



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 12:07 PM BST

PDB ID : 2F3T
Title : Crystal Structure Of E.coli Guanylate Kinase In Complex With Ganciclovir monophosphate
Authors : Hible, G.; Cherfils, J.
Deposited on : 2005-11-22
Resolution : 3.16 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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 : 2.13.1
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) : 2.13.1

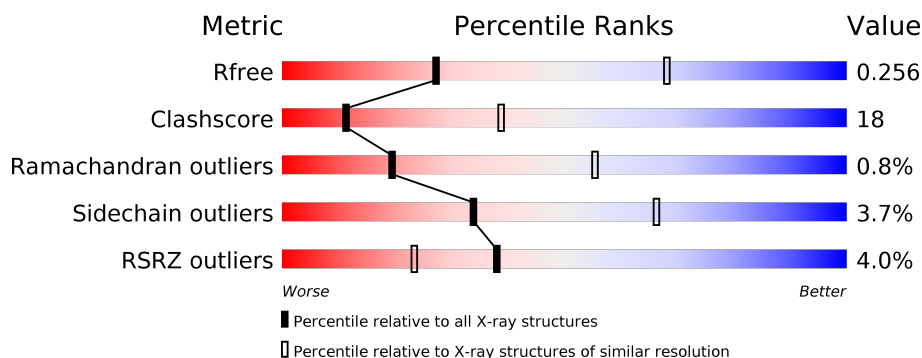
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.16 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	207	<div> <div>7%</div> <div>65%</div> <div>33%</div> <div>..</div> </div>
1	B	207	<div> <div>%</div> <div>67%</div> <div>29%</div> <div>..</div> </div>
1	C	207	<div> <div>6%</div> <div>63%</div> <div>32%</div> <div>..</div> </div>
1	D	207	<div> <div>2%</div> <div>69%</div> <div>29%</div> <div>..</div> </div>
1	E	207	<div> <div>%</div> <div>68%</div> <div>30%</div> <div>.</div> </div>
1	F	207	<div> <div>7%</div> <div>61%</div> <div>37%</div> <div>..</div> </div>

2 Entry composition [i](#)

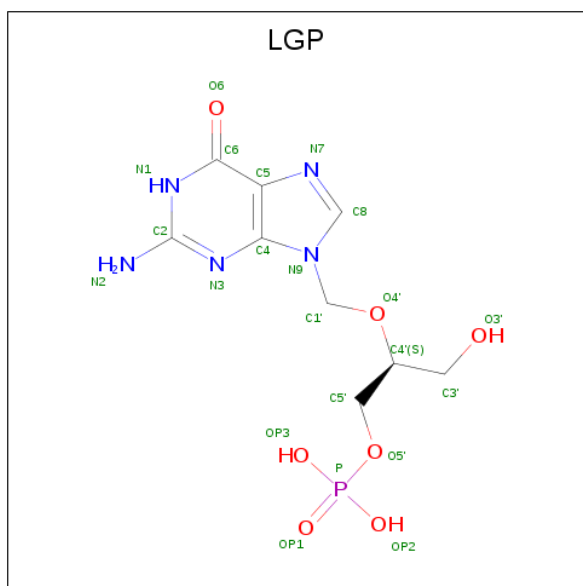
There are 3 unique types of molecules in this entry. The entry contains 9925 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Guanylate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1645	1034	296	310	5			
1	B	203	Total	C	N	O	S	0	0	0
			1632	1027	293	307	5			
1	C	201	Total	C	N	O	S	0	0	0
			1617	1019	288	305	5			
1	D	205	Total	C	N	O	S	0	0	0
			1640	1031	294	310	5			
1	E	204	Total	C	N	O	S	0	0	0
			1640	1031	295	309	5			
1	F	205	Total	C	N	O	S	0	0	0
			1638	1030	295	308	5			

- Molecule 2 is N9-1-HYDROXY-PROP-2-OXYMETHYL-GUANINE-3'-MONOPHOSPHATE (three-letter code: LGP) (formula: $C_9H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	9	5	7	1		
2	A	1	Total	C	N	O	P	0	0
			22	9	5	7	1		
2	A	1	Total	C	N	O	P	0	0
			22	9	5	7	1		
2	A	1	Total	C	N	O	P	0	0
			22	9	5	7	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	O	0	0
			3	3		
3	B	2	Total	O	0	0
			2	2		
3	C	5	Total	O	0	0
			5	5		
3	D	4	Total	O	0	0
			4	4		
3	E	6	Total	O	0	0
			6	6		
3	F	5	Total	O	0	0
			5	5		

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.

Chain A:

7% 65% 33%

MET A2 A11 A15 G16 K17 L20 L25 Q28 P29 L30 Y31 D32 T33 V35 S36 H39 T40 T41 R42 Q43 P44 R45 G46 G47 E48 V49 E52 F55 F56 F62 M65 I66 S67 R68 D69 A70 F71 L72 E73 H74 V77 F78 G79 N80 Y81 Y82 R86 I89 E90 Q91 V92 L93 A94 V97 F100 L101 D102 I103 D104 H105 Q106 Q110 I111 R112 Q113 P116 S120 I123 L135 R136 G137 Q140 D141 S142 E143 E144 V145 I146 M150 V154 Y163 L166 N169 D173 T181 I182 R183 R184 P192

Chain B:

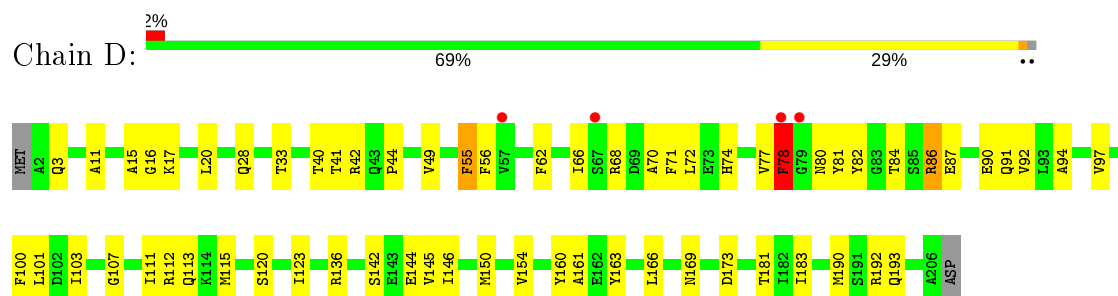
67% 29%

••

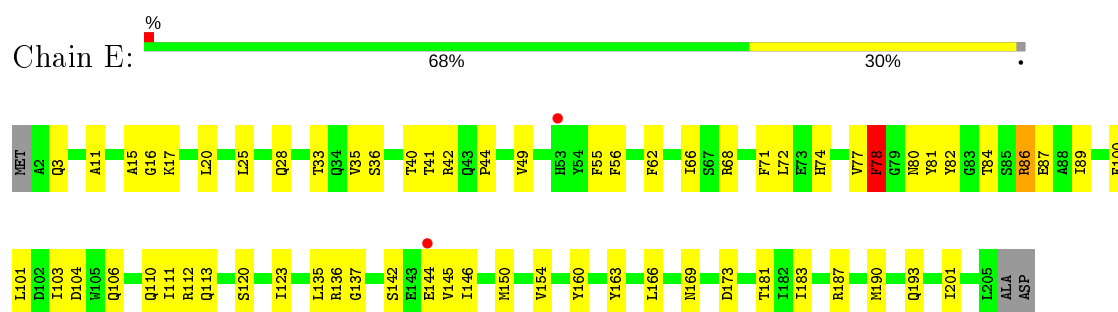
MET A2 Q3 A11 A15 G16 K17 L20 L25 Q28 P29 D32 T33 Q34 V35 T41 R42 Q43 P44 V49 Y54 F55 F56 F62 I66 S67 R68 F71 L72 E73 V77 F78 G79 N80 Y81 Y82 G83 T84 S85 R86 E87 A88 I89 E90 Q91 Y92 I93 G96 F100 F101 L101 D102 I103 G107 I111 R112 S120 I123 R136 G137 R138 GLY ASP S142 V145 I146 R149 M150 V154 Y160 Y163 M169 D170 D171 F172 D173 L179 R180 T181 I182 I183 M190 S191 R192 Q193 E207

Chain C:

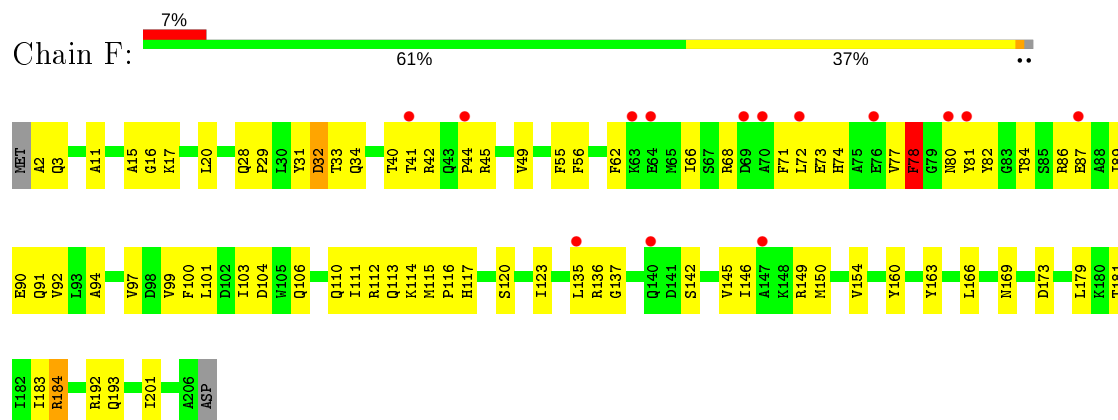
- Molecule 1: Guanylate kinase



- Molecule 1: Guanylate kinase



- Molecule 1: Guanylate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	107.75Å 107.75Å 272.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 3.16 29.89 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.96-3.16) 92.4 (29.89-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.268 , 0.290 0.237 , 0.256	Depositor DCC
R_{free} test set	1456 reflections (3.89%)	wwPDB-VP
Wilson B-factor (Å ²)	63.5	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9925	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.71% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LGP

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	0.45	0/1677	0.76	7/2264 (0.3%)
1	B	0.46	0/1663	0.97	6/2244 (0.3%)
1	C	0.46	0/1648	0.79	7/2225 (0.3%)
1	D	0.43	0/1671	0.76	6/2256 (0.3%)
1	E	0.47	0/1672	1.23	6/2257 (0.3%)
1	F	0.47	1/1670 (0.1%)	1.34	12/2255 (0.5%)
All	All	0.46	1/10001 (0.0%)	1.00	44/13501 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	192	ARG	CD-NE	-5.37	1.37	1.46

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	184	ARG	NE-CZ-NH1	-28.61	105.99	120.30
1	F	184	ARG	NE-CZ-NH2	26.48	133.54	120.30
1	E	112	ARG	NE-CZ-NH1	-25.30	107.65	120.30
1	E	112	ARG	NE-CZ-NH2	24.82	132.71	120.30
1	F	192	ARG	NE-CZ-NH1	-23.11	108.75	120.30

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	1645	0	1626	57	0
1	B	1632	0	1614	52	0
1	C	1617	0	1598	55	0
1	D	1640	0	1621	53	0
1	E	1640	0	1621	56	0
1	F	1638	0	1610	86	0
2	A	88	0	48	15	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
3	C	5	0	0	1	0
3	D	4	0	0	0	0
3	E	6	0	0	0	0
3	F	5	0	0	0	0
All	All	9925	0	9738	349	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 18.

The worst 5 of 349 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:GLN:HG2	1:C:33:THR:HB	1.43	0.99
1:F:72:LEU:HD21	1:F:115:MET:SD	2.03	0.98
2:A:302:LGP:C5'	2:A:302:LGP:H8	1.93	0.97
2:A:302:LGP:C8	2:A:302:LGP:H5''	1.94	0.97
2:A:302:LGP:H8	2:A:302:LGP:H5''	1.00	0.97

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	203/207 (98%)	182 (90%)	19 (9%)	2 (1%)	15	51
1	B	199/207 (96%)	184 (92%)	14 (7%)	1 (0%)	29	65
1	C	197/207 (95%)	180 (91%)	15 (8%)	2 (1%)	15	51
1	D	203/207 (98%)	187 (92%)	15 (7%)	1 (0%)	29	65
1	E	202/207 (98%)	184 (91%)	16 (8%)	2 (1%)	15	51
1	F	203/207 (98%)	186 (92%)	15 (7%)	2 (1%)	15	51
All	All	1207/1242 (97%)	1103 (91%)	94 (8%)	10 (1%)	19	55

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	PHE
1	B	78	PHE
1	C	78	PHE
1	D	78	PHE
1	E	78	PHE

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	175/177 (99%)	170 (97%)	5 (3%)	42	72
1	B	174/177 (98%)	166 (95%)	8 (5%)	27	60
1	C	173/177 (98%)	164 (95%)	9 (5%)	23	55
1	D	174/177 (98%)	168 (97%)	6 (3%)	37	68
1	E	175/177 (99%)	170 (97%)	5 (3%)	42	72
1	F	172/177 (97%)	166 (96%)	6 (4%)	36	67
All	All	1043/1062 (98%)	1004 (96%)	39 (4%)	34	66

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	86	ARG

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Mol	Chain	Res	Type
1	C	173	ASP
1	F	78	PHE
1	C	113	GLN
1	C	115	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	169	ASN
1	D	80	ASN
1	F	152	GLN
1	C	197	HIS
1	D	28	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	LGP	A	303	-	19,23,23	1.66	3 (15%)	20,33,33	2.35	5 (25%)
2	LGP	A	301	-	19,23,23	1.65	3 (15%)	20,33,33	2.30	6 (30%)
2	LGP	A	302	-	19,23,23	1.65	3 (15%)	20,33,33	2.38	6 (30%)
2	LGP	A	300	-	19,23,23	1.64	3 (15%)	20,33,33	2.33	9 (45%)

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	LGP	A	303	-	-	5/11/13/13	0/2/2/2
2	LGP	A	301	-	-	3/11/13/13	0/2/2/2
2	LGP	A	302	-	-	6/11/13/13	0/2/2/2
2	LGP	A	300	-	-	7/11/13/13	0/2/2/2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	303	LGP	C6-N1	4.41	1.40	1.33
2	A	300	LGP	C6-N1	4.38	1.40	1.33
2	A	301	LGP	C6-N1	4.28	1.40	1.33
2	A	302	LGP	C6-N1	4.18	1.40	1.33
2	A	301	LGP	P-OP1	3.52	1.61	1.50

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	302	LGP	C2-N3-C4	5.85	122.03	115.36
2	A	302	LGP	N3-C2-N1	-5.71	119.61	127.22
2	A	301	LGP	N3-C2-N1	-5.68	119.64	127.22
2	A	300	LGP	N3-C2-N1	-5.37	120.06	127.22
2	A	303	LGP	C2-N3-C4	5.25	121.36	115.36

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	303	LGP	C5'-O5'-P-OP1
2	A	303	LGP	C5'-O5'-P-OP2

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Mol	Chain	Res	Type	Atoms
2	A	303	LGP	C5'-O5'-P-OP3
2	A	303	LGP	C5'-C4'-O4'-C1'
2	A	301	LGP	C3'-C4'-O4'-C1'

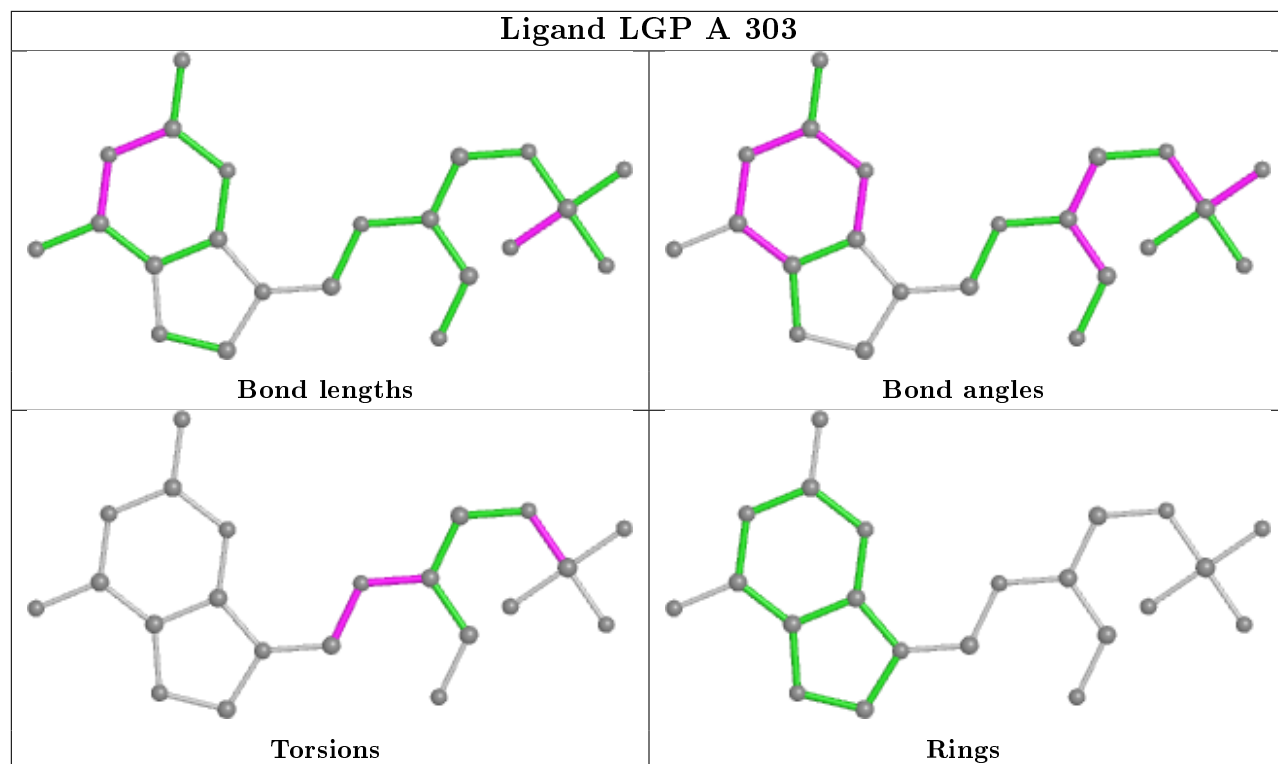
There are no ring outliers.

4 monomers are involved in 15 short contacts:

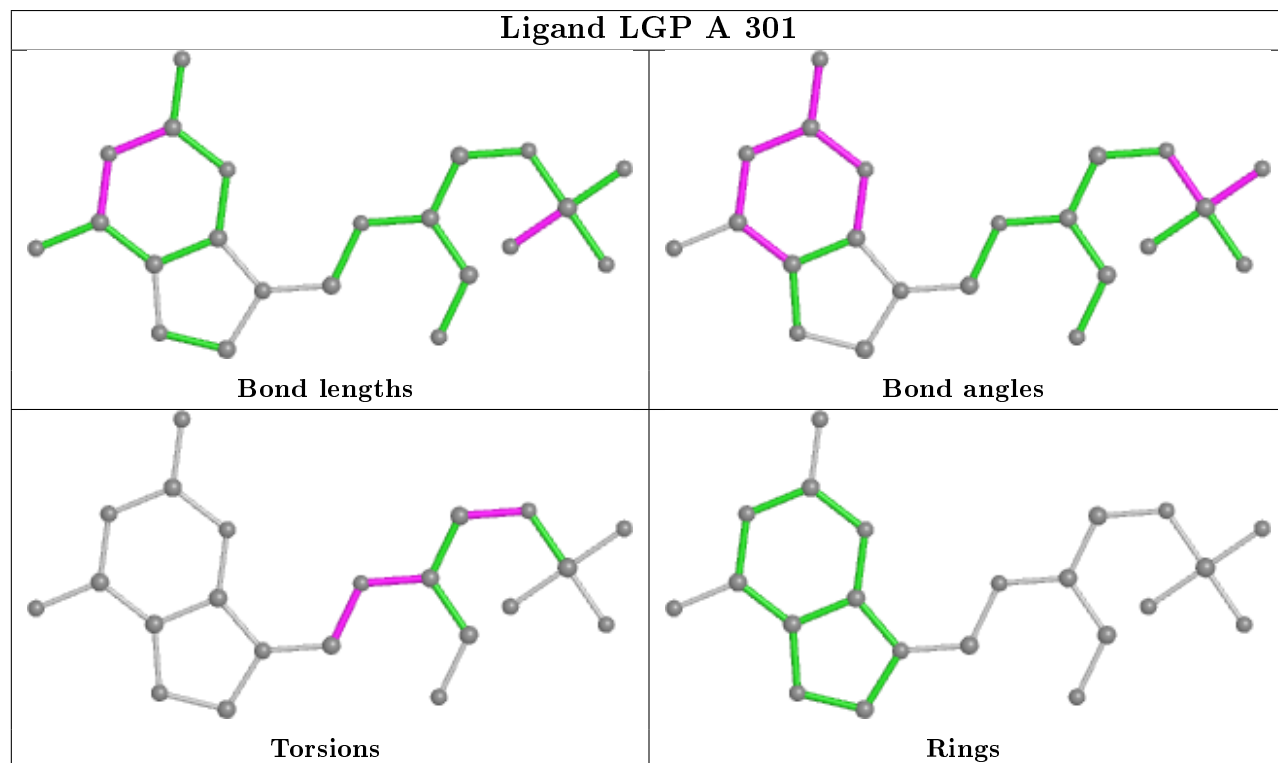
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	303	LGP	1	0
2	A	301	LGP	6	0
2	A	302	LGP	4	0
2	A	300	LGP	4	0

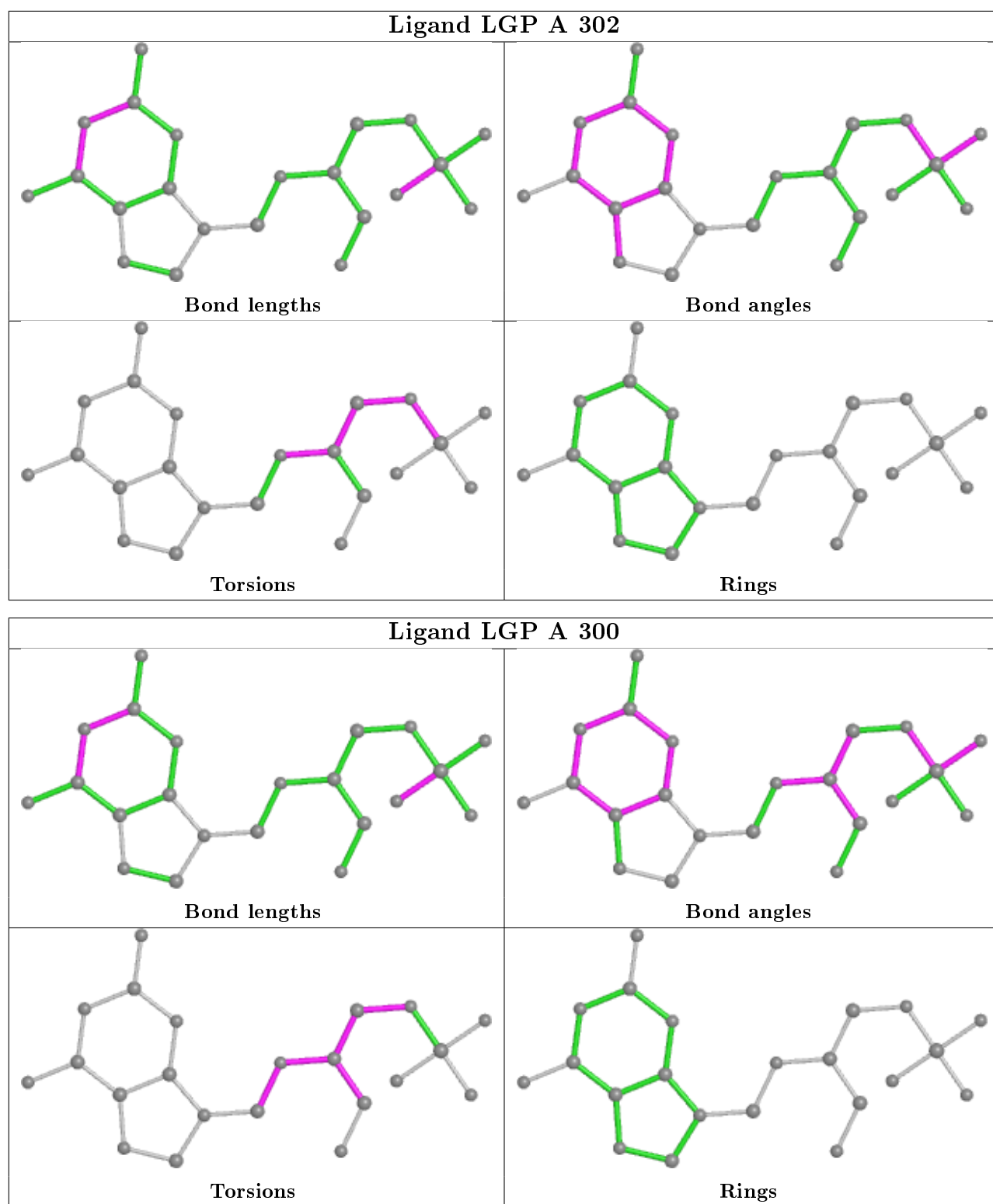
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand LGP A 303



Ligand LGP A 301





5.7 Other polymers [i](#)

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 [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, 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	205/207 (99%)	0.22	15 (7%) 15 8	22, 55, 78, 84	0
1	B	203/207 (98%)	-0.11	2 (0%) 82 73	23, 51, 76, 82	0
1	C	201/207 (97%)	0.21	12 (5%) 21 11	23, 53, 79, 85	0
1	D	205/207 (99%)	-0.00	4 (1%) 65 50	24, 57, 79, 88	0
1	E	204/207 (98%)	-0.05	2 (0%) 82 73	23, 50, 76, 82	0
1	F	205/207 (99%)	0.24	14 (6%) 17 9	23, 56, 80, 88	0
All	All	1223/1242 (98%)	0.08	49 (4%) 38 23	22, 54, 79, 88	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70	ALA	6.0
1	C	48	GLU	5.4
1	F	81	TYR	5.3
1	A	78	PHE	4.5
1	F	87	GLU	4.3

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](#)

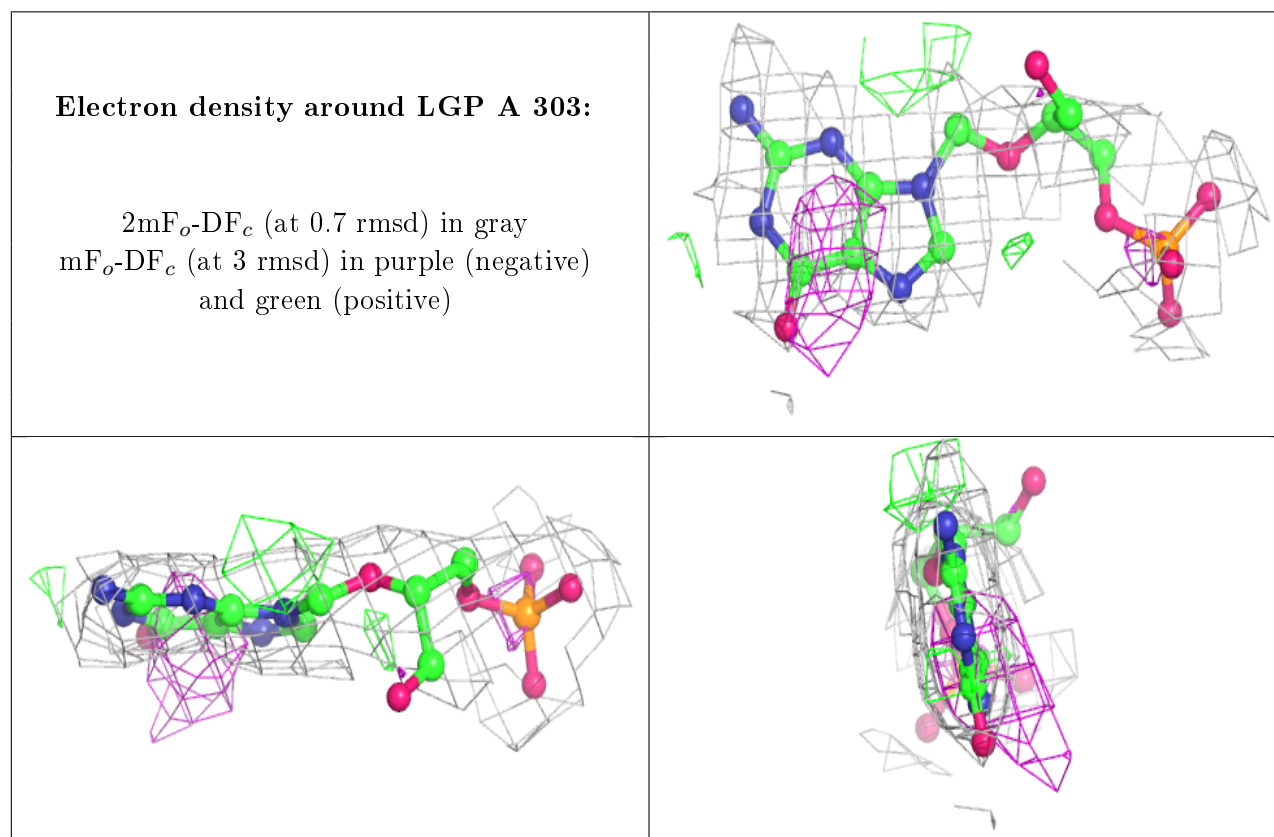
There are no monosaccharides in this entry.

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, 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.

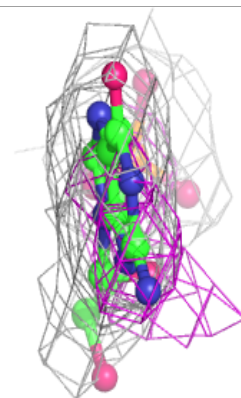
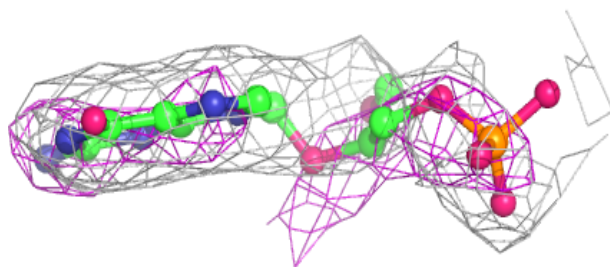
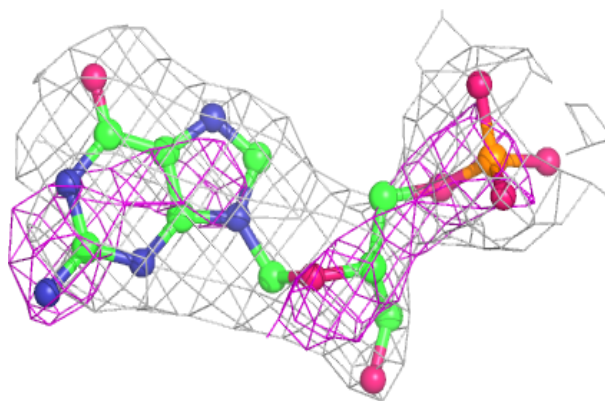
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	LGP	A	303	22/22	0.82	0.23	54,57,70,72	0
2	LGP	A	301	22/22	0.89	0.20	26,33,45,46	0
2	LGP	A	300	22/22	0.89	0.19	55,57,63,64	0
2	LGP	A	302	22/22	0.95	0.13	29,33,49,51	0

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.

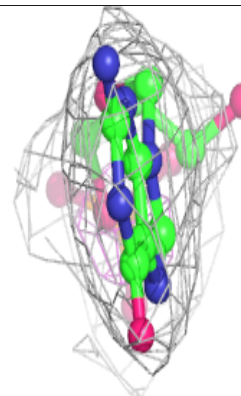
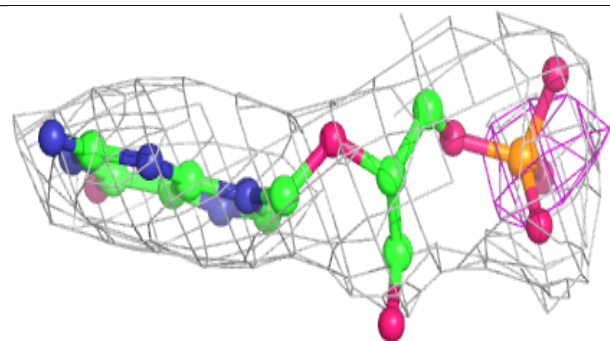
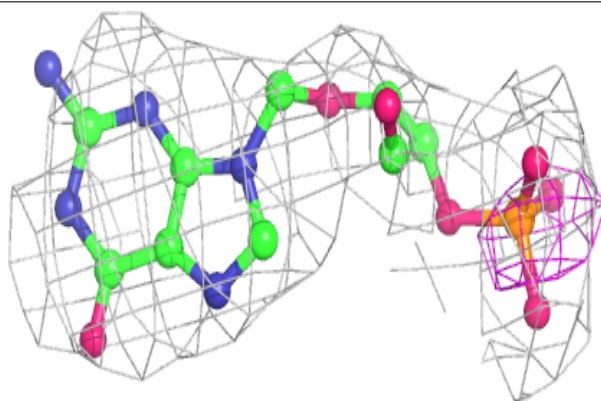


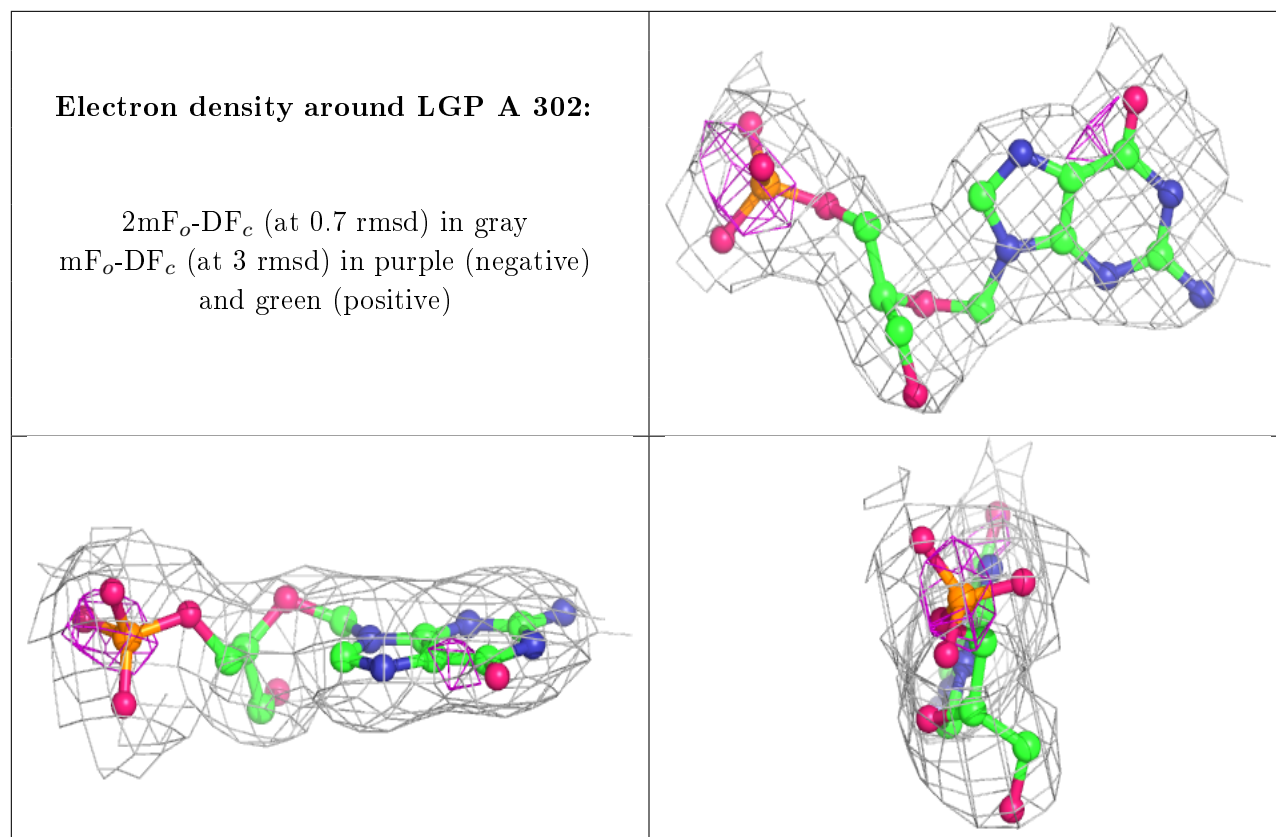
Electron density around LGP A 301:

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

**Electron density around LGP A 300:**

$2mF_o-DF_c$ (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.