WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 9, 2023 – 10:41 PM EDT

PDB ID	:	7LNF
Title	:	3'-deoxy modification at 3' end of RNA primer complex with guanosine dinucleotide ligand G(5')ppp(5')G
Authors	:	Fang, Z.; Giurgiu, C.; Szostak, J.W.
Deposited on	:	2021-02-07
Resolution	:	1.65 Å(reported)

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

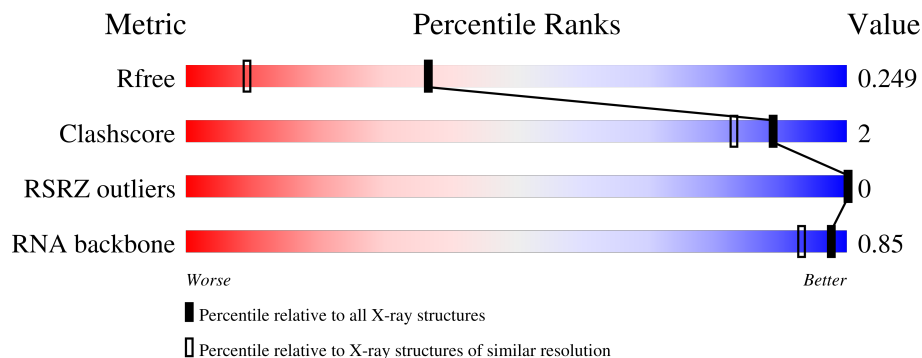|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.65 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	Percentile Ranks	Value
Rfree		0.249
Clashscore		2
RSRZ outliers		0
RNA backbone		0.85

Worse *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)
RNA backbone	3102	1011 (2.36-0.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

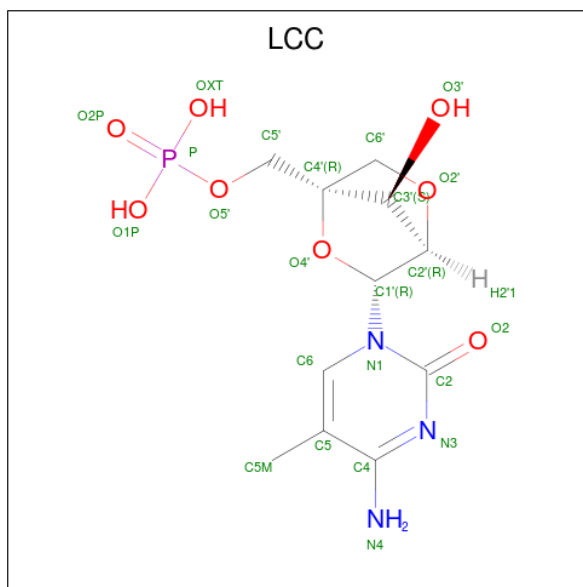| Mol	Chain	Length	Quality of chain
1	A	14	64% 36%
1	B	14	64% 36%

2 Entry composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 831 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 RNA chain called RNA (5'-R(*(LCC)P*(LCC)P*(LCC)P*(LCG)P*AP*CP *UP*UP*AP*AP*GP*UP*CP*(GDO))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	9	Total	C	N	O	P	0	0	0
			189	85	32	63	9			
1	B	9	Total	C	N	O	P	0	0	0
			189	85	32	63	9			

- Molecule 2 is [(1R,3R,4R,7S)-7-HYDROXY-3-(5-METHYLCYTOSIN-1-YL)-2,5-DIOXA BICYCLO[2.2.1]HEPT-1-YL]METHYL DIHYDROGEN PHOSPHATE (three-letter code: LCC) (formula: $C_{11}H_{16}N_3O_8P$).
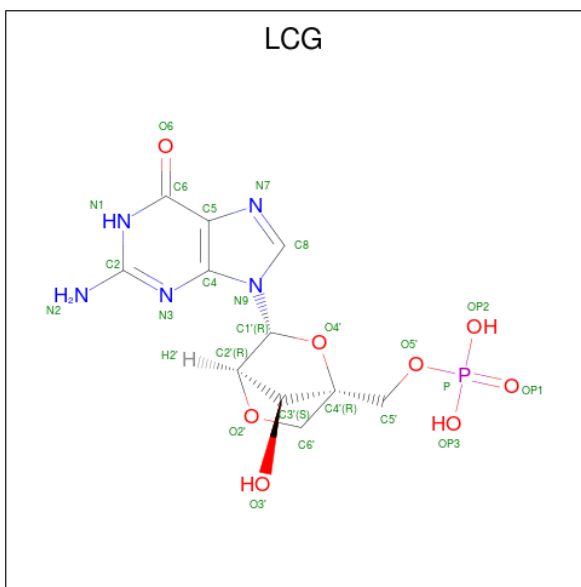

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	11	3	7	1		
2	A	1	Total	C	N	O	P	0	0
			22	11	3	7	1		
2	B	1	Total	C	N	O	P	0	0
			22	11	3	7	1		

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WORLDWIDE
PDB
PROTEIN DATA BANK

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	B	1	22	11	3	7	1	0	0

- Molecule 3 is [(1R,3R,4R,7S)-7-HYDROXY-3-(GUANIN-9-YL)-2,5-DIOXABICYCLO[2.2.1]HEPT-1-YL]METHYL DIHYDROGEN PHOSPHATE (three-letter code: LCG) (formula: $C_{11}H_{14}N_5O_8P$).
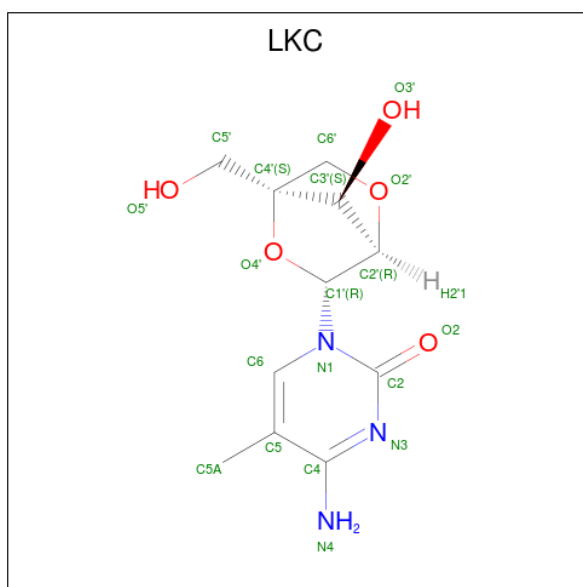

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	24	11	5	7	1	0	0
3	B	1	24	11	5	7	1	0	0

- Molecule 4 is 3'-deoxy-guanosine 5'-monophosphate (three-letter code: GDO) (formula: $C_{10}H_{14}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).

GDO
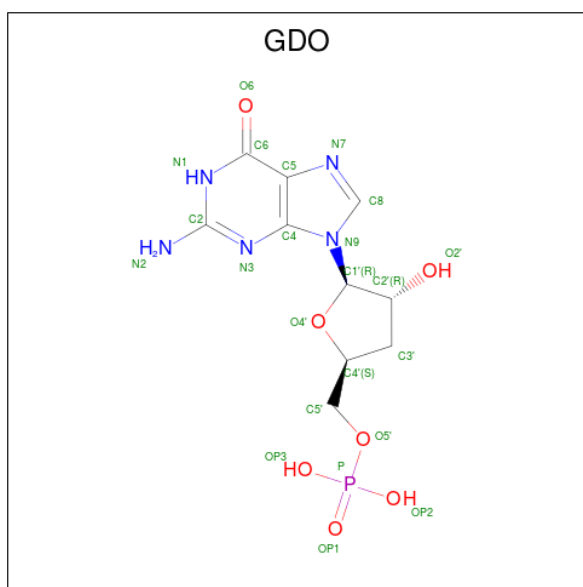
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
4	B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

- Molecule 5 is 4-AMINO-1-[(1S,3R,4R,7S)-7-HYDROXY-1-(HYDROXYMETHYL)-2,5-DIO
 XABICYCLO[2.2.1]HEPT-3-YL]-5-METHYLPYRIMIDIN-2(1H)-ONE (three-letter code:
  LKC) (formula: $C_{11}H_{15}N_3O_5$).

LKC

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			19	11	3	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total 19	C 11	N 3	O 5	0	0

- Molecule 6 is DIGUANOSINE-5'-TRIPHOSPHATE (three-letter code: GP3) (formula: $C_{20}H_{27}N_{10}O_{18}P_3$) (labeled as "Ligand of Interest" by depositor).
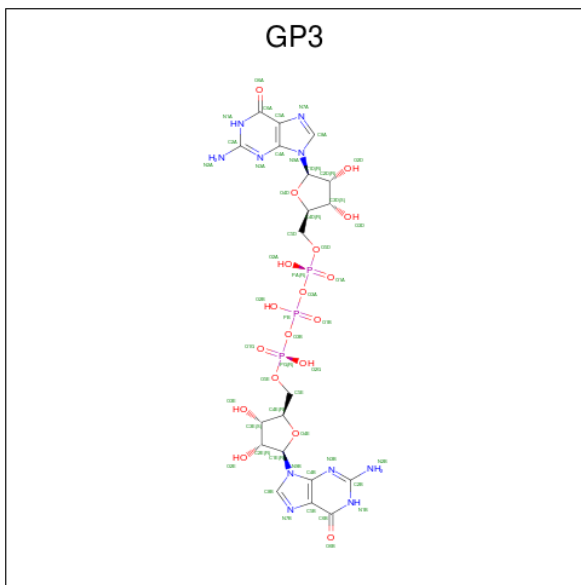
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 51	C 20	N 10	O 18	P 3	0	0
6	B	1	Total 51	C 20	N 10	O 18	P 3	0	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	4	Total 4	Mg 4	0	0
7	B	4	Total 4	Mg 4	0	0

- Molecule 8 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total 1	Co 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total 1	Co 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	60	Total 60	O 60	0	0
9	B	63	Total 63	O 63	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: RNA (5'-R(*(LCC)P*(LCC)P*(LCC)P*(LCG)P*AP*CP*UP*UP*AP*AP*GP*U P*CP*(GDO))-3')

Chain A:

• Molecule 1: RNA (5'-R(*(LCC)P*(LCC)P*(LCC)P*(LCG)P*AP*CP*UP*UP*AP*AP*GP*U P*CP*(GDO))-3')

Chain B:
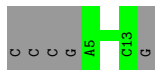
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α, β, γ	46.82Å 46.82Å 83.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.75 – 1.65 27.73 – 1.65	Depositor EDS
% Data completeness (in resolution range)	89.0 (27.75-1.65) 89.0 (27.73-1.65)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.32 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.208 , 0.239 0.212 , 0.249	Depositor DCC
R_{free} test set	553 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å^2)	9.0	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 34.4	EDS
L-test for twinning[2]	$< |L| > = 0.52, < L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.466 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	831	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.68% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GP3, LCG, MG, LCC, GDO, LKC, CO

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	0.57	0/210	0.94	0/324
1	B	0.56	0/210	0.94	0/324
All	All	0.57	0/420	0.94	0/648

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	189	0	96	0	0
1	B	189	0	96	0	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
3	A	24	0	11	0	0
3	B	24	0	11	0	0
4	A	22	0	13	0	0
4	B	22	0	13	0	0
5	A	19	0	14	0	0
5	B	19	0	14	0	0
6	A	51	0	22	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	51	0	22	1	0
7	A	4	0	0	0	0
7	B	4	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	60	0	0	1	0
9	B	63	0	0	1	0
All	All	831	0	364	2	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 (2) 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)
6:B:103:GP3:N7A	9:B:201:HOH:O	2.33	0.54
6:A:106:GP3:N7A	9:A:201:HOH:O	2.35	0.47

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein molecules in this entry.

5.3.2 Protein sidechains ⓘ

There are no protein molecules in this entry.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	8/14 (57%)	0	0
1	B	8/14 (57%)	0	0
All	All	16/28 (57%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 10 are monoatomic - leaving 12 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	$\#|Z| > 2$
2	LCC	B	104	2,3	20,24,25	2.74	10 (50%)	28,37,40	1.89	6 (21%)
5	LKC	A	104	2	20,21,21	1.94	5 (25%)	30,33,33	1.70	6 (20%)
6	GP3	B	103	7,8	44,56,56	2.02	11 (25%)	49,88,88	1.63	9 (18%)
2	LCC	A	101	2,3	20,24,25	2.44	8 (40%)	28,37,40	1.86	8 (28%)
4	GDO	B	106	1	17,24,25	2.25	4 (23%)	16,35,38	2.49	7 (43%)
2	LCC	A	105	2,5	20,24,25	1.99	4 (20%)	28,37,40	1.49	7 (25%)
3	LCG	A	102	1,2	19,27,28	2.14	7 (36%)	22,42,45	1.76	6 (27%)
3	LCG	B	105	1,2	19,27,28	2.41	7 (36%)	22,42,45	1.63	5 (22%)
5	LKC	B	101	2	20,21,21	1.84	4 (20%)	30,33,33	1.74	7 (23%)
6	GP3	A	106	7,8	44,56,56	1.91	8 (18%)	49,88,88	1.69	11 (22%)
4	GDO	A	103	1	17,24,25	2.36	6 (35%)	16,35,38	2.34	7 (43%)
2	LCC	B	102	2,5	20,24,25	2.19	5 (25%)	28,37,40	1.54	6 (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	LCC	B	104	2,3	-	0/8/35/36	0/4/3/3
5	LKC	A	104	2	-	0/7/32/32	0/4/3/3
6	GP3	B	103	7,8	-	1/24/64/64	0/6/6/6
2	LCC	A	101	2,3	-	0/8/35/36	0/4/3/3
4	GDO	B	106	1	-	0/3/21/22	0/3/3/3
2	LCC	A	105	2,5	-	0/8/35/36	0/4/3/3
3	LCG	A	102	1,2	-	0/4/35/36	0/5/4/4
3	LCG	B	105	1,2	-	0/4/35/36	0/5/4/4
5	LKC	B	101	2	-	0/7/32/32	0/4/3/3
6	GP3	A	106	7,8	-	2/24/64/64	0/6/6/6
4	GDO	A	103	1	-	0/3/21/22	0/3/3/3
2	LCC	B	102	2,5	-	0/8/35/36	0/4/3/3

The worst 5 of 79 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	106	GP3	C5B-C6B	-6.55	1.34	1.47
6	B	103	GP3	C5B-C6B	-6.53	1.34	1.47
2	B	104	LCC	O2'-C6'	6.39	1.55	1.43
4	B	106	GDO	C5-C6	-6.25	1.34	1.47
2	A	101	LCC	O2'-C6'	6.18	1.55	1.43

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	104	LCC	C5-C6-N1	-6.35	116.80	123.34
2	A	101	LCC	C5-C6-N1	-5.63	117.55	123.34
6	A	106	GP3	O6A-C6A-N1A	-5.49	114.16	120.65
4	B	106	GDO	O6-C6-N1	-5.31	114.38	120.65
4	B	106	GDO	C4'-O4'-C1'	-4.99	102.88	109.75

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	103	GP3	PB-O3A-PA-O2A
6	A	106	GP3	PB-O3A-PA-O1A
6	A	106	GP3	C5D-O5D-PA-O1A

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	103	GP3	1	0
6	A	106	GP3	1	0

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

Ligand LCC B 104

Bond lengths

Bond angles

Torsions

Rings

Ligand LKC A 104

Bond lengths

Bond angles

Torsions

Rings

Ligand GP3 B 103

Bond lengths

Bond angles

Torsions

Rings

wwPDB X-ray Structure Validation Summary Report

Ligand LCC A 101

Bond lengths

Bond angles

Torsions

Rings

Ligand GDO B 106

Bond lengths

Bond angles

Torsions

Rings

Ligand LCC A 105

Bond lengths

Bond angles

Torsions

Rings

Ligand LCG A 102

Bond lengths

Bond angles

Torsions

Rings

Ligand LCG B 105

Bond lengths

Bond angles

Torsions

Rings

Ligand LKC B 101

Bond lengths

Bond angles

Torsions

Rings

Ligand GP3 A 106

Bond lengths

Bond angles

Torsions

Rings

Ligand GDO A 103

Bond lengths

Bond angles

Torsions

Rings

Ligand LCC B 102

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	9/14 (64%)	-0.27	0	100	100	7, 16, 26, 28	0
1	B	9/14 (64%)	-0.38	0	100	100	7, 16, 26, 27	0
All	All	18/28 (64%)	-0.32	0	100	100	7, 20, 27, 28	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	MG	A	109	1/1	0.67	0.13	41,41,41,41	0
7	MG	A	110	1/1	0.71	0.19	47,47,47,47	0
7	MG	B	110	1/1	0.85	0.09	47,47,47,47	0
7	MG	B	108	1/1	0.90	0.11	38,38,38,38	0
6	GP3	A	106	51/51	0.94	0.09	8,12,35,36	0
6	GP3	B	103	51/51	0.94	0.09	8,12,34,36	0
8	CO	B	111	1/1	0.94	0.08	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	LKC	B	101	19/19	0.95	0.08	9,11,14,14	0
5	LKC	A	104	19/19	0.95	0.08	9,11,14,15	0
2	LCC	B	102	22/23	0.96	0.07	8,9,12,13	0
4	GDO	A	103	22/23	0.96	0.07	7,9,17,21	0
4	GDO	B	106	22/23	0.96	0.07	7,9,17,20	0
2	LCC	B	104	22/23	0.97	0.08	6,7,9,11	0
2	LCC	A	105	22/23	0.97	0.06	8,9,12,14	0
8	CO	A	111	1/1	0.97	0.06	28,28,28,28	0
2	LCC	A	101	22/23	0.97	0.08	6,7,9,10	0
7	MG	A	107	1/1	0.98	0.05	13,13,13,13	1
3	LCG	A	102	24/25	0.98	0.07	6,6,7,8	0
3	LCG	B	105	24/25	0.98	0.07	6,6,7,8	0
7	MG	B	107	1/1	0.98	0.09	11,11,11,11	1
7	MG	B	109	1/1	0.99	0.04	8,8,8,8	0
7	MG	A	108	1/1	0.99	0.05	8,8,8,8	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.

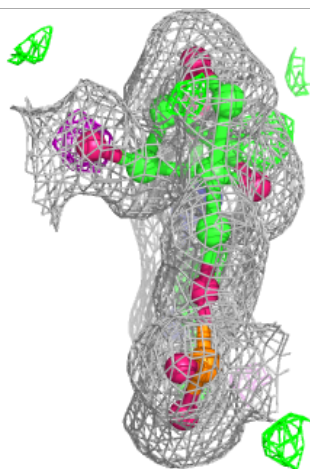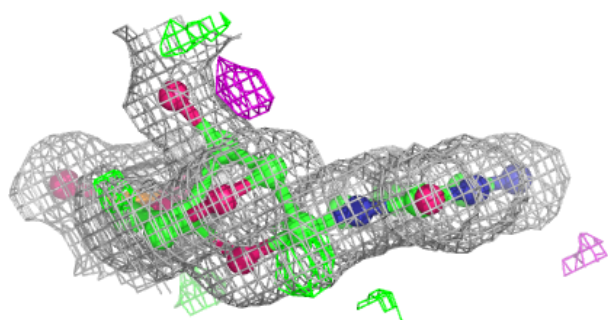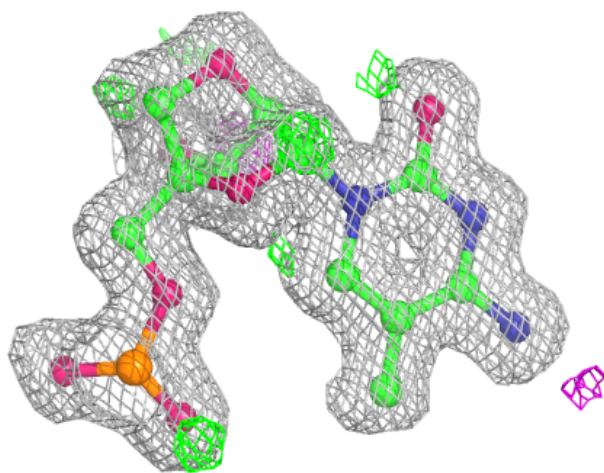**Electron density around GP3 A 106:**

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
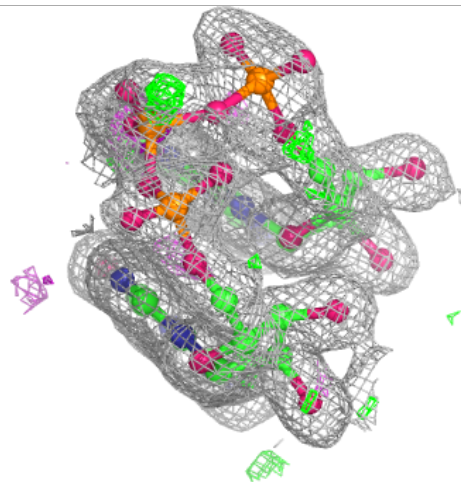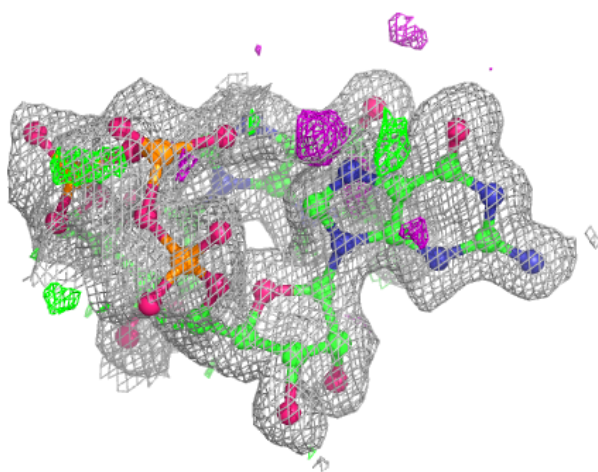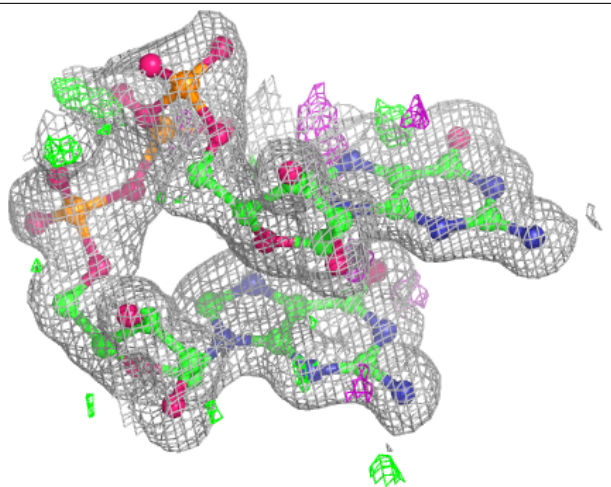
Electron density around GP3 B 103:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
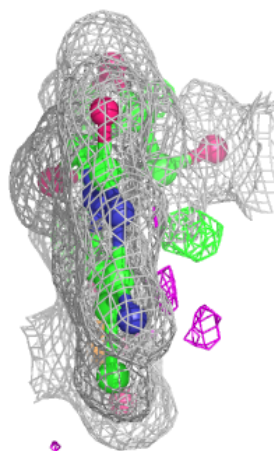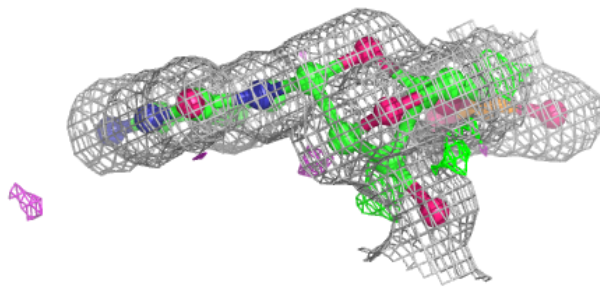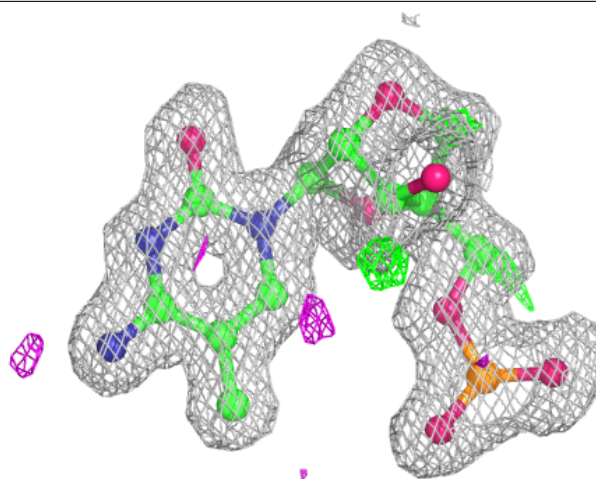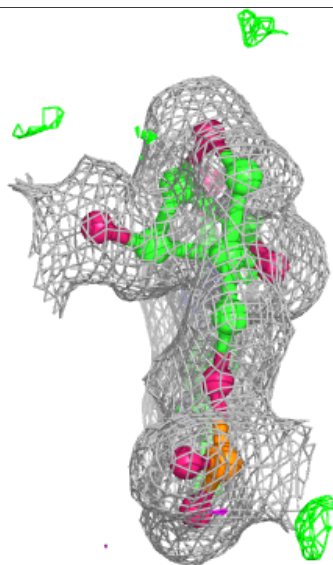$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
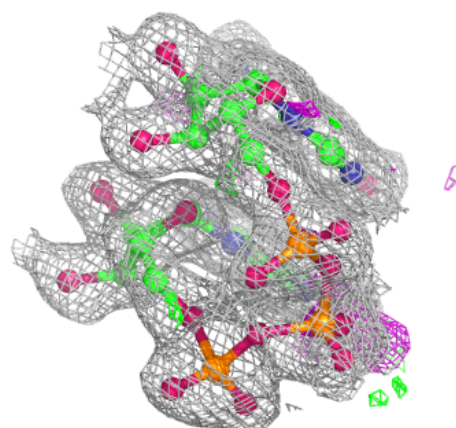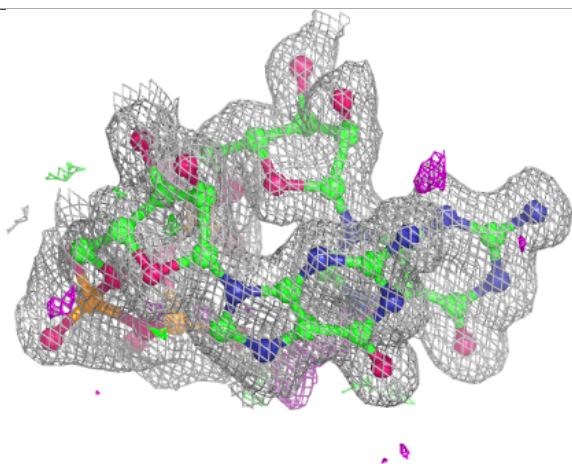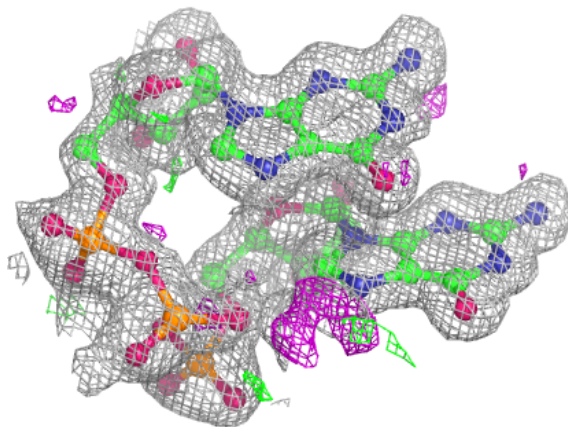
Electron density around LKC B 101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
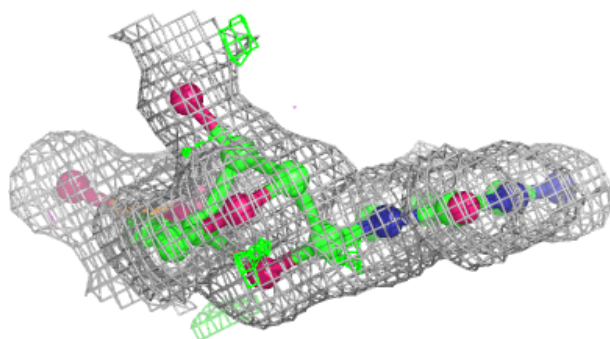mF_o-DF_c (at 3 rmsd) in purple (negative)
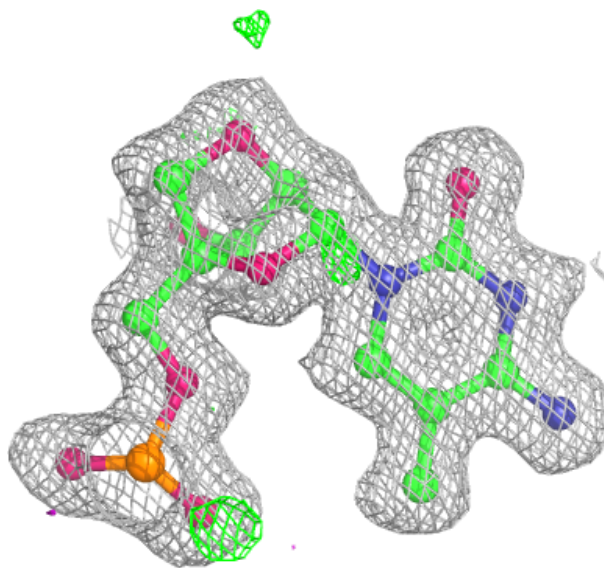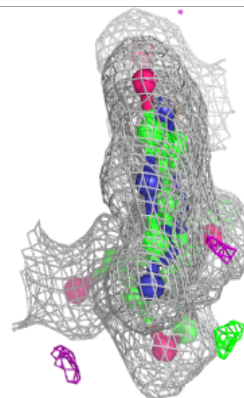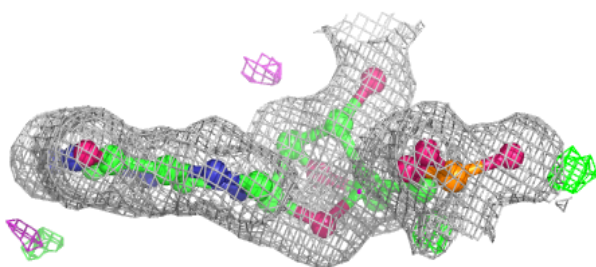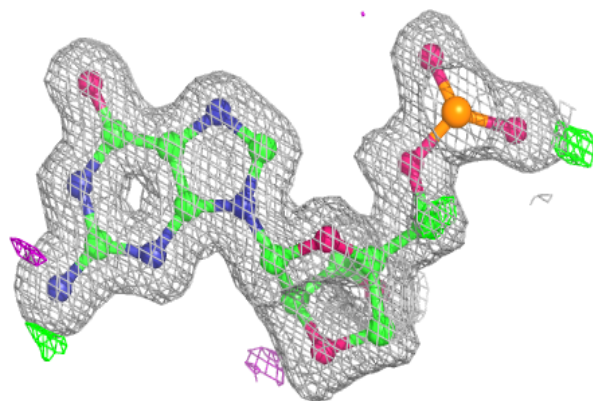and green (positive)
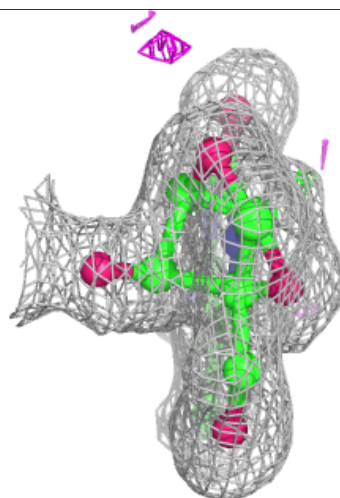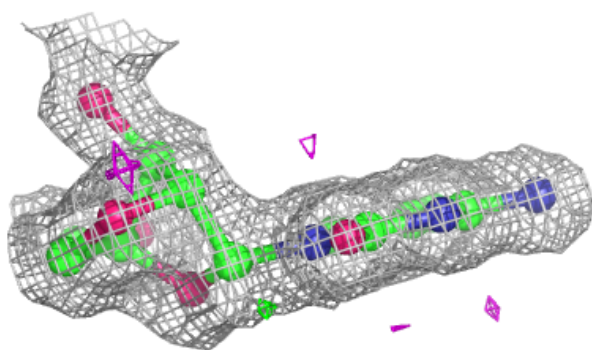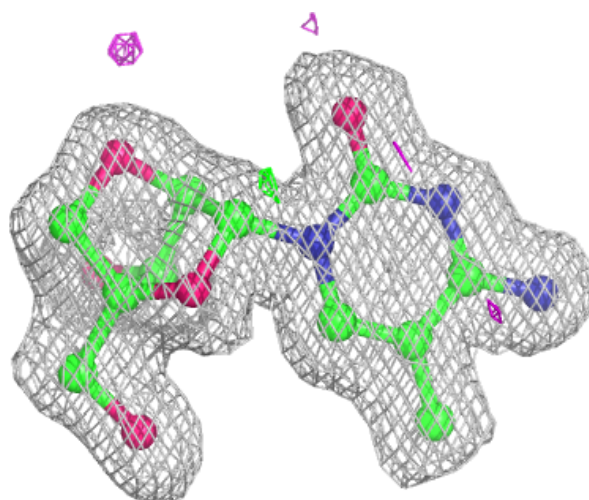
Electron density around LKC A 104:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
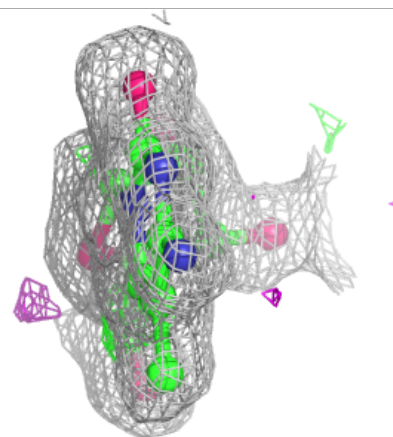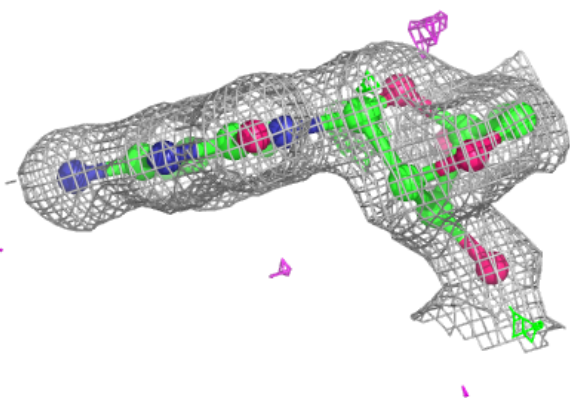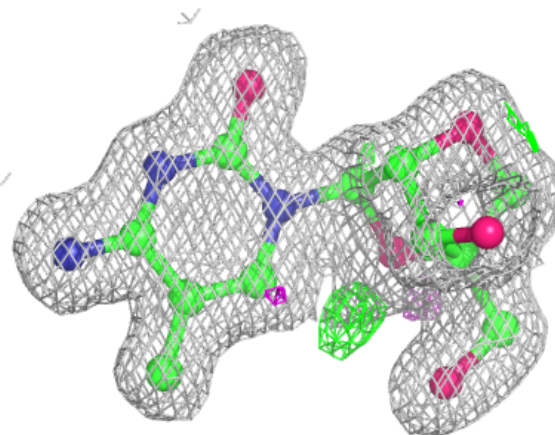
Electron density around LCC B 102:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
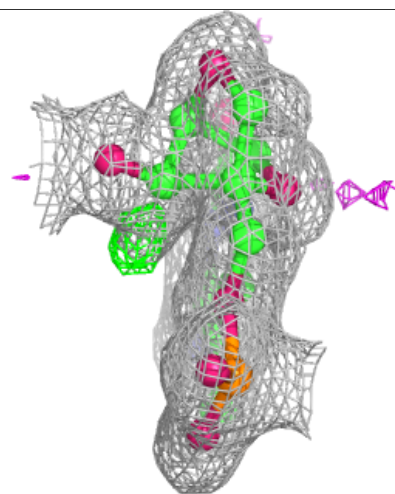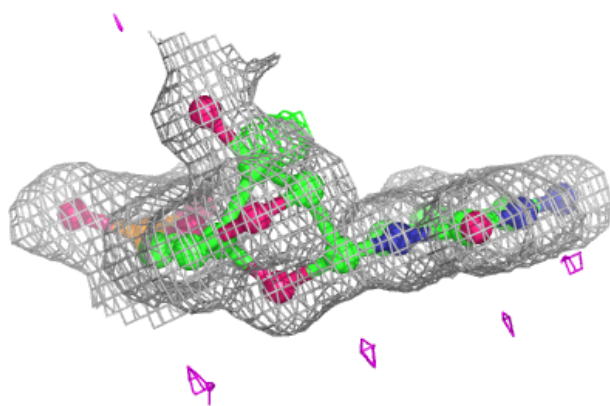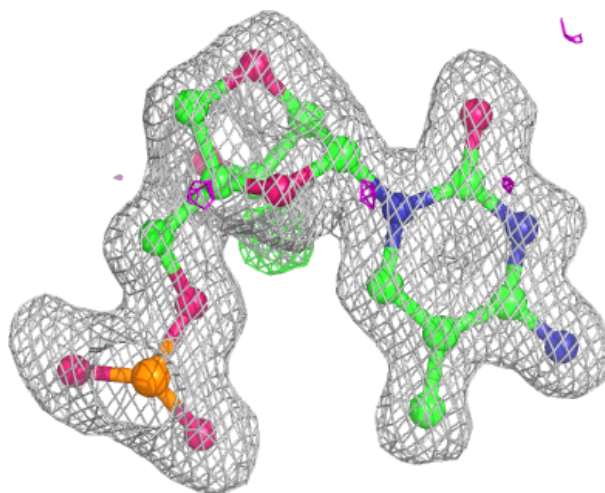
Electron density around GDO A 103:

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

Electron density around GDO B 106:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
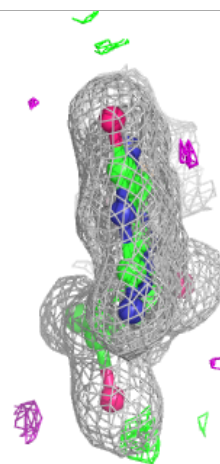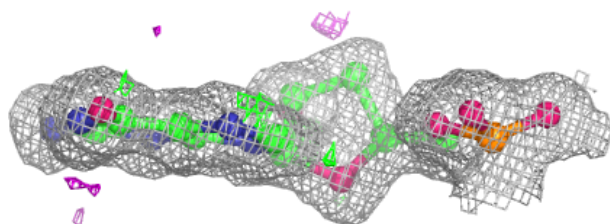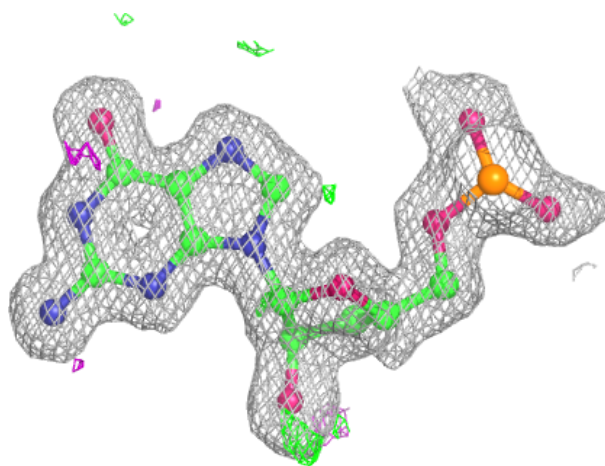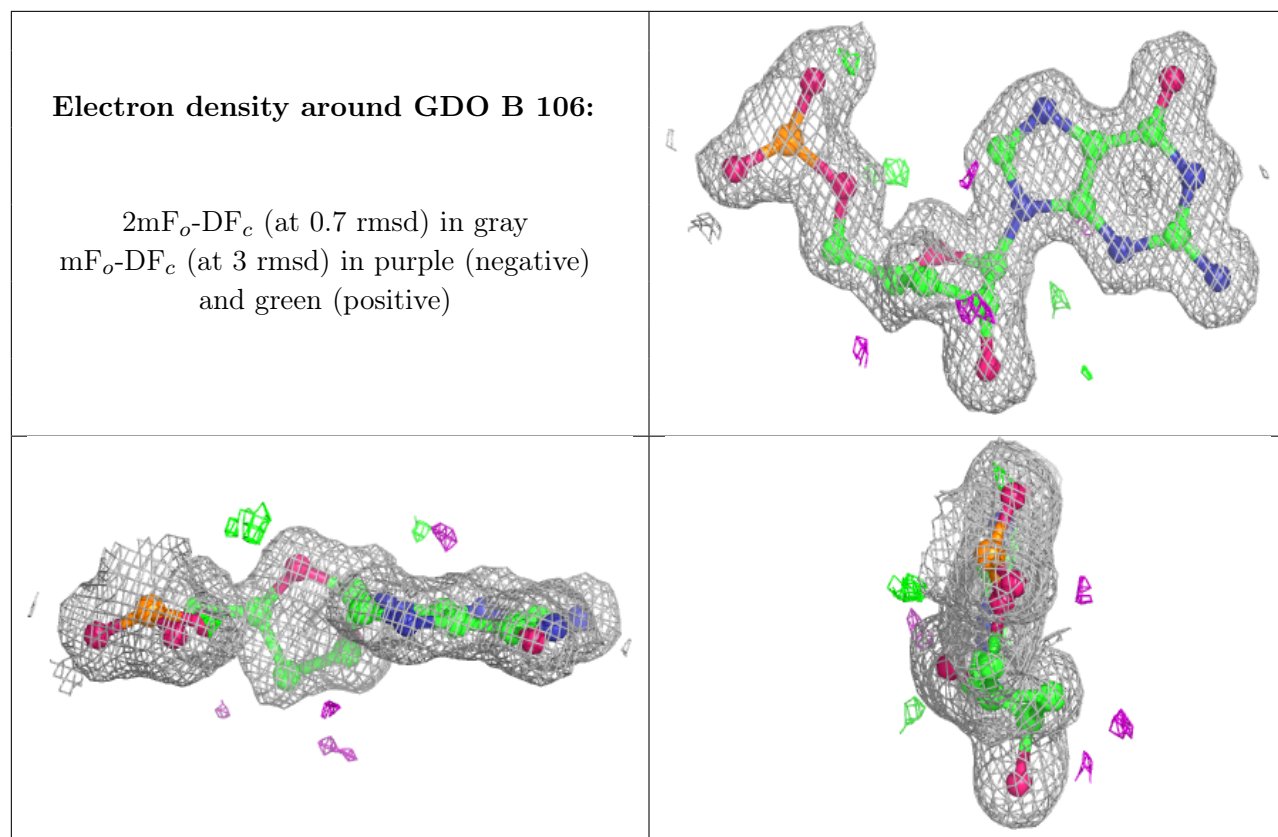
Electron density around LCC B 104:

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

Electron density around LCC A 105:

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

Electron density around LCC A 101:

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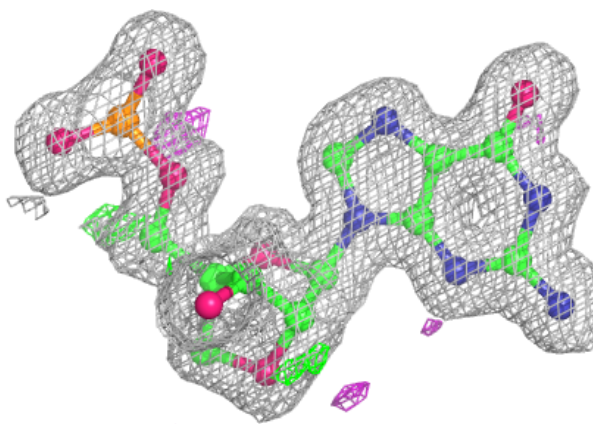and green (positive)

Electron density around LCG A 102:

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

Electron density around LCG B 105:

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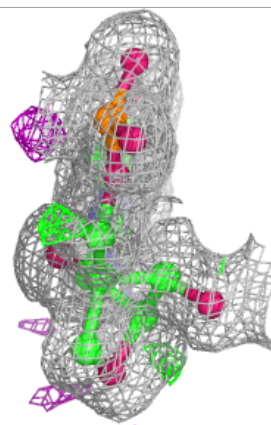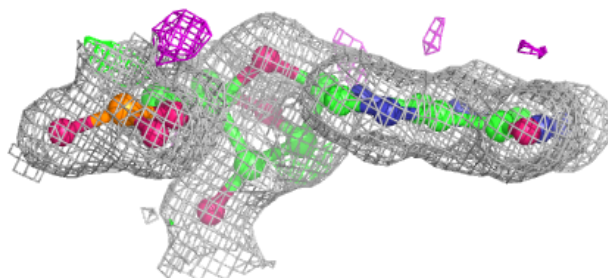
6.5 Other polymers (i)

There are no such residues in this entry.