



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:00 PM UTC

PDB ID : 9EMJ / pdb_00009emj
Title : SARS-CoV-2 methyltransferase nsp10-16 in complex with Toyocamycin and m7GpppA (Cap0-analog)
Authors : Kremling, V.; Sprenger, J.; Oberthuer, D.; Kiene, A.
Deposited on : 2024-03-08
Resolution : 1.79 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

A user guide is available at

<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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

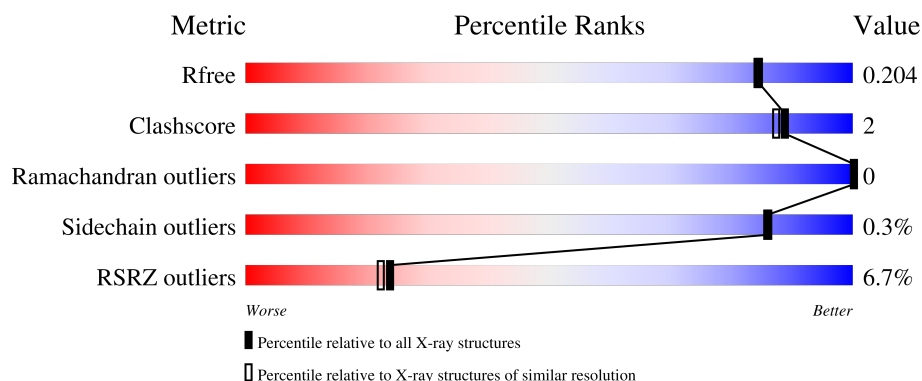
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	303	3% 94% 5%
2	B	140	13% 81% 17%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7053 atoms, of which 3291 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 2'-O-methyltransferase nsp16.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	300	Total	C	H	N	O	S	0	7	0
			4800	1533	2392	406	452	17			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6797	SER	-	expression tag	UNP P0DTD1
A	6798	ASN	-	expression tag	UNP P0DTD1
A	7097	GLU	-	expression tag	UNP P0DTD1
A	7098	ASN	-	expression tag	UNP P0DTD1
A	7099	LEU	-	expression tag	UNP P0DTD1

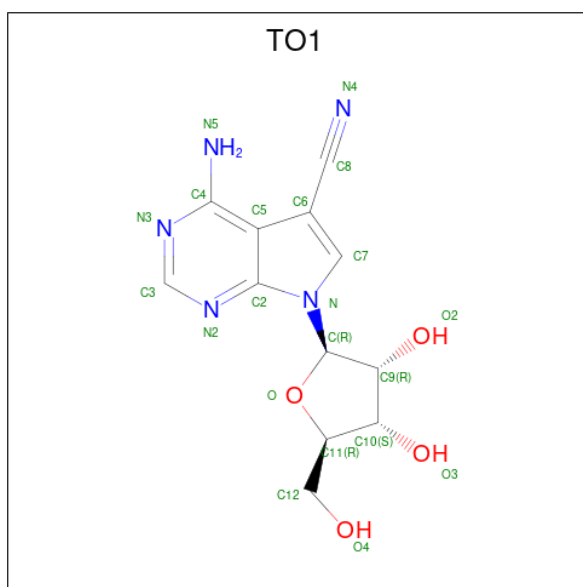
- Molecule 2 is a protein called Non-structural protein 10.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	116	Total	C	H	N	O	S	0	3	0
			1680	534	819	145	166	16			

There is a discrepancy between the modelled and reference sequences:

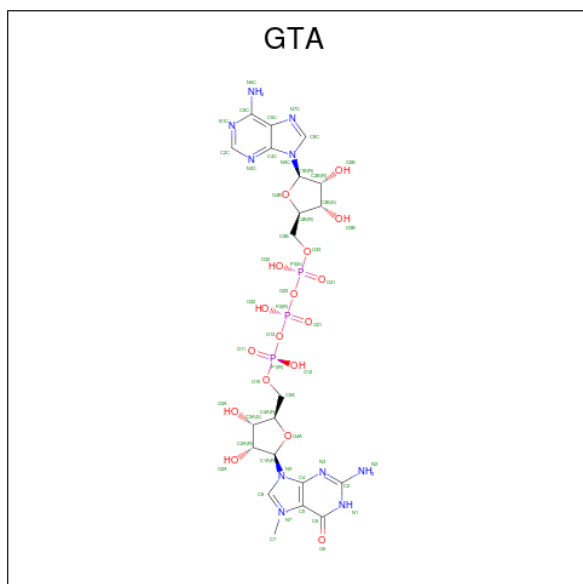
Chain	Residue	Modelled	Actual	Comment	Reference
B	4253	GLY	-	expression tag	UNP P0DTD1

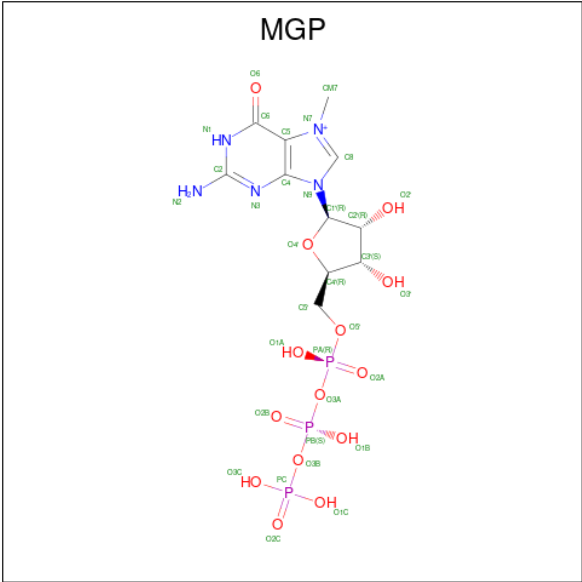
- Molecule 3 is 4-amino-7-(beta-D-ribofuranosyl)-7H-pyrrolo[2,3-d]pyrimidine-5-carbonitrile (CCD ID: TO1) (formula: C₁₂H₁₃N₅O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	1
			68	24	26	10	8		

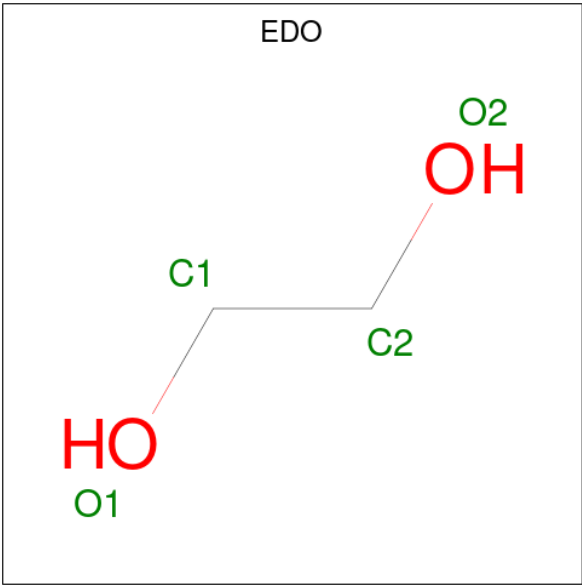
- Molecule 4 is P1-7-METHYLGUANOSINE-P3-ADENOSINE-5',5'-TRIPHOSPHATE (CCD ID: GTA) (formula: $C_{21}H_{30}N_{10}O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	A	1	Total	C	H	N	O	P	0	0
			40	11	15	5	8	1		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	H	O	0	0
			10	2	6	2		
6	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total 2	Zn 2	0	0

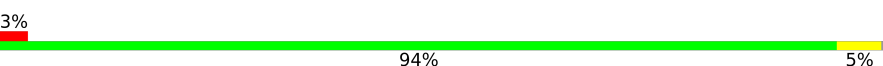
- Molecule 8 is water.

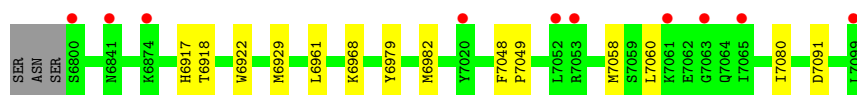
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	280	Total 280	O 280	0	0
8	B	85	Total 85	O 85	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

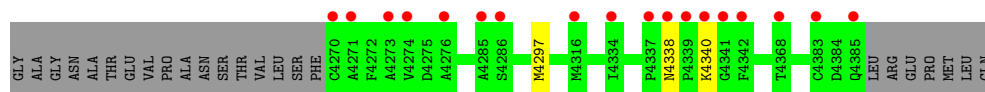
- Molecule 1: 2'-O-methyltransferase nsp16

Chain A: 



- Molecule 2: Non-structural protein 10

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.70Å 168.70Å 52.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.42 – 1.79 44.42 – 1.79	Depositor EDS
% Data completeness (in resolution range)	99.2 (44.42-1.79) 86.8 (44.42-1.79)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.33 (at 1.77Å)	Xtriage
Refinement program	PHENIX 1.19.2-4158	Depositor
R, R_{free}	0.181 , 0.207 0.181 , 0.204	Depositor DCC
R_{free} test set	1075 reflections (1.30%)	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7053	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: TO1, GTA, ZN, MGP, EDO

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	0.50	1/2465 (0.0%)	0.63	0/3343
2	B	0.39	0/893	0.59	0/1212
All	All	0.48	1/3358 (0.0%)	0.62	0/4555

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	6929	MET	SD-CE	-5.28	1.66	1.79

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	2408	2392	2381	7	0
2	B	861	819	804	3	0
3	A	42	26	23	1	0
4	A	51	27	27	0	0
5	A	25	15	13	2	0
6	B	8	12	12	0	0
7	B	2	0	0	0	0
8	A	280	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	85	0	0	0	0
All	All	3762	3291	3260	13	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 (13) 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:A:7101[B]:TO1:C	3:A:7101[B]:TO1:O	1.65	1.27
5:A:7103:MGP:C4'	5:A:7103:MGP:O4'	1.64	1.18
2:B:4338:ASN:OD1	2:B:4340:LYS:N	2.29	0.65
5:A:7103:MGP:O4'	5:A:7103:MGP:C5'	2.55	0.49
1:A:6979:TYR:O	1:A:6982:MET:HB2	2.14	0.48
1:A:7048:PHE:N	1:A:7049:PRO:CD	2.78	0.47
1:A:6918:THR:HG21	1:A:6922:TRP:HE1	1.82	0.44
1:A:7058:MET:CE	1:A:7060:LEU:HD11	2.48	0.44
1:A:6917:HIS:CE1	1:A:7091:ASP:OD2	2.72	0.43
1:A:6961:LEU:HB2	1:A:7080:ILE:HB	2.00	0.43
2:B:4338:ASN:OD1	2:B:4338:ASN:C	2.63	0.41
2:B:4297:MET:HE3	2:B:4297:MET:HB3	1.95	0.41
1:A:6917:HIS:HE1	1:A:7091:ASP:OD2	2.04	0.40

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	305/303 (101%)	298 (98%)	7 (2%)	0	100	100
2	B	117/140 (84%)	115 (98%)	2 (2%)	0	100	100
All	All	422/443 (95%)	413 (98%)	9 (2%)	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	267/263 (102%)	266 (100%)	1 (0%)	84	83
2	B	97/113 (86%)	97 (100%)	0	100	100
All	All	364/376 (97%)	363 (100%)	1 (0%)	86	86

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6968	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6917	HIS
1	A	7008	ASN
1	A	7016	GLN
1	A	7033	ASN
2	B	4289	GLN
2	B	4293	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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
5	MGP	A	7103	-	27,27,35	4.26	16 (59%)	41,42,56	1.69	9 (21%)
6	EDO	B	4404	-	3,3,3	0.60	0	2,2,2	0.15	0
4	GTA	A	7102	-	56,56,56	3.05	22 (39%)	83,88,88	1.64	15 (18%)
3	TO1	A	7101[B]	-	22,23,23	3.87	9 (40%)	29,34,34	2.41	8 (27%)
6	EDO	B	4401	-	3,3,3	0.45	0	2,2,2	0.42	0
3	TO1	A	7101[A]	-	22,23,23	3.62	9 (40%)	29,34,34	2.53	10 (34%)

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
5	MGP	A	7103	-	-	2/10/26/38	0/3/3/3
6	EDO	B	4404	-	-	0/1/1/1	-
4	GTA	A	7102	-	-	1/32/64/64	0/6/6/6
3	TO1	A	7101[B]	-	-	2/6/24/24	0/3/3/3
6	EDO	B	4401	-	-	1/1/1/1	-
3	TO1	A	7101[A]	-	-	0/6/24/24	0/3/3/3

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	7103	MGP	C3'-C4'	-10.69	1.25	1.53
3	A	7101[B]	TO1	O-C	9.94	1.65	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	7101[A]	TO1	O-C	9.19	1.63	1.42
5	A	7103	MGP	O4'-C4'	8.60	1.64	1.45
3	A	7101[B]	TO1	C8-C6	8.11	1.57	1.44
4	A	7102	GTA	C3B-C4B	-8.07	1.32	1.53
4	A	7102	GTA	O4A-C1A	7.94	1.60	1.42
3	A	7101[A]	TO1	C8-C6	7.69	1.56	1.44
4	A	7102	GTA	C2A-C1A	-7.14	1.31	1.53
4	A	7102	GTA	O4B-C4B	6.78	1.60	1.45
3	A	7101[B]	TO1	C9-C	-6.77	1.32	1.53
3	A	7101[B]	TO1	O-C11	-6.70	1.30	1.45
4	A	7102	GTA	O4A-C4A	-6.58	1.30	1.45
5	A	7103	MGP	C2'-C3'	6.54	1.71	1.53
5	A	7103	MGP	C4-N3	6.45	1.49	1.34
3	A	7101[A]	TO1	C9-C	-6.31	1.33	1.53
5	A	7103	MGP	C2'-C1'	-6.27	1.33	1.53
5	A	7103	MGP	C2-N3	6.13	1.48	1.33
3	A	7101[A]	TO1	O-C11	-5.89	1.31	1.45
4	A	7102	GTA	O4B-C1B	-5.71	1.28	1.42
3	A	7101[B]	TO1	C4-N5	5.62	1.48	1.34
5	A	7103	MGP	O4'-C1'	5.34	1.54	1.42
4	A	7102	GTA	C5-N7	-5.25	1.33	1.39
3	A	7101[A]	TO1	C4-N5	5.23	1.47	1.34
4	A	7102	GTA	C4-N3	5.15	1.46	1.34
4	A	7102	GTA	C2-N3	4.64	1.44	1.33
5	A	7103	MGP	C2-N2	4.47	1.44	1.34
5	A	7103	MGP	C5-N7	-4.27	1.34	1.39
5	A	7103	MGP	O6-C6	-4.26	1.15	1.23
4	A	7102	GTA	C6C-N6C	4.07	1.44	1.34
5	A	7103	MGP	C5-C6	3.76	1.53	1.43
4	A	7102	GTA	C2-N2	3.72	1.42	1.34
5	A	7103	MGP	C2-N1	3.27	1.45	1.37
4	A	7102	GTA	O2A-C2A	3.24	1.51	1.43
4	A	7102	GTA	O3B-C3B	3.11	1.50	1.43
5	A	7103	MGP	PA-O3A	3.11	1.66	1.54
3	A	7101[A]	TO1	O3-C10	-3.01	1.35	1.43
4	A	7102	GTA	C5-C6	2.96	1.51	1.43
3	A	7101[B]	TO1	O3-C10	-2.90	1.35	1.43
4	A	7102	GTA	C4-N9	-2.51	1.31	1.38
4	A	7102	GTA	C8C-N9C	-2.51	1.33	1.37
4	A	7102	GTA	O3A-C3A	-2.43	1.36	1.43
5	A	7103	MGP	C6-N1	2.36	1.43	1.38
3	A	7101[B]	TO1	O2-C9	2.34	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	7102	GTA	P3-O23	2.33	1.62	1.59
4	A	7102	GTA	O2B-C2B	-2.31	1.37	1.43
3	A	7101[A]	TO1	O2-C9	2.25	1.48	1.43
4	A	7102	GTA	P1-O13	2.24	1.61	1.59
3	A	7101[A]	TO1	C10-C11	2.20	1.58	1.53
5	A	7103	MGP	C4-N9	-2.17	1.32	1.38
3	A	7101[B]	TO1	C10-C11	2.15	1.58	1.53
3	A	7101[A]	TO1	C8-N4	-2.11	1.11	1.14
5	A	7103	MGP	O3'-C3'	2.09	1.48	1.43
3	A	7101[B]	TO1	C3-N3	-2.05	1.30	1.33
4	A	7102	GTA	O6-C6	-2.03	1.19	1.23
4	A	7102	GTA	C5C-N7C	-2.01	1.35	1.39

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	7101[A]	TO1	C5-C2-N2	-8.38	118.08	126.97
3	A	7101[B]	TO1	C5-C2-N2	-7.59	118.91	126.97
3	A	7101[A]	TO1	C4-C5-C2	5.25	119.67	115.74
4	A	7102	GTA	N3C-C2C-N1C	-5.05	120.94	128.58
4	A	7102	GTA	C5C-C4C-N3C	-4.64	120.32	126.72
3	A	7101[B]	TO1	N3-C3-N2	-4.54	121.72	128.58
3	A	7101[B]	TO1	C2-N-C7	4.35	109.88	108.08
5	A	7103	MGP	C5-C6-N1	4.14	120.41	111.84
5	A	7103	MGP	O6-C6-C5	-4.10	118.85	128.01
3	A	7101[B]	TO1	C4-C5-C2	3.94	118.69	115.74
3	A	7101[A]	TO1	N3-C3-N2	-3.89	122.69	128.58
3	A	7101[B]	TO1	C3-N2-C2	3.79	121.09	111.83
5	A	7103	MGP	C2-N3-C4	3.77	118.80	112.30
4	A	7102	GTA	C2C-N3C-C4C	3.71	120.89	111.83
3	A	7101[A]	TO1	C3-N2-C2	3.62	120.68	111.83
3	A	7101[A]	TO1	C12-C11-C10	-3.36	107.15	115.10
4	A	7102	GTA	N3C-C4C-N9C	3.32	132.82	127.17
4	A	7102	GTA	N9C-C8C-N7C	-3.25	109.32	113.94
3	A	7101[A]	TO1	N2-C2-N	3.22	132.64	127.17
5	A	7103	MGP	C5-C4-N3	-3.17	122.15	128.15
4	A	7102	GTA	C7-N7-C5	-3.12	122.91	126.80
4	A	7102	GTA	C4C-N9C-C8C	3.02	108.91	105.74
3	A	7101[B]	TO1	C11-O-C	-3.01	102.82	109.47
3	A	7101[B]	TO1	N2-C2-N	2.85	132.02	127.17
5	A	7103	MGP	C2-N1-C6	-2.84	119.96	125.11
5	A	7103	MGP	C2'-C1'-N9	-2.75	105.60	113.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	7102	GTA	O12-P1-O13	2.71	114.59	107.27
5	A	7103	MGP	C4'-O4'-C1'	-2.68	103.54	109.47
3	A	7101[A]	TO1	O-C11-C12	2.63	114.78	109.22
4	A	7102	GTA	C5-C4-N3	-2.61	123.21	128.15
3	A	7101[A]	TO1	C2-N-C7	2.53	109.12	108.08
4	A	7102	GTA	C7-N7-C8	2.45	128.51	124.79
4	A	7102	GTA	C4C-C5C-N7C	-2.45	107.78	110.58
5	A	7103	MGP	O3A-PA-O5'	2.39	112.91	106.67
5	A	7103	MGP	N9-C4-N3	2.36	130.68	125.95
4	A	7102	GTA	C5C-N7C-C8C	2.34	107.12	103.45
4	A	7102	GTA	C3A-C2A-C1A	2.33	105.88	101.46
3	A	7101[B]	TO1	C12-C11-C10	-2.29	109.69	115.10
3	A	7101[A]	TO1	C10-C9-C	2.19	105.61	101.46
4	A	7102	GTA	C2B-C1B-N9C	-2.09	108.12	113.30
4	A	7102	GTA	C2-N3-C4	2.08	115.88	112.30
3	A	7101[A]	TO1	O-C-C9	-2.03	102.26	106.62

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	7102	GTA	C5A-O15-P1-O11
5	A	7103	MGP	O4'-C4'-C5'-O5'
3	A	7101[B]	TO1	O-C11-C12-O4
5	A	7103	MGP	C3'-C4'-C5'-O5'
3	A	7101[B]	TO1	C10-C11-C12-O4
6	B	4401	EDO	O1-C1-C2-O2

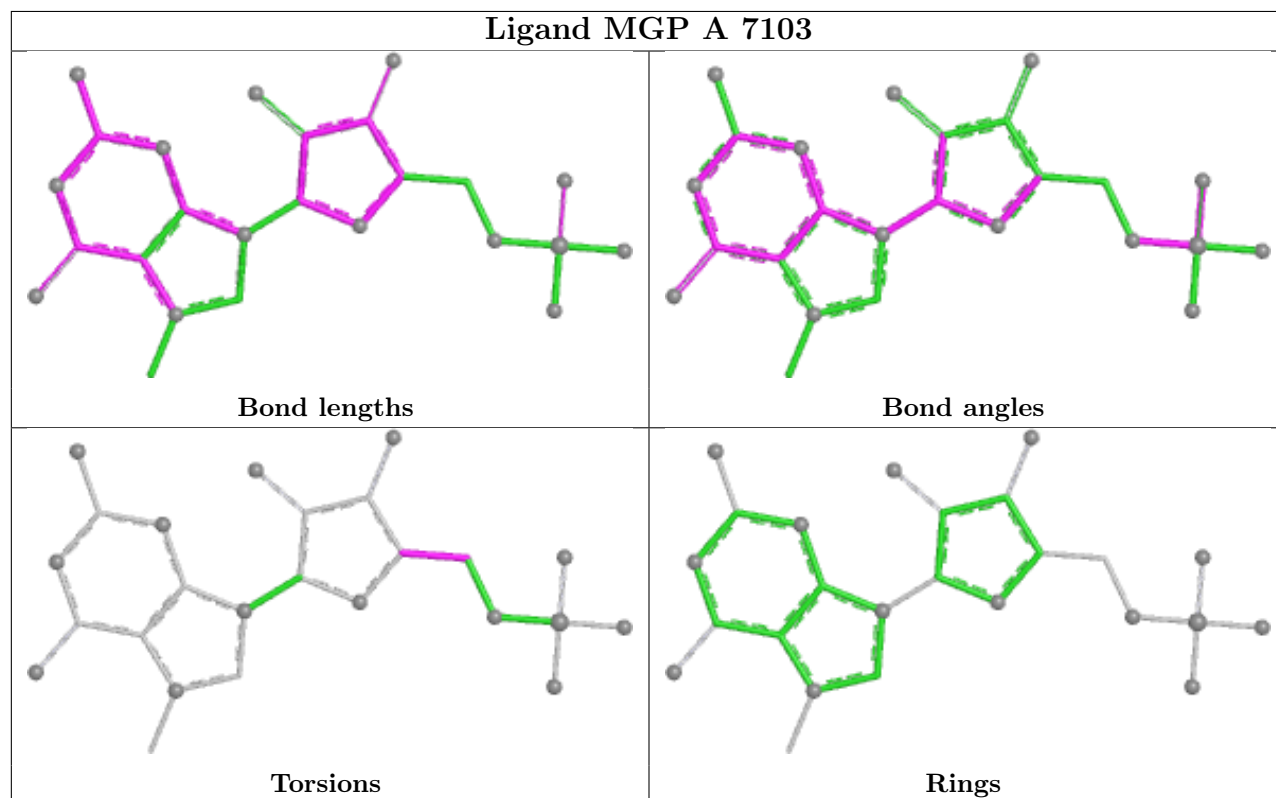
There are no ring outliers.

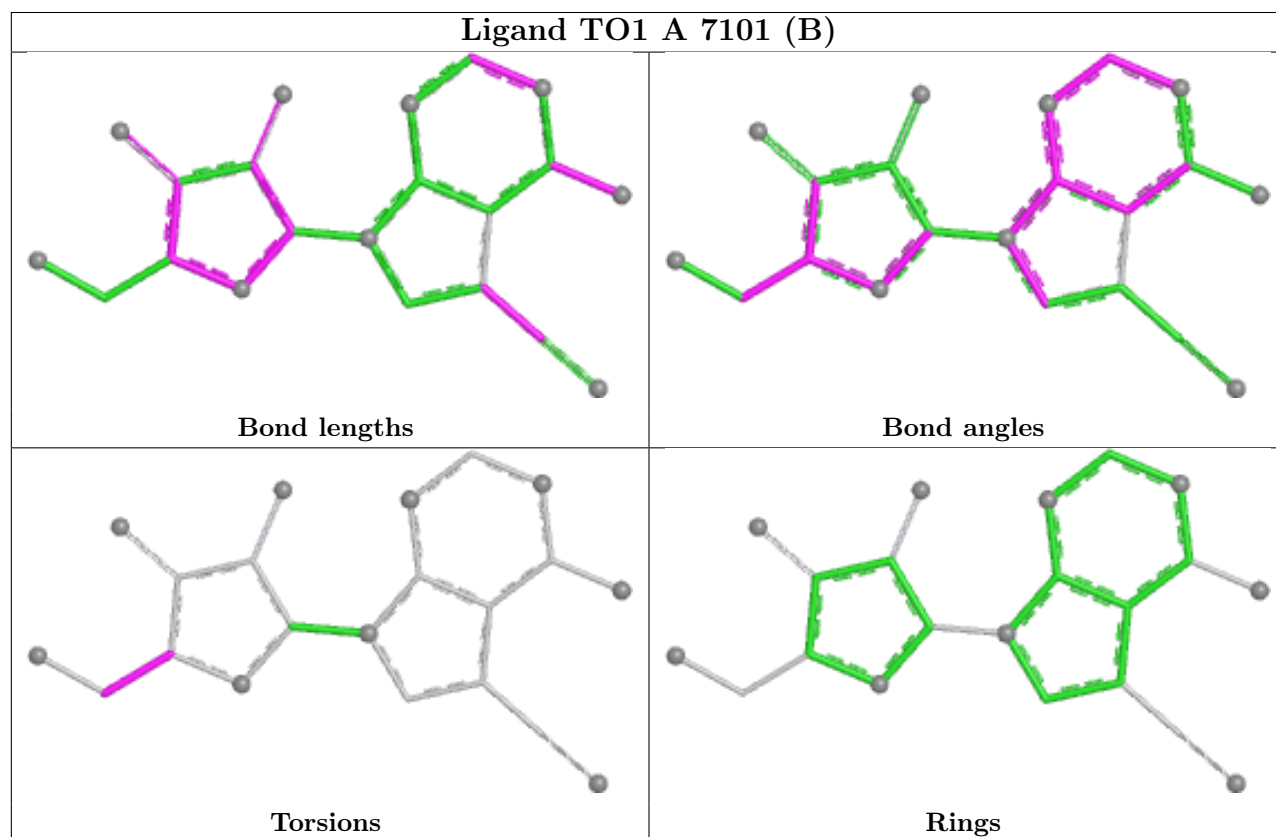
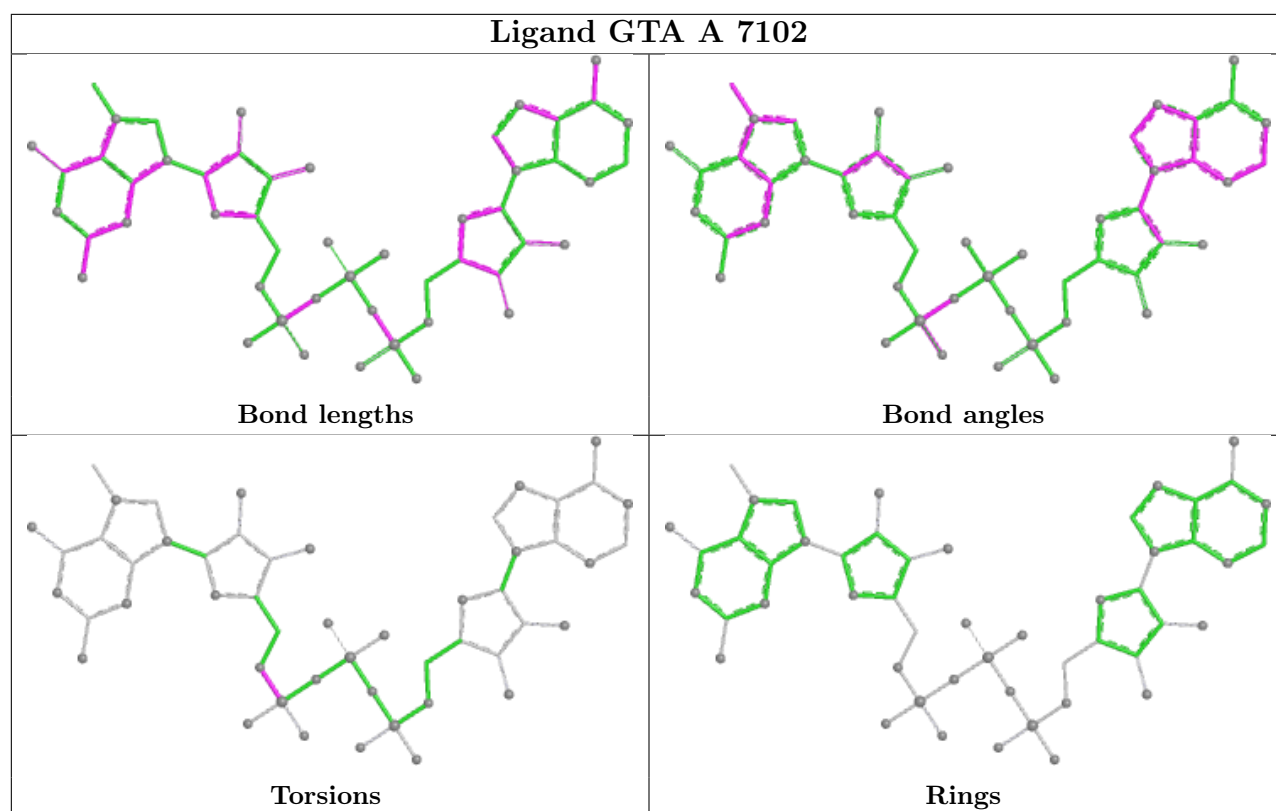
2 monomers are involved in 3 short contacts:

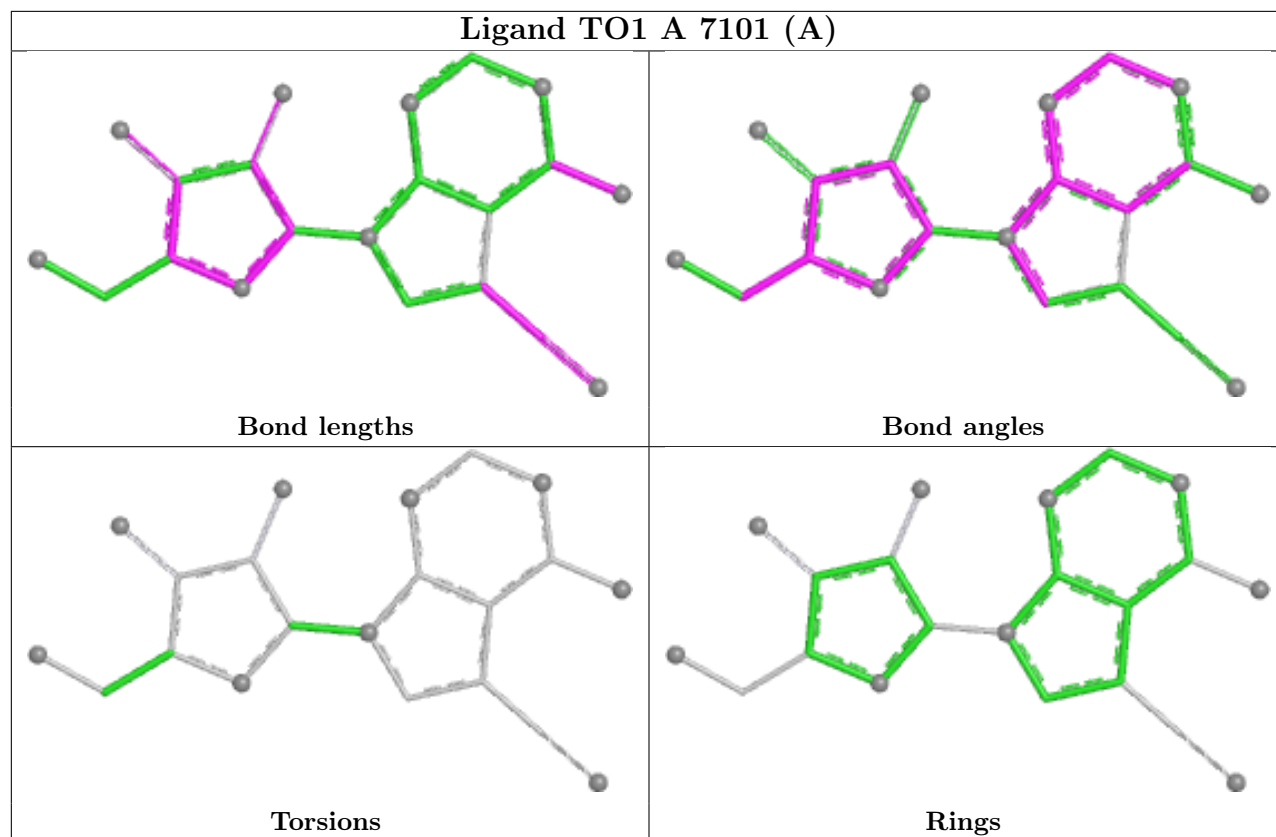
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	7103	MGP	2	0
3	A	7101[B]	TO1	1	0

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

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	300/303 (99%)	-0.11	10 (3%) 49 49	15, 32, 62, 103	6 (2%)
2	B	116/140 (82%)	0.58	18 (15%) 5 4	23, 42, 73, 104	1 (0%)
All	All	416/443 (93%)	0.08	28 (6%) 24 22	15, 35, 69, 104	7 (1%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7099	LEU	9.7
2	B	4270	CYS	4.0
2	B	4385	GLN	4.0
2	B	4342	PHE	3.9
2	B	4339	PRO	3.6
2	B	4340	LYS	3.4
2	B	4338	ASN	3.3
1	A	7061	LYS	3.1
1	A	7052	LEU	3.1
2	B	4271	ALA	2.9
2	B	4316	MET	2.9
1	A	6800	SER	2.8
2	B	4274	VAL	2.7
2	B	4341	GLY	2.7
2	B	4285	ALA	2.7
1	A	7063	GLY	2.5
1	A	7065	ILE	2.5
1	A	7053[A]	ARG	2.4
1	A	7020	TYR	2.4
2	B	4334	ILE	2.3
2	B	4286	SER	2.3
2	B	4337	PRO	2.2
2	B	4276	ALA	2.1
2	B	4383	CYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	6841[A]	ASN	2.1
2	B	4368[A]	THR	2.1
2	B	4273	ALA	2.0
1	A	6874	LYS	2.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

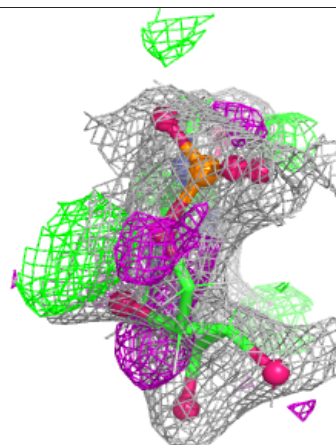
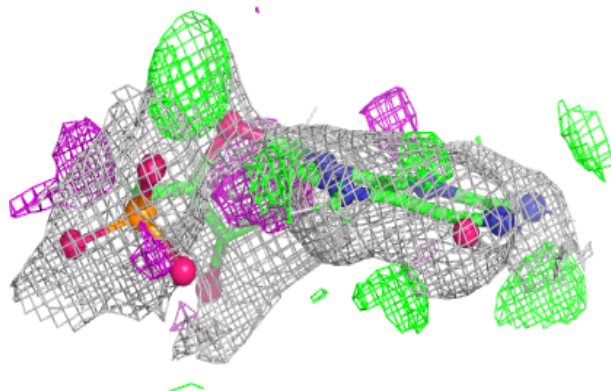
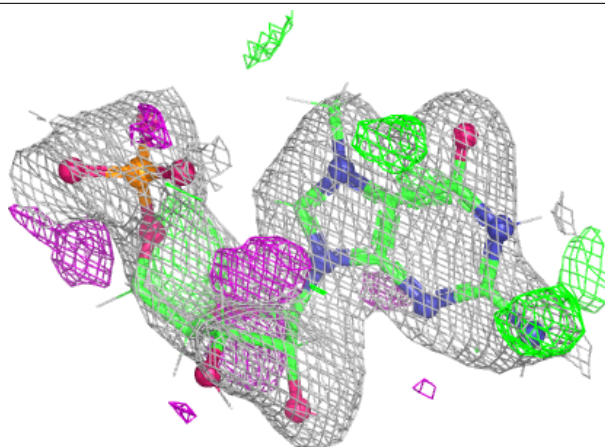
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EDO	B	4401	4/4	0.81	0.26	46,60,72,73	0
5	MGP	A	7103	25/33	0.82	0.18	35,71,98,106	0
6	EDO	B	4404	4/4	0.87	0.17	55,66,78,81	0
3	TO1	A	7101[B]	21/21	0.95	0.07	23,29,35,36	34
3	TO1	A	7101[A]	21/21	0.95	0.07	22,29,36,43	34
7	ZN	B	4403	1/1	0.96	0.06	48,48,48,48	0
4	GTA	A	7102	51/51	0.98	0.07	21,33,61,73	0
7	ZN	B	4402	1/1	0.99	0.03	34,34,34,34	0

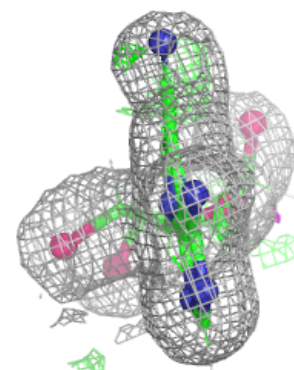
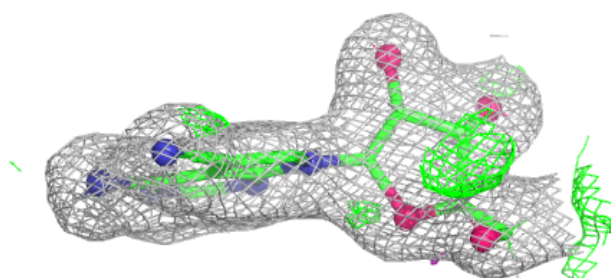
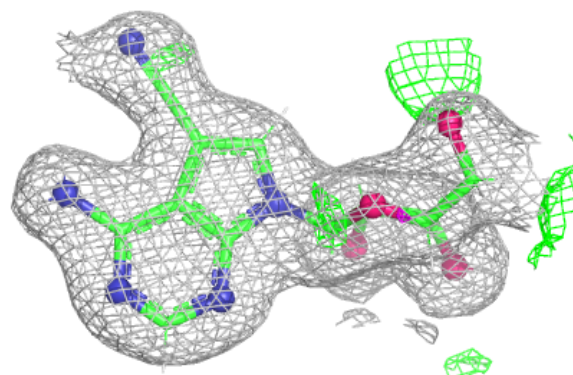
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MGP A 7103:

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

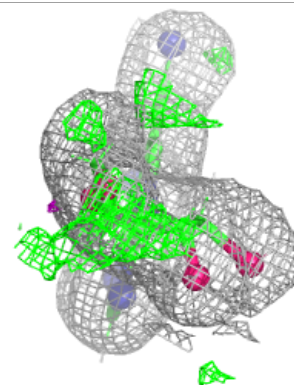
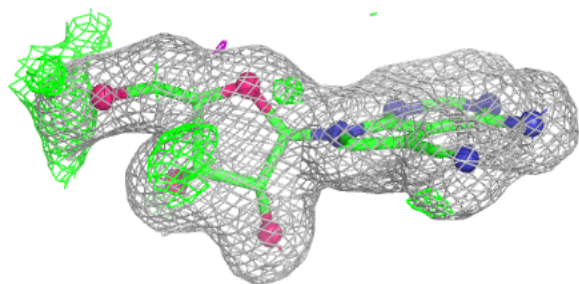
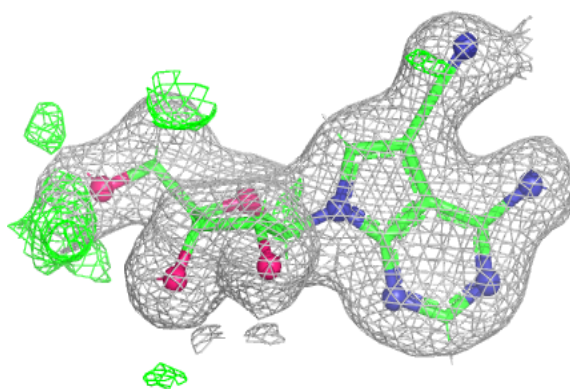
**Electron density around TO1 A 7101 (B):**

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

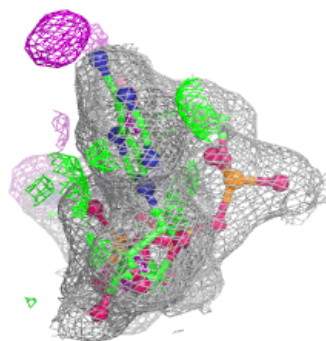
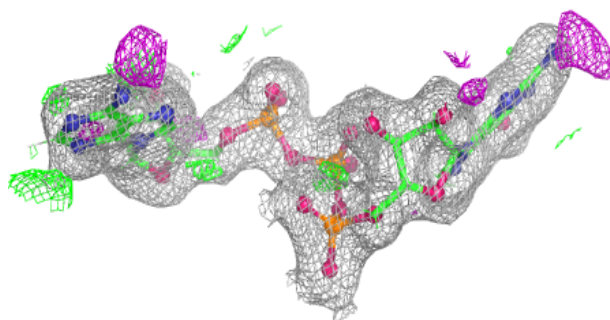
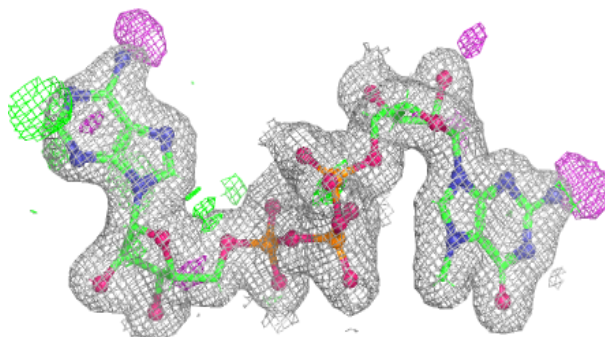


Electron density around TO1 A 7101 (A):

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

**Electron density around GTA A 7102:**

$2mF_o-DF_c$ (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.