wwPDB X-ray Structure Validation Summary Report (i)

Mar 9, 2021 – 07:48 pm GMT

PDB ID	:	7BLE
Title	:	Co-crystal structure of Human Nicotinamide N-methyltransferase (NNMT) with the tricyclic inhibitor (3)
Authors	:	Schreuder, H.A.; Liesum, A.
Deposited on	:	2021-01-18
Resolution	:	2.81 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 following versions of software and data (see references (i)) were used in the production of this report:

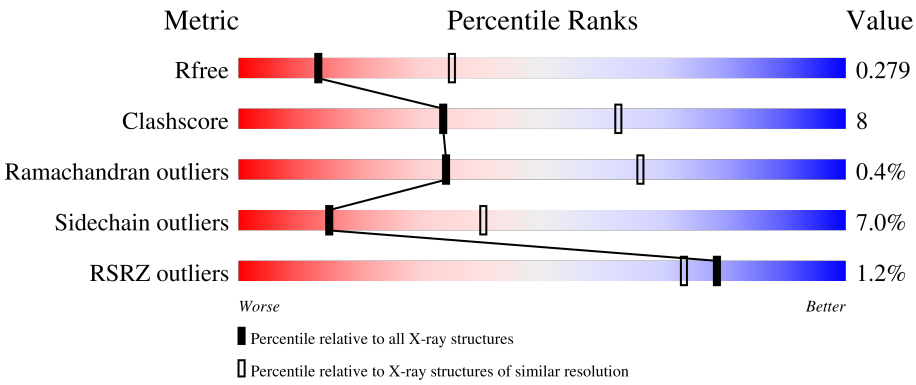
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.17.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.17.1

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 2.81 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	283	72% 20% • 6%
1	B	283	76% 15% • 7%
1	C	283	% 68% 18% • 11%
1	D	283	3% 61% 25% • 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8460 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 Nicotinamide N-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	265	2049	1315	330	392	12	0	0	0
1	B	263	2035	1306	327	390	12	0	0	0
1	C	252	1969	1267	317	374	11	0	0	0
1	D	252	1969	1267	317	374	11	0	0	0

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP P40261
A	-17	GLY	-	expression tag	UNP P40261
A	-16	SER	-	expression tag	UNP P40261
A	-15	SER	-	expression tag	UNP P40261
A	-14	HIS	-	expression tag	UNP P40261
A	-13	HIS	-	expression tag	UNP P40261
A	-12	HIS	-	expression tag	UNP P40261
A	-11	HIS	-	expression tag	UNP P40261
A	-10	HIS	-	expression tag	UNP P40261
A	-9	HIS	-	expression tag	UNP P40261
A	-8	SER	-	expression tag	UNP P40261
A	-7	SER	-	expression tag	UNP P40261
A	-6	GLY	-	expression tag	UNP P40261
A	-5	LEU	-	expression tag	UNP P40261
A	-4	VAL	-	expression tag	UNP P40261
A	-3	PRO	-	expression tag	UNP P40261
A	-2	ARG	-	expression tag	UNP P40261
A	-1	GLY	-	expression tag	UNP P40261
A	0	SER	-	expression tag	UNP P40261
A	100	ALA	LYS	engineered mutation	UNP P40261
A	101	ALA	GLU	engineered mutation	UNP P40261

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Chain	Residue	Modelled	Actual	Comment	Reference
A	103	ALA	GLU	engineered mutation	UNP P40261
B	-18	MET	-	initiating methionine	UNP P40261
B	-17	GLY	-	expression tag	UNP P40261
B	-16	SER	-	expression tag	UNP P40261
B	-15	SER	-	expression tag	UNP P40261
B	-14	HIS	-	expression tag	UNP P40261
B	-13	HIS	-	expression tag	UNP P40261
B	-12	HIS	-	expression tag	UNP P40261
B	-11	HIS	-	expression tag	UNP P40261
B	-10	HIS	-	expression tag	UNP P40261
B	-9	HIS	-	expression tag	UNP P40261
B	-8	SER	-	expression tag	UNP P40261
B	-7	SER	-	expression tag	UNP P40261
B	-6	GLY	-	expression tag	UNP P40261
B	-5	LEU	-	expression tag	UNP P40261
B	-4	VAL	-	expression tag	UNP P40261
B	-3	PRO	-	expression tag	UNP P40261
B	-2	ARG	-	expression tag	UNP P40261
B	-1	GLY	-	expression tag	UNP P40261
B	0	SER	-	expression tag	UNP P40261
B	100	ALA	LYS	engineered mutation	UNP P40261
B	101	ALA	GLU	engineered mutation	UNP P40261
B	103	ALA	GLU	engineered mutation	UNP P40261
C	-18	MET	-	initiating methionine	UNP P40261
C	-17	GLY	-	expression tag	UNP P40261
C	-16	SER	-	expression tag	UNP P40261
C	-15	SER	-	expression tag	UNP P40261
C	-14	HIS	-	expression tag	UNP P40261
C	-13	HIS	-	expression tag	UNP P40261
C	-12	HIS	-	expression tag	UNP P40261
C	-11	HIS	-	expression tag	UNP P40261
C	-10	HIS	-	expression tag	UNP P40261
C	-9	HIS	-	expression tag	UNP P40261
C	-8	SER	-	expression tag	UNP P40261
C	-7	SER	-	expression tag	UNP P40261
C	-6	GLY	-	expression tag	UNP P40261
C	-5	LEU	-	expression tag	UNP P40261
C	-4	VAL	-	expression tag	UNP P40261
C	-3	PRO	-	expression tag	UNP P40261
C	-2	ARG	-	expression tag	UNP P40261
C	-1	GLY	-	expression tag	UNP P40261
C	0	SER	-	expression tag	UNP P40261

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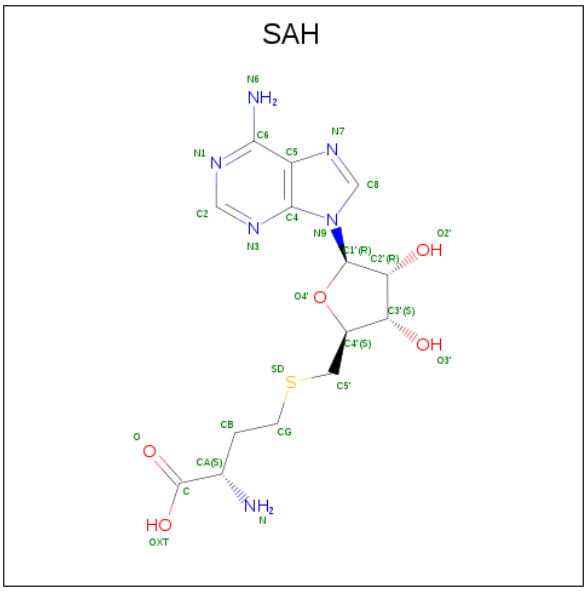
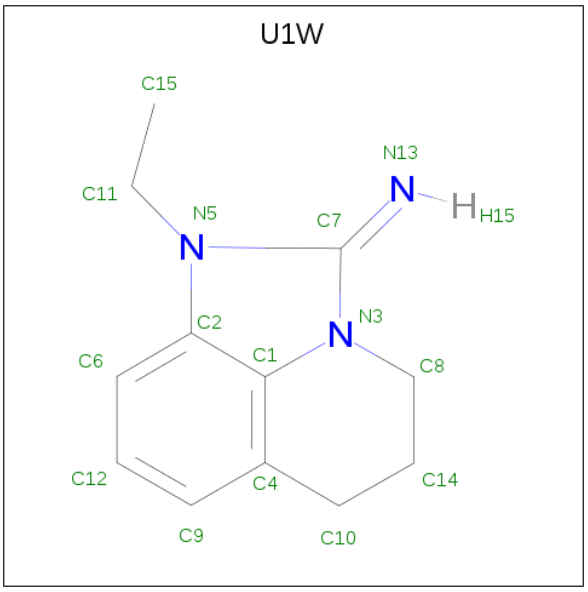
Chain	Residue	Modelled	Actual	Comment	Reference
C	100	ALA	LYS	engineered mutation	UNP P40261
C	101	ALA	GLU	engineered mutation	UNP P40261
C	103	ALA	GLU	engineered mutation	UNP P40261
D	-18	MET	-	initiating methionine	UNP P40261
D	-17	GLY	-	expression tag	UNP P40261
D	-16	SER	-	expression tag	UNP P40261
D	-15	SER	-	expression tag	UNP P40261
D	-14	HIS	-	expression tag	UNP P40261
D	-13	HIS	-	expression tag	UNP P40261
D	-12	HIS	-	expression tag	UNP P40261
D	-11	HIS	-	expression tag	UNP P40261
D	-10	HIS	-	expression tag	UNP P40261
D	-9	HIS	-	expression tag	UNP P40261
D	-8	SER	-	expression tag	UNP P40261
D	-7	SER	-	expression tag	UNP P40261
D	-6	GLY	-	expression tag	UNP P40261
D	-5	LEU	-	expression tag	UNP P40261
D	-4	VAL	-	expression tag	UNP P40261
D	-3	PRO	-	expression tag	UNP P40261
D	-2	ARG	-	expression tag	UNP P40261
D	-1	GLY	-	expression tag	UNP P40261
D	0	SER	-	expression tag	UNP P40261
D	100	ALA	LYS	engineered mutation	UNP P40261
D	101	ALA	GLU	engineered mutation	UNP P40261
D	103	ALA	GLU	engineered mutation	UNP P40261

- 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		

- Molecule 3 is 3-ethyl-1,3-diazatricyclo[6.3.1.0^{4,12}]dodeca-4,6,8(12)-trien-2-imine (three-letter code: U1W) (formula: $C_{12}H_{15}N_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
3	A	1	15	12	3	0	0
3	B	1	15	12	3	0	0
3	C	1	15	12	3	0	0
3	D	1	15	12	3	0	0

- Molecule 4 is water.

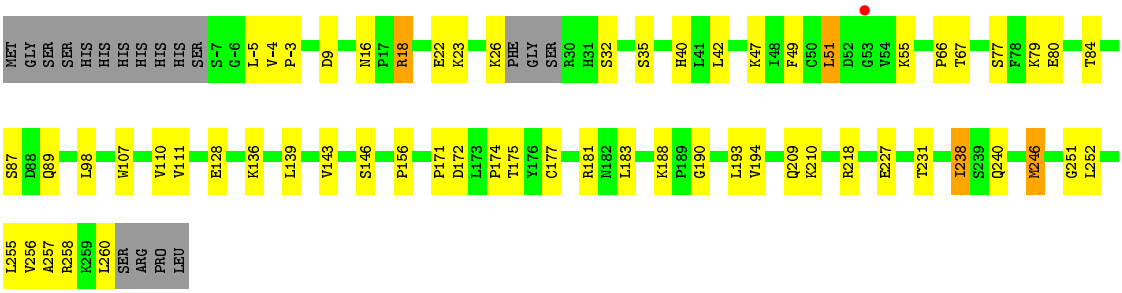
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	69	69	69	0	0
4	B	85	85	85	0	0
4	C	56	56	56	0	0
4	D	64	64	64	0	0

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.

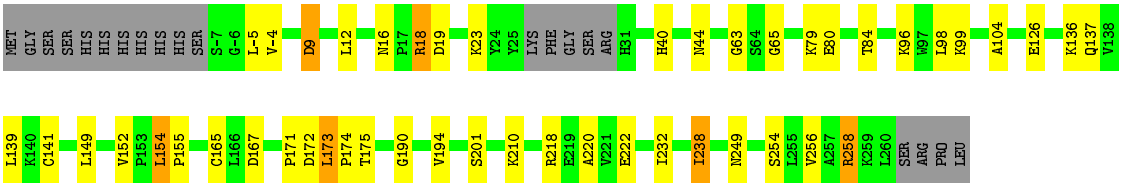
- Molecule 1: Nicotinamide N-methyltransferase

Chain A:



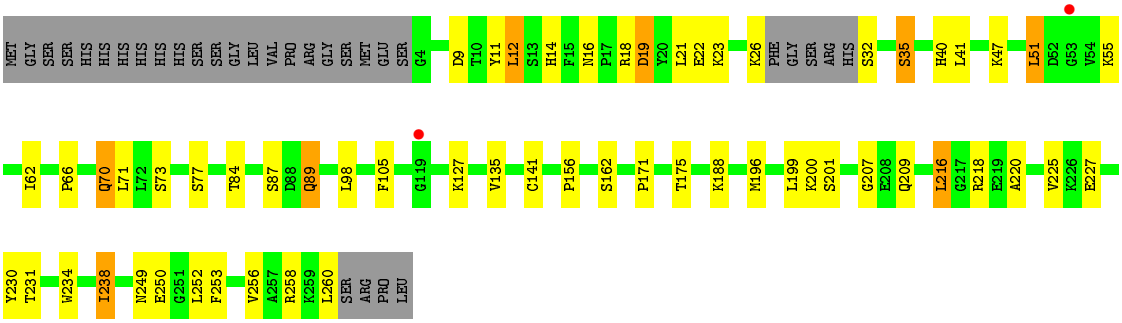
- Molecule 1: Nicotinamide N-methyltransferase

Chain B:



- Molecule 1: Nicotinamide N-methyltransferase

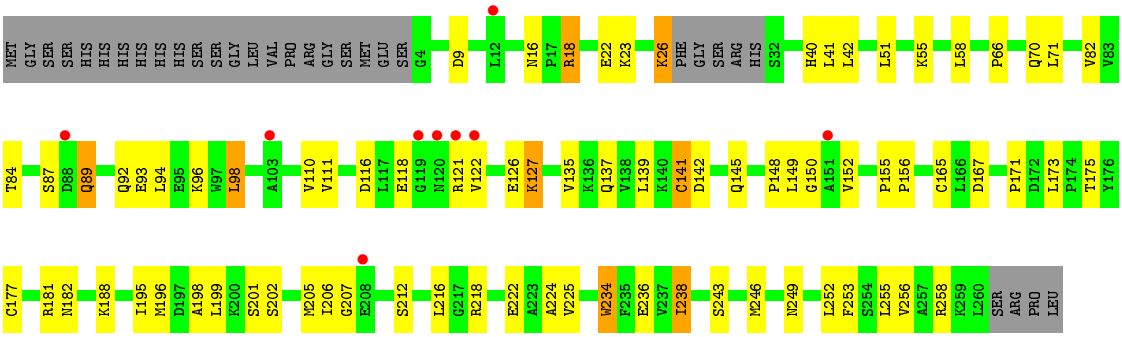
Chain C:



- Molecule 1: Nicotinamide N-methyltransferase

Chain D:

3%
61%
25%
11%


MET GLY SER SER HIS HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER MET GLU SER G4 D9 L12 N16 P17 R18 E22 K23 K26 PHE GLY SER ARG HIS S32 H40 L41 L42 L51 K55 L58 P66 Q70 L71 V82 V83
T84 S87 D88 Q89 Q92 E93 L94 E95 K96 W97 L98 A103 V110 V111 D116 L117 E118 G119 N120 R121 V122 E126 K127 V135 K136 Q137 V138 L139 K140 C141 D142 Q145 P148 L149 G150 A151 V152 P155 P156 C165 L166 D167 P171 D172 L173 P174 T175 Y176
C177 R181 N182 K188 I195 M196 D197 A198 L199 K200 S201 S202 M205 I206 G207 E208 S212 L216 G217 R218 E222 A223 A224 V225 W234 F235 E236 V237 I238 S243 M246 N249 L252 F253 S254 L255 V256 A257 R258 K259 L260 SER ARG PRO LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	45.71Å 62.19Å 107.69Å 91.51° 98.09° 111.54°	Depositor
Resolution (Å)	57.64 – 2.81 57.64 – 2.81	Depositor EDS
% Data completeness (in resolution range)	97.0 (57.64-2.81) 97.0 (57.64-2.81)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.20 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.11.7 (6-FEB-2020)	Depositor
R, R_{free}	0.186 , 0.270 0.189 , 0.279	Depositor DCC
R_{free} test set	1295 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	32.1	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 65.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8460	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 5.52% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SAH, U1W

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	0.44	0/2091	0.63	0/2832
1	B	0.43	0/2077	0.63	0/2814
1	C	0.42	0/2010	0.62	0/2722
1	D	0.41	0/2010	0.62	0/2722
All	All	0.43	0/8188	0.63	0/11090

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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2049	0	2053	33	0
1	B	2035	0	2038	29	0
1	C	1969	0	1981	33	0
1	D	1969	0	1981	47	0
2	A	26	0	19	0	0
2	B	26	0	19	1	0
2	C	26	0	19	1	0
2	D	26	0	19	1	0
3	A	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	15	0	0	0	0
3	C	15	0	0	0	0
3	D	15	0	0	0	0
4	A	69	0	0	0	0
4	B	85	0	0	1	0
4	C	56	0	0	0	0
4	D	64	0	0	1	0
All	All	8460	0	8129	138	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 8.

The worst 5 of 138 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:16:ASN:HD21	1:A:18:ARG:NH2	1.60	0.99
1:A:16:ASN:HD21	1:A:18:ARG:HH22	1.12	0.96
1:D:234:TRP:HE1	1:D:256:VAL:HG23	1.31	0.96
1:D:234:TRP:HD1	1:D:256:VAL:HB	1.39	0.88
1:B:84:THR:HB	1:B:141:CYS:HB2	1.60	0.81

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	261/283 (92%)	245 (94%)	15 (6%)	1 (0%)	34	66
1	B	259/283 (92%)	247 (95%)	12 (5%)	0	100	100
1	C	248/283 (88%)	238 (96%)	10 (4%)	0	100	100
1	D	248/283 (88%)	225 (91%)	20 (8%)	3 (1%)	13	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1016/1132 (90%)	955 (94%)	57 (6%)	4 (0%)	34 66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	150	GLY
1	A	32	SER
1	D	207	GLY
1	D	66	PRO

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	226/245 (92%)	212 (94%)	14 (6%)	18 47
1	B	225/245 (92%)	213 (95%)	12 (5%)	22 54
1	C	218/245 (89%)	204 (94%)	14 (6%)	17 45
1	D	218/245 (89%)	196 (90%)	22 (10%)	7 22
All	All	887/980 (90%)	825 (93%)	62 (7%)	15 40

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	22	GLU
1	D	212	SER
1	C	127	LYS
1	D	202	SER
1	D	238	ILE

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	C	209	GLN

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Mol	Chain	Res	Type
1	D	145	GLN
1	D	240	GLN
1	B	137	GLN
1	C	14	HIS

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)

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	C	4001	-	21,28,28	0.57	0	20,40,40	1.19	2 (10%)
3	U1W	A	4002	-	12,17,17	1.16	1 (8%)	11,25,25	1.92	3 (27%)
3	U1W	D	4002	-	12,17,17	1.54	3 (25%)	11,25,25	1.93	4 (36%)
3	U1W	B	4002	-	12,17,17	1.29	1 (8%)	11,25,25	2.13	4 (36%)
3	U1W	C	4002	-	12,17,17	1.53	3 (25%)	11,25,25	2.00	4 (36%)
2	SAH	B	4001	-	21,28,28	0.65	0	20,40,40	1.06	2 (10%)
2	SAH	A	4001	-	21,28,28	0.61	0	20,40,40	1.17	2 (10%)
2	SAH	D	4001	-	21,28,28	0.58	0	20,40,40	1.25	3 (15%)

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	C	4001	-	-	1/7/31/31	0/3/3/3
3	U1W	A	4002	-	-	1/2/8/8	0/2/3/3
3	U1W	D	4002	-	-	1/2/8/8	0/2/3/3
3	U1W	B	4002	-	-	1/2/8/8	0/2/3/3
3	U1W	C	4002	-	-	0/2/8/8	0/2/3/3
2	SAH	B	4001	-	-	0/7/31/31	0/3/3/3
2	SAH	A	4001	-	-	1/7/31/31	0/3/3/3
2	SAH	D	4001	-	-	1/7/31/31	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4002	U1W	C4-C1	-3.28	1.37	1.42
3	C	4002	U1W	C9-C4	3.27	1.43	1.37
3	D	4002	U1W	C9-C4	2.74	1.42	1.37
3	B	4002	U1W	C4-C1	-2.30	1.39	1.42
3	C	4002	U1W	C10-C4	2.29	1.52	1.50

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	4002	U1W	C2-C1-N3	3.70	110.68	105.77
2	C	4001	SAH	CB-CG-SD	-3.61	105.21	113.31
3	A	4002	U1W	C2-C1-N3	3.57	110.51	105.77
2	A	4001	SAH	CB-CG-SD	-3.53	105.38	113.31
3	D	4002	U1W	C2-C1-N3	3.52	110.45	105.77

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	4002	U1W	C15-C11-N5-C7
2	C	4001	SAH	CB-CG-SD-C5'
3	D	4002	U1W	C15-C11-N5-C2
2	A	4001	SAH	CB-CG-SD-C5'
2	D	4001	SAH	CB-CG-SD-C5'

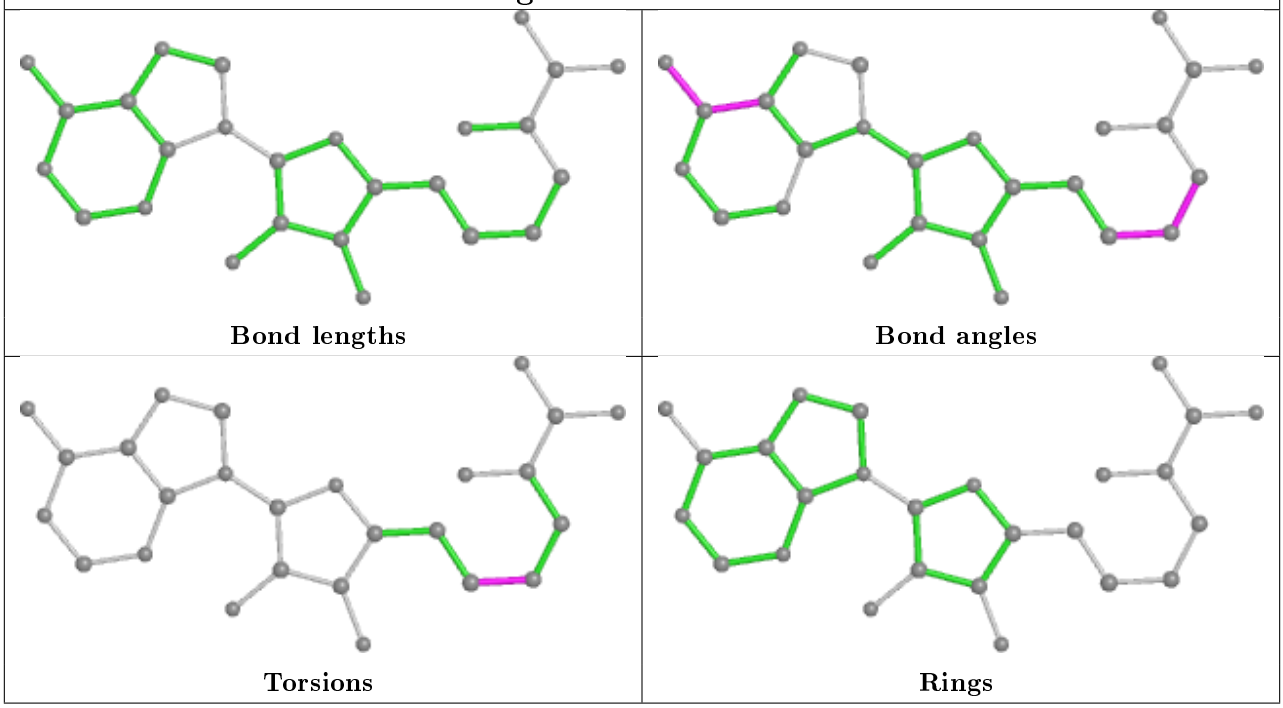
There are no ring outliers.

3 monomers are involved in 3 short contacts:

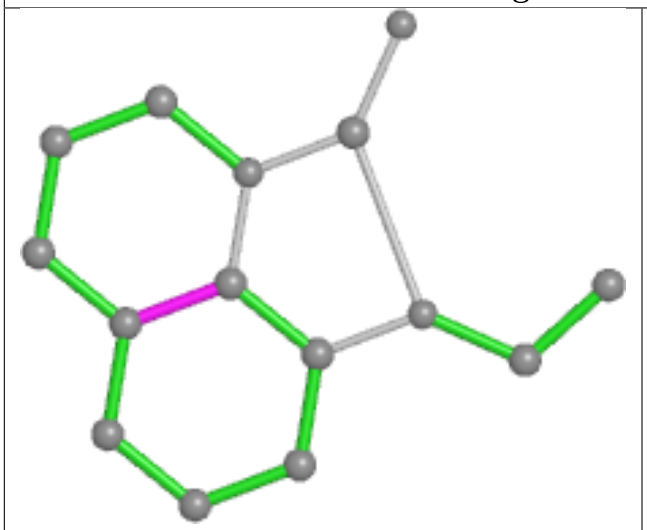
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	4001	SAH	1	0
2	B	4001	SAH	1	0
2	D	4001	SAH	1	0

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.

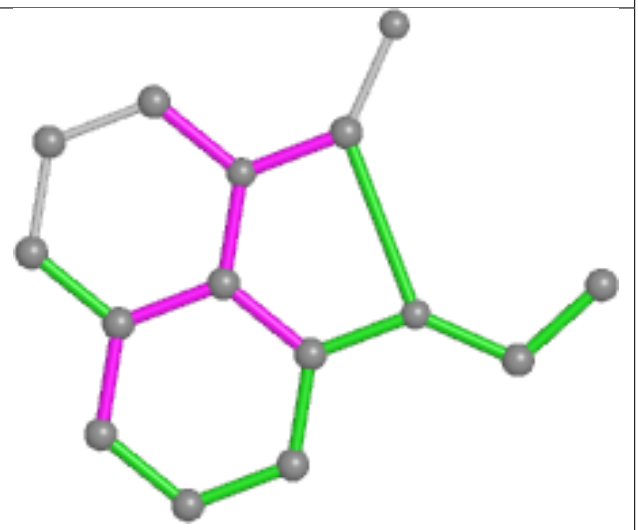
Ligand SAH C 4001



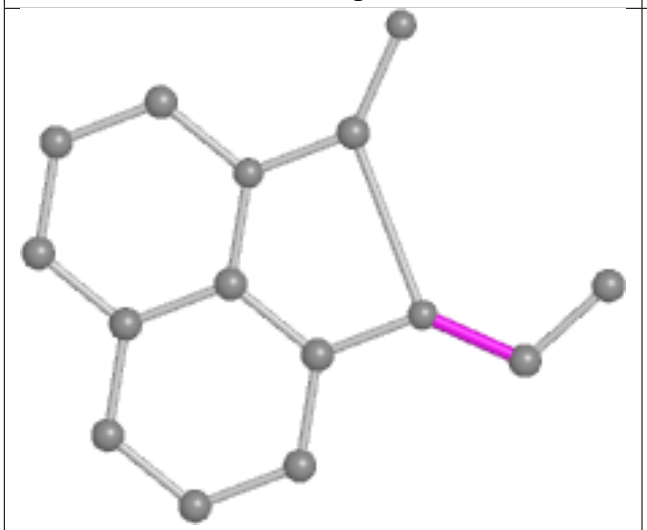
Ligand U1W A 4002



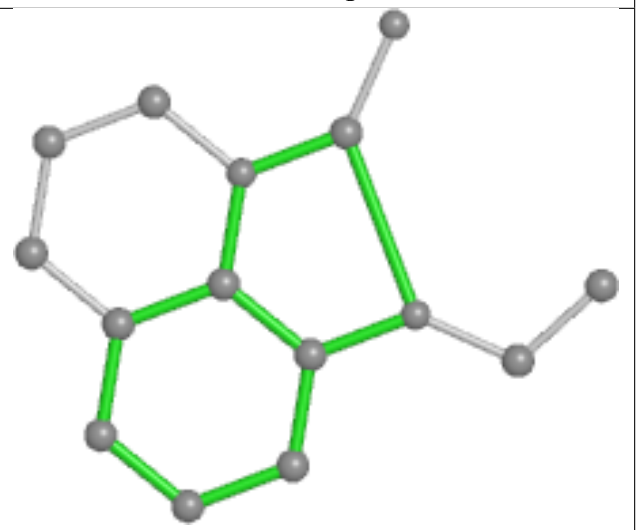
Bond lengths



Bond angles

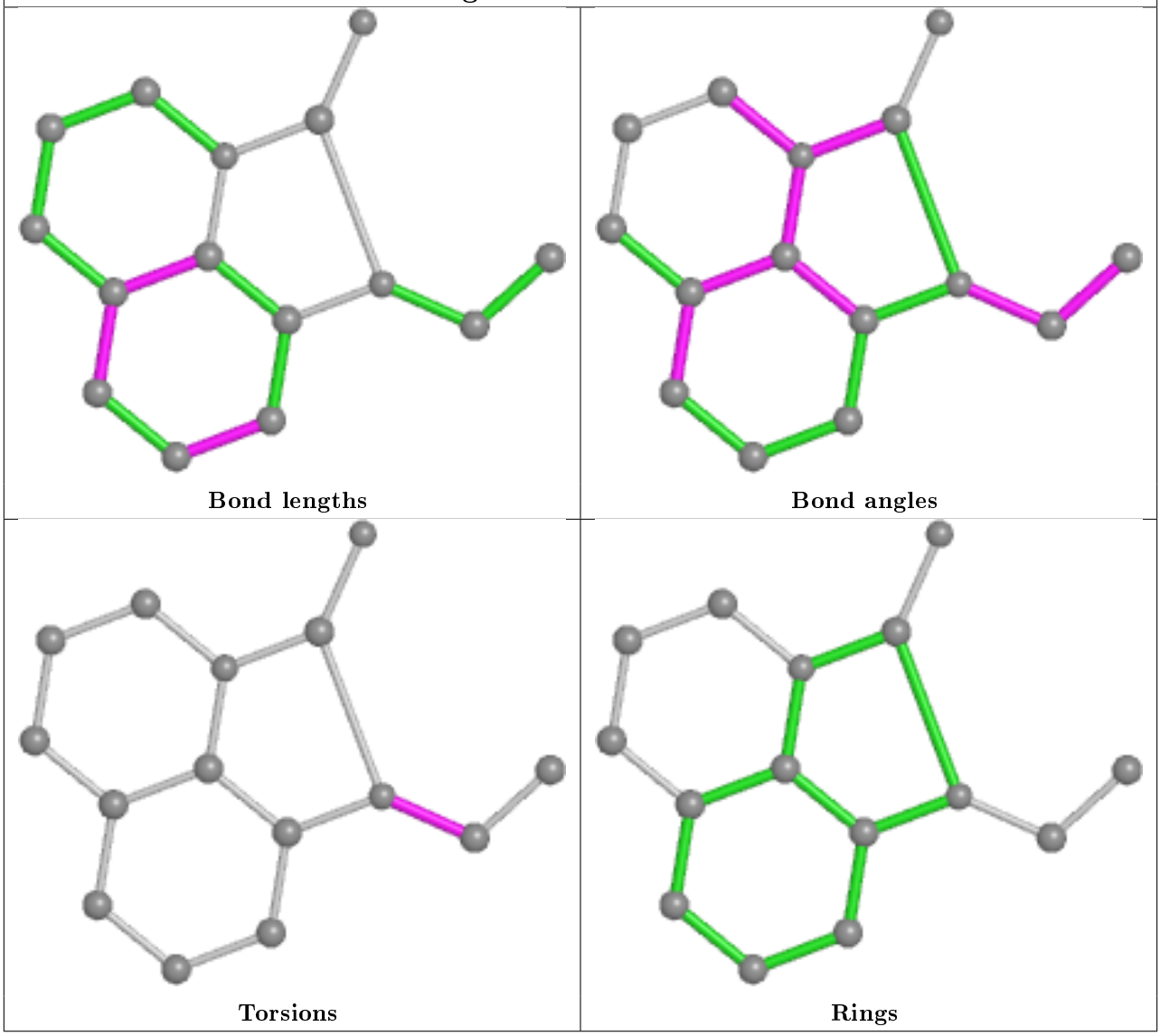


Torsions

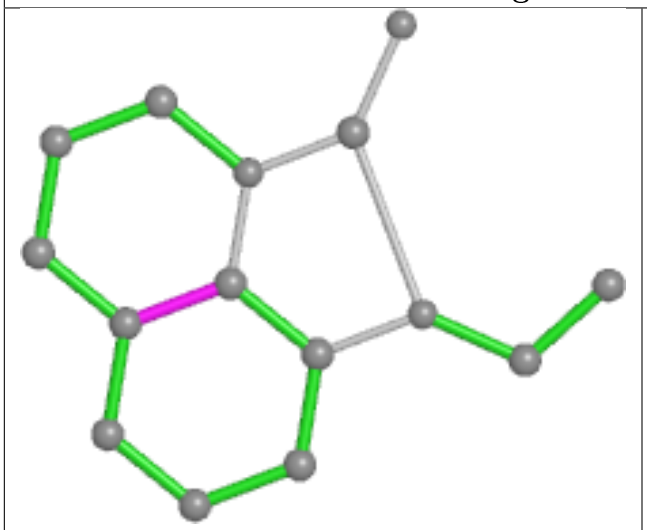


Rings

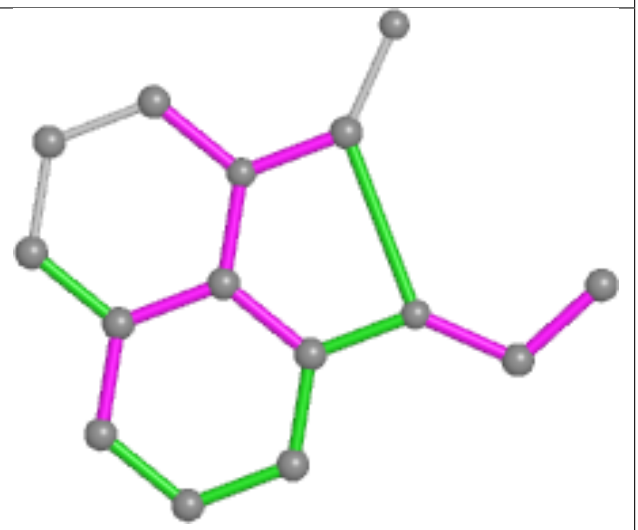
Ligand U1W D 4002



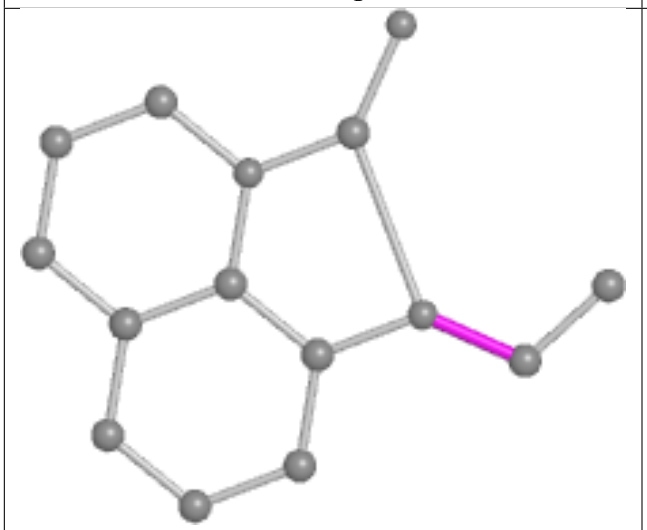
Ligand U1W B 4002



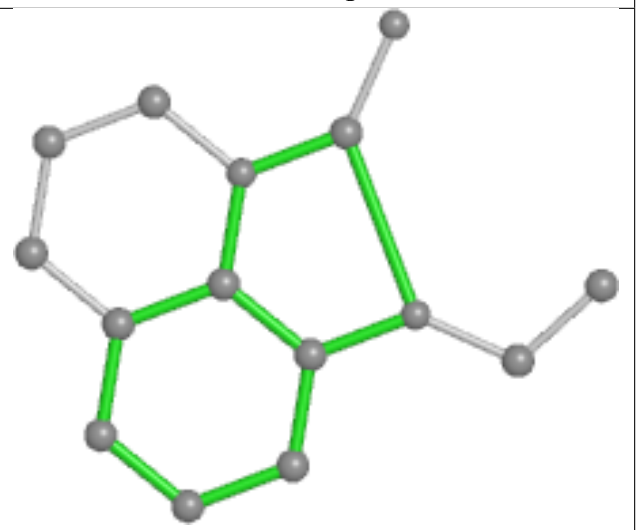
Bond lengths



Bond angles

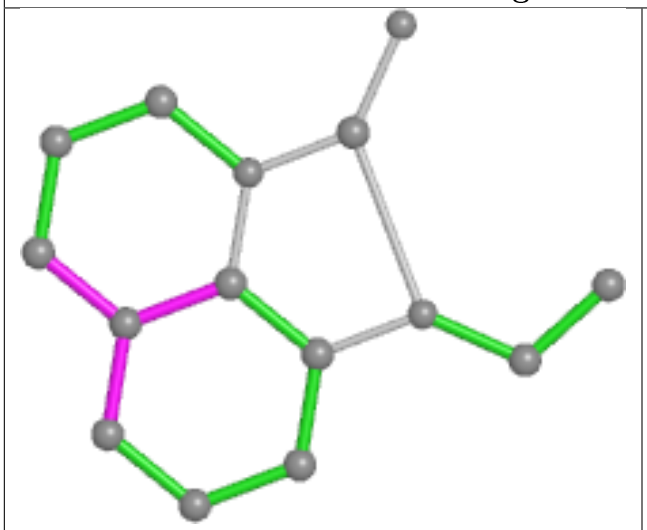


Torsions

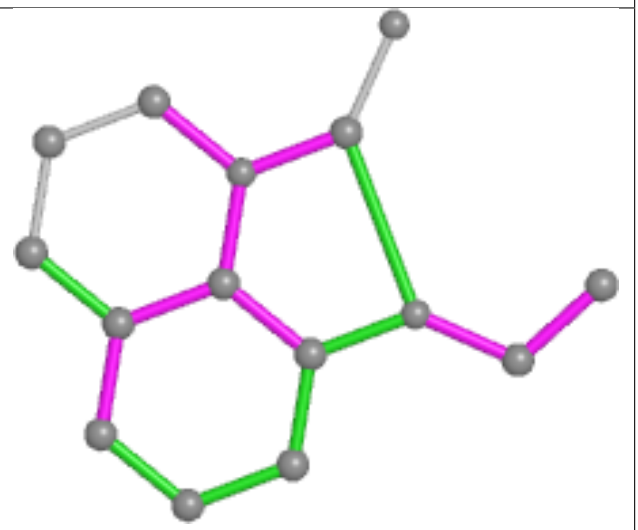


Rings

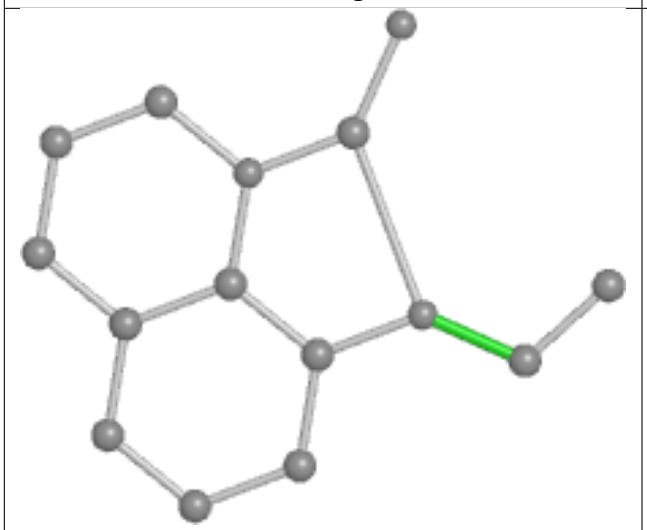
Ligand U1W C 4002



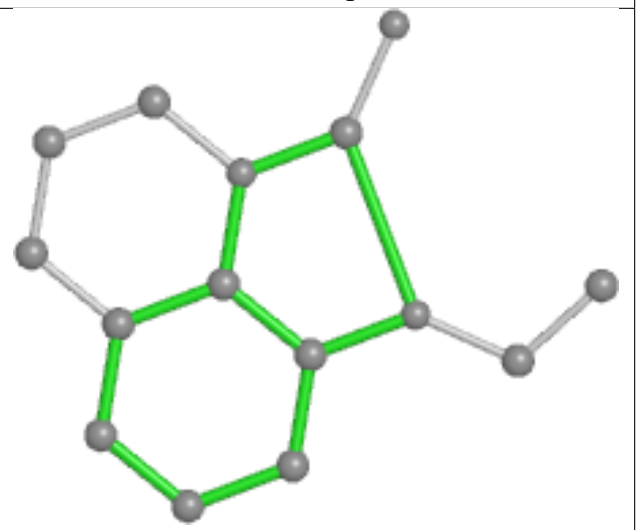
Bond lengths



Bond angles

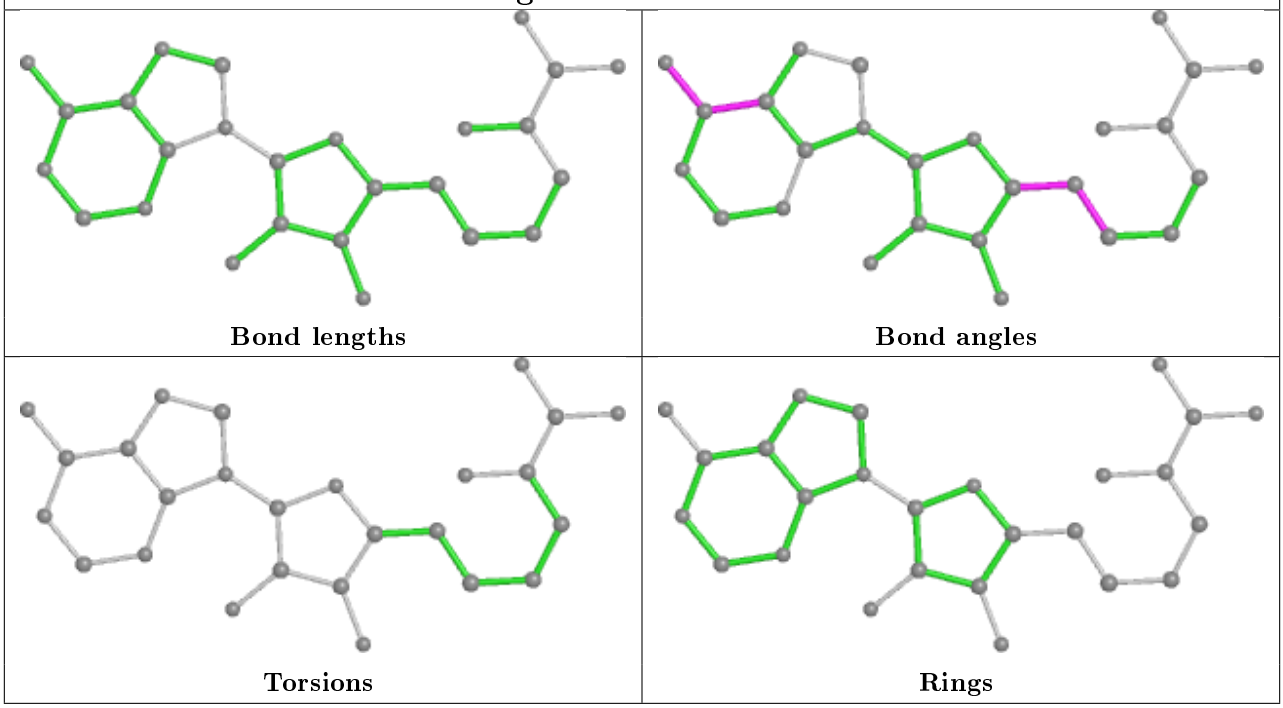


Torsions

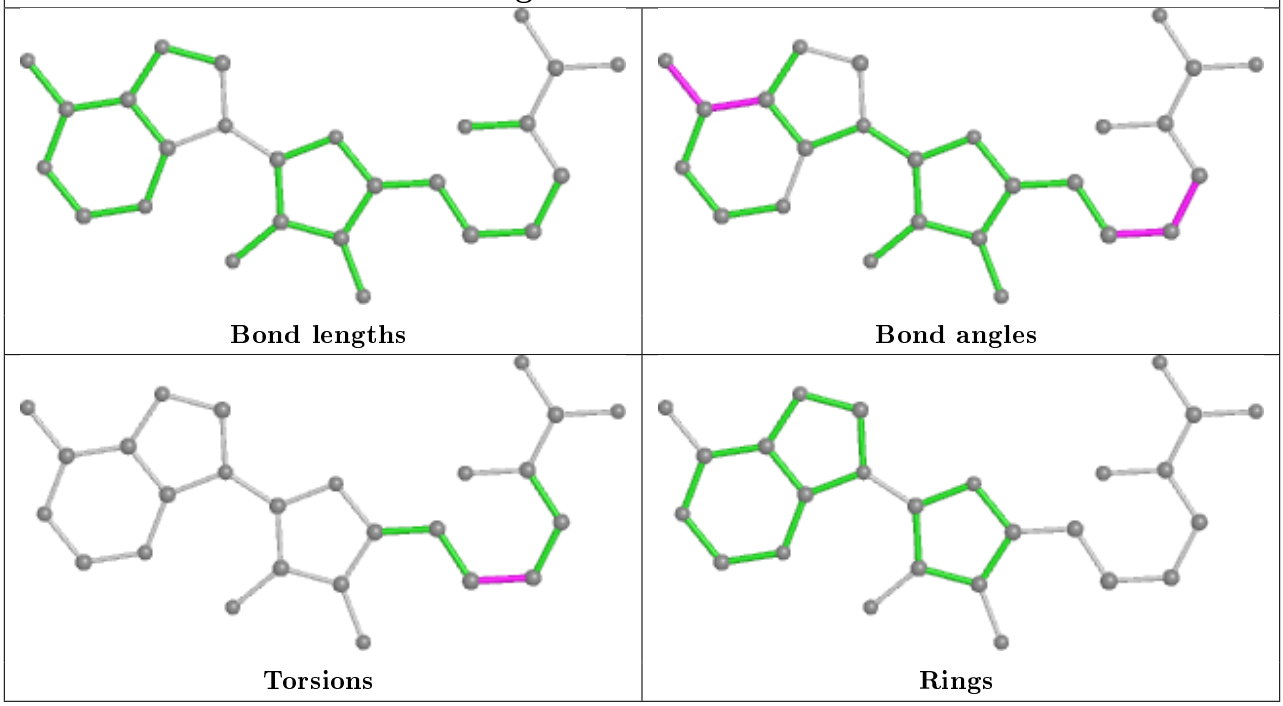


Rings

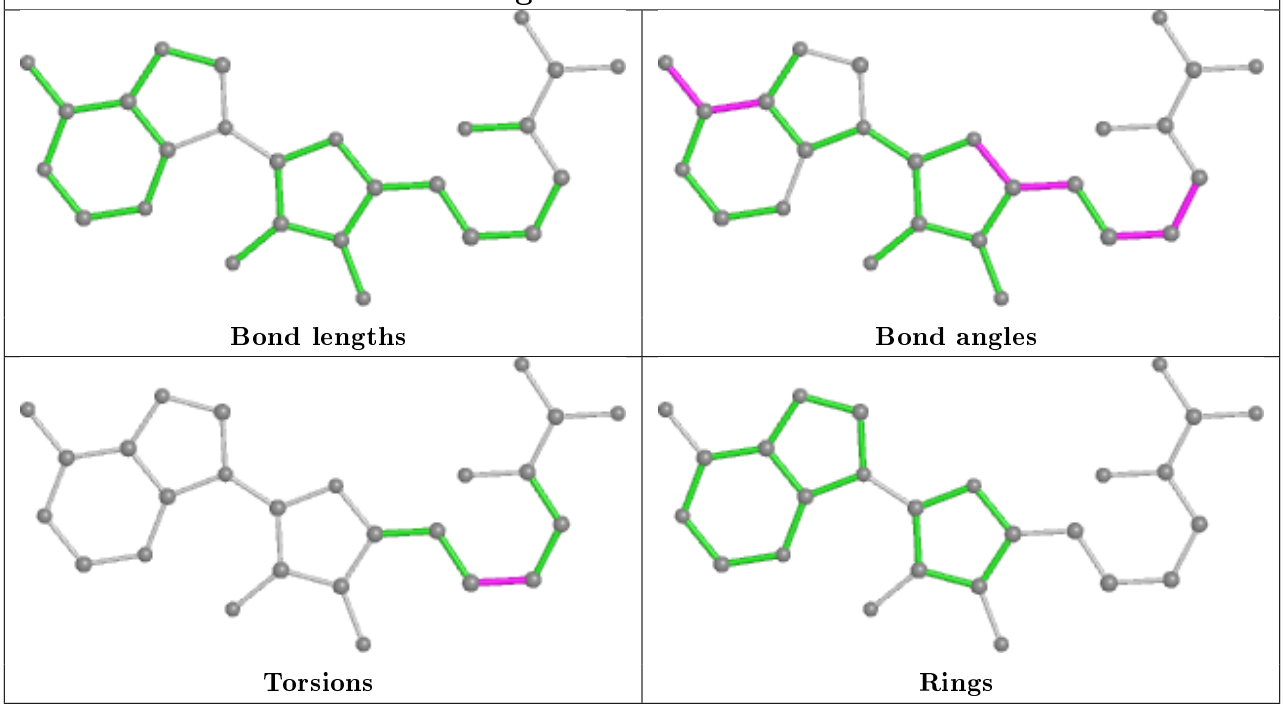
Ligand SAH B 4001



Ligand SAH A 4001



Ligand SAH D 4001



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	265/283 (93%)	-0.37	1 (0%) 92 91	15, 28, 41, 56	0
1	B	263/283 (92%)	-0.39	0 100 100	16, 28, 40, 53	0
1	C	252/283 (89%)	0.04	2 (0%) 86 81	18, 33, 46, 61	0
1	D	252/283 (89%)	0.09	9 (3%) 42 32	17, 33, 49, 66	0
All	All	1032/1132 (91%)	-0.16	12 (1%) 79 73	15, 29, 45, 66	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	151	ALA	3.3
1	D	122	VAL	2.7
1	D	103	ALA	2.6
1	D	119	GLY	2.6
1	D	12	LEU	2.5

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

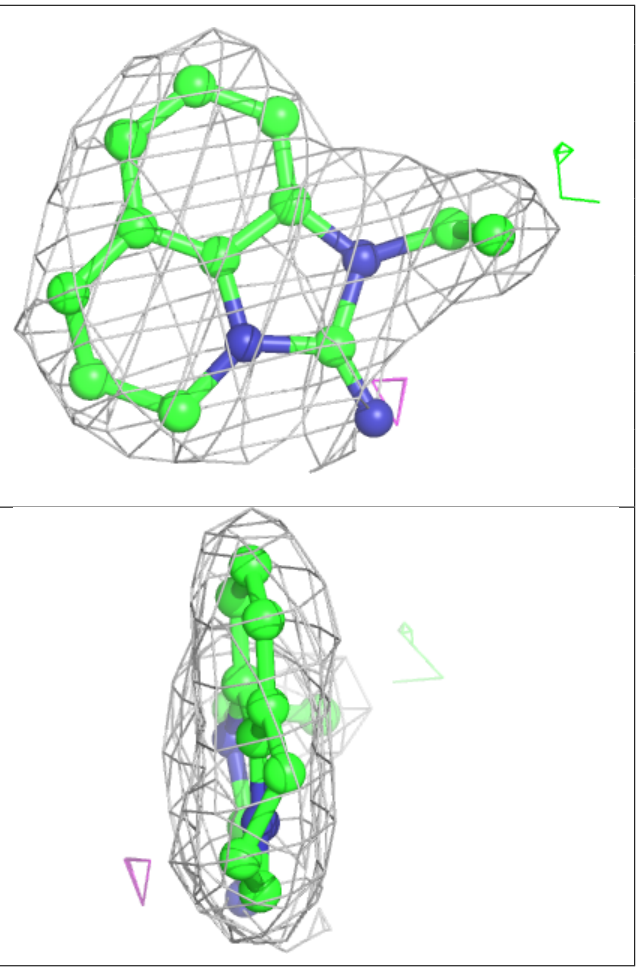
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	U1W	A	4002	15/15	0.95	0.17	11,12,12,13	0
3	U1W	D	4002	15/15	0.95	0.18	19,19,21,21	0
2	SAH	B	4001	26/26	0.96	0.17	17,18,25,26	0
2	SAH	D	4001	26/26	0.96	0.20	23,23,25,25	0
2	SAH	C	4001	26/26	0.97	0.17	20,21,22,23	0
3	U1W	B	4002	15/15	0.97	0.15	11,11,11,11	15
3	U1W	C	4002	15/15	0.97	0.18	21,22,22,23	0
2	SAH	A	4001	26/26	0.97	0.14	10,11,17,18	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.

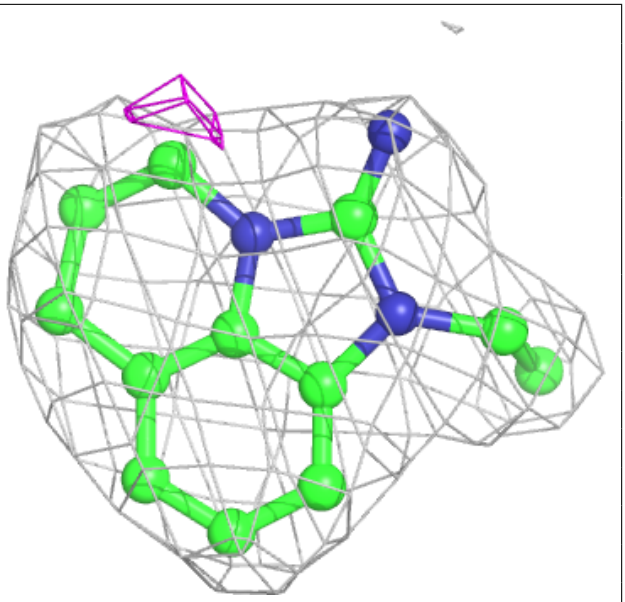
Electron density around U1W A 4002:

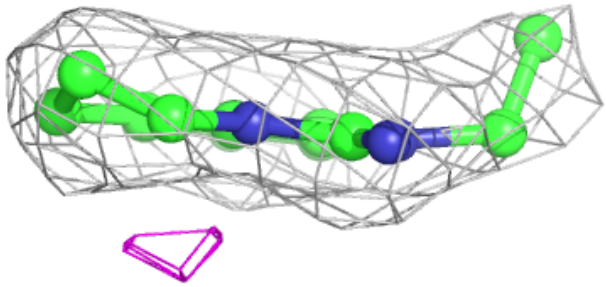
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

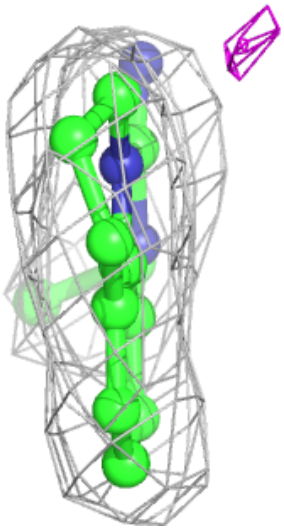


Electron density around U1W D 4002:

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

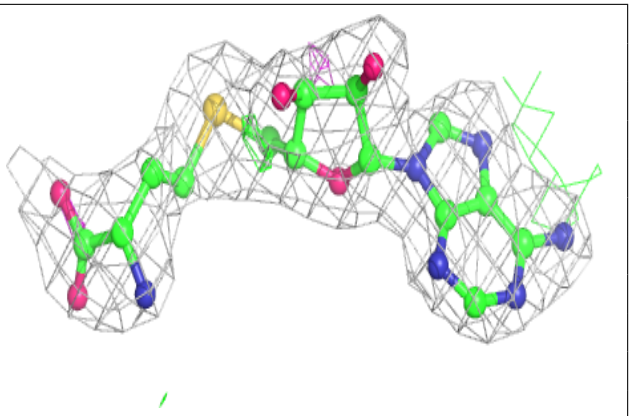


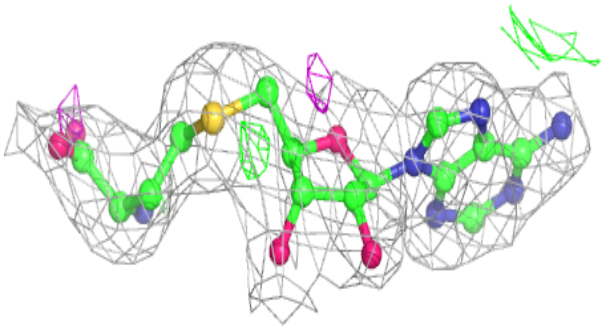


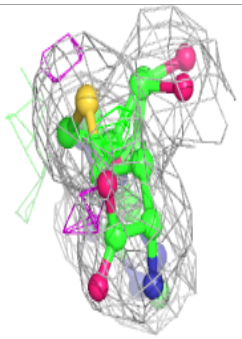


Electron density around SAH B 4001:

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

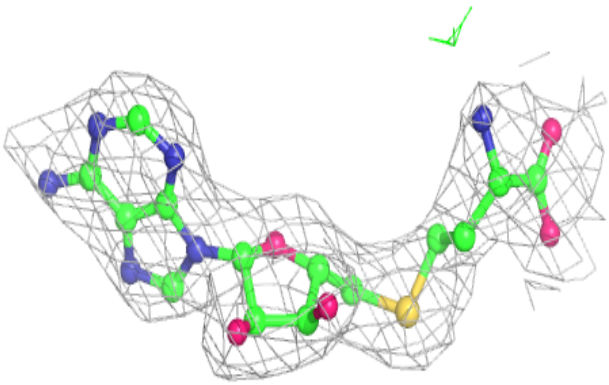


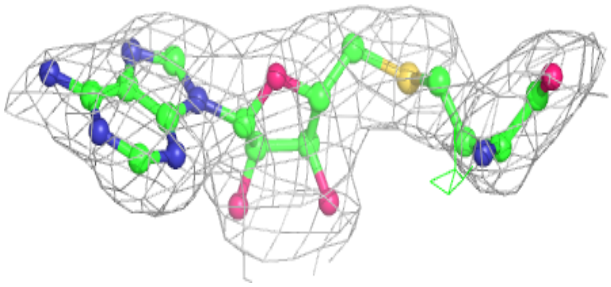


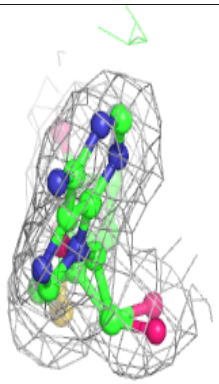


Electron density around SAH D 4001:

$2mF_o$-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 4001:

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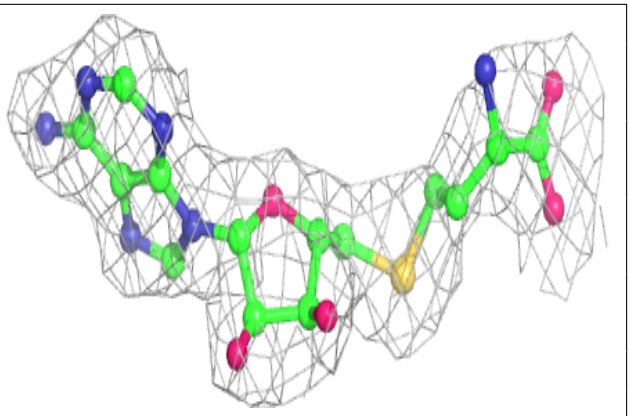
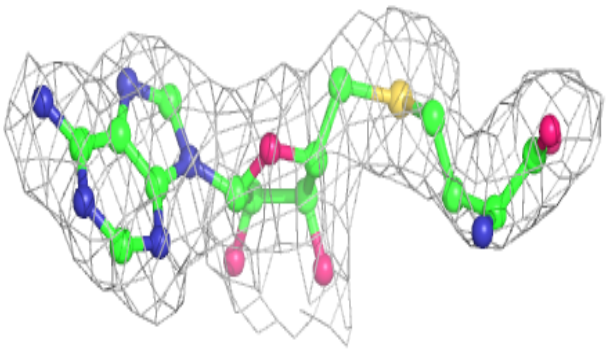
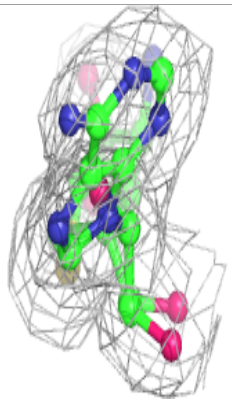
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around U1W B 4002:

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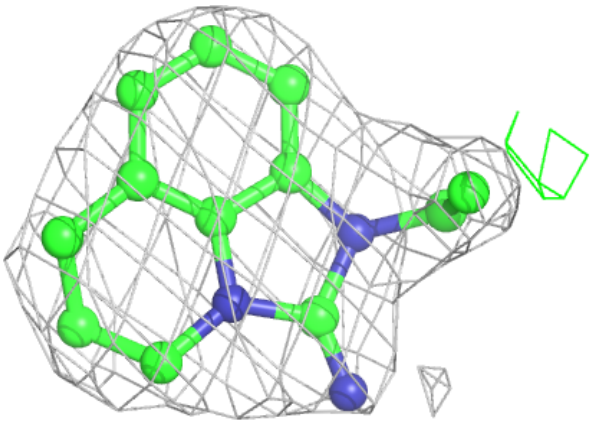
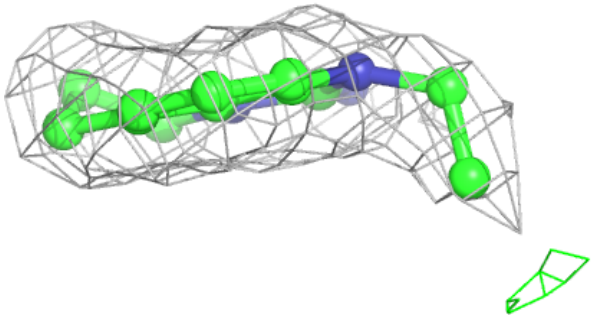
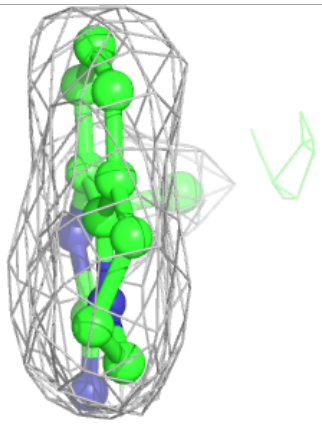
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around U1W C 4002:

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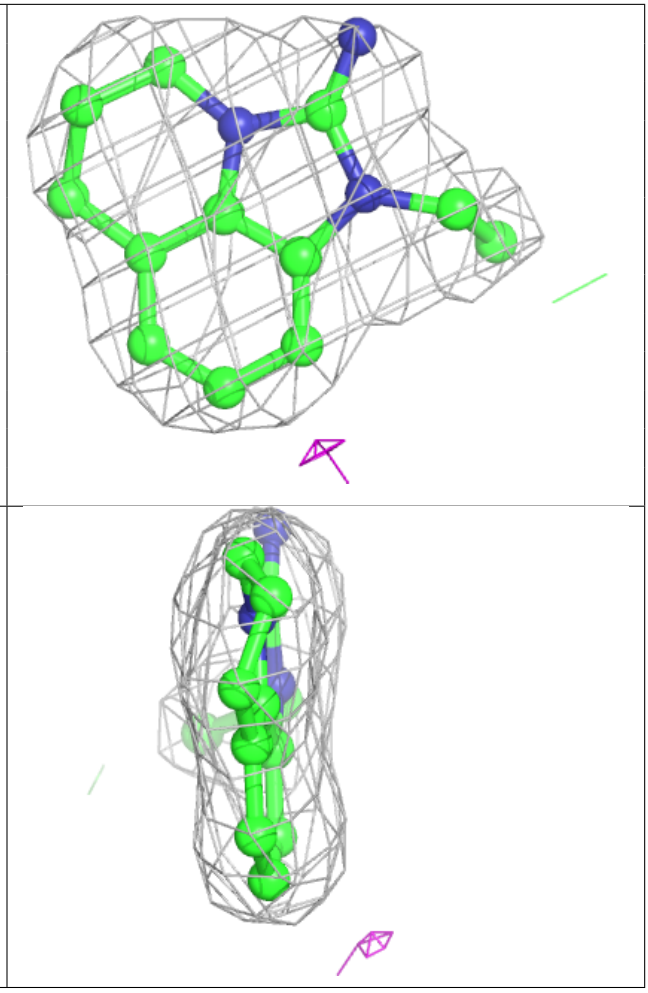
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SAH A 4001:

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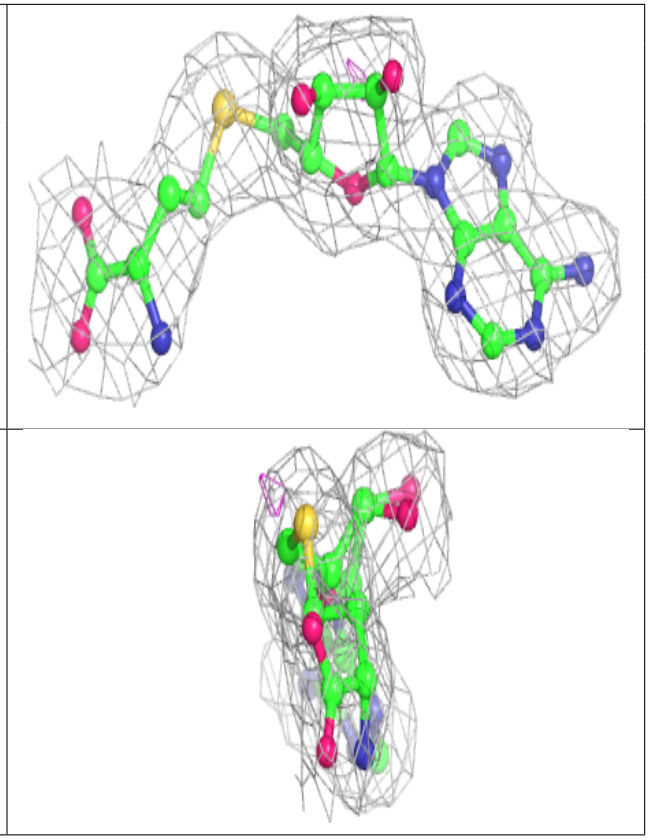
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.