wwPDB X-ray Structure Validation Summary Report (i)

Jun 23, 2024 – 09:44 AM EDT

PDB ID	:	5GP1
Title	:	Crystal structure of ZIKV NS5 Methyltransferase in complex with GTP and SAH
Authors	:	Zhang, C.; Jin, T.
Deposited on	:	2016-07-30
Resolution	:	2.44 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:

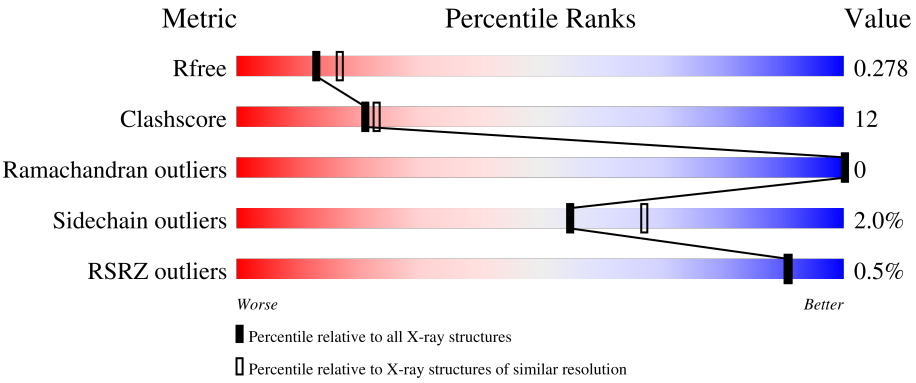
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.44 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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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	269	% 70% 27%
1	B	269	72% 24%
1	C	269	74% 22%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6440 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.

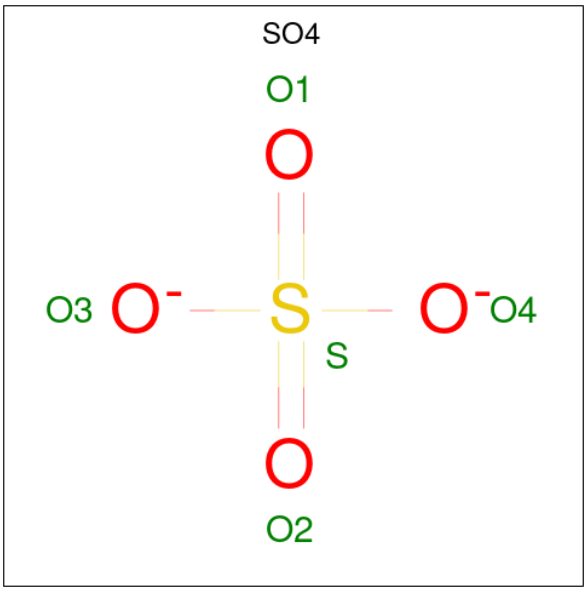
- Molecule 1 is a protein called RNA-directed RNA polymerase NS5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	0	0
			2038	1274	369	381	14			
1	B	260	Total	C	N	O	S	0	0	0
			2027	1268	367	378	14			
1	C	261	Total	C	N	O	S	0	0	0
			2033	1271	368	380	14			

There are 21 discrepancies between the modelled and reference sequences:

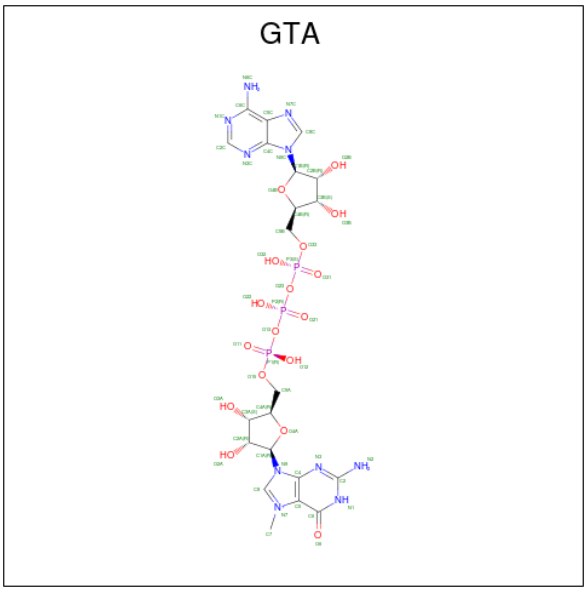
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP H9A910
A	1	SER	-	expression tag	UNP H9A910
A	2	VAL	-	expression tag	UNP H9A910
A	3	ASP	-	expression tag	UNP H9A910
A	266	ALA	-	expression tag	UNP H9A910
A	267	ALA	-	expression tag	UNP H9A910
A	268	SER	-	expression tag	UNP H9A910
B	0	GLY	-	expression tag	UNP H9A910
B	1	SER	-	expression tag	UNP H9A910
B	2	VAL	-	expression tag	UNP H9A910
B	3	ASP	-	expression tag	UNP H9A910
B	266	ALA	-	expression tag	UNP H9A910
B	267	ALA	-	expression tag	UNP H9A910
B	268	SER	-	expression tag	UNP H9A910
C	0	GLY	-	expression tag	UNP H9A910
C	1	SER	-	expression tag	UNP H9A910
C	2	VAL	-	expression tag	UNP H9A910
C	3	ASP	-	expression tag	UNP H9A910
C	266	ALA	-	expression tag	UNP H9A910
C	267	ALA	-	expression tag	UNP H9A910
C	268	SER	-	expression tag	UNP H9A910

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



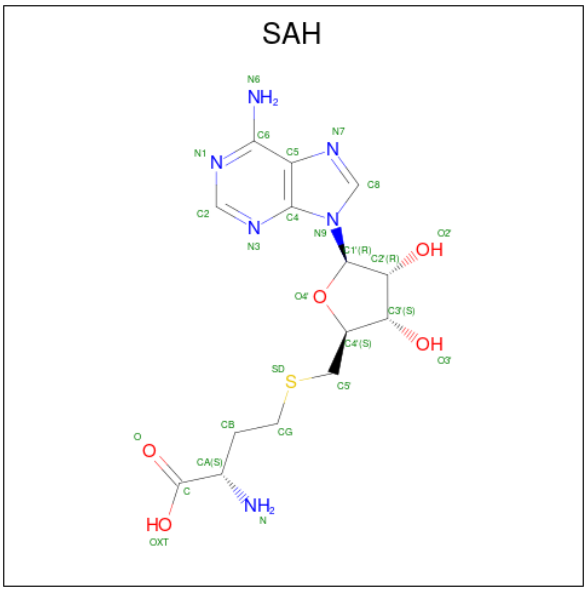
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0

- Molecule 3 is P1-7-METHYLGUANOSINE-P3-ADENOSINE-5',5'-TRIPHOSPHATE (three-letter code: GTA) (formula: $C_{21}H_{30}N_{10}O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			51	21	10	17	3		
3	B	1	Total	C	N	O	P	0	0
			51	21	10	17	3		
3	C	1	Total	C	N	O	P	0	0
			51	21	10	17	3		

- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



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

- Molecule 5 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Ni	0	0
			1	1		

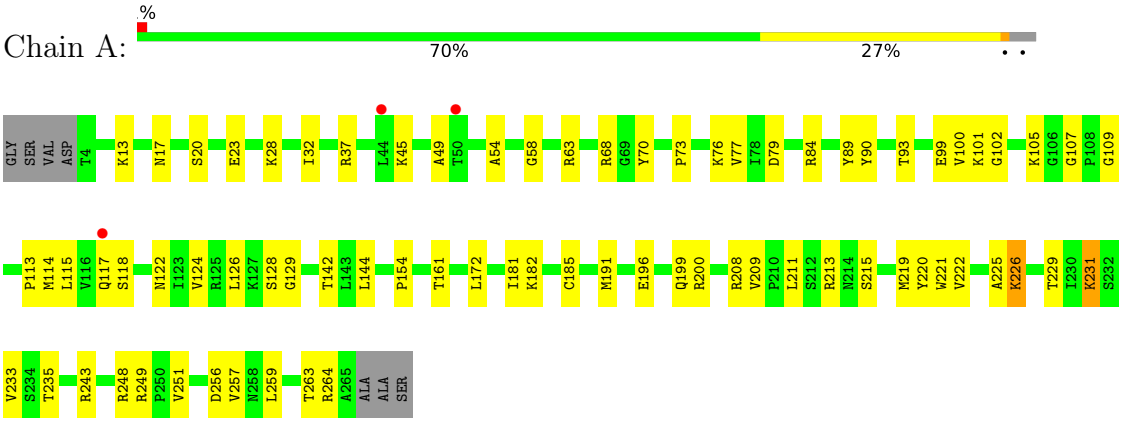
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	31	Total	O	0	0
			31	31		
6	B	19	Total	O	0	0
			19	19		
6	C	20	Total	O	0	0
			20	20		

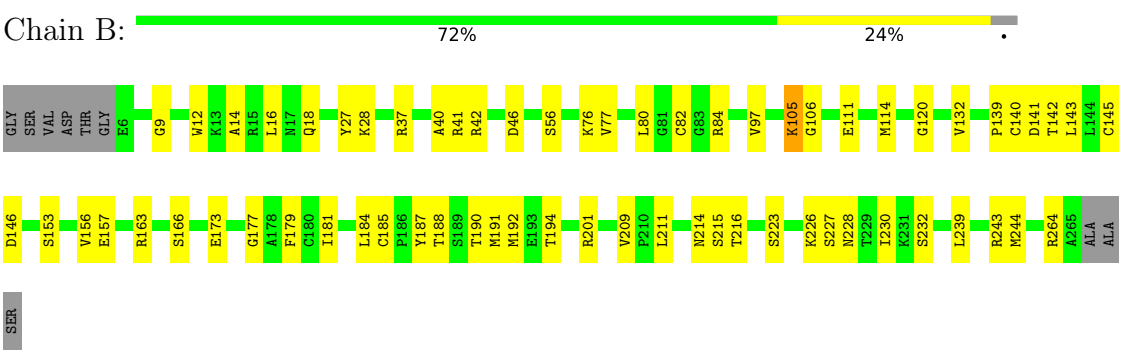
3 Residue-property plots (i)

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.

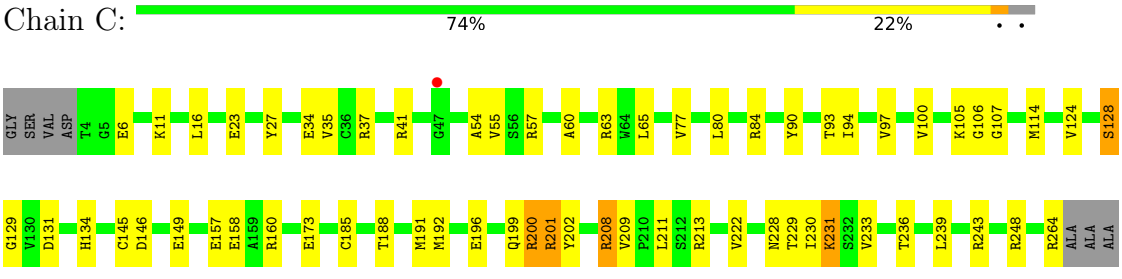
• Molecule 1: RNA-directed RNA polymerase NS5



• Molecule 1: RNA-directed RNA polymerase NS5



• Molecule 1: RNA-directed RNA polymerase NS5



SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	123.77Å 123.77Å 119.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.89 – 2.44 48.89 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.89-2.44) 91.3 (48.89-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.85 (at 2.45Å)	Xtriage
Refinement program	PHENIX (dev_2481: ???)	Depositor
R, R_{free}	0.237 , 0.280 0.238 , 0.278	Depositor DCC
R_{free} test set	1985 reflections (5.26%)	wwPDB-VP
Wilson B-factor (Å^2)	34.9	Xtriage
Anisotropy	0.593	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 21.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.468 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6440	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.44 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.4614e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: NI, SAH, SO4, GTA

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	0.26	0/2078	0.44	0/2800
1	B	0.24	0/2067	0.43	0/2785
1	C	0.25	0/2073	0.43	0/2793
All	All	0.25	0/6218	0.43	0/8378

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	107	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2038	0	2039	51	0
1	B	2027	0	2031	46	0
1	C	2033	0	2036	45	0
2	A	25	0	0	1	0
2	B	10	0	0	1	0
2	C	5	0	0	1	0
3	A	51	0	26	4	0
3	B	51	0	26	6	0
3	C	51	0	26	4	0
4	A	26	0	19	1	0
4	B	26	0	19	4	0
4	C	26	0	19	1	0
5	C	1	0	0	0	0
6	A	31	0	0	1	0
6	B	19	0	0	1	0
6	C	20	0	0	3	0
All	All	6440	0	6241	152	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 12.

The worst 5 of 152 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)
3:B:303:GTA:O4A	3:B:303:GTA:C1A	1.66	1.25
3:C:303:GTA:C1A	3:C:303:GTA:O4A	1.66	1.24
3:A:306:GTA:O4A	3:A:306:GTA:C1A	1.66	1.23
1:C:199:GLN:HE21	1:C:200:ARG:HH22	1.15	0.90
1:C:208:ARG:NH1	6:C:401:HOH:O	2.03	0.90

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	260/269 (97%)	250 (96%)	10 (4%)	0	100	100
1	B	258/269 (96%)	249 (96%)	9 (4%)	0	100	100
1	C	259/269 (96%)	249 (96%)	10 (4%)	0	100	100
All	All	777/807 (96%)	748 (96%)	29 (4%)	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	217/221 (98%)	212 (98%)	5 (2%)	50	63
1	B	216/221 (98%)	213 (99%)	3 (1%)	67	78
1	C	217/221 (98%)	212 (98%)	5 (2%)	50	63
All	All	650/663 (98%)	637 (98%)	13 (2%)	55	67

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	105	LYS
1	C	128	SER
1	C	231	LYS
1	C	201	ARG
1	C	208	ARG

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	117	GLN
1	C	199	GLN
1	C	228	ASN
1	B	18	GLN
1	B	199	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GTA	C	303	-	46,56,56	5.41	23 (50%)	46,88,88	2.13	8 (17%)
3	GTA	B	303	-	46,56,56	5.43	22 (47%)	46,88,88	2.19	8 (17%)
4	SAH	B	304	-	24,28,28	1.19	3 (12%)	25,40,40	1.65	4 (16%)
4	SAH	C	304	-	24,28,28	1.19	3 (12%)	25,40,40	1.70	4 (16%)
2	SO4	A	305	-	4,4,4	0.14	0	6,6,6	0.05	0
3	GTA	A	306	-	46,56,56	5.39	23 (50%)	46,88,88	2.18	8 (17%)
2	SO4	A	303	-	4,4,4	0.17	0	6,6,6	0.06	0
2	SO4	B	302	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	C	301	-	4,4,4	0.15	0	6,6,6	0.08	0
4	SAH	A	307	-	24,28,28	1.20	3 (12%)	25,40,40	1.68	5 (20%)
2	SO4	B	301	-	4,4,4	0.13	0	6,6,6	0.08	0
2	SO4	A	302	1	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	A	301	1	4,4,4	0.38	0	6,6,6	0.21	0
2	SO4	A	304	-	4,4,4	0.14	0	6,6,6	0.06	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
3	GTA	C	303	-	-	7/24/64/64	0/6/6/6
4	SAH	C	304	-	-	4/11/31/31	0/3/3/3
4	SAH	B	304	-	-	2/11/31/31	0/3/3/3
3	GTA	A	306	-	-	6/24/64/64	0/6/6/6
4	SAH	A	307	-	-	3/11/31/31	0/3/3/3
3	GTA	B	303	-	-	10/24/64/64	0/6/6/6

The worst 5 of 77 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	303	GTA	O4A-C1A	18.50	1.66	1.41
3	C	303	GTA	O4A-C1A	18.07	1.66	1.41
3	A	306	GTA	O4A-C1A	17.91	1.66	1.41
3	C	303	GTA	C2B-C1B	-16.26	1.29	1.53
3	B	303	GTA	C2B-C1B	-16.07	1.29	1.53

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	303	GTA	C5C-C6C-N6C	9.05	134.11	120.35
3	B	303	GTA	C5C-C6C-N6C	8.96	133.96	120.35
3	A	306	GTA	C5C-C6C-N6C	8.92	133.90	120.35
3	C	303	GTA	N6C-C6C-N1C	-6.13	105.85	118.57
3	A	306	GTA	N6C-C6C-N1C	-6.09	105.94	118.57

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	306	GTA	P2-O23-P3-O33
3	B	303	GTA	C3A-C4A-C5A-O15
3	B	303	GTA	O4A-C4A-C5A-O15
3	B	303	GTA	C5A-O15-P1-O11
3	B	303	GTA	C5A-O15-P1-O12

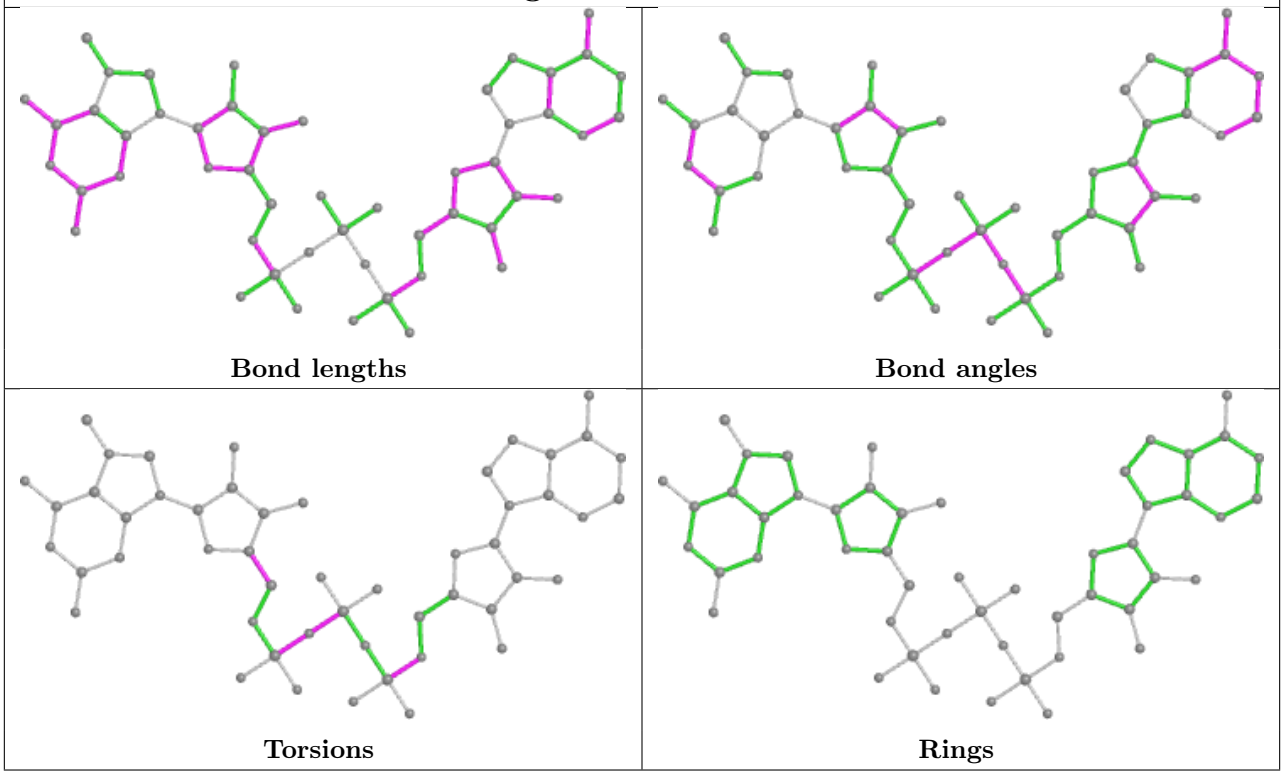
There are no ring outliers.

9 monomers are involved in 23 short contacts:

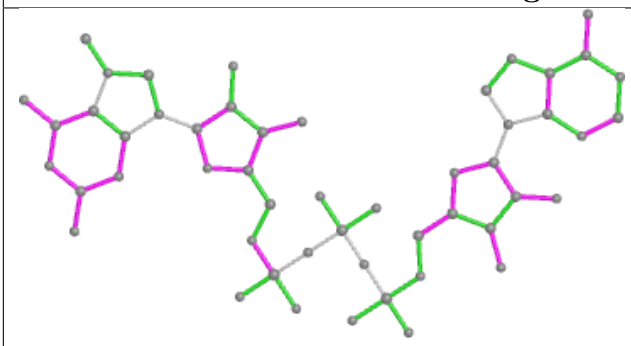
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	303	GTA	4	0
3	B	303	GTA	6	0
4	B	304	SAH	4	0
4	C	304	SAH	1	0
3	A	306	GTA	4	0
2	B	302	SO4	1	0
2	C	301	SO4	1	0
4	A	307	SAH	1	0
2	A	301	SO4	1	0

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.

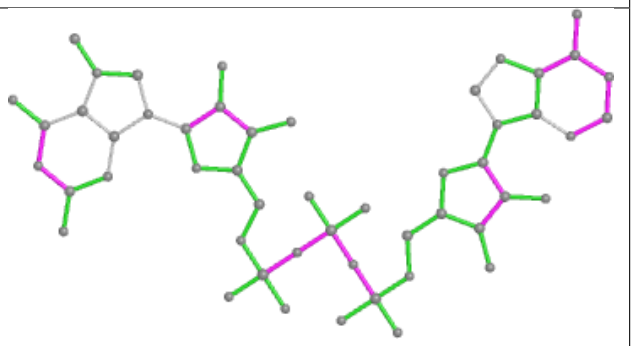
Ligand GTA C 303



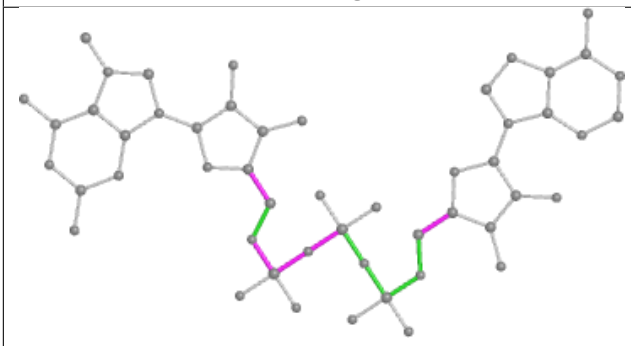
Ligand GTA B 303



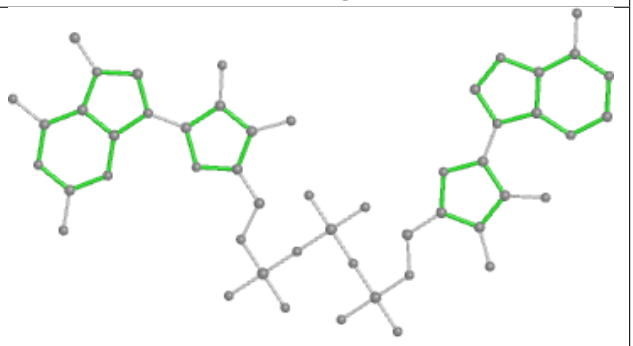
Bond lengths



Bond angles

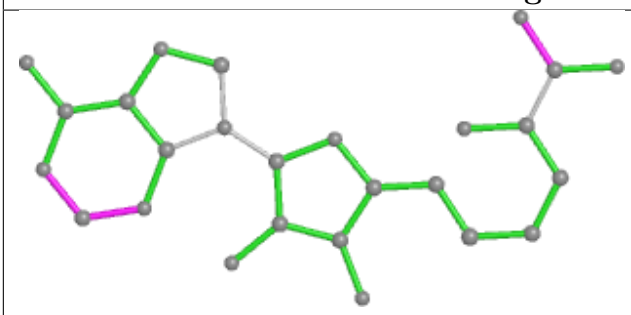


Torsions

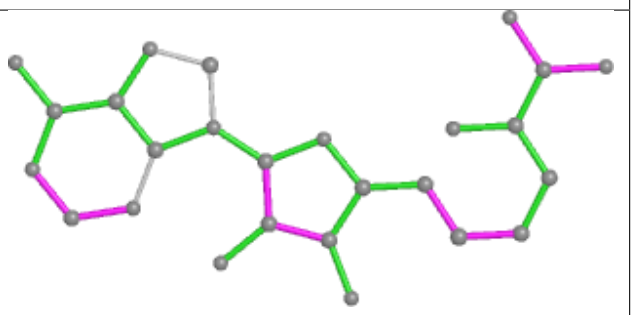


Rings

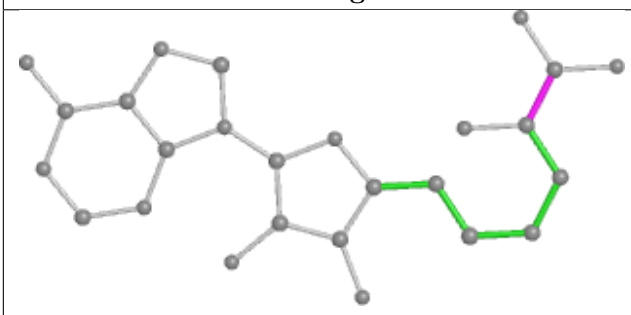
Ligand SAH B 304



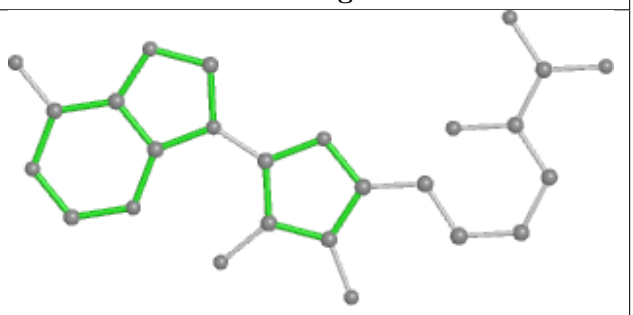
Bond lengths



Bond angles

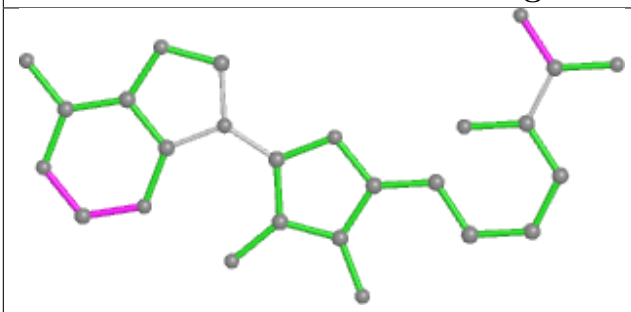


Torsions

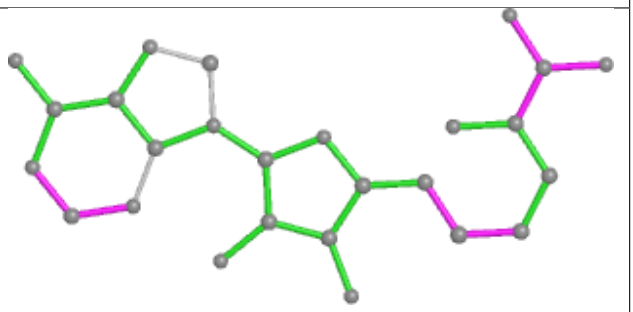


Rings

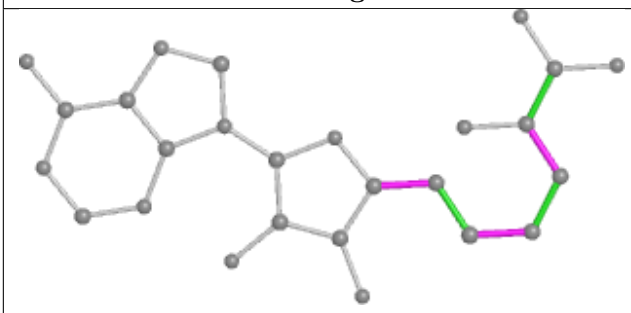
Ligand SAH C 304



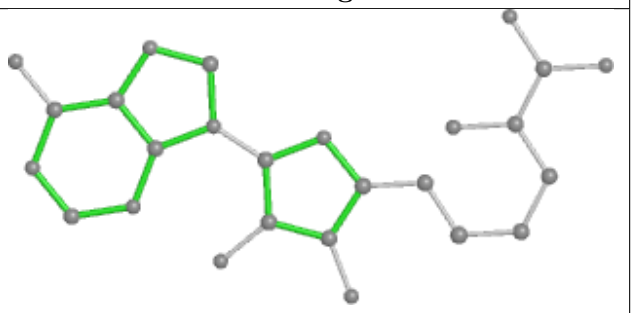
Bond lengths



Bond angles

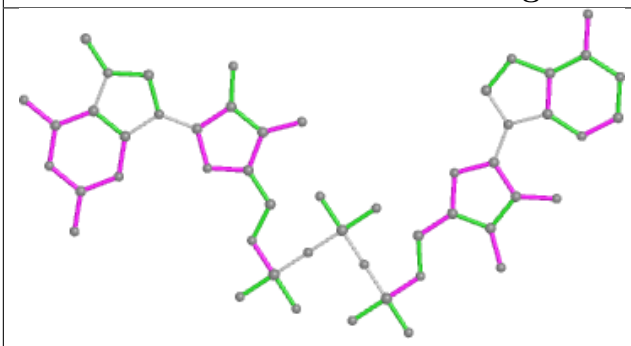


Torsions

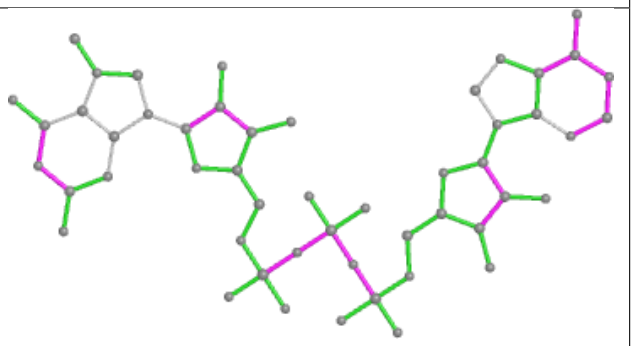


Rings

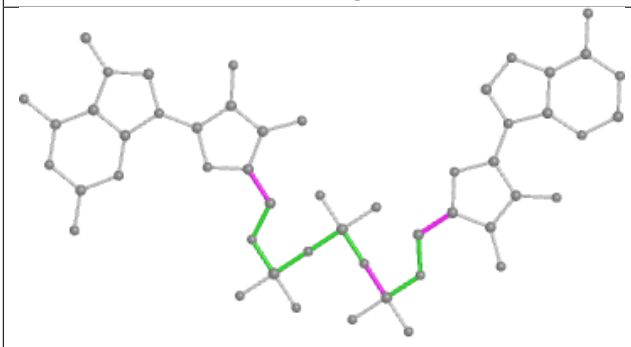
Ligand GTA A 306



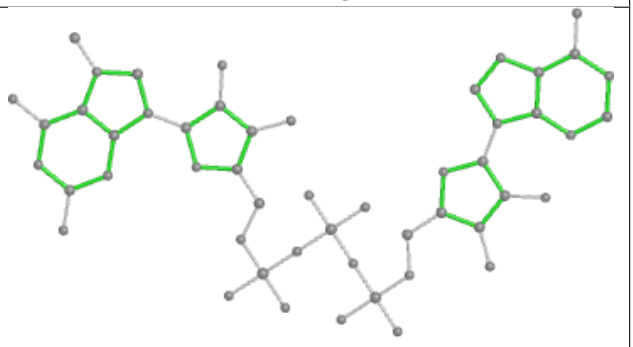
Bond lengths



Bond angles

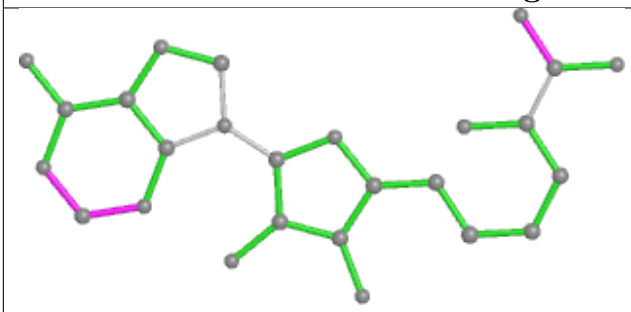


Torsions

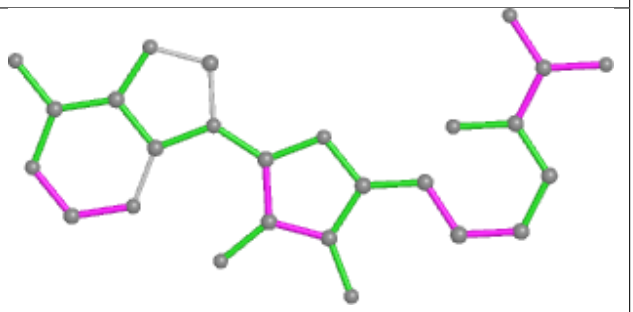


Rings

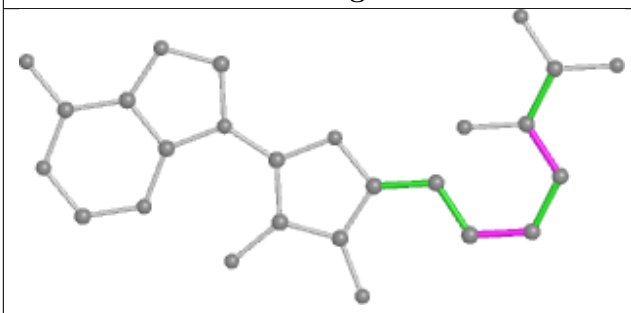
Ligand SAH A 307



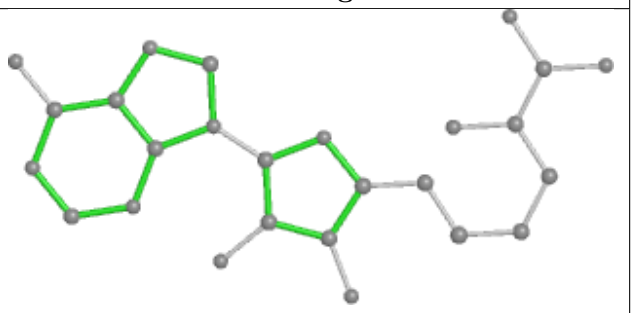
Bond lengths



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	262/269 (97%)	0.01	3 (1%) 80 79	34, 50, 78, 110	0
1	B	260/269 (96%)	-0.37	0 100 100	26, 38, 60, 93	0
1	C	261/269 (97%)	-0.28	1 (0%) 92 92	28, 43, 67, 98	0
All	All	783/807 (97%)	-0.21	4 (0%) 91 91	26, 43, 71, 110	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	44	LEU	5.2
1	C	47	GLY	2.5
1	A	50	THR	2.4
1	A	117	GLN	2.3

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 monosaccharides in this entry.

6.4 Ligands

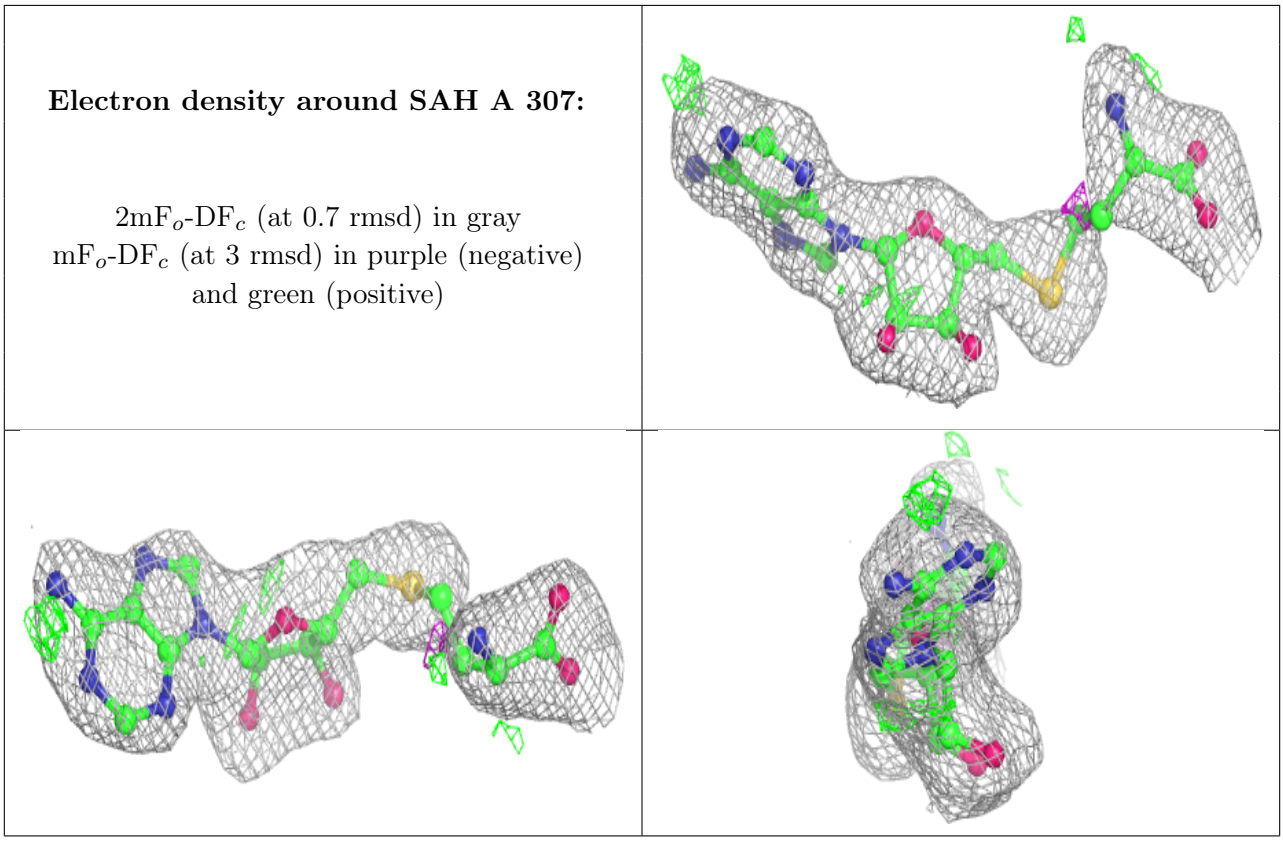
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	SO4	A	303	5/5	0.90	0.22	52,66,72,73	0
2	SO4	A	301	5/5	0.91	0.10	41,59,61,62	0
4	SAH	A	307	26/26	0.92	0.17	30,44,50,52	0
3	GTA	B	303	51/51	0.94	0.14	18,53,74,75	0
3	GTA	A	306	51/51	0.94	0.12	18,35,66,69	0
3	GTA	C	303	51/51	0.95	0.12	19,48,76,78	0
2	SO4	A	305	5/5	0.95	0.13	68,68,72,72	0
4	SAH	C	304	26/26	0.95	0.13	21,31,40,46	0
2	SO4	B	302	5/5	0.96	0.09	64,65,68,74	0
4	SAH	B	304	26/26	0.96	0.12	20,32,42,44	0
2	SO4	A	304	5/5	0.96	0.11	36,46,52,53	0
5	NI	C	302	1/1	0.96	0.12	77,77,77,77	0
2	SO4	C	301	5/5	0.97	0.10	48,57,58,64	0
2	SO4	A	302	5/5	0.98	0.09	29,33,41,50	0
2	SO4	B	301	5/5	0.99	0.09	33,37,52,53	0

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

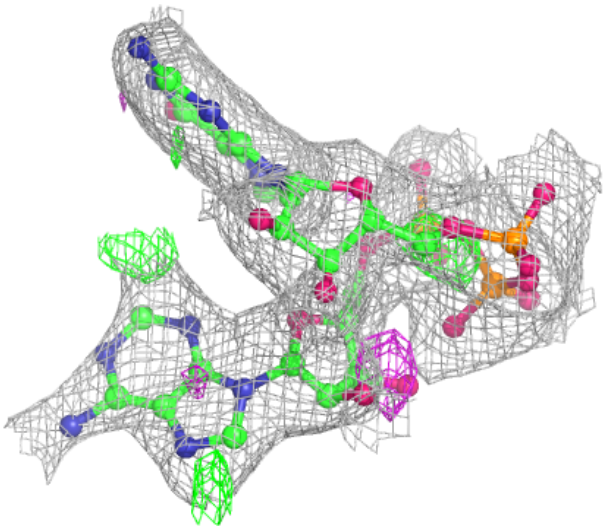
Electron density around SAH A 307:

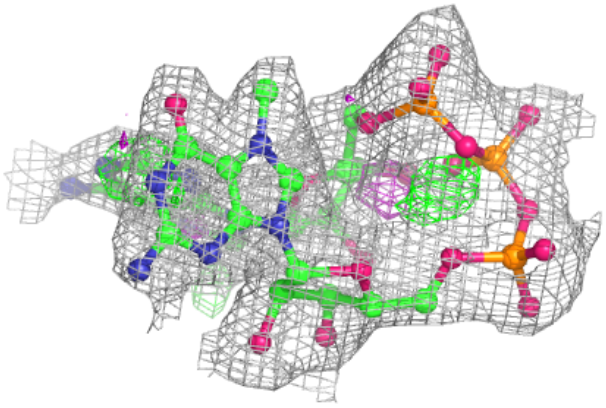
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

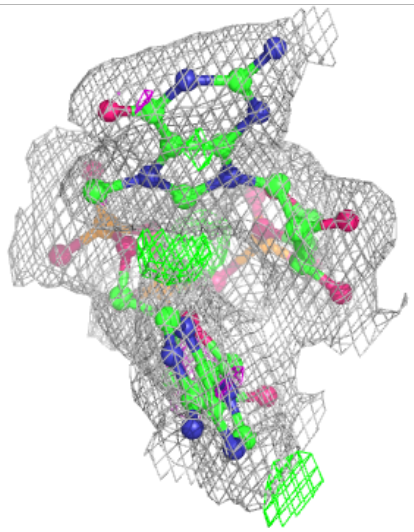


Electron density around GTA B 303:

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

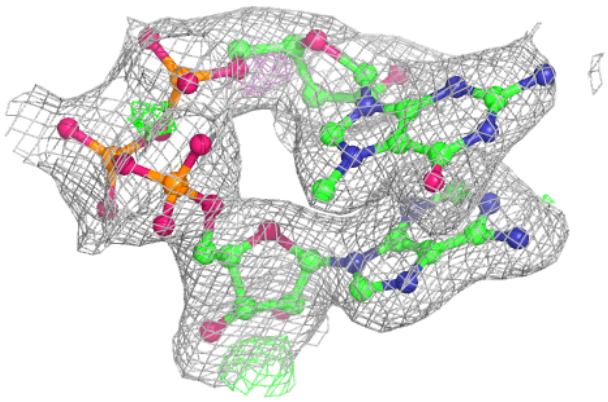


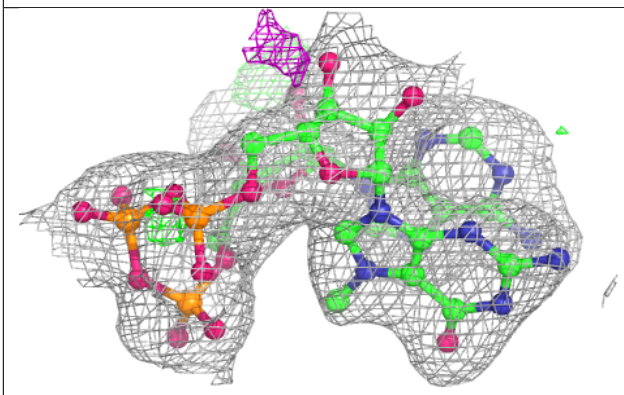


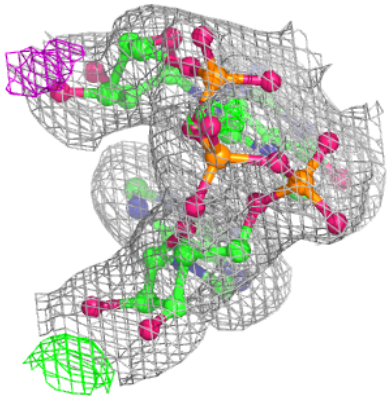


Electron density around GTA A 306:

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

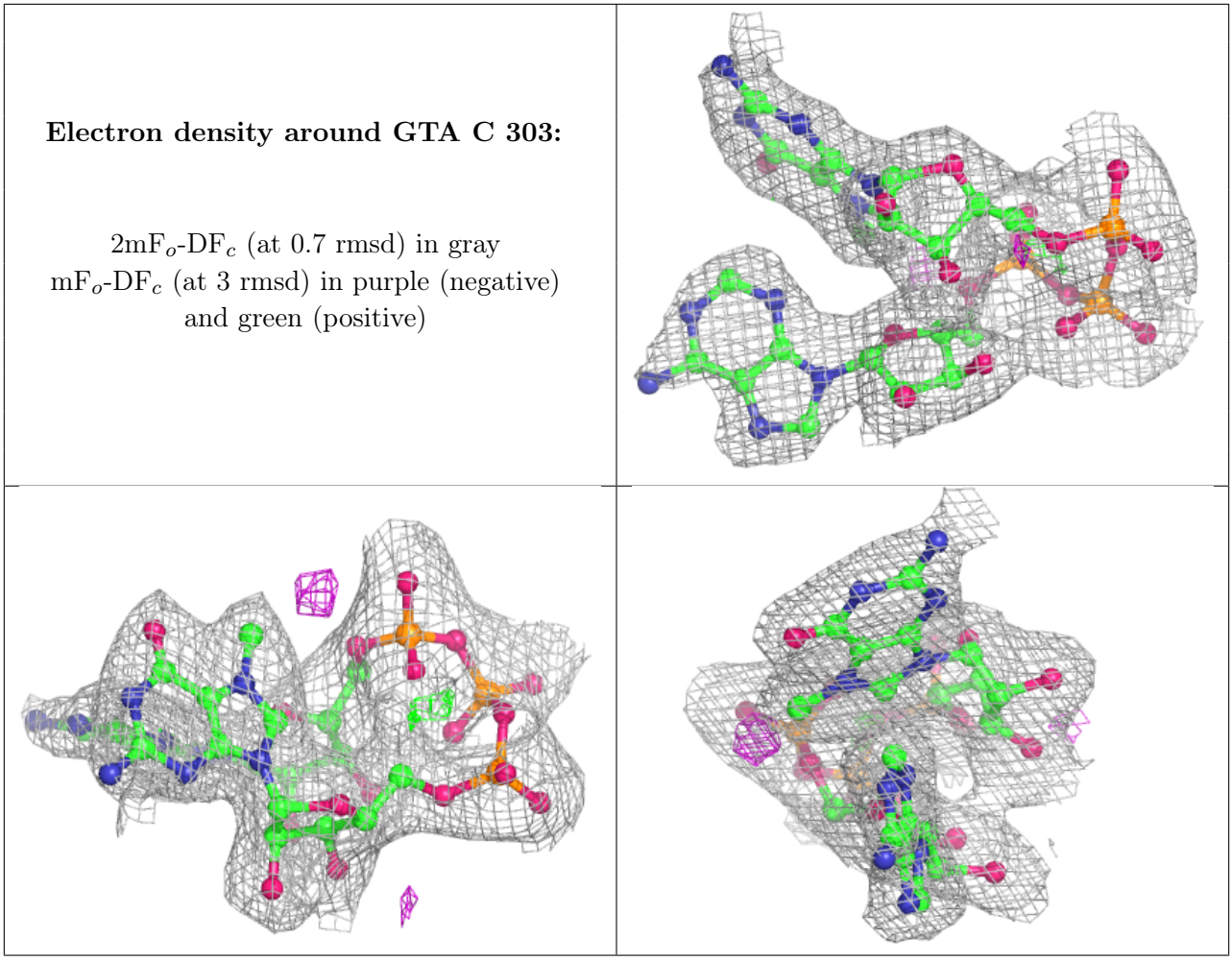






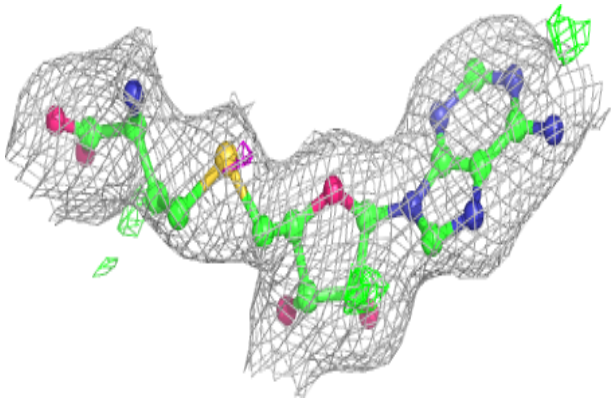
Electron density around GTA C 303:

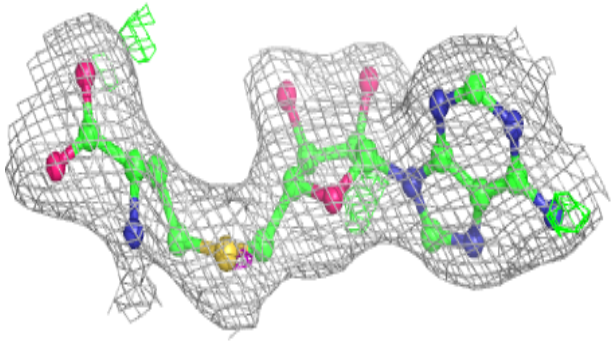
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

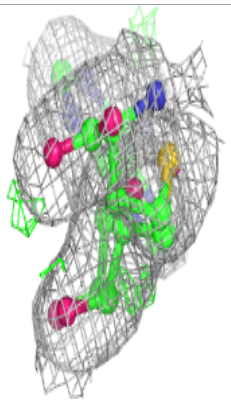


Electron density around SAH C 304:

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

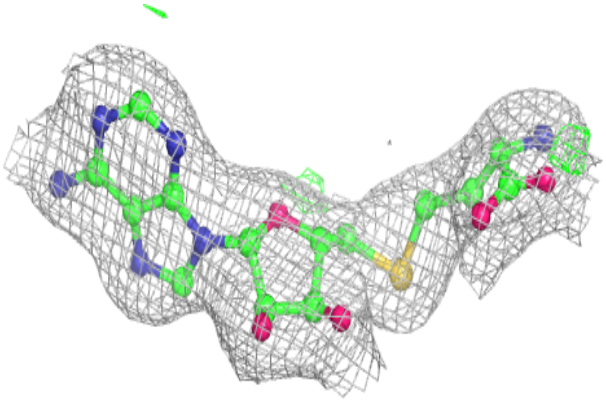


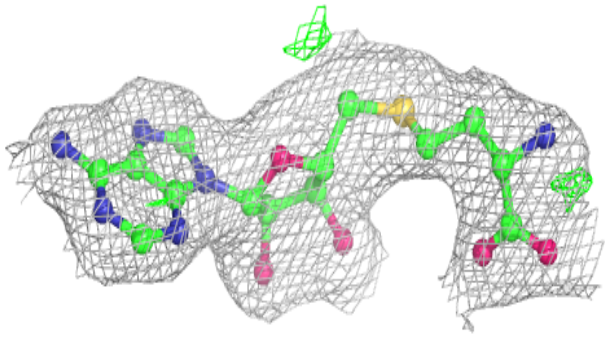


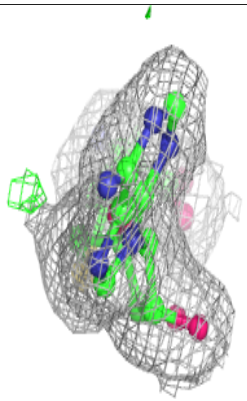


Electron density around SAH B 304:

$2mF_o$-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.