



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 06:00 am BST

PDB ID : 2PX8  
Title : Crystal structure of the Murray Valley Encephalitis Virus NS5 2'-O Methyltransferase domain in complex with SAH and 7M-GTP  
Authors : Assenberg, R.; Ren, J.; Verma, A.; Walter, T.S.; Alderton, D.; Hurrelbrink, R.J.; Fuller, S.D.; Owens, R.J.; Stuart, D.I.; Grimes, J.M.; Oxford Protein Production Facility (OPPF)  
Deposited on : 2007-05-14  
Resolution : 2.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

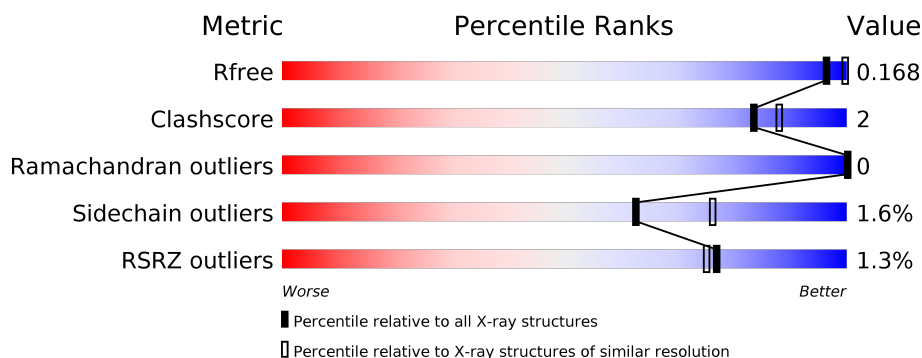
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>9%</div> <div></div> </div> <div></div> </div>
1	B	269	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>6%</div> <div></div> </div> <div></div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4823 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.

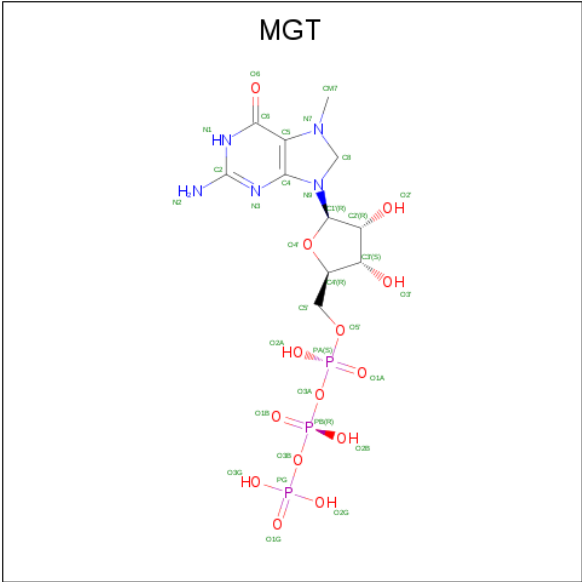
- Molecule 1 is a protein called Genome polyprotein [Contains: Capsid protein C (Core protein); Envelope protein M (Matrix protein); Major envelope protein E; Non-structural protein 1 (NS1); Non-structural protein 2A (NS2A); Flavivirin protease NS2B regulatory subunit; Flavivirin protease NS3 catalytic subunit; Non-structural protein 4A (NS4A); Non-structural protein 4B (NS4B); RNA-directed RNA polymerase (EC 2.7.7.48) (NS5)].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2098	1322	380	382	14			
1	B	265	Total	C	N	O	S	0	0	0
			2108	1328	382	384	14			

There are 8 discrepancies between the modelled and reference sequences:

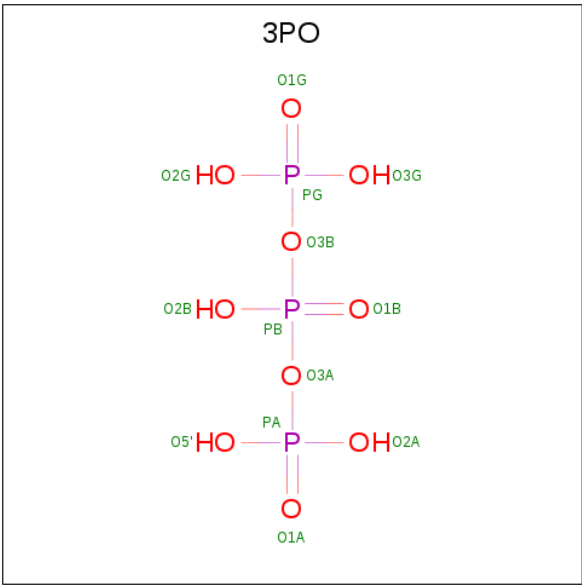
Chain	Residue	Modelled	Actual	Comment	Reference
A	15	MLY	LYS	MODIFIED RESIDUE	UNP P05769
A	76	MLY	LYS	MODIFIED RESIDUE	UNP P05769
A	95	MLY	LYS	MODIFIED RESIDUE	UNP P05769
A	105	MLY	LYS	MODIFIED RESIDUE	UNP P05769
B	15	MLY	LYS	MODIFIED RESIDUE	UNP P05769
B	76	MLY	LYS	MODIFIED RESIDUE	UNP P05769
B	95	MLY	LYS	MODIFIED RESIDUE	UNP P05769
B	105	MLY	LYS	MODIFIED RESIDUE	UNP P05769

- Molecule 2 is 7N-METHYL-8-HYDROGUANOSINE-5'-TRIPHOSPHATE (three-letter code: MGT) (formula: C<sub>11</sub>H<sub>20</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			33	11	5	14	3		
2	B	1	Total	C	N	O	P	0	0
			33	11	5	14	3		
2	B	1	Total	C	N	O	P	0	0
			33	11	5	14	3		

- Molecule 3 is TRIPHOSPHATE (three-letter code: 3PO) (formula: H<sub>5</sub>O<sub>10</sub>P<sub>3</sub>).



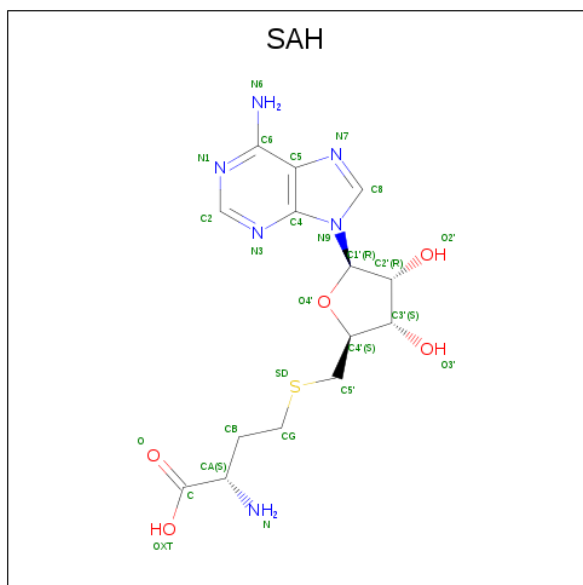
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			13	10	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	P	0	0
			13	10	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		

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



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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		

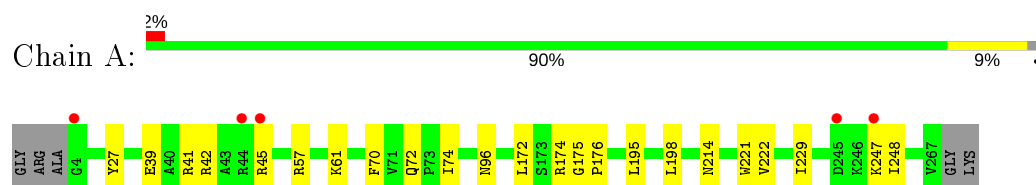
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	212	Total	O	0	0
			212	212		
7	B	215	Total	O	0	0
			215	215		

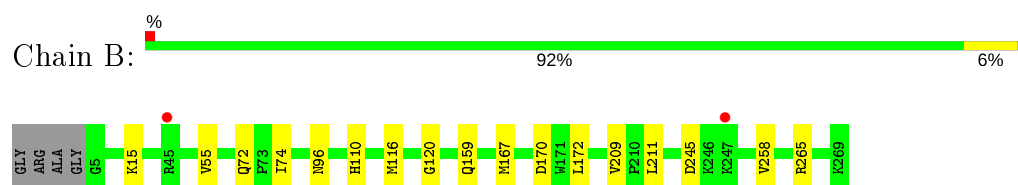
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Genome polyprotein [Contains: Capsid protein C (Core protein); Envelope protein M (Matrix protein); Major envelope protein E; Non-structural protein 1 (NS1); Non-structural protein 2A (NS2A); Flavivirin protease NS2B regulatory subunit; Flavivirin protease NS3 catalytic subunit; Non-structural protein 4A (NS4A); Non-structural protein 4B (NS4B); RNA-directed RNA polymerase (EC 2.7.7.48) (NS5)]



- Molecule 1: Genome polyprotein [Contains: Capsid protein C (Core protein); Envelope protein M (Matrix protein); Major envelope protein E; Non-structural protein 1 (NS1); Non-structural protein 2A (NS2A); Flavivirin protease NS2B regulatory subunit; Flavivirin protease NS3 catalytic subunit; Non-structural protein 4A (NS4A); Non-structural protein 4B (NS4B); RNA-directed RNA polymerase (EC 2.7.7.48) (NS5)]



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.58Å 87.44Å 100.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 43.72 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.2 (30.00-2.20) 82.8 (43.72-2.00)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.166 , 0.217 0.172 , 0.168	Depositor DCC
$R_{free}$ test set	1726 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.3	Xtriage
Anisotropy	1.118	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4823	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	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 22.11 % 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 6.0910e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: GOL, SAH, CL, 3PO, MGT, MLY

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	0.36	0/2097	0.48	0/2823
1	B	0.36	0/2107	0.49	0/2834
All	All	0.36	0/4204	0.48	0/5657

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	2098	0	2110	13	0
1	B	2108	0	2123	7	0
2	A	33	0	16	0	0
2	B	66	0	32	1	0
3	A	13	0	0	0	0
3	B	13	0	0	0	0
4	A	26	0	19	0	0
4	B	26	0	19	1	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
6	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	212	0	0	2	0
7	B	215	0	0	1	0
All	All	4823	0	4335	21	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 2.

All (21) 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:42:ARG:HA	1:A:45:ARG:HE	1.67	0.58
1:B:120:GLY:HA2	1:B:265:ARG:HG2	1.93	0.50
1:B:15:MLY:HH12	1:B:245:ASP:OD2	2.12	0.49
1:A:175:GLY:N	1:A:176:PRO:HD2	2.28	0.49
1:B:74:ILE:HG13	1:B:96:ASN:HB3	1.95	0.48
1:A:39:GLU:O	1:A:42:ARG:HG3	2.14	0.48
1:B:110:HIS:HD2	4:B:500:SAH:O2'	1.98	0.47
1:B:55:VAL:CG1	1:B:116:MET:HG3	2.45	0.47
1:A:195:LEU:HB3	1:A:229:ILE:HD13	1.96	0.46
1:A:61:LYS:NZ	7:A:877:HOH:O	2.49	0.46
1:A:247:LYS:HG3	1:A:248:ILE:H	1.80	0.46
1:A:72:GLN:HG2	7:A:1054:HOH:O	2.15	0.45
1:A:198:LEU:HB3	1:A:221:TRP:CH2	2.52	0.45
1:A:70:PHE:HB3	1:A:222:VAL:HG21	2.00	0.43
1:A:41:ARG:HH22	1:A:57:ARG:HH21	1.68	0.42
1:A:27:TYR:CZ	1:A:214:ASN:HB3	2.55	0.42
1:A:74:ILE:HG13	1:A:96:ASN:HB3	2.02	0.42
2:B:402:MGT:H82	2:B:402:MGT:O5'	2.19	0.41
1:B:209:VAL:HG12	1:B:211:LEU:H	1.86	0.41
1:A:175:GLY:N	1:A:176:PRO:CD	2.83	0.40
1:B:72:GLN:HG2	7:B:572:HOH:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	258/269 (96%)	256 (99%)	2 (1%)	0	100	100
1	B	259/269 (96%)	257 (99%)	2 (1%)	0	100	100
All	All	517/538 (96%)	513 (99%)	4 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	219/221 (99%)	217 (99%)	2 (1%)	78	88
1	B	220/221 (100%)	215 (98%)	5 (2%)	50	63
All	All	439/442 (99%)	432 (98%)	7 (2%)	62	76

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	LEU
1	A	174	ARG
1	B	159	GLN
1	B	167	MET
1	B	170	ASP
1	B	172	LEU
1	B	258	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	96	ASN
1	B	98	GLN

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Mol	Chain	Res	Type
1	B	110	HIS
1	B	117	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	MLY	B	15	1	9,10,11	0.56	0	6,11,13	1.77	1 (16%)
1	MLY	B	105	1	9,10,11	0.46	0	6,11,13	0.94	1 (16%)
1	MLY	A	95	1	9,10,11	0.51	0	6,11,13	0.55	0
1	MLY	A	76	1	9,10,11	0.51	0	6,11,13	0.61	0
1	MLY	B	76	1	9,10,11	0.44	0	6,11,13	0.71	0
1	MLY	A	105	1	9,10,11	0.51	0	6,11,13	0.58	0
1	MLY	A	15	1	9,10,11	0.57	0	6,11,13	0.59	0
1	MLY	B	95	1	9,10,11	0.45	0	6,11,13	0.61	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
1	MLY	B	15	1	-	5/8/9/11	-
1	MLY	B	105	1	-	3/8/9/11	-
1	MLY	A	95	1	-	3/8/9/11	-
1	MLY	A	76	1	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	B	76	1	-	2/8/9/11	-
1	MLY	A	105	1	-	1/8/9/11	-
1	MLY	A	15	1	-	2/8/9/11	-
1	MLY	B	95	1	-	3/8/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	15	MLY	CD-CE-NZ	-3.71	103.75	113.79
1	B	105	MLY	CD-CE-NZ	-2.19	107.86	113.79

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	15	MLY	C-CA-CB-CG
1	B	95	MLY	O-C-CA-CB
1	B	15	MLY	CD-CE-NZ-CH1
1	B	15	MLY	CD-CE-NZ-CH2
1	B	105	MLY	CD-CE-NZ-CH1
1	A	95	MLY	CD-CE-NZ-CH1
1	A	95	MLY	CG-CD-CE-NZ
1	A	15	MLY	CG-CD-CE-NZ
1	B	105	MLY	CD-CE-NZ-CH2
1	B	95	MLY	CD-CE-NZ-CH2
1	A	95	MLY	CD-CE-NZ-CH2
1	B	95	MLY	CG-CD-CE-NZ
1	A	76	MLY	CD-CE-NZ-CH2
1	A	76	MLY	CD-CE-NZ-CH1
1	B	15	MLY	CG-CD-CE-NZ
1	A	105	MLY	CE-CD-CG-CB
1	B	15	MLY	N-CA-CB-CG
1	B	76	MLY	CD-CE-NZ-CH1
1	B	105	MLY	CE-CD-CG-CB
1	A	15	MLY	C-CA-CB-CG
1	B	76	MLY	CD-CE-NZ-CH2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	15	MLY	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 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$
4	SAH	A	500	-	21,28,28	1.26	2 (9%)	20,40,40	1.67	2 (10%)
5	GOL	A	463	-	5,5,5	0.30	0	5,5,5	0.44	0
2	MGT	A	401	-	30,35,35	1.62	4 (13%)	41,56,56	2.31	10 (24%)
3	3PO	A	451	-	8,12,12	0.68	0	15,20,20	1.36	2 (13%)
4	SAH	B	500	-	21,28,28	1.19	2 (9%)	20,40,40	1.63	2 (10%)
3	3PO	B	452	-	8,12,12	0.71	0	15,20,20	1.26	2 (13%)
5	GOL	B	468	-	5,5,5	0.75	0	5,5,5	0.10	0
2	MGT	B	403	-	30,35,35	1.60	4 (13%)	41,56,56	2.42	12 (29%)
2	MGT	B	402	-	30,35,35	1.61	4 (13%)	41,56,56	2.28	11 (26%)

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
4	SAH	A	500	-	-	0/7/31/31	0/3/3/3
5	GOL	A	463	-	-	4/4/4/4	-
2	MGT	A	401	-	-	3/22/50/50	0/3/3/3
3	3PO	A	451	-	-	2/12/12/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SAH	B	500	-	-	0/7/31/31	0/3/3/3
3	3PO	B	452	-	-	1/12/12/12	-
5	GOL	B	468	-	-	0/4/4/4	-
2	MGT	B	403	-	-	5/22/50/50	0/3/3/3
2	MGT	B	402	-	-	0/22/50/50	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	MGT	C6-C5	4.79	1.48	1.41
2	B	403	MGT	C6-C5	4.79	1.48	1.41
2	A	401	MGT	C6-C5	4.78	1.48	1.41
2	A	401	MGT	C5-C4	4.56	1.48	1.39
2	B	403	MGT	C5-C4	4.53	1.48	1.39
2	B	402	MGT	C5-C4	4.44	1.47	1.39
4	A	500	SAH	C2-N3	4.07	1.38	1.32
4	B	500	SAH	C2-N3	3.81	1.38	1.32
2	B	402	MGT	C5-N7	-3.62	1.33	1.39
2	A	401	MGT	C5-N7	-3.55	1.33	1.39
2	B	403	MGT	C5-N7	-3.47	1.33	1.39
4	A	500	SAH	C2-N1	2.62	1.38	1.33
2	A	401	MGT	C4-N9	-2.59	1.33	1.38
2	B	402	MGT	C4-N9	-2.51	1.33	1.38
4	B	500	SAH	C2-N1	2.37	1.38	1.33
2	B	403	MGT	C4-N9	-2.16	1.34	1.38

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	403	MGT	N3-C4-N9	9.00	138.47	126.91
2	B	402	MGT	N3-C4-N9	8.54	137.88	126.91
2	A	401	MGT	N3-C4-N9	8.28	137.55	126.91
4	A	500	SAH	N3-C2-N1	-5.64	119.87	128.68
4	B	500	SAH	N3-C2-N1	-5.52	120.05	128.68
2	B	403	MGT	N7-C8-N9	-5.11	96.06	103.38
2	B	403	MGT	C5-C4-N3	-5.03	118.28	126.49
2	A	401	MGT	N7-C8-N9	-4.91	96.35	103.38
2	B	402	MGT	C5-C4-N3	-4.84	118.59	126.49
2	B	402	MGT	N7-C8-N9	-4.82	96.49	103.38
2	A	401	MGT	C6-N1-C2	4.79	123.54	115.93
2	A	401	MGT	C5-C4-N3	-4.78	118.69	126.49
2	B	403	MGT	C6-N1-C2	4.40	122.91	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	402	MGT	C6-N1-C2	4.35	122.85	115.93
2	B	403	MGT	C6-C5-C4	3.95	119.44	115.20
2	A	401	MGT	C5-C6-N1	-3.66	115.61	123.14
2	A	401	MGT	C6-C5-C4	3.66	119.13	115.20
2	B	403	MGT	C5-C6-N1	-3.48	115.99	123.14
2	B	402	MGT	C5-C6-N1	-3.37	116.22	123.14
2	B	402	MGT	C6-C5-C4	3.35	118.79	115.20
4	A	500	SAH	C5'-SD-CG	-3.06	93.07	102.27
2	A	401	MGT	PA-O3A-PB	-2.97	122.63	132.83
2	B	403	MGT	PB-O3B-PG	-2.80	123.20	132.83
2	B	402	MGT	PB-O3B-PG	-2.69	123.58	132.83
2	B	402	MGT	C8-N7-C5	2.59	115.68	108.94
2	B	403	MGT	C8-N7-C5	2.59	115.67	108.94
2	A	401	MGT	PB-O3B-PG	-2.56	124.05	132.83
3	A	451	3PO	PB-O3B-PG	-2.52	124.17	132.83
2	A	401	MGT	C8-N7-C5	2.52	115.50	108.94
2	B	403	MGT	PA-O3A-PB	-2.48	124.32	132.83
3	A	451	3PO	PB-O3A-PA	-2.44	124.47	132.83
3	B	452	3PO	PB-O3A-PA	-2.34	124.79	132.83
4	B	500	SAH	C5'-SD-CG	-2.31	95.34	102.27
2	B	403	MGT	C5-C4-N9	-2.28	103.24	106.44
2	B	402	MGT	C2-N3-C4	2.26	120.13	113.89
3	B	452	3PO	PB-O3B-PG	-2.22	125.20	132.83
2	B	403	MGT	C2-N3-C4	2.18	119.93	113.89
2	B	402	MGT	CM7-N7-C5	2.16	132.31	124.01
2	A	401	MGT	C2-N3-C4	2.13	119.77	113.89
2	B	402	MGT	C5-C4-N9	-2.08	103.52	106.44
2	B	403	MGT	C3'-C2'-C1'	2.07	105.36	101.43

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	463	GOL	O1-C1-C2-C3
5	A	463	GOL	C1-C2-C3-O3
5	A	463	GOL	O1-C1-C2-O2
5	A	463	GOL	O2-C2-C3-O3
3	A	451	3PO	PG-O3B-PB-O1B
2	B	403	MGT	PB-O3A-PA-O1A
2	B	403	MGT	C5'-O5'-PA-O3A
2	A	401	MGT	PG-O3B-PB-O2B
3	B	452	3PO	PG-O3B-PB-O2B

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Mol	Chain	Res	Type	Atoms
2	B	403	MGT	PG-O3B-PB-O1B
2	A	401	MGT	PG-O3B-PB-O1B
2	B	403	MGT	PB-O3A-PA-O2A
2	B	403	MGT	PG-O3B-PB-O2B
3	A	451	3PO	PG-O3B-PB-O2B
2	A	401	MGT	C5'-O5'-PA-O1A

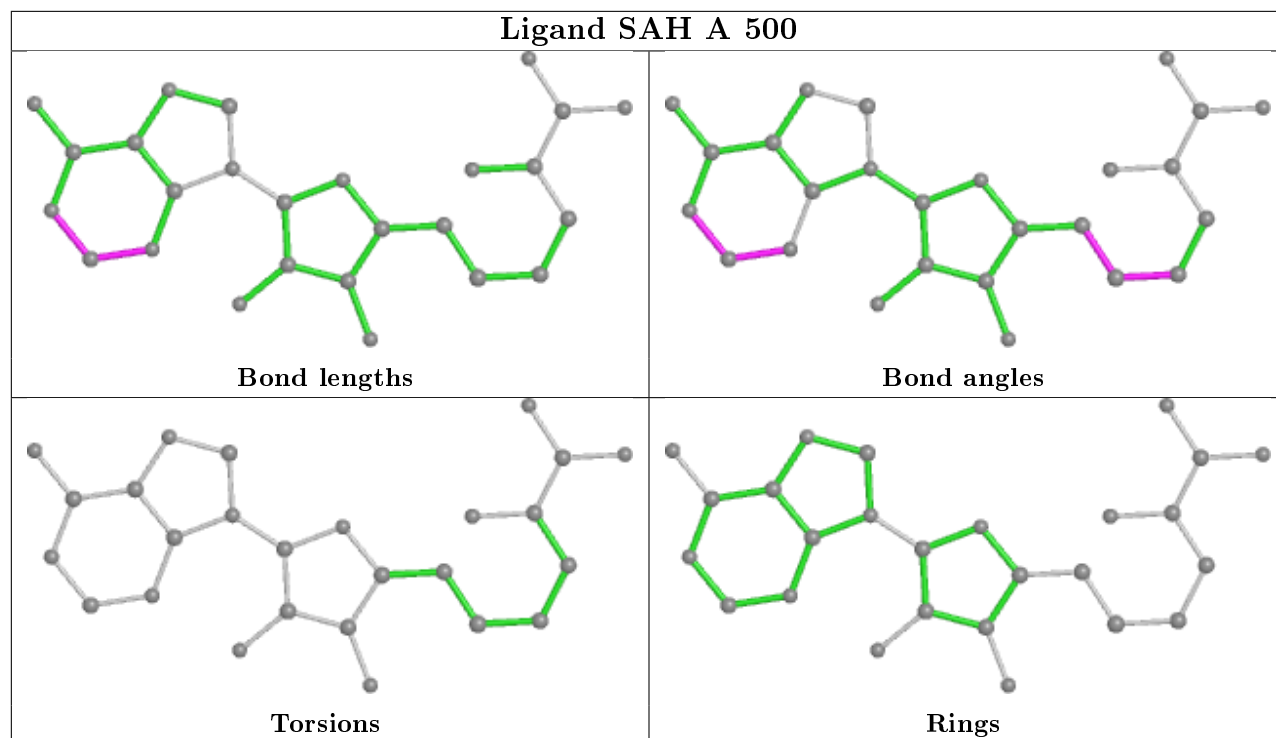
There are no ring outliers.

2 monomers are involved in 2 short contacts:

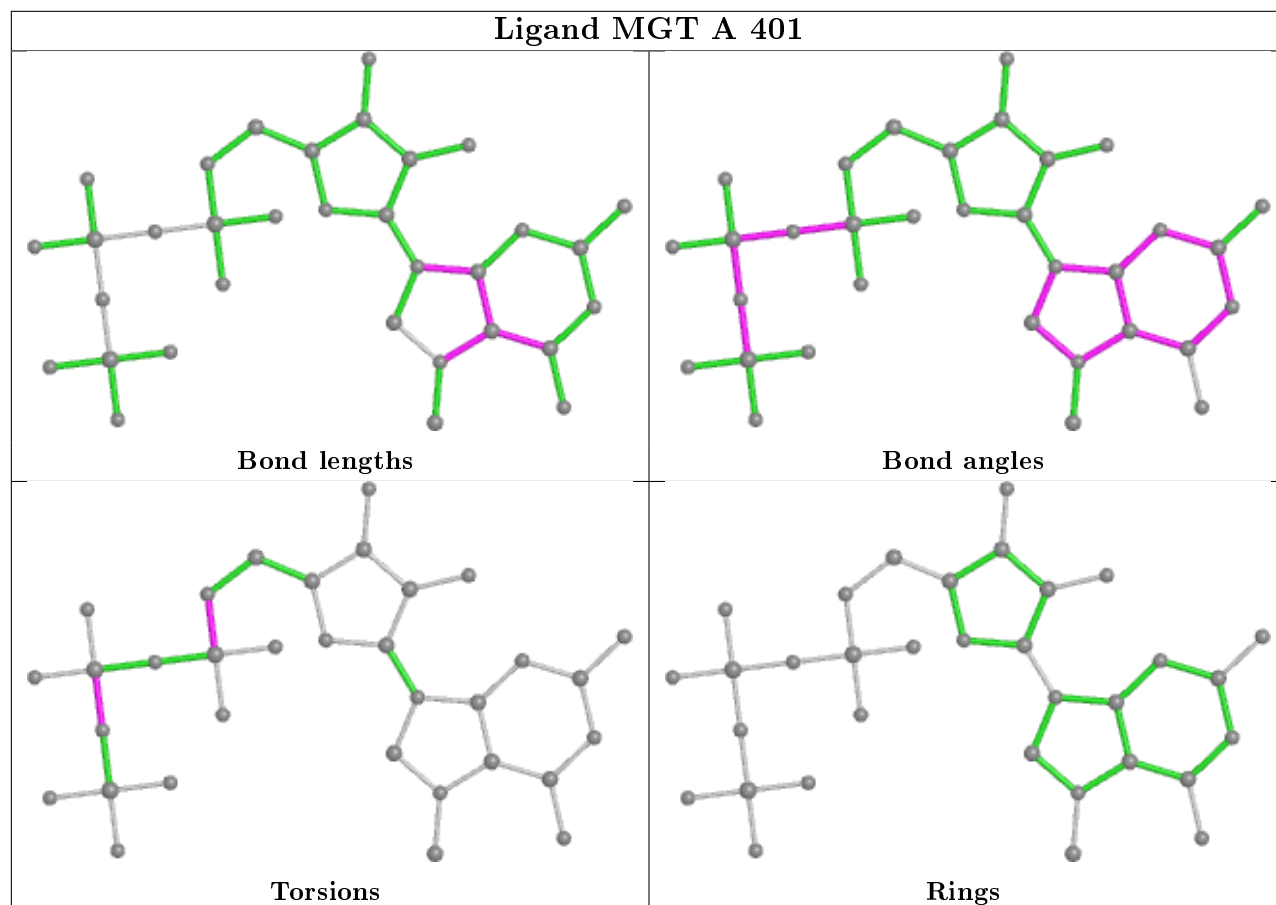
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	500	SAH	1	0
2	B	402	MGT	1	0

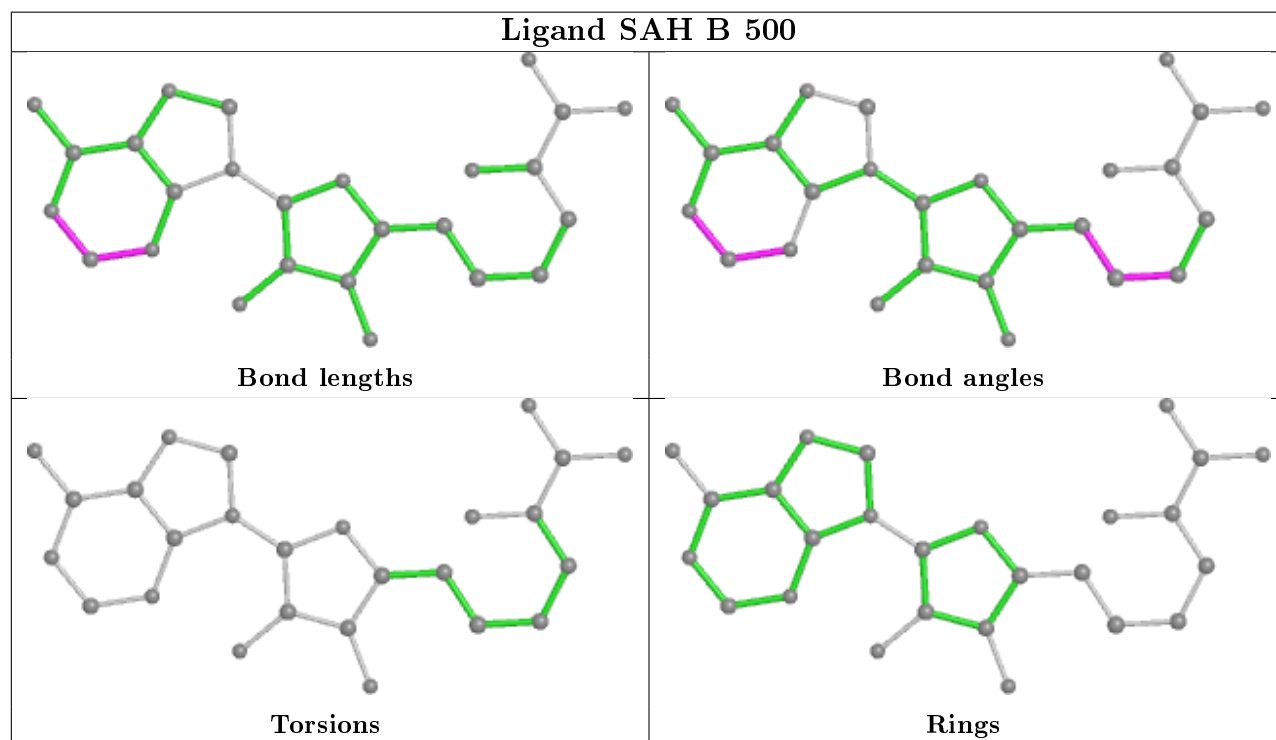
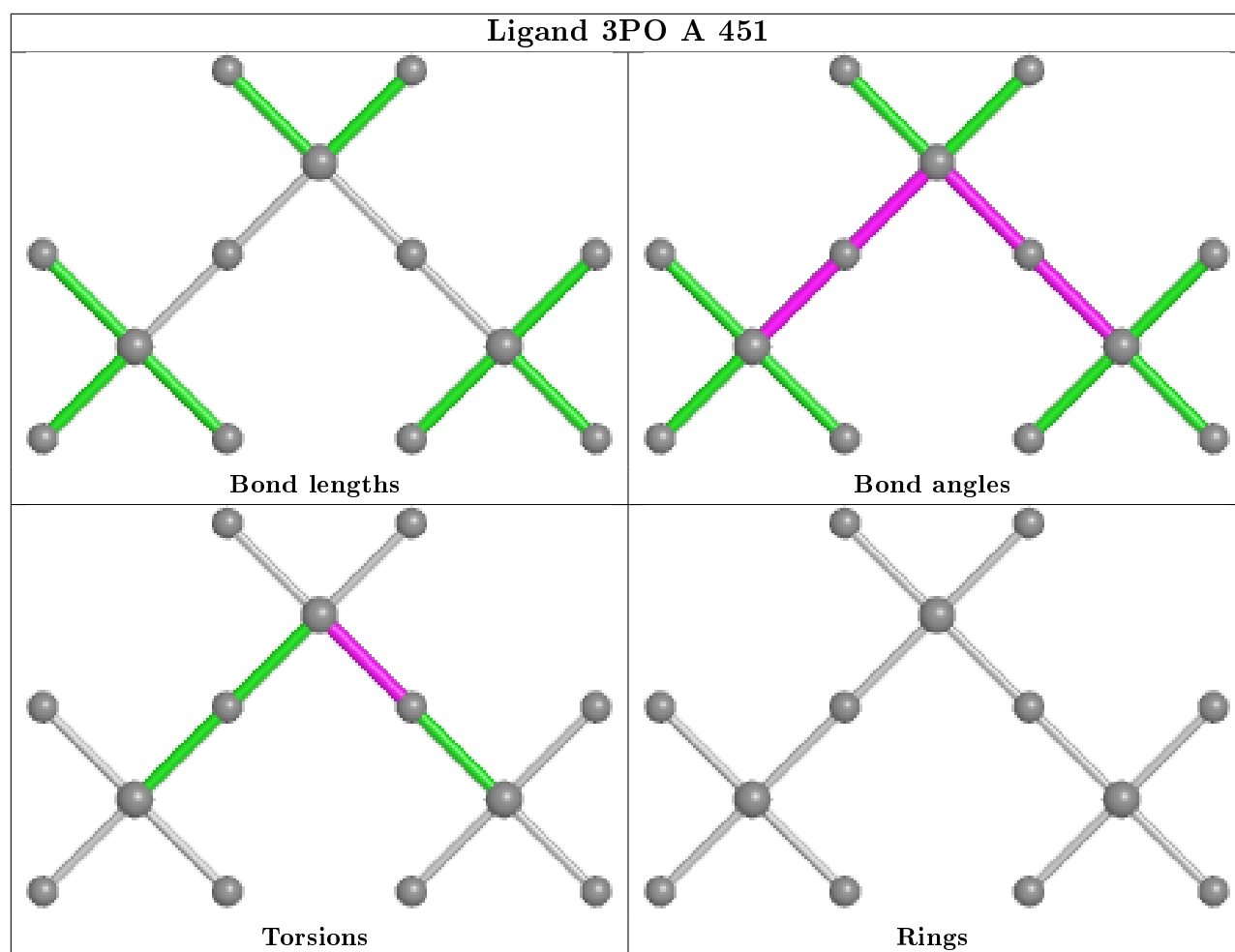
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

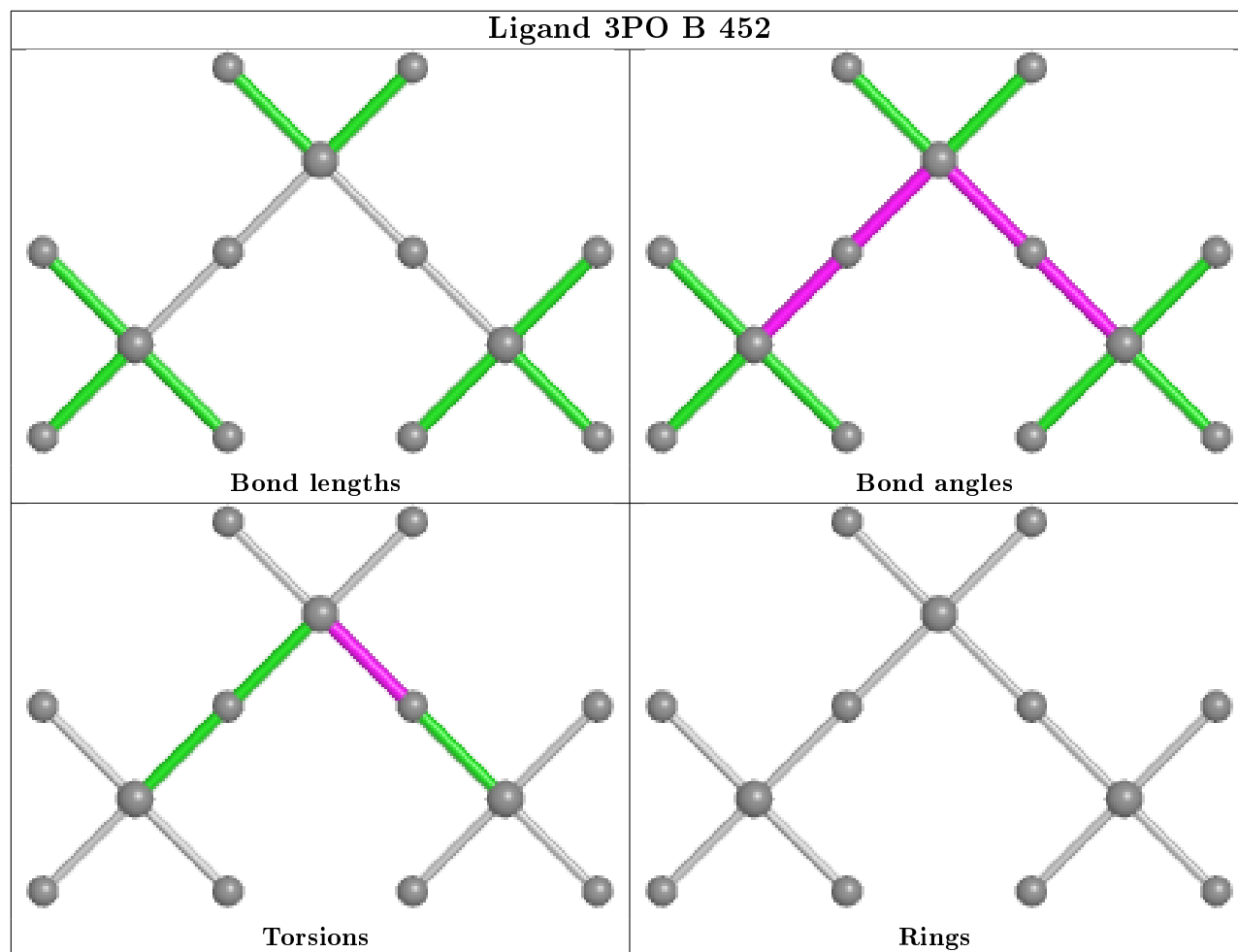
## Ligand SAH A 500

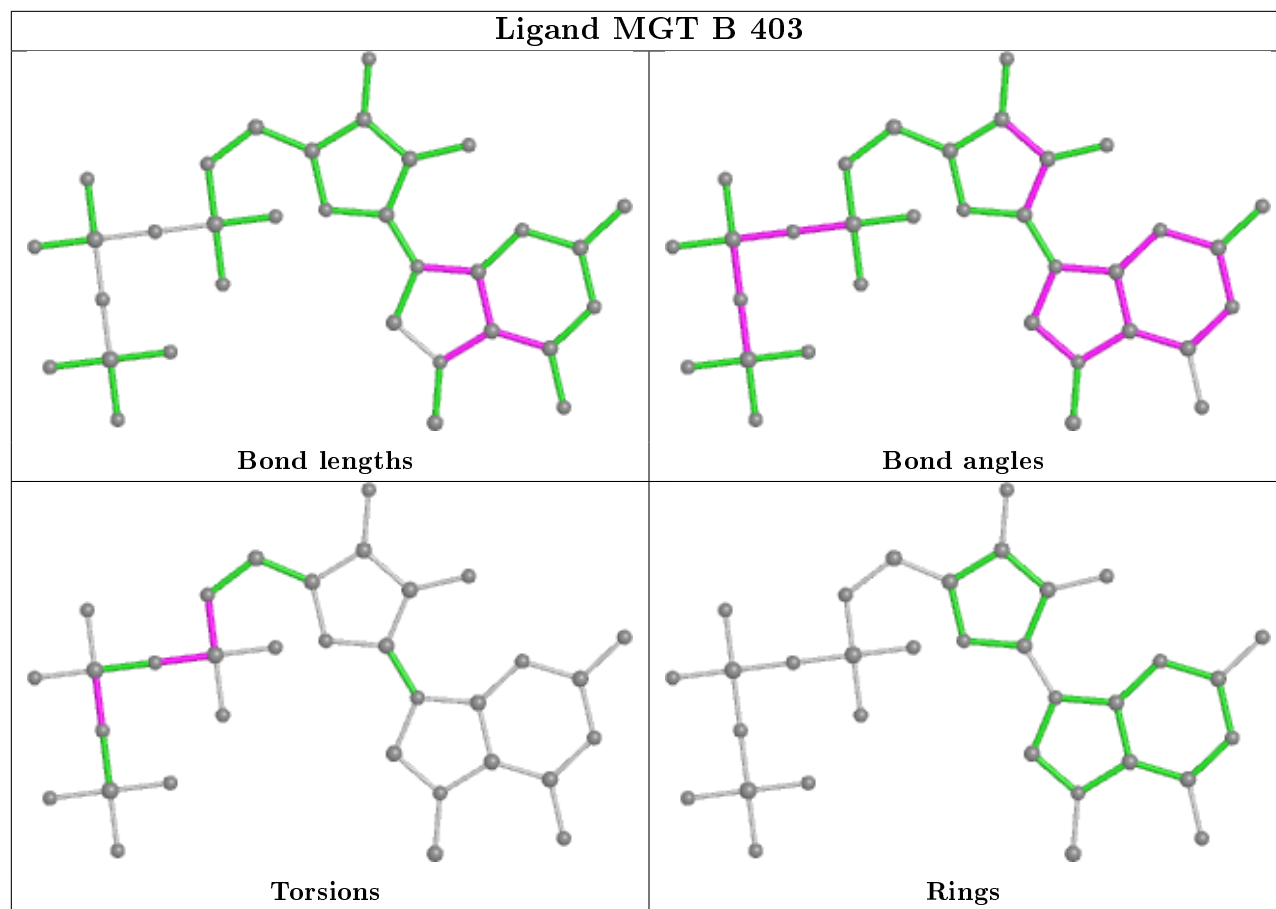


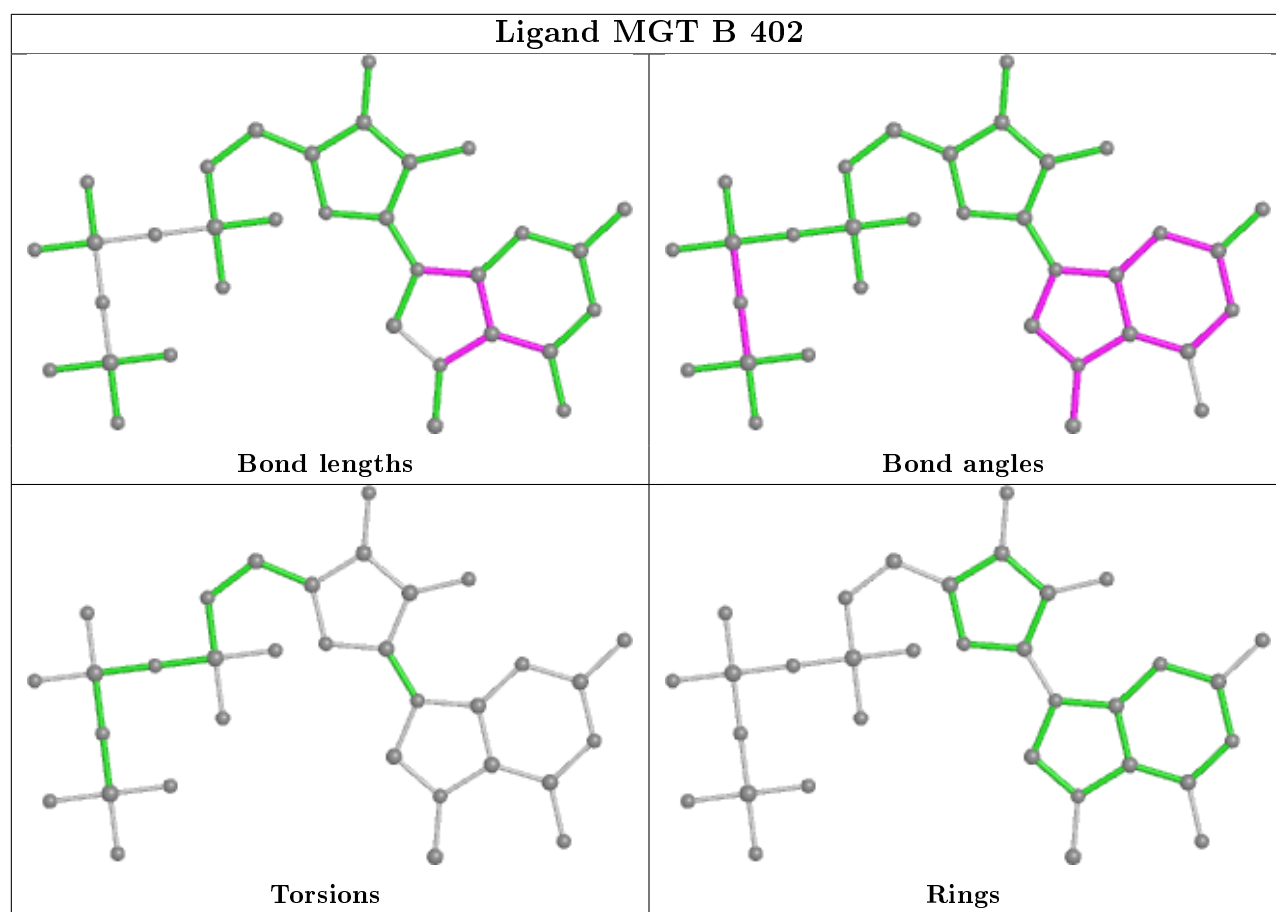
## Ligand MGT A 401











## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	260/269 (96%)	-0.02	5 (1%) 66 65	23, 32, 50, 71	0
1	B	261/269 (97%)	-0.08	2 (0%) 86 85	23, 32, 51, 68	0
All	All	521/538 (96%)	-0.05	7 (1%) 77 75	23, 32, 51, 71	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	44	ARG	4.0
1	A	4	GLY	3.8
1	A	45	ARG	3.0
1	B	247	LYS	3.0
1	A	245	ASP	2.2
1	B	45	ARG	2.1
1	A	247	LYS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	MLY	B	105	11/12	0.86	0.16	27,31,57,60	0
1	MLY	A	15	11/12	0.89	0.21	29,35,60,60	0
1	MLY	A	95	11/12	0.91	0.17	32,35,55,60	0
1	MLY	A	105	11/12	0.92	0.13	27,32,42,43	0
1	MLY	B	15	11/12	0.93	0.14	26,31,39,42	0
1	MLY	B	76	11/12	0.94	0.14	31,32,59,63	0
1	MLY	B	95	11/12	0.95	0.15	26,30,46,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MLY	A	76	11/12	0.97	0.12	27,29,47,53	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

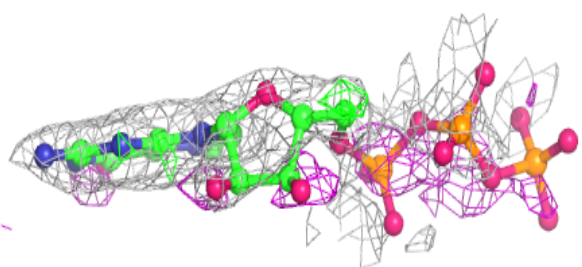
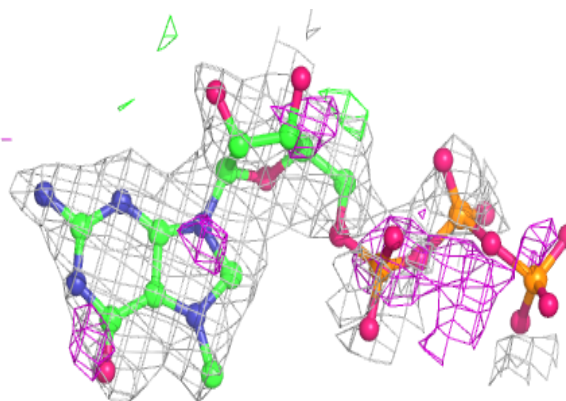
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MGT	B	403	33/33	0.71	0.36	46,73,146,146	0
5	GOL	A	463	6/6	0.81	0.16	45,47,48,56	0
3	3PO	B	452	13/13	0.88	0.30	60,70,78,79	0
2	MGT	B	402	33/33	0.90	0.16	18,26,94,96	0
3	3PO	A	451	13/13	0.94	0.26	47,55,76,79	0
2	MGT	A	401	33/33	0.94	0.16	22,31,102,104	0
4	SAH	A	500	26/26	0.96	0.12	17,23,27,29	0
5	GOL	B	468	6/6	0.97	0.15	17,19,27,27	0
6	CL	B	502	1/1	0.98	0.05	35,35,35,35	0
4	SAH	B	500	26/26	0.98	0.14	14,21,24,25	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.

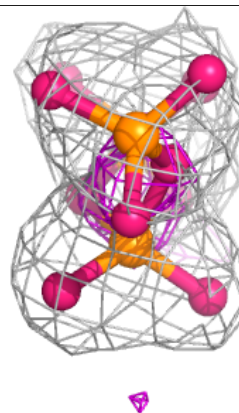
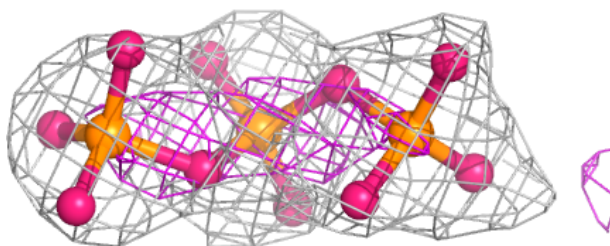
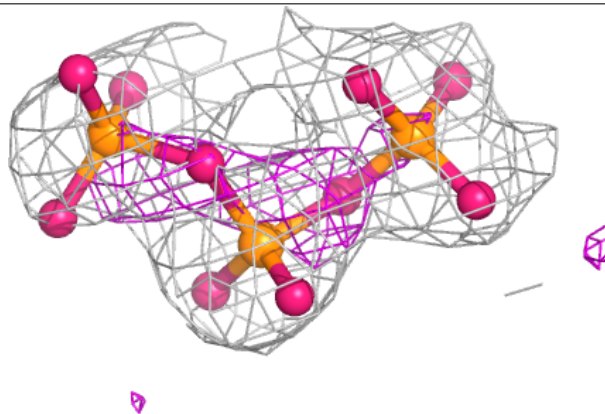


**Electron density around MGT B 403:**

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

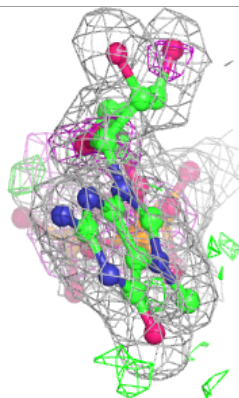
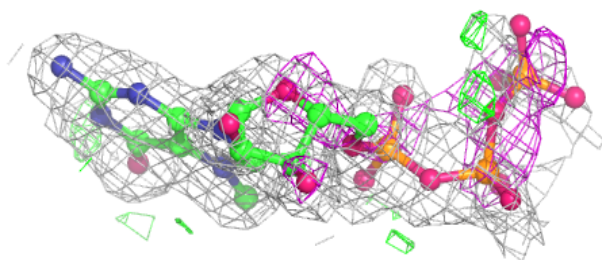
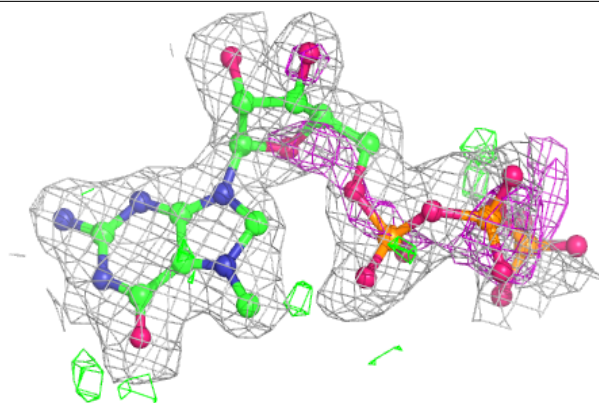
**Electron density around 3PO B 452:**

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

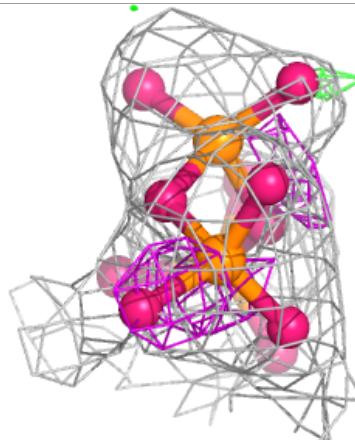
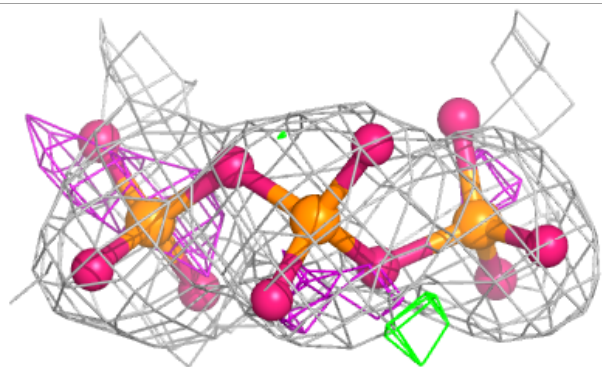
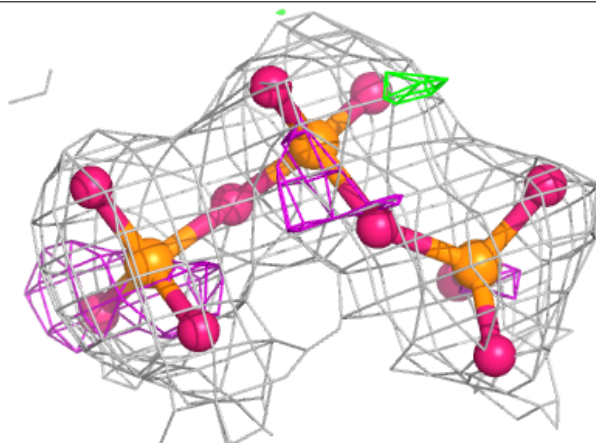


**Electron density around MGT B 402:**

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

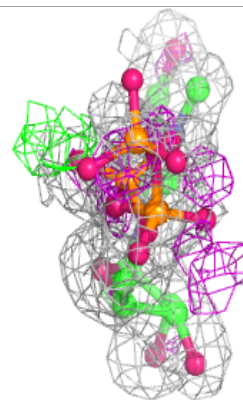
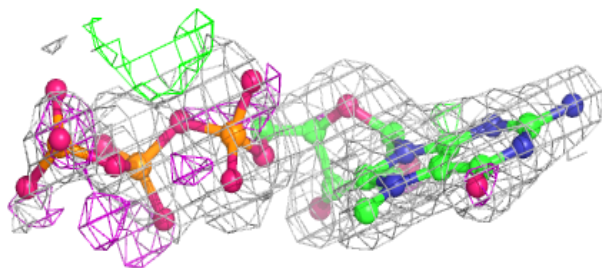
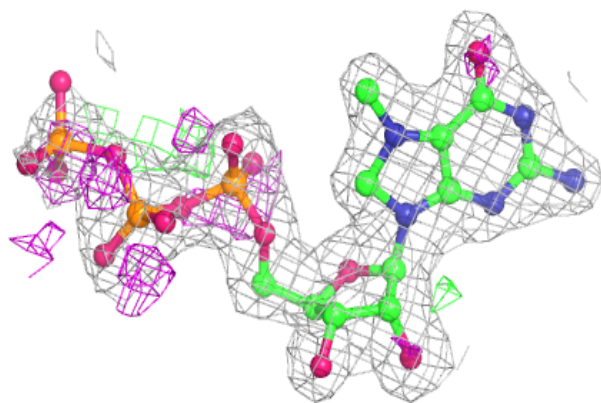
**Electron density around 3PO A 451:**

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

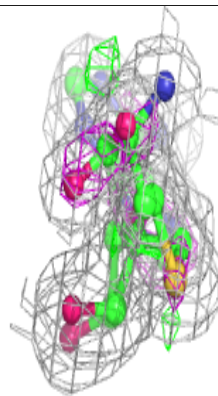
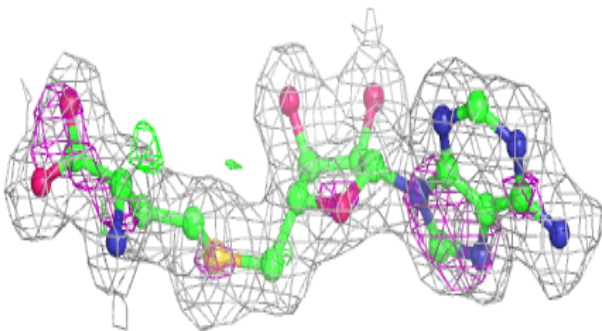
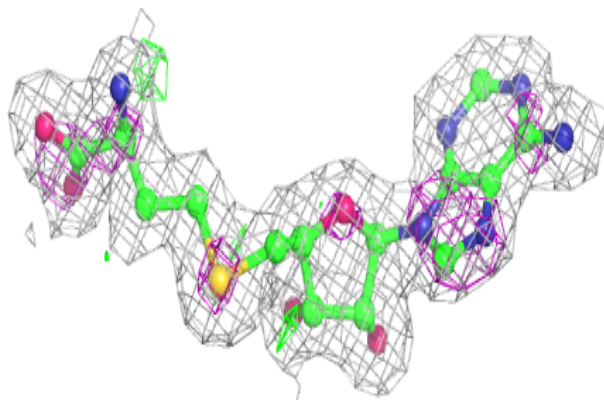


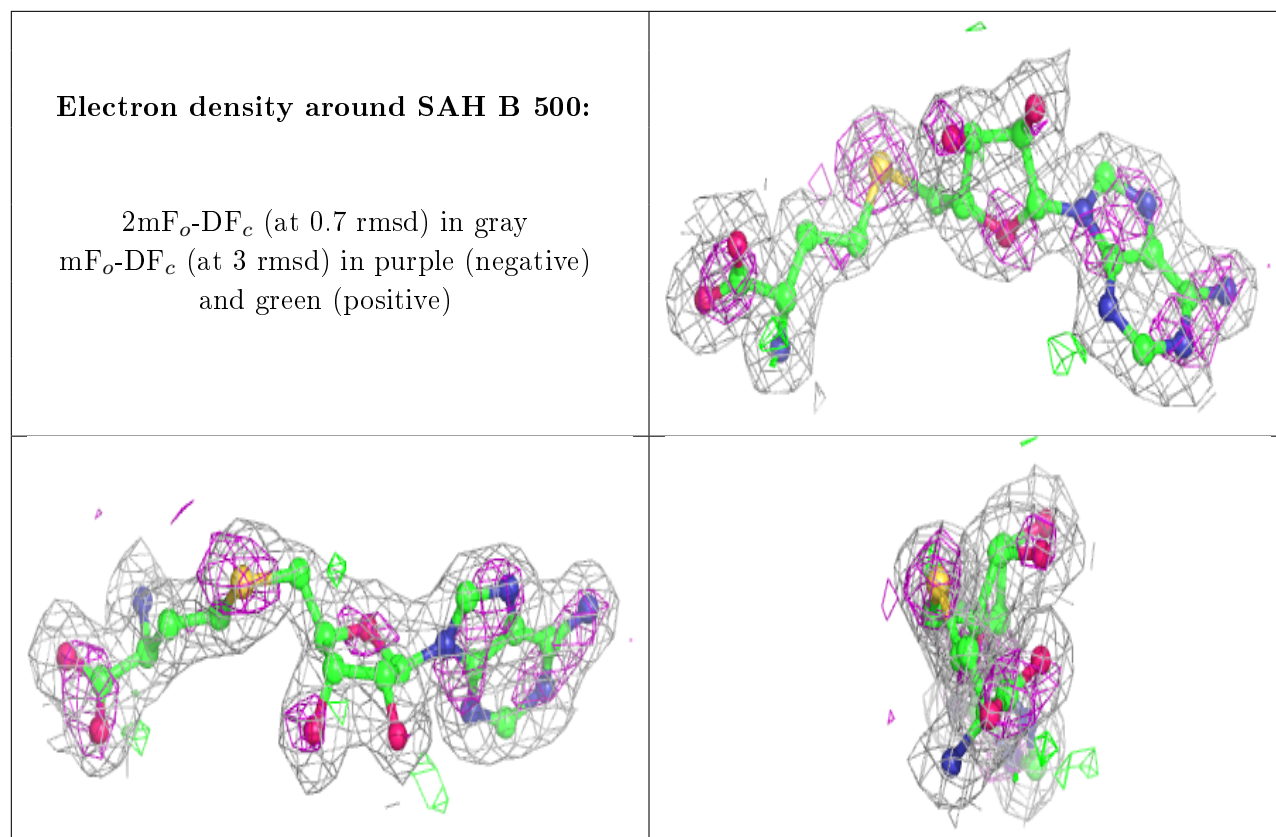
**Electron density around MGT A 401:**

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

**Electron density around SAH A 500:**

$2mF_o-DF_c$  (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.