



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 10:48 PM EDT

PDB ID : 7LNG  
Title : TNA 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 : 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.

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 : 4.02b-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

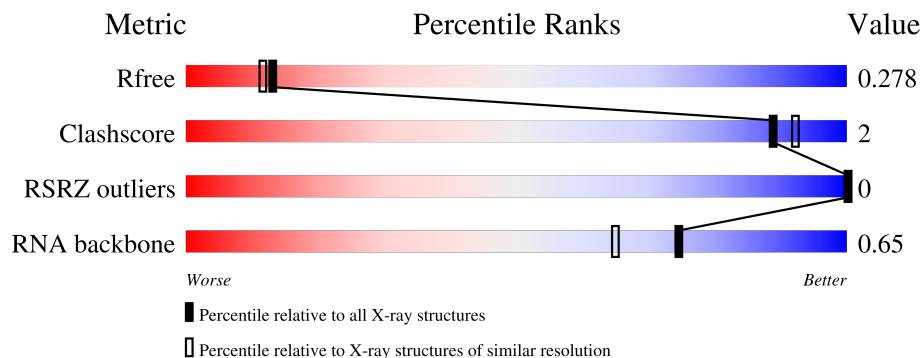
# 1 Overall quality at a glance i

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)
RSRZ outliers	127900	4800 (2.20-2.20)
RNA backbone	3102	1032 (2.60-1.80)

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  $\geq 3$ , 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	14	 57% 7% 36%
1	B	14	 50% 14% 36%

## 2 Entry composition [i](#)

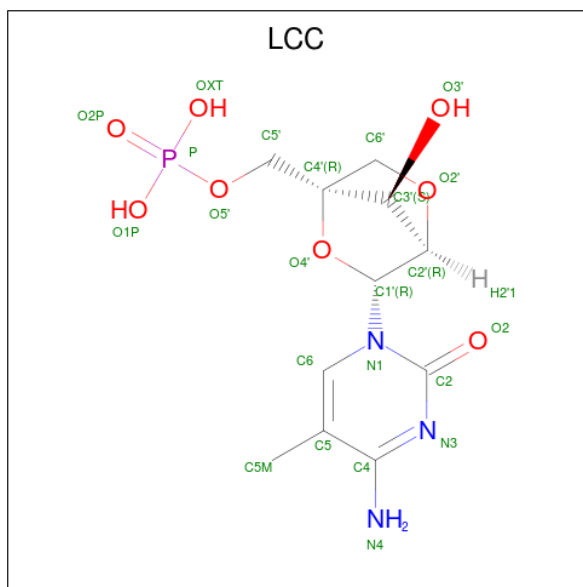
There are 6 unique types of molecules in this entry. The entry contains 696 atoms, of which 0 are hydrogens and 0 are deuteriums.

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\*(TG))-3').

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

- 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<sub>11</sub>H<sub>16</sub>N<sub>3</sub>O<sub>8</sub>P).



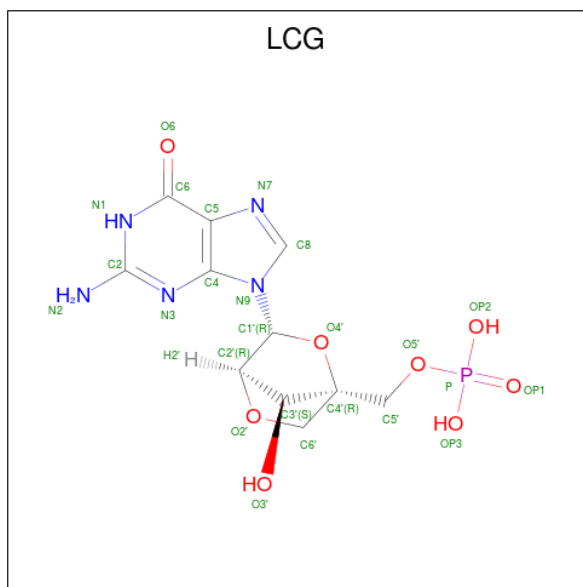
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 22	C 11	N 3	O 7	P 1	0	0
2	A	1	Total 22	C 11	N 3	O 7	P 1	0	0
2	A	1	Total 22	C 11	N 3	O 7	P 1	0	0

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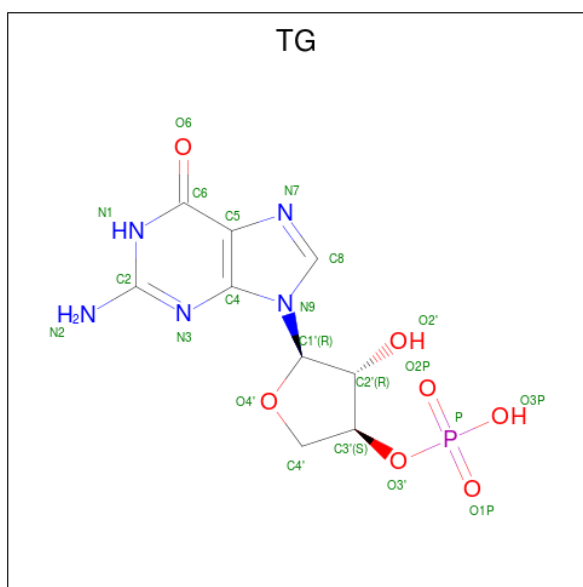
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	B	1	22	11	3	7	1	0	0

- 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<sub>11</sub>H<sub>14</sub>N<sub>5</sub>O<sub>8</sub>P).



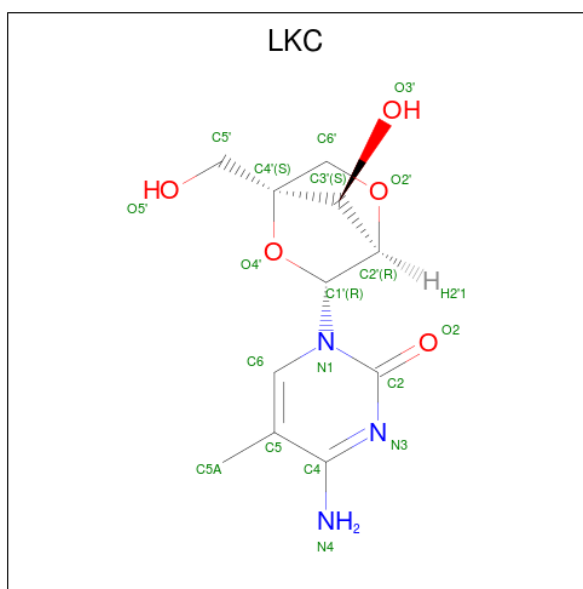
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	24	11	5	7	1	0	0
3	B	1	24	11	5	7	1	0	0

- Molecule 4 is 2-azanyl-9-[(2 {R},3 {R},4 {S})-3-oxidanyl-4-[oxidanyl-bis(oxidanylidene)-\$1^{\wedge}\{6\}\$-phosphanyl]oxy-oxolan-2-yl]-1 {H}-purin-6-one (three-letter code: TG) (formula: C<sub>9</sub>H<sub>11</sub>N<sub>5</sub>O<sub>7</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	21	9	5	6	1	0	0
4	B	1	21	9	5	6	1	0	0

- Molecule 5 is 4-AMINO-1-[(1S,3R,4R,7S)-7-HYDROXY-1-(HYDROXYMETHYL)-2,5-DIOXABICYCLO[2.2.1]HEPT-3-YL]-5-METHYLPYRIMIDIN-2(1H)-ONE (three-letter code: LKC) (formula: C<sub>11</sub>H<sub>15</sub>N<sub>3</sub>O<sub>5</sub>).



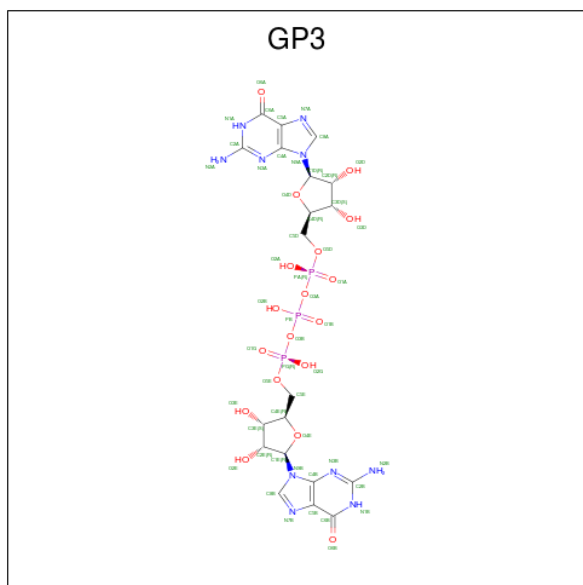
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	19	11	3	5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	B	1	19	11	3	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
			Total	C	N	O	P		
6	A	1	51	20	10	18	3	0	0
6	B	1	51	20	10	18	3	0	0

### 3 Residue-property plots

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.

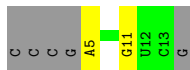
- Molecule 1: RNA (5'-R\*(LCC)P\*(LCC)P\*(LCC)P\*(LCG)P\*AP\*CP\*UP\*UP\*AP\*AP\*GP\*UP\*CP\*(TG))-3')

Chain A: 



- Molecule 1: RNA (5'-R\*(LCC)P\*(LCC)P\*(LCC)P\*(LCG)P\*AP\*CP\*UP\*UP\*AP\*AP\*GP\*UP\*CP\*(TG))-3')

Chain B: 



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.16Å 45.16Å 82.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	82.83 – 2.20 82.83 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (82.83-2.20) 99.7 (82.83-2.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.225 , 0.275 0.233 , 0.278	Depositor DCC
$R_{free}$ test set	290 reflections (5.45%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.9	Xtrriage
Anisotropy	0.113	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 20.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	0.437 for -h,-k,l	Xtrriage
Reported twinning fraction	0.565 for H, K, L 0.435 for -K, -H, -L	Depositor
Outliers	1 of 5325 reflections (0.019%)	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	696	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.05% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.54	0/210	0.86	0/324
1	B	0.75	2/210 (1.0%)	1.20	2/324 (0.6%)
All	All	0.65	2/420 (0.5%)	1.04	2/648 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	5	A	P-OP1	5.19	1.57	1.49
1	B	11	G	P-O5'	5.14	1.64	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	5	A	OP1-P-OP2	-11.61	102.19	119.60
1	B	5	A	O5'-P-OP1	-8.31	98.22	105.70

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	66	0	39	0	0
2	B	22	0	13	1	0
3	A	24	0	11	0	0
3	B	24	0	11	0	0
4	A	21	0	0	0	0
4	B	21	0	0	0	0
5	A	19	0	14	0	0
5	B	19	0	14	0	0
6	A	51	0	24	1	0
6	B	51	0	24	0	0
All	All	696	0	342	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:A:107:GP3:H3D	6:A:107:GP3:O4E	2.17	0.45
2:B:102:LCC:H41	2:B:102:LCC:H5M1	1.67	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	8/14 (57%)	1 (12%)	0
1	B	8/14 (57%)	0	0
All	All	16/28 (57%)	1 (6%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	13	C

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

12 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	LCC	A	101	3,2	20,24,25	2.30	5 (25%)	28,37,40	2.23	7 (25%)
4	TG	A	103	1	16,23,24	2.24	4 (25%)	16,34,37	1.75	5 (31%)
3	LCG	B	104	1,2	19,27,28	3.00	6 (31%)	22,42,45	1.93	8 (36%)
2	LCC	B	102	5,2	20,24,25	2.02	6 (30%)	28,37,40	1.81	7 (25%)
3	LCG	A	102	1,2	19,27,28	2.69	7 (36%)	22,42,45	1.81	7 (31%)
5	LKC	B	101	2	20,21,21	2.33	9 (45%)	30,33,33	2.34	12 (40%)
6	GP3	A	107	-	44,56,56	1.91	7 (15%)	49,88,88	1.49	11 (22%)
2	LCC	A	105	5,2	20,24,25	2.09	7 (35%)	28,37,40	2.82	9 (32%)
5	LKC	A	104	2	20,21,21	1.91	8 (40%)	30,33,33	1.95	10 (33%)
6	GP3	B	103	-	44,56,56	1.96	9 (20%)	49,88,88	1.50	9 (18%)
2	LCC	A	106	3,2	20,24,25	2.60	7 (35%)	28,37,40	1.96	8 (28%)
4	TG	B	105	1	16,23,24	2.04	3 (18%)	16,34,37	1.67	3 (18%)

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	A	101	3,2	-	3/8/35/36	0/4/3/3
4	TG	A	103	1	-	0/1/21/22	0/3/3/3
3	LCG	B	104	1,2	-	0/4/35/36	0/5/4/4
2	LCC	B	102	5,2	-	3/8/35/36	0/4/3/3
3	LCG	A	102	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	107	-	-	10/24/64/64	0/6/6/6
2	LCC	A	105	5,2	-	0/8/35/36	0/4/3/3
5	LKC	A	104	2	-	4/7/32/32	0/4/3/3
6	GP3	B	103	-	-	8/24/64/64	0/6/6/6
2	LCC	A	106	3,2	-	3/8/35/36	0/4/3/3
4	TG	B	105	1	-	1/1/21/22	0/3/3/3

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	103	GP3	C5A-C6A	-7.67	1.31	1.47
3	B	104	LCG	C5-C6	-7.30	1.32	1.47
3	A	102	LCG	C5-C6	-7.00	1.33	1.47
2	A	106	LCC	O3'-C3'	-6.85	1.29	1.42
6	A	107	GP3	C5B-C6B	-6.53	1.34	1.47
4	A	103	TG	C5-C6	-6.44	1.34	1.47
4	B	105	TG	C5-C6	-6.32	1.34	1.47
3	B	104	LCG	O5'-C5'	-6.13	1.29	1.44
5	B	101	LKC	O4'-C1'	6.12	1.51	1.42
6	A	107	GP3	C5A-C6A	-6.03	1.35	1.47
3	B	104	LCG	C4'-C3'	-5.54	1.47	1.53
2	A	101	LCC	C4'-C3'	-5.40	1.47	1.53
6	B	103	GP3	C5B-C6B	-5.36	1.36	1.47
3	A	102	LCG	C4'-C3'	-5.24	1.47	1.53
2	A	101	LCC	O2'-C6'	4.81	1.52	1.43
2	A	101	LCC	C5M-C5	-4.76	1.38	1.50
5	B	101	LKC	C5A-C5	-4.55	1.39	1.50
2	A	105	LCC	O4'-C1'	4.51	1.49	1.42
5	A	104	LKC	C5A-C5	-4.47	1.39	1.50
6	A	107	GP3	O4E-C1E	4.35	1.47	1.41
2	B	102	LCC	C5M-C5	-4.33	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	102	LCG	O2'-C6'	4.28	1.51	1.43
2	A	106	LCC	C5M-C5	-4.25	1.40	1.50
2	A	106	LCC	C4'-C3'	-4.11	1.48	1.53
2	A	105	LCC	C5M-C5	-4.11	1.40	1.50
2	B	102	LCC	O4'-C1'	3.98	1.48	1.42
2	A	106	LCC	C2'-C3'	-3.95	1.44	1.53
2	A	106	LCC	O4'-C1'	3.85	1.48	1.42
3	B	104	LCG	C5-C4	-3.77	1.33	1.43
2	A	105	LCC	C6-C5	3.71	1.40	1.34
2	A	105	LCC	O3'-C3'	3.70	1.50	1.42
6	B	103	GP3	C5A-C4A	-3.69	1.33	1.43
3	B	104	LCG	O2'-C6'	3.47	1.50	1.43
6	A	107	GP3	C5B-C4B	-3.34	1.34	1.43
3	A	102	LCG	C5-C4	-3.25	1.34	1.43
2	A	101	LCC	C6-C5	3.18	1.39	1.34
4	A	103	TG	O4'-C1'	3.17	1.46	1.41
6	A	107	GP3	C5A-C4A	-3.16	1.35	1.43
4	A	103	TG	C6-N1	3.16	1.42	1.37
2	B	102	LCC	O2'-C6'	3.12	1.49	1.43
6	B	103	GP3	O4E-C1E	3.06	1.45	1.41
5	A	104	LKC	O2'-C6'	3.04	1.49	1.43
5	A	104	LKC	C2'-C3'	-2.99	1.46	1.53
2	B	102	LCC	C6-N1	2.87	1.42	1.38
4	A	103	TG	C5-C4	-2.86	1.35	1.43
6	A	107	GP3	O2D-C2D	2.86	1.49	1.43
5	B	101	LKC	C4'-C3'	-2.80	1.50	1.53
5	A	104	LKC	C6-C5	2.77	1.39	1.34
6	B	103	GP3	C5B-C4B	-2.73	1.36	1.43
5	B	101	LKC	O3'-C3'	2.59	1.47	1.42
5	A	104	LKC	C4'-C3'	-2.59	1.50	1.53
6	B	103	GP3	C2E-C1E	-2.58	1.49	1.53
4	B	105	TG	C5-C4	-2.58	1.36	1.43
6	B	103	GP3	C2E-C3E	-2.57	1.46	1.53
3	A	102	LCG	O3'-C3'	2.56	1.47	1.42
2	A	101	LCC	C6-N1	2.55	1.42	1.38
2	A	106	LCC	O2'-C6'	2.50	1.48	1.43
2	B	102	LCC	C6-C5	2.38	1.38	1.34
5	B	101	LKC	O4'-C4'	2.37	1.49	1.45
6	B	103	GP3	PA-O5D	2.32	1.68	1.59
5	B	101	LKC	C6'-C4'	2.27	1.57	1.53
5	B	101	LKC	O2'-C6'	2.26	1.48	1.43
2	A	105	LCC	C2-N1	-2.21	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	101	LKC	C6-C5	2.20	1.38	1.34
4	B	105	TG	O3'-C3'	-2.20	1.42	1.45
3	B	104	LCG	C2'-C3'	-2.19	1.48	1.53
5	B	101	LKC	O2'-C2'	2.17	1.48	1.43
3	A	102	LCG	C2'-C3'	-2.17	1.48	1.53
5	A	104	LKC	O4'-C1'	2.14	1.45	1.42
2	B	102	LCC	C2-N3	-2.13	1.32	1.36
2	A	106	LCC	C2-N1	-2.13	1.35	1.40
5	A	104	LKC	O2'-C2'	2.09	1.48	1.43
6	A	107	GP3	O4D-C1D	2.08	1.44	1.41
5	A	104	LKC	C2-N1	-2.08	1.35	1.40
2	A	105	LCC	O2'-C6'	2.05	1.47	1.43
2	A	105	LCC	C6-N1	2.03	1.41	1.38
6	B	103	GP3	O4D-C1D	2.02	1.43	1.41
3	A	102	LCG	O4'-C1'	2.00	1.45	1.42

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	105	LCC	O4'-C1'-N1	11.26	123.26	108.77
2	A	101	LCC	C5-C6-N1	-5.67	117.51	123.34
2	A	101	LCC	C5M-C5-C6	-5.60	115.36	122.85
5	B	101	LKC	O4'-C4'-C3'	-5.30	95.20	102.22
2	A	101	LCC	O4'-C1'-N1	-4.82	102.56	108.77
5	B	101	LKC	O5'-C5'-C4'	-4.59	102.45	111.71
2	A	106	LCC	O3'-C3'-C4'	-4.23	101.22	112.52
5	A	104	LKC	O5'-C5'-C4'	-4.11	103.42	111.71
2	B	102	LCC	C5-C6-N1	-4.05	119.17	123.34
5	B	101	LKC	C5-C6-N1	-3.99	119.23	123.34
2	A	106	LCC	O4'-C4'-C5'	3.91	120.42	108.82
5	B	101	LKC	C4'-O4'-C1'	-3.88	100.80	107.58
5	A	104	LKC	O2'-C6'-C4'	-3.87	96.28	103.78
2	B	102	LCC	O2-C2-N3	-3.86	116.05	122.33
2	A	105	LCC	C5-C6-N1	-3.85	119.38	123.34
3	A	102	LCG	C2-N1-C6	-3.75	118.20	125.10
5	A	104	LKC	C5-C6-N1	-3.73	119.50	123.34
3	B	104	LCG	C2-N1-C6	-3.73	118.24	125.10
3	B	104	LCG	O2'-C6'-C4'	-3.70	96.61	103.78
4	B	105	TG	O4'-C4'-C3'	-3.69	97.92	104.52
6	B	103	GP3	C8B-N7B-C5B	3.67	109.99	102.99
2	A	105	LCC	O4'-C4'-C3'	-3.63	97.41	102.22
2	A	105	LCC	O4'-C4'-C5'	3.52	119.27	108.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	101	LKC	C5-C4-N4	-3.52	116.22	121.48
6	B	103	GP3	O6B-C6B-N1B	-3.48	116.54	120.65
6	A	107	GP3	C2B-N1B-C6B	-3.37	118.90	125.10
4	B	105	TG	C8-N7-C5	3.29	109.25	102.99
4	A	103	TG	C2-N1-C6	-3.26	119.09	125.10
3	A	102	LCG	O2'-C6'-C4'	-3.23	97.52	103.78
3	B	104	LCG	C5-C6-N1	3.19	119.58	113.95
2	A	106	LCC	C5-C4-N4	-3.18	116.72	121.48
5	A	104	LKC	O2-C2-N3	-3.17	117.17	122.33
6	B	103	GP3	C5A-C6A-N1A	3.14	119.50	113.95
2	A	101	LCC	O4'-C4'-C6'	3.08	112.48	105.97
3	B	104	LCG	N2-C2-N1	3.08	123.27	116.71
6	A	107	GP3	C5B-C6B-N1B	3.05	119.33	113.95
6	B	103	GP3	C2B-N1B-C6B	-3.01	119.56	125.10
6	A	107	GP3	C8A-N7A-C5A	3.00	108.71	102.99
2	A	105	LCC	C5M-C5-C6	-2.99	118.85	122.85
5	B	101	LKC	C6'-O2'-C2'	-2.96	102.22	107.65
6	A	107	GP3	C2A-N1A-C6A	-2.87	119.81	125.10
2	B	102	LCC	O4'-C1'-N1	2.86	112.44	108.77
3	A	102	LCG	C5-C6-N1	2.85	118.99	113.95
4	A	103	TG	C5-C6-N1	2.84	118.97	113.95
5	B	101	LKC	C5A-C5-C6	-2.82	119.08	122.85
4	B	105	TG	C2-N1-C6	-2.80	119.95	125.10
2	A	106	LCC	C5M-C5-C6	-2.78	119.14	122.85
5	A	104	LKC	C5-C4-N4	-2.74	117.39	121.48
2	B	102	LCC	O2-C2-N1	2.73	124.54	118.89
2	A	106	LCC	O2'-C6'-C4'	-2.73	98.48	103.78
5	B	101	LKC	O4'-C1'-N1	2.73	112.28	108.77
3	B	104	LCG	O6-C6-C5	-2.73	119.05	124.37
6	A	107	GP3	PG-O3B-PB	-2.71	123.53	132.83
2	A	106	LCC	C4'-O4'-C1'	-2.68	102.90	107.58
6	B	103	GP3	PG-O3B-PB	-2.66	123.71	132.83
6	B	103	GP3	N1A-C2A-N3A	-2.65	118.38	123.32
6	B	103	GP3	C2A-N1A-C6A	-2.64	120.23	125.10
2	A	105	LCC	O2-C2-N3	-2.62	118.07	122.33
3	A	102	LCG	N2-C2-N1	2.61	122.28	116.71
2	A	106	LCC	N4-C4-N3	2.60	123.22	118.48
5	B	101	LKC	N4-C4-N3	2.60	123.22	118.48
2	B	102	LCC	C5-C4-N4	-2.58	117.61	121.48
4	A	103	TG	C8-N7-C5	2.58	107.91	102.99
5	A	104	LKC	C5'-C4'-C3'	-2.58	110.41	117.07
6	A	107	GP3	N2A-C2A-N1A	2.56	122.17	116.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	103	TG	N1-C2-N3	-2.54	118.57	123.32
3	A	102	LCG	C8-N7-C5	2.53	107.81	102.99
3	B	104	LCG	C8-N7-C5	2.52	107.80	102.99
5	B	101	LKC	C1'-N1-C6	-2.51	116.94	121.12
2	A	105	LCC	N1-C2-N3	2.46	123.29	118.81
6	A	107	GP3	C3D-C2D-C1D	-2.45	97.29	100.98
5	A	104	LKC	O4'-C4'-C5'	2.41	113.33	108.97
4	A	103	TG	O4'-C4'-C3'	-2.39	100.24	104.52
3	B	104	LCG	N1-C2-N3	-2.38	118.87	123.32
2	A	106	LCC	O4'-C1'-N1	2.37	111.82	108.77
3	B	104	LCG	C4'-O4'-C1'	-2.37	103.45	107.58
2	A	101	LCC	O2'-C6'-C4'	-2.35	99.22	103.78
6	A	107	GP3	C8B-N7B-C5B	2.33	107.44	102.99
2	A	105	LCC	C4'-O4'-C1'	-2.33	103.51	107.58
2	B	102	LCC	O2'-C6'-C4'	-2.31	99.31	103.78
2	A	101	LCC	O2-C2-N3	-2.30	118.59	122.33
5	B	101	LKC	O4'-C4'-C5'	2.30	113.13	108.97
3	A	102	LCG	C4'-O4'-C1'	-2.28	103.60	107.58
2	A	101	LCC	O2'-C2'-C1'	2.27	112.58	105.66
6	A	107	GP3	N1B-C2B-N3B	-2.26	119.10	123.32
2	B	102	LCC	O4'-C4'-C5'	2.25	115.50	108.82
6	A	107	GP3	N1A-C2A-N3A	-2.25	119.11	123.32
3	A	102	LCG	O4'-C4'-C6'	2.24	110.71	105.97
6	A	107	GP3	C5A-C6A-N1A	2.23	117.89	113.95
5	A	104	LKC	C4'-O4'-C1'	-2.20	103.73	107.58
6	B	103	GP3	C5B-C6B-N1B	2.17	117.78	113.95
6	B	103	GP3	N2A-C2A-N1A	2.14	121.28	116.71
5	A	104	LKC	C5A-C5-C6	-2.14	119.99	122.85
5	B	101	LKC	O2-C2-N3	-2.08	118.94	122.33
2	A	105	LCC	O3'-C3'-C4'	2.06	118.02	112.52
5	A	104	LKC	N4-C4-N3	2.05	122.21	118.48

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	101	LCC	C6'-C4'-C5'-O5'
5	A	104	LKC	C3'-C4'-C5'-O5'
5	A	104	LKC	O4'-C4'-C5'-O5'
5	A	104	LKC	C6'-C4'-C5'-O5'
6	A	107	GP3	PB-O3B-PG-O5E
6	A	107	GP3	C5E-O5E-PG-O3B

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Mol	Chain	Res	Type	Atoms
6	B	103	GP3	C5D-O5D-PA-O3A
6	A	107	GP3	O4E-C4E-C5E-O5E
6	A	107	GP3	C3E-C4E-C5E-O5E
6	B	103	GP3	O4E-C4E-C5E-O5E
6	B	103	GP3	C3E-C4E-C5E-O5E
6	A	107	GP3	PA-O3A-PB-O1B
6	A	107	GP3	C3D-C4D-C5D-O5D
6	B	103	GP3	PB-O3B-PG-O5E
6	A	107	GP3	O4D-C4D-C5D-O5D
6	B	103	GP3	PA-O3A-PB-O2B
2	A	101	LCC	O4'-C4'-C5'-O5'
2	A	101	LCC	C3'-C4'-C5'-O5'
2	A	106	LCC	O4'-C4'-C5'-O5'
2	B	102	LCC	O4'-C4'-C5'-O5'
2	B	102	LCC	C3'-C4'-C5'-O5'
6	A	107	GP3	C5E-O5E-PG-O1G
6	B	103	GP3	C5D-O5D-PA-O1A
2	B	102	LCC	C6'-C4'-C5'-O5'
6	A	107	GP3	PA-O3A-PB-O2B
6	B	103	GP3	PG-O3B-PB-O1B
6	B	103	GP3	O4D-C4D-C5D-O5D
2	A	106	LCC	C2'-C1'-N1-C6
4	B	105	TG	C2'-C3'-O3'-P
2	A	106	LCC	C2'-C1'-N1-C2
5	A	104	LKC	C2'-C1'-N1-C2
6	A	107	GP3	C5E-O5E-PG-O2G

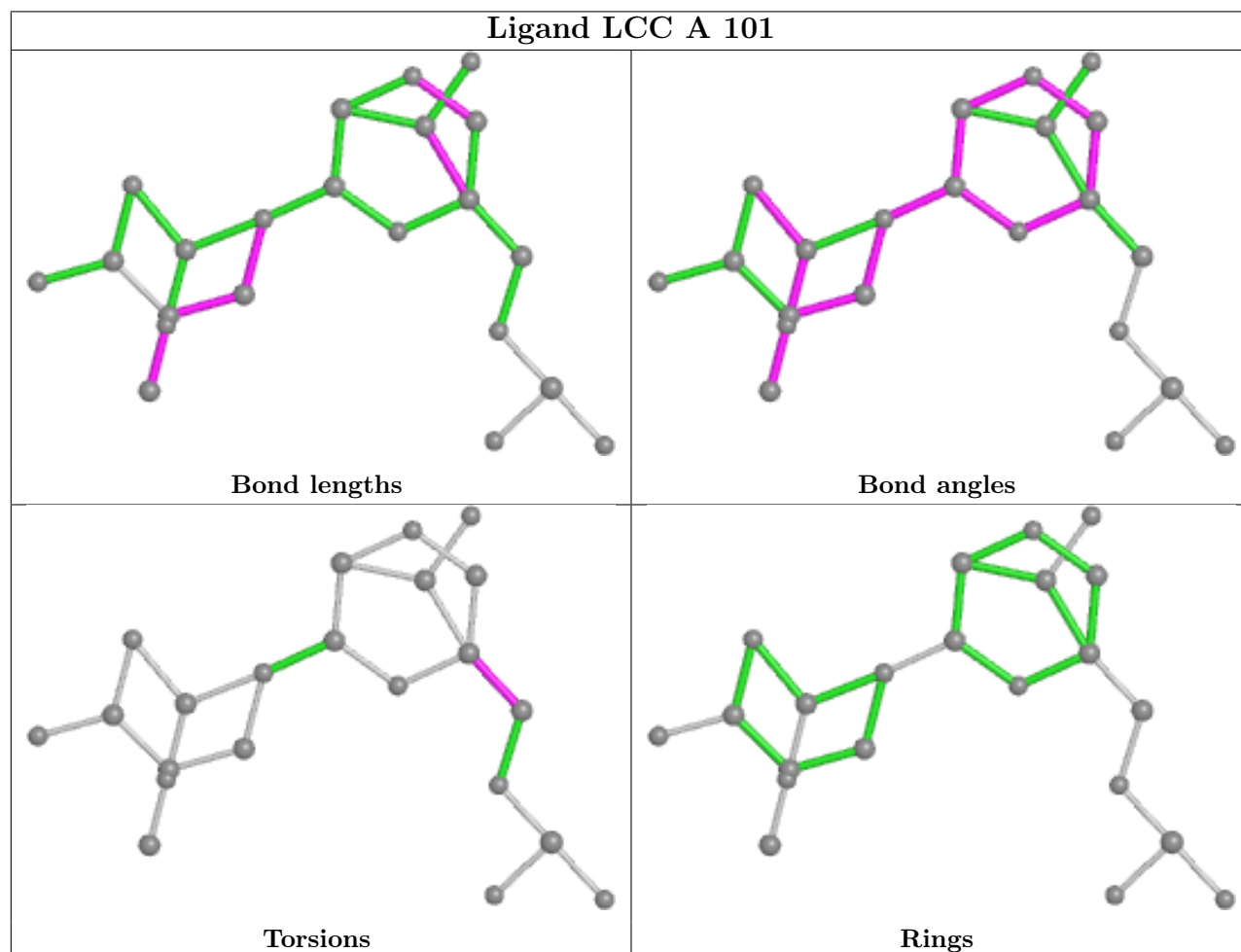
There are no ring outliers.

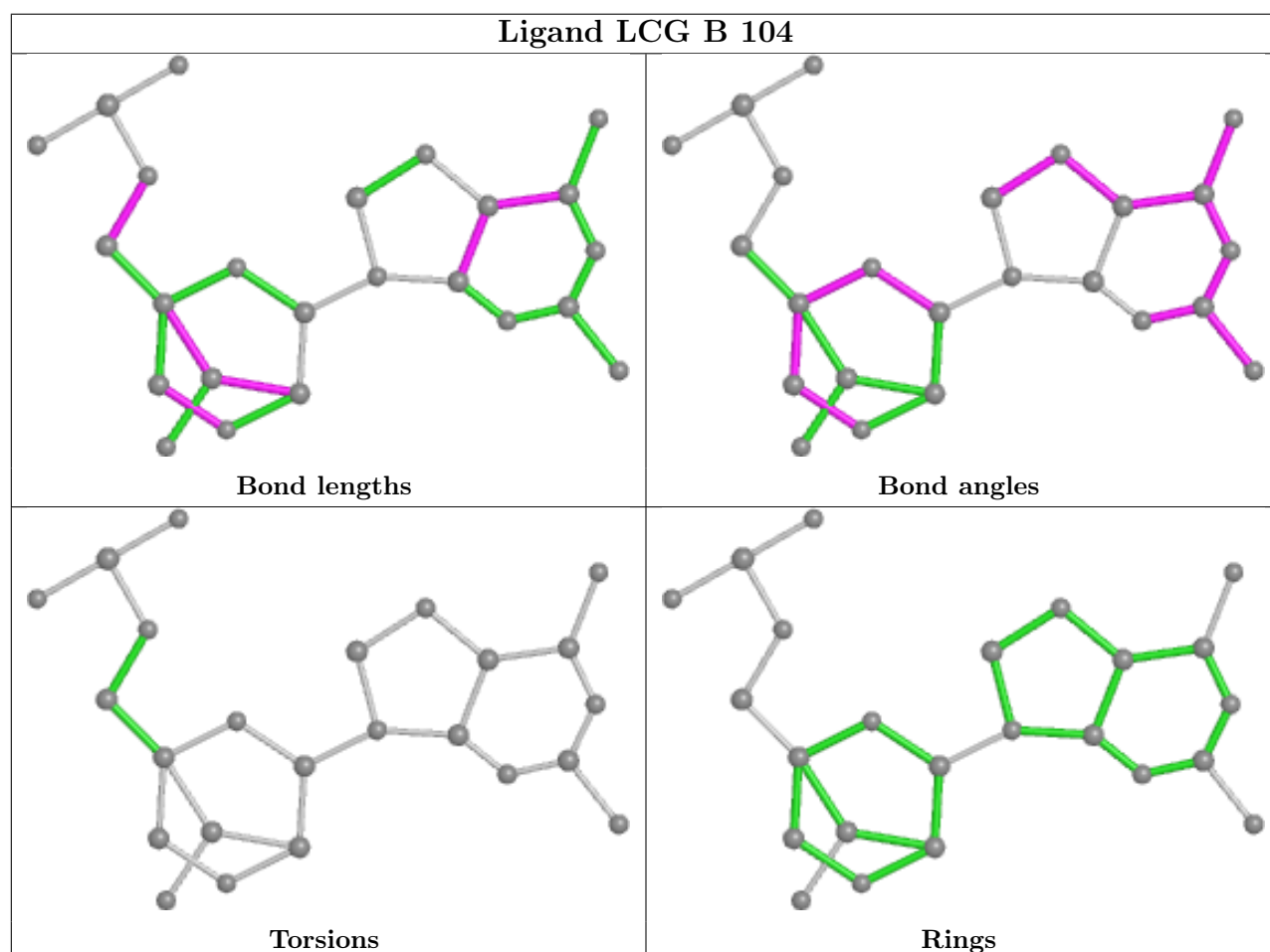
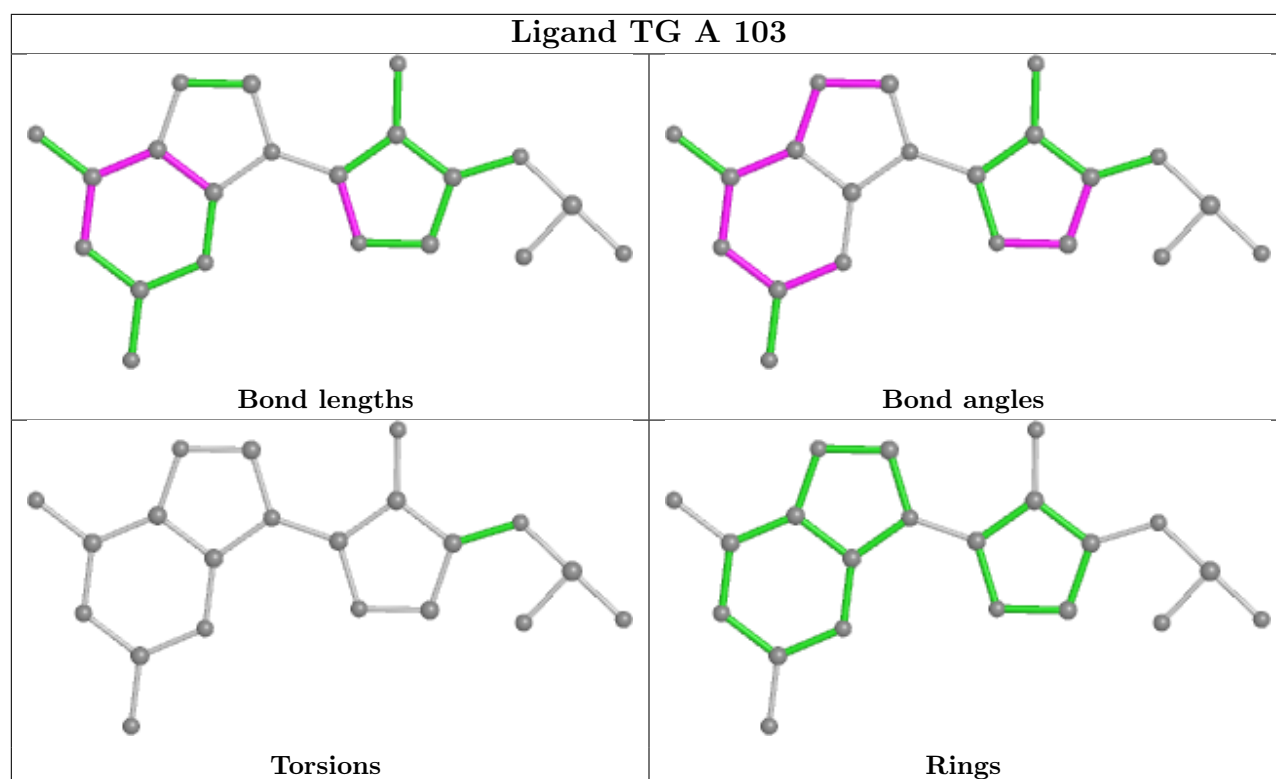
2 monomers are involved in 2 short contacts:

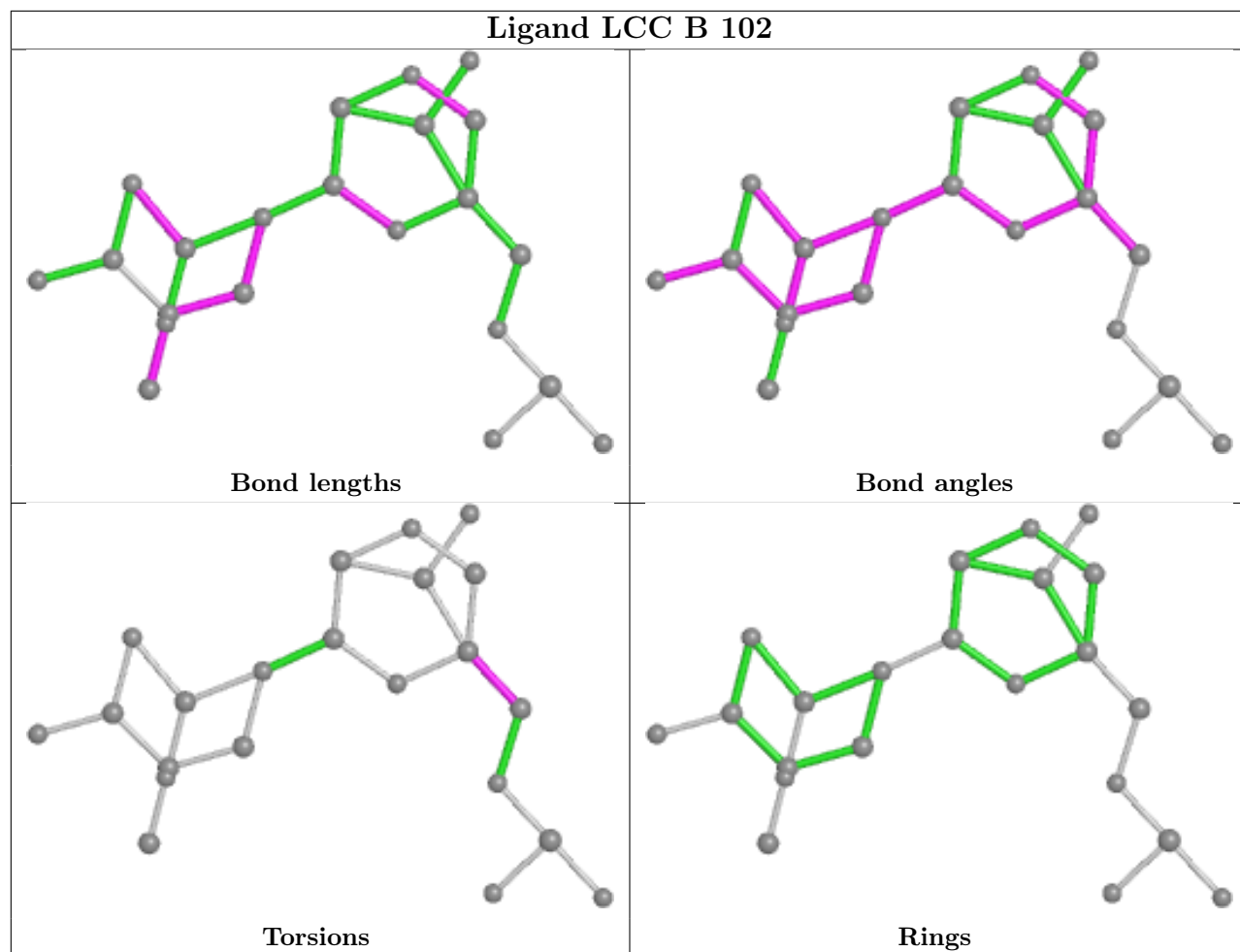
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	102	LCC	1	0
6	A	107	GP3	1	0

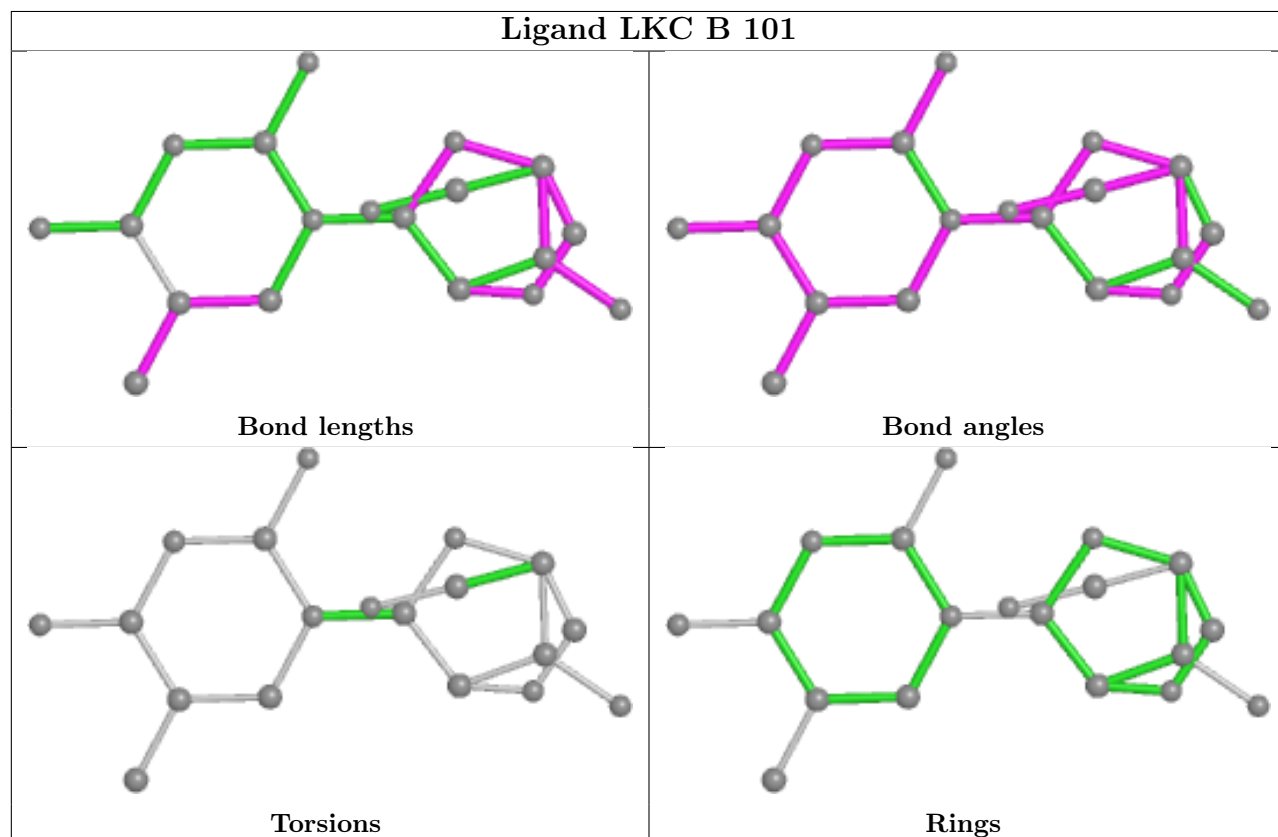
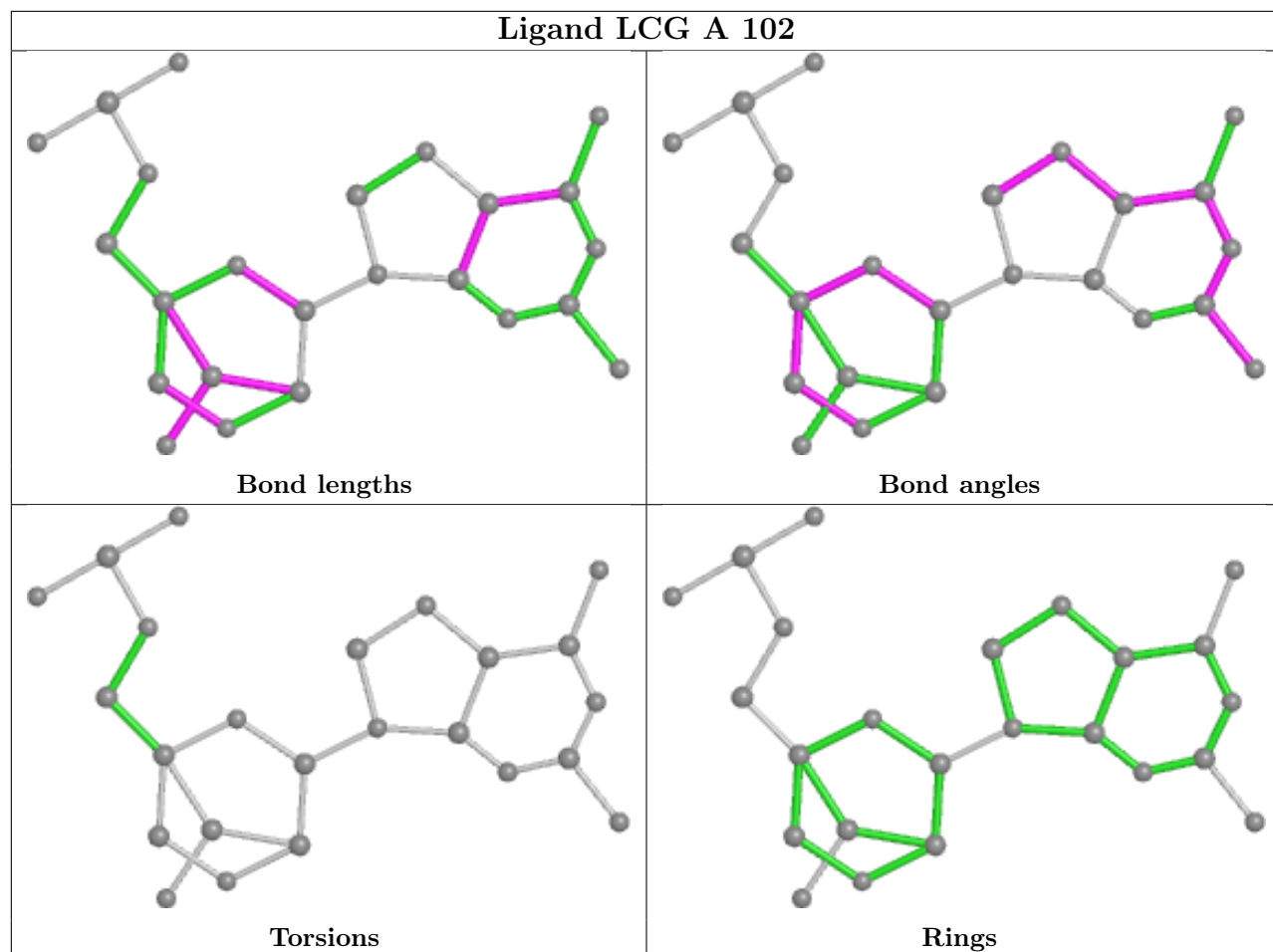
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

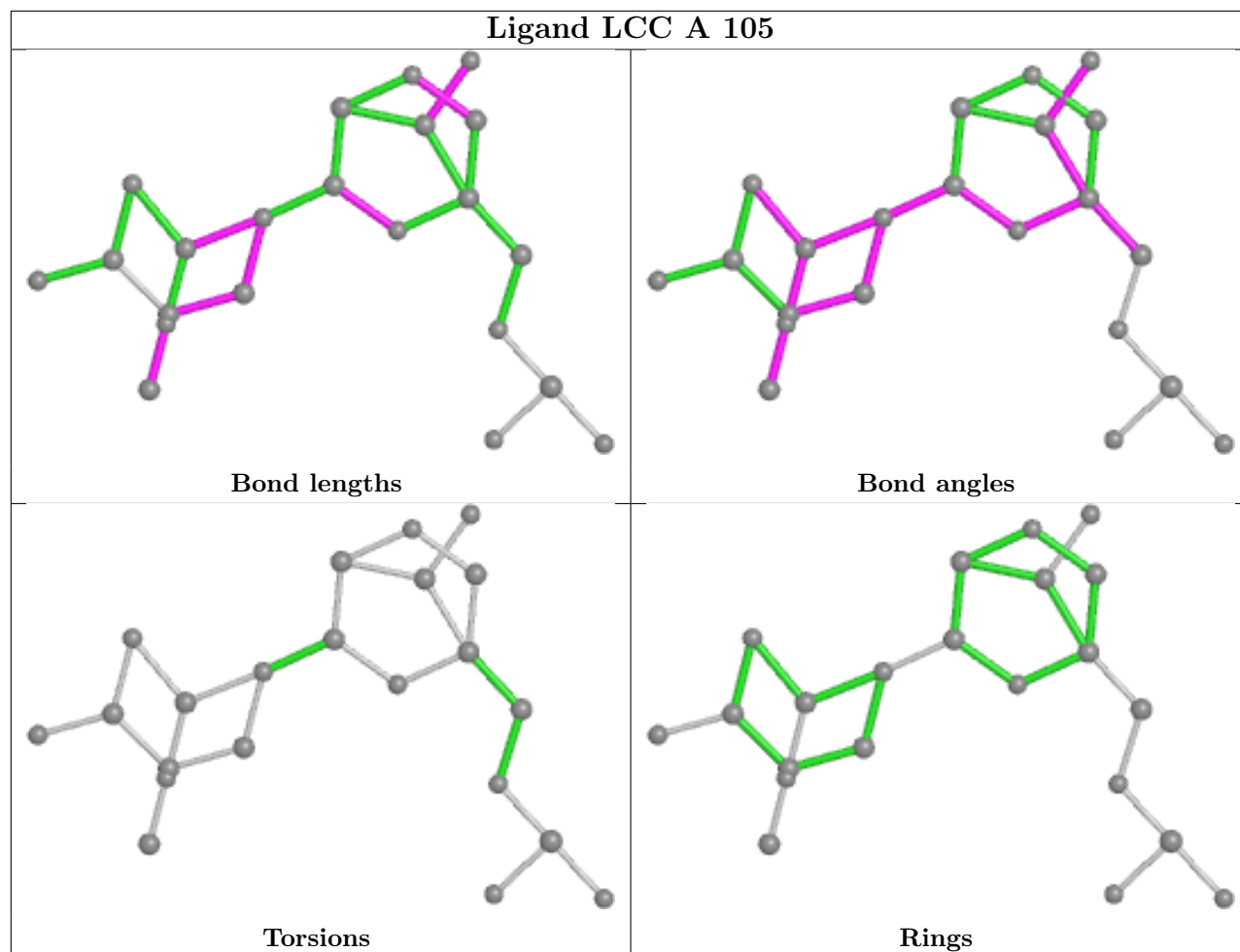
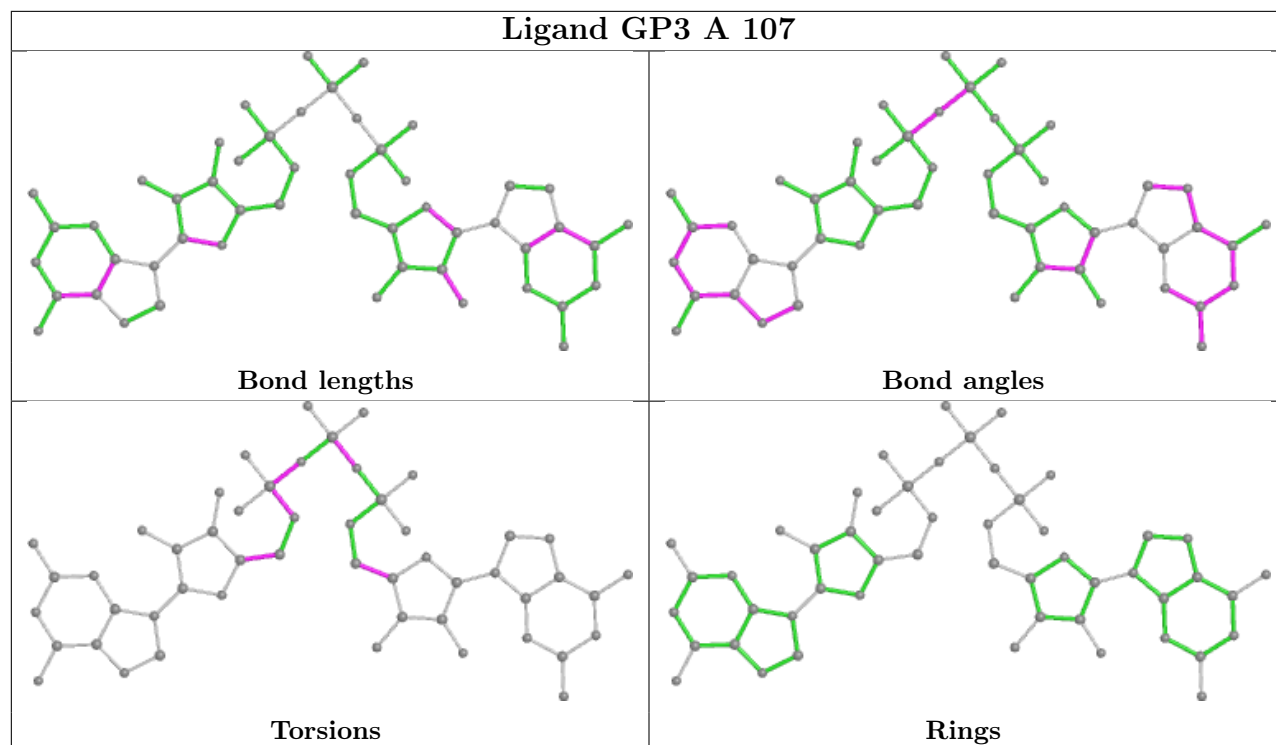
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

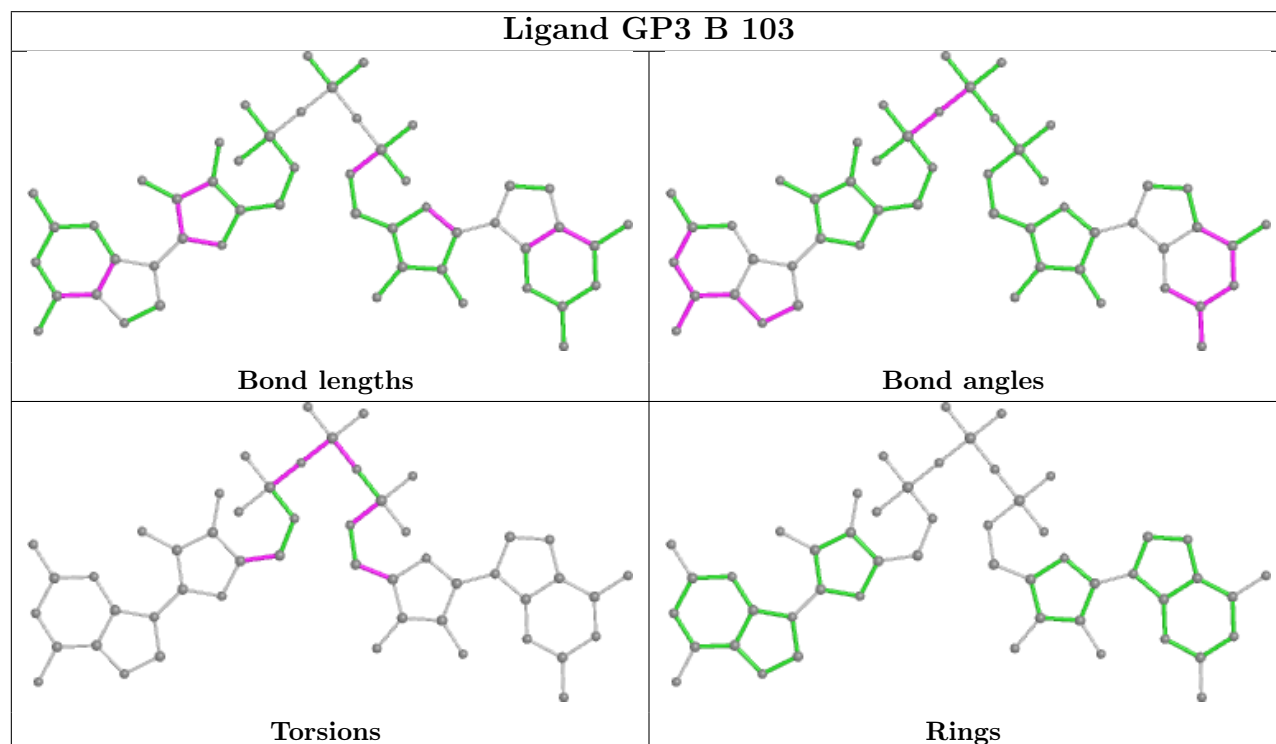
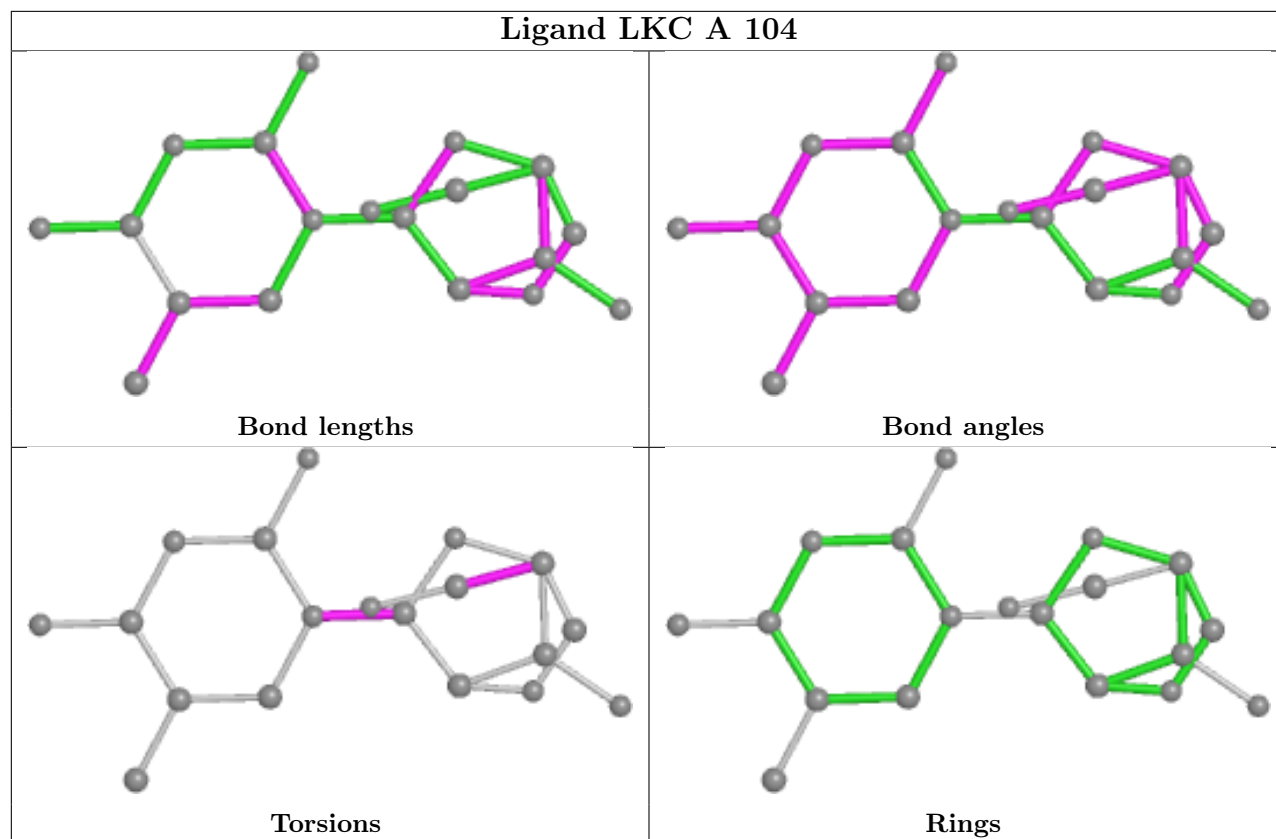


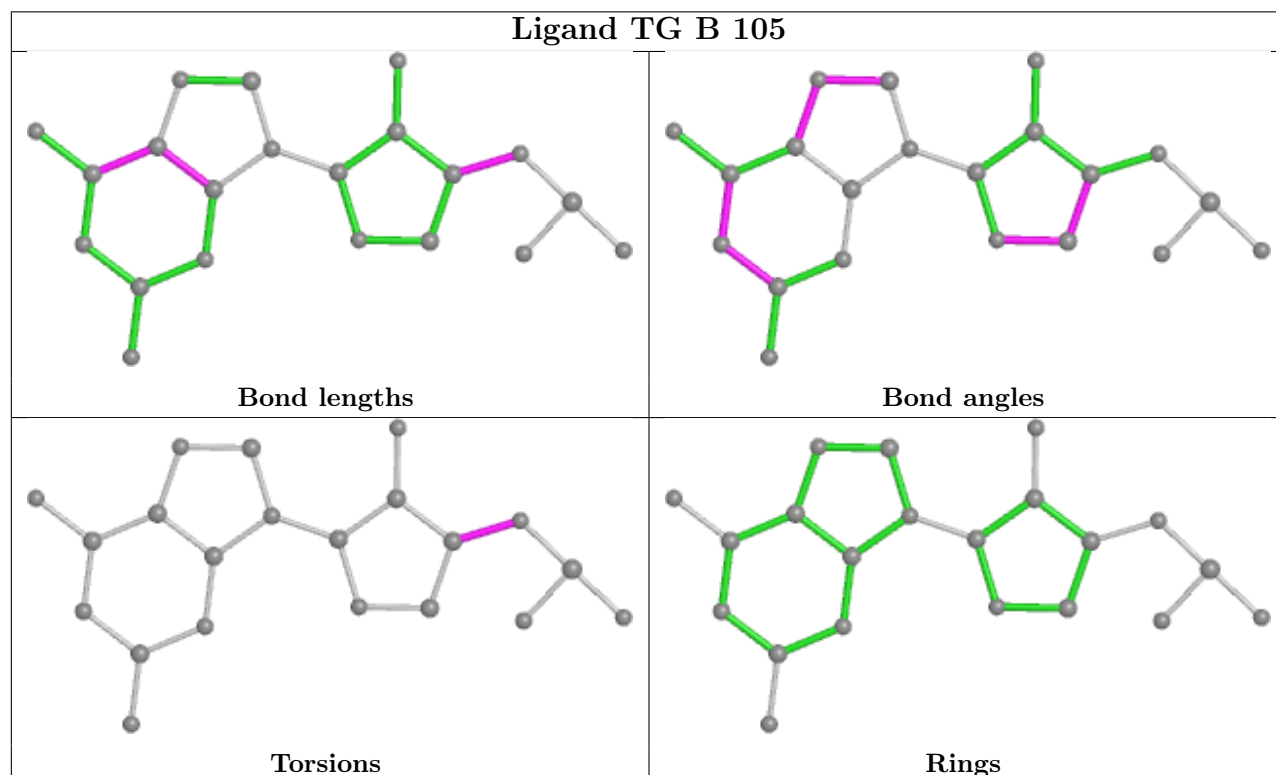
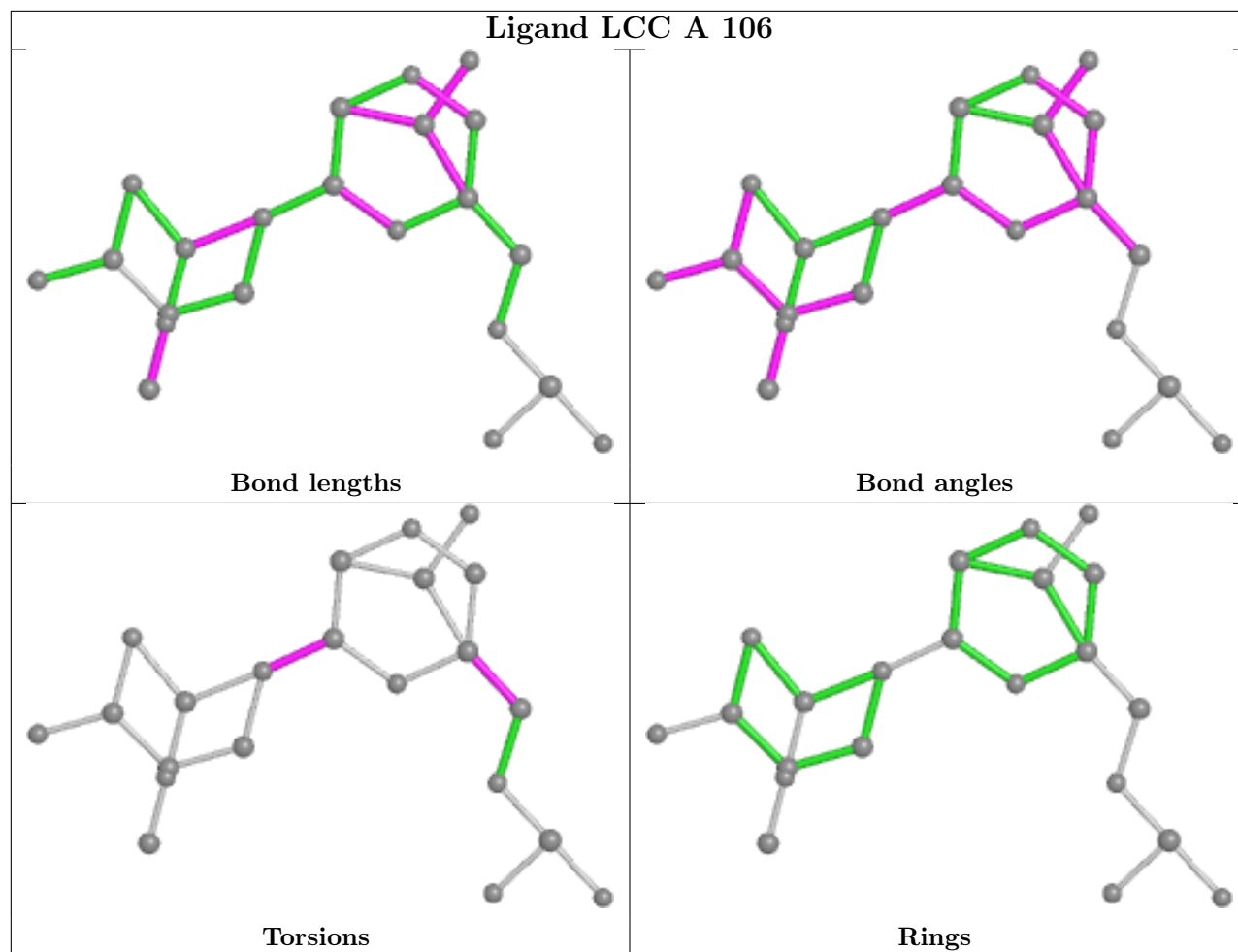














## 5.7 Other polymers [i](#)

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	9/14 (64%)	0.14	0 <a href="#">100</a> <a href="#">100</a>	37, 58, 68, 71	0
1	B	9/14 (64%)	0.08	0 <a href="#">100</a> <a href="#">100</a>	49, 51, 57, 57	0
All	All	18/28 (64%)	0.11	0 <a href="#">100</a> <a href="#">100</a>	37, 55, 68, 71	0

There are no RSRZ outliers to report.

### 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.

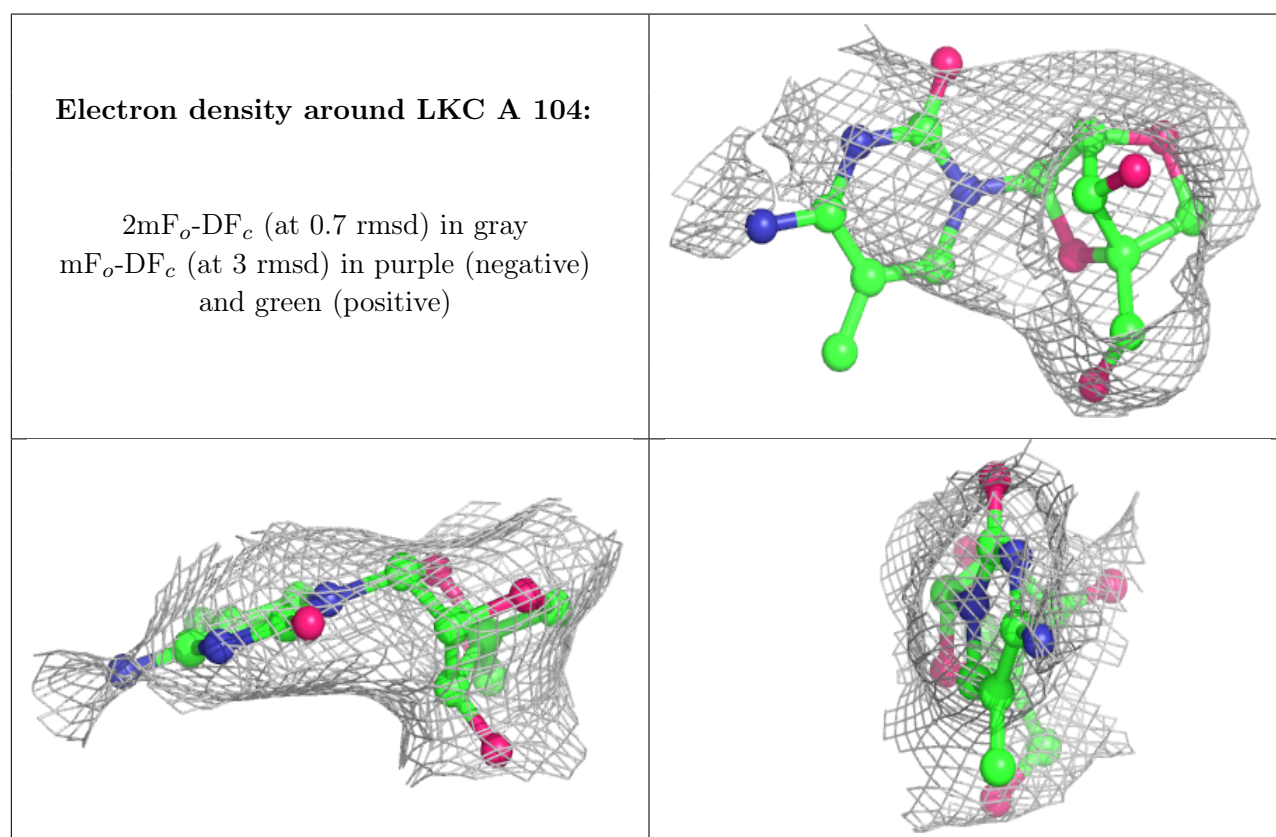
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	LKC	A	104	19/19	0.75	0.26	88,105,113,119	0
2	LCC	A	105	22/23	0.81	0.22	65,85,109,112	0
2	LCC	A	106	22/23	0.82	0.20	48,64,87,99	0
6	GP3	A	107	51/51	0.84	0.17	55,80,112,121	0
5	LKC	B	101	19/19	0.85	0.20	38,43,62,67	0
4	TG	A	103	21/22	0.87	0.18	57,67,73,80	0
3	LCG	B	104	24/25	0.89	0.16	53,65,69,71	0

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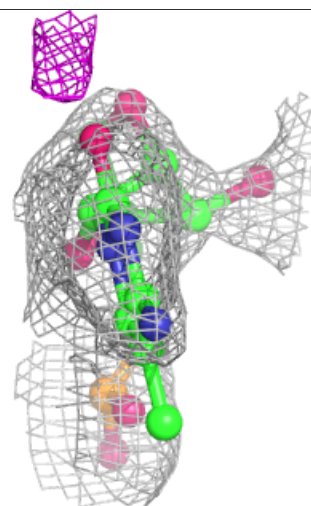
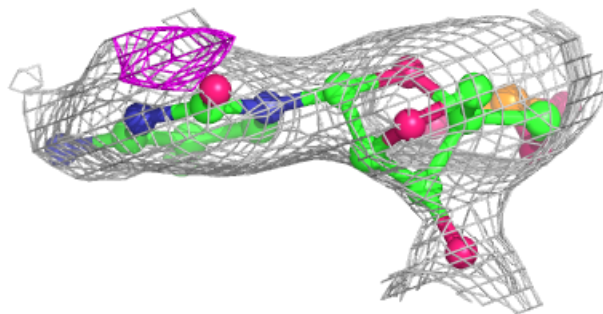
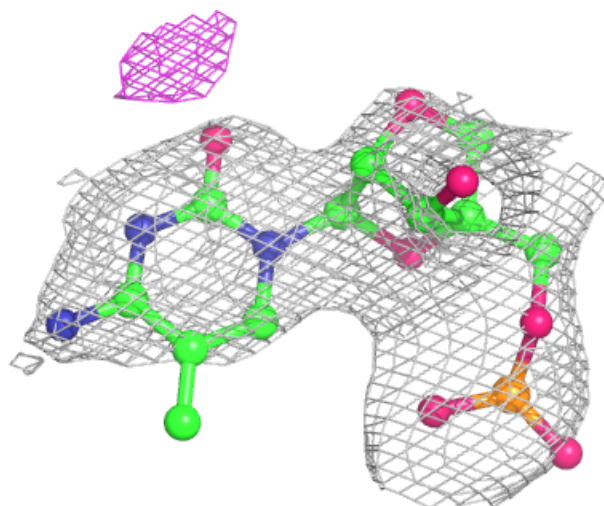
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	GP3	B	103	51/51	0.90	0.14	32,45,58,63	0
2	LCC	A	101	22/23	0.92	0.14	33,41,47,55	0
3	LCG	A	102	24/25	0.93	0.12	31,39,44,46	0
2	LCC	B	102	22/23	0.94	0.10	36,44,50,56	0
4	TG	B	105	21/22	0.95	0.12	35,42,47,52	0

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.



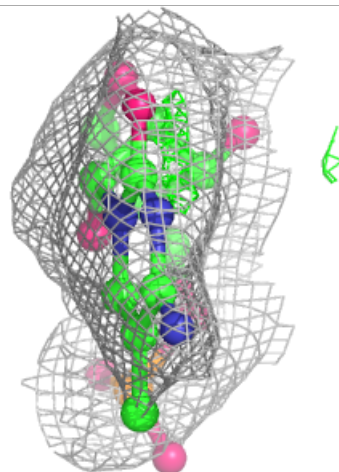
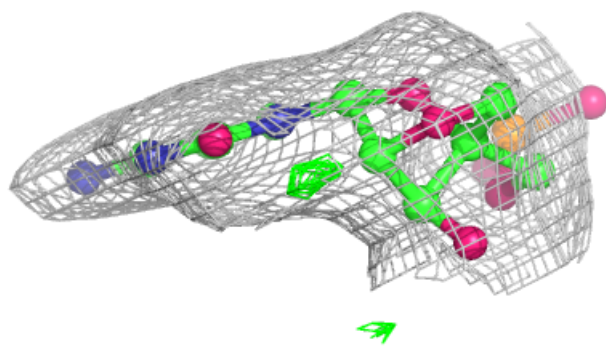
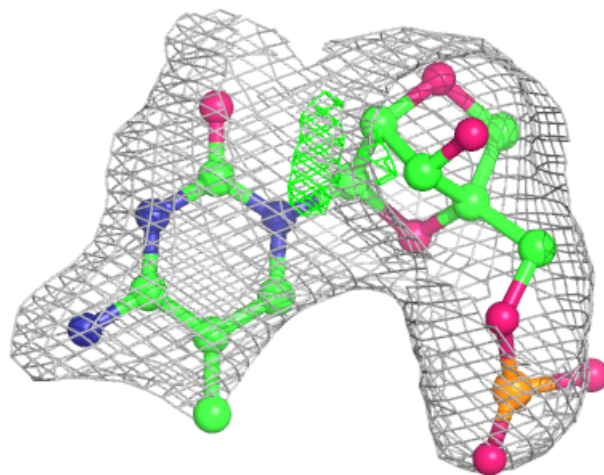
**Electron density around LCC A 105:**

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



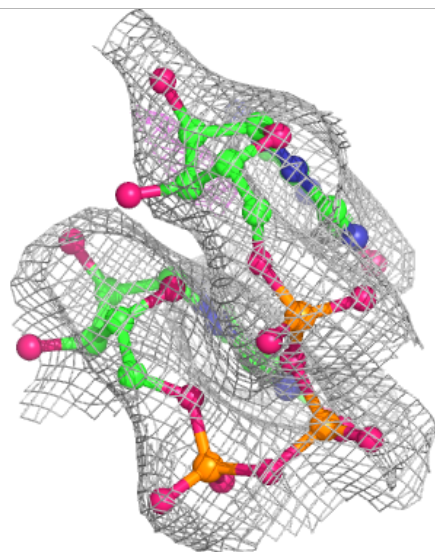
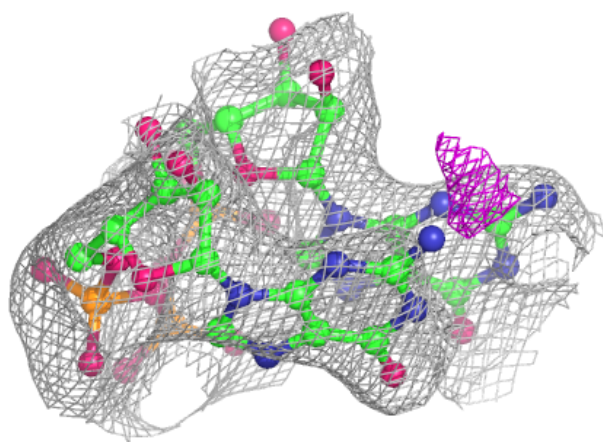
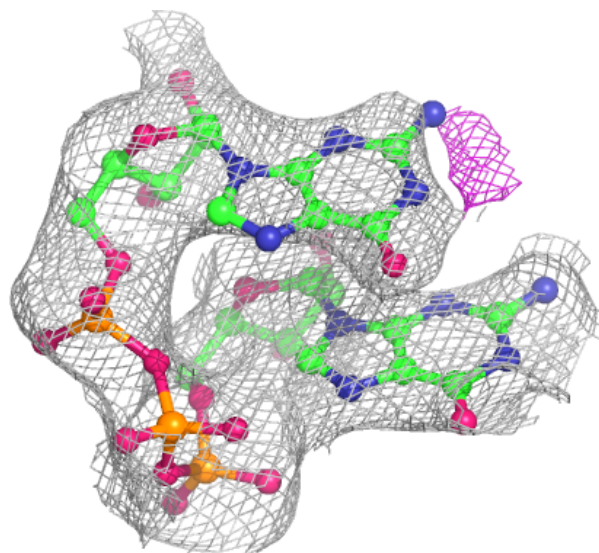
**Electron density around LCC A 106:**

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



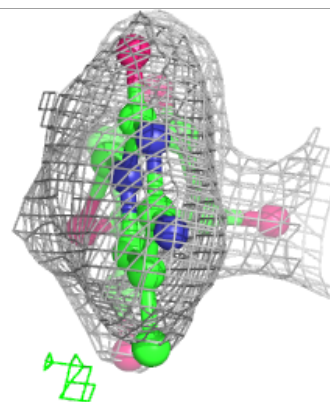
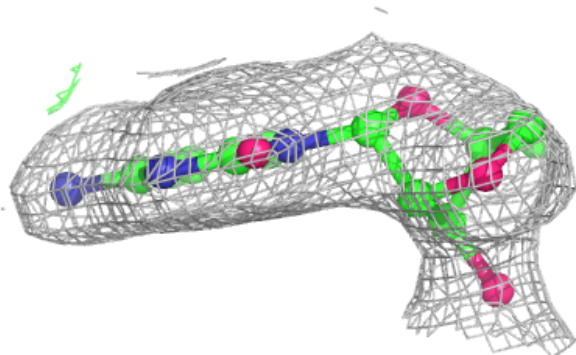
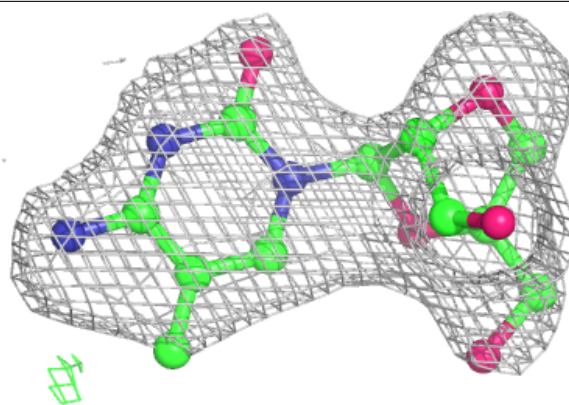
**Electron density around GP3 A 107:**

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

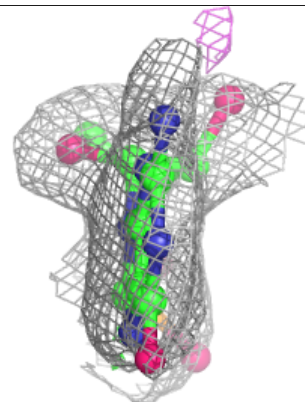
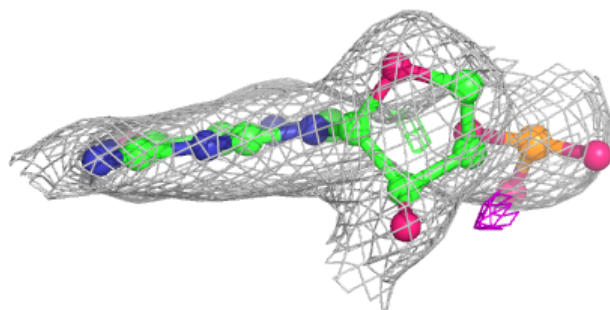
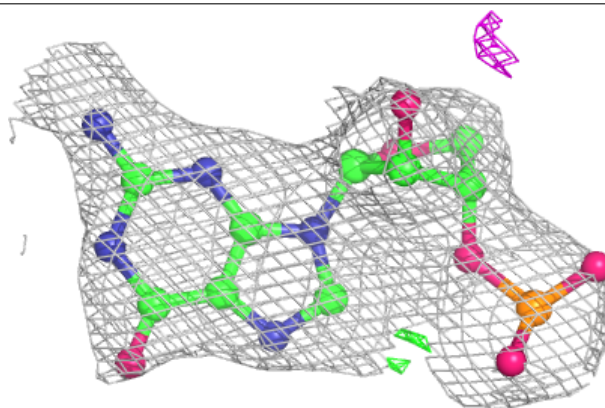


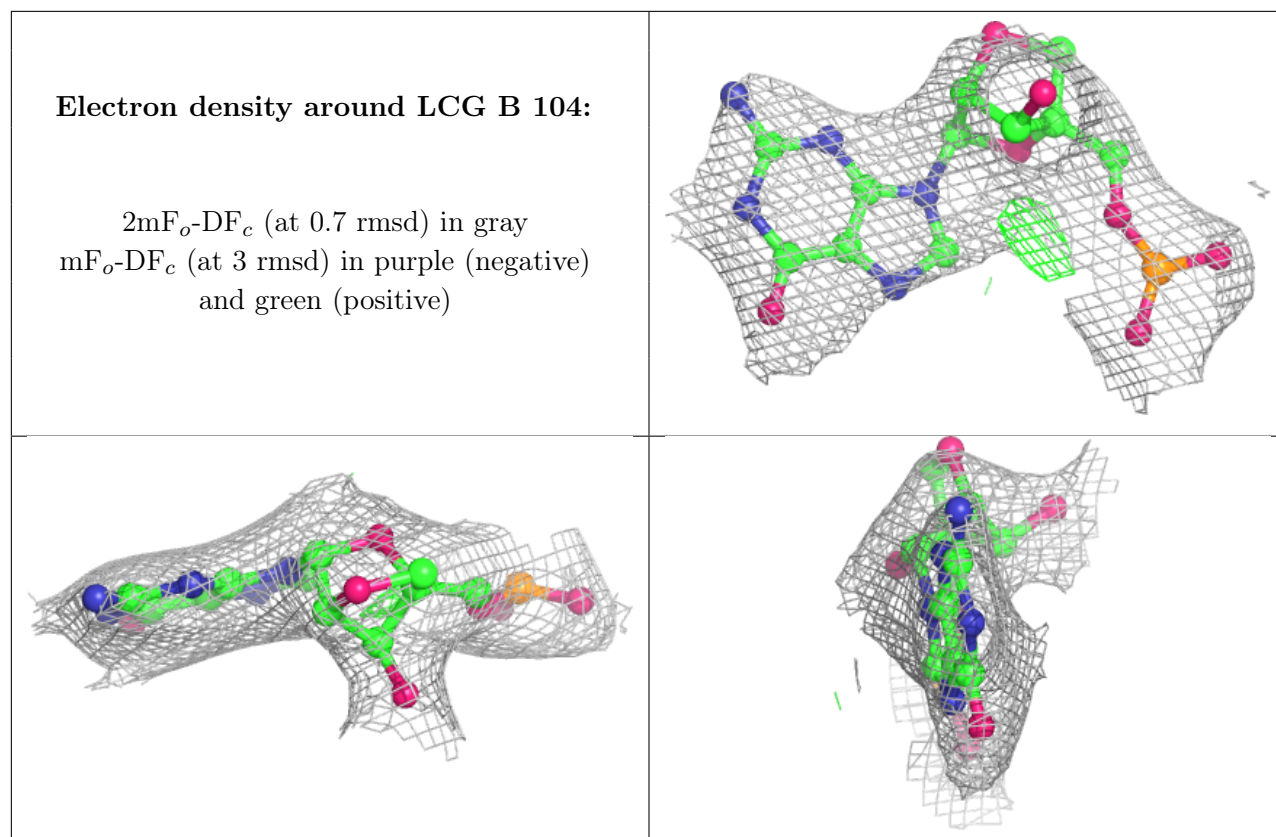
**Electron density around LKC B 101:**

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

**Electron density around TG A 103:**

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

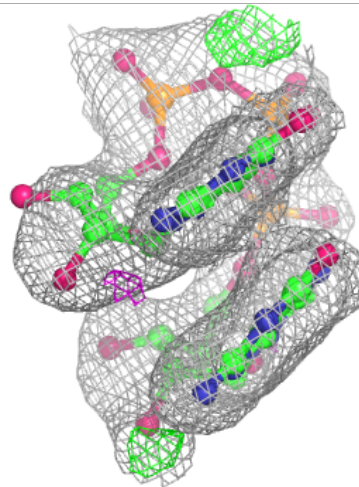
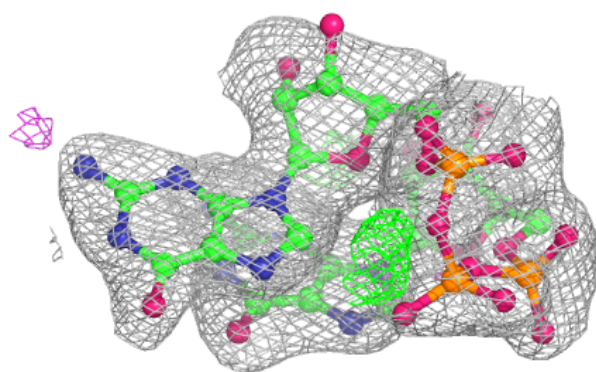
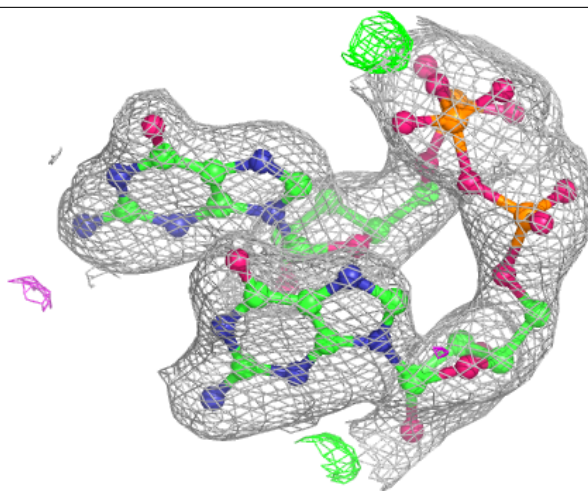






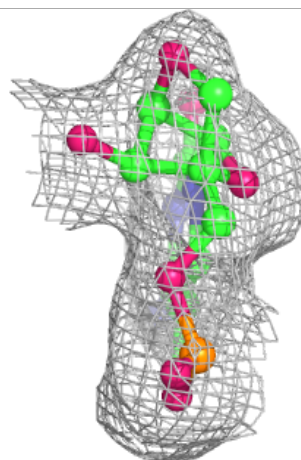
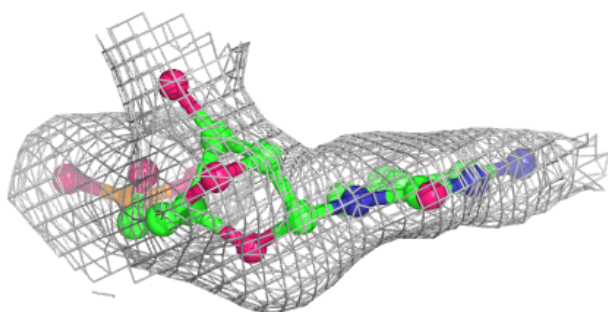
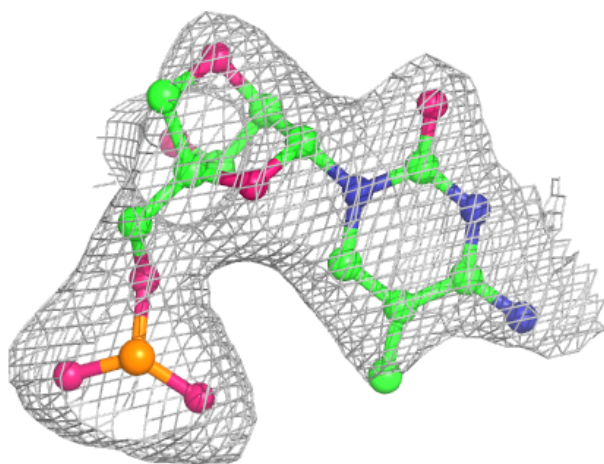
**Electron density around GP3 B 103:**

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



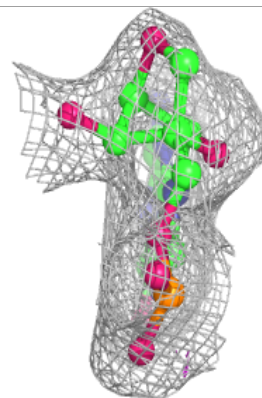
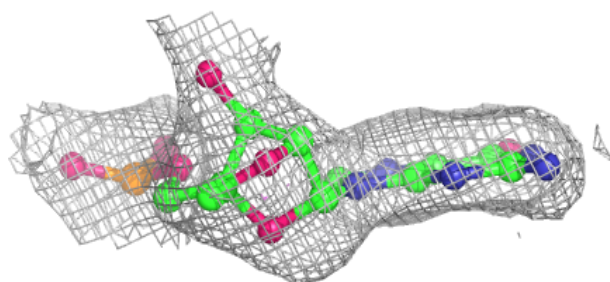
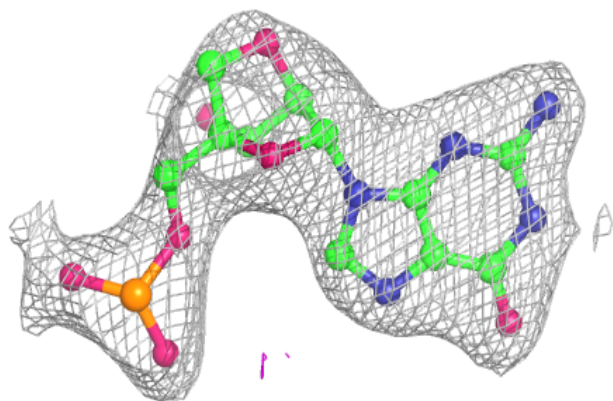
**Electron density around LCC A 101:**

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

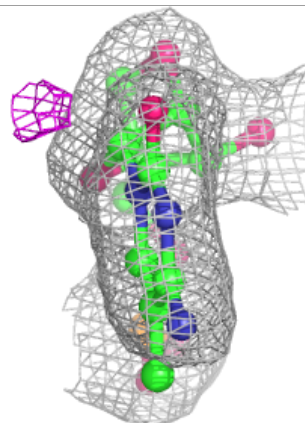
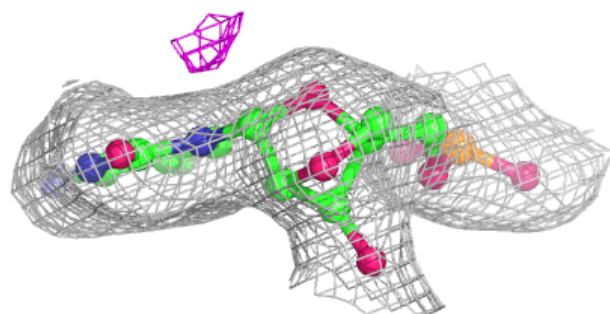
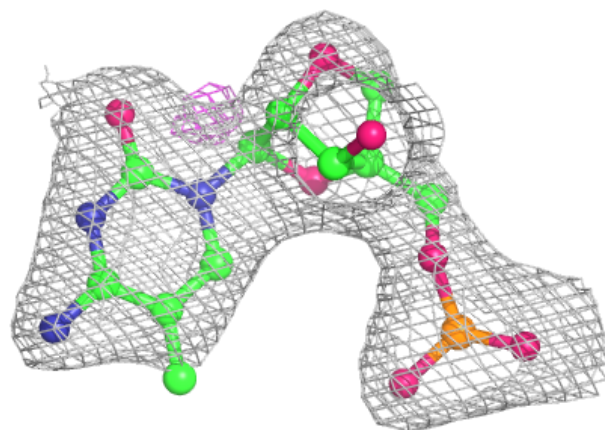


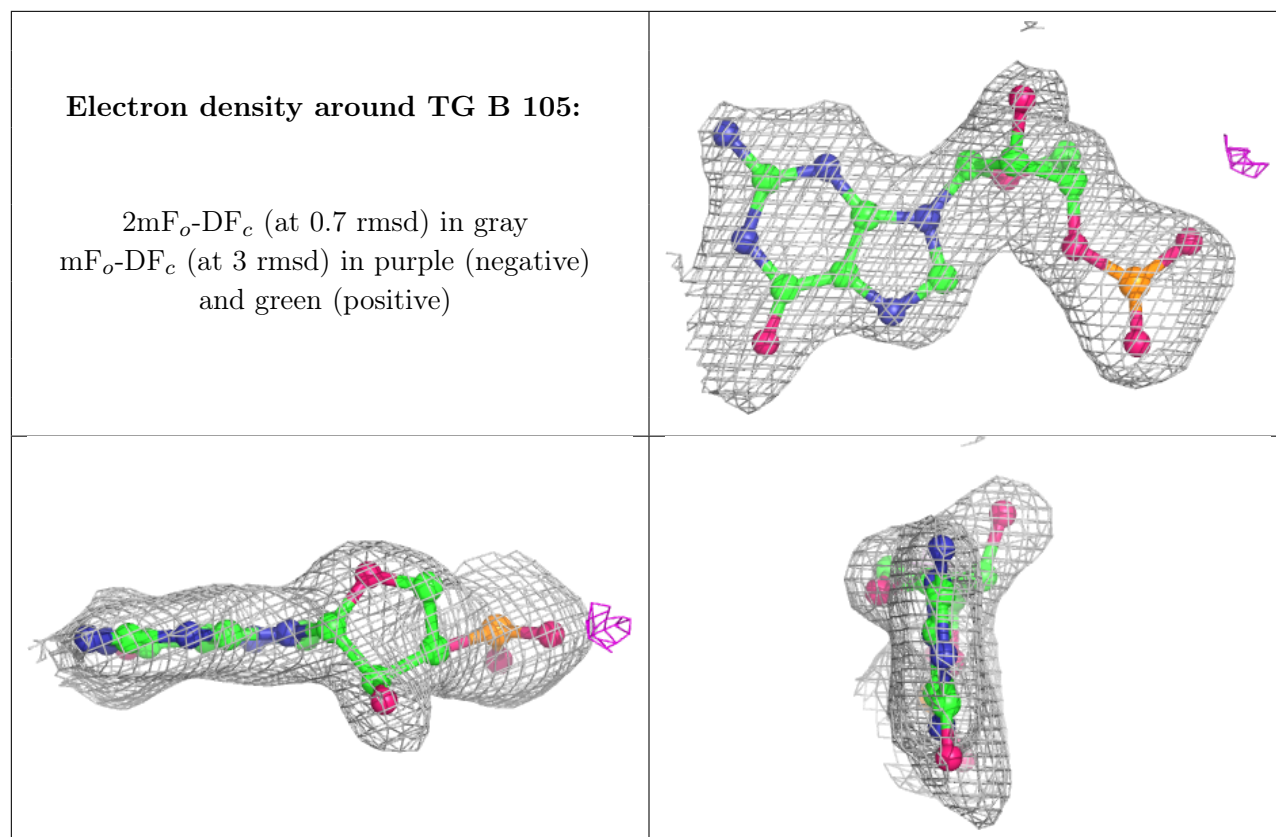
**Electron density around LCG A 102:**

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

**Electron density around 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.