Full wwPDB X-ray Structure Validation Report ⓘ

Aug 19, 2024 – 12:31 PM JST

PDB ID	:	8XTG
Title	:	Crystal structure of methyltransferase MpaG' in complex with SAH and DMMPA
Authors	:	You, C.; Pan, Y.J.; Li, S.Y.; Feng, Y.G.
Deposited on	:	2024-01-10
Resolution	:	2.00 Å(reported)

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

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

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

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

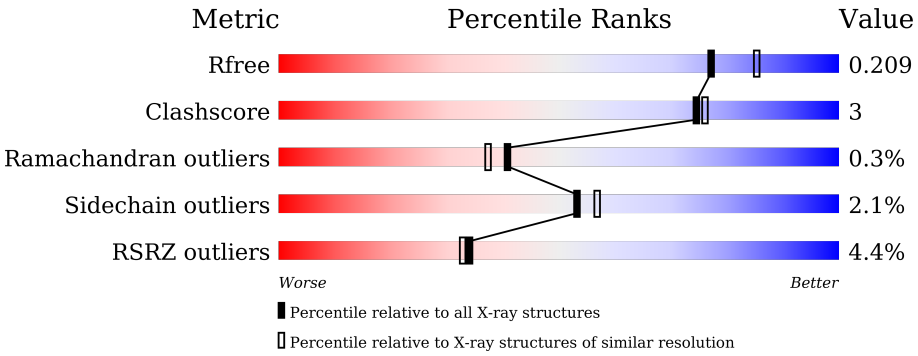
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	400	88% 10%
1	B	400	89% 10%
1	C	400	90% 8%
1	D	400	89% 10%
1	E	400	9% 86% 12%
1	F	400	11% 87% 10%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 20311 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 O-methyltransferase mpaG'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	0	0
			3048	1932	526	579	11			
1	B	395	Total	C	N	O	S	0	1	0
			3061	1940	528	581	12			
1	C	393	Total	C	N	O	S	0	0	0
			3042	1929	525	577	11			
1	D	395	Total	C	N	O	S	0	0	0
			3053	1935	527	580	11			
1	E	391	Total	C	N	O	S	0	0	0
			3030	1921	523	575	11			
1	F	389	Total	C	N	O	S	0	0	0
			3013	1912	521	569	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0A0B5L781
A	0	ALA	-	expression tag	UNP A0A0B5L781
A	1	MET	-	expression tag	UNP A0A0B5L781
A	2	GLY	-	expression tag	UNP A0A0B5L781
B	-1	GLY	-	expression tag	UNP A0A0B5L781
B	0	ALA	-	expression tag	UNP A0A0B5L781
B	1	MET	-	expression tag	UNP A0A0B5L781
B	2	GLY	-	expression tag	UNP A0A0B5L781
C	-1	GLY	-	expression tag	UNP A0A0B5L781
C	0	ALA	-	expression tag	UNP A0A0B5L781
C	1	MET	-	expression tag	UNP A0A0B5L781
C	2	GLY	-	expression tag	UNP A0A0B5L781
D	-1	GLY	-	expression tag	UNP A0A0B5L781
D	0	ALA	-	expression tag	UNP A0A0B5L781
D	1	MET	-	expression tag	UNP A0A0B5L781
D	2	GLY	-	expression tag	UNP A0A0B5L781
E	-1	GLY	-	expression tag	UNP A0A0B5L781

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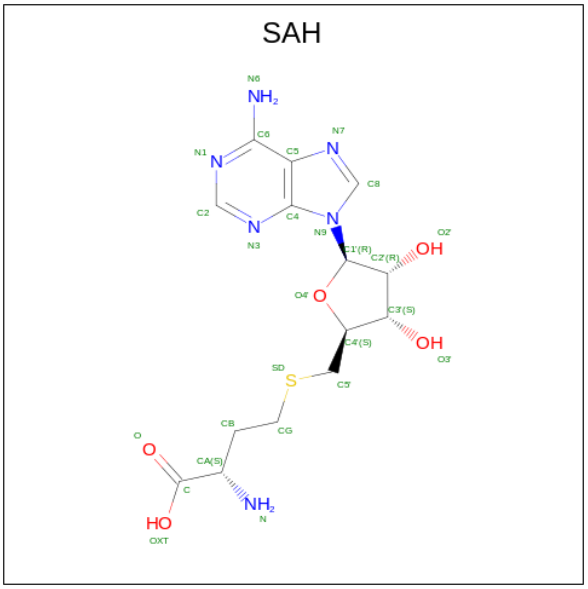
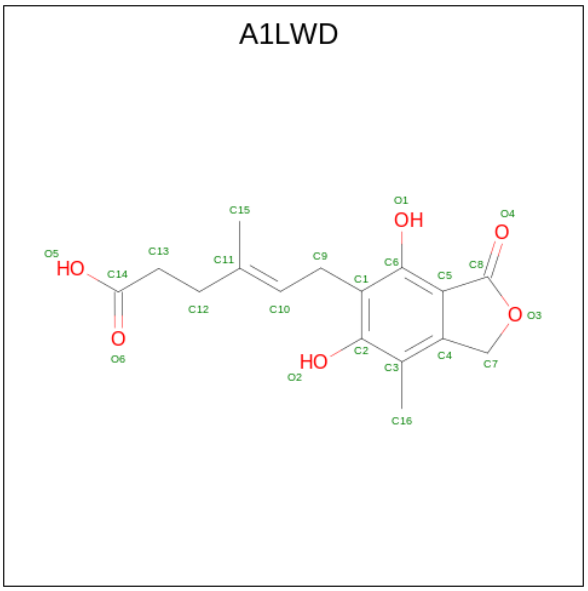
Chain	Residue	Modelled	Actual	Comment	Reference
E	0	ALA	-	expression tag	UNP A0A0B5L781
E	1	MET	-	expression tag	UNP A0A0B5L781
E	2	GLY	-	expression tag	UNP A0A0B5L781
F	-1	GLY	-	expression tag	UNP A0A0B5L781
F	0	ALA	-	expression tag	UNP A0A0B5L781
F	1	MET	-	expression tag	UNP A0A0B5L781
F	2	GLY	-	expression tag	UNP A0A0B5L781

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



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

- Molecule 3 is O-desmethyl mycophenolic acid (three-letter code: A1LWD) (formula: $C_{16}H_{18}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 22 16 6	0	0
3	B	1	Total C O 22 16 6	0	0
3	C	1	Total C O 22 16 6	0	0
3	D	1	Total C O 22 16 6	0	0
3	E	1	Total C O 22 16 6	0	0
3	F	1	Total C O 22 16 6	0	0

- Molecule 4 is water.

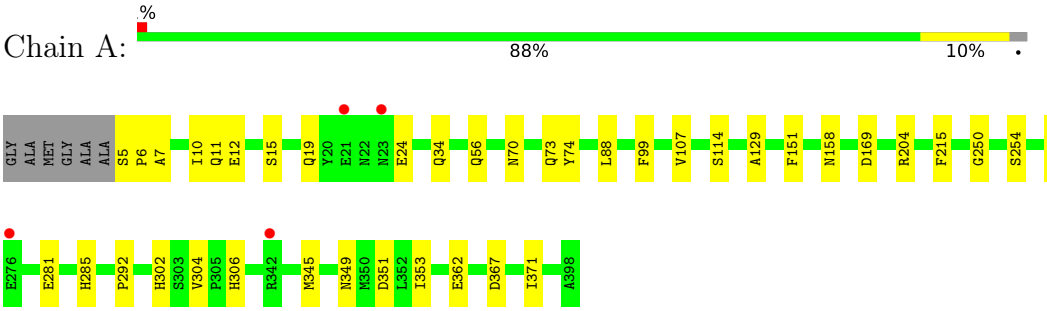
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	382	Total O 382 382	0	0
4	B	407	Total O 407 407	0	0
4	C	383	Total O 383 383	0	0
4	D	356	Total O 356 356	0	0
4	E	142	Total O 142 142	0	0
4	F	106	Total O 106 106	0	0

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.

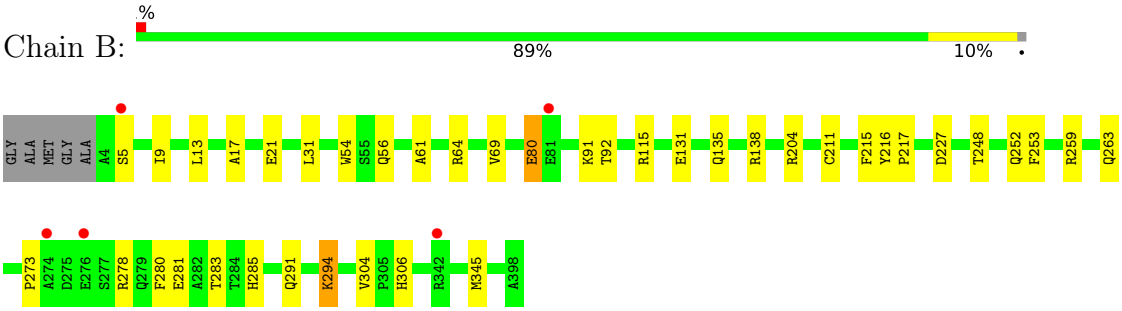
• Molecule 1: O-methyltransferase mpaG'

Chain A:



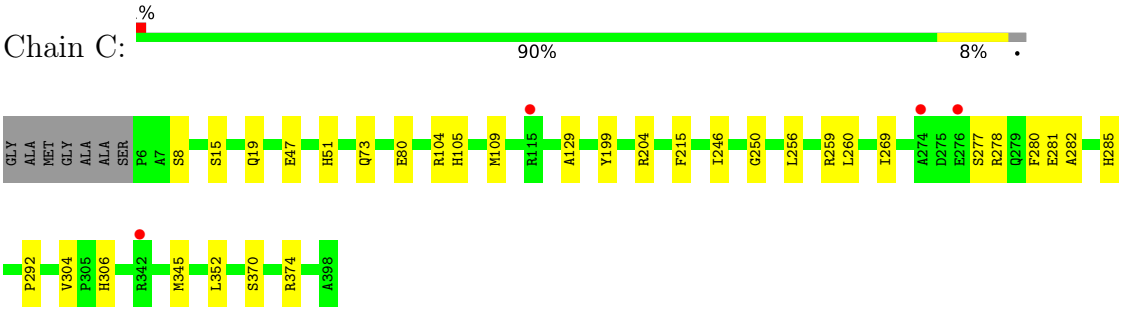
• Molecule 1: O-methyltransferase mpaG'

Chain B:



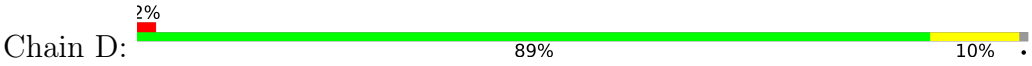
• Molecule 1: O-methyltransferase mpaG'

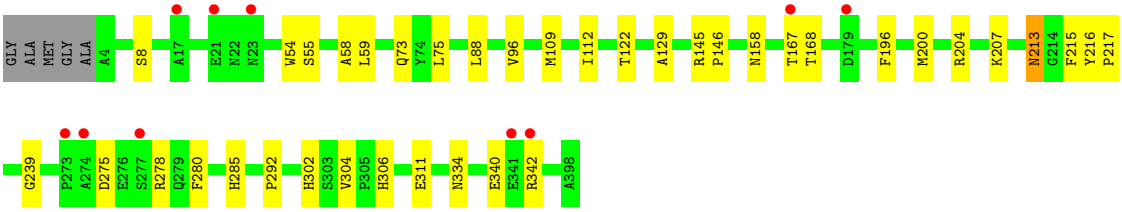
Chain C:



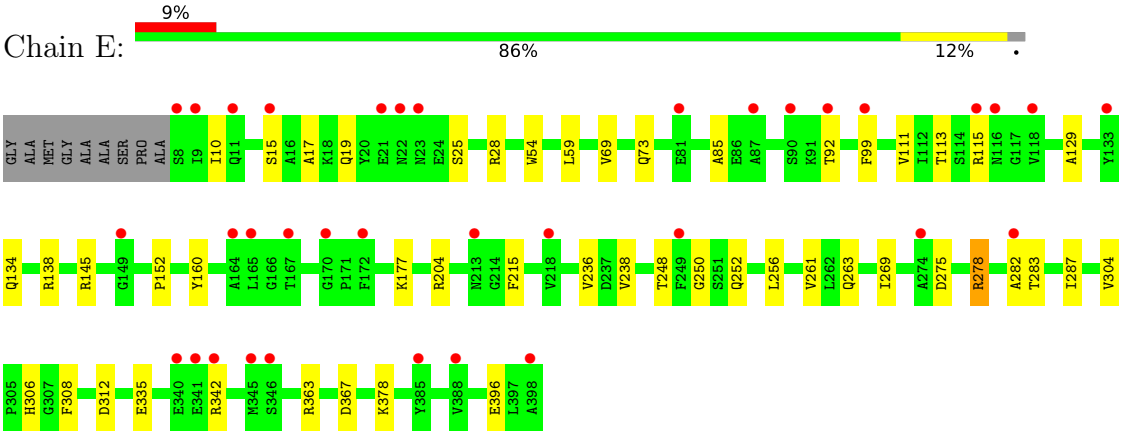
• Molecule 1: O-methyltransferase mpaG'

Chain D:

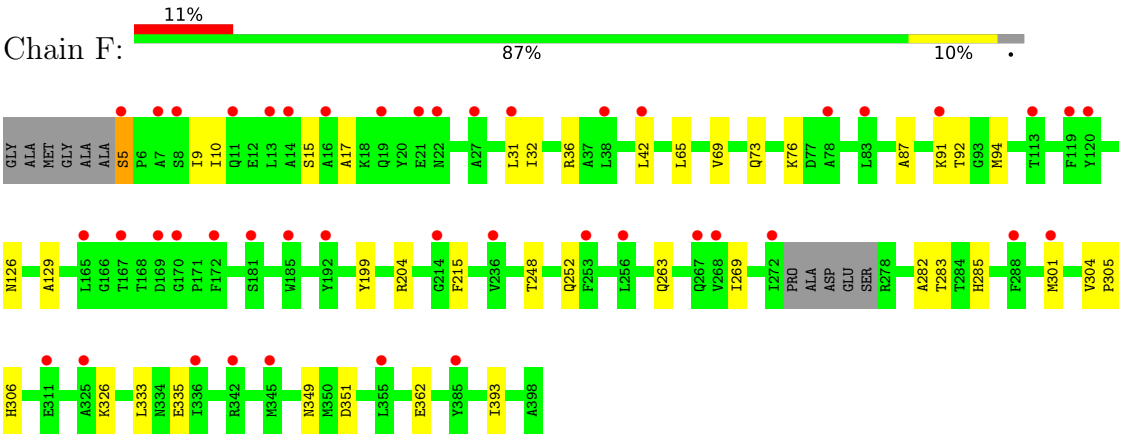




• Molecule 1: O-methyltransferase mpaG'



• Molecule 1: O-methyltransferase mpaG'



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	199.54Å 199.54Å 67.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.93 – 2.00 47.93 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.93-2.00) 99.9 (47.93-2.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	153.50 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.162 , 0.211 0.160 , 0.209	Depositor DCC
R_{free} test set	10410 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	23.4	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 31.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l 0.389 for h,-h-k,-l 0.028 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	20311	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 3.06% 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: A1LWD, SAH

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.29	0/3120	0.51	0/4239
1	B	0.28	0/3133	0.52	0/4256
1	C	0.28	0/3114	0.51	0/4230
1	D	0.28	0/3125	0.51	0/4246
1	E	0.27	0/3101	0.48	0/4212
1	F	0.27	0/3083	0.48	0/4186
All	All	0.28	0/18676	0.50	0/25369

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	3048	0	2967	23	0
1	B	3061	0	2980	22	0
1	C	3042	0	2963	19	0
1	D	3053	0	2972	26	0
1	E	3030	0	2950	26	0
1	F	3013	0	2939	21	0
2	A	26	0	19	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	26	0	19	0	0
2	C	26	0	19	0	0
2	D	26	0	19	2	0
2	E	26	0	19	0	0
2	F	26	0	19	1	0
3	A	22	0	0	0	0
3	B	22	0	0	0	0
3	C	22	0	0	0	0
3	D	22	0	0	0	0
3	E	22	0	0	0	0
3	F	22	0	0	0	0
4	A	382	0	0	2	0
4	B	407	0	0	2	0
4	C	383	0	0	1	0
4	D	356	0	0	4	0
4	E	142	0	0	2	0
4	F	106	0	0	0	0
All	All	20311	0	17885	118	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 3.

All (118) 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:D:73:GLN:HG3	1:D:129:ALA:HB1	1.68	0.75
1:C:73:GLN:HG3	1:C:129:ALA:HB1	1.71	0.73
1:D:145:ARG:NH2	4:D:504:HOH:O	2.26	0.68
1:F:301:MET:HE3	1:F:305:PRO:HD3	1.76	0.65
1:C:345:MET:HG3	1:D:109:MET:HE3	1.80	0.64
1:E:145:ARG:NH2	4:E:505:HOH:O	2.32	0.61
1:B:291:GLN:O	1:B:294:LYS:NZ	2.30	0.61
1:D:167:THR:HG23	1:D:168:THR:HG23	1.83	0.61
1:C:47:GLU:OE2	1:D:207:LYS:NZ	2.35	0.59
1:C:278:ARG:HD2	1:C:280:PHE:CZ	2.38	0.59
1:A:56:GLN:NE2	4:A:509:HOH:O	2.32	0.57
1:A:367:ASP:O	1:A:371:ILE:HD12	2.05	0.57
1:E:275:ASP:HB3	1:E:278:ARG:HB3	1.87	0.56
1:F:269:ILE:HG23	1:F:282:ALA:HB1	1.87	0.55
1:E:54:TRP:HE1	1:F:199:TYR:HH	1.54	0.55
1:D:213:ASN:ND2	4:D:520:HOH:O	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:GLN:HB3	1:B:285:HIS:HB3	1.90	0.53
1:E:308:PHE:HB3	1:E:312:ASP:HB2	1.91	0.53
1:A:7:ALA:O	1:A:11:GLN:HG3	2.09	0.53
1:D:278:ARG:HD2	1:D:280:PHE:CZ	2.45	0.52
1:C:345:MET:HE3	1:D:55:SER:OG	2.10	0.51
1:B:80:GLU:H	1:B:80:GLU:CD	2.14	0.51
1:C:269:ILE:HG23	1:C:282:ALA:HB1	1.93	0.51
1:E:269:ILE:HG23	1:E:282:ALA:HB1	1.93	0.50
1:C:259:ARG:HD2	1:C:281:GLU:OE2	2.12	0.50
1:A:285:HIS:CE1	1:A:292:PRO:HD3	2.46	0.49
1:B:13:LEU:HD12	1:B:31:LEU:HD12	1.93	0.49
1:E:152:PRO:HA	1:F:65:LEU:HD12	1.93	0.49
1:B:17:ALA:O	1:B:21:GLU:HG3	2.11	0.49
1:E:363:ARG:HB3	1:E:367:ASP:HB2	1.94	0.49
1:E:248:THR:O	1:E:252:GLN:HG3	2.11	0.48
1:A:70:ASN:HB3	1:A:74:TYR:CE2	2.48	0.48
1:A:19:GLN:HB3	1:A:24:GLU:OE1	2.13	0.48
1:A:302:HIS:O	2:A:401:SAH:N	2.47	0.48
1:A:6:PRO:O	1:A:10:ILE:HG13	2.14	0.47
1:C:199:TYR:HH	1:D:54:TRP:HE1	1.62	0.47
1:B:259:ARG:HD2	1:B:281:GLU:OE2	2.14	0.47
1:D:75:LEU:HD21	1:D:88:LEU:HD11	1.96	0.47
1:B:263:GLN:HA	1:B:283:THR:O	2.14	0.47
1:F:87:ALA:O	1:F:91:LYS:HG3	2.14	0.47
1:D:239:GLY:O	2:D:401:SAH:N	2.48	0.47
1:E:160:TYR:HB3	1:F:94:MET:HG2	1.97	0.47
1:C:285:HIS:CE1	1:C:292:PRO:HD3	2.49	0.46
1:E:85:ALA:HA	1:E:99:PHE:HE2	1.80	0.46
1:F:285:HIS:O	2:F:401:SAH:H2	2.16	0.46
1:F:69:VAL:HB	1:F:92:THR:HB	1.96	0.46
1:F:32:ILE:O	1:F:36:ARG:HG3	2.16	0.46
1:C:345:MET:HG3	1:D:109:MET:CE	2.45	0.46
1:E:73:GLN:HG3	1:E:129:ALA:HB1	1.98	0.46
1:E:238:VAL:HG12	1:E:287:ILE:HG22	1.98	0.46
1:F:73:GLN:HG3	1:F:129:ALA:HB1	1.98	0.46
1:A:285:HIS:O	2:A:401:SAH:H2	2.16	0.45
1:E:335:GLU:OE1	4:E:501:HOH:O	2.21	0.45
1:A:259:ARG:HD2	1:A:281:GLU:OE2	2.16	0.45
1:F:333:LEU:HB3	1:F:393:ILE:HB	1.99	0.45
1:A:151:PHE:HB2	1:B:61:ALA:HB1	1.99	0.44
1:B:273:PRO:O	1:B:278:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:76:LYS:HD2	1:F:126:ASN:HB3	1.99	0.44
1:B:131:GLU:HG3	1:B:135:GLN:HE21	1.82	0.44
1:A:351:ASP:HA	1:A:362:GLU:HG2	2.00	0.44
1:F:5:SER:O	1:F:9:ILE:HG13	2.17	0.44
1:C:15:SER:O	1:C:19:GLN:HG3	2.17	0.44
1:E:378:LYS:NZ	1:E:396:GLU:OE2	2.49	0.44
1:C:105:HIS:O	1:C:109:MET:HG2	2.17	0.44
1:F:305:PRO:HD2	1:F:335:GLU:OE2	2.18	0.44
1:B:64:ARG:CZ	1:B:138:ARG:HG2	2.48	0.44
1:A:107:VAL:HG21	1:A:114:SER:HB2	1.99	0.43
1:D:59:LEU:HD13	1:D:109:MET:HG3	2.00	0.43
1:D:96:VAL:HG23	4:D:669:HOH:O	2.18	0.43
1:D:275:ASP:HB3	1:D:278:ARG:HB2	2.01	0.43
1:B:211:CYS:HB2	1:B:253:PHE:HE2	1.84	0.43
1:A:56:GLN:NE2	1:B:56:GLN:HG3	2.33	0.43
1:A:259:ARG:NH2	4:A:538:HOH:O	2.52	0.43
1:E:28:ARG:NH1	1:F:42:LEU:O	2.52	0.43
1:D:302:HIS:HD2	1:D:334:ASN:O	2.02	0.42
1:E:134:GLN:O	1:E:138:ARG:HG3	2.19	0.42
1:B:91:LYS:NZ	4:B:555:HOH:O	2.52	0.42
1:F:263:GLN:HA	1:F:283:THR:O	2.19	0.42
1:F:351:ASP:HA	1:F:362:GLU:HG2	2.01	0.42
1:F:248:THR:O	1:F:252:GLN:HG3	2.20	0.42
1:B:216:TYR:CD1	1:B:217:PRO:HD2	2.54	0.42
1:B:248:THR:O	1:B:252:GLN:HG3	2.19	0.42
1:C:246:ILE:HD11	1:C:260:LEU:HB3	2.00	0.42
1:C:370:SER:O	1:C:374:ARG:HD3	2.19	0.42
1:D:340:GLU:OE2	4:D:501:HOH:O	2.21	0.42
1:C:51:HIS:ND1	4:C:507:HOH:O	2.34	0.41
1:D:216:TYR:CD1	1:D:217:PRO:HD2	2.55	0.41
1:E:236:VAL:HG22	1:E:261:VAL:HB	2.01	0.41
1:A:15:SER:O	1:A:19:GLN:HG3	2.20	0.41
1:E:113:THR:OG1	1:E:115:ARG:NH2	2.53	0.41
1:B:5:SER:O	1:B:9:ILE:HG13	2.20	0.41
1:B:227:ASP:OD2	4:B:501:HOH:O	2.21	0.41
1:C:250:GLY:HA2	1:C:256:LEU:HD21	2.02	0.41
1:D:285:HIS:O	2:D:401:SAH:H2	2.21	0.41
1:D:285:HIS:CE1	1:D:292:PRO:HD3	2.55	0.41
1:A:169:ASP:N	1:A:169:ASP:OD1	2.53	0.41
1:A:12:GLU:HG3	1:A:34:GLN:CD	2.40	0.41
1:A:73:GLN:HG3	1:A:129:ALA:HB1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:GLY:O	1:A:254:SER:OG	2.27	0.41
1:B:278:ARG:HG2	1:B:280:PHE:H	1.86	0.41
1:C:352:LEU:HD12	1:D:58:ALA:HB1	2.02	0.41
1:E:69:VAL:HB	1:E:92:THR:HB	2.03	0.41
1:C:104:ARG:CZ	1:D:340:GLU:HG2	2.51	0.41
1:C:199:TYR:OH	1:D:54:TRP:NE1	2.52	0.41
1:E:10:ILE:HD13	1:F:17:ALA:HB1	2.03	0.41
1:B:69:VAL:HB	1:B:92:THR:HB	2.02	0.40
1:E:17:ALA:HB1	1:F:10:ILE:HD13	2.03	0.40
1:E:59:LEU:HD11	1:E:111:VAL:HG21	2.02	0.40
1:A:349:ASN:HB3	1:B:54:TRP:HE3	1.86	0.40
1:E:263:GLN:HA	1:E:283:THR:O	2.22	0.40
1:E:15:SER:O	1:E:19:GLN:HG3	2.21	0.40
1:A:88:LEU:HD13	1:A:99:PHE:HZ	1.87	0.40
1:A:353:ILE:HG13	1:B:54:TRP:CD2	2.57	0.40
1:D:112:ILE:HA	1:D:122:THR:HG23	2.03	0.40
1:D:196:PHE:O	1:D:200:MET:HG2	2.20	0.40
1:E:54:TRP:HE3	1:F:349:ASN:HB3	1.86	0.40
1:E:250:GLY:HA2	1:E:256:LEU:HD21	2.04	0.40
1:D:145:ARG:HB3	1:D:146:PRO:HD3	2.02	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	392/400 (98%)	382 (97%)	9 (2%)	1 (0%)	41	37
1	B	394/400 (98%)	384 (98%)	9 (2%)	1 (0%)	41	37
1	C	391/400 (98%)	383 (98%)	7 (2%)	1 (0%)	41	37
1	D	393/400 (98%)	383 (98%)	9 (2%)	1 (0%)	41	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	389/400 (97%)	379 (97%)	9 (2%)	1 (0%)	41 37
1	F	385/400 (96%)	369 (96%)	15 (4%)	1 (0%)	41 37
All	All	2344/2400 (98%)	2280 (97%)	58 (2%)	6 (0%)	41 37

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	304	VAL
1	B	304	VAL
1	C	304	VAL
1	D	304	VAL
1	E	304	VAL
1	F	304	VAL

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	321/322 (100%)	315 (98%)	6 (2%)	57 61
1	B	322/322 (100%)	314 (98%)	8 (2%)	47 49
1	C	320/322 (99%)	314 (98%)	6 (2%)	57 61
1	D	321/322 (100%)	313 (98%)	8 (2%)	47 49
1	E	319/322 (99%)	312 (98%)	7 (2%)	52 55
1	F	317/322 (98%)	310 (98%)	7 (2%)	52 55
All	All	1920/1932 (99%)	1878 (98%)	42 (2%)	53 55

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	158	ASN
1	A	204	ARG
1	A	215	PHE

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Mol	Chain	Res	Type
1	A	306	HIS
1	A	345	MET
1	B	80	GLU
1	B	115	ARG
1	B	204	ARG
1	B	215	PHE
1	B	294	LYS
1	B	306	HIS
1	B	345[A]	MET
1	B	345[B]	MET
1	C	8	SER
1	C	80	GLU
1	C	204	ARG
1	C	215	PHE
1	C	277	SER
1	C	306	HIS
1	D	8	SER
1	D	158	ASN
1	D	204	ARG
1	D	213	ASN
1	D	215	PHE
1	D	306	HIS
1	D	311	GLU
1	D	342	ARG
1	E	25	SER
1	E	177	LYS
1	E	204	ARG
1	E	215	PHE
1	E	278	ARG
1	E	306	HIS
1	E	342	ARG
1	F	5	SER
1	F	15	SER
1	F	31	LEU
1	F	204	ARG
1	F	215	PHE
1	F	306	HIS
1	F	326	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	213	ASN
1	C	349	ASN
1	D	213	ASN
1	D	349	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)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	A1LWD	B	402	-	23,23,23	0.63	0	33,33,33	0.82	1 (3%)
2	SAH	E	401	-	24,28,28	1.18	3 (12%)	25,40,40	1.61	4 (16%)
2	SAH	C	401	-	24,28,28	1.18	3 (12%)	25,40,40	1.52	3 (12%)
3	A1LWD	F	402	-	23,23,23	0.61	0	33,33,33	0.74	1 (3%)
2	SAH	A	401	-	24,28,28	1.15	3 (12%)	25,40,40	1.49	4 (16%)
3	A1LWD	C	402	-	23,23,23	0.61	0	33,33,33	0.86	2 (6%)
2	SAH	F	401	-	24,28,28	1.19	3 (12%)	25,40,40	1.60	4 (16%)
3	A1LWD	D	402	-	23,23,23	0.60	0	33,33,33	0.81	1 (3%)
2	SAH	D	401	-	24,28,28	1.12	2 (8%)	25,40,40	1.58	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	A1LWD	E	402	-	23,23,23	0.60	0	33,33,33	0.79	1 (3%)
2	SAH	B	401	-	24,28,28	1.13	3 (12%)	25,40,40	1.55	4 (16%)
3	A1LWD	A	402	-	23,23,23	0.60	0	33,33,33	0.82	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1LWD	B	402	-	-	0/10/19/19	0/2/2/2
2	SAH	E	401	-	-	0/11/31/31	0/3/3/3
2	SAH	C	401	-	-	0/11/31/31	0/3/3/3
3	A1LWD	F	402	-	-	0/10/19/19	0/2/2/2
2	SAH	A	401	-	-	0/11/31/31	0/3/3/3
3	A1LWD	C	402	-	-	1/10/19/19	0/2/2/2
2	SAH	F	401	-	-	3/11/31/31	0/3/3/3
3	A1LWD	D	402	-	-	0/10/19/19	0/2/2/2
2	SAH	D	401	-	-	2/11/31/31	0/3/3/3
3	A1LWD	E	402	-	-	2/10/19/19	0/2/2/2
2	SAH	B	401	-	-	0/11/31/31	0/3/3/3
3	A1LWD	A	402	-	-	0/10/19/19	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	SAH	C2-N3	3.98	1.38	1.32
2	F	401	SAH	C2-N3	3.95	1.38	1.32
2	E	401	SAH	C2-N3	3.86	1.38	1.32
2	B	401	SAH	C2-N3	3.79	1.38	1.32
2	D	401	SAH	C2-N3	3.74	1.38	1.32
2	A	401	SAH	C2-N3	3.70	1.38	1.32
2	F	401	SAH	C2-N1	2.51	1.38	1.33
2	A	401	SAH	C2-N1	2.47	1.38	1.33
2	C	401	SAH	C2-N1	2.47	1.38	1.33
2	E	401	SAH	C2-N1	2.45	1.38	1.33
2	B	401	SAH	C2-N1	2.34	1.38	1.33
2	D	401	SAH	C2-N1	2.32	1.38	1.33
2	E	401	SAH	OXT-C	-2.14	1.23	1.30
2	A	401	SAH	OXT-C	-2.01	1.24	1.30
2	F	401	SAH	OXT-C	-2.01	1.24	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	SAH	OXT-C	-2.01	1.24	1.30
2	B	401	SAH	OXT-C	-2.01	1.24	1.30

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	401	SAH	N3-C2-N1	-5.44	120.18	128.68
2	B	401	SAH	N3-C2-N1	-5.35	120.31	128.68
2	C	401	SAH	N3-C2-N1	-5.32	120.36	128.68
2	D	401	SAH	N3-C2-N1	-5.27	120.44	128.68
2	A	401	SAH	N3-C2-N1	-5.17	120.60	128.68
2	F	401	SAH	N3-C2-N1	-5.16	120.62	128.68
2	F	401	SAH	C5'-SD-CG	-3.55	91.62	102.27
2	E	401	SAH	C5'-SD-CG	-3.16	92.78	102.27
2	C	401	SAH	C5'-SD-CG	-3.15	92.81	102.27
2	D	401	SAH	C5'-SD-CG	-3.11	92.92	102.27
2	B	401	SAH	C5'-SD-CG	-3.02	93.20	102.27
2	E	401	SAH	OXT-C-O	-2.80	117.73	124.09
3	C	402	A1LWD	C1-C9-C10	2.57	116.24	112.17
2	F	401	SAH	OXT-C-O	-2.56	118.28	124.09
2	A	401	SAH	OXT-C-O	-2.54	118.33	124.09
2	D	401	SAH	OXT-C-O	-2.54	118.33	124.09
2	A	401	SAH	C5'-SD-CG	-2.52	94.72	102.27
3	A	402	A1LWD	C1-C9-C10	2.49	116.10	112.17
3	B	402	A1LWD	C1-C9-C10	2.44	116.04	112.17
2	D	401	SAH	OXT-C-CA	2.42	121.64	113.38
2	B	401	SAH	OXT-C-O	-2.40	118.64	124.09
2	F	401	SAH	OXT-C-CA	2.37	121.47	113.38
2	C	401	SAH	OXT-C-O	-2.34	118.78	124.09
3	D	402	A1LWD	C1-C9-C10	2.33	115.85	112.17
2	E	401	SAH	OXT-C-CA	2.29	121.19	113.38
3	E	402	A1LWD	C1-C9-C10	2.22	115.68	112.17
2	B	401	SAH	OXT-C-CA	2.19	120.83	113.38
2	A	401	SAH	OXT-C-CA	2.13	120.64	113.38
3	F	402	A1LWD	C6-C5-C4	-2.04	120.65	121.85
3	C	402	A1LWD	C6-C5-C4	-2.04	120.66	121.85

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	401	SAH	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	F	401	SAH	CB-CG-SD-C5'
2	D	401	SAH	O-C-CA-N
3	E	402	A1LWD	C12-C13-C14-O5
2	D	401	SAH	OXT-C-CA-N
2	F	401	SAH	N-CA-CB-CG
3	E	402	A1LWD	C12-C13-C14-O6
3	C	402	A1LWD	C12-C13-C14-O5

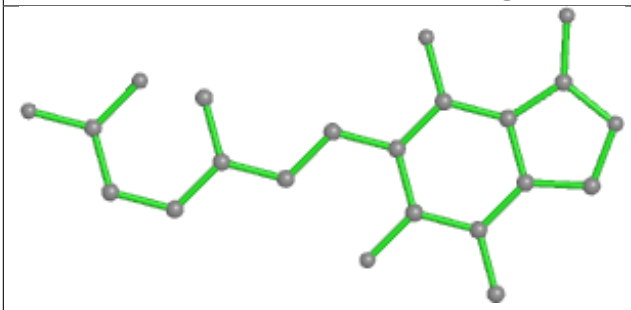
There are no ring outliers.

3 monomers are involved in 5 short contacts:

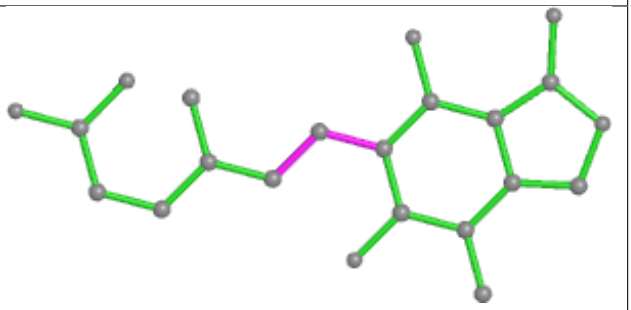
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	SAH	2	0
2	F	401	SAH	1	0
2	D	401	SAH	2	0

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.

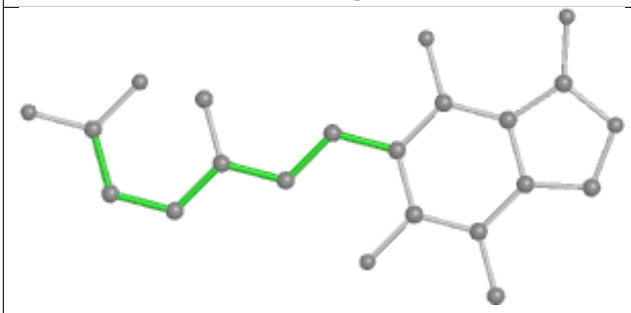
Ligand A1LWD B 402



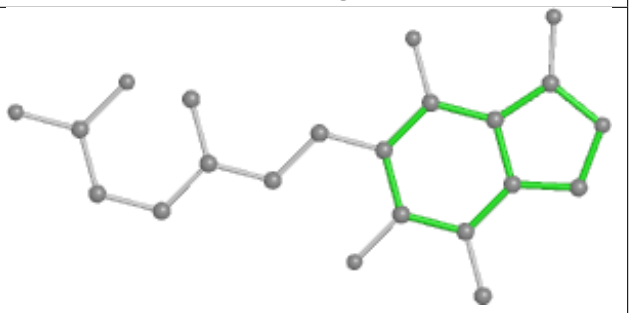
Bond lengths



Bond angles

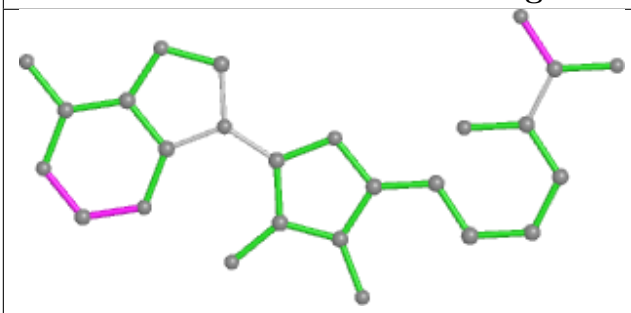


Torsions



Rings

Ligand SAH E 401



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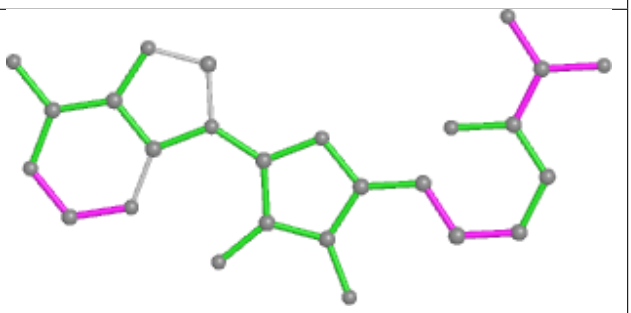
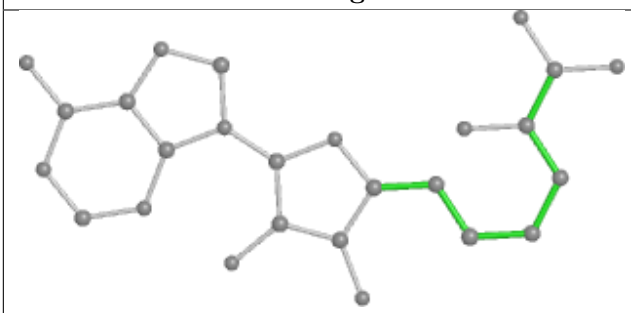


Bond angles



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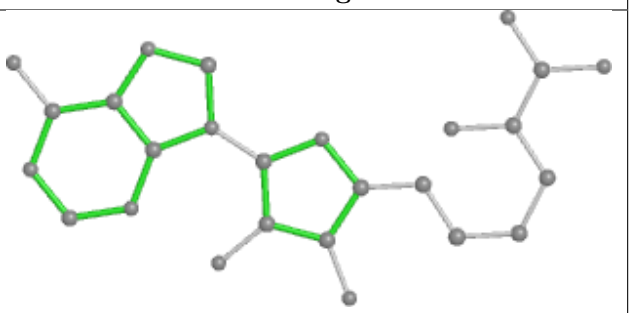
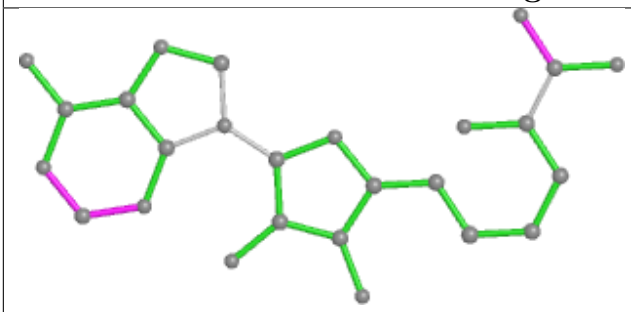


Rings

Ligand SAH C 401



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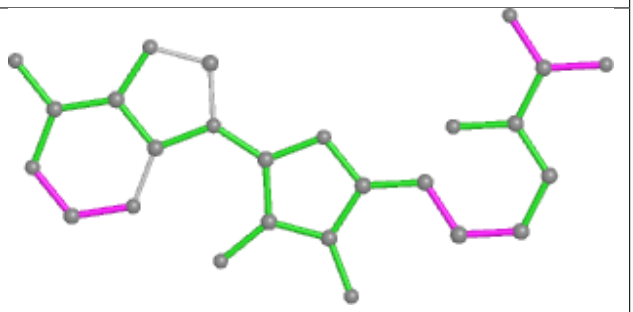

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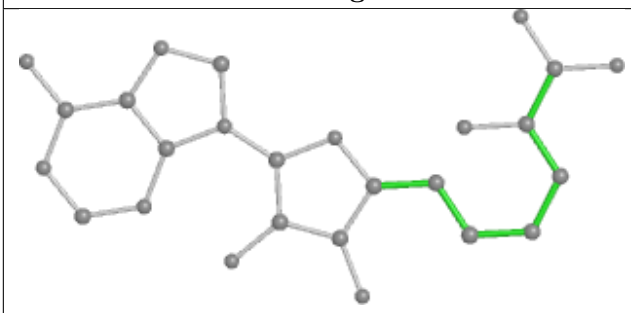
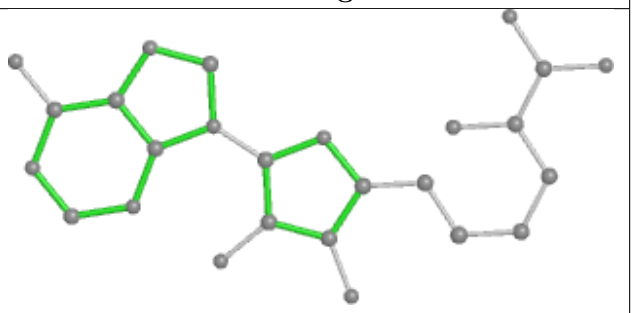
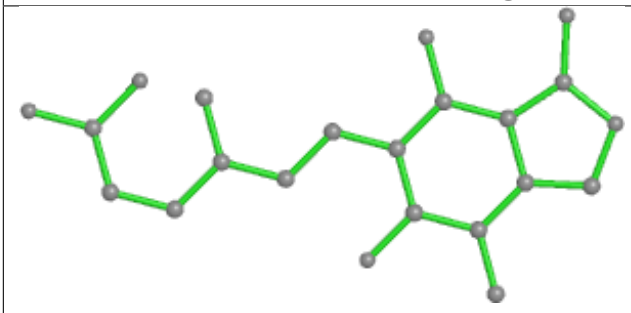


Torsions

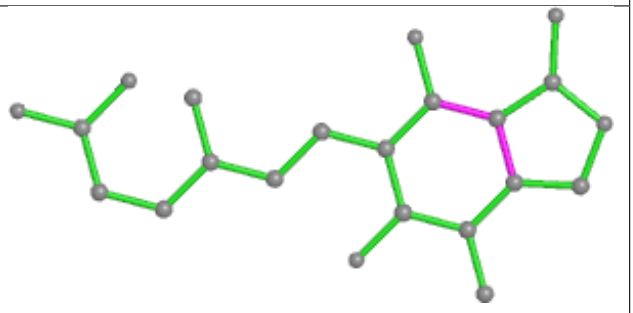


Rings

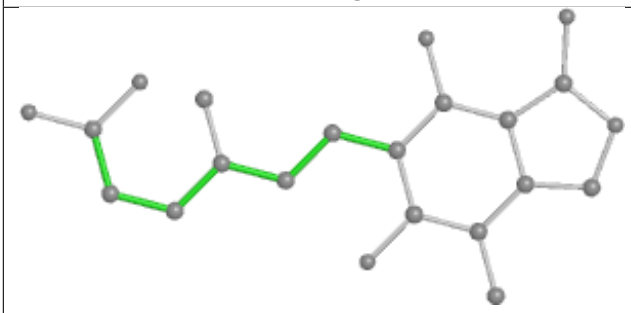
Ligand A1LWD F 402



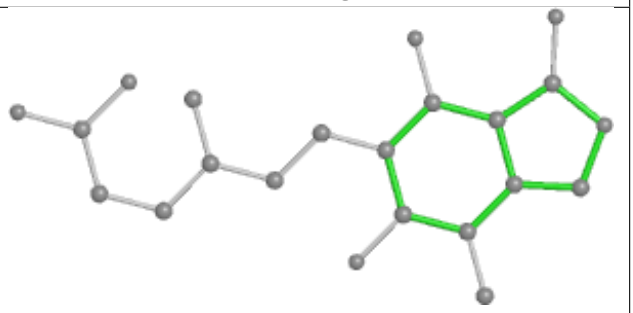
Bond lengths



Bond angles

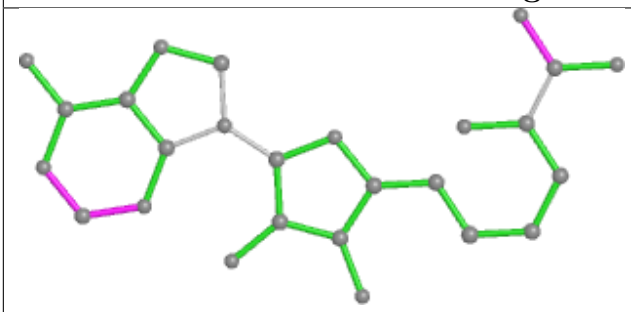


Torsions

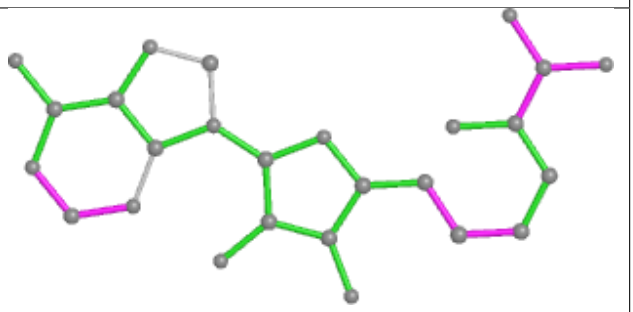


Rings

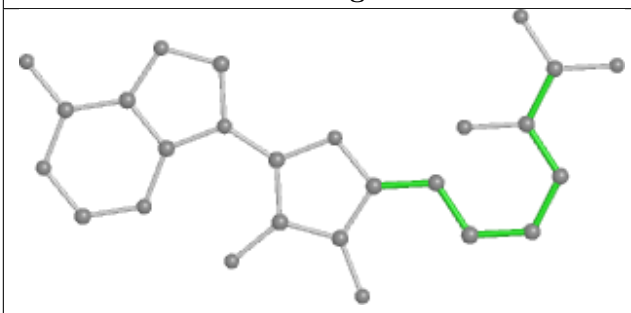
Ligand SAH A 401



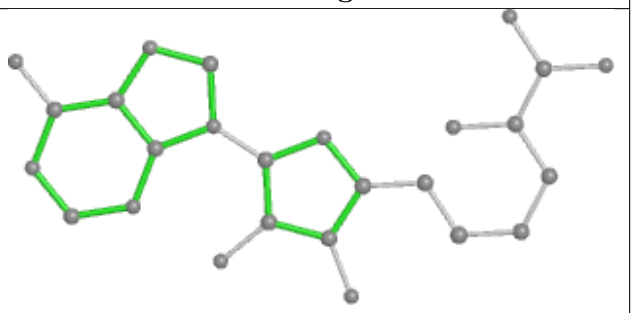
Bond lengths



Bond angles

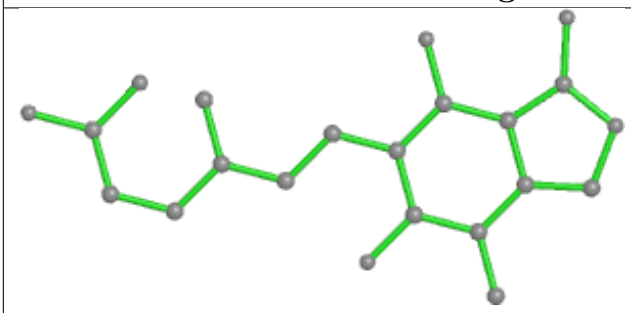


Torsions

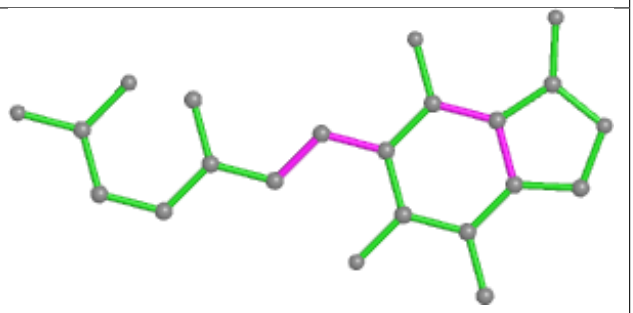


Rings

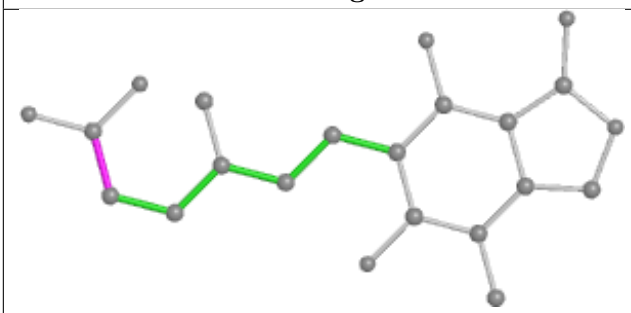
Ligand A1LWD C 402



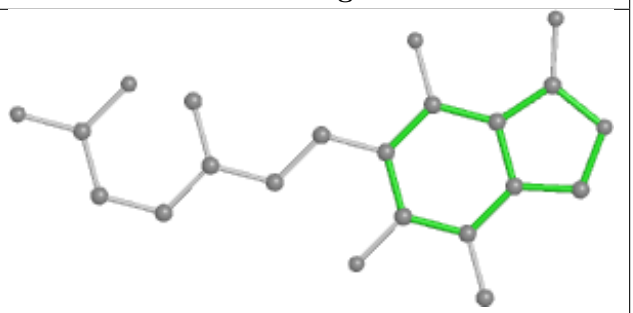
Bond lengths



Bond angles

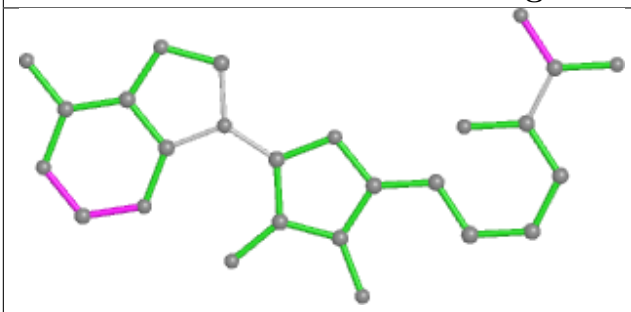


Torsions

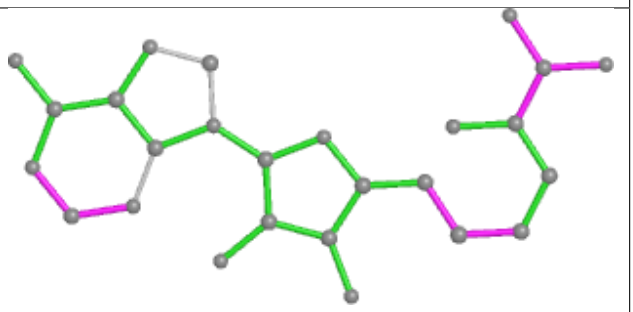


Rings

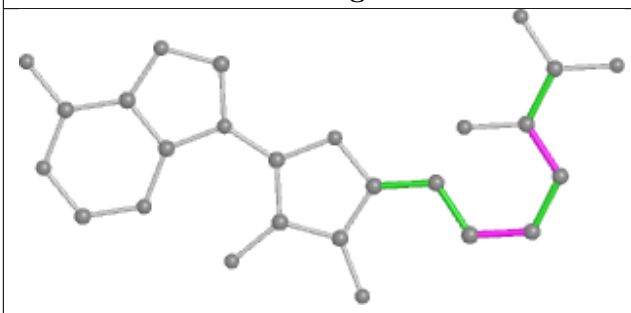
Ligand SAH F 401



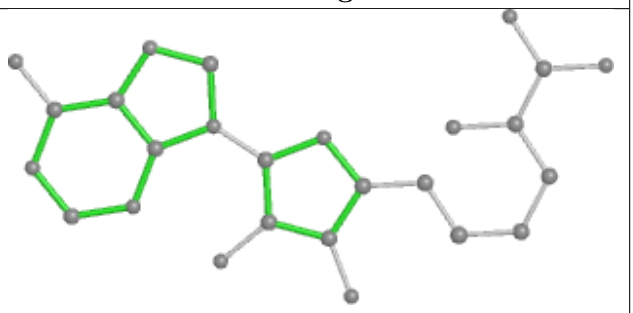
Bond lengths



Bond angles

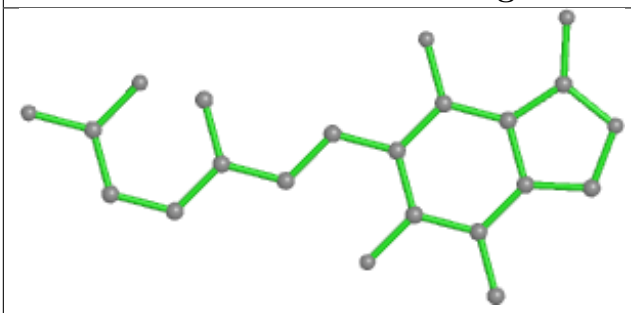


Torsions



Rings

Ligand A1LWD D 402



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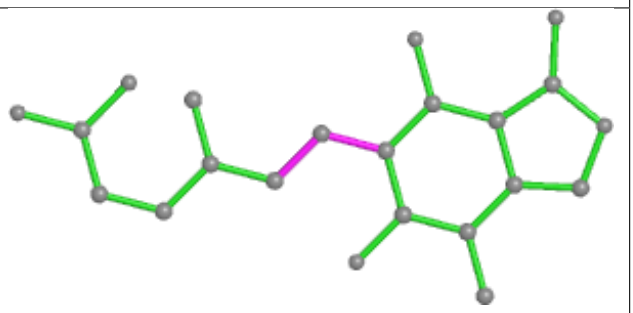
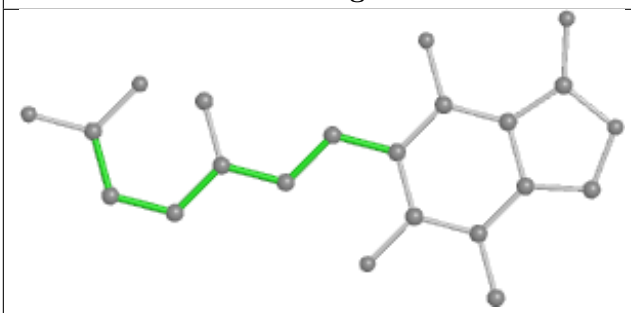
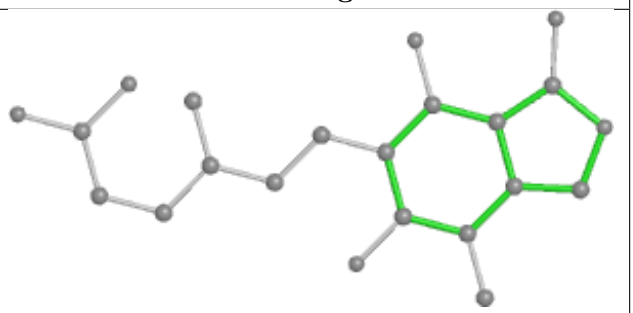


Bond angles

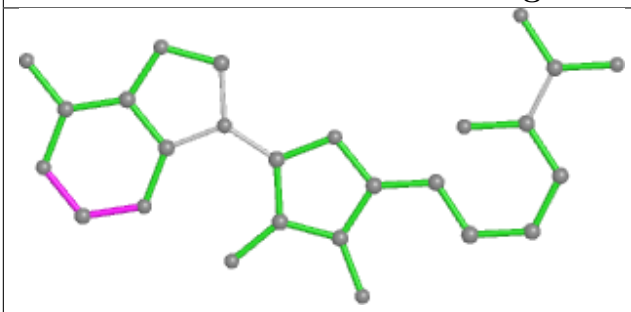


Torsions



Rings

Ligand SAH D 401



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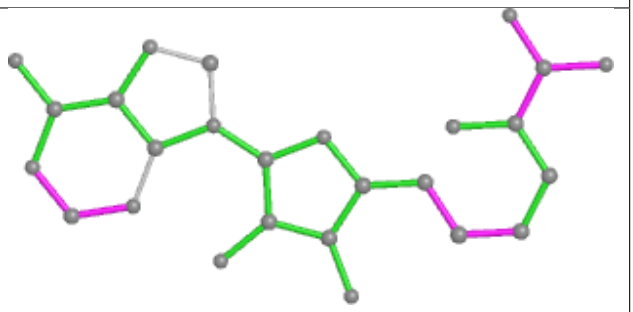
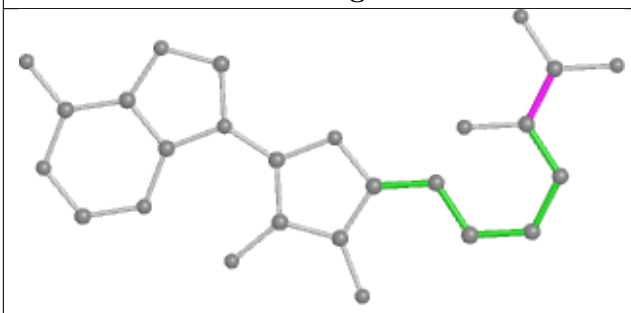


Bond angles



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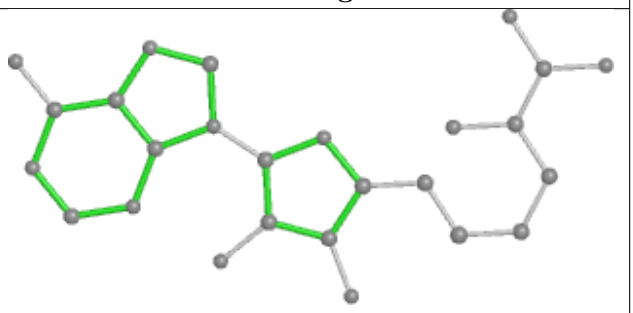
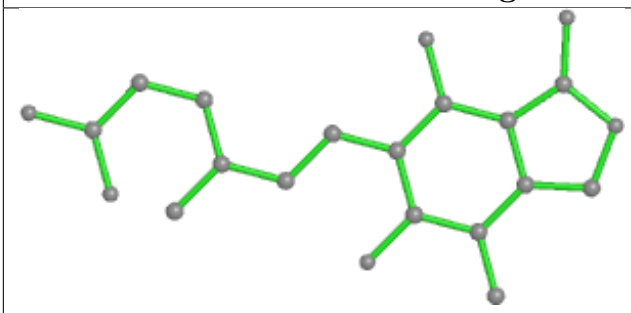
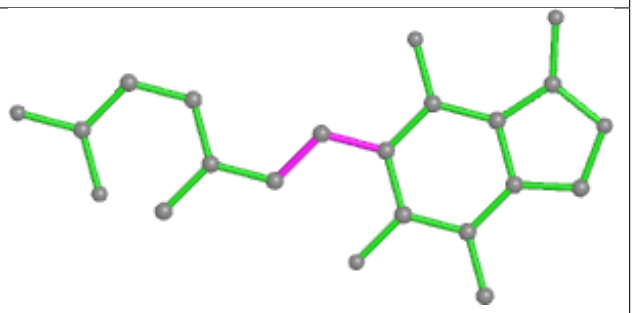


Rings

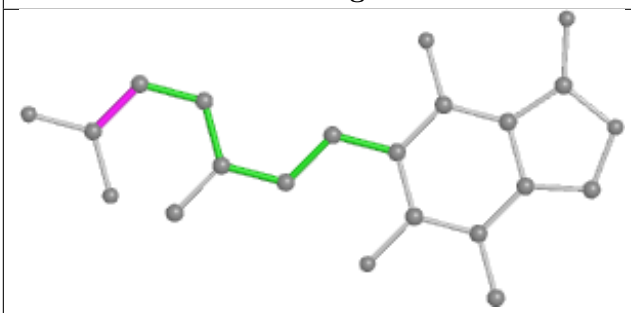
Ligand A1LWD E 402



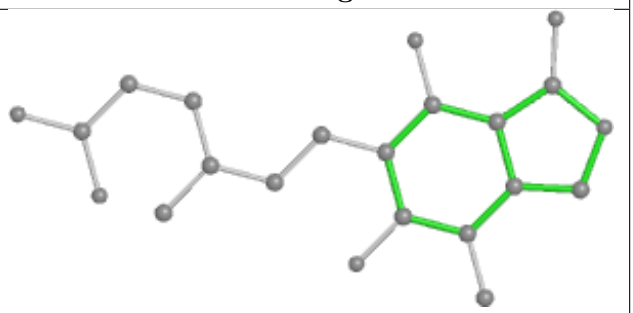
Bond lengths



Bond angles

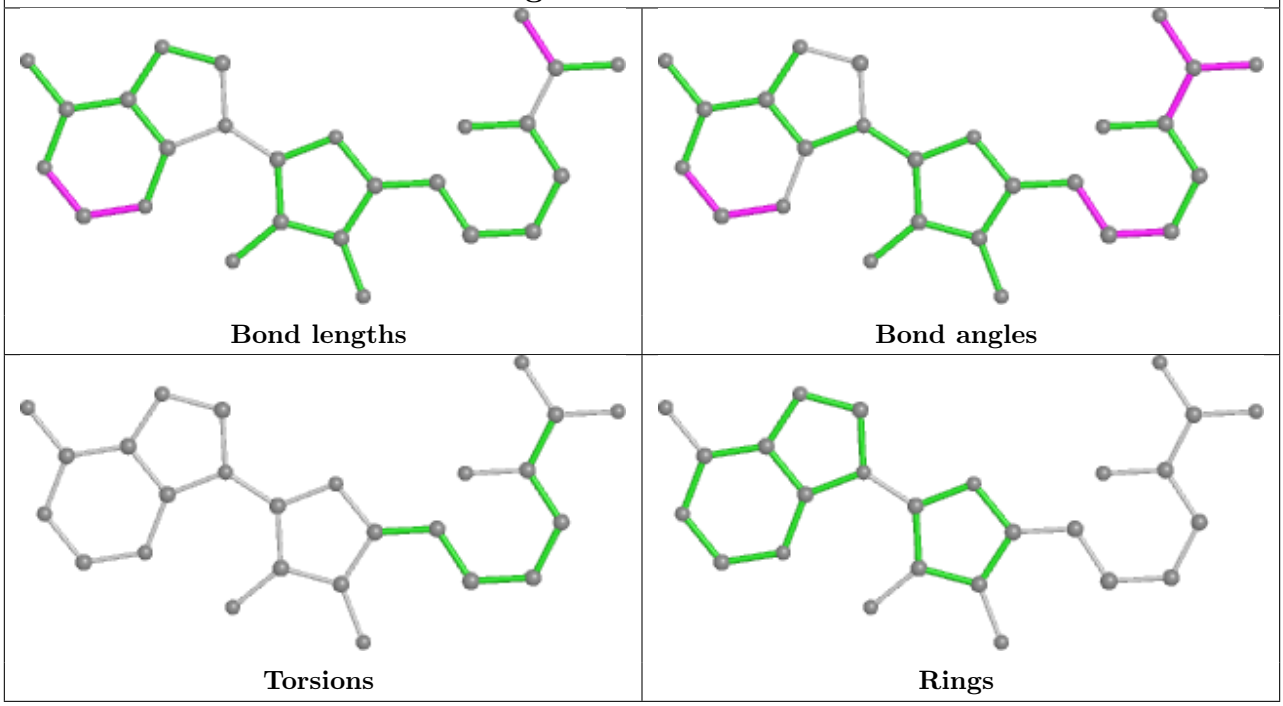


Torsions

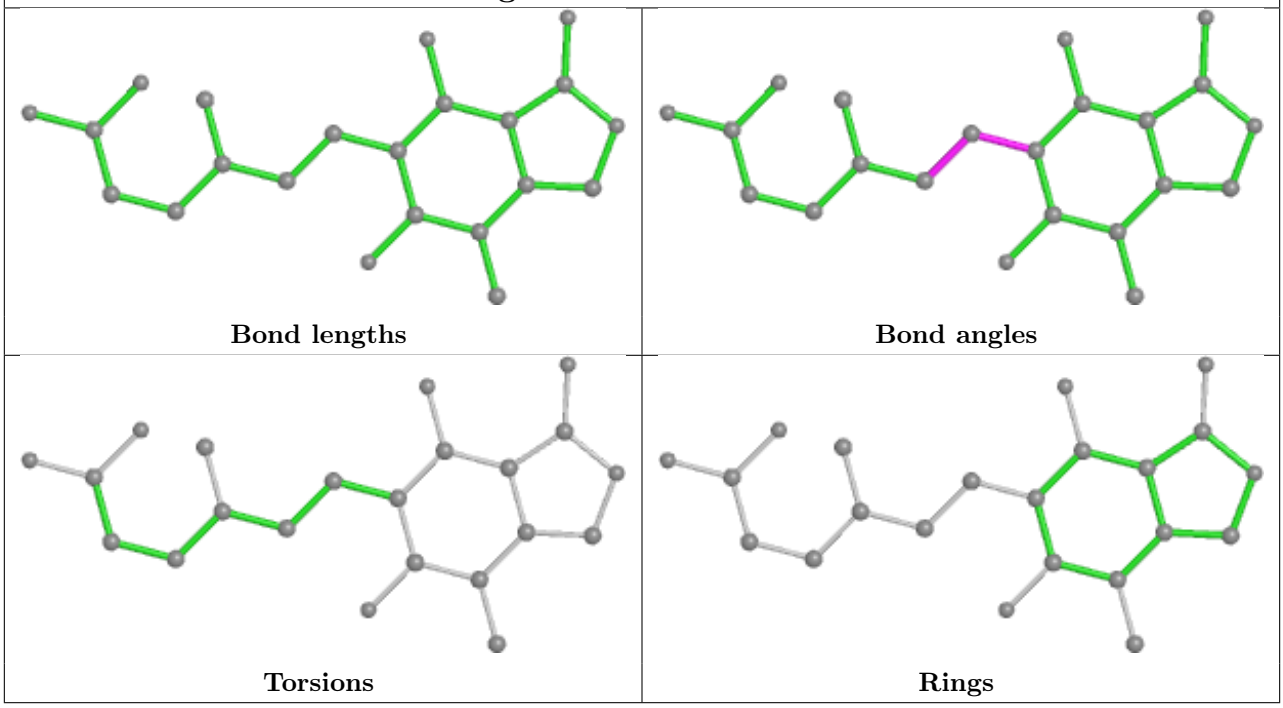


Rings

Ligand SAH B 401



Ligand A1LWD A 402



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	394/400 (98%)	0.41	5 (1%) 77 76	16, 22, 45, 72	0
1	B	395/400 (98%)	0.35	5 (1%) 77 76	15, 21, 43, 73	0
1	C	393/400 (98%)	0.37	4 (1%) 82 81	16, 22, 41, 75	0
1	D	395/400 (98%)	0.40	10 (2%) 57 56	17, 22, 44, 75	0
1	E	391/400 (97%)	1.04	35 (8%) 9 8	32, 40, 65, 94	0
1	F	389/400 (97%)	1.16	44 (11%) 5 4	32, 43, 71, 91	0
All	All	2357/2400 (98%)	0.62	103 (4%) 34 33	15, 25, 56, 94	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	274	ALA	4.0
1	F	83	LEU	3.9
1	E	15	SER	3.8
1	C	276	GLU	3.6
1	D	23	ASN	3.5
1	F	345	MET	3.5
1	B	274	ALA	3.4
1	D	277	SER	3.4
1	F	342	ARG	3.4
1	F	185	TRP	3.3
1	E	170	GLY	3.1
1	F	169	ASP	3.1
1	E	23	ASN	3.1
1	E	341	GLU	3.0
1	E	385	TYR	3.0
1	D	273	PRO	3.0
1	E	81	GLU	3.0
1	F	42	LEU	3.0
1	F	336	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	276	GLU	2.9
1	F	5	SER	2.9
1	E	388	VAL	2.9
1	F	253	PHE	2.9
1	F	170	GLY	2.9
1	E	99	PHE	2.8
1	F	355	LEU	2.8
1	D	274	ALA	2.8
1	E	342	ARG	2.8
1	F	8	SER	2.8
1	D	21	GLU	2.8
1	E	164	ALA	2.8
1	F	31	LEU	2.8
1	E	213	ASN	2.7
1	E	87	ALA	2.7
1	F	91	LYS	2.6
1	F	16	ALA	2.6
1	F	27	ALA	2.6
1	A	21	GLU	2.6
1	E	116	ASN	2.6
1	D	167	THR	2.6
1	F	13	LEU	2.6
1	F	7	ALA	2.6
1	E	398	ALA	2.6
1	E	11	GLN	2.5
1	E	21	GLU	2.5
1	F	38	LEU	2.5
1	D	17	ALA	2.5
1	F	256	LEU	2.4
1	F	22	ASN	2.4
1	E	282	ALA	2.4
1	D	341	GLU	2.4
1	D	342	ARG	2.4
1	E	115	ARG	2.4
1	E	9	ILE	2.4
1	E	133	TYR	2.4
1	E	345	MET	2.4
1	E	118	VAL	2.4
1	E	167	THR	2.4
1	F	167	THR	2.3
1	E	165	LEU	2.3
1	F	385	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	249	PHE	2.3
1	E	22	ASN	2.3
1	B	342	ARG	2.3
1	E	346	SER	2.3
1	A	23	ASN	2.3
1	F	19	GLN	2.3
1	F	192	TYR	2.2
1	F	113	THR	2.2
1	F	236	VAL	2.2
1	F	214	GLY	2.2
1	B	276	GLU	2.2
1	C	342	ARG	2.2
1	E	92	THR	2.2
1	F	272	ILE	2.2
1	E	340	GLU	2.2
1	F	288	PHE	2.2
1	F	165	LEU	2.2
1	F	181	SER	2.2
1	C	115	ARG	2.2
1	F	267	GLN	2.1
1	F	325	ALA	2.1
1	D	179	ASP	2.1
1	F	268	VAL	2.1
1	F	172	PHE	2.1
1	F	301	MET	2.1
1	B	5	SER	2.1
1	F	119	PHE	2.1
1	F	78	ALA	2.1
1	E	274	ALA	2.1
1	B	81	GLU	2.1
1	E	8	SER	2.1
1	F	11	GLN	2.1
1	F	14	ALA	2.1
1	E	90	SER	2.0
1	C	274	ALA	2.0
1	E	172	PHE	2.0
1	E	149	GLY	2.0
1	F	21	GLU	2.0
1	F	120	TYR	2.0
1	E	218	VAL	2.0
1	F	311	GLU	2.0
1	A	342	ARG	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)

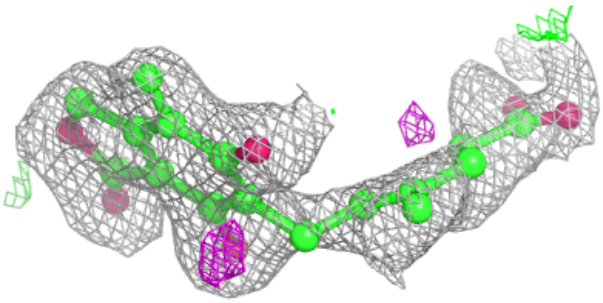
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

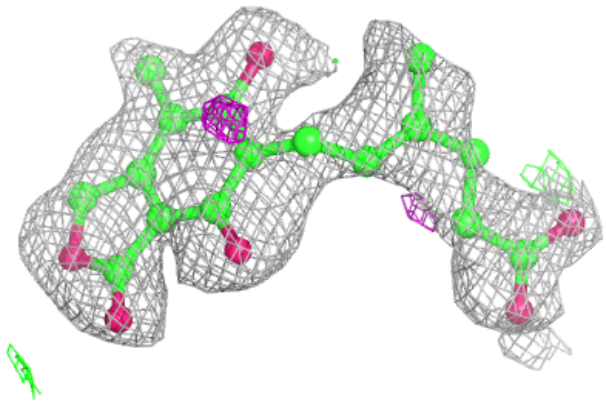
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	A1LWD	F	402	22/22	0.79	0.23	39,42,47,48	0
3	A1LWD	E	402	22/22	0.80	0.16	32,36,41,46	0
3	A1LWD	D	402	22/22	0.82	0.19	17,19,25,31	0
3	A1LWD	A	402	22/22	0.83	0.18	18,21,26,32	0
2	SAH	E	401	26/26	0.85	0.16	29,33,37,38	0
2	SAH	F	401	26/26	0.85	0.19	31,41,46,47	0
3	A1LWD	C	402	22/22	0.86	0.16	14,17,19,20	0
2	SAH	D	401	26/26	0.88	0.15	16,19,21,25	0
2	SAH	C	401	26/26	0.89	0.14	13,18,22,22	0
3	A1LWD	B	402	22/22	0.89	0.14	13,18,21,24	0
2	SAH	B	401	26/26	0.90	0.14	15,18,20,20	0
2	SAH	A	401	26/26	0.91	0.14	14,19,21,23	0

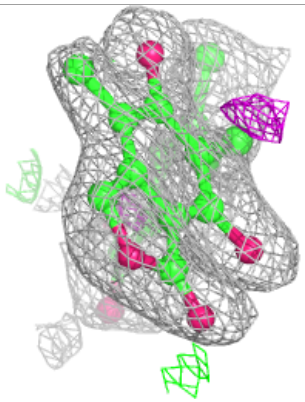
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1LWD 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)

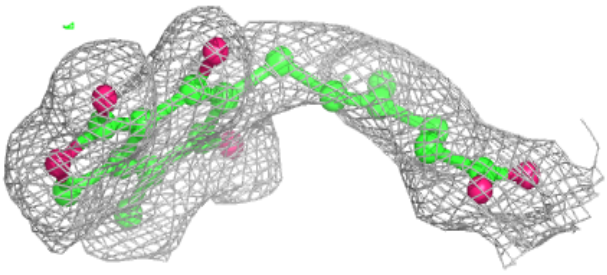


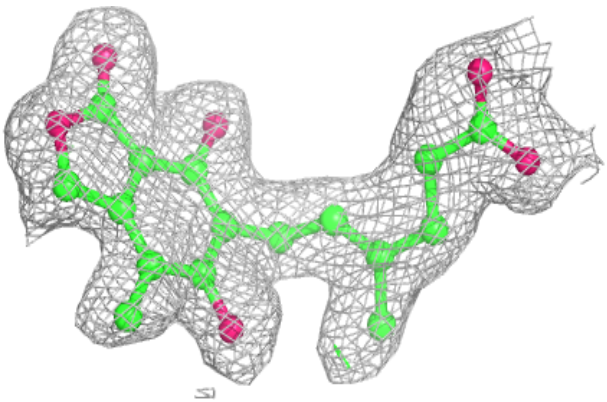


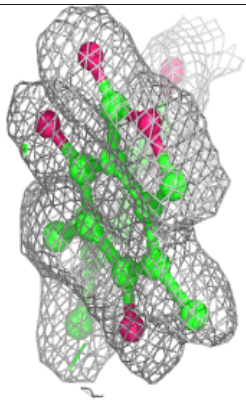


Electron density around A1LWD E 402:

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

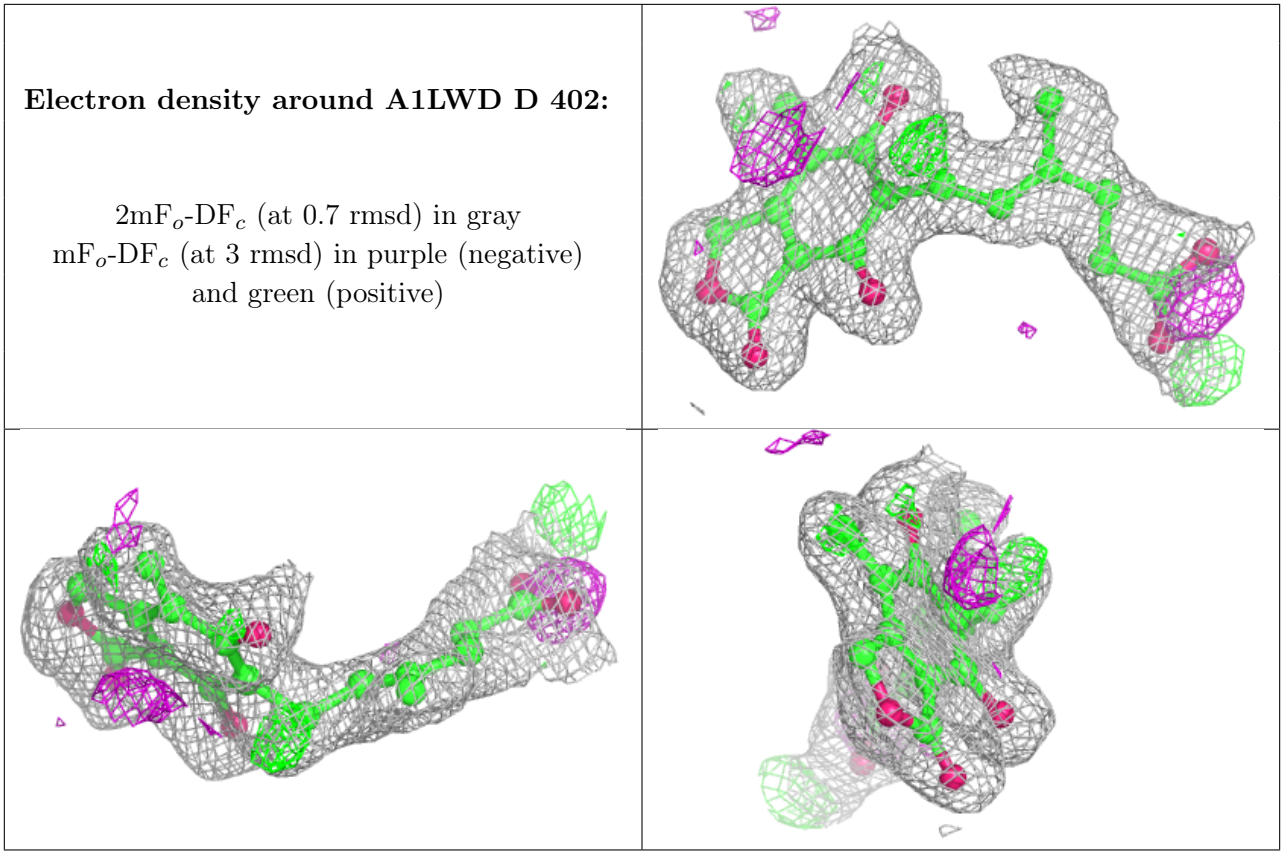






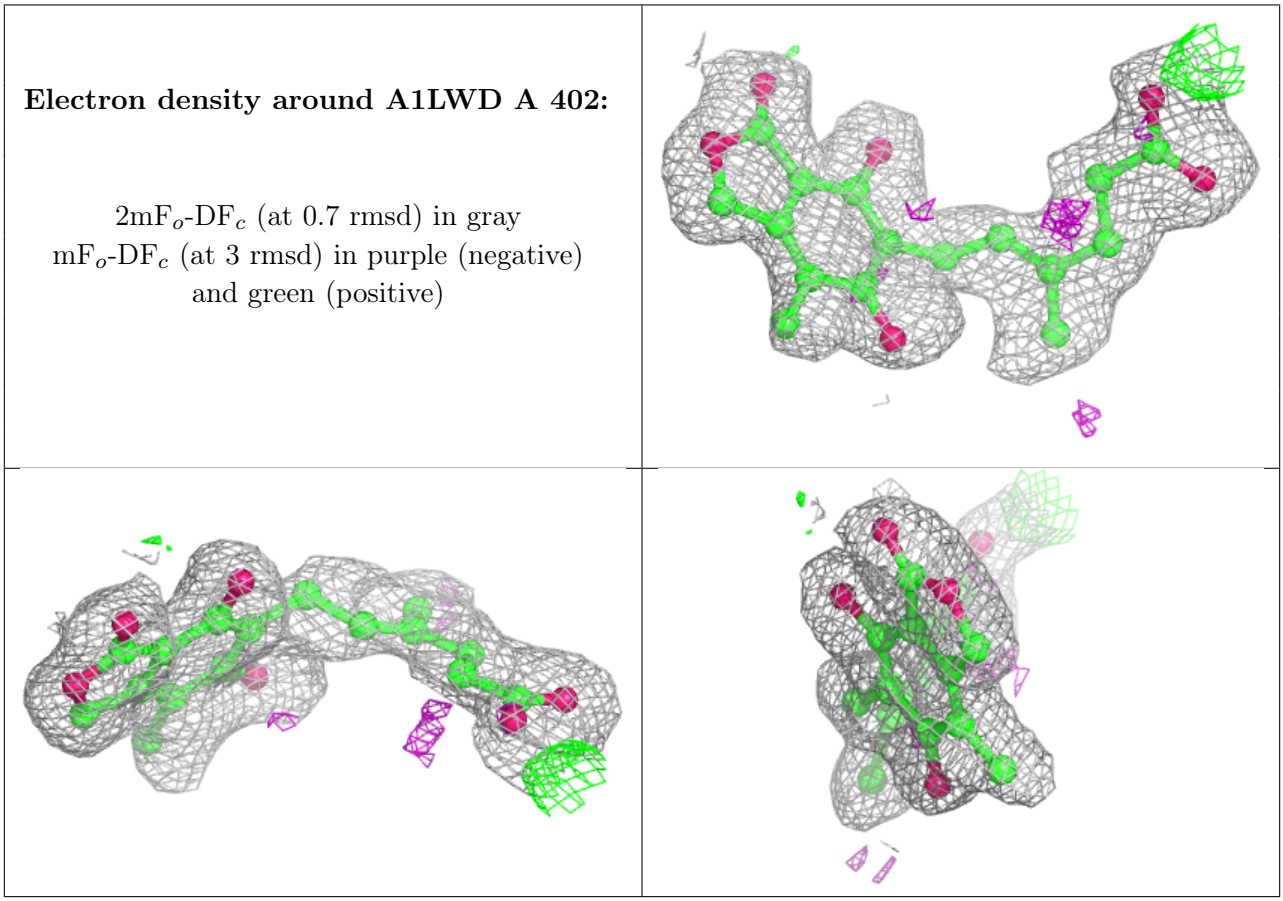
Electron density around A1LWD D 402:

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



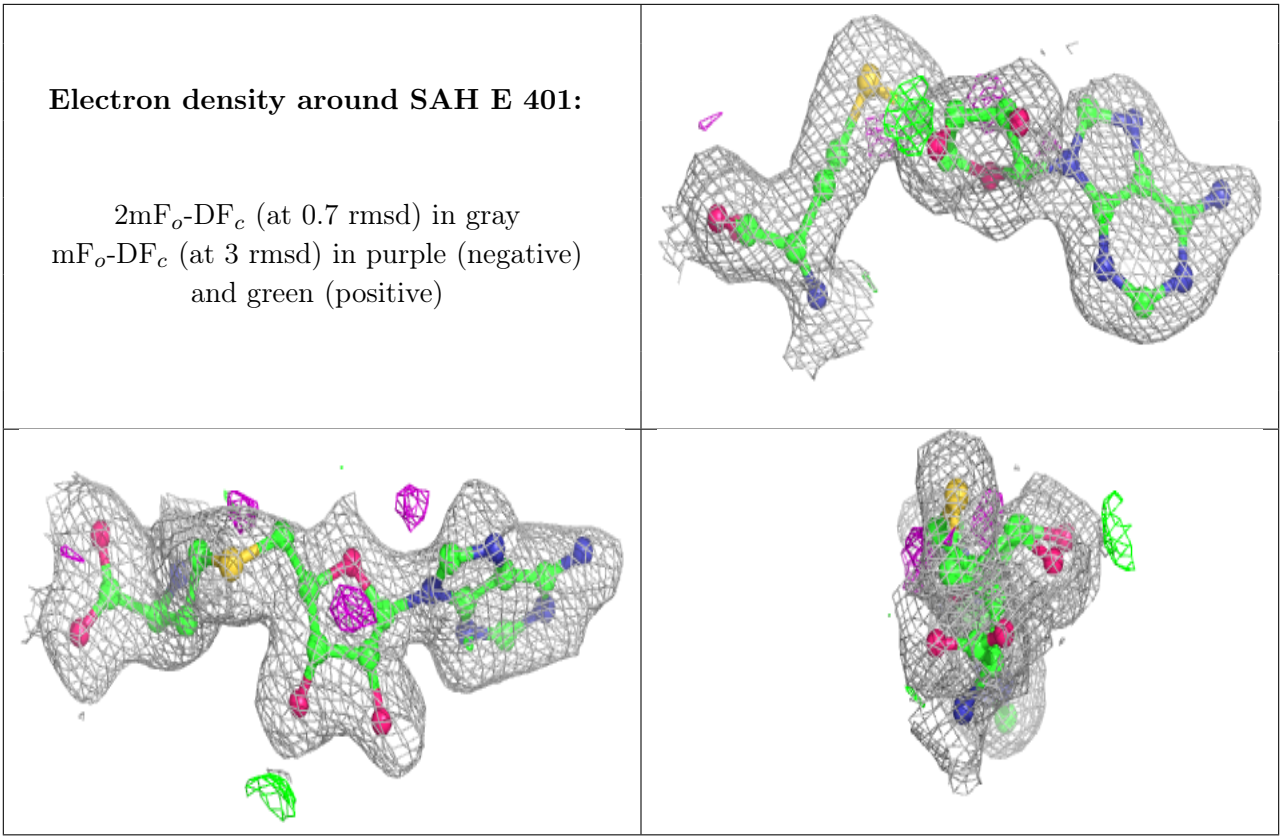
Electron density around A1LWD A 402:

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



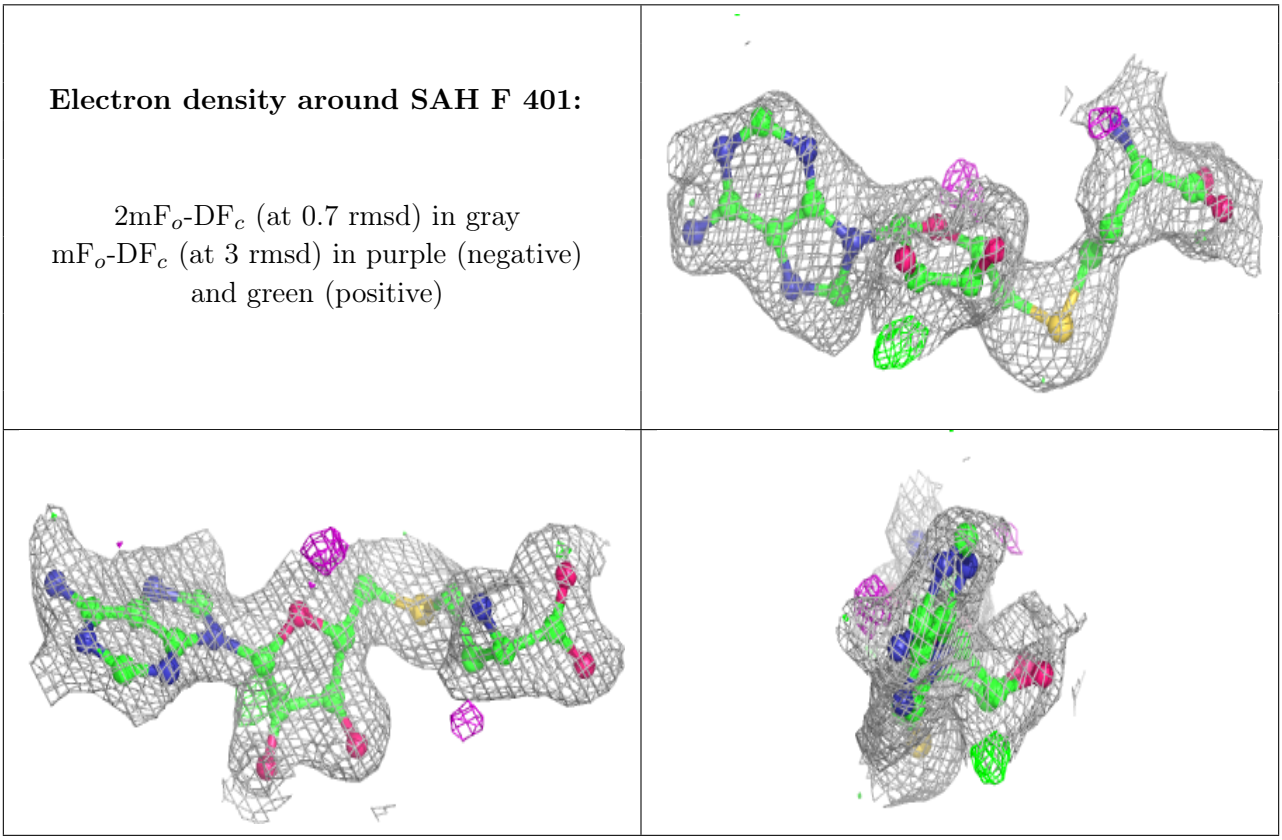
Electron density around SAH E 401:

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



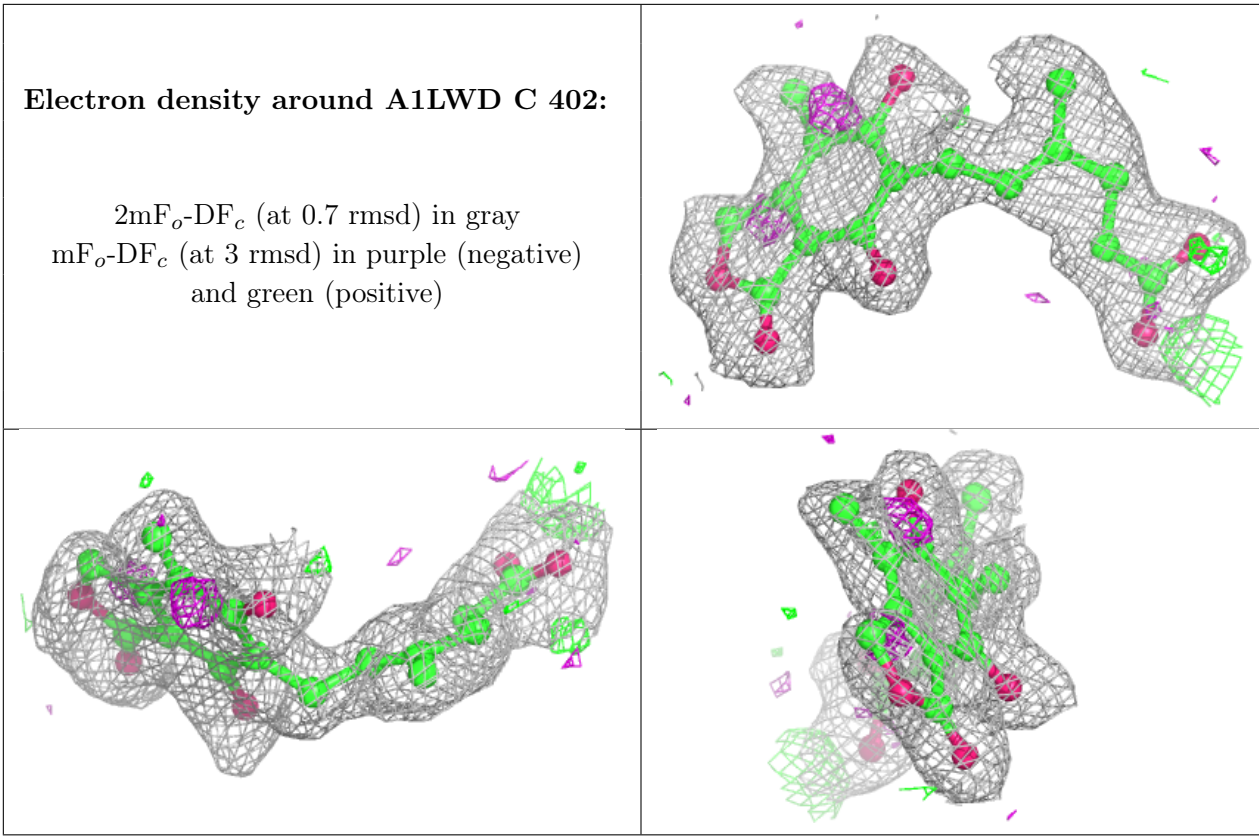
Electron density around SAH F 401:

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



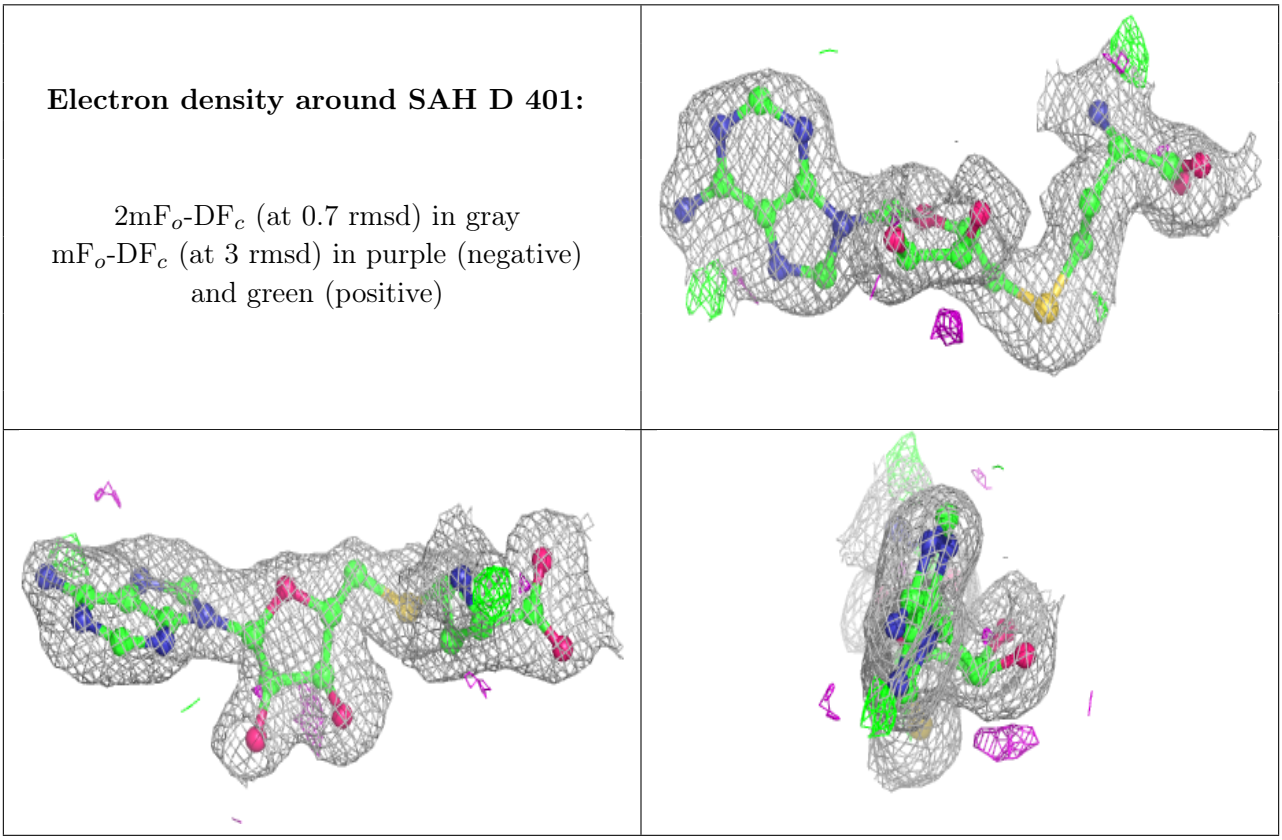
Electron density around A1LWD C 402:

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



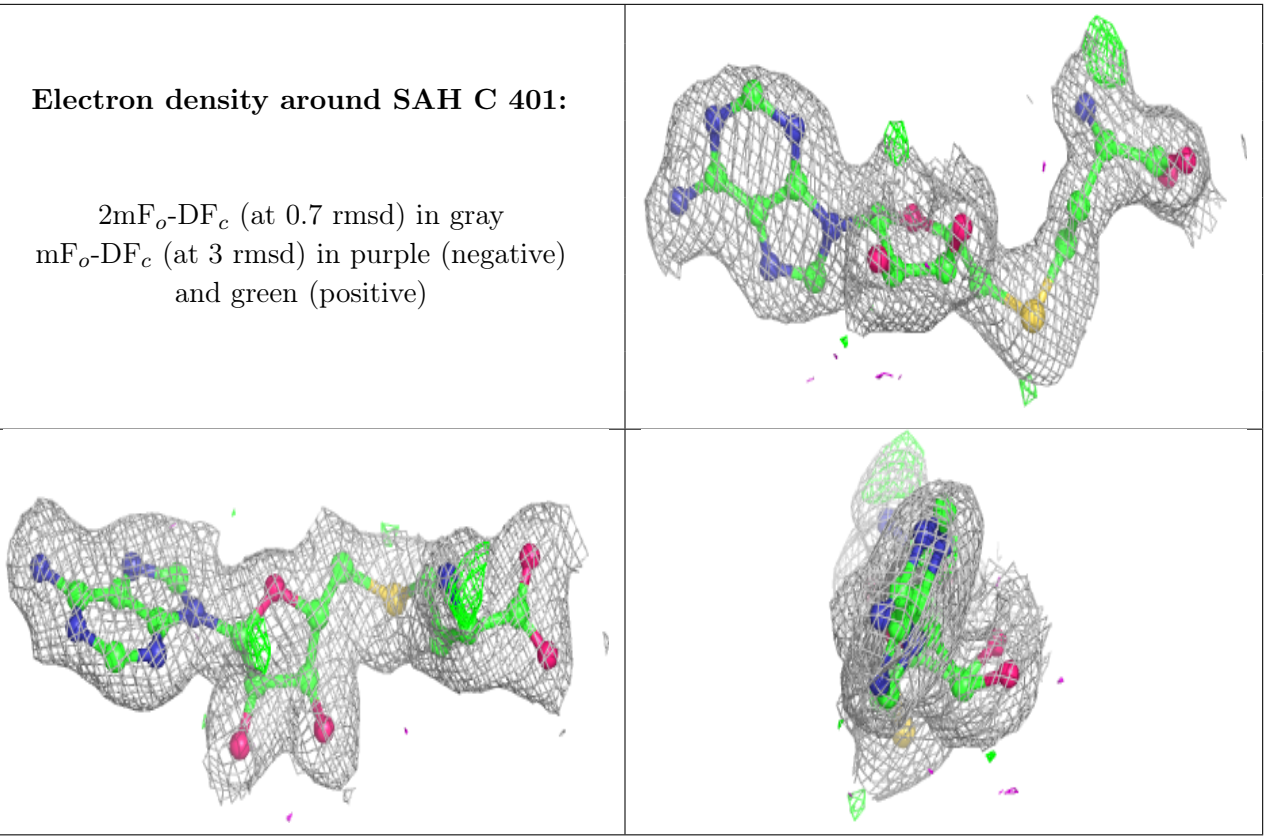
Electron density around SAH D 401:

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



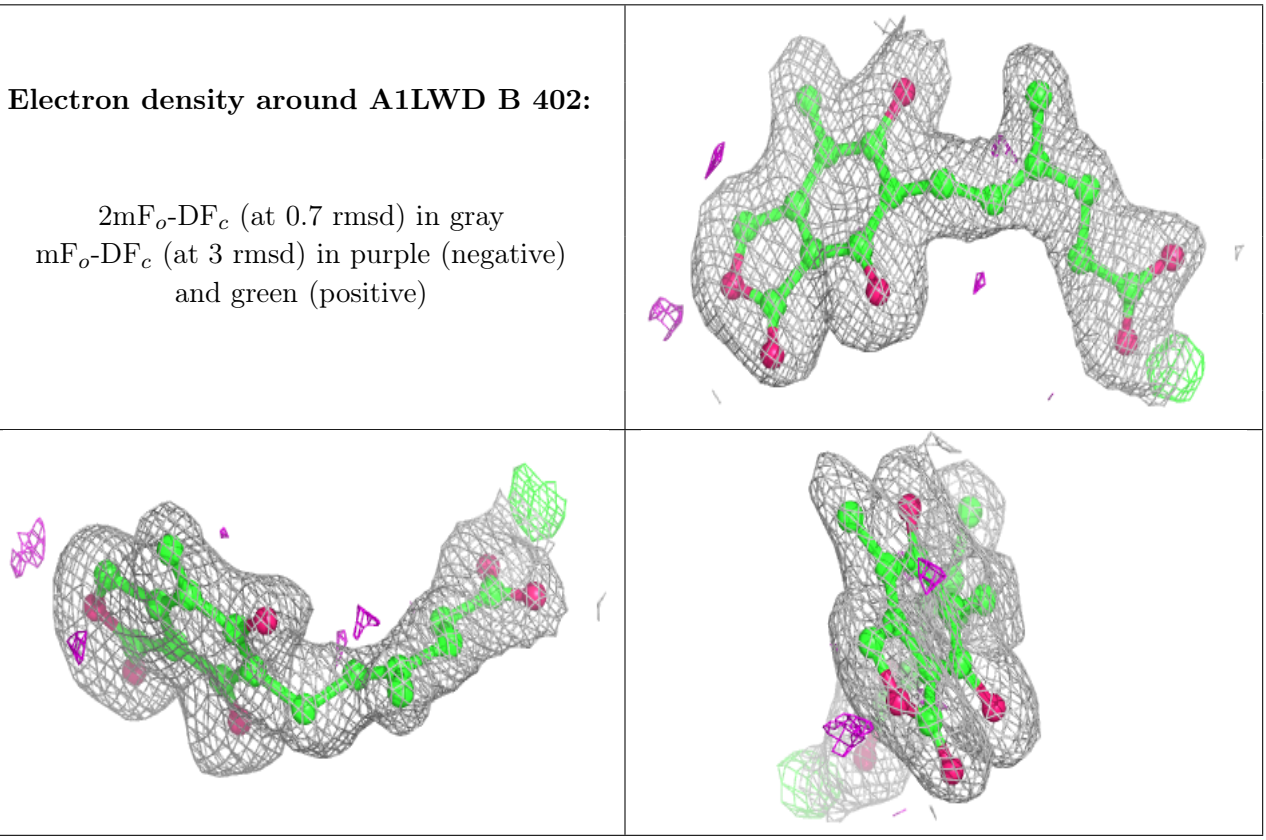
Electron density around SAH C 401:

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



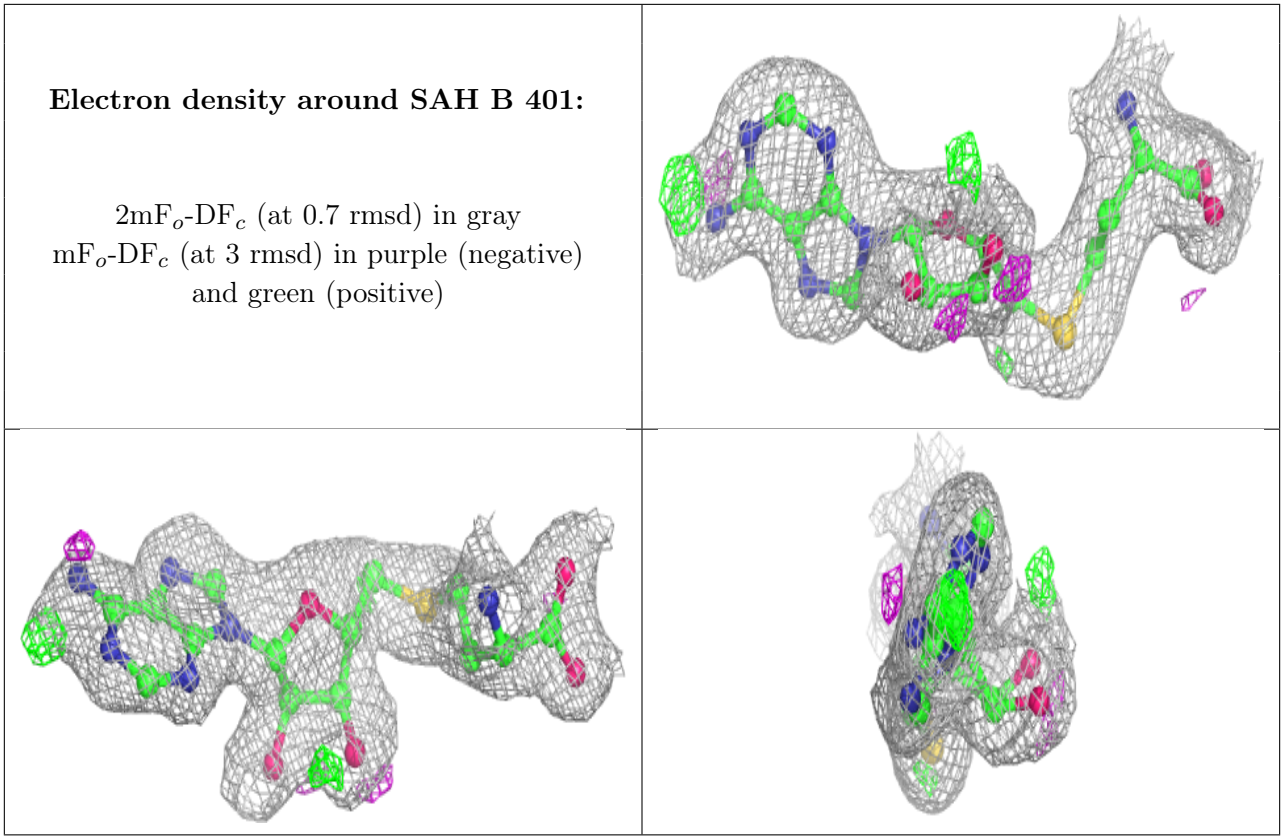
Electron density around A1LWD B 402:

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



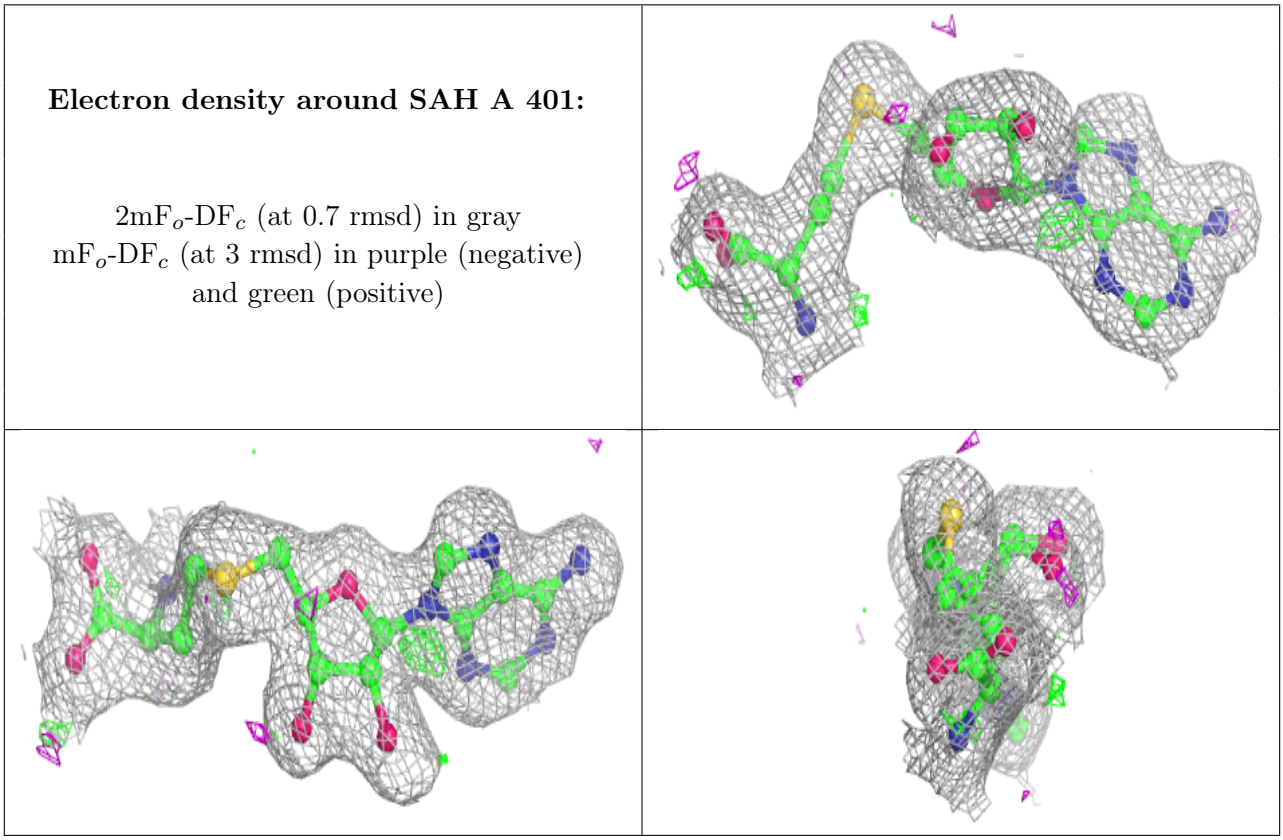
Electron density around SAH B 401:

$2mF_o$-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 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)



6.5 Other polymers (i)

There are no such residues in this entry.