wwPDB X-ray Structure Validation Summary Report (i)

Oct 7, 2026 – 03:30 PM JST

PDB ID	:	9WJ8 / pdb_00009wj8
Title	:	N-methyltransferase 1 complexed with SAH and NCM in Chimonanthus praecox
Authors	:	Zhang, A.; Luo, Y.; Hong, B.
Deposited on	:	2025-08-30
Resolution	:	2.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

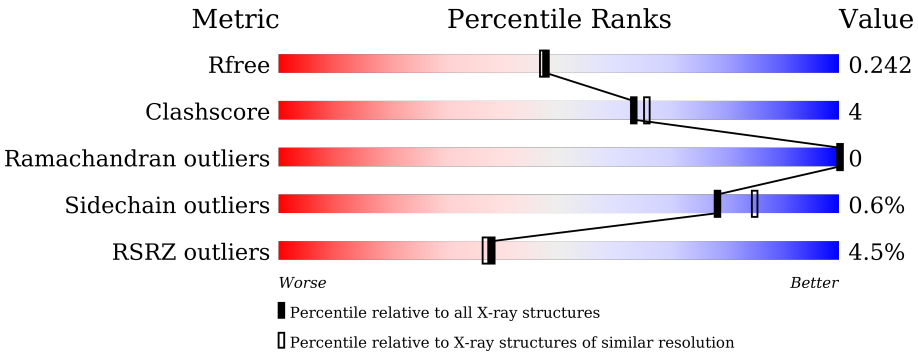
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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	368	4% 81% 12% 7%
1	B	368	2% 85% 8% 8%
1	C	368	6% 85% 8% 8%
1	D	368	4% 81% 11% 8%

2 Entry composition (i)

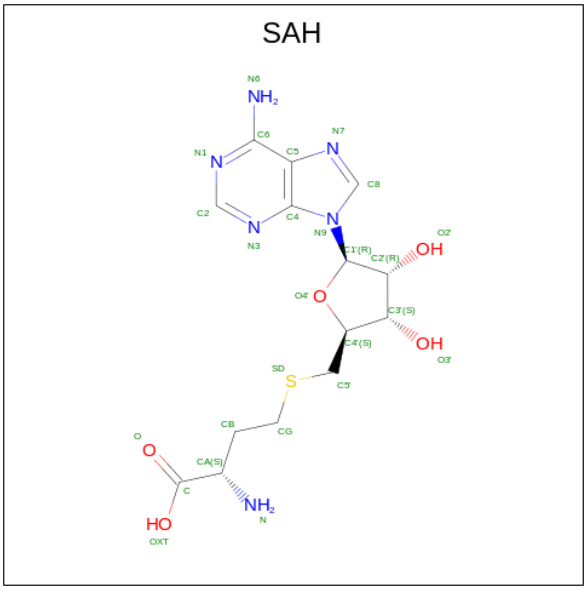
There are 4 unique types of molecules in this entry. The entry contains 11839 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 N-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	340	Total	C	N	O	S	0	0	0
			2744	1769	447	510	18			
1	A	342	Total	C	N	O	S	0	0	0
			2761	1778	450	515	18			
1	C	340	Total	C	N	O	S	0	0	0
			2746	1770	447	511	18			
1	D	338	Total	C	N	O	S	0	0	0
			2727	1757	445	507	18			

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



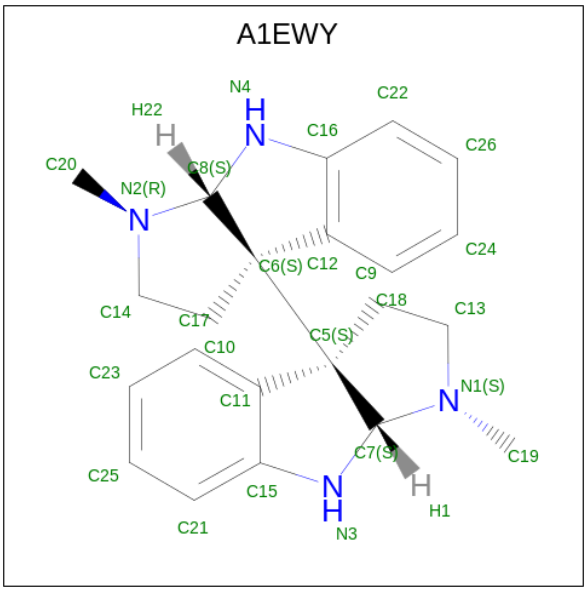
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

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

- Molecule 3 is (3 {a} {S},8 {b} {S})-8 {b}-[(3 {a} {S},8 {b} {S})-3-methyl-1,2,3 {a},4-tetrahydropyrrolo[2,3-b]indol-8 {b}-yl]-3-methyl-1,2,3 {a},4-tetrahydropyrrolo[2,3-b]indole (CCD ID: A1EWY) (formula: $C_{22}H_{26}N_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N 26 22 4	0	0
3	A	1	Total C N 26 22 4	0	0
3	C	1	Total C N 26 22 4	0	0
3	D	1	Total C N 26 22 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	182	Total O 182 182	0	0
4	A	149	Total O 149 149	0	0

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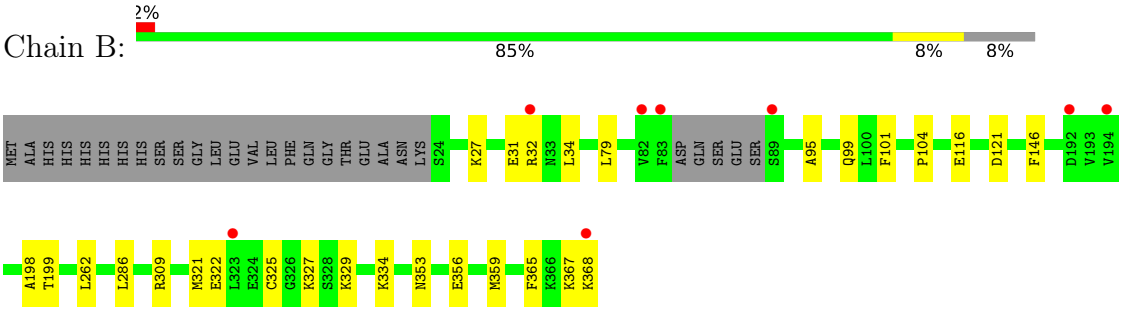
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	130	Total O 130 130	0	0
4	D	192	Total O 192 192	0	0

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.

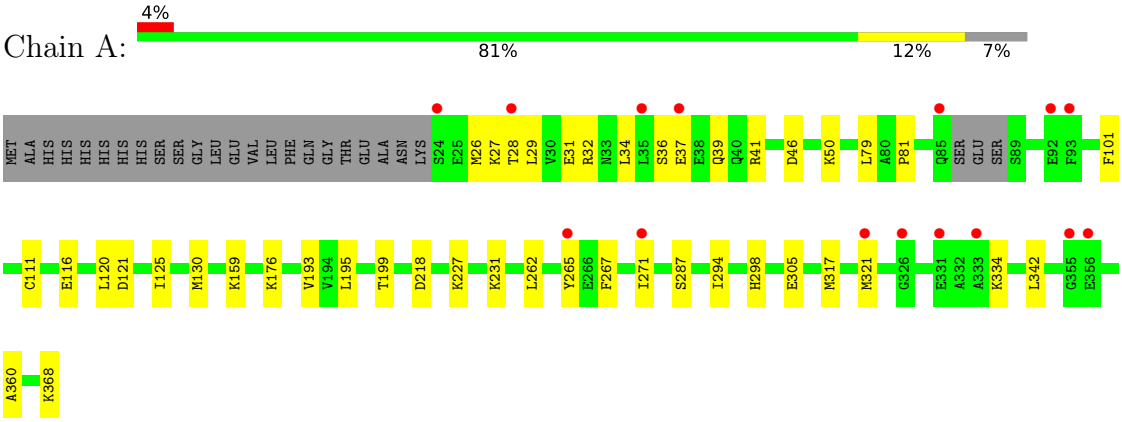
• Molecule 1: N-methyltransferase

Chain B:



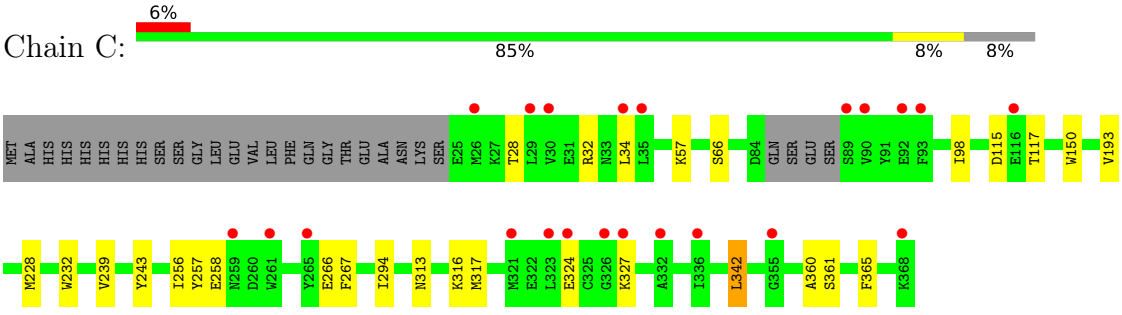
• Molecule 1: N-methyltransferase

Chain A:



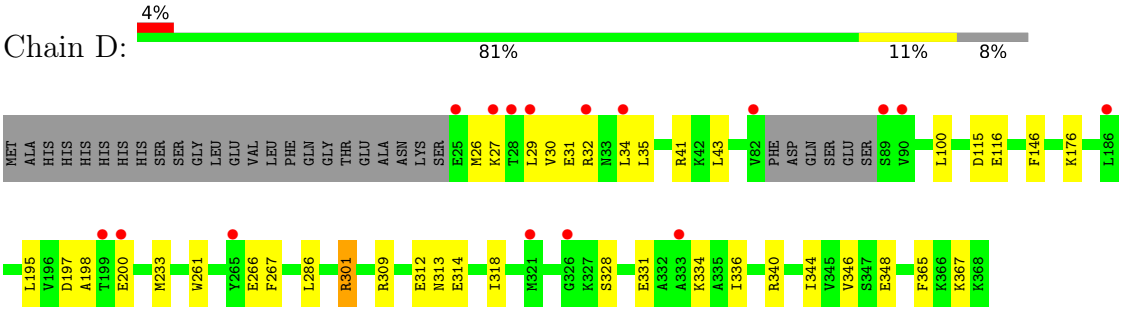
• Molecule 1: N-methyltransferase

Chain C:



• Molecule 1: N-methyltransferase

Chain D:


4%
81%
11%
8%
MET ALA HIS HIS HIS HIS HIS SER SER GLY LEU GLU VAL LEU PHE GLN GLY THR GLU ALA ASN LYS SER E25 M26 K27 T28 L29 V30 E31 R32 N33 L34 L35 R41 K42 L43 V82 PHE ASP GLN SER GLU SER S89 V90 L100 D115 E116 F146 K176 L186
L195 V196 D197 A198 T199 E200 M233 W261 Y265 E266 F267 L286 R301 R309 E312 N313 E314 I318 M321 G326 K327 S328 E331 A332 A333 K334 A335 I336 R340 I344 V345 V346 S347 E348 F365 K366 K367 K368

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	50.33Å 88.84Å 92.27Å 75.88° 89.97° 76.28°	Depositor
Resolution (Å)	20.88 – 2.00 20.88 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.1 (20.88-2.00) 96.0 (20.88-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.06 (at 2.01Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.208 , 0.242 0.208 , 0.242	Depositor DCC
R_{free} test set	4899 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	31.8	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 47.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.069 for h,h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11839	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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, A1EWY

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	0.10	0/2821	0.27	0/3804
1	B	0.11	0/2804	0.30	0/3781
1	C	0.15	0/2806	0.30	0/3784
1	D	0.18	0/2786	0.33	0/3757
All	All	0.14	0/11217	0.30	0/15126

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	2761	0	2738	26	0
1	B	2744	0	2726	17	0
1	C	2746	0	2725	20	0
1	D	2727	0	2712	25	0
2	A	26	0	19	0	0
2	B	26	0	19	0	0
2	C	26	0	19	1	0
2	D	26	0	19	0	0
3	A	26	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	26	0	0	0	0
3	C	26	0	0	1	0
3	D	26	0	0	1	0
4	A	149	0	0	0	0
4	B	182	0	0	0	0
4	C	130	0	0	0	0
4	D	192	0	0	0	0
All	All	11839	0	10977	89	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 89 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:GLU:HB3	1:A:41:ARG:HH12	1.36	0.88
1:B:367:LYS:HG2	1:B:368:LYS:HG2	1.59	0.83
1:A:116:GLU:H	1:A:116:GLU:CD	2.03	0.67
1:C:266:GLU:O	1:C:342:LEU:HD22	1.97	0.65
1:A:287:SER:OG	1:A:368:LYS:HG2	1.98	0.64

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	338/368 (92%)	332 (98%)	6 (2%)	0	100	100
1	B	336/368 (91%)	330 (98%)	6 (2%)	0	100	100
1	C	336/368 (91%)	329 (98%)	7 (2%)	0	100	100
1	D	334/368 (91%)	324 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1344/1472 (91%)	1315 (98%)	29 (2%)	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	302/324 (93%)	300 (99%)	2 (1%)	76 82
1	B	300/324 (93%)	300 (100%)	0	100 100
1	C	300/324 (93%)	298 (99%)	2 (1%)	76 82
1	D	298/324 (92%)	295 (99%)	3 (1%)	68 75
All	All	1200/1296 (93%)	1193 (99%)	7 (1%)	78 85

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	342	LEU
1	D	35	LEU
1	D	301	ARG
1	D	266	GLU
1	C	193	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	39	GLN
1	D	277	ASN
1	D	313	ASN
1	A	202	GLN
1	A	204	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SAH	B	401	-	27,28,28	0.20	0	38,40,40	0.45	0
2	SAH	A	401	-	27,28,28	0.30	0	38,40,40	0.43	0
3	A1EWY	D	402	-	29,31,31	0.18	0	44,50,50	0.34	0
3	A1EWY	B	402	-	29,31,31	0.19	0	44,50,50	0.43	0
3	A1EWY	C	402	-	29,31,31	0.27	0	44,50,50	0.83	2 (4%)
3	A1EWY	A	402	-	29,31,31	0.24	0	44,50,50	0.69	2 (4%)
2	SAH	D	401	-	27,28,28	0.20	0	38,40,40	0.51	0
2	SAH	C	401	-	27,28,28	0.32	0	38,40,40	0.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAH	B	401	-	-	0/15/31/31	0/3/3/3
2	SAH	A	401	-	-	2/15/31/31	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1EWY	D	402	-	-	0/9/61/61	0/6/6/6
3	A1EWY	B	402	-	-	0/9/61/61	0/6/6/6
3	A1EWY	C	402	-	-	0/9/61/61	0/6/6/6
3	A1EWY	A	402	-	-	0/9/61/61	0/6/6/6
2	SAH	D	401	-	-	0/15/31/31	0/3/3/3
2	SAH	C	401	-	-	1/15/31/31	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	402	A1EWY	C14-N2-C8	3.14	109.55	105.74
3	C	402	A1EWY	C13-N1-C7	2.98	109.36	105.74
3	A	402	A1EWY	C13-N1-C7	2.61	108.91	105.74
3	A	402	A1EWY	C13-C9-C5	-2.10	101.95	104.92

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	SAH	O-C-CA-N
2	A	401	SAH	O-C-CA-CB
2	A	401	SAH	OXT-C-CA-CB

There are no ring outliers.

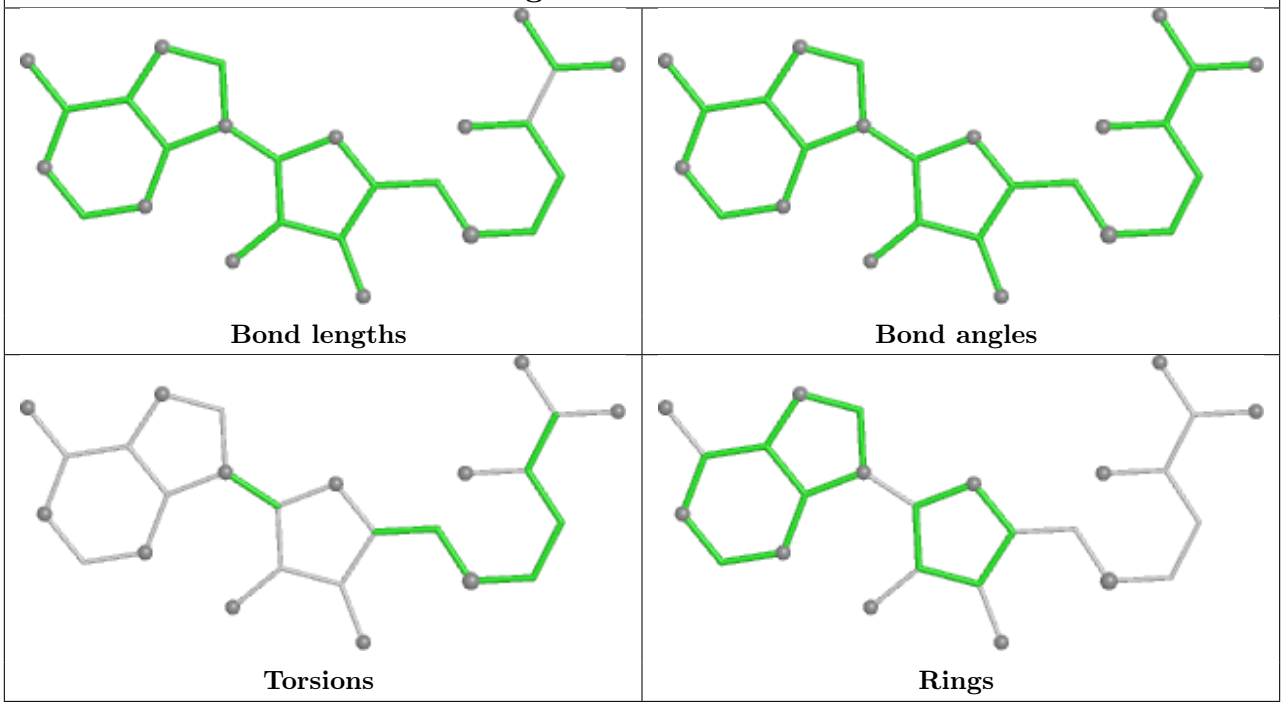
3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	402	A1EWY	1	0
3	C	402	A1EWY	1	0
2	C	401	SAH	1	0

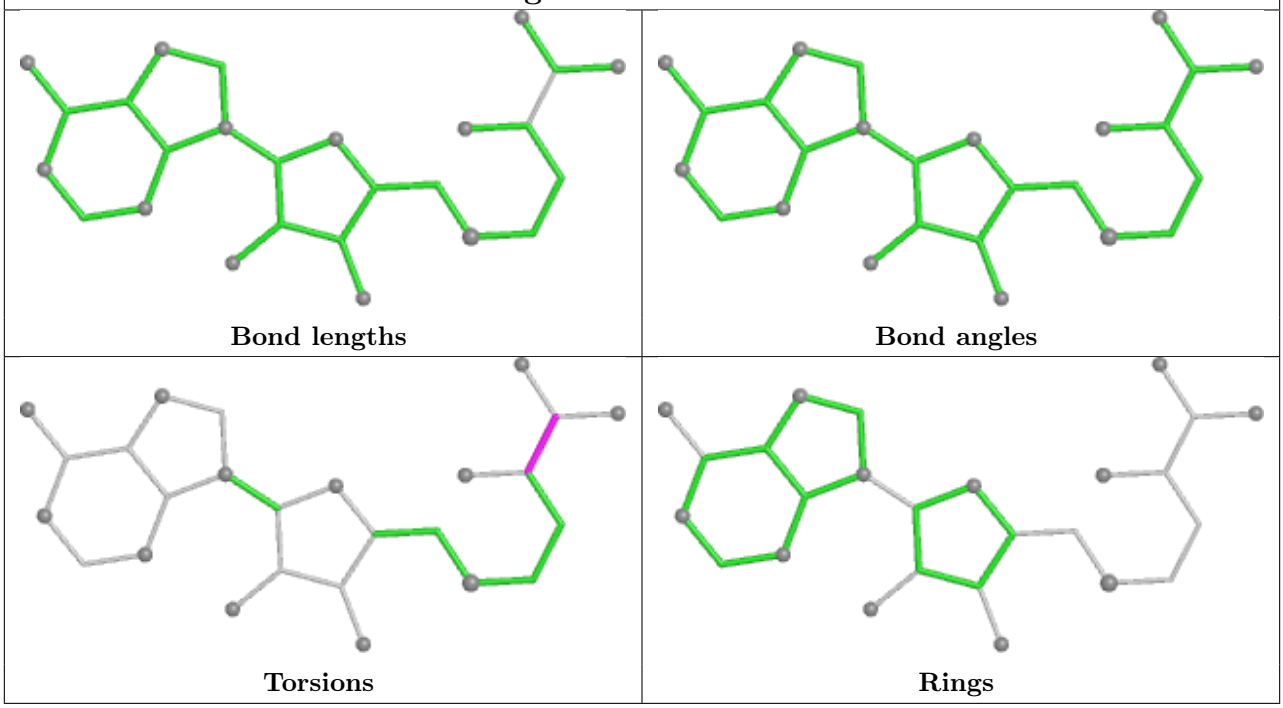
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

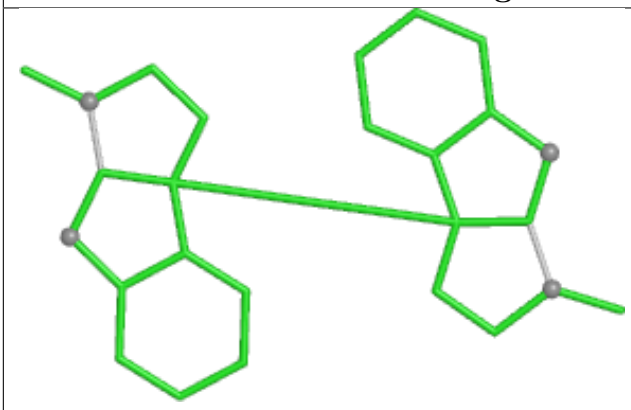
Ligand SAH B 401



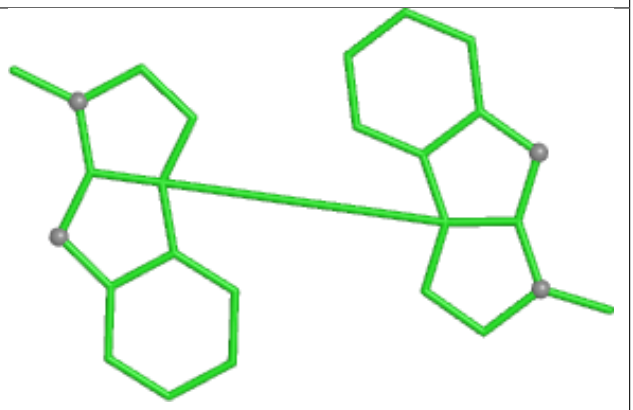
Ligand SAH A 401



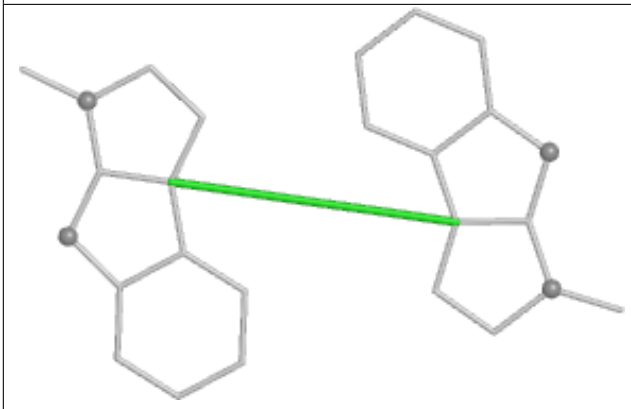
Ligand A1EWY D 402



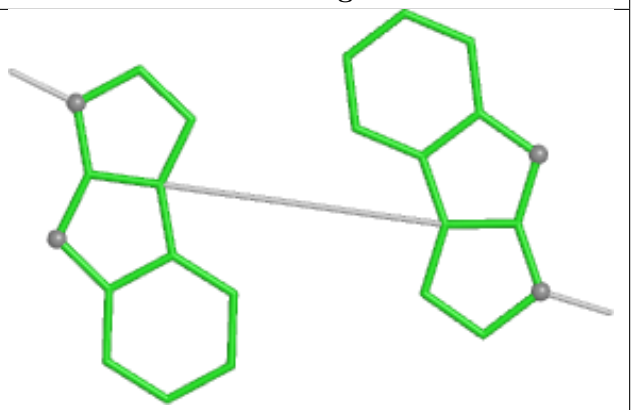
Bond lengths



Bond angles

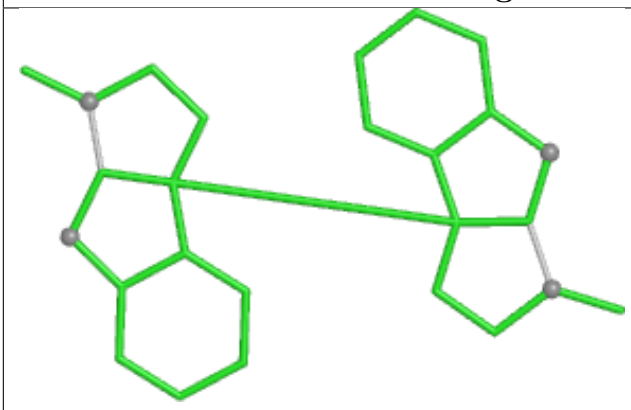


Torsions

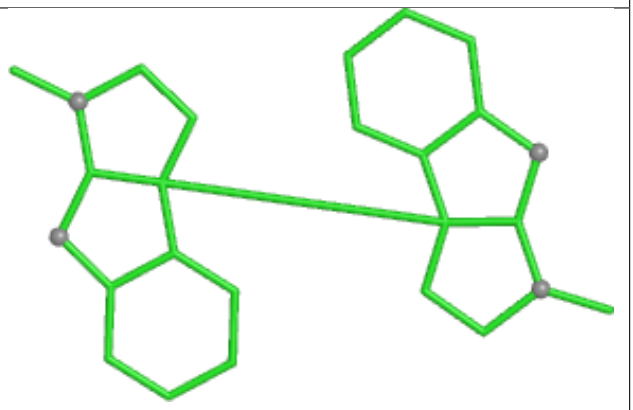


Rings

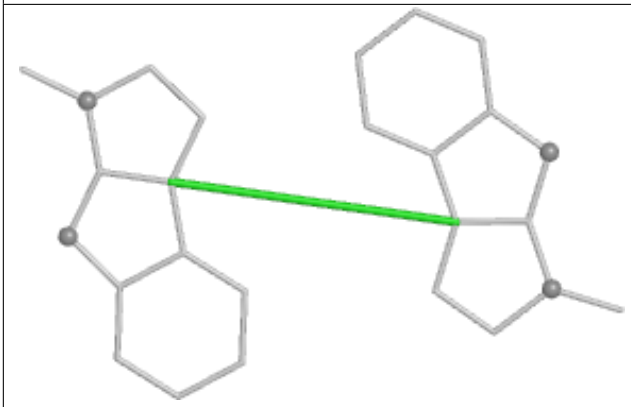
Ligand A1EWY B 402



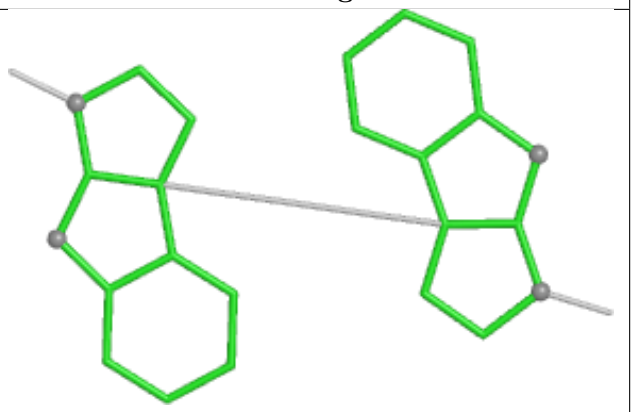
Bond lengths



Bond angles

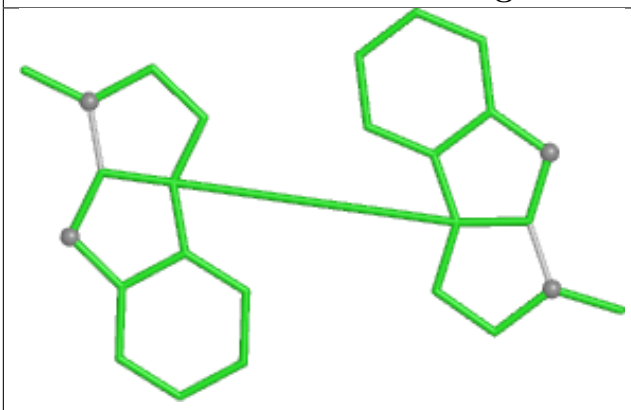


Torsions

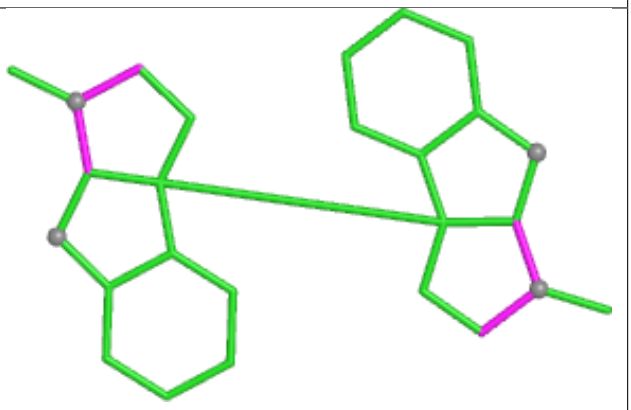


Rings

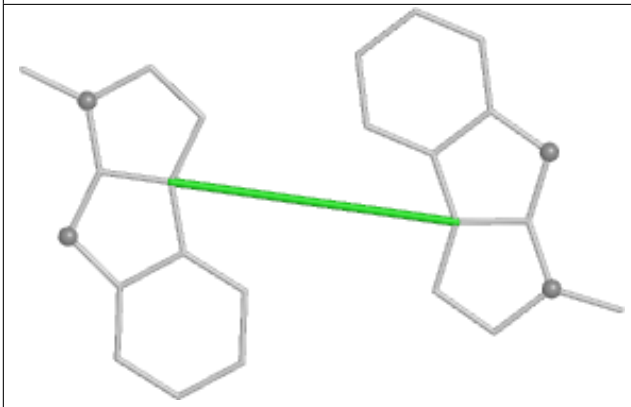
Ligand A1EWY C 402



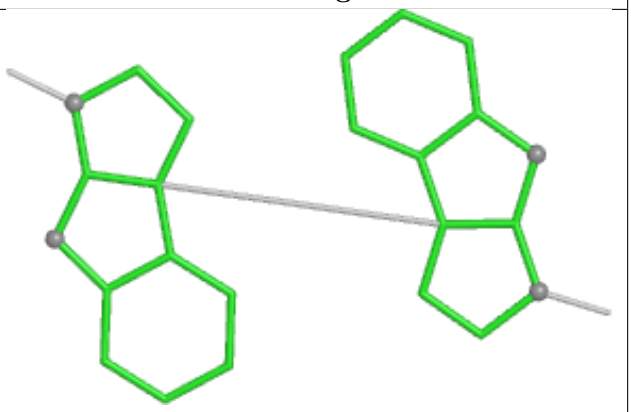
Bond lengths



Bond angles

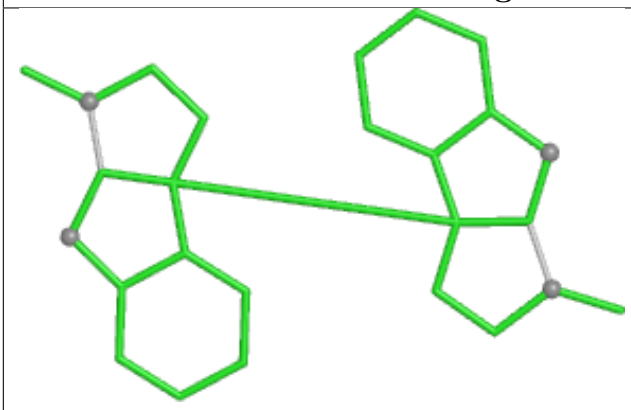


Torsions

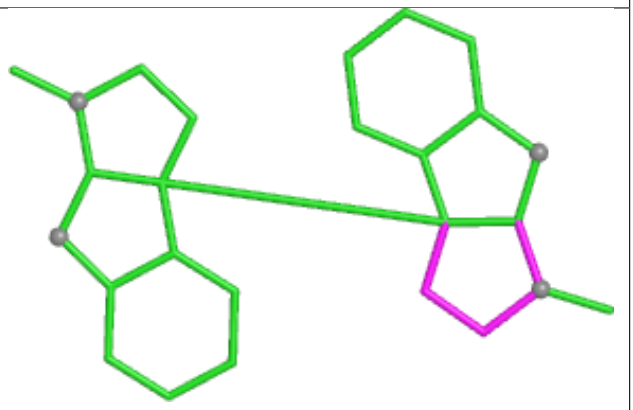


Rings

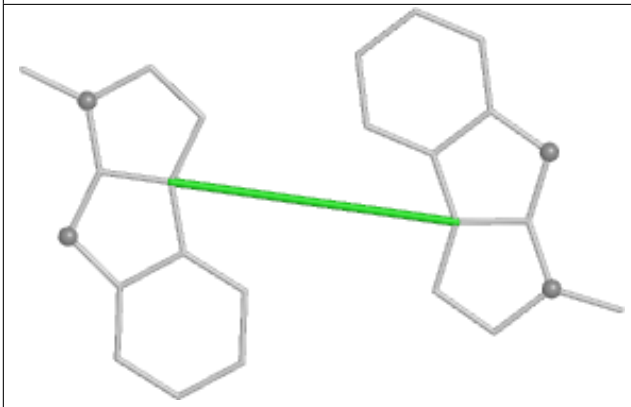
Ligand A1EWY A 402



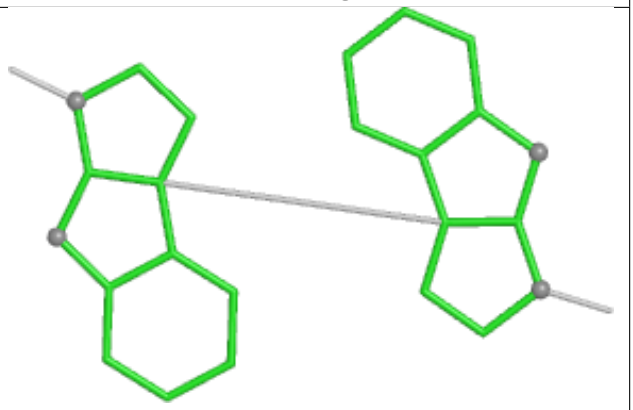
Bond lengths



Bond angles

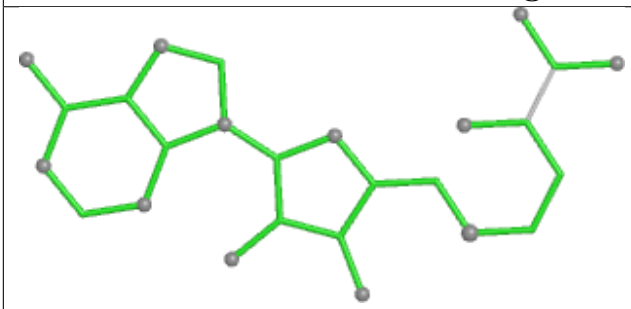


Torsions

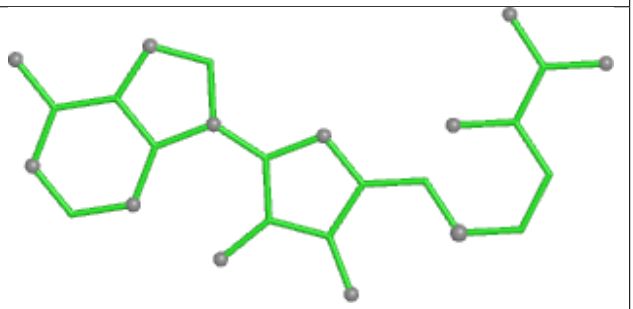


Rings

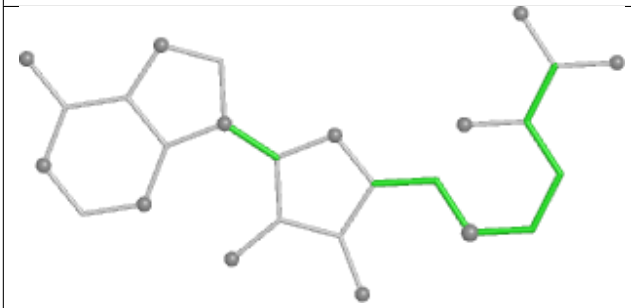
Ligand SAH D 401



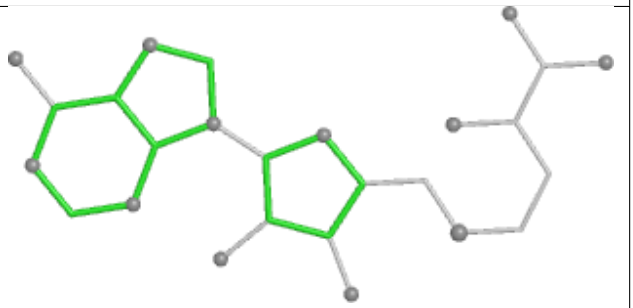
Bond lengths



Bond angles

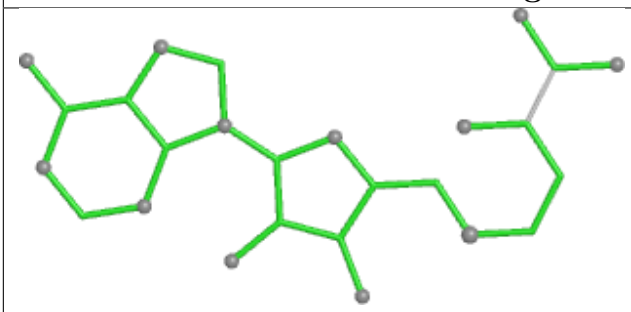


Torsions

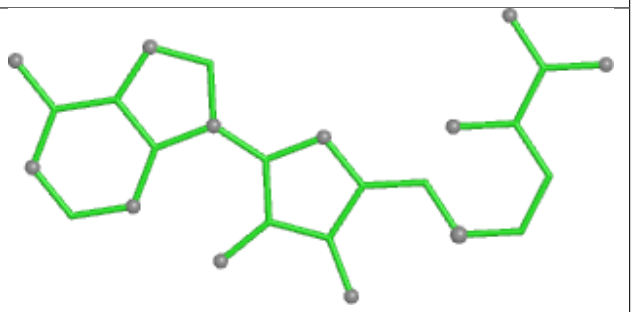


Rings

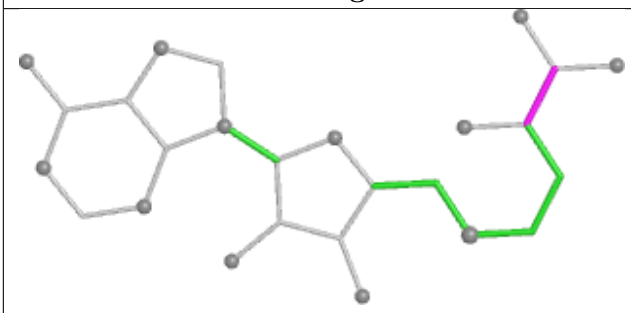
Ligand SAH C 401



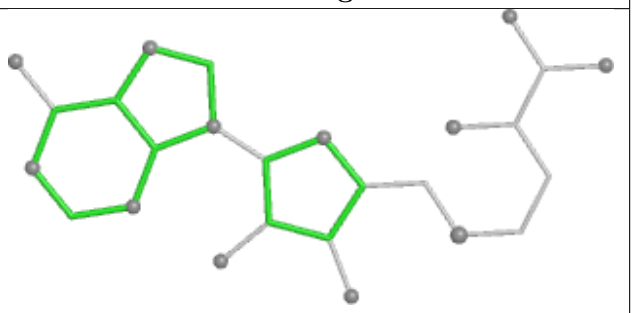
Bond lengths



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	342/368 (92%)	0.44	15 (4%)	39	38	24, 37, 79, 97	0
1	B	340/368 (92%)	0.37	8 (2%)	59	59	22, 36, 66, 86	0
1	C	340/368 (92%)	0.49	22 (6%)	25	23	24, 37, 83, 101	0
1	D	338/368 (91%)	0.42	16 (4%)	36	35	23, 37, 77, 105	0
All	All	1360/1472 (92%)	0.43	61 (4%)	38	37	22, 37, 79, 105	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	25	GLU	5.2
1	A	326	GLY	4.4
1	C	265	TYR	4.2
1	C	332	ALA	3.4
1	A	265	TYR	3.3

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

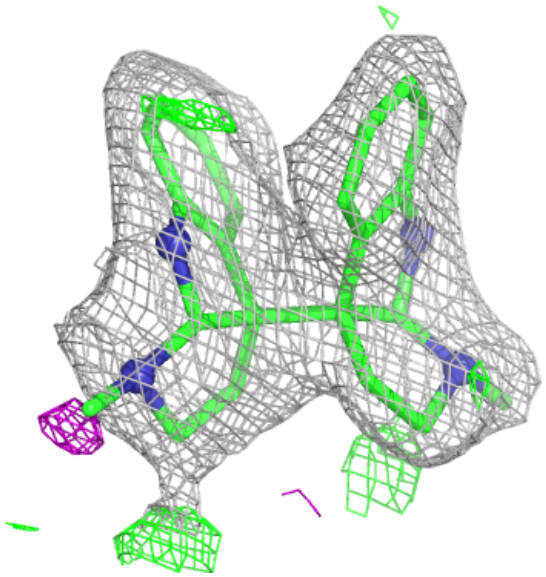
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

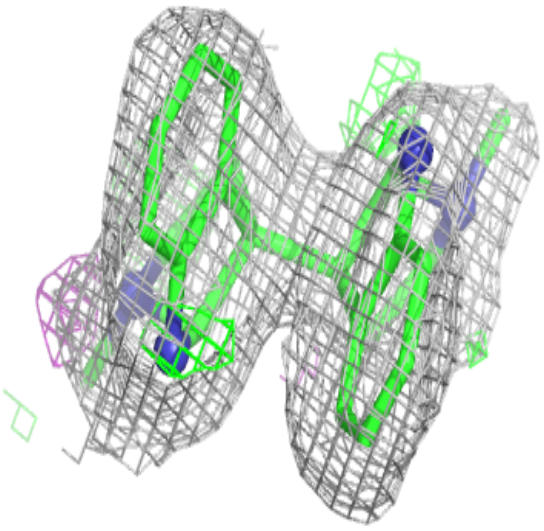
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	A1EWY	D	402	26/26	0.82	0.12	38,46,52,57	0
3	A1EWY	A	402	26/26	0.86	0.11	31,45,52,57	0
3	A1EWY	C	402	26/26	0.86	0.11	32,47,58,64	0
3	A1EWY	B	402	26/26	0.86	0.10	30,41,47,49	0
2	SAH	B	401	26/26	0.92	0.08	29,37,41,45	0
2	SAH	D	401	26/26	0.92	0.09	30,36,43,45	0
2	SAH	C	401	26/26	0.94	0.08	27,31,40,50	0
2	SAH	A	401	26/26	0.94	0.07	23,32,36,41	0

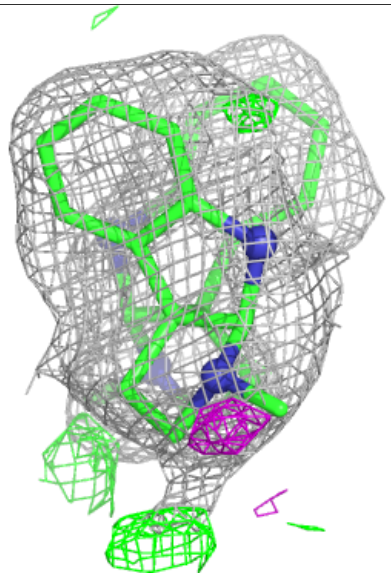
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1EWY 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)

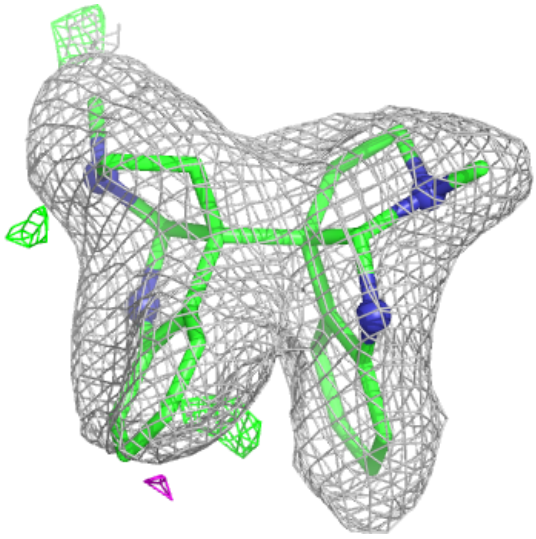


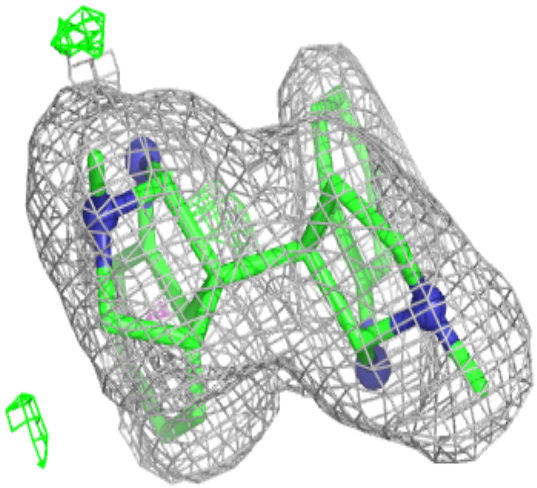


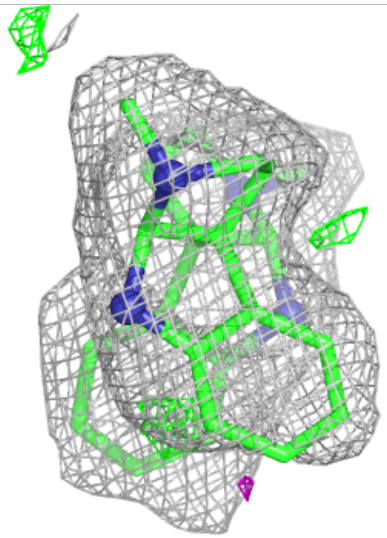


Electron density around A1EWY A 402:

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

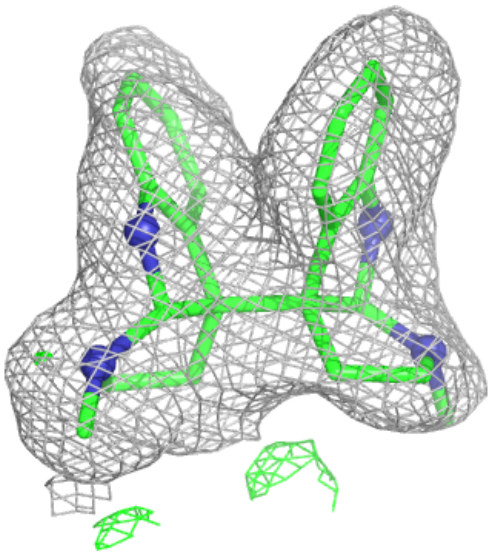


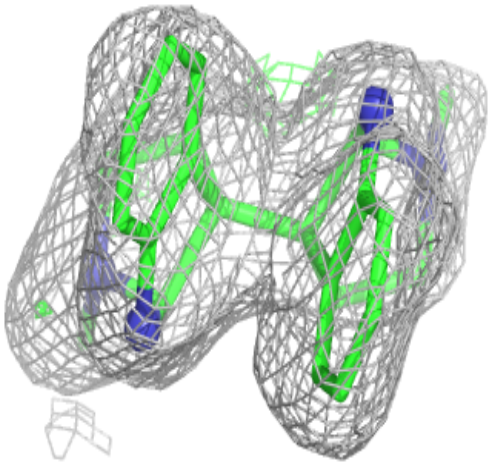


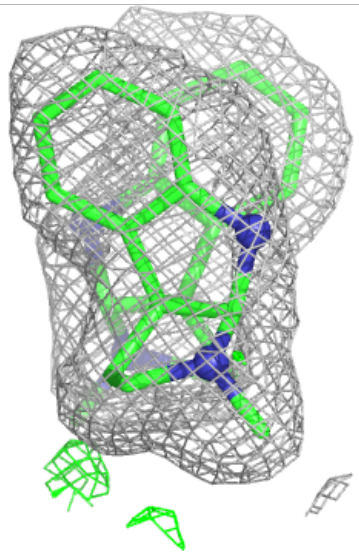


Electron density around A1EWY C 402:

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

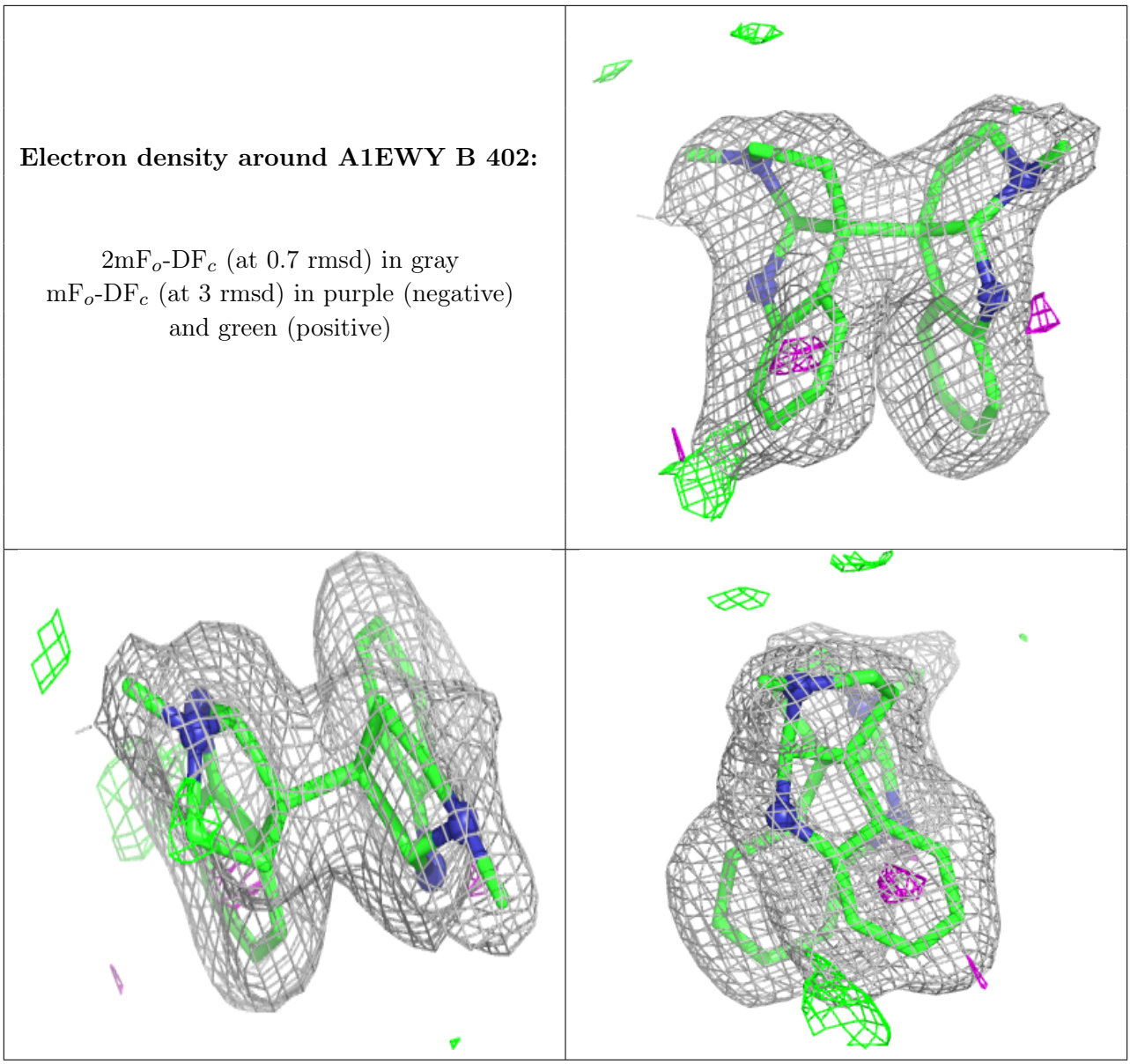






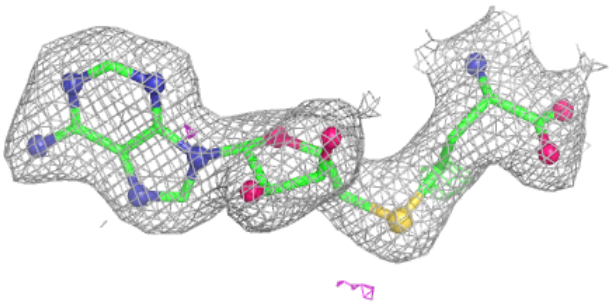
Electron density around A1EWY B 402:

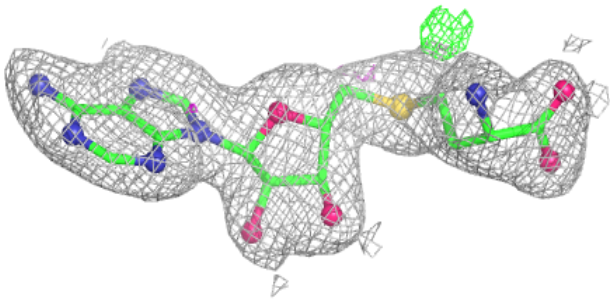
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

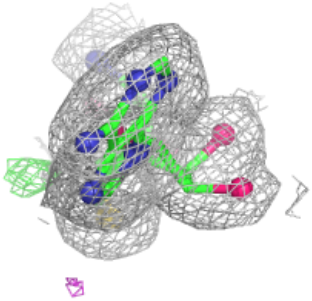


Electron density around SAH B 401:

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

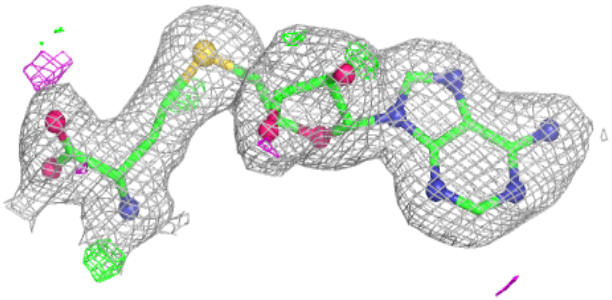


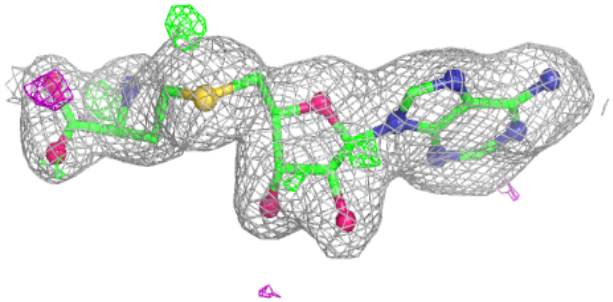


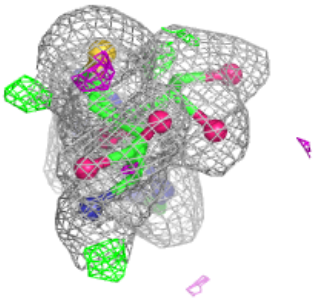


Electron density around SAH D 401:

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

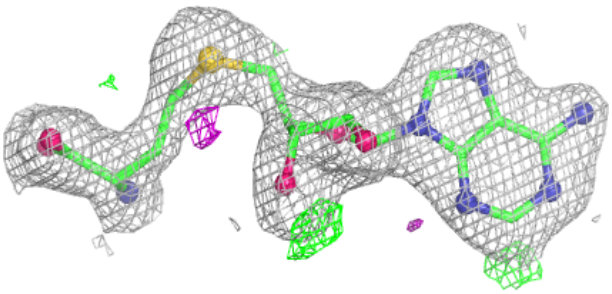


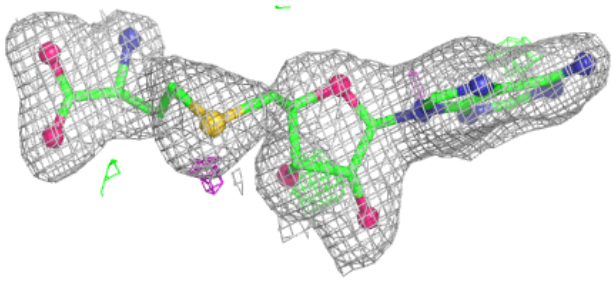


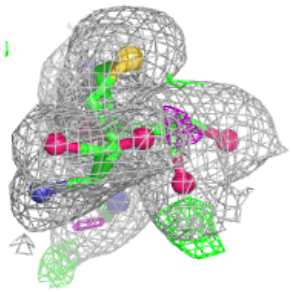


Electron density around SAH C 401:

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

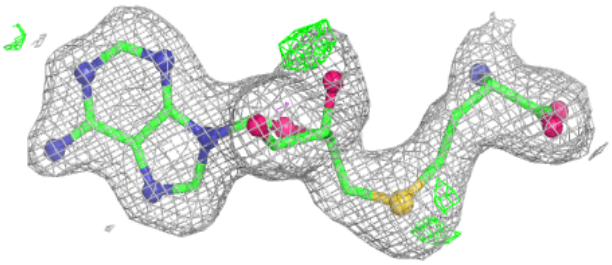


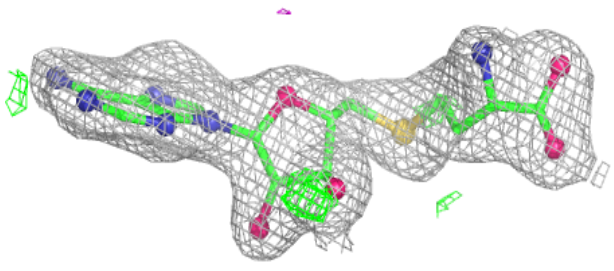


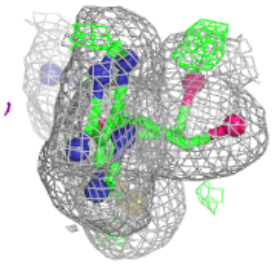


Electron density around SAH A 401:

$2mF_o$-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.