



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 28, 2025 – 08:42 PM JST

PDB ID : 7XII / pdb\_00007xii  
Title : Crystal structure of the aminopropyltransferase, SpeE from hyperthermophilic crenarchaeon, Pyrobaculum calidifontis in complex with 5'-methylthioadenosine (MTA) & aminopropylagmatine  
Authors : Mizohata, E.; Yasuda, Y.  
Deposited on : 2022-04-13  
Resolution : 2.25 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](mailto:validation@mail.wwpdb.org)

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

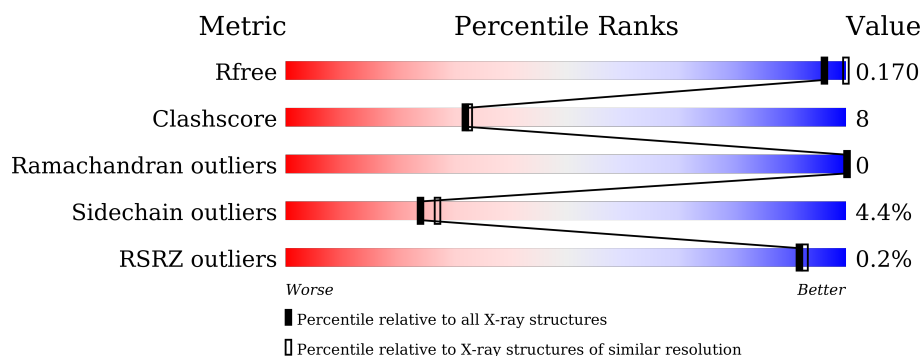
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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))
$R_{free}$	164625	1763 (2.26-2.26)
Clashscore	180529	1919 (2.26-2.26)
Ramachandran outliers	177936	1884 (2.26-2.26)
Sidechain outliers	177891	1885 (2.26-2.26)
RSRZ outliers	164620	1763 (2.26-2.26)

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  $\geq 3$ , 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	309	<div> <div>79%</div> <div>12%</div> <div>• 7%</div> </div>
1	B	309	<div> <div>80%</div> <div>12%</div> <div>• 7%</div> </div>
1	C	309	<div> <div>77%</div> <div>13%</div> <div>• 7%</div> </div>
1	D	309	<div> <div>80%</div> <div>11%</div> <div>• 7%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AG3	A	302	-	-	X	-
3	AG3	C	302	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9834 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 Polyamine aminopropyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2276	1460	385	424	7			
1	B	288	Total	C	N	O	S	0	0	0
			2296	1472	391	426	7			
1	C	286	Total	C	N	O	S	0	0	0
			2276	1460	385	424	7			
1	D	288	Total	C	N	O	S	0	0	0
			2296	1472	391	426	7			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A3MU81
A	-18	GLY	-	expression tag	UNP A3MU81
A	-17	SER	-	expression tag	UNP A3MU81
A	-16	SER	-	expression tag	UNP A3MU81
A	-15	HIS	-	expression tag	UNP A3MU81
A	-14	HIS	-	expression tag	UNP A3MU81
A	-13	HIS	-	expression tag	UNP A3MU81
A	-12	HIS	-	expression tag	UNP A3MU81
A	-11	HIS	-	expression tag	UNP A3MU81
A	-10	HIS	-	expression tag	UNP A3MU81
A	-9	SER	-	expression tag	UNP A3MU81
A	-8	SER	-	expression tag	UNP A3MU81
A	-7	GLY	-	expression tag	UNP A3MU81
A	-6	LEU	-	expression tag	UNP A3MU81
A	-5	VAL	-	expression tag	UNP A3MU81
A	-4	PRO	-	expression tag	UNP A3MU81
A	-3	ARG	-	expression tag	UNP A3MU81
A	-2	GLY	-	expression tag	UNP A3MU81
A	-1	SER	-	expression tag	UNP A3MU81
A	0	HIS	-	expression tag	UNP A3MU81
B	-19	MET	-	initiating methionine	UNP A3MU81

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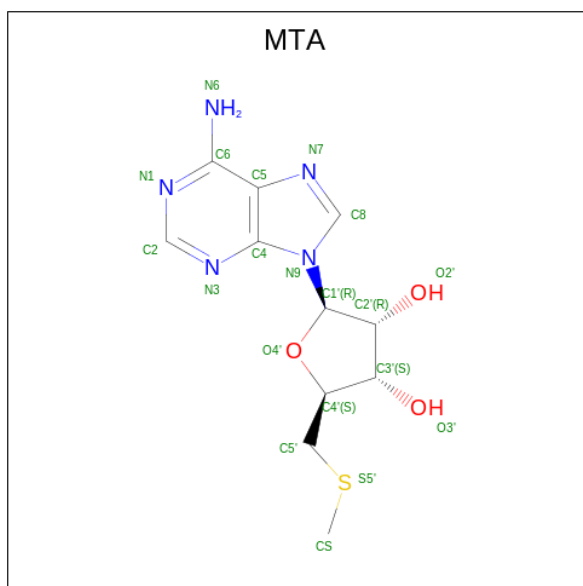
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP A3MU81
B	-17	SER	-	expression tag	UNP A3MU81
B	-16	SER	-	expression tag	UNP A3MU81
B	-15	HIS	-	expression tag	UNP A3MU81
B	-14	HIS	-	expression tag	UNP A3MU81
B	-13	HIS	-	expression tag	UNP A3MU81
B	-12	HIS	-	expression tag	UNP A3MU81
B	-11	HIS	-	expression tag	UNP A3MU81
B	-10	HIS	-	expression tag	UNP A3MU81
B	-9	SER	-	expression tag	UNP A3MU81
B	-8	SER	-	expression tag	UNP A3MU81
B	-7	GLY	-	expression tag	UNP A3MU81
B	-6	LEU	-	expression tag	UNP A3MU81
B	-5	VAL	-	expression tag	UNP A3MU81
B	-4	PRO	-	expression tag	UNP A3MU81
B	-3	ARG	-	expression tag	UNP A3MU81
B	-2	GLY	-	expression tag	UNP A3MU81
B	-1	SER	-	expression tag	UNP A3MU81
B	0	HIS	-	expression tag	UNP A3MU81
C	-19	MET	-	initiating methionine	UNP A3MU81
C	-18	GLY	-	expression tag	UNP A3MU81
C	-17	SER	-	expression tag	UNP A3MU81
C	-16	SER	-	expression tag	UNP A3MU81
C	-15	HIS	-	expression tag	UNP A3MU81
C	-14	HIS	-	expression tag	UNP A3MU81
C	-13	HIS	-	expression tag	UNP A3MU81
C	-12	HIS	-	expression tag	UNP A3MU81
C	-11	HIS	-	expression tag	UNP A3MU81
C	-10	HIS	-	expression tag	UNP A3MU81
C	-9	SER	-	expression tag	UNP A3MU81
C	-8	SER	-	expression tag	UNP A3MU81
C	-7	GLY	-	expression tag	UNP A3MU81
C	-6	LEU	-	expression tag	UNP A3MU81
C	-5	VAL	-	expression tag	UNP A3MU81
C	-4	PRO	-	expression tag	UNP A3MU81
C	-3	ARG	-	expression tag	UNP A3MU81
C	-2	GLY	-	expression tag	UNP A3MU81
C	-1	SER	-	expression tag	UNP A3MU81
C	0	HIS	-	expression tag	UNP A3MU81
D	-19	MET	-	initiating methionine	UNP A3MU81
D	-18	GLY	-	expression tag	UNP A3MU81
D	-17	SER	-	expression tag	UNP A3MU81

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP A3MU81
D	-15	HIS	-	expression tag	UNP A3MU81
D	-14	HIS	-	expression tag	UNP A3MU81
D	-13	HIS	-	expression tag	UNP A3MU81
D	-12	HIS	-	expression tag	UNP A3MU81
D	-11	HIS	-	expression tag	UNP A3MU81
D	-10	HIS	-	expression tag	UNP A3MU81
D	-9	SER	-	expression tag	UNP A3MU81
D	-8	SER	-	expression tag	UNP A3MU81
D	-7	GLY	-	expression tag	UNP A3MU81
D	-6	LEU	-	expression tag	UNP A3MU81
D	-5	VAL	-	expression tag	UNP A3MU81
D	-4	PRO	-	expression tag	UNP A3MU81
D	-3	ARG	-	expression tag	UNP A3MU81
D	-2	GLY	-	expression tag	UNP A3MU81
D	-1	SER	-	expression tag	UNP A3MU81
D	0	HIS	-	expression tag	UNP A3MU81

- Molecule 2 is 5'-DEOXY-5'-METHYLTHIOADENOSINE (CCD ID: MTA) (formula:  $C_{11}H_{15}N_5O_3S$ ) (labeled as "Ligand of Interest" by depositor).



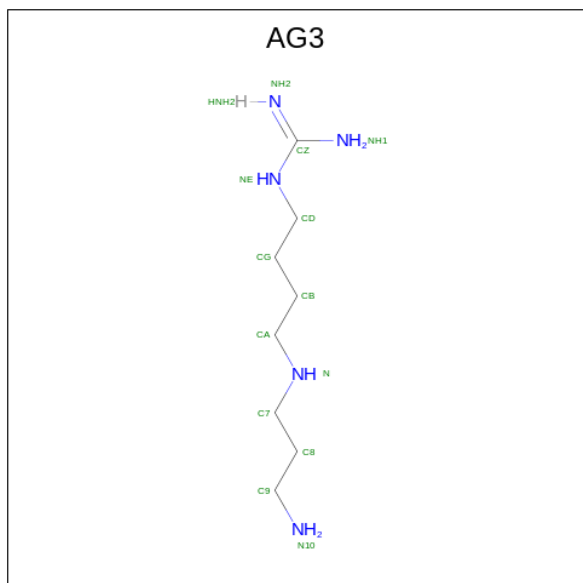
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
2	B	1	Total	C	N	O	S	0	0
			20	11	5	3	1		

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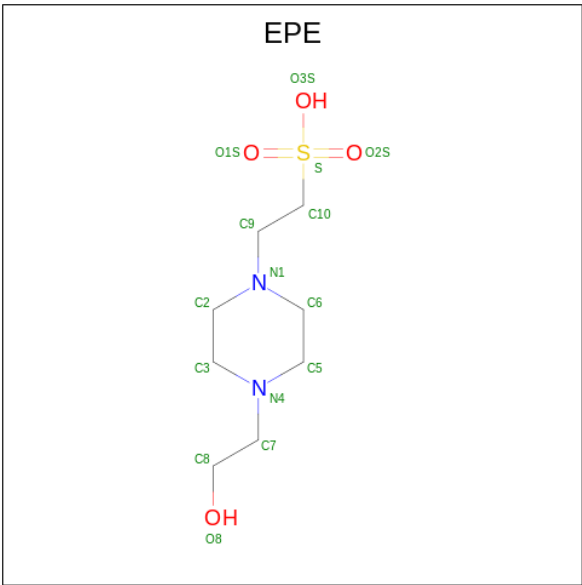
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
2	D	1	Total	C	N	O	S	0	0
			20	11	5	3	1		

- Molecule 3 is 1-{4-[(3-aminopropyl)amino]butyl}guanidine (CCD ID: AG3) (formula:  $C_8H_{21}N_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			13	8	5		
3	B	1	Total	C	N	0	0
			13	8	5		
3	C	1	Total	C	N	0	0
			13	8	5		
3	D	1	Total	C	N	0	0
			13	8	5		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula:  $C_8H_{18}N_2O_4S$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	162	Total	O	0	0
			162	162		
5	B	125	Total	O	0	0
			125	125		
5	C	131	Total	O	0	0
			131	131		
5	D	125	Total	O	0	0
			125	125		





- Molecule 1: Polyamine aminopropyltransferase



K176	
R180	
D193	
G194	
V195	
Q199	
A200	
G201	
N202	
S203	
Y236	
N239	
Y247	
D248	
P249	
T253	
P254	
S255	
E259	
R262	
Y271	
R274	
V275	
H276	
N281	
R289	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.16Å 57.17Å 97.31Å 77.19° 78.32° 88.49°	Depositor
Resolution (Å)	46.51 – 2.25 46.51 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.51-2.25) 99.6 (46.51-2.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.16 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.149 , 0.170 0.149 , 0.170	Depositor DCC
$R_{free}$ test set	2624 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.6	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 33.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9834	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: AG3, MTA, EPE

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	0.75	2/2329 (0.1%)	1.10	4/3164 (0.1%)
1	B	0.68	0/2349	1.05	4/3189 (0.1%)
1	C	0.71	2/2329 (0.1%)	1.06	4/3164 (0.1%)
1	D	0.69	0/2349	1.07	4/3189 (0.1%)
All	All	0.71	4/9356 (0.0%)	1.07	16/12706 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	262	ARG	NE-CZ	6.66	1.40	1.33
1	C	4	VAL	N-CA	5.33	1.56	1.46
1	C	276	HIS	CE1-NE2	5.31	1.37	1.32
1	A	4	VAL	N-CA	5.10	1.55	1.46

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	ARG	CB-CG-CD	10.37	135.15	111.30
1	A	262	ARG	CD-NE-CZ	-9.16	111.58	124.40
1	B	262	ARG	CG-CD-NE	-8.57	93.14	112.00
1	B	215	GLU	CB-CA-C	-6.88	98.98	110.68
1	D	4	VAL	CB-CA-C	6.61	118.78	111.18

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	2276	0	2265	37	0
1	B	2296	0	2291	35	0
1	C	2276	0	2265	48	0
1	D	2296	0	2291	36	0
2	A	20	0	15	2	0
2	B	20	0	15	1	0
2	C	20	0	15	1	0
2	D	20	0	15	1	0
3	A	13	0	20	11	0
3	B	13	0	20	6	0
3	C	13	0	20	7	0
3	D	13	0	20	6	0
4	A	15	0	18	1	0
5	A	162	0	0	4	0
5	B	125	0	0	3	0
5	C	131	0	0	3	0
5	D	125	0	0	0	0
All	All	9834	0	9270	147	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 147 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:C:9:THR:HG21	1:C:21:LEU:CD2	1.37	1.51
1:C:9:THR:CG2	1:C:21:LEU:CD2	2.08	1.27
1:C:181:GLU:HG2	5:C:476:HOH:O	1.43	1.16
1:C:9:THR:HG21	1:C:21:LEU:HD21	1.28	1.09
1:C:20:LEU:HD23	1:D:20:LEU:HD23	1.36	1.07

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	284/309 (92%)	276 (97%)	8 (3%)	0	100	100
1	B	286/309 (93%)	279 (98%)	7 (2%)	0	100	100
1	C	284/309 (92%)	276 (97%)	8 (3%)	0	100	100
1	D	286/309 (93%)	279 (98%)	7 (2%)	0	100	100
All	All	1140/1236 (92%)	1110 (97%)	30 (3%)	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	245/265 (92%)	234 (96%)	11 (4%)	23	26
1	B	247/265 (93%)	236 (96%)	11 (4%)	23	26
1	C	245/265 (92%)	236 (96%)	9 (4%)	29	35
1	D	247/265 (93%)	235 (95%)	12 (5%)	21	23
All	All	984/1060 (93%)	941 (96%)	43 (4%)	24	27

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	199	GLN
1	D	61	VAL
1	C	255	SER

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Mol	Chain	Res	Type
1	D	32	LYS
1	D	127	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	239	ASN
1	D	199	GLN
1	C	57	GLN
1	D	276	HIS
1	D	17	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

9 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	MTA	B	301	-	19,22,22	1.57	4 (21%)	19,32,32	2.03	10 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MTA	C	301	-	19,22,22	1.13	1 (5%)	19,32,32	1.96	7 (36%)
3	AG3	D	302	-	12,12,12	0.61	0	11,12,12	1.68	1 (9%)
4	EPE	A	303	-	15,15,15	1.73	1 (6%)	18,20,20	2.11	6 (33%)
3	AG3	A	302	-	12,12,12	0.40	0	11,12,12	1.26	1 (9%)
2	MTA	A	301	-	19,22,22	1.40	3 (15%)	19,32,32	1.88	6 (31%)
3	AG3	B	302	-	12,12,12	0.36	0	11,12,12	0.92	1 (9%)
3	AG3	C	302	-	12,12,12	0.48	0	11,12,12	1.07	1 (9%)
2	MTA	D	301	-	19,22,22	1.29	2 (10%)	19,32,32	1.87	4 (21%)

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	MTA	B	301	-	-	2/3/23/23	0/3/3/3
2	MTA	C	301	-	-	2/3/23/23	0/3/3/3
3	AG3	D	302	-	-	4/10/10/10	-
4	EPE	A	303	-	-	4/9/19/19	0/1/1/1
3	AG3	A	302	-	-	6/10/10/10	-
2	MTA	A	301	-	-	2/3/23/23	0/3/3/3
3	AG3	B	302	-	-	7/10/10/10	-
3	AG3	C	302	-	-	7/10/10/10	-
2	MTA	D	301	-	-	2/3/23/23	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	303	EPE	C10-S	-5.96	1.69	1.77
2	B	301	MTA	C2-N3	3.46	1.37	1.32
2	B	301	MTA	C5-C4	3.04	1.49	1.40
2	B	301	MTA	C2'-C1'	-2.97	1.49	1.53
2	D	301	MTA	C5'-S5'	-2.85	1.76	1.80

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	303	EPE	O1S-S-C10	5.86	113.97	106.92

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302	AG3	CG-CD-NE	-5.11	97.61	112.21
2	D	301	MTA	O4'-C1'-C2'	-4.91	99.75	106.93
2	D	301	MTA	N3-C2-N1	-4.65	121.41	128.68
2	A	301	MTA	N3-C2-N1	-4.36	121.86	128.68

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

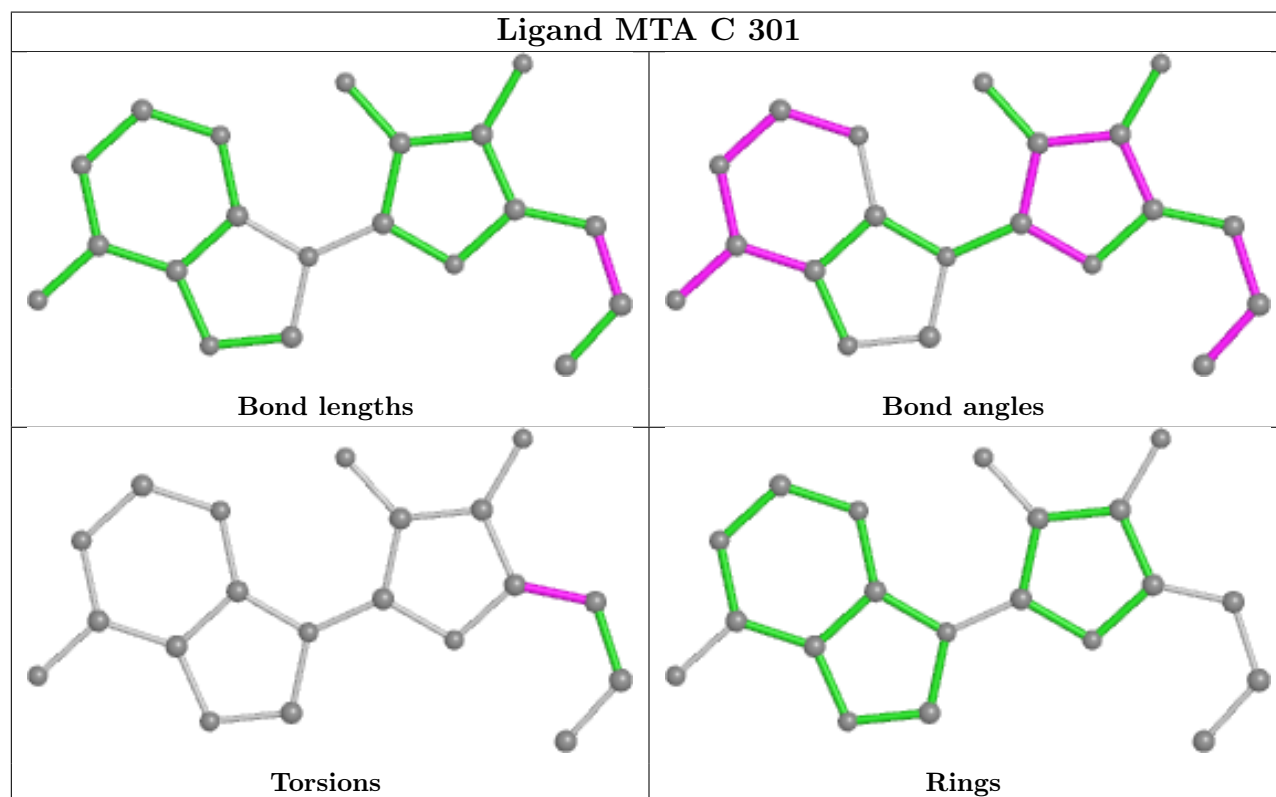
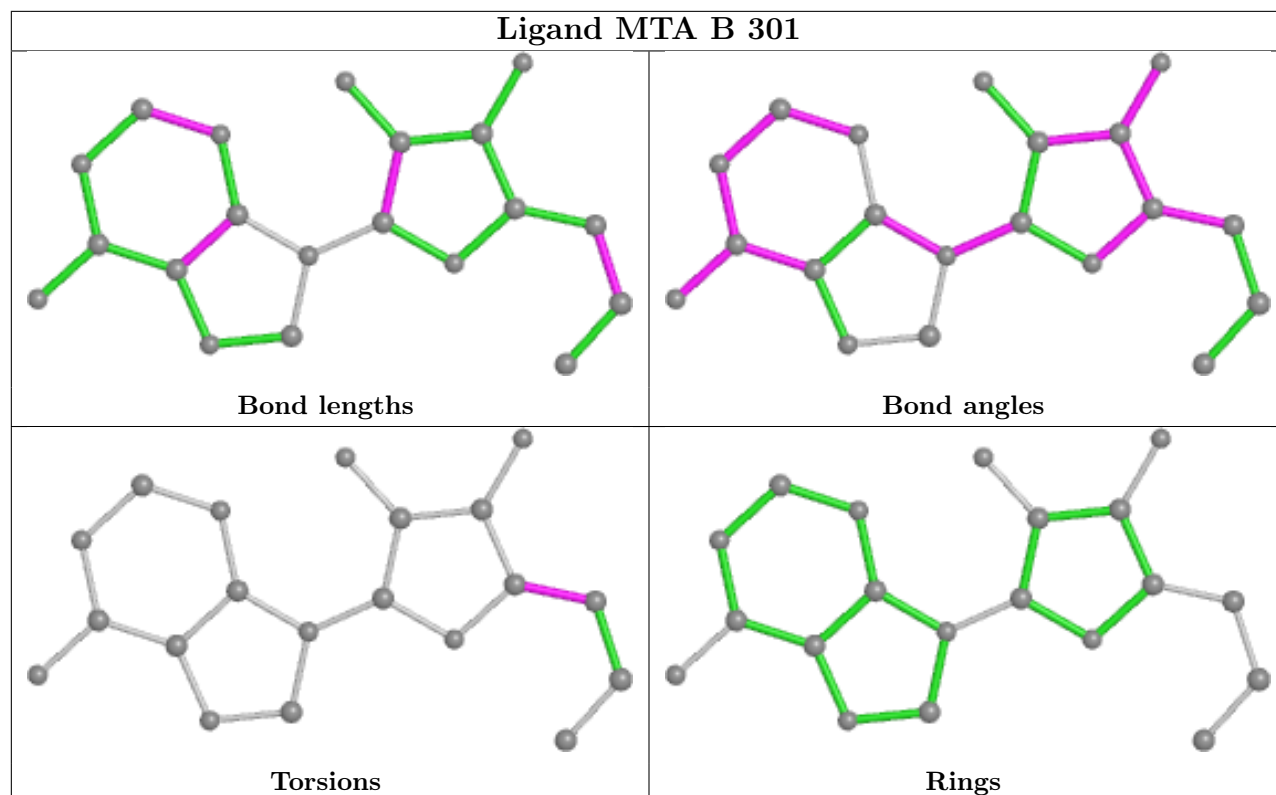
Mol	Chain	Res	Type	Atoms
2	A	301	MTA	O4'-C4'-C5'-S5'
2	A	301	MTA	C3'-C4'-C5'-S5'
2	B	301	MTA	O4'-C4'-C5'-S5'
2	B	301	MTA	C3'-C4'-C5'-S5'
2	C	301	MTA	O4'-C4'-C5'-S5'

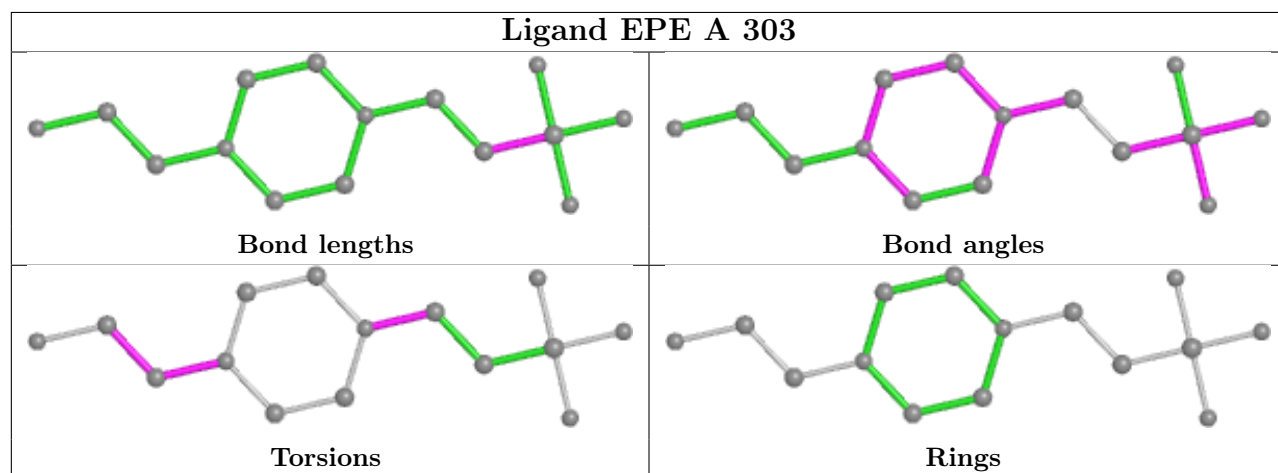
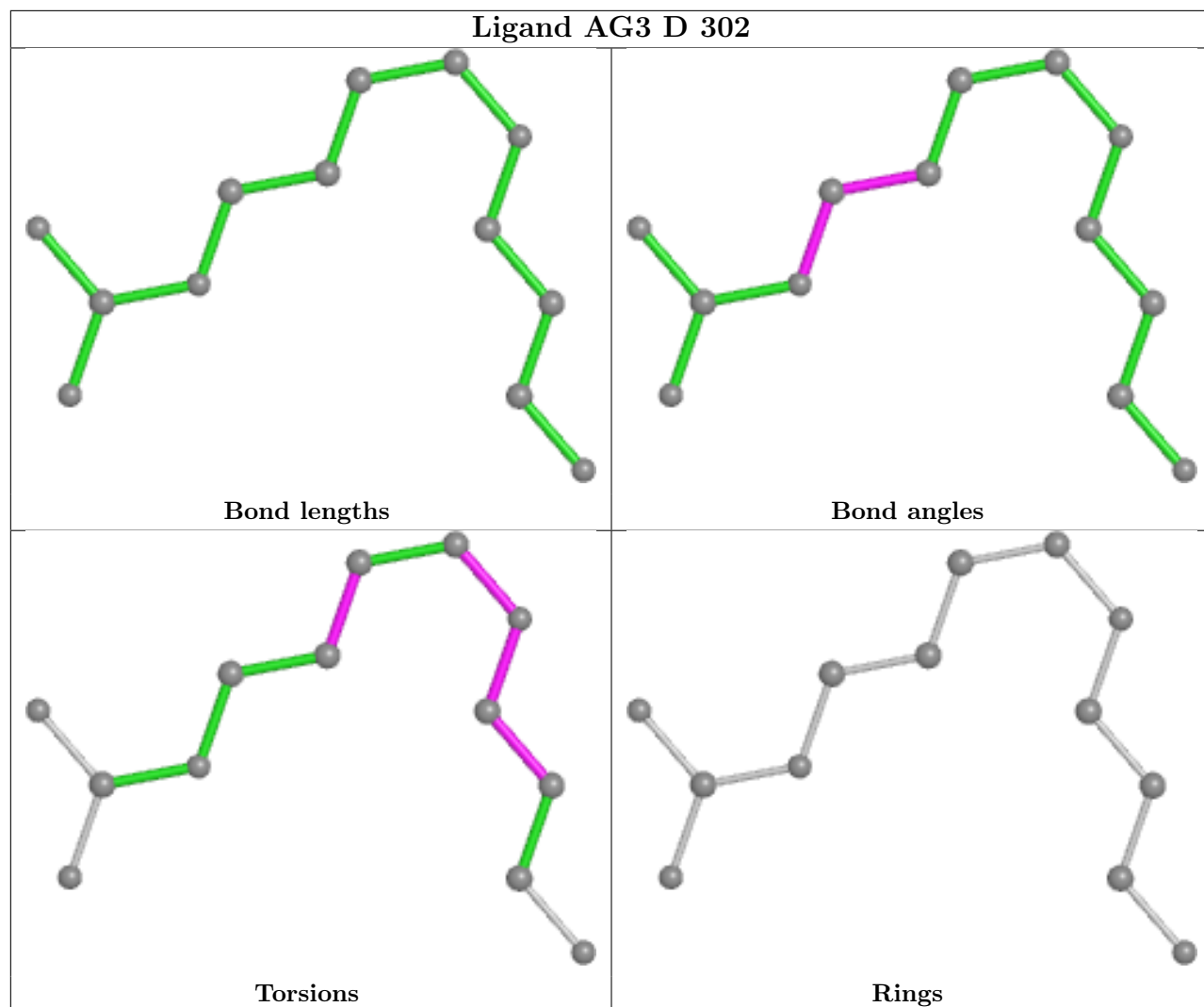
There are no ring outliers.

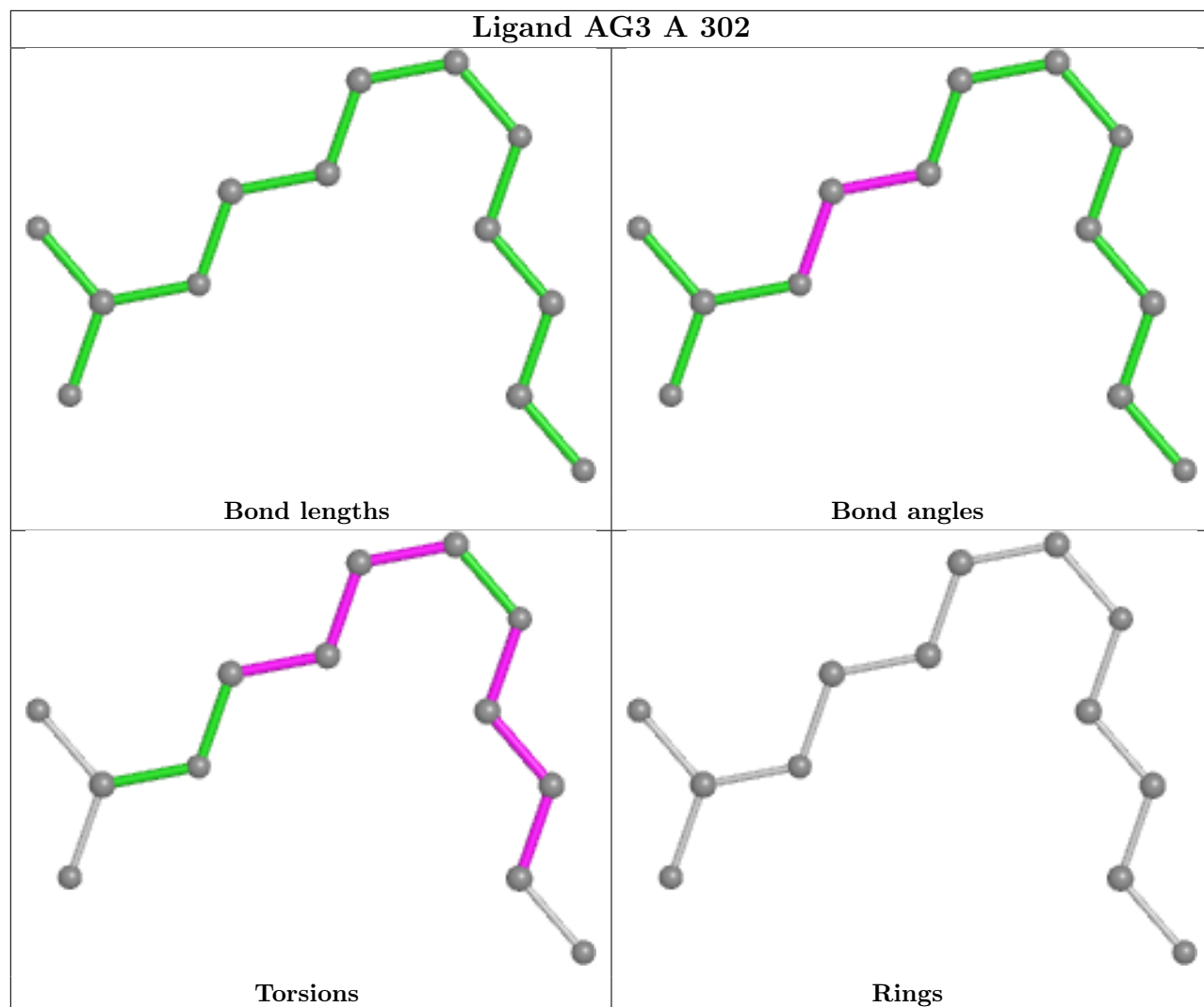
9 monomers are involved in 31 short contacts:

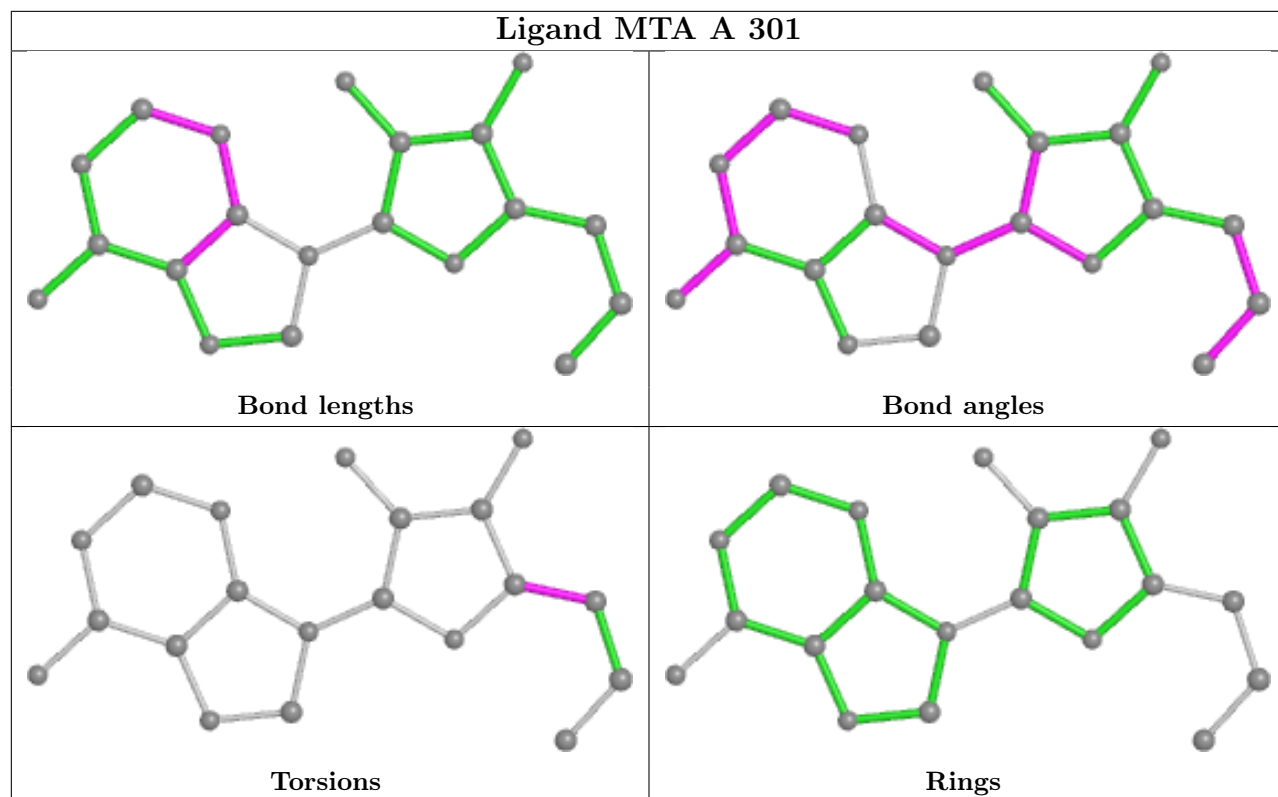
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	MTA	1	0
2	C	301	MTA	1	0
3	D	302	AG3	6	0
4	A	303	EPE	1	0
3	A	302	AG3	11	0
2	A	301	MTA	2	0
3	B	302	AG3	6	0
3	C	302	AG3	7	0
2	D	301	MTA	1	0

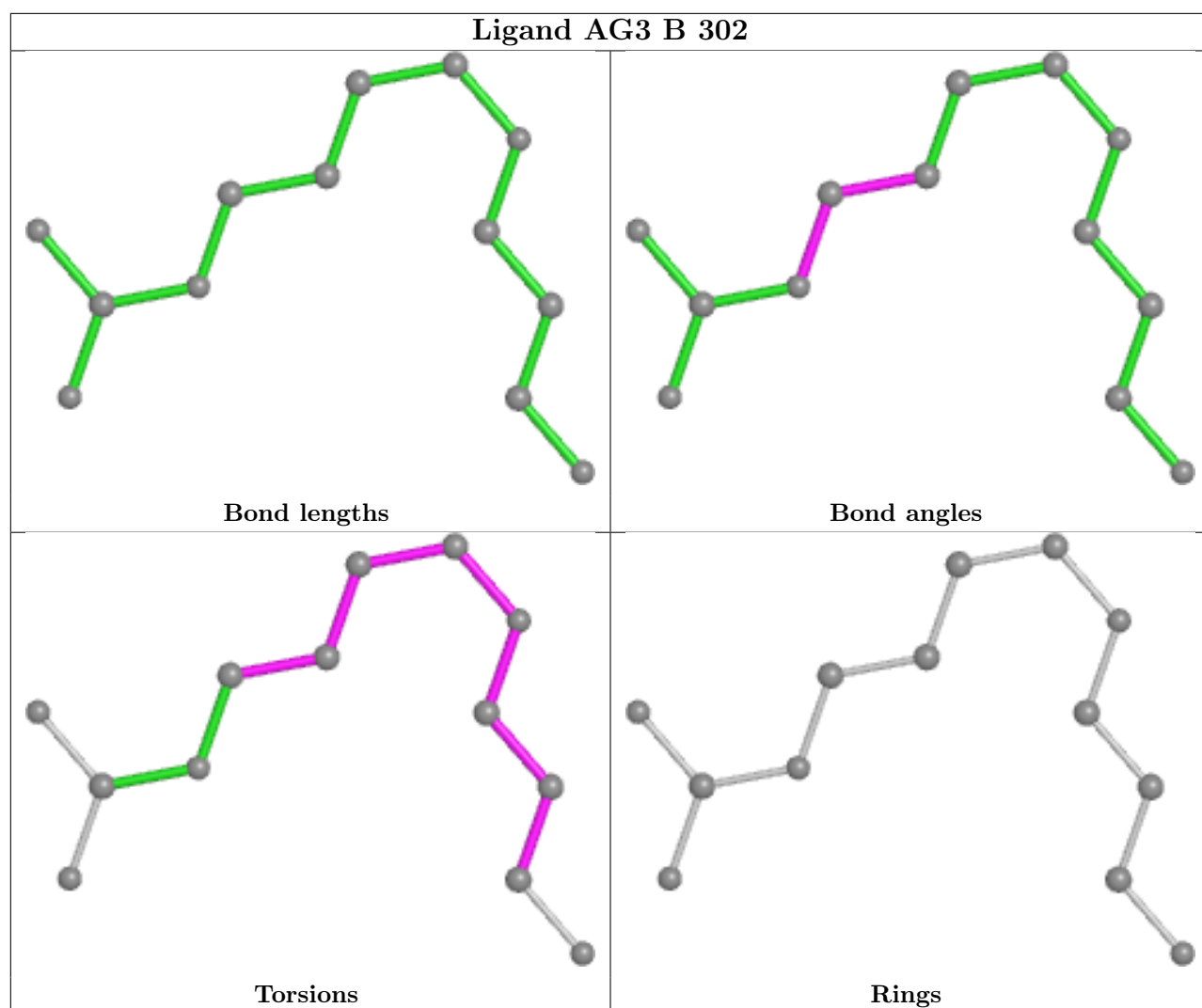
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

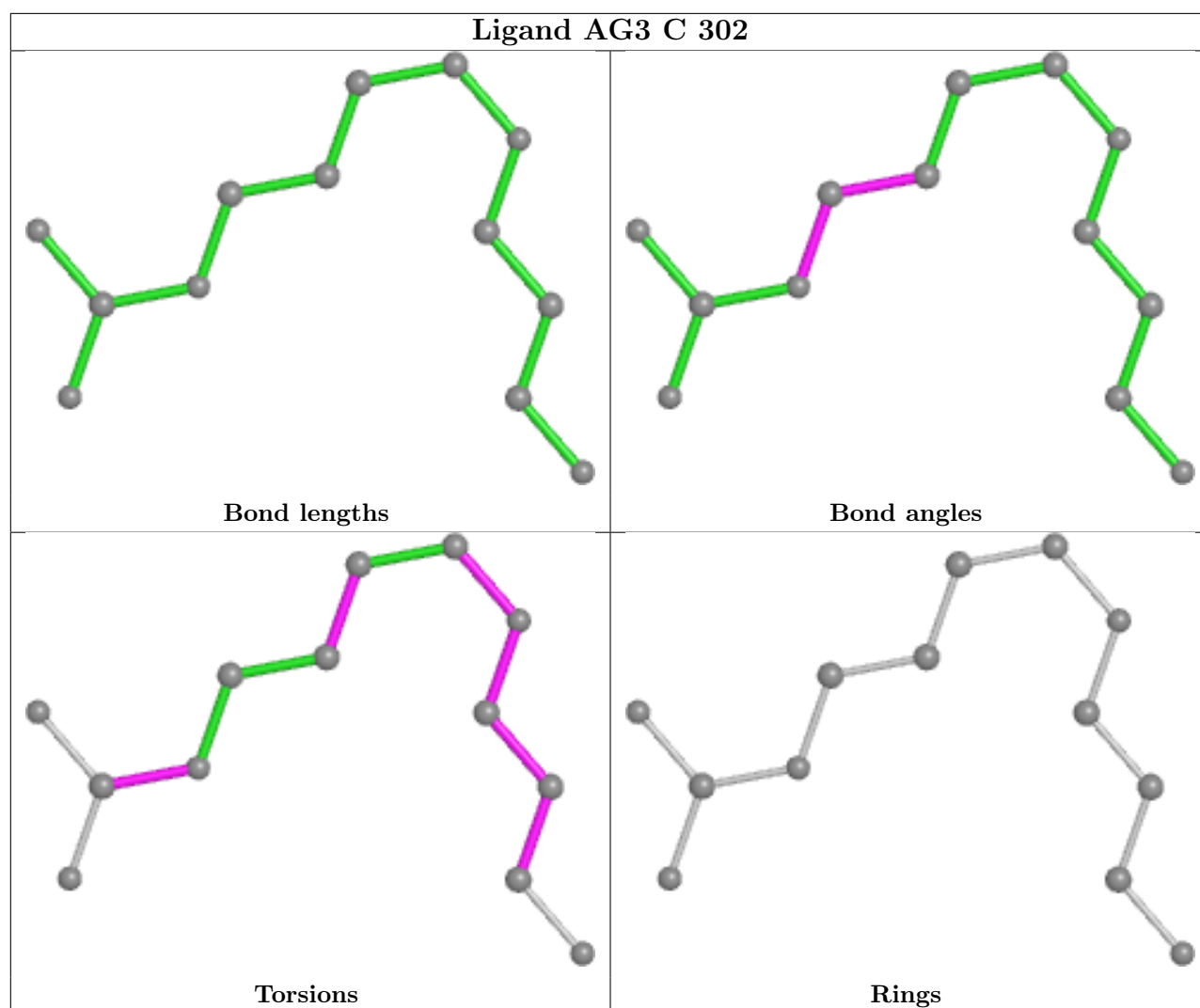


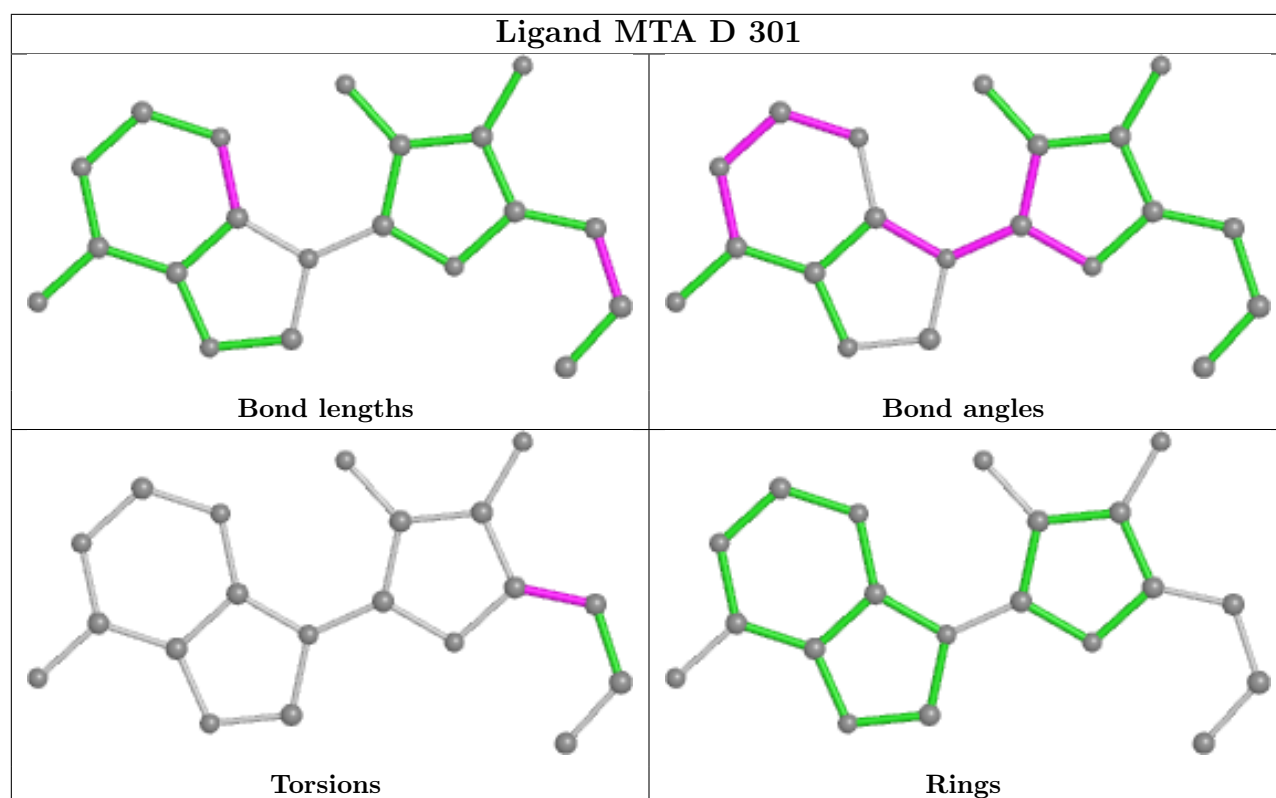












## 5.7 Other polymers [i](#)

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	286/309 (92%)	-0.73	1 (0%) 90 91	10, 20, 35, 48	0
1	B	288/309 (93%)	-0.62	0 100 100	11, 22, 43, 58	0
1	C	286/309 (92%)	-0.58	1 (0%) 90 91	11, 22, 40, 58	0
1	D	288/309 (93%)	-0.63	0 100 100	11, 22, 42, 55	0
All	All	1148/1236 (92%)	-0.64	2 (0%) 92 93	10, 22, 41, 58	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	4	VAL	3.2
1	A	4	VAL	3.1

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

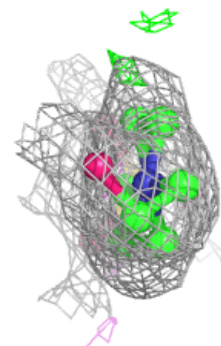
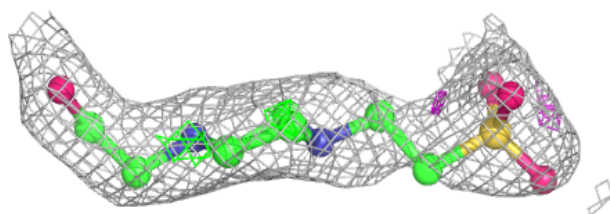
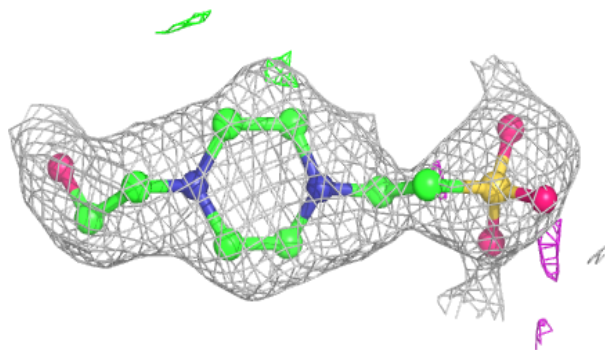
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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
4	EPE	A	303	15/15	0.88	0.12	34,40,64,69	0
3	AG3	C	302	13/13	0.94	0.08	17,21,34,36	0
3	AG3	D	302	13/13	0.95	0.08	19,25,38,40	0
3	AG3	A	302	13/13	0.95	0.09	20,26,44,44	0
3	AG3	B	302	13/13	0.96	0.08	19,22,35,38	0
2	MTA	C	301	20/20	0.97	0.05	16,19,21,23	0
2	MTA	D	301	20/20	0.98	0.04	17,21,24,25	0
2	MTA	B	301	20/20	0.98	0.04	17,18,20,24	0
2	MTA	A	301	20/20	0.98	0.04	13,15,19,22	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.

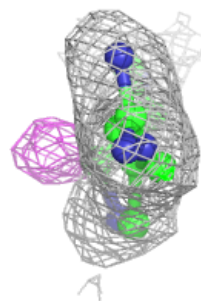
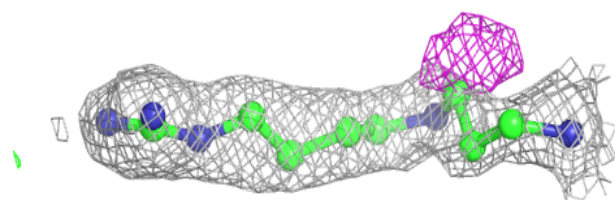
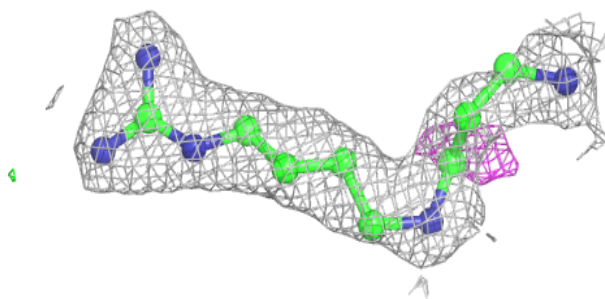
**Electron density around EPE A 303:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

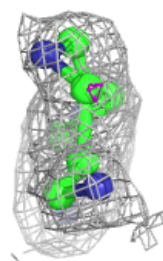
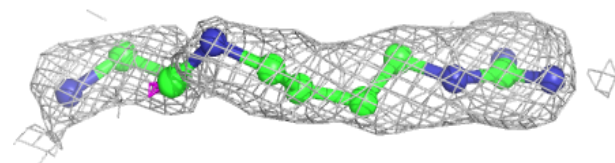
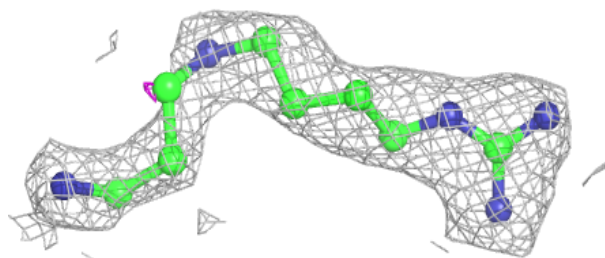


**Electron density around AG3 C 302:**

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

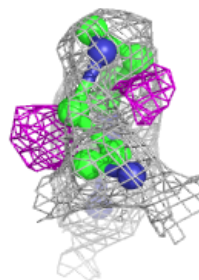
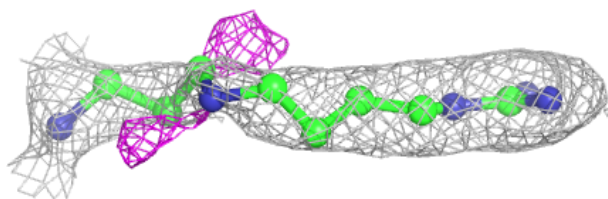
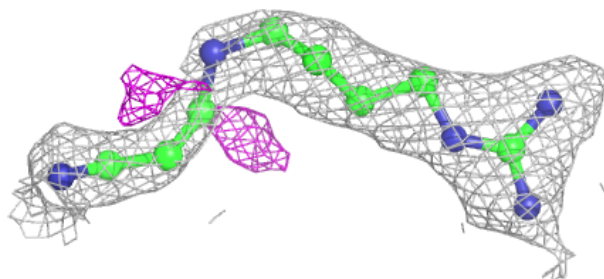
**Electron density around AG3 D 302:**

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

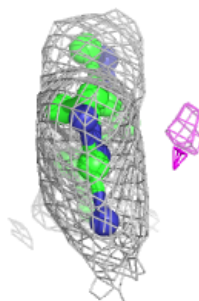
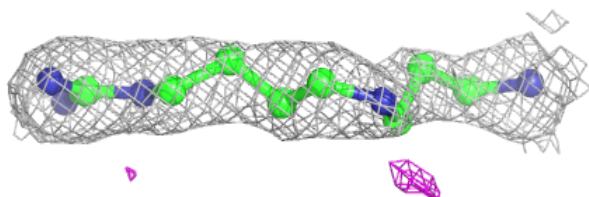
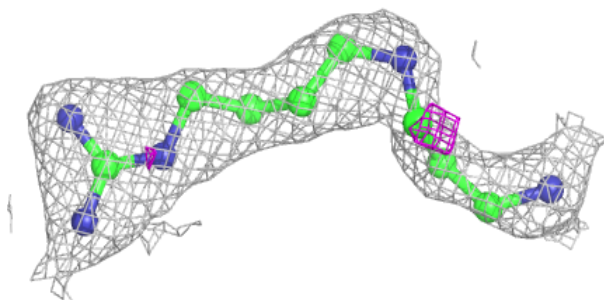


**Electron density around AG3 A 302:**

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

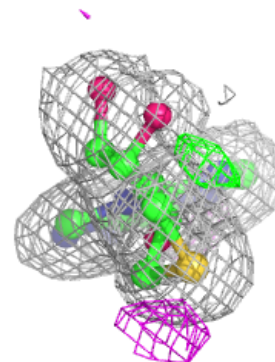
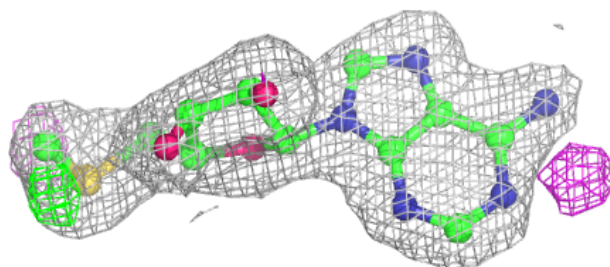
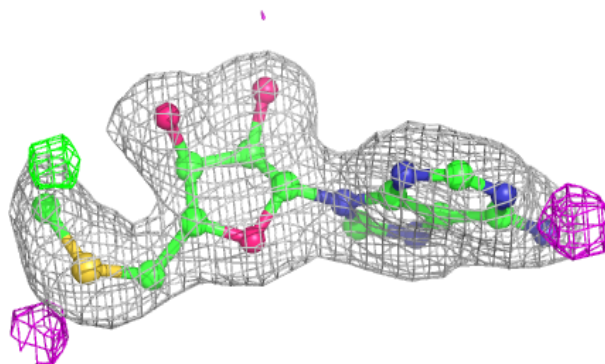
**Electron density around AG3 B 302:**

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

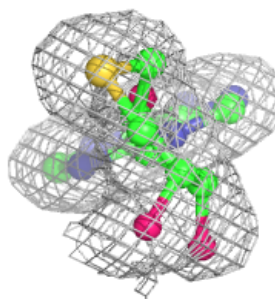
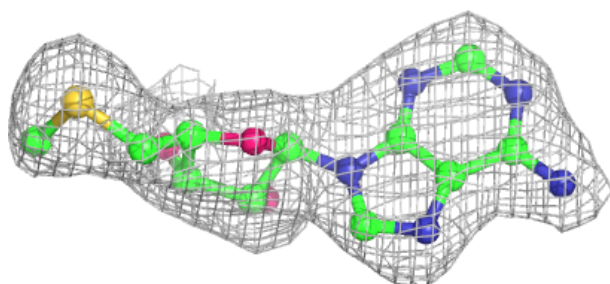
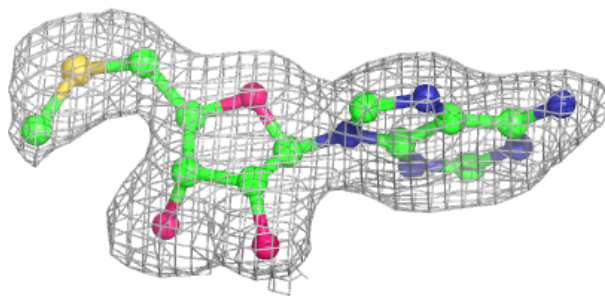


**Electron density around MTA C 301:**

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

**Electron density around MTA D 301:**

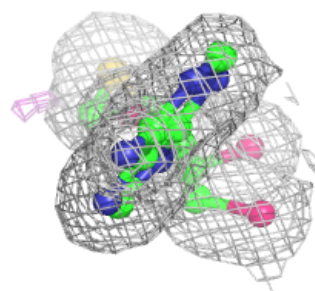
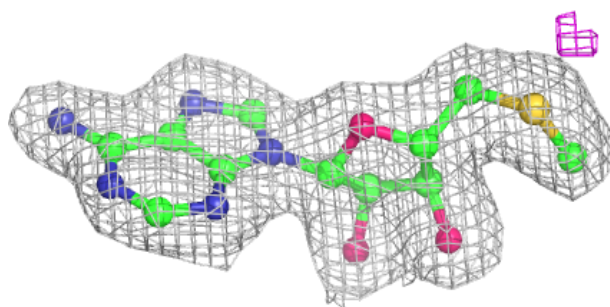
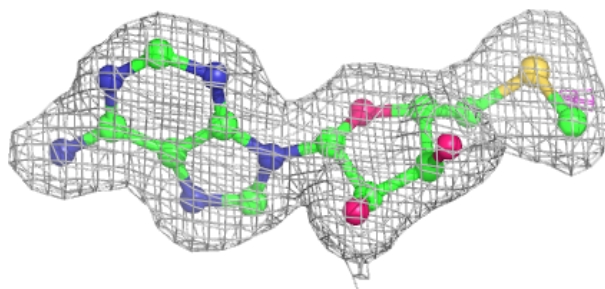
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



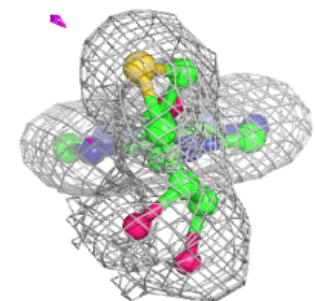
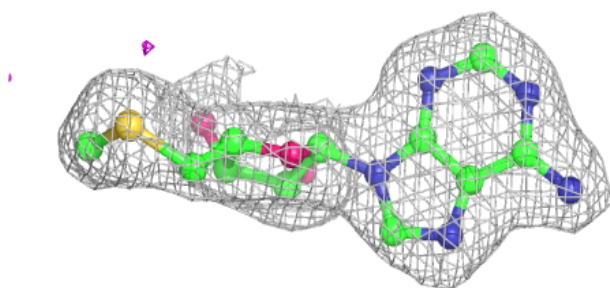
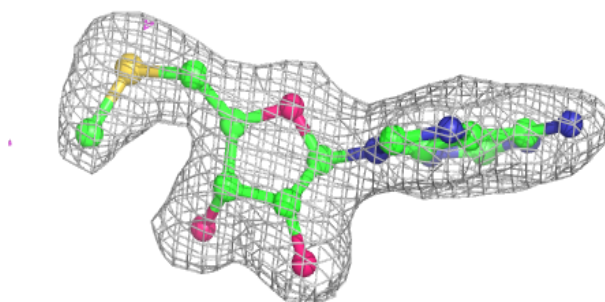


**Electron density around MTA B 301:**

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

**Electron density around MTA A 301:**

$2mF_o-DF_c$  (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.