HD11	2.38	0.59
1:G:78:PHE:CE1	1:G:89:ILE:HD11	2.40	0.56
1:I:13:ALA:HB1	1:J:101:TRP:CE3	2.40	0.56
1:D:225:LYS:HA	1:D:256:ILE:O	2.06	0.55
1:L:165[B]:ARG:NH2	1:L:165[B]:ARG:CB	2.70	0.55
1:H:225:LYS:HA	1:H:256:ILE:O	2.06	0.55
1:J:106:LYS:NZ	1:L:130:ASP:O	2.39	0.55
1:E:78:PHE:CE1	1:E:89:ILE:HD11	2.42	0.54
1:I:210:ASN:OD1	2:I:401:SAH:N6	2.41	0.54
1:D:37:GLU:HA	1:D:40:ARG:HD2	1.89	0.53
1:H:296:VAL:HG13	1:H:318:LYS:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:225:LYS:HA	1:J:256:ILE:O	2.08	0.52
1:D:78:PHE:CE1	1:D:89:ILE:HD11	2.45	0.51
1:L:225:LYS:HA	1:L:256:ILE:O	2.11	0.51
1:A:78:PHE:CE1	1:A:89:ILE:HD11	2.45	0.51
1:B:13:ALA:HB1	1:E:101:TRP:CE3	2.45	0.51
1:G:143:MET:SD	3:G:402:QOT:C26	2.99	0.51
1:B:2:LEU:HD11	1:E:78:PHE:CZ	2.46	0.50
1:C:130:ASP:O	1:E:106:LYS:NZ	2.39	0.50
1:B:22:GLY:O	1:B:25:THR:OG1	2.27	0.50
1:G:225:LYS:HA	1:G:256:ILE:O	2.12	0.49
1:J:56:LEU:HA	1:J:59:MET:HE3	1.96	0.48
1:H:78:PHE:CE1	1:H:89:ILE:HD11	2.48	0.47
1:K:254:LEU:HD22	1:K:312:PHE:CZ	2.50	0.47
1:F:141:ALA:O	1:F:145:ARG:HG2	2.14	0.46
1:F:296:VAL:HG13	1:F:318:LYS:HG2	1.97	0.46
1:E:225:LYS:HA	1:E:256:ILE:O	2.16	0.46
1:E:258:MET:HE1	1:E:268:PHE:CZ	2.50	0.46
1:I:32:TYR:CE1	1:I:65:ASN:HB2	2.51	0.46
1:B:78:PHE:CE1	1:B:89:ILE:HD11	2.51	0.46
1:B:221:LEU:HD11	1:B:254:LEU:HG	1.98	0.46
1:I:225:LYS:HA	1:I:256:ILE:O	2.16	0.45
1:K:266:ARG:NE	1:K:280:GLU:OE1	2.44	0.45
1:A:193:ASP:HB3	1:A:195:TYR:CZ	2.51	0.45
1:C:56:LEU:HA	1:C:59:MET:HE3	1.99	0.45
1:F:258:MET:HE1	1:F:268:PHE:CZ	2.51	0.45
1:F:93:ILE:O	1:H:102:LEU:HD21	2.18	0.44
1:K:78:PHE:CE1	1:K:89:ILE:HD11	2.52	0.44
1:F:147:SER:O	1:F:151:VAL:HG23	2.18	0.44
1:F:225:LYS:HA	1:F:256:ILE:O	2.17	0.44
1:E:249:LYS:NZ	7:E:501:HOH:O	2.50	0.43
1:G:56:LEU:HD23	1:G:59:MET:HE3	2.00	0.43
1:L:165[B]:ARG:HB3	1:L:165[B]:ARG:CZ	2.47	0.43
1:A:13:ALA:HB1	1:L:101:TRP:CE3	2.54	0.43
1:B:101:TRP:CE3	1:E:13:ALA:HB1	2.53	0.43
1:H:126:PHE:CD2	2:H:401:SAH:H8	2.54	0.42
1:K:147:SER:O	1:K:151:VAL:HG23	2.18	0.42
1:A:258:MET:HE1	1:A:268:PHE:CZ	2.54	0.42
1:B:61:VAL:HA	1:B:75:CYS:SG	2.60	0.42
1:I:229:HIS:HE2	3:I:402:QOT:C26	2.32	0.42
1:H:193:ASP:HB3	1:H:195:TYR:CZ	2.55	0.42
1:G:16:HIS:HA	1:G:89:ILE:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:225:LYS:HA	1:K:256:ILE:O	2.19	0.42
1:H:141:ALA:O	1:H:145:ARG:HG2	2.19	0.41
1:C:78:PHE:CZ	1:G:2:LEU:HD11	2.54	0.41
3:C:402:QOT:O18	3:C:402:QOT:O8	2.38	0.41
1:G:296:VAL:HG13	1:G:318:LYS:HG2	2.02	0.41
1:H:152:GLU:OE1	1:H:152:GLU:N	2.40	0.41
1:A:78:PHE:CZ	1:L:2:LEU:HD11	2.55	0.41
1:I:230:ASN:O	1:I:276:PHE:HB3	2.21	0.41
4:A:403:CL:CL	1:C:36:SER:OG	2.76	0.41
1:B:170:GLY:O	2:B:401:SAH:N	2.54	0.41
1:D:36:SER:O	1:D:40:ARG:HG3	2.21	0.41
1:D:157:ILE:O	1:D:301:LYS:NZ	2.53	0.41
3:H:402:QOT:O8	3:H:402:QOT:O18	2.37	0.41
1:I:229:HIS:NE2	3:I:402:QOT:C26	2.84	0.40
1:H:56:LEU:HA	1:H:59:MET:HE3	2.04	0.40
1:C:147:SER:O	1:C:151:VAL:HG23	2.21	0.40
3:I:402:QOT:O18	3:I:402:QOT:O8	2.36	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	317/319 (99%)	307 (97%)	10 (3%)	0	100	100
1	B	317/319 (99%)	307 (97%)	10 (3%)	0	100	100
1	C	317/319 (99%)	312 (98%)	5 (2%)	0	100	100
1	D	317/319 (99%)	311 (98%)	6 (2%)	0	100	100
1	E	317/319 (99%)	311 (98%)	6 (2%)	0	100	100
1	F	317/319 (99%)	308 (97%)	9 (3%)	0	100	100
1	G	317/319 (99%)	308 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	317/319 (99%)	304 (96%)	13 (4%)	0	100	100
1	I	317/319 (99%)	305 (96%)	12 (4%)	0	100	100
1	J	317/319 (99%)	311 (98%)	6 (2%)	0	100	100
1	K	317/319 (99%)	308 (97%)	9 (3%)	0	100	100
1	L	318/319 (100%)	310 (98%)	8 (2%)	0	100	100
All	All	3805/3828 (99%)	3702 (97%)	103 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	287/287 (100%)	283 (99%)	4 (1%)	67	82
1	B	287/287 (100%)	283 (99%)	4 (1%)	67	82
1	C	287/287 (100%)	282 (98%)	5 (2%)	60	78
1	D	287/287 (100%)	282 (98%)	5 (2%)	60	78
1	E	287/287 (100%)	280 (98%)	7 (2%)	49	68
1	F	287/287 (100%)	281 (98%)	6 (2%)	53	72
1	G	287/287 (100%)	284 (99%)	3 (1%)	76	88
1	H	287/287 (100%)	284 (99%)	3 (1%)	76	88
1	I	287/287 (100%)	282 (98%)	5 (2%)	60	78
1	J	287/287 (100%)	279 (97%)	8 (3%)	43	63
1	K	287/287 (100%)	281 (98%)	6 (2%)	53	72
1	L	288/287 (100%)	278 (96%)	10 (4%)	36	55
All	All	3445/3444 (100%)	3379 (98%)	66 (2%)	57	75

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	PHE
1	A	185	LYS
1	A	211	PHE
1	A	229	HIS
1	B	211	PHE
1	B	220	ASP
1	B	229	HIS
1	B	257	ASN
1	C	73	ASP
1	C	82	GLU
1	C	198	LEU
1	C	211	PHE
1	C	229	HIS
1	D	84	PHE
1	D	185	LYS
1	D	211	PHE
1	D	220	ASP
1	D	229	HIS
1	E	84	PHE
1	E	179	ARG
1	E	198	LEU
1	E	211	PHE
1	E	229	HIS
1	E	257	ASN
1	E	318	LYS
1	F	84	PHE
1	F	106	LYS
1	F	185	LYS
1	F	211	PHE
1	F	229	HIS
1	F	296	VAL
1	G	84	PHE
1	G	211	PHE
1	G	229	HIS
1	H	84	PHE
1	H	211	PHE
1	H	229	HIS
1	I	67	ASN
1	I	84	PHE
1	I	142	LEU
1	I	211	PHE
1	I	229	HIS
1	J	185	LYS

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Mol	Chain	Res	Type
1	J	198	LEU
1	J	211	PHE
1	J	229	HIS
1	J	257	ASN
1	J	261	GLU
1	J	279	LYS
1	J	296	VAL
1	K	40	ARG
1	K	84	PHE
1	K	185	LYS
1	K	211	PHE
1	K	220	ASP
1	K	229	HIS
1	L	73	ASP
1	L	84	PHE
1	L	133	LYS
1	L	136	LYS
1	L	165[A]	ARG
1	L	165[B]	ARG
1	L	185	LYS
1	L	198	LEU
1	L	229	HIS
1	L	257	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	226	ASN
1	K	203	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)

Of 29 ligands modelled in this entry, 6 are monoatomic - leaving 23 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	A	401	-	24,28,28	0.71	1 (4%)	25,40,40	0.97	3 (12%)
3	QOT	A	402	-	23,23,23	1.56	4 (17%)	34,34,34	1.00	4 (11%)
2	SAH	B	401	-	24,28,28	0.71	1 (4%)	25,40,40	0.91	3 (12%)
2	SAH	C	401	-	24,28,28	0.70	1 (4%)	25,40,40	0.95	3 (12%)
2	SAH	F	401	-	24,28,28	0.69	1 (4%)	25,40,40	0.99	3 (12%)
2	SAH	D	401	-	24,28,28	0.71	1 (4%)	25,40,40	1.03	3 (12%)
3	QOT	E	402	-	23,23,23	1.50	4 (17%)	34,34,34	1.18	2 (5%)
3	QOT	H	402	-	23,23,23	1.59	4 (17%)	34,34,34	0.75	1 (2%)
3	QOT	D	402	-	23,23,23	1.53	4 (17%)	34,34,34	0.92	2 (5%)
5	GOL	C	403	-	5,5,5	0.08	0	5,5,5	0.23	0
5	GOL	D	403	-	5,5,5	0.09	0	5,5,5	0.26	0
2	SAH	E	401	-	24,28,28	0.71	1 (4%)	25,40,40	0.96	3 (12%)
2	SAH	G	401	-	24,28,28	0.71	1 (4%)	25,40,40	0.96	3 (12%)
3	QOT	F	402	-	23,23,23	1.47	4 (17%)	34,34,34	0.82	2 (5%)
2	SAH	L	900	-	24,28,28	0.71	1 (4%)	25,40,40	0.95	3 (12%)
3	QOT	C	402	-	23,23,23	1.50	4 (17%)	34,34,34	1.03	3 (8%)
2	SAH	K	401	-	24,28,28	0.70	1 (4%)	25,40,40	1.02	3 (12%)
2	SAH	I	401	-	24,28,28	0.69	0	25,40,40	0.98	3 (12%)
3	QOT	G	402	-	23,23,23	1.52	4 (17%)	34,34,34	1.11	2 (5%)
3	QOT	I	402	-	23,23,23	1.54	4 (17%)	34,34,34	0.89	1 (2%)
2	SAH	H	401	-	24,28,28	0.70	1 (4%)	25,40,40	0.96	3 (12%)
3	QOT	B	402	-	23,23,23	1.52	4 (17%)	34,34,34	1.11	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SAH	J	900	-	24,28,28	0.71	1 (4%)	25,40,40	0.96	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	A	401	-	-	0/11/31/31	0/3/3/3
3	QOT	A	402	-	-	4/4/20/20	0/3/3/3
2	SAH	B	401	-	-	0/11/31/31	0/3/3/3
2	SAH	C	401	-	-	0/11/31/31	0/3/3/3
2	SAH	F	401	-	-	1/11/31/31	0/3/3/3
2	SAH	D	401	-	-	4/11/31/31	0/3/3/3
3	QOT	E	402	-	-	4/4/20/20	0/3/3/3
3	QOT	H	402	-	-	4/4/20/20	0/3/3/3
3	QOT	D	402	-	-	4/4/20/20	0/3/3/3
5	GOL	C	403	-	-	0/4/4/4	-
5	GOL	D	403	-	-	0/4/4/4	-
2	SAH	E	401	-	-	4/11/31/31	0/3/3/3
2	SAH	G	401	-	-	0/11/31/31	0/3/3/3
3	QOT	F	402	-	-	4/4/20/20	0/3/3/3
2	SAH	L	900	-	-	0/11/31/31	0/3/3/3
3	QOT	C	402	-	-	4/4/20/20	0/3/3/3
2	SAH	K	401	-	-	0/11/31/31	0/3/3/3
2	SAH	I	401	-	-	0/11/31/31	0/3/3/3
3	QOT	G	402	-	-	4/4/20/20	0/3/3/3
3	QOT	I	402	-	-	4/4/20/20	0/3/3/3
2	SAH	H	401	-	-	0/11/31/31	0/3/3/3
3	QOT	B	402	-	-	4/4/20/20	0/3/3/3
2	SAH	J	900	-	-	0/11/31/31	0/3/3/3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	402	QOT	C4-C10	-4.37	1.39	1.48
3	A	402	QOT	C20-C10	-4.35	1.39	1.48
3	B	402	QOT	C4-C10	-4.23	1.39	1.48
3	A	402	QOT	C4-C10	-4.11	1.39	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	402	QOT	C4-C10	-4.11	1.39	1.48
3	G	402	QOT	C4-C10	-4.11	1.39	1.48
3	H	402	QOT	C20-C10	-4.08	1.39	1.48
3	C	402	QOT	C4-C10	-4.06	1.39	1.48
3	B	402	QOT	C20-C10	-4.04	1.39	1.48
3	D	402	QOT	C20-C10	-4.02	1.40	1.48
3	E	402	QOT	C4-C10	-4.02	1.40	1.48
3	G	402	QOT	C20-C10	-3.96	1.40	1.48
3	D	402	QOT	C4-C10	-3.95	1.40	1.48
3	F	402	QOT	C4-C10	-3.90	1.40	1.48
3	I	402	QOT	C20-C10	-3.90	1.40	1.48
3	C	402	QOT	C20-C10	-3.90	1.40	1.48
3	E	402	QOT	C20-C10	-3.89	1.40	1.48
3	F	402	QOT	C20-C10	-3.87	1.40	1.48
3	I	402	QOT	C9-C21	-3.36	1.39	1.47
3	H	402	QOT	C9-C21	-3.31	1.39	1.47
3	D	402	QOT	C9-C21	-3.30	1.39	1.47
3	C	402	QOT	C9-C21	-3.25	1.39	1.47
3	A	402	QOT	C9-C21	-3.22	1.40	1.47
3	E	402	QOT	C9-C21	-3.18	1.40	1.47
3	G	402	QOT	C9-C21	-3.17	1.40	1.47
3	F	402	QOT	C9-C21	-3.12	1.40	1.47
3	B	402	QOT	C9-C21	-3.00	1.40	1.47
3	G	402	QOT	C3-C21	-2.95	1.40	1.47
3	I	402	QOT	C3-C21	-2.92	1.40	1.47
3	D	402	QOT	C3-C21	-2.85	1.40	1.47
3	H	402	QOT	C3-C21	-2.84	1.40	1.47
3	E	402	QOT	C3-C21	-2.80	1.41	1.47
3	F	402	QOT	C3-C21	-2.79	1.41	1.47
3	C	402	QOT	C3-C21	-2.66	1.41	1.47
3	B	402	QOT	C3-C21	-2.66	1.41	1.47
3	A	402	QOT	C3-C21	-2.64	1.41	1.47
2	E	401	SAH	OXT-C	-2.18	1.23	1.30
2	J	900	SAH	OXT-C	-2.14	1.23	1.30
2	B	401	SAH	OXT-C	-2.13	1.23	1.30
2	C	401	SAH	OXT-C	-2.12	1.23	1.30
2	G	401	SAH	OXT-C	-2.12	1.23	1.30
2	F	401	SAH	OXT-C	-2.10	1.23	1.30
2	H	401	SAH	OXT-C	-2.10	1.23	1.30
2	L	900	SAH	OXT-C	-2.09	1.23	1.30
2	K	401	SAH	OXT-C	-2.09	1.23	1.30
2	D	401	SAH	OXT-C	-2.07	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	SAH	OXT-C	-2.06	1.23	1.30

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	402	QOT	C26-O17-C2	-4.97	110.03	117.53
3	G	402	QOT	C26-O17-C2	-4.65	110.51	117.53
3	B	402	QOT	C26-O17-C2	-4.56	110.65	117.53
3	C	402	QOT	C26-O17-C2	-3.14	112.78	117.53
3	D	402	QOT	C17-O19-C12	-2.84	111.34	117.51
3	C	402	QOT	C17-O19-C12	-2.80	111.43	117.51
3	A	402	QOT	C26-O17-C2	-2.79	113.32	117.53
2	K	401	SAH	OXT-C-O	-2.77	117.79	124.09
2	L	900	SAH	OXT-C-O	-2.73	117.89	124.09
2	D	401	SAH	OXT-C-O	-2.70	117.96	124.09
2	G	401	SAH	OXT-C-O	-2.63	118.13	124.09
3	B	402	QOT	O17-C2-C1	-2.62	119.88	124.37
3	A	402	QOT	C17-O19-C12	-2.51	112.06	117.51
2	I	401	SAH	OXT-C-O	-2.50	118.41	124.09
2	C	401	SAH	OXT-C-O	-2.47	118.47	124.09
2	B	401	SAH	OXT-C-O	-2.46	118.50	124.09
2	A	401	SAH	OXT-C-O	-2.45	118.52	124.09
2	F	401	SAH	OXT-C-O	-2.44	118.56	124.09
2	J	900	SAH	OXT-C-O	-2.43	118.56	124.09
2	D	401	SAH	OXT-C-CA	2.41	121.61	113.38
2	F	401	SAH	OXT-C-CA	2.41	121.58	113.38
2	K	401	SAH	OXT-C-CA	2.39	121.54	113.38
2	I	401	SAH	OXT-C-CA	2.39	121.53	113.38
3	I	402	QOT	C17-O19-C12	-2.38	112.34	117.51
3	A	402	QOT	O17-C2-C1	-2.37	120.30	124.37
3	H	402	QOT	C26-O17-C2	-2.36	113.97	117.53
2	L	900	SAH	OXT-C-CA	2.35	121.40	113.38
2	A	401	SAH	OXT-C-CA	2.28	121.14	113.38
2	E	401	SAH	OXT-C-O	-2.27	118.93	124.09
2	H	401	SAH	OXT-C-CA	2.27	121.12	113.38
3	E	402	QOT	O17-C2-C1	-2.25	120.51	124.37
3	G	402	QOT	O17-C2-C1	-2.24	120.53	124.37
2	J	900	SAH	OXT-C-CA	2.22	120.95	113.38
2	H	401	SAH	OXT-C-O	-2.22	119.04	124.09
2	G	401	SAH	OXT-C-CA	2.21	120.93	113.38
2	E	401	SAH	C5-C6-N6	2.21	123.70	120.35
2	F	401	SAH	C5-C6-N6	2.20	123.70	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	401	SAH	C5-C6-N6	2.19	123.68	120.35
2	B	401	SAH	C5-C6-N6	2.19	123.68	120.35
3	C	402	QOT	O17-C2-C1	-2.19	120.62	124.37
2	H	401	SAH	C5-C6-N6	2.18	123.67	120.35
2	C	401	SAH	OXT-C-CA	2.17	120.79	113.38
2	J	900	SAH	C5-C6-N6	2.15	123.62	120.35
2	A	401	SAH	C5-C6-N6	2.15	123.61	120.35
2	L	900	SAH	C5-C6-N6	2.14	123.60	120.35
2	G	401	SAH	C5-C6-N6	2.14	123.60	120.35
2	C	401	SAH	C5-C6-N6	2.13	123.59	120.35
2	K	401	SAH	C5-C6-N6	2.13	123.59	120.35
2	B	401	SAH	OXT-C-CA	2.12	120.59	113.38
2	D	401	SAH	C5-C6-N6	2.12	123.57	120.35
3	F	402	QOT	O17-C2-C1	-2.12	120.74	124.37
2	E	401	SAH	OXT-C-CA	2.09	120.51	113.38
3	D	402	QOT	C26-O17-C2	-2.07	114.41	117.53
3	F	402	QOT	C26-O17-C2	-2.04	114.44	117.53
3	A	402	QOT	O18-C14-C9	-2.00	117.40	121.14

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	402	QOT	C13-C12-O19-C17
3	C	402	QOT	C11-C12-O19-C17
3	D	402	QOT	C13-C12-O19-C17
3	D	402	QOT	C11-C12-O19-C17
3	I	402	QOT	C13-C12-O19-C17
3	I	402	QOT	C11-C12-O19-C17
3	A	402	QOT	C13-C12-O19-C17
3	A	402	QOT	C11-C12-O19-C17
3	E	402	QOT	C13-C12-O19-C17
3	E	402	QOT	C11-C12-O19-C17
3	H	402	QOT	C13-C12-O19-C17
3	G	402	QOT	C13-C12-O19-C17
3	H	402	QOT	C11-C12-O19-C17
3	G	402	QOT	C11-C12-O19-C17
3	F	402	QOT	C13-C12-O19-C17
3	F	402	QOT	C11-C12-O19-C17
3	B	402	QOT	C11-C12-O19-C17
3	G	402	QOT	C3-C2-O17-C26
3	B	402	QOT	C13-C12-O19-C17

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Mol	Chain	Res	Type	Atoms
3	B	402	QOT	C3-C2-O17-C26
3	C	402	QOT	C3-C2-O17-C26
3	D	402	QOT	C3-C2-O17-C26
3	I	402	QOT	C3-C2-O17-C26
3	A	402	QOT	C3-C2-O17-C26
3	E	402	QOT	C3-C2-O17-C26
3	F	402	QOT	C1-C2-O17-C26
3	G	402	QOT	C1-C2-O17-C26
3	B	402	QOT	C1-C2-O17-C26
3	D	402	QOT	C1-C2-O17-C26
3	E	402	QOT	C1-C2-O17-C26
3	C	402	QOT	C1-C2-O17-C26
3	F	402	QOT	C3-C2-O17-C26
3	A	402	QOT	C1-C2-O17-C26
3	I	402	QOT	C1-C2-O17-C26
3	H	402	QOT	C1-C2-O17-C26
3	H	402	QOT	C3-C2-O17-C26
2	D	401	SAH	C-CA-CB-CG
2	E	401	SAH	C-CA-CB-CG
2	D	401	SAH	O-C-CA-N
2	E	401	SAH	O-C-CA-N
2	D	401	SAH	N-CA-CB-CG
2	E	401	SAH	N-CA-CB-CG
2	D	401	SAH	OXT-C-CA-N
2	E	401	SAH	OXT-C-CA-N
2	F	401	SAH	C-CA-CB-CG

There are no ring outliers.

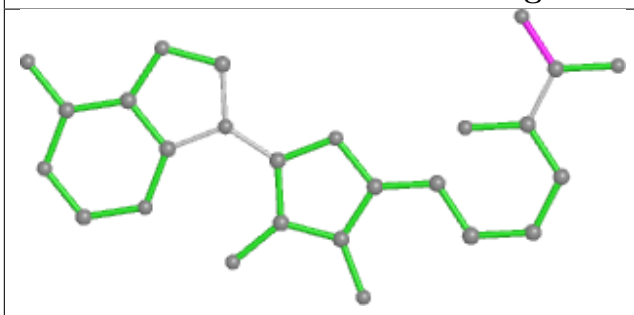
7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	SAH	1	0
3	H	402	QOT	1	0
3	C	402	QOT	1	0
2	I	401	SAH	1	0
3	G	402	QOT	1	0
3	I	402	QOT	3	0
2	H	401	SAH	1	0

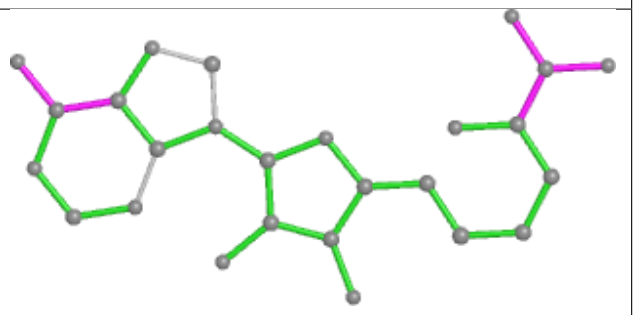
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

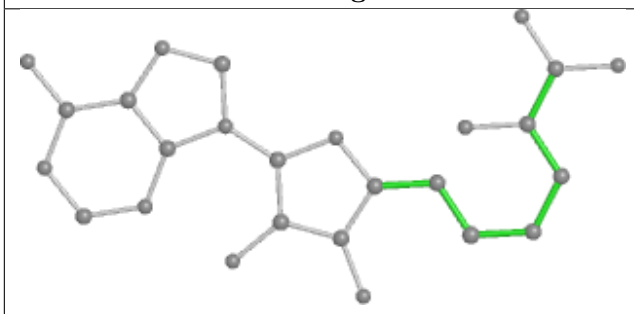
Ligand SAH A 401



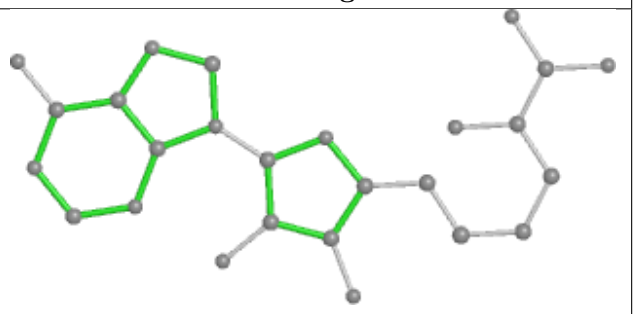
Bond lengths



Bond angles

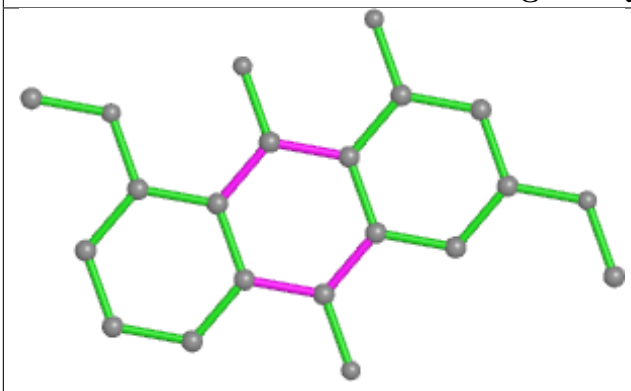


Torsions

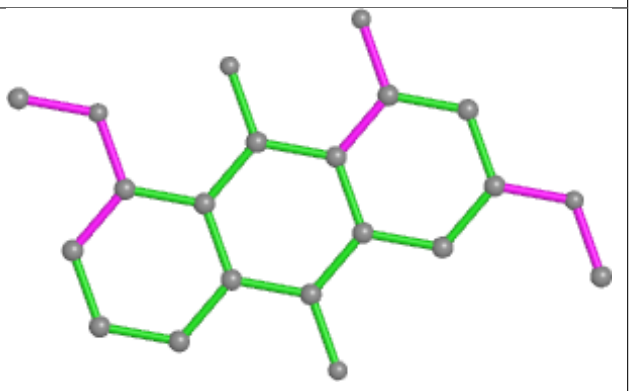


Rings

Ligand QOT A 402



Bond lengths



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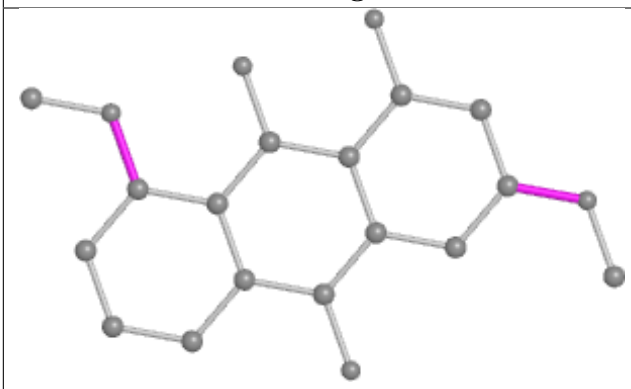

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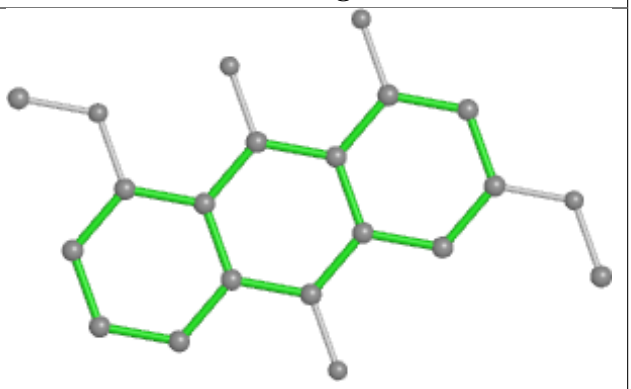
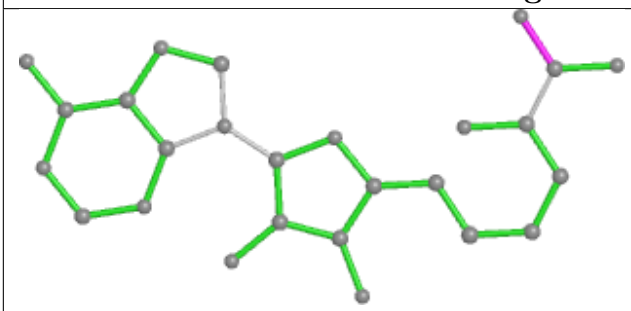
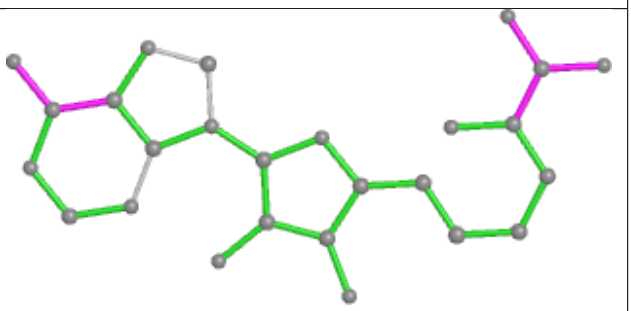


Rings

Ligand SAH B 401



Bond lengths



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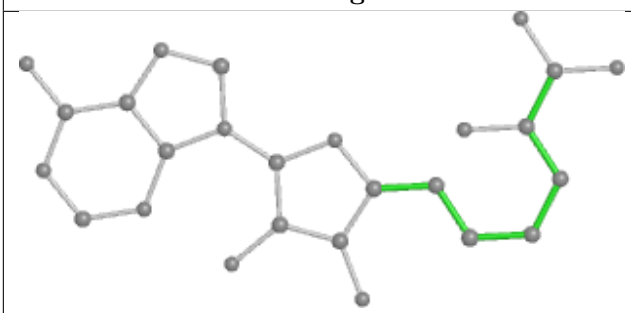

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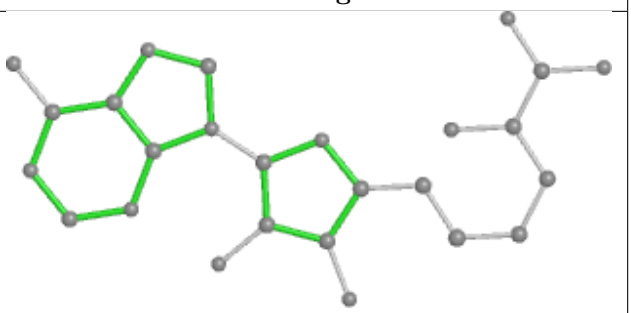
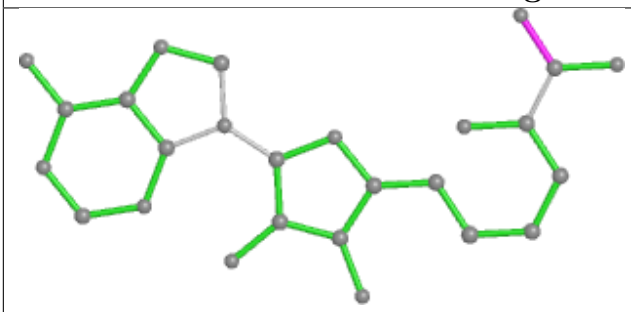


Rings

Ligand SAH C 401



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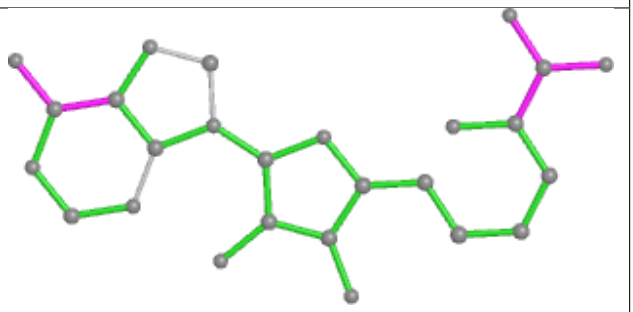

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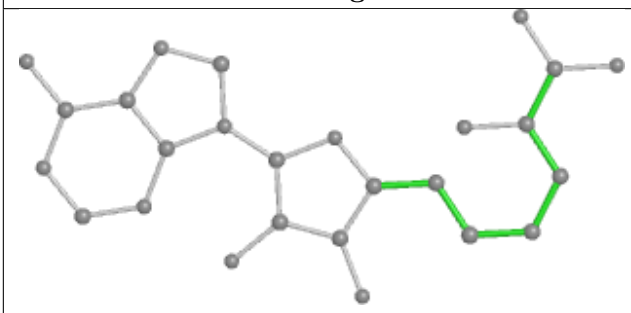

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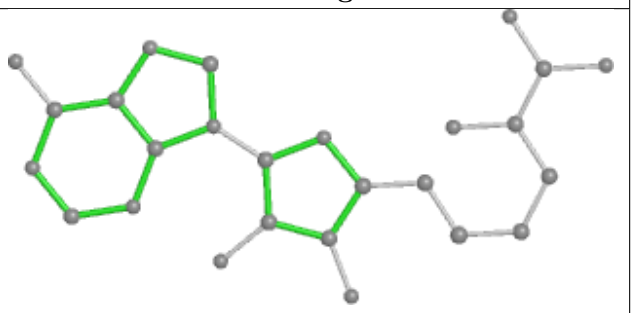
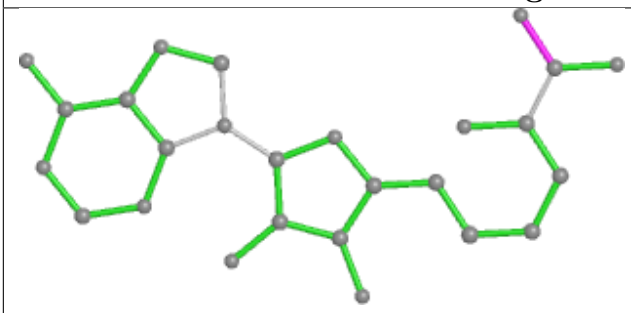


Rings

Ligand SAH F 401



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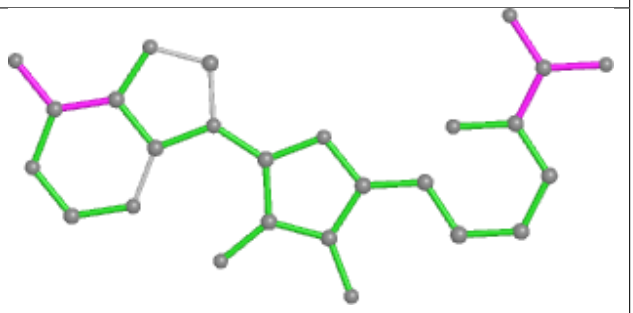

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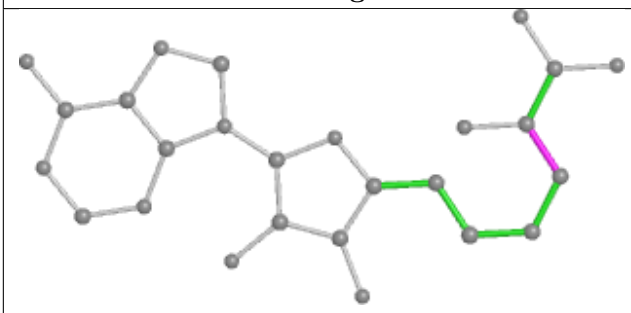

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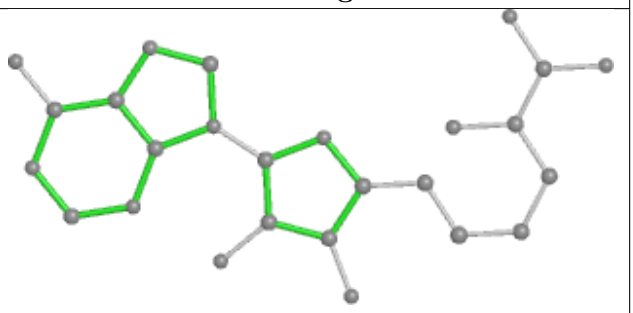
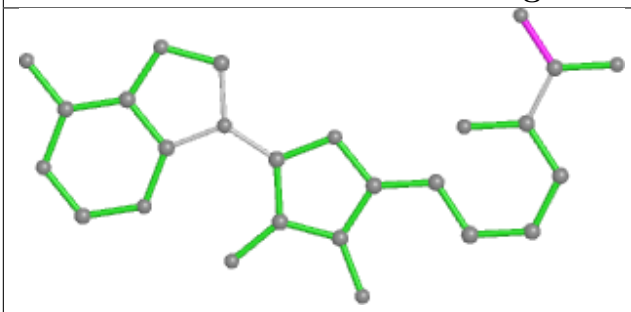


Rings

Ligand SAH D 401



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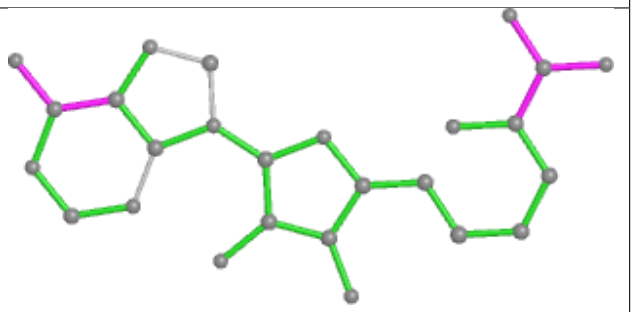
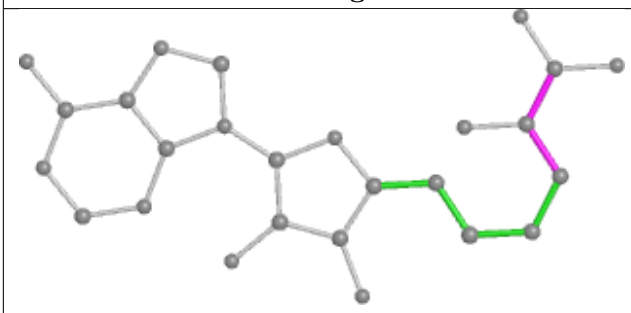


Bond angles



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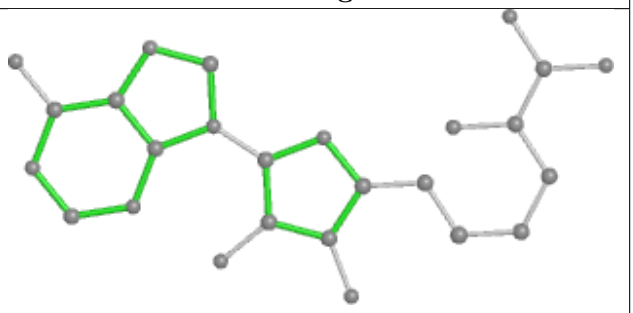
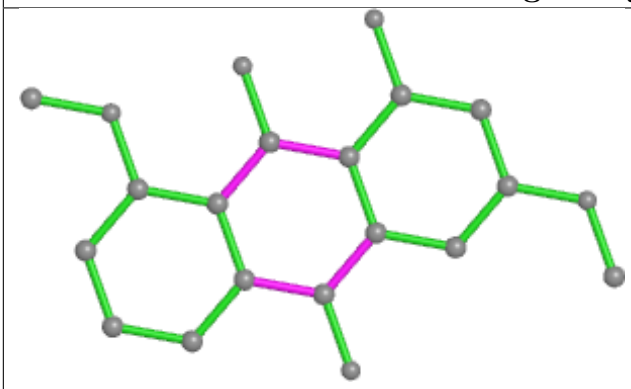


Rings

Ligand QOT E 402



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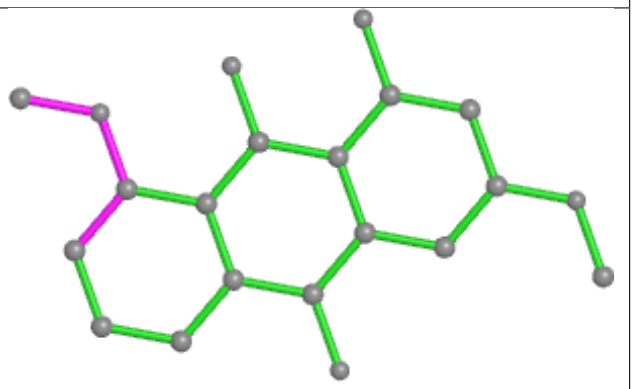

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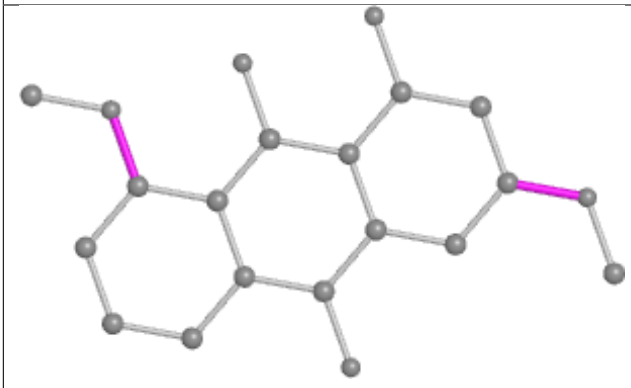

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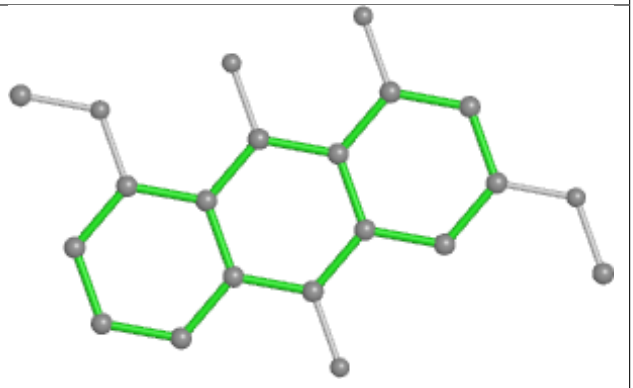
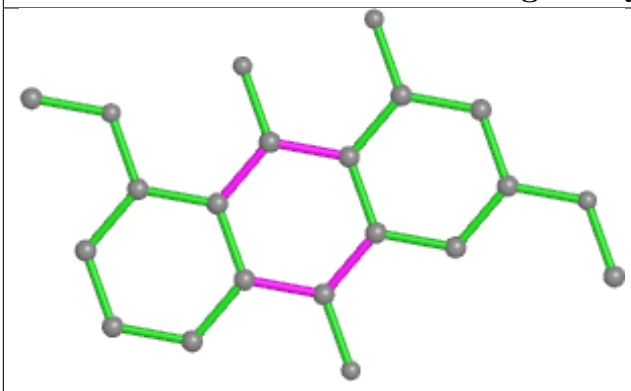


Rings

Ligand QOT H 402



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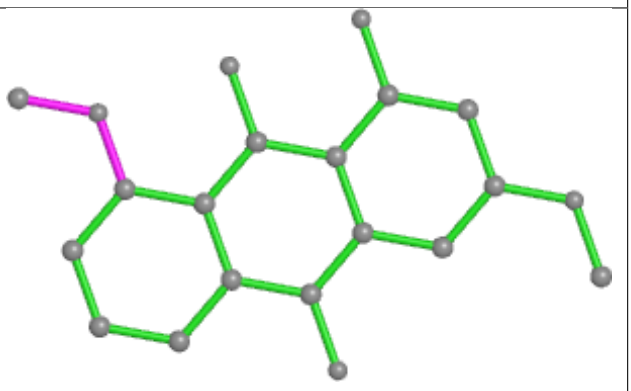

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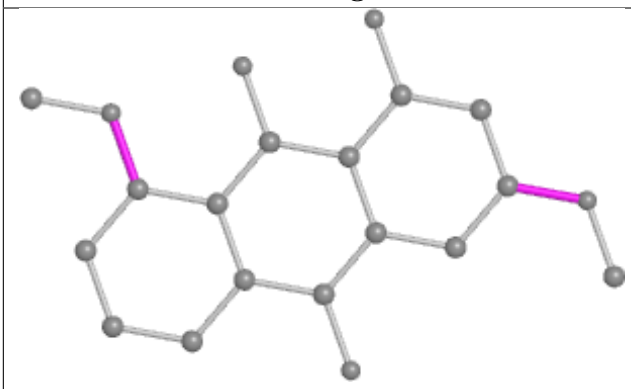

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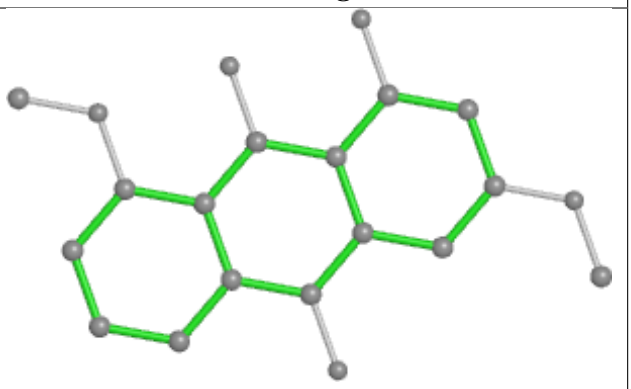
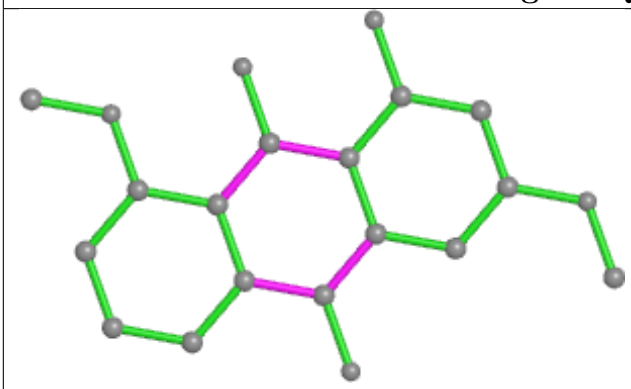
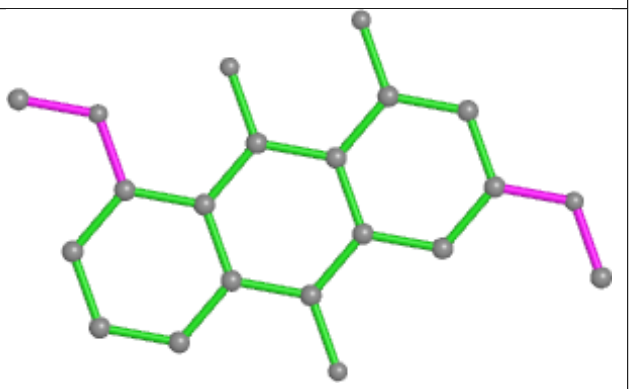


Rings

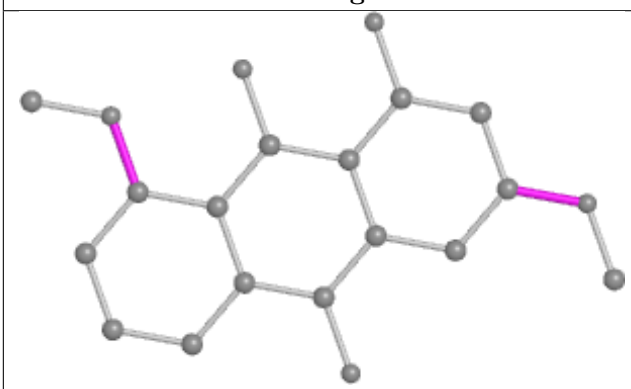
Ligand QOT D 402



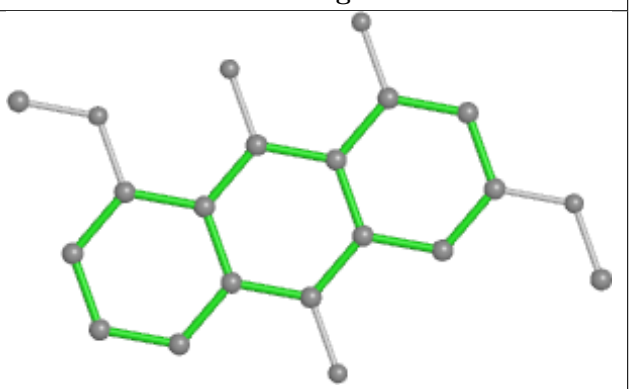
Bond lengths



Bond angles

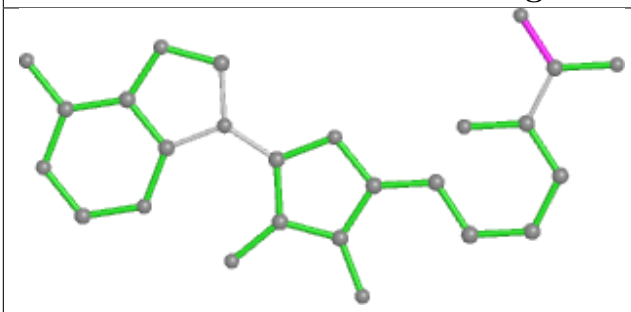


Torsions



Rings

Ligand SAH E 401



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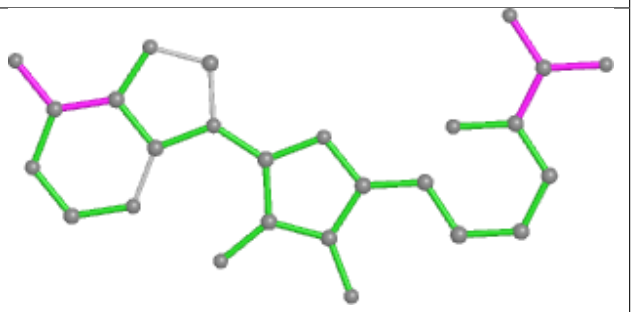

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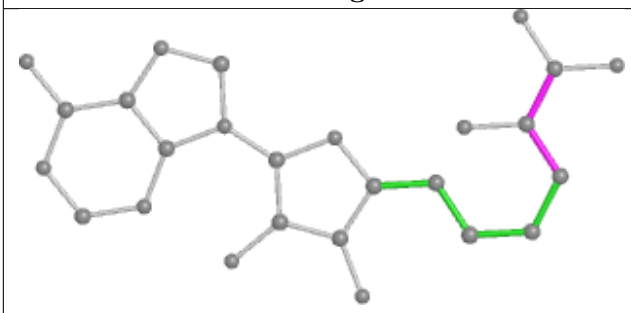

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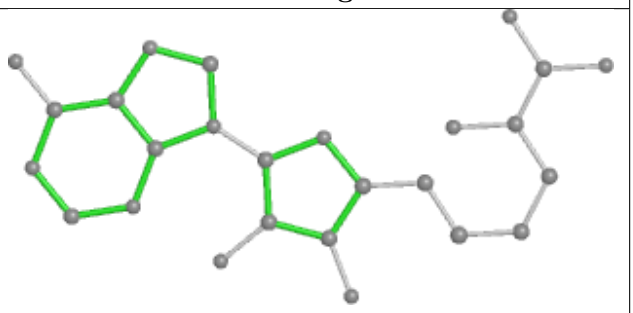
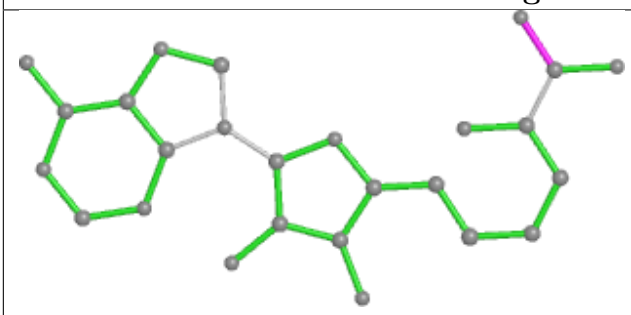


Rings

Ligand SAH G 401



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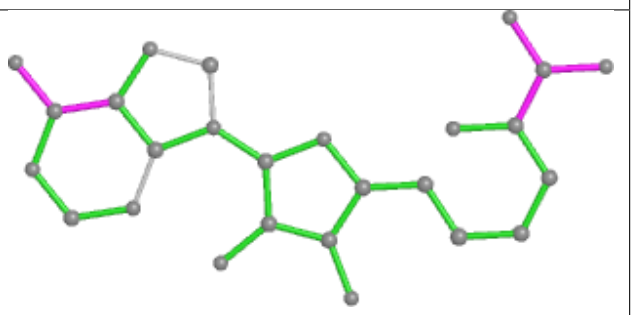

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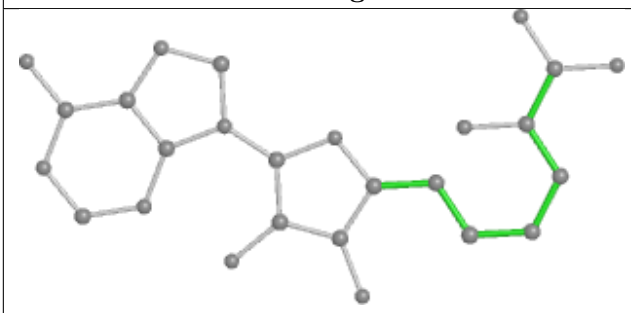

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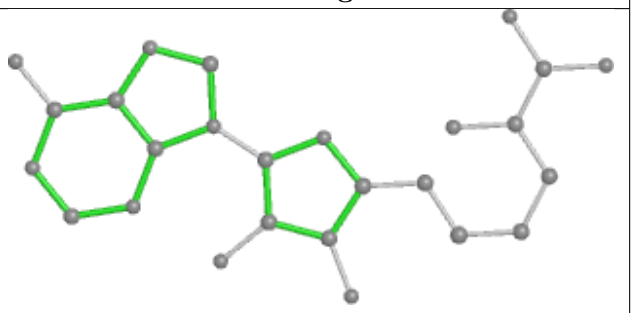
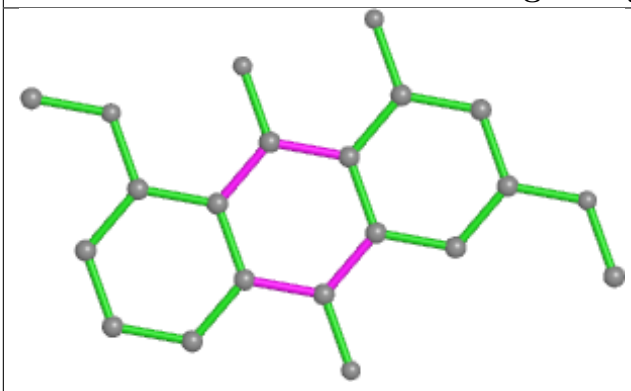


Rings

Ligand QOT F 402



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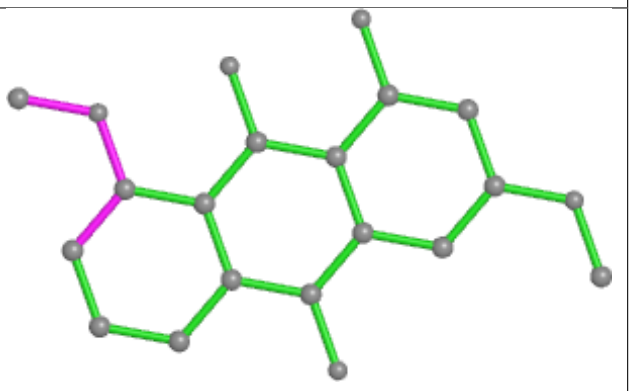
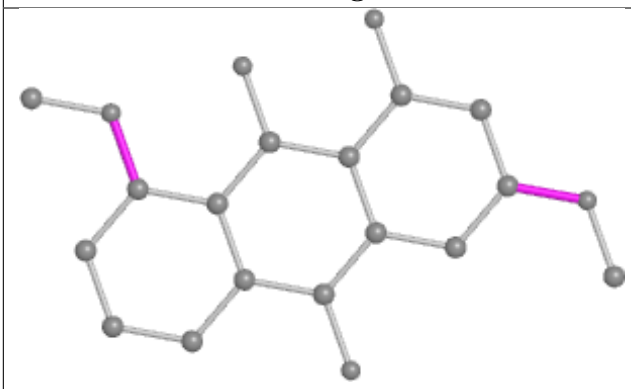


Bond angles



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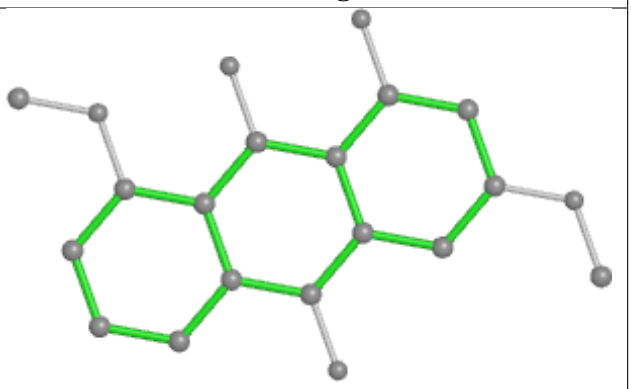
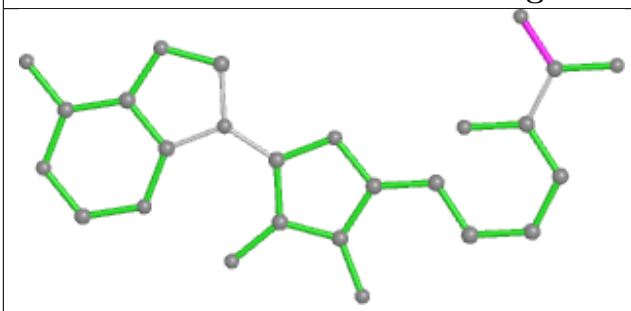


Rings

Ligand SAH L 900



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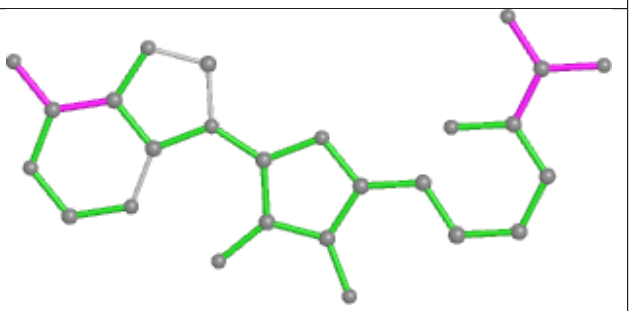

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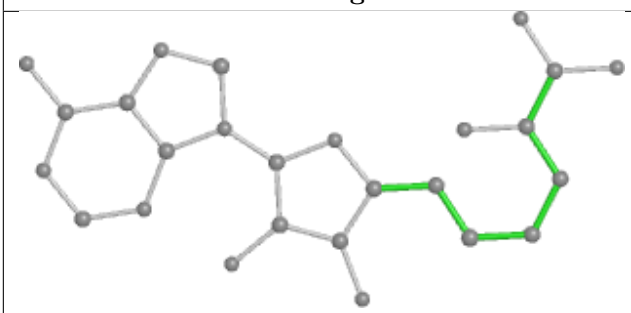
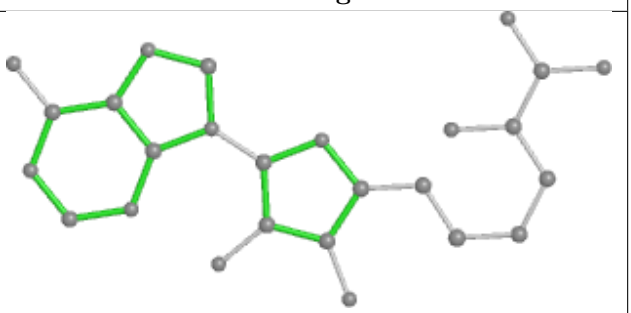
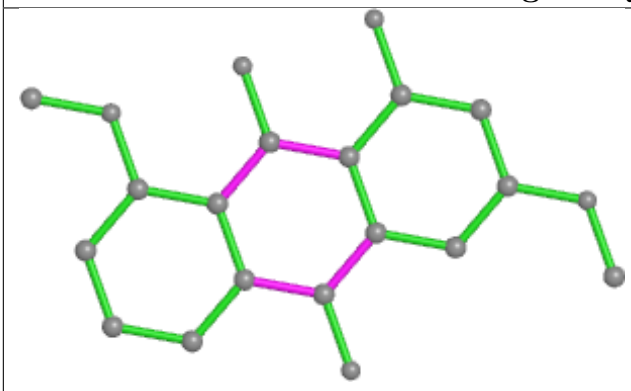


Torsions

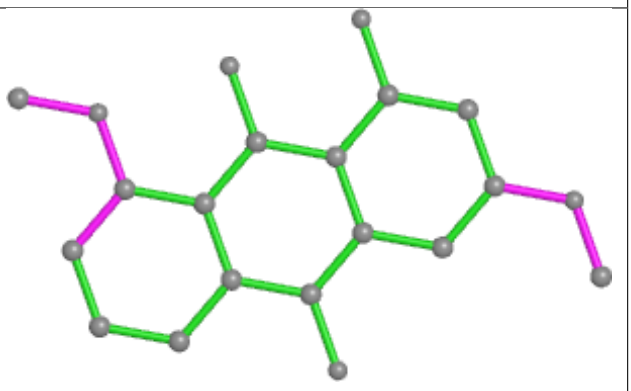


Rings

Ligand QOT C 402



Bond lengths



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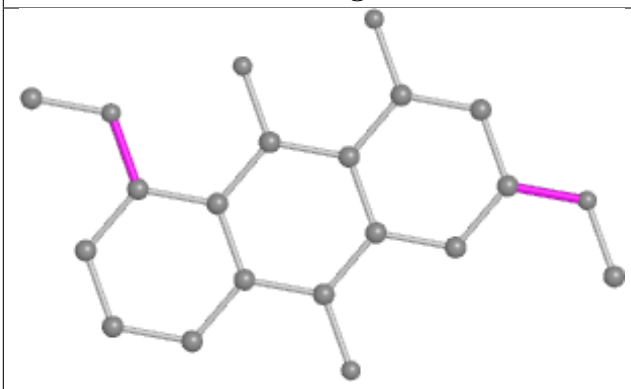

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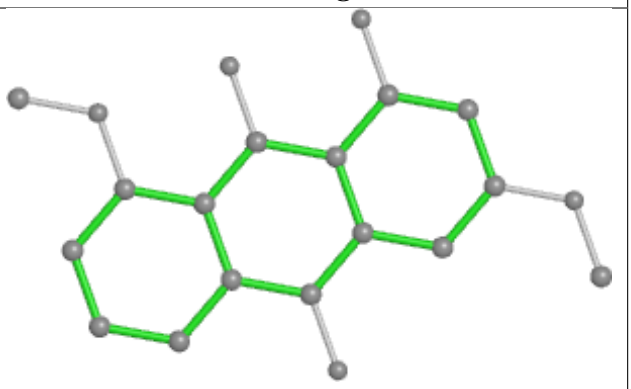
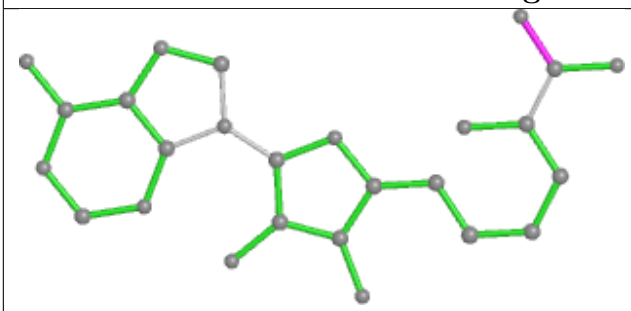


Rings

Ligand SAH K 401



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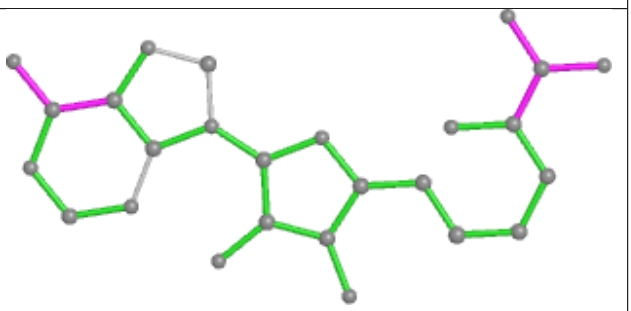
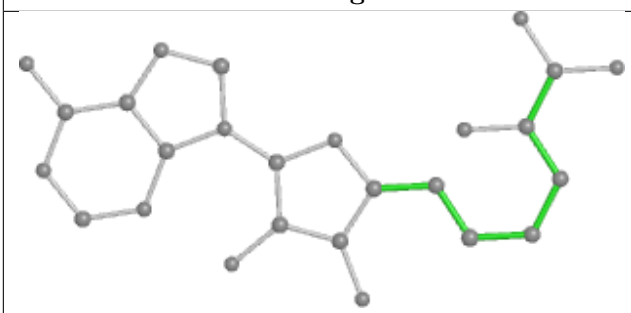


Bond angles



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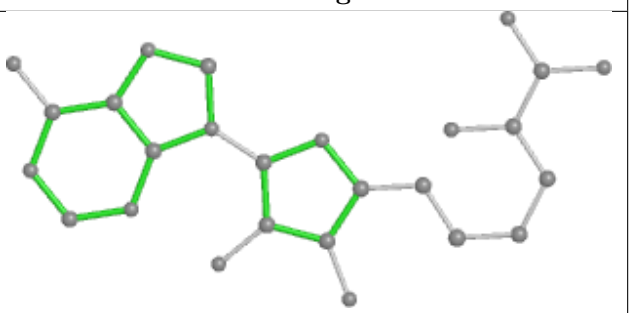
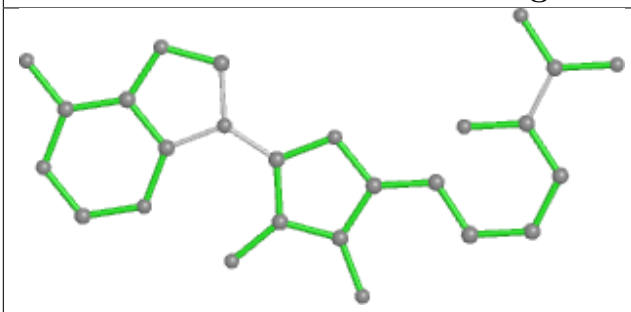


Rings

Ligand SAH I 401



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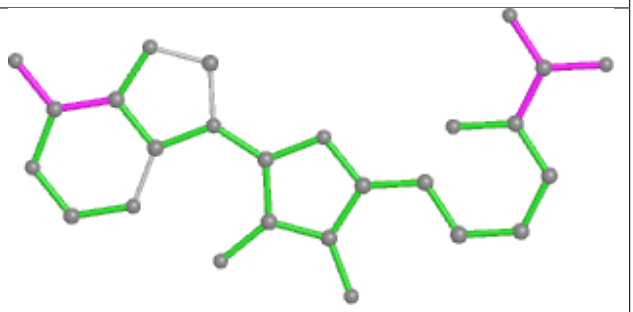
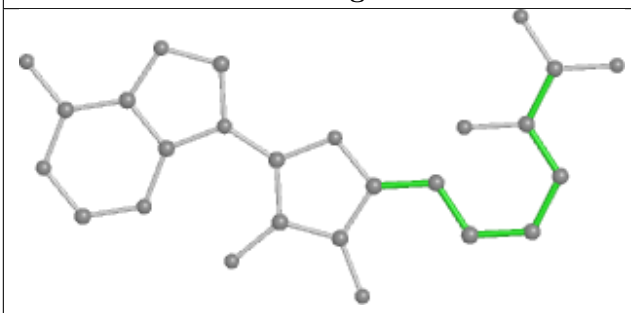


Bond angles



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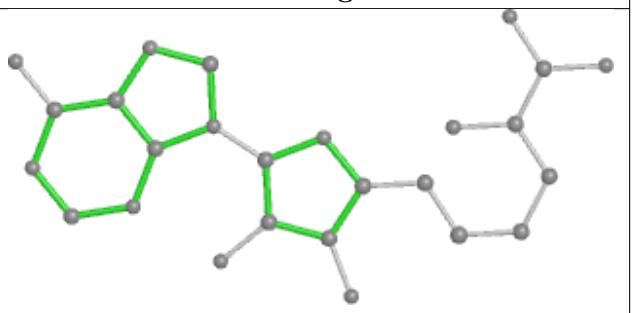
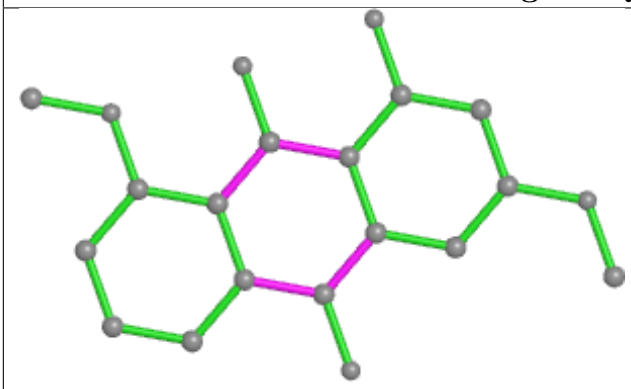


Rings

Ligand QOT G 402



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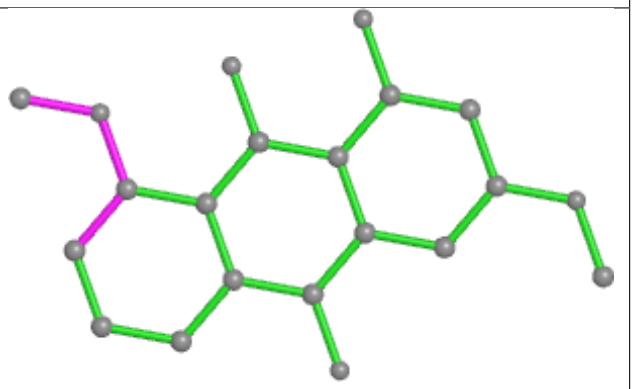

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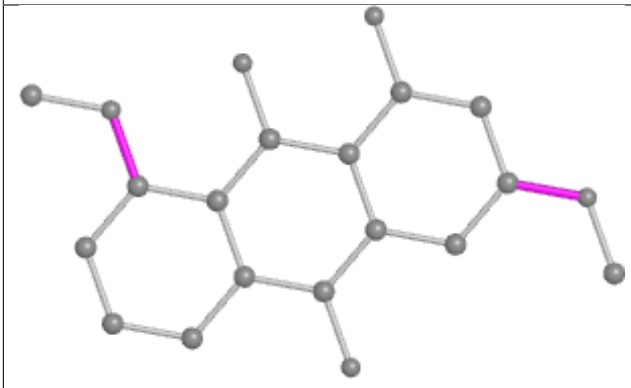

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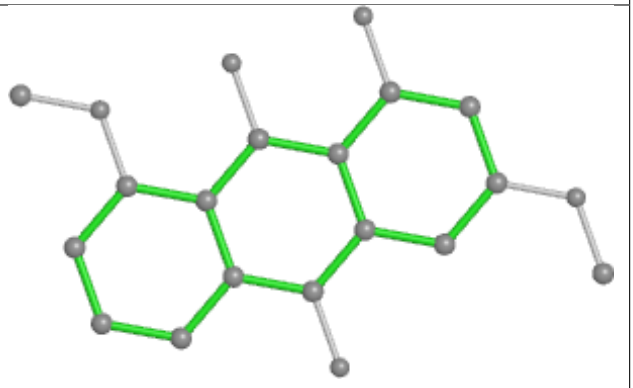
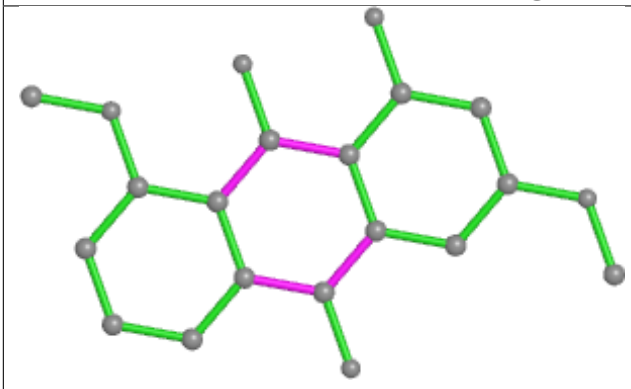


Rings

Ligand QOT I 402



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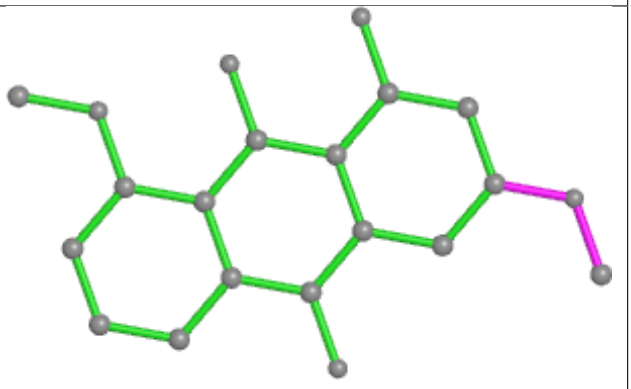
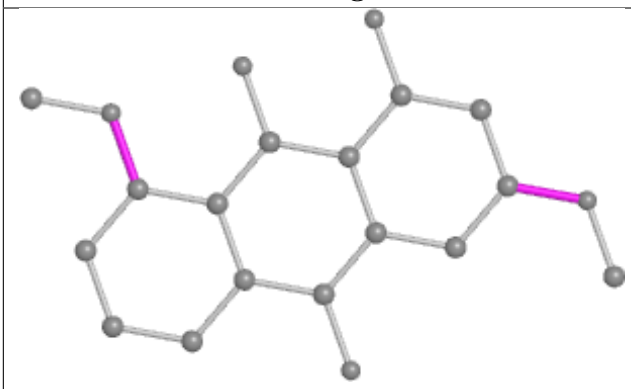
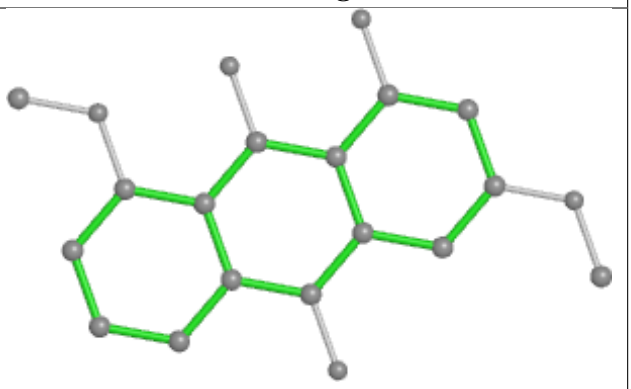


Bond angles

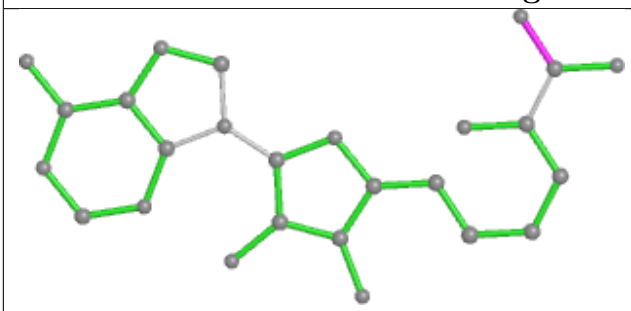


Torsions

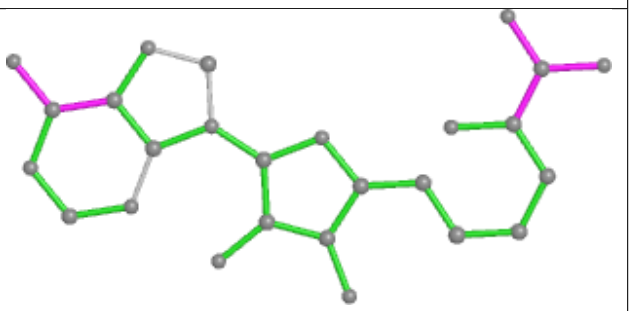


Rings

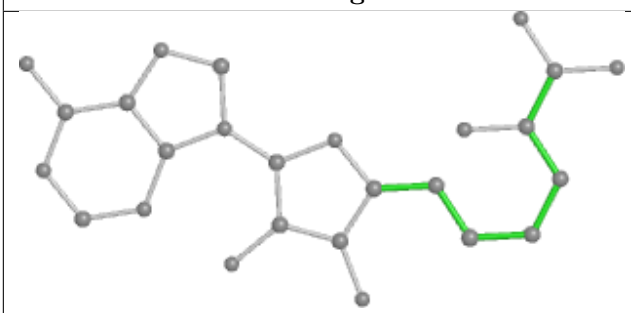
Ligand SAH H 401



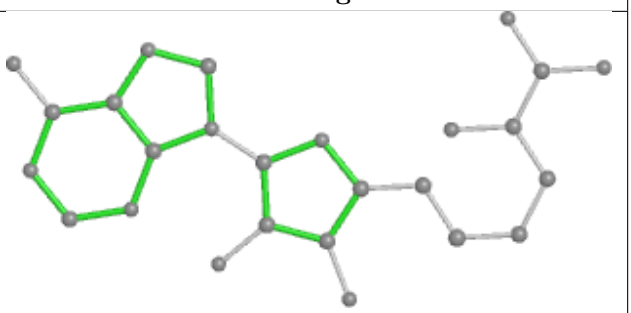
Bond lengths



Bond angles

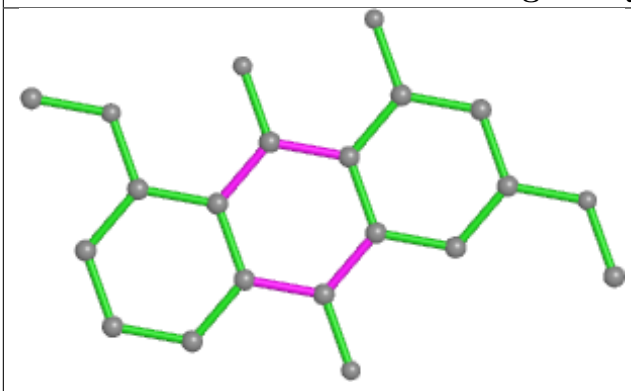


Torsions

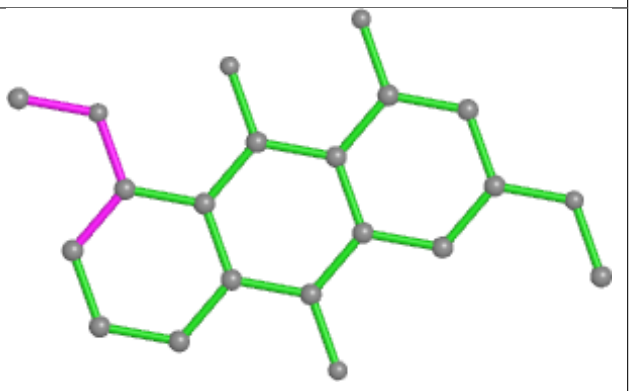


Rings

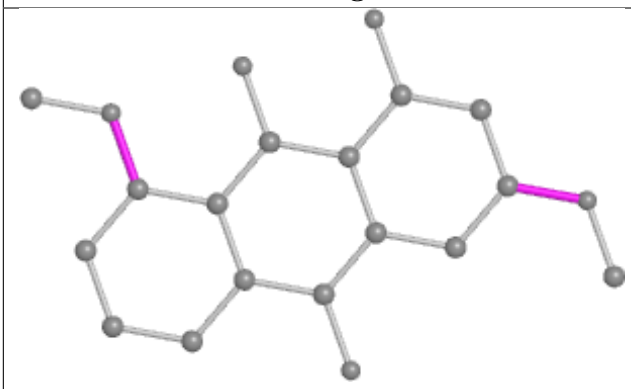
Ligand QOT B 402



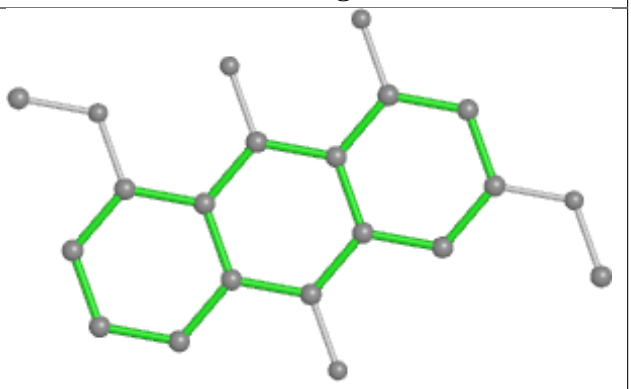
Bond lengths



Bond angles

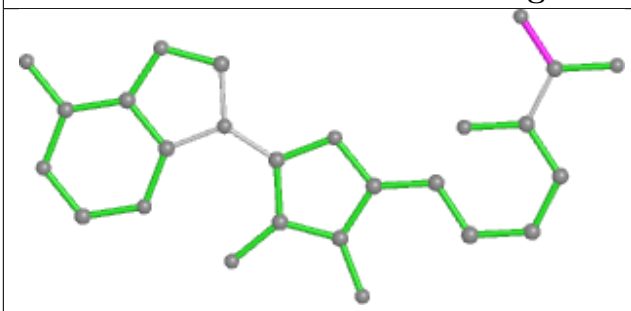


Torsions

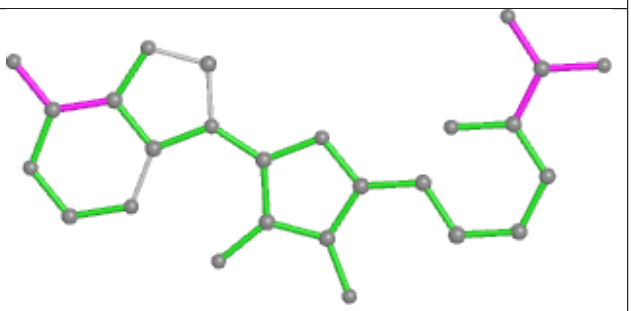


Rings

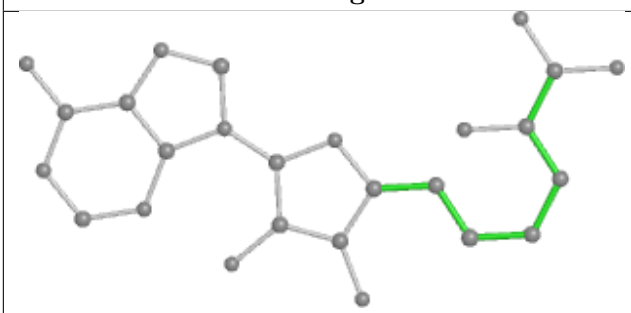
Ligand SAH J 900



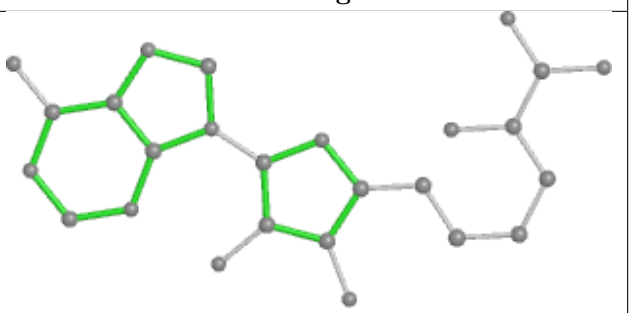
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	319/319 (100%)	-0.08	1 (0%)	94	93	39, 52, 69, 86	0
1	B	319/319 (100%)	0.05	5 (1%)	72	70	39, 54, 70, 80	0
1	C	319/319 (100%)	0.07	5 (1%)	72	70	42, 61, 78, 90	0
1	D	319/319 (100%)	-0.04	2 (0%)	89	88	42, 53, 68, 96	0
1	E	319/319 (100%)	-0.04	4 (1%)	77	75	39, 53, 71, 100	0
1	F	319/319 (100%)	-0.01	3 (0%)	84	82	35, 57, 80, 90	0
1	G	319/319 (100%)	-0.00	1 (0%)	94	93	42, 56, 70, 83	0
1	H	319/319 (100%)	0.01	1 (0%)	94	93	37, 56, 76, 87	0
1	I	319/319 (100%)	-0.03	0	100	100	39, 53, 66, 74	0
1	J	319/319 (100%)	0.10	5 (1%)	72	70	38, 58, 80, 90	0
1	K	319/319 (100%)	0.19	7 (2%)	62	60	41, 63, 86, 101	0
1	L	319/319 (100%)	0.33	15 (4%)	31	30	40, 66, 101, 113	0
All	All	3828/3828 (100%)	0.05	49 (1%)	77	75	35, 56, 80, 113	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	218	GLY	4.5
1	B	0	SER	4.3
1	J	203	ASN	3.9
1	L	189	TYR	3.4
1	L	166	ILE	3.3
1	L	196	SER	3.2
1	K	200	VAL	3.2
1	K	218	GLY	3.1
1	E	200	VAL	3.1
1	B	28	LYS	3.0
1	E	110	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	160	PHE	3.0
1	K	204	ILE	2.9
1	J	111	ASP	2.8
1	L	238	LEU	2.8
1	L	142	LEU	2.7
1	B	42	SER	2.7
1	C	186	GLY	2.7
1	J	318	LYS	2.7
1	L	204	ILE	2.6
1	G	31	ILE	2.6
1	E	111	ASP	2.6
1	L	203	ASN	2.6
1	L	306	SER	2.5
1	C	318	LYS	2.5
1	L	245	LYS	2.5
1	F	250	ASN	2.5
1	B	160	PHE	2.5
1	L	207	ILE	2.4
1	C	0	SER	2.4
1	F	1	MET	2.4
1	L	1	MET	2.4
1	F	200	VAL	2.3
1	C	89	ILE	2.3
1	D	23	LEU	2.3
1	K	33	VAL	2.3
1	J	1	MET	2.3
1	L	215	ILE	2.3
1	L	249	LYS	2.3
1	L	198	LEU	2.2
1	E	203	ASN	2.2
1	K	203	ASN	2.2
1	B	69	PHE	2.2
1	J	0	SER	2.2
1	K	296	VAL	2.2
1	D	42	SER	2.1
1	K	66	ASP	2.1
1	A	42	SER	2.1
1	C	288	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no 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.

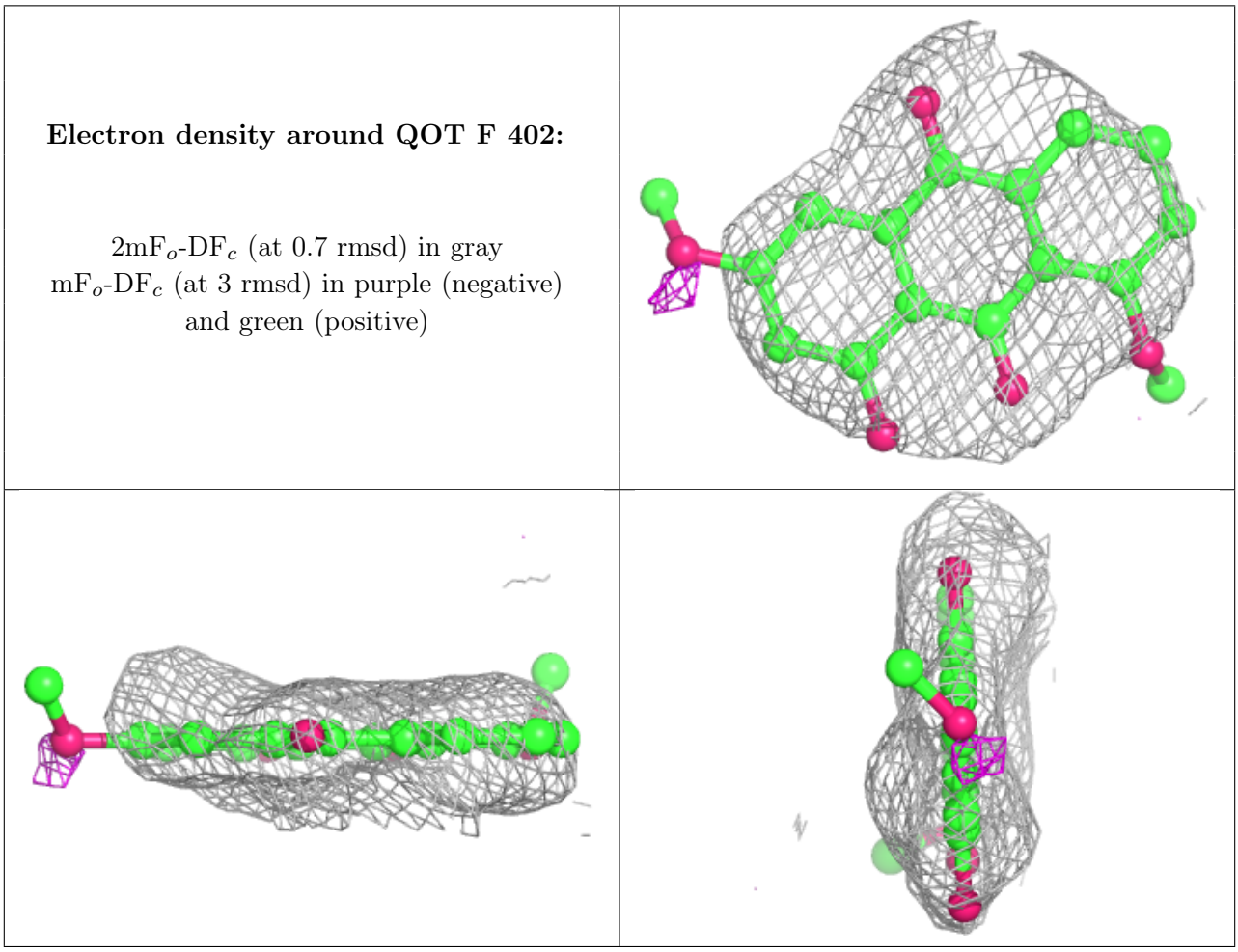
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NA	H	403	1/1	0.60	0.20	66,66,66,66	0
4	CL	C	404	1/1	0.72	0.13	69,69,69,69	0
3	QOT	F	402	21/21	0.76	0.30	94,95,96,97	0
4	CL	A	403	1/1	0.80	0.28	98,98,98,98	0
3	QOT	H	402	21/21	0.81	0.24	65,67,69,70	0
3	QOT	D	402	21/21	0.81	0.24	82,83,84,86	0
3	QOT	C	402	21/21	0.82	0.28	82,83,84,84	0
3	QOT	I	402	21/21	0.84	0.17	69,70,71,71	0
3	QOT	A	402	21/21	0.86	0.20	69,69,70,71	0
3	QOT	E	402	21/21	0.86	0.26	79,80,80,81	0
3	QOT	B	402	21/21	0.87	0.26	76,77,78,80	0
2	SAH	L	900	26/26	0.88	0.17	74,77,82,82	0
5	GOL	D	403	6/6	0.89	0.15	65,66,66,67	0
3	QOT	G	402	21/21	0.90	0.22	82,82,83,84	0
5	GOL	C	403	6/6	0.90	0.14	51,51,51,51	0
4	CL	C	406	1/1	0.91	0.07	69,69,69,69	0
2	SAH	C	401	26/26	0.91	0.14	66,68,69,69	0
2	SAH	H	401	26/26	0.92	0.13	49,50,51,52	0
6	NA	K	402	1/1	0.92	0.47	59,59,59,59	0
2	SAH	J	900	26/26	0.93	0.15	53,55,56,56	0
2	SAH	K	401	26/26	0.94	0.15	62,63,65,65	0
2	SAH	E	401	26/26	0.94	0.12	46,46,47,48	0
2	SAH	F	401	26/26	0.94	0.12	53,54,56,56	0
2	SAH	B	401	26/26	0.94	0.12	49,50,52,52	0
2	SAH	I	401	26/26	0.94	0.15	46,47,48,48	0
2	SAH	A	401	26/26	0.94	0.12	42,43,46,46	0
4	CL	C	405	1/1	0.95	0.05	77,77,77,77	0
2	SAH	D	401	26/26	0.95	0.12	43,44,45,45	0
2	SAH	G	401	26/26	0.95	0.11	48,49,53,53	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.

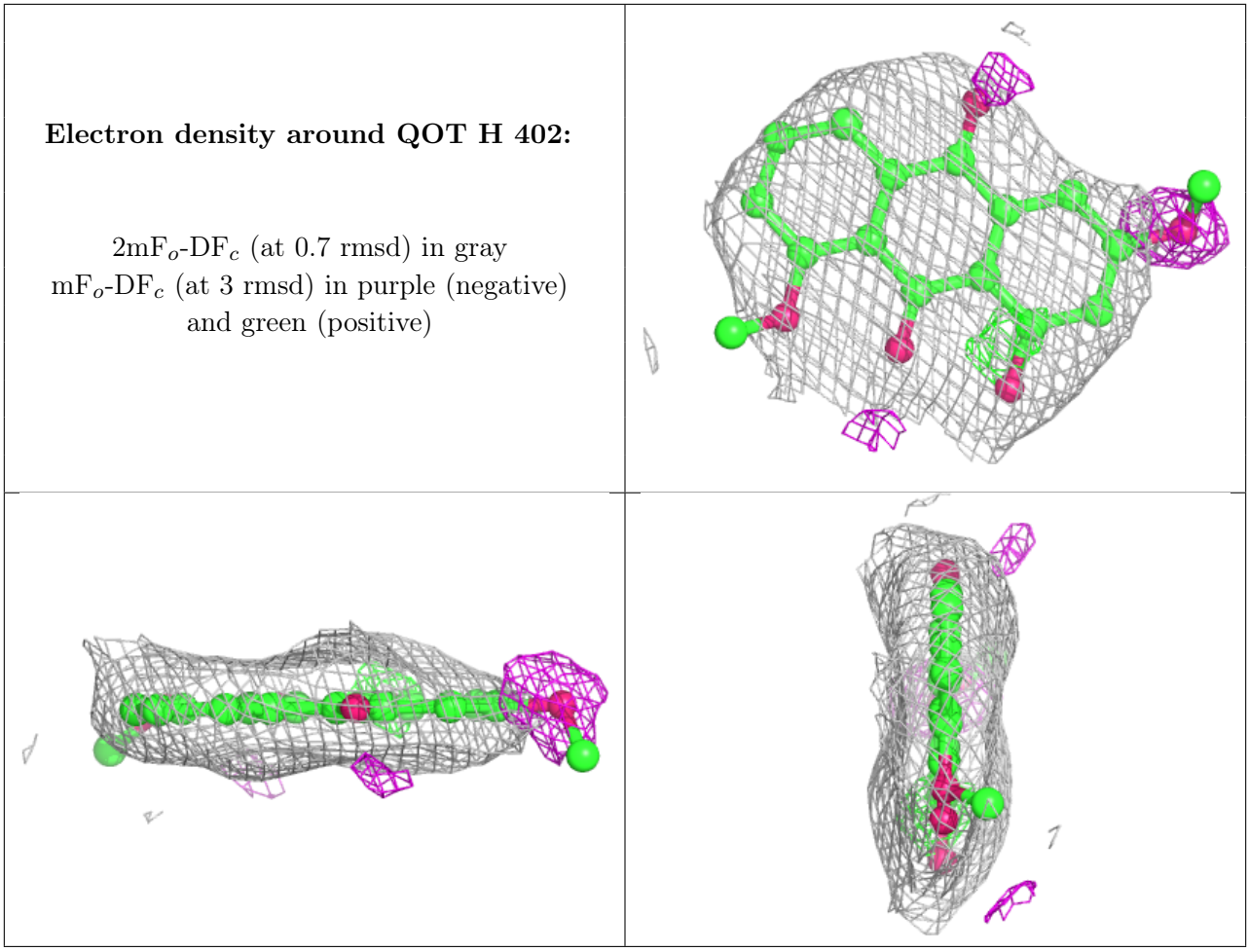
Electron density around QOT F 402:

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



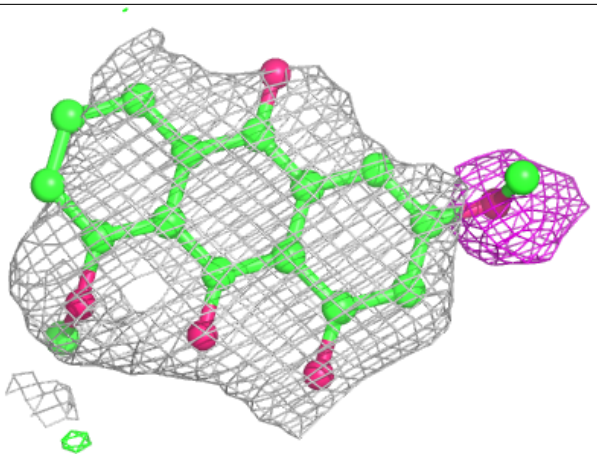
Electron density around QOT H 402:

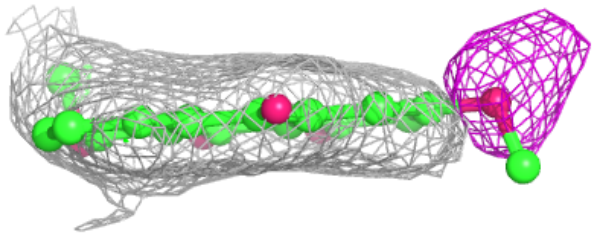
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

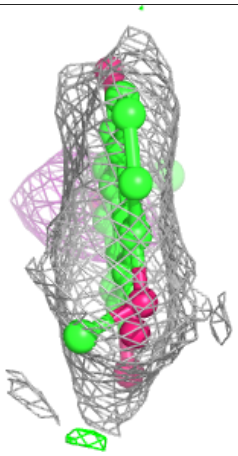


Electron density around QOT D 402:

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

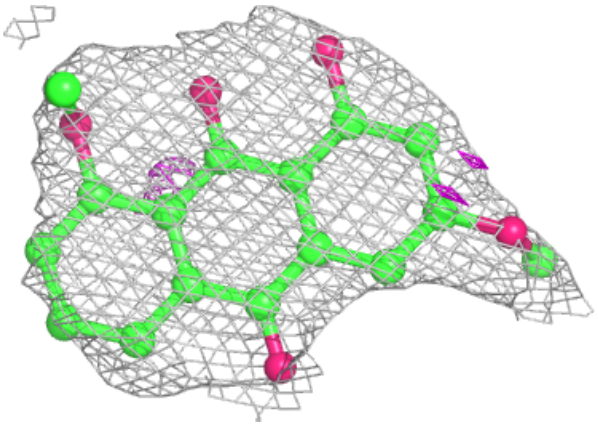


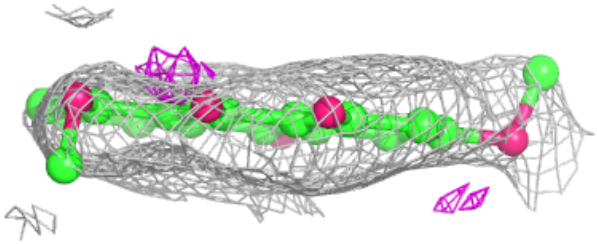


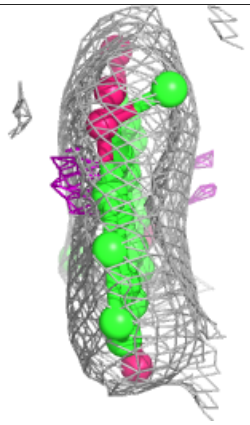


Electron density around QOT C 402:

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

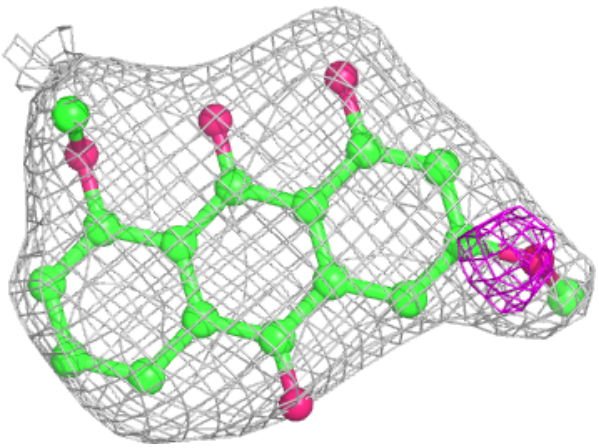


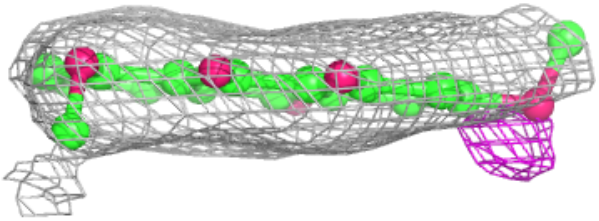


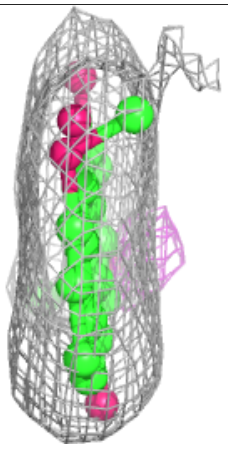


Electron density around QOT I 402:

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

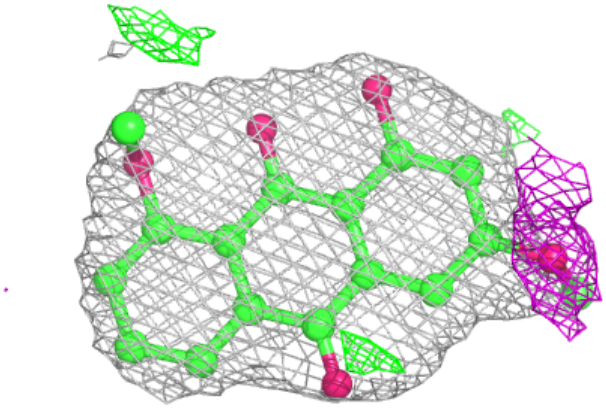


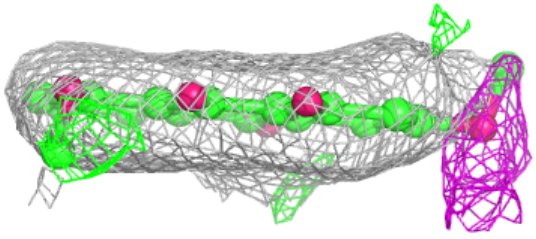


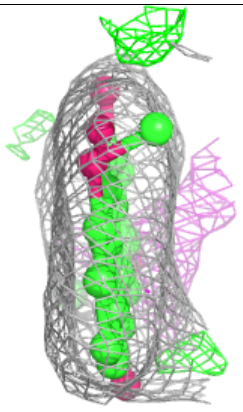


Electron density around QOT A 402:

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

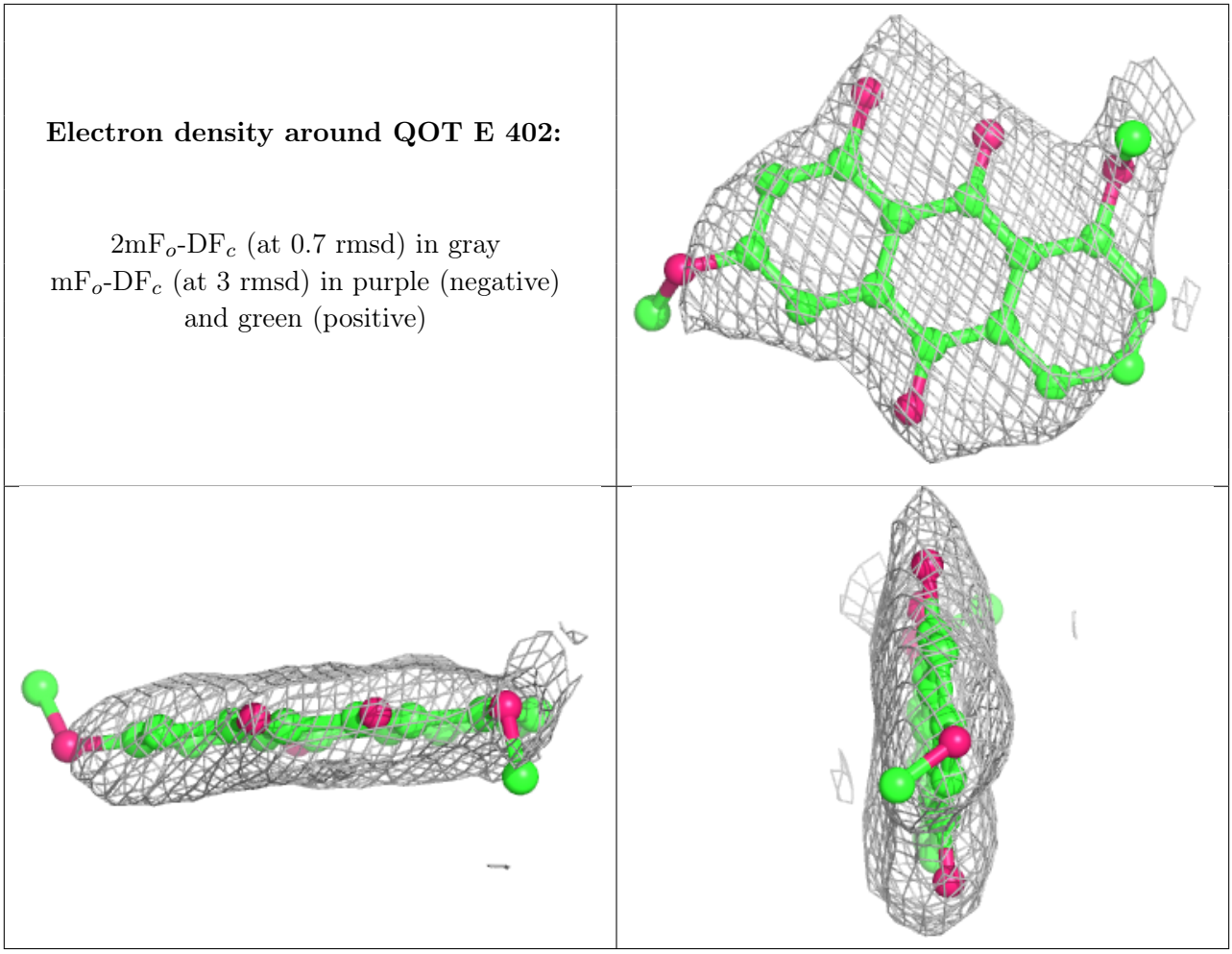






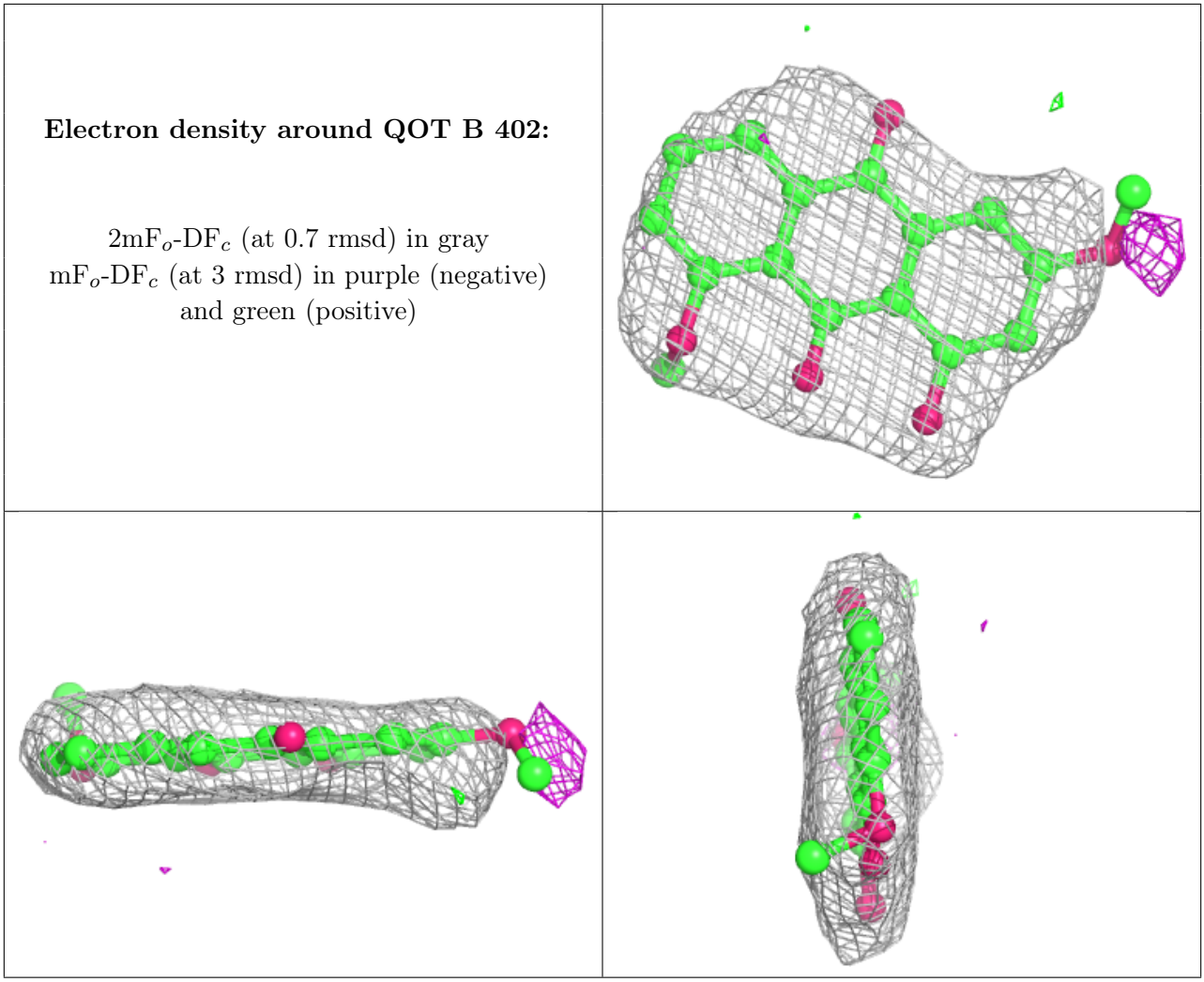
Electron density around QOT E 402:

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



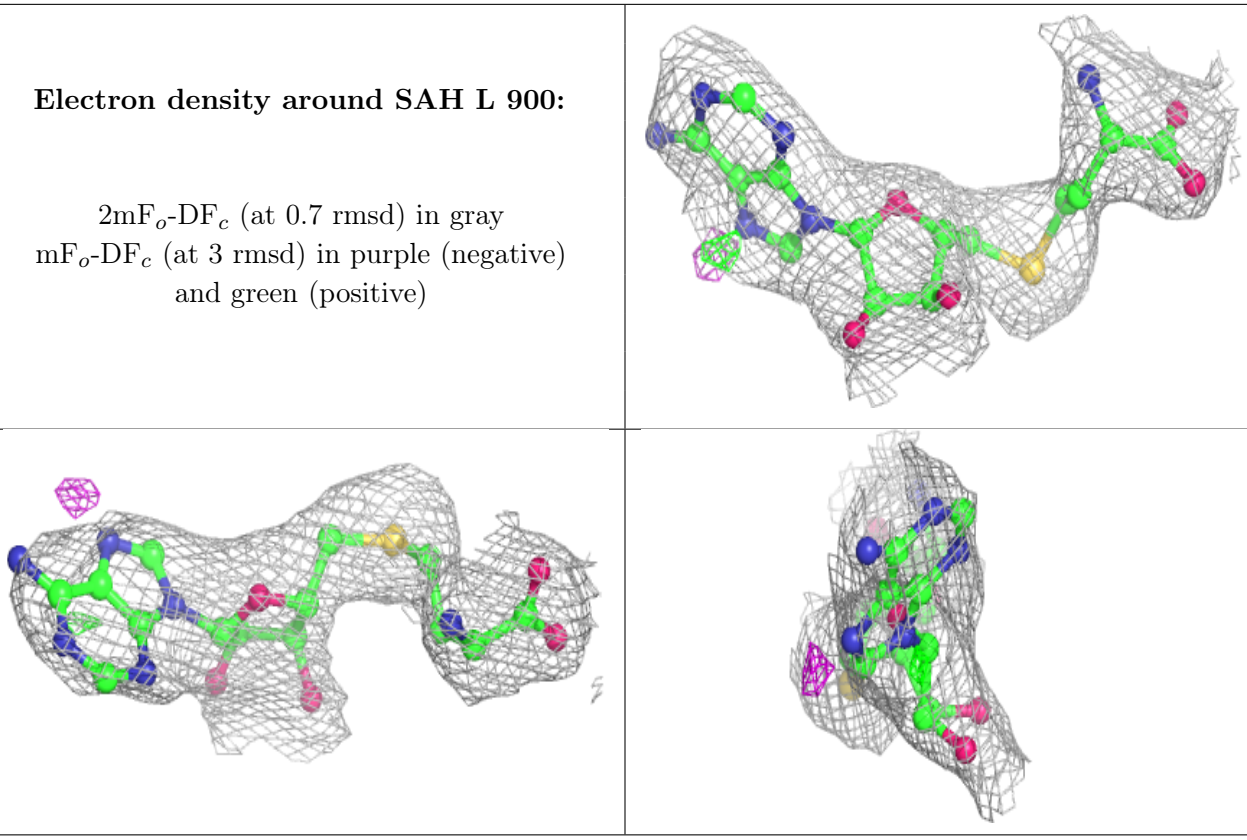
Electron density around QOT B 402:

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



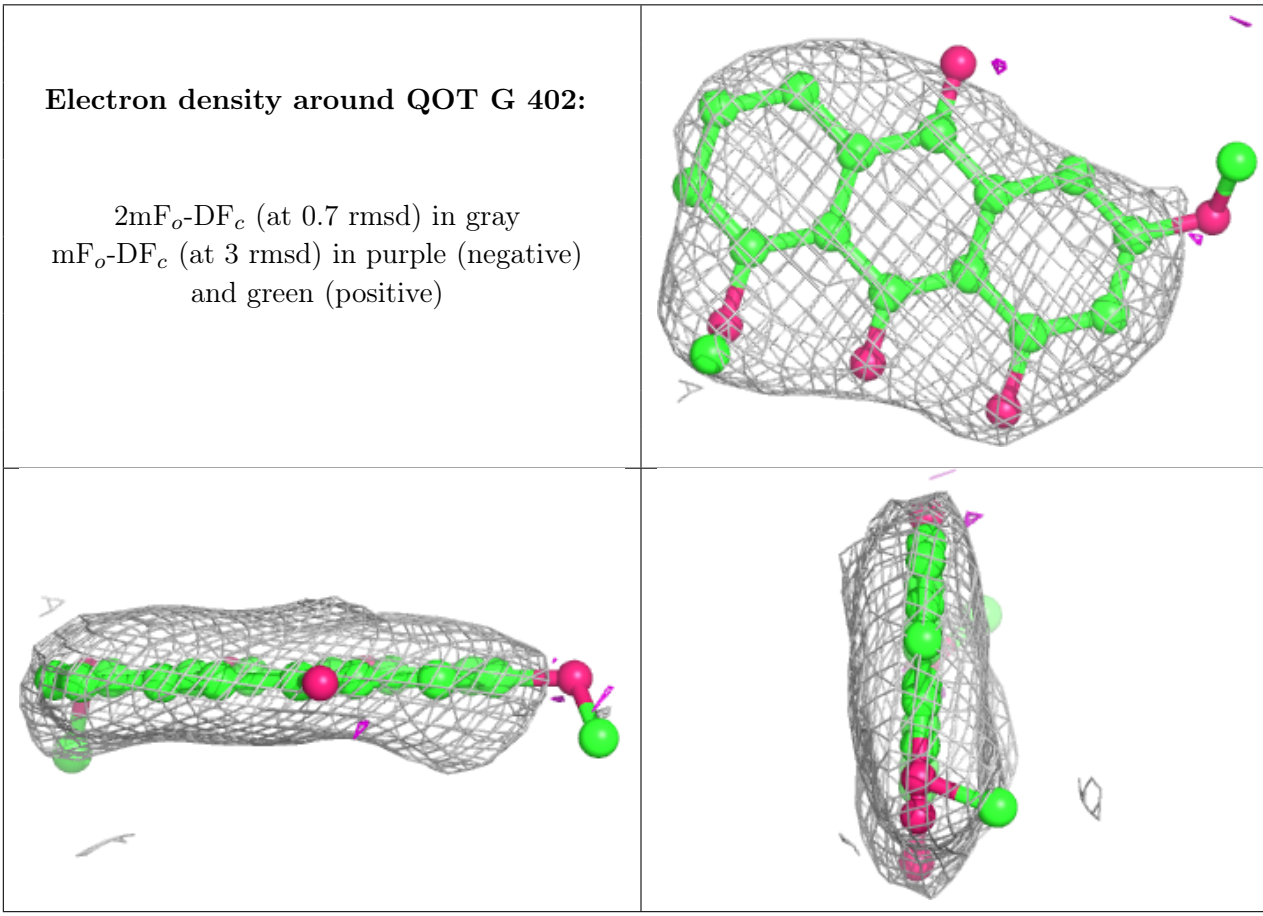
Electron density around SAH L 900:

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



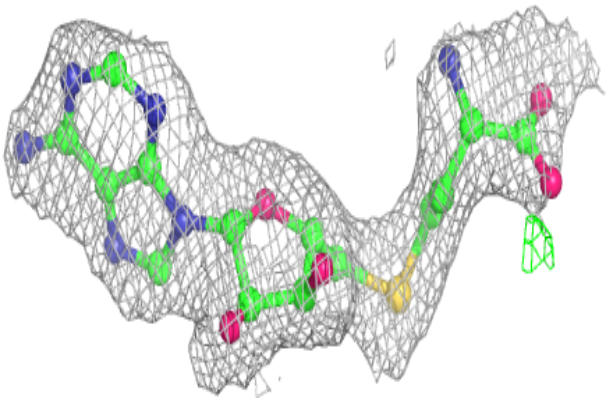
Electron density around QOT G 402:

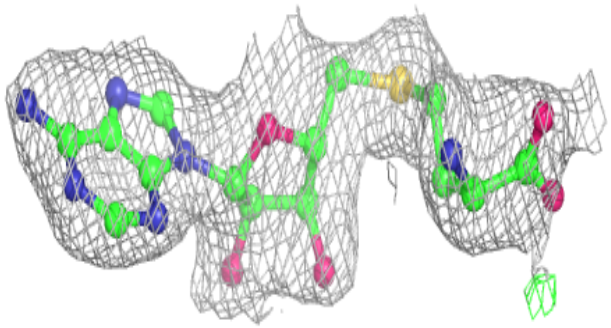
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

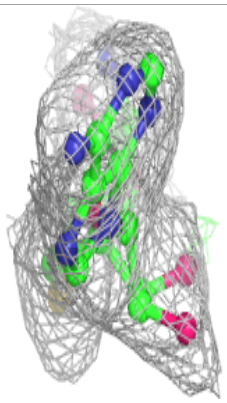


Electron density around SAH C 401:

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

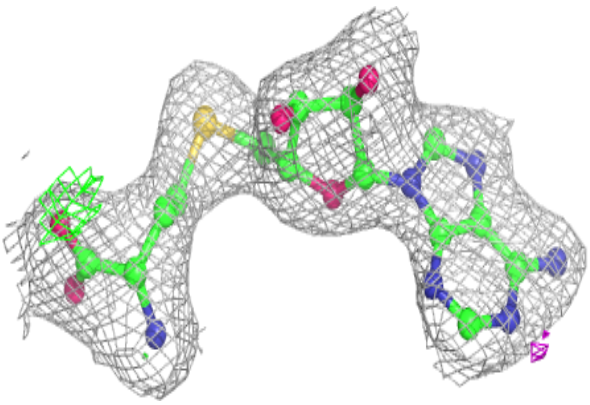


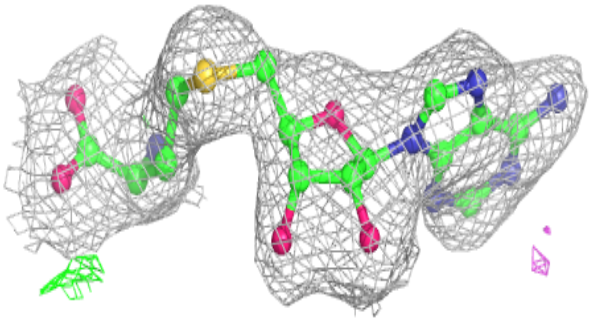


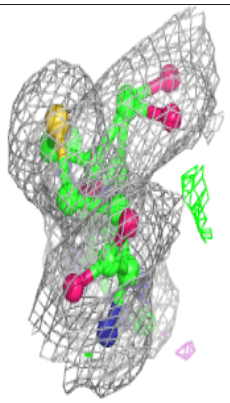


Electron density around SAH H 401:

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

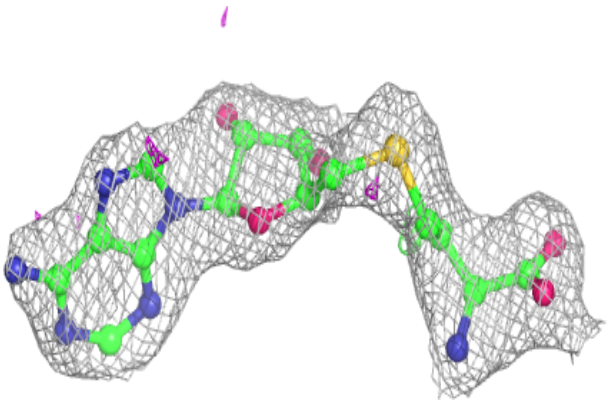


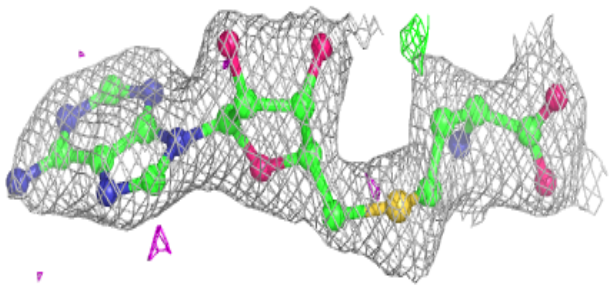


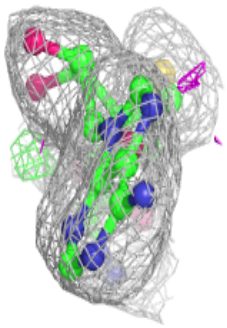


Electron density around SAH J 900:

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

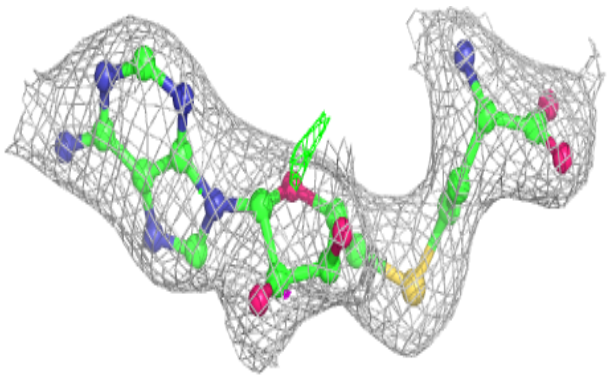


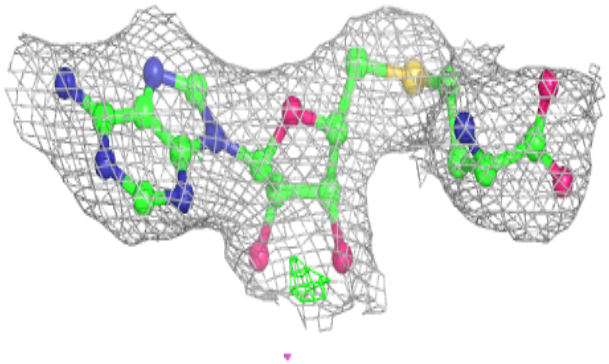


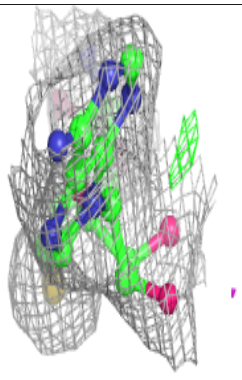


Electron density around SAH K 401:

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

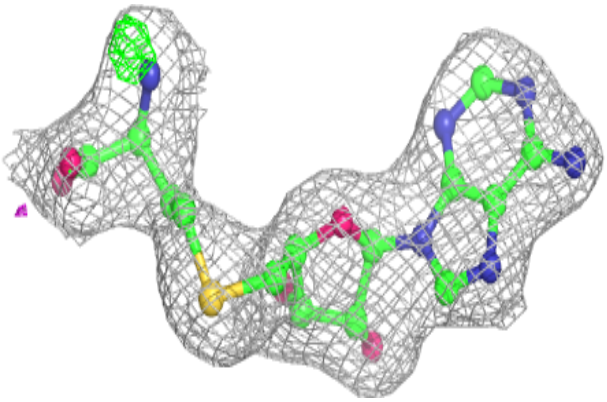


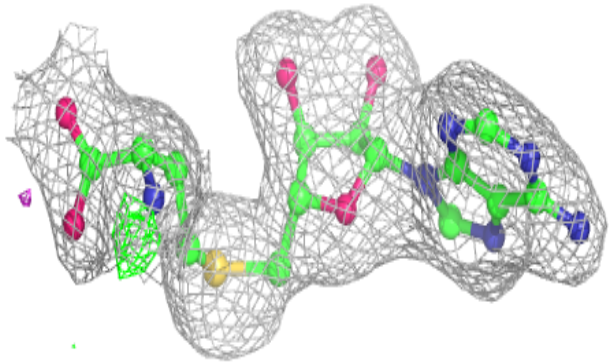


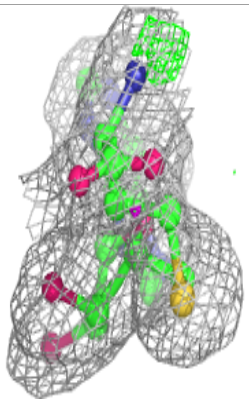


Electron density around SAH E 401:

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

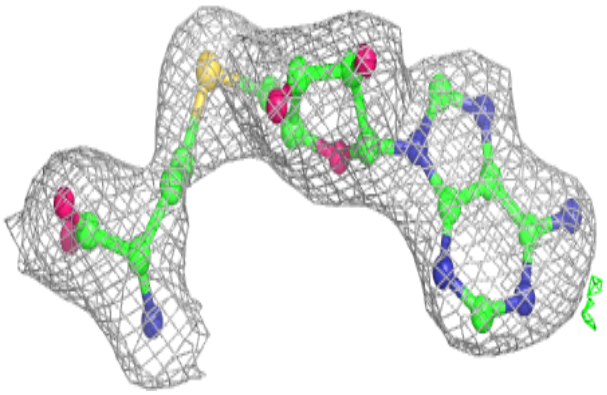


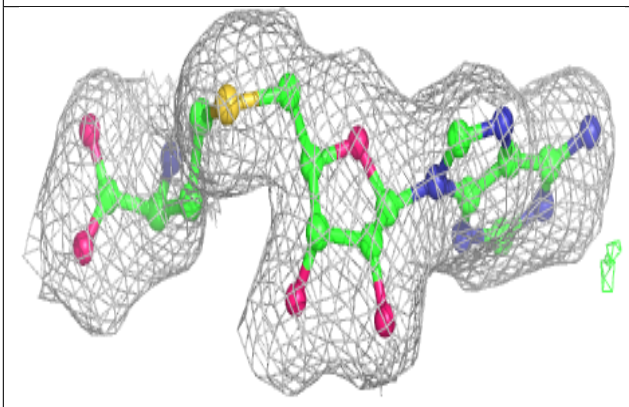


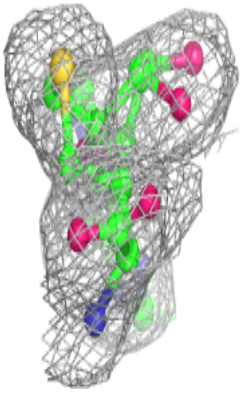


Electron density around SAH F 401:

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

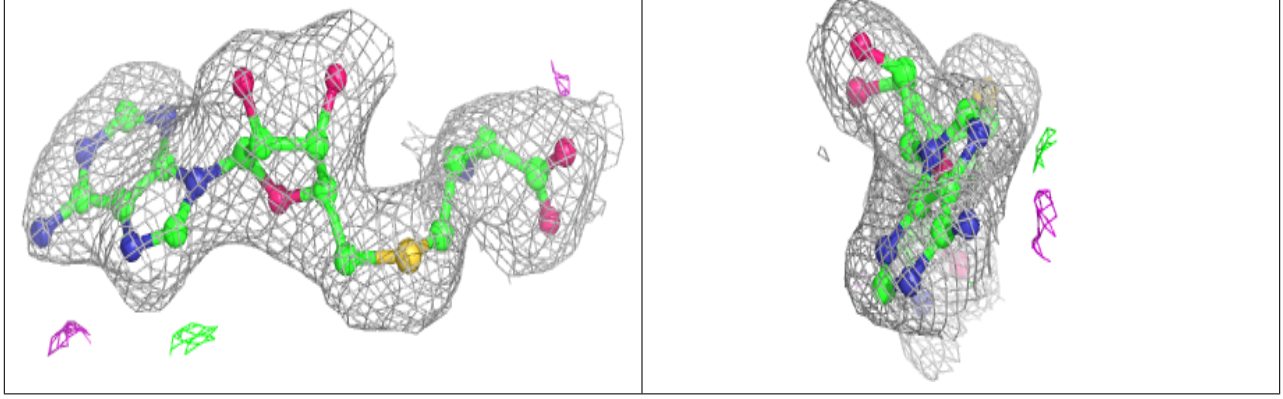






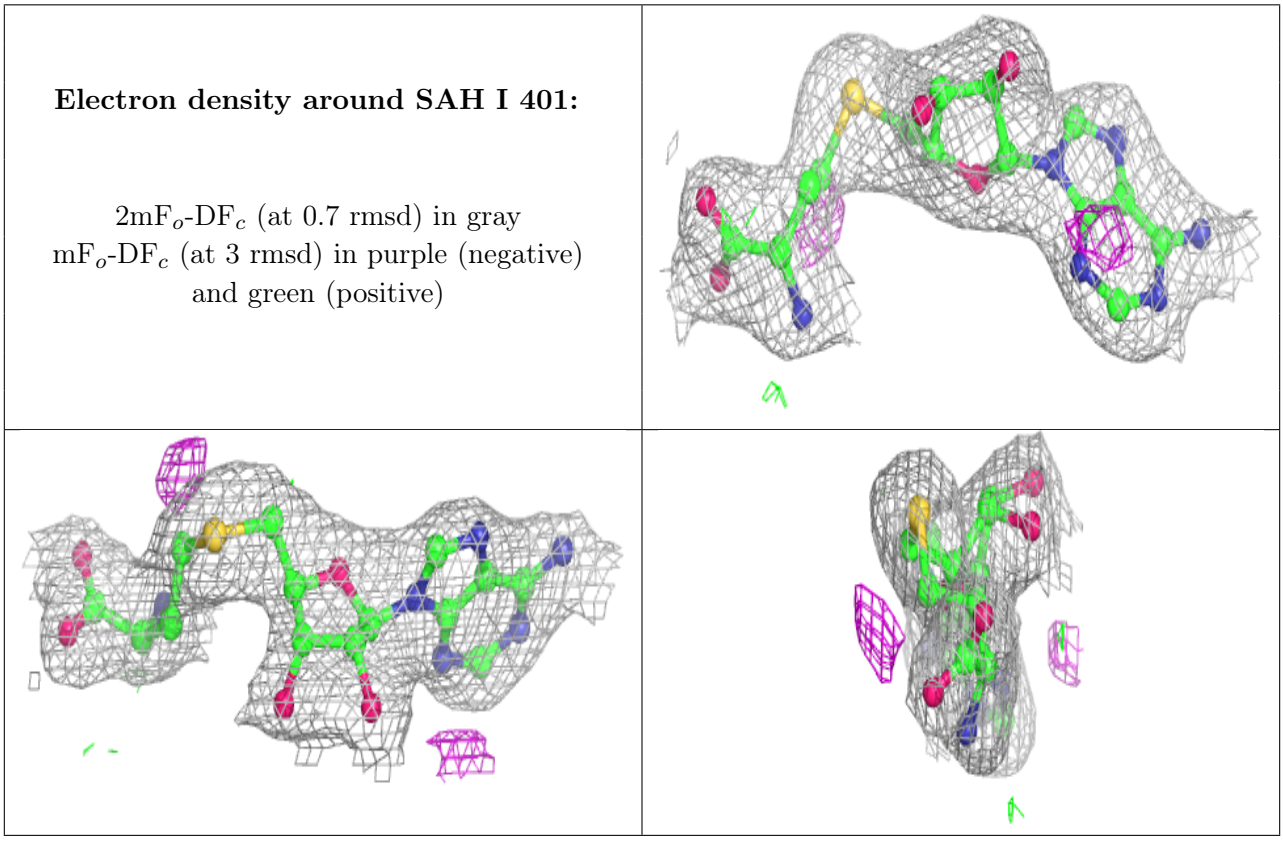
Electron density around SAH B 401:

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



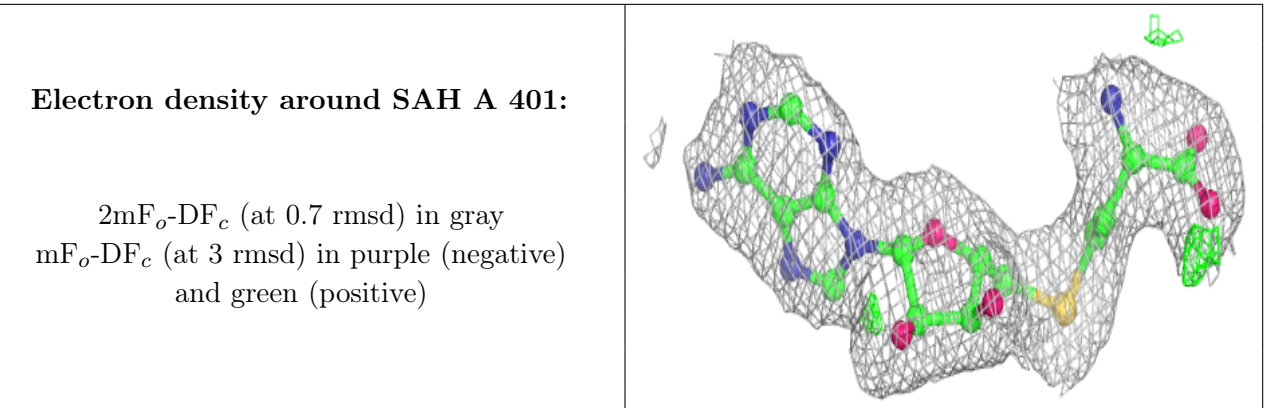
Electron density around SAH I 401:

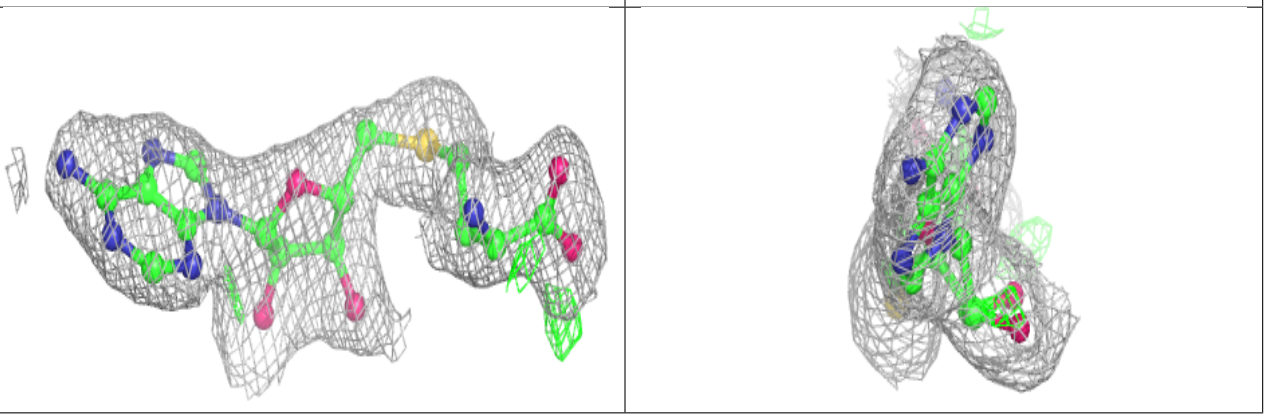
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around SAH A 401:

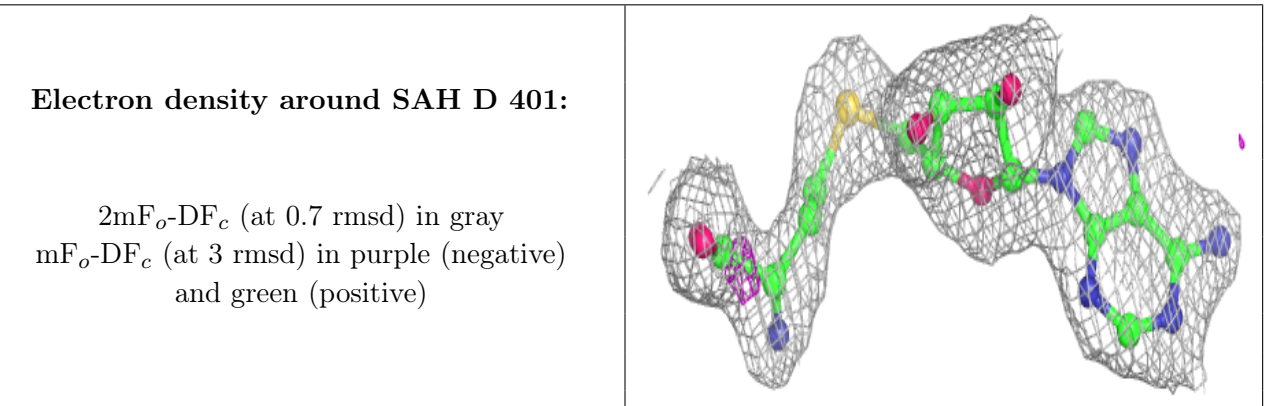
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

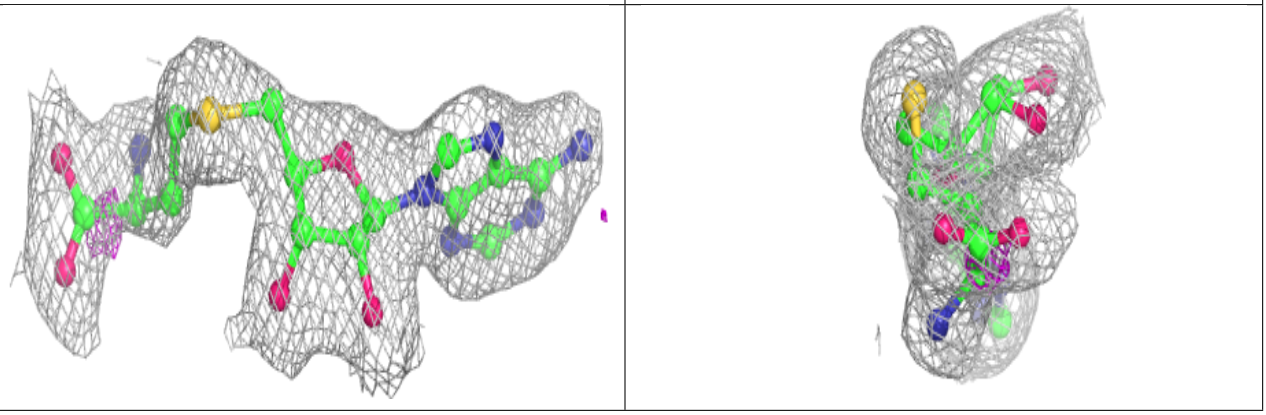




Electron density around SAH D 401:

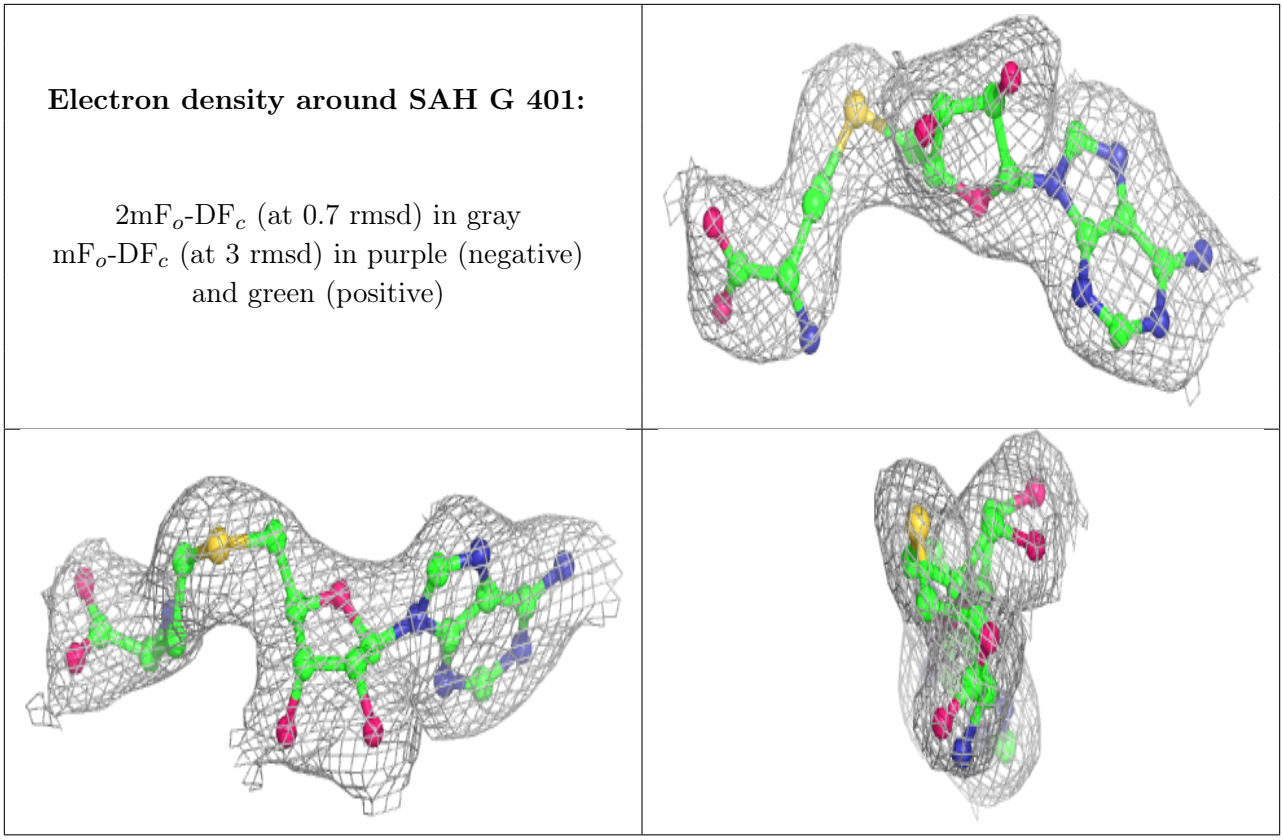
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around SAH G 401:

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



6.5 Other polymers (i)

There are no such residues in this entry.