



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 3, 2023 – 01:40 pm GMT

PDB ID : 2C2H
Title : CRYSTAL STRUCTURE OF THE HUMAN RAC3 IN COMPLEX WITH GDP
Authors : Debreczeni, J.E.; Yang, X.; Zao, Y.; Elkins, J.; Gileadi, C.; Burgess, N.; Colebrook, S.; Gileadi, O.; Fedorov, O.; Bunkoczi, G.; von Delft, F.; Doyle, D.; Sundstrom, M.; Arrowsmith, C.; Weigelt, J.; Edwards, A.
Deposited on : 2005-09-29
Resolution : 1.85 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

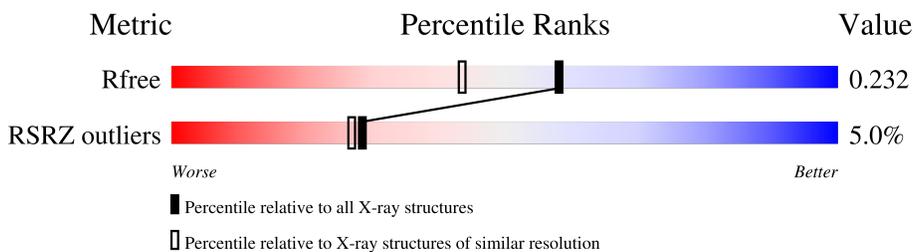
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

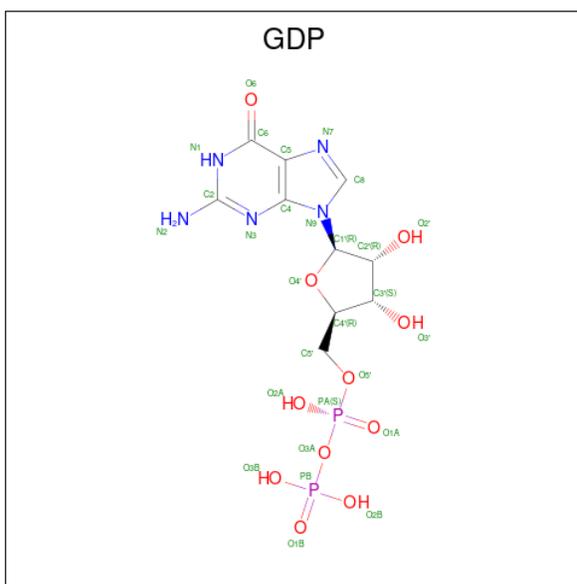
There are 6 unique types of molecules in this entry. The entry contains 3027 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RAS-RELATED C3 BOTULINUM TOXIN SUBSTRATE 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	168	Total	C	N	O	S	0	3	0
			1280	826	215	232	7			
1	B	173	Total	C	N	O	S	0	1	0
			1283	829	210	236	8			

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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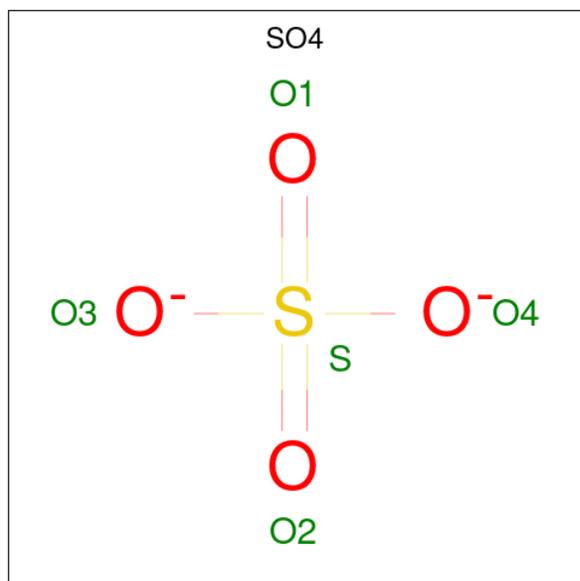
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
2	A	1	Total 37	C 10	N 5	O 18	P 4	0	1
2	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
2	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
2	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
2	B	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	6	Total Ca 6 6	0	0
3	B	6	Total Ca 6 6	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total Mg 3 3	0	0
5	B	2	Total Mg 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	105	Total O 105 105	0	0
6	B	61	Total O 61 61	0	0

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3 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	110.32Å 110.32Å 81.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	62.14 – 1.85 27.07 – 1.85	Depositor EDS
% Data completeness (in resolution range)	90.5 (62.14-1.85) 90.6 (27.07-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 1.85Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.194 , 0.229 0.198 , 0.232	Depositor DCC
R_{free} test set	1461 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtrriage
Anisotropy	0.034	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3027	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 17 are monoatomic - leaving 14 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	GDP	A	1178	5	24,30,30	1.07	1 (4%)	30,47,47	1.06	3 (10%)
2	GDP	B	1181	3	24,30,30	0.99	1 (4%)	30,47,47	1.45	7 (23%)
4	SO4	B	1187	3	4,4,4	0.44	0	6,6,6	0.34	0
2	GDP	A	1180	3,5	24,30,30	0.79	0	30,47,47	1.28	4 (13%)
4	SO4	A	1188	3	4,4,4	0.33	0	6,6,6	0.56	0
2	GDP	B	1180	3,5	24,30,30	1.07	2 (8%)	30,47,47	1.86	9 (30%)
4	SO4	B	1188	3	4,4,4	0.30	0	6,6,6	0.46	0
2	GDP	A	1182[A]	-	24,30,30	0.93	0	30,47,47	1.20	2 (6%)
2	GDP	A	1179	3,5	24,30,30	0.96	2 (8%)	30,47,47	1.44	5 (16%)
2	GDP	A	1182[B]	-	24,30,30	0.95	0	30,47,47	1.09	2 (6%)
2	GDP	B	1179	3,5	24,30,30	0.85	1 (4%)	30,47,47	1.39	5 (16%)
4	SO4	A	1189	3	4,4,4	0.70	0	6,6,6	0.43	0
2	GDP	B	1178	5	24,30,30	0.86	0	30,47,47	1.21	5 (16%)
2	GDP	A	1181	3	24,30,30	1.19	1 (4%)	30,47,47	1.13	2 (6%)

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	GDP	A	1178	5	-	0/12/32/32	0/3/3/3
2	GDP	B	1181	3	-	0/12/32/32	0/3/3/3
2	GDP	A	1180	3,5	-	1/12/32/32	0/3/3/3
2	GDP	B	1180	3,5	-	6/12/32/32	0/3/3/3
2	GDP	A	1182[A]	-	-	0/12/32/32	0/3/3/3
2	GDP	A	1179	3,5	-	0/12/32/32	0/3/3/3
2	GDP	A	1182[B]	-	-	3/12/32/32	0/3/3/3
2	GDP	B	1179	3,5	-	0/12/32/32	0/3/3/3
2	GDP	B	1178	5	-	2/12/32/32	0/3/3/3
2	GDP	A	1181	3	-	0/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1181	GDP	O4'-C1'	3.84	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1178	GDP	C6-N1	-2.96	1.33	1.37
2	B	1180	GDP	O5'-C5'	-2.93	1.33	1.44
2	B	1180	GDP	C6-N1	-2.79	1.33	1.37
2	B	1179	GDP	C6-N1	-2.33	1.34	1.37
2	A	1179	GDP	C6-N1	-2.27	1.34	1.37
2	B	1181	GDP	O4'-C1'	2.18	1.44	1.41
2	A	1179	GDP	O4'-C1'	2.02	1.43	1.41

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1180	GDP	C5'-C4'-C3'	-5.10	96.07	115.18
2	B	1179	GDP	PA-O3A-PB	-3.72	120.07	132.83
2	A	1179	GDP	O3B-PB-O3A	3.29	115.67	104.64
2	B	1180	GDP	O2A-PA-O5'	-3.26	92.59	107.75
2	A	1182[A]	GDP	PA-O3A-PB	-3.14	122.06	132.83
2	B	1180	GDP	O4'-C4'-C3'	3.14	111.32	105.11
2	A	1180	GDP	O6-C6-C5	-3.02	118.47	124.37
2	B	1181	GDP	O6-C6-C5	-2.96	118.58	124.37
2	B	1180	GDP	C8-N7-C5	2.89	108.50	102.99
2	B	1180	GDP	O3'-C3'-C2'	2.89	121.17	111.82
2	B	1178	GDP	PA-O3A-PB	-2.86	123.00	132.83
2	A	1180	GDP	C5-C6-N1	2.79	118.87	113.95
2	B	1180	GDP	C5-C6-N1	2.74	118.79	113.95
2	A	1178	GDP	PA-O3A-PB	-2.74	123.42	132.83
2	A	1179	GDP	O4'-C1'-C2'	-2.74	102.93	106.93
2	A	1178	GDP	C8-N7-C5	2.62	107.98	102.99
2	B	1179	GDP	O6-C6-C5	-2.58	119.34	124.37
2	A	1179	GDP	C5-C6-N1	2.52	118.40	113.95
2	A	1179	GDP	O6-C6-C5	-2.50	119.49	124.37
2	A	1179	GDP	PA-O3A-PB	-2.49	124.27	132.83
2	B	1181	GDP	PA-O3A-PB	-2.48	124.33	132.83
2	B	1181	GDP	O3A-PB-O1B	-2.41	97.82	111.19
2	B	1178	GDP	O3B-PB-O3A	2.41	112.71	104.64
2	B	1181	GDP	O6-C6-N1	2.41	123.49	120.65
2	B	1179	GDP	C5-C6-N1	2.39	118.18	113.95
2	A	1180	GDP	N2-C2-N3	-2.35	115.17	119.74
2	A	1181	GDP	O3B-PB-O2B	2.33	116.55	107.64
2	A	1181	GDP	C5-C6-N1	2.30	118.02	113.95
2	B	1180	GDP	O5'-PA-O1A	2.29	118.03	109.07
2	A	1182[A]	GDP	N2-C2-N1	2.26	121.53	116.71
2	A	1182[B]	GDP	N2-C2-N1	2.26	121.53	116.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1181	GDP	C5-C6-N1	2.25	117.92	113.95
2	B	1179	GDP	O2B-PB-O3A	2.23	112.13	104.64
2	B	1181	GDP	O3B-PB-O3A	2.19	111.99	104.64
2	A	1178	GDP	N2-C2-N3	-2.19	115.47	119.74
2	B	1181	GDP	O2B-PB-O3A	2.18	111.96	104.64
2	B	1178	GDP	C5-C6-N1	2.11	117.69	113.95
2	A	1180	GDP	N2-C2-N1	2.09	121.16	116.71
2	B	1178	GDP	O6-C6-C5	-2.09	120.30	124.37
2	B	1179	GDP	C8-N7-C5	2.08	106.95	102.99
2	B	1180	GDP	C2-N1-C6	-2.06	121.30	125.10
2	A	1182[B]	GDP	O3B-PB-O3A	2.06	111.53	104.64
2	B	1178	GDP	C8-N7-C5	2.02	106.84	102.99
2	B	1180	GDP	O2B-PB-O1B	2.01	118.57	110.68

There are no chirality outliers.

All (12) torsion outliers are listed below:

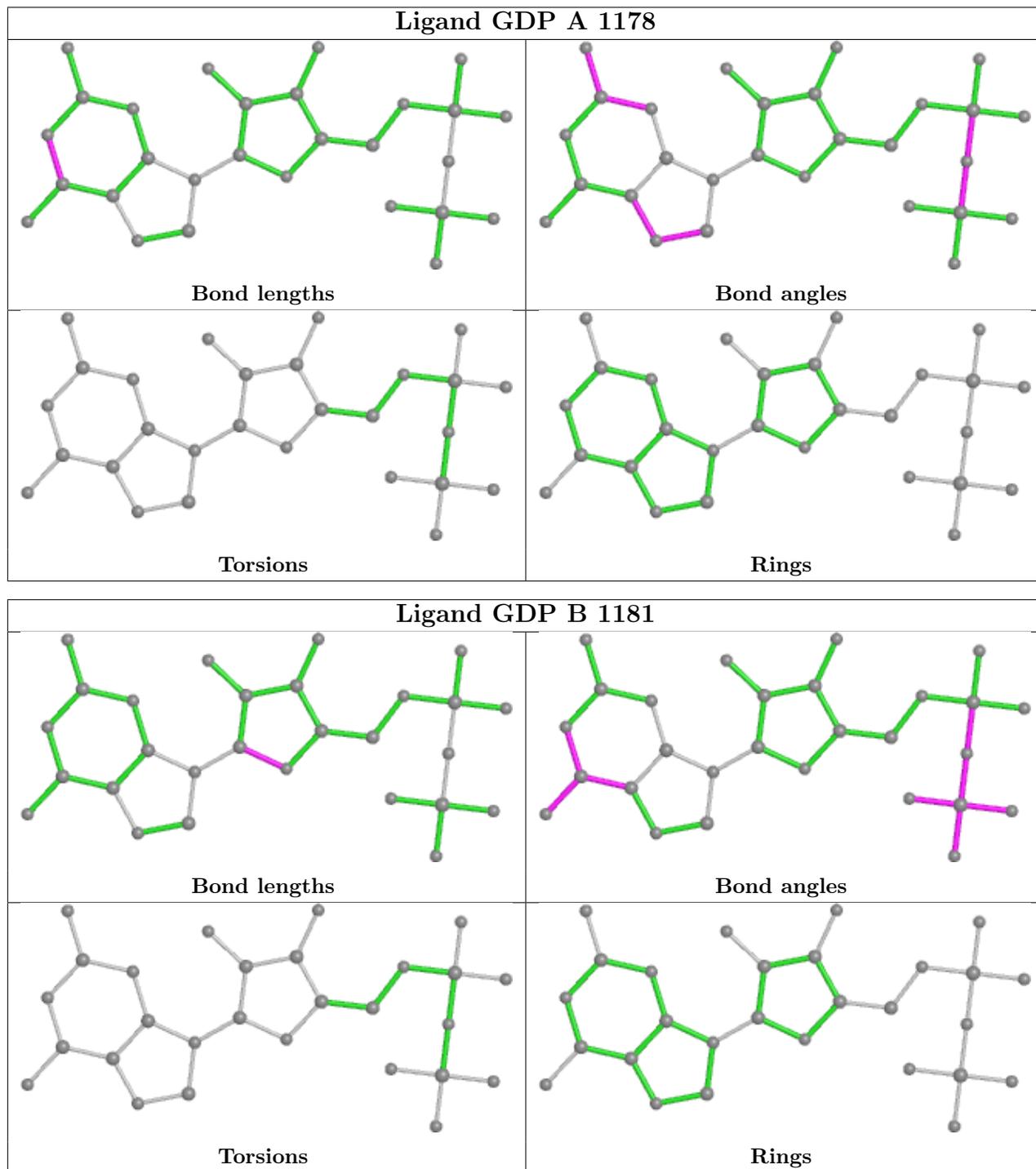
Mol	Chain	Res	Type	Atoms
2	A	1180	GDP	PA-O3A-PB-O3B
2	A	1182[B]	GDP	C5'-O5'-PA-O3A
2	A	1182[B]	GDP	C5'-O5'-PA-O1A
2	A	1182[B]	GDP	C5'-O5'-PA-O2A
2	B	1180	GDP	PA-O3A-PB-O3B
2	B	1178	GDP	PA-O3A-PB-O1B
2	B	1178	GDP	PA-O3A-PB-O2B
2	B	1180	GDP	C5'-O5'-PA-O3A
2	B	1180	GDP	C5'-O5'-PA-O1A
2	B	1180	GDP	C5'-O5'-PA-O2A
2	B	1180	GDP	PA-O3A-PB-O1B
2	B	1180	GDP	PA-O3A-PB-O2B

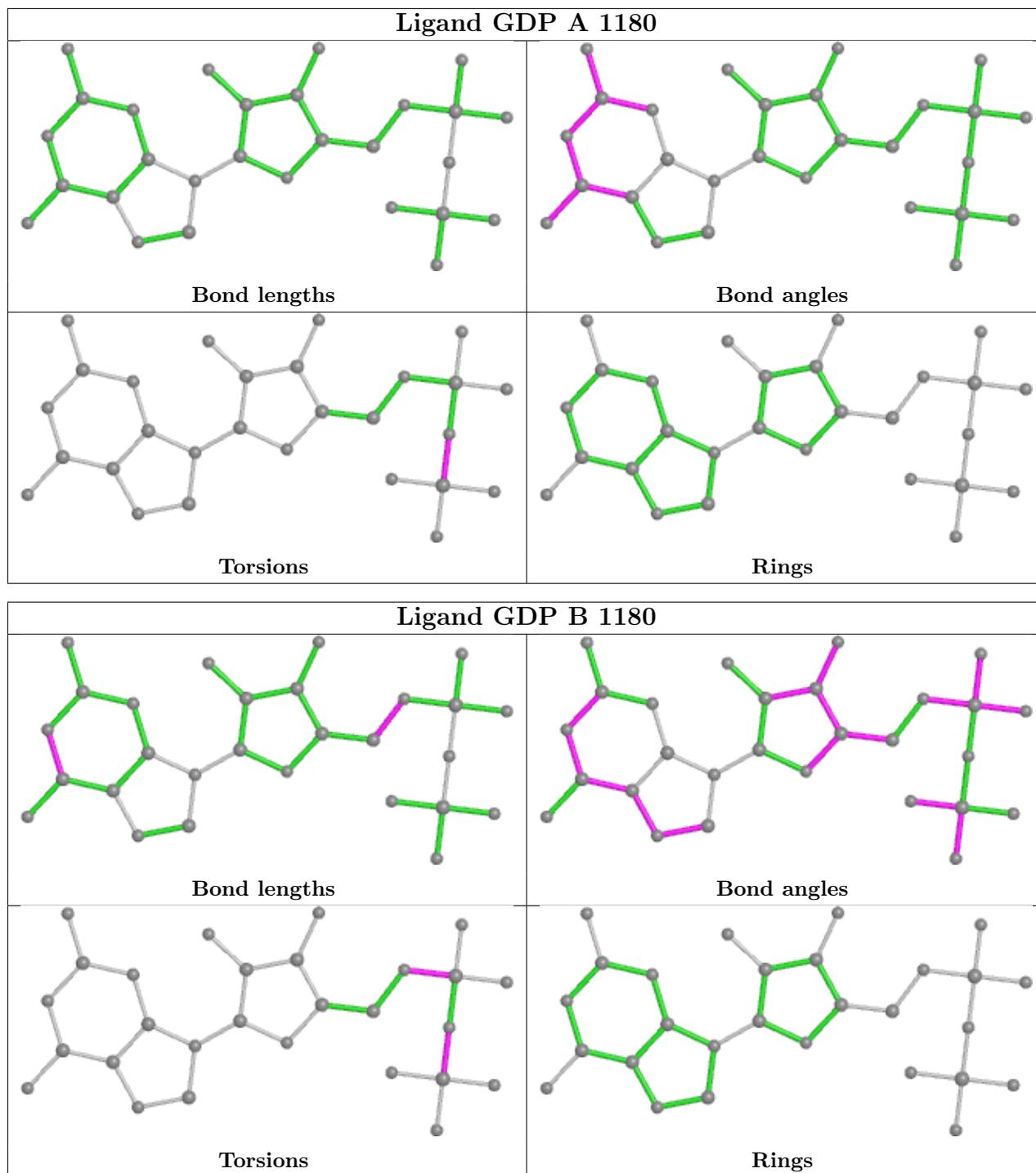
There are no ring outliers.

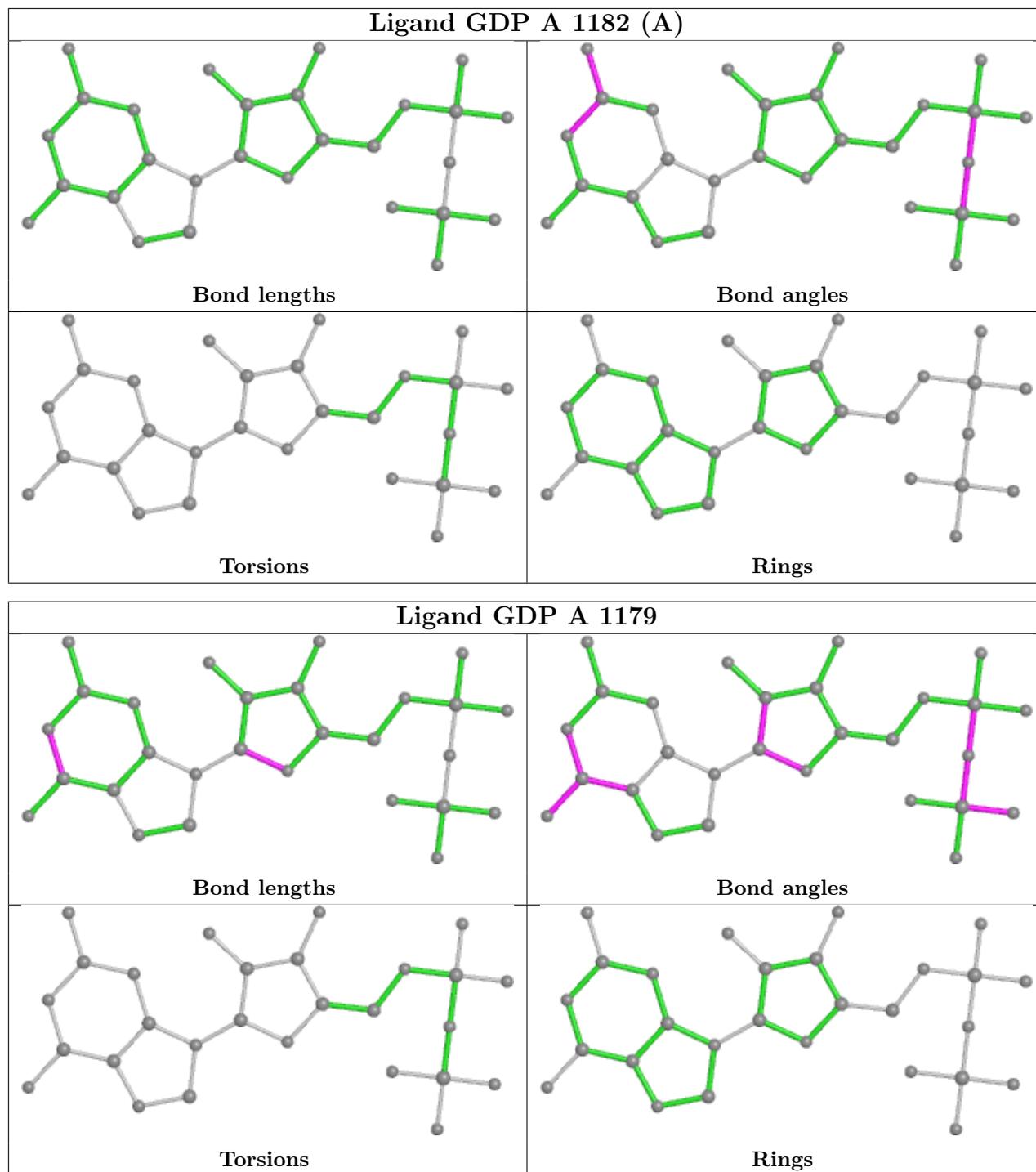
No monomer is involved in short contacts.

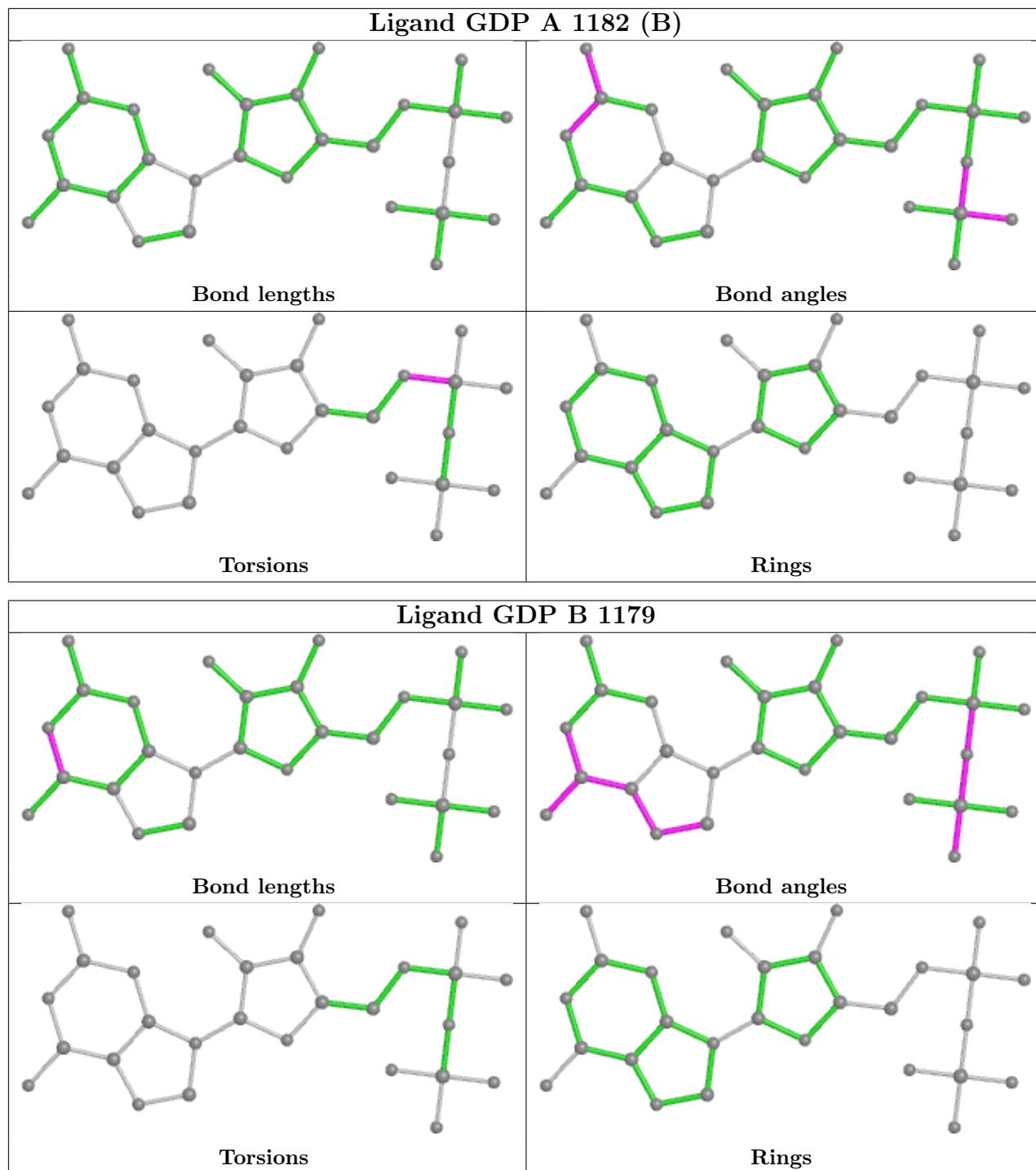
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

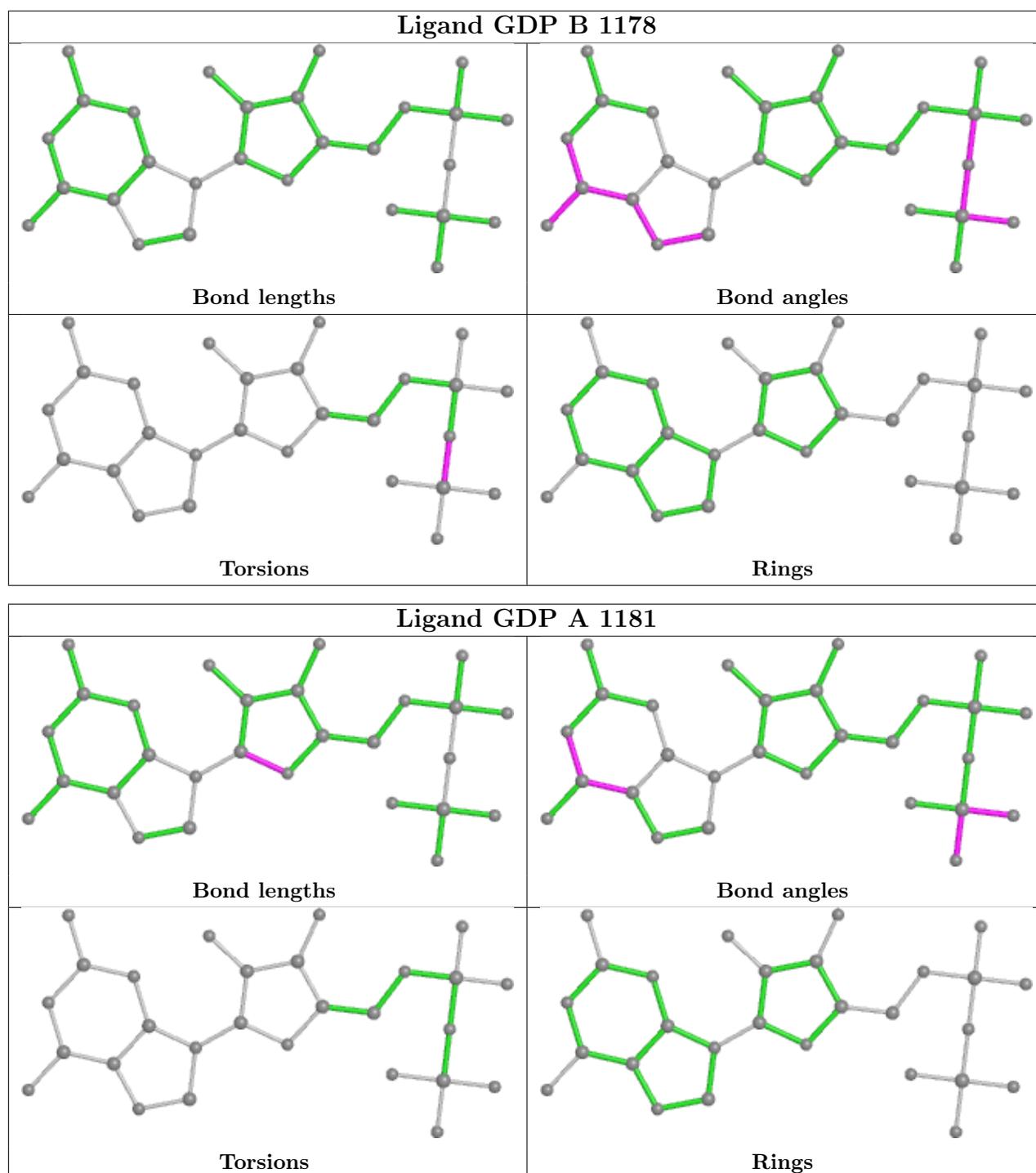
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents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











4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 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	168/192 (87%)	0.30	6 (3%) 42 40	19, 25, 33, 36	0
1	B	173/192 (90%)	0.47	11 (6%) 19 18	20, 25, 32, 43	0
All	All	341/384 (88%)	0.38	17 (4%) 28 27	19, 25, 33, 43	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	32	TYR	3.6
1	A	131	ASP	3.4
1	B	131	ASP	2.9
1	B	1	MET	2.8
1	B	48	GLY	2.6
1	B	130	ARG	2.6
1	A	30	GLY	2.6
1	B	80	ILE	2.6
1	A	80	ILE	2.5
1	B	128	ARG	2.4
1	A	113	VAL	2.4
1	A	9	VAL	2.4
1	A	7	VAL	2.3
1	B	121	ASP	2.3
1	B	126	ILE	2.1
1	B	129	LEU	2.1
1	B	79	LEU	2.1

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

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

5.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.4 Ligands [i](#)

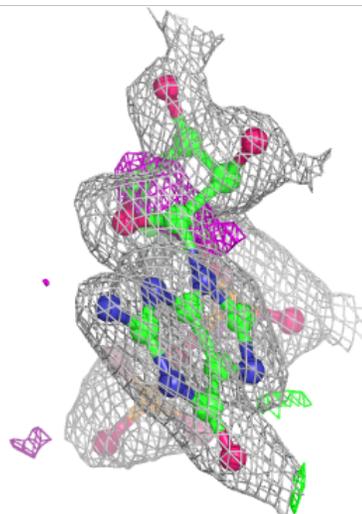
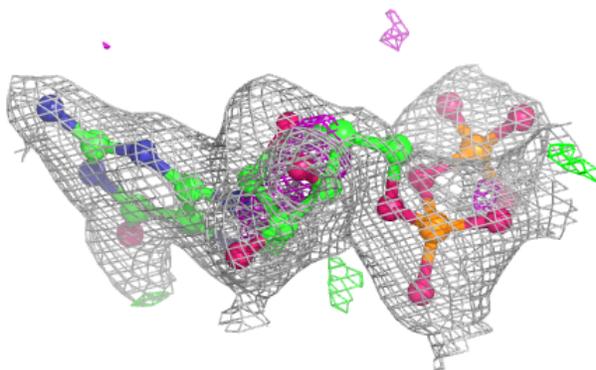
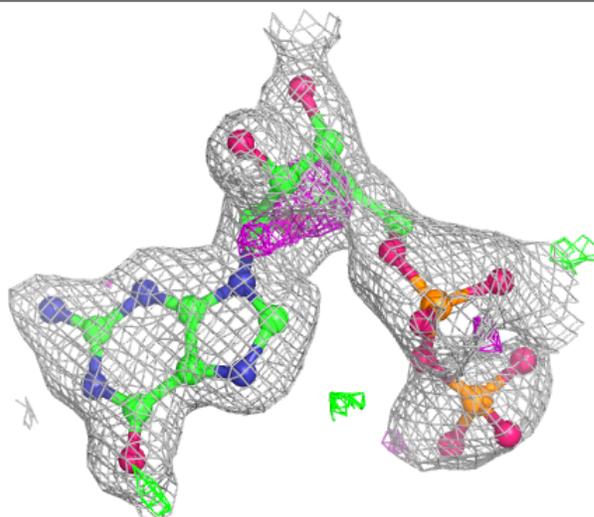
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GDP	A	1182[A]	28/28	0.87	0.19	39,43,56,56	9
2	GDP	A	1182[B]	28/28	0.87	0.19	39,43,54,54	9
2	GDP	B	1179	28/28	0.94	0.19	26,42,43,45	0
4	SO4	B	1187	5/5	0.94	0.14	25,26,27,30	0
5	MG	B	1189	1/1	0.94	0.09	30,30,30,30	0
5	MG	B	1190	1/1	0.95	0.05	26,26,26,26	0
4	SO4	A	1188	5/5	0.96	0.16	18,20,22,23	0
2	GDP	B	1180	28/28	0.96	0.08	21,24,27,29	0
2	GDP	A	1179	28/28	0.97	0.14	17,31,34,38	0
5	MG	A	1191	1/1	0.97	0.12	20,20,20,20	0
2	GDP	A	1180	28/28	0.97	0.06	13,16,21,22	0
2	GDP	B	1178	28/28	0.97	0.07	25,33,34,34	0
4	SO4	A	1189	5/5	0.98	0.12	15,19,21,21	0
2	GDP	A	1178	28/28	0.98	0.05	17,19,22,24	0
4	SO4	B	1188	5/5	0.98	0.17	30,30,34,34	0
5	MG	A	1190	1/1	0.98	0.03	17,17,17,17	0
2	GDP	B	1181	28/28	0.98	0.07	16,21,23,23	0
3	CA	A	1187	1/1	0.98	0.05	24,24,24,24	1
2	GDP	A	1181	28/28	0.98	0.07	14,15,18,18	0
3	CA	B	1182	1/1	0.99	0.06	14,14,14,14	0
3	CA	B	1183	1/1	0.99	0.08	12,12,12,12	0
3	CA	B	1184	1/1	0.99	0.03	24,24,24,24	0
3	CA	B	1185	1/1	0.99	0.07	14,14,14,14	0
3	CA	B	1186	1/1	0.99	0.12	30,30,30,30	1
5	MG	A	1192	1/1	0.99	0.15	23,23,23,23	0
3	CA	B	1191	1/1	0.99	0.04	17,17,17,17	0
3	CA	A	1183	1/1	0.99	0.05	17,17,17,17	0
3	CA	A	1193	1/1	1.00	0.03	10,10,10,10	0
3	CA	A	1185	1/1	1.00	0.10	6,6,6,6	0
3	CA	A	1186	1/1	1.00	0.06	8,8,8,8	0
3	CA	A	1184	1/1	1.00	0.07	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.

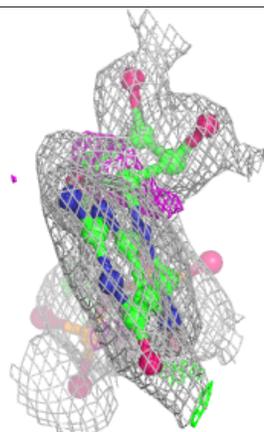
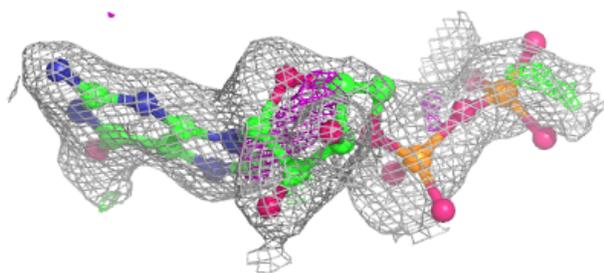
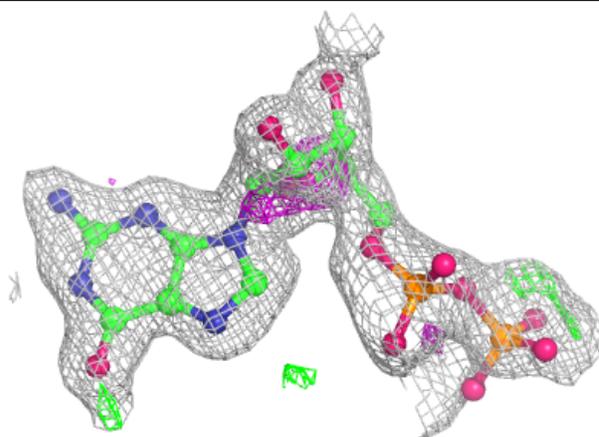
Electron density around GDP A 1182 (A):

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

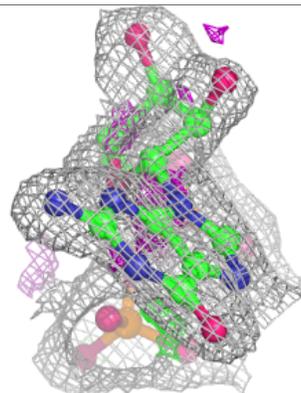
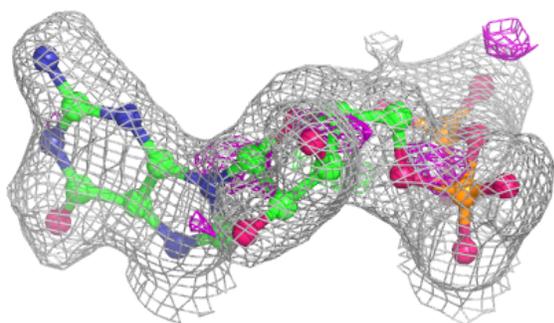
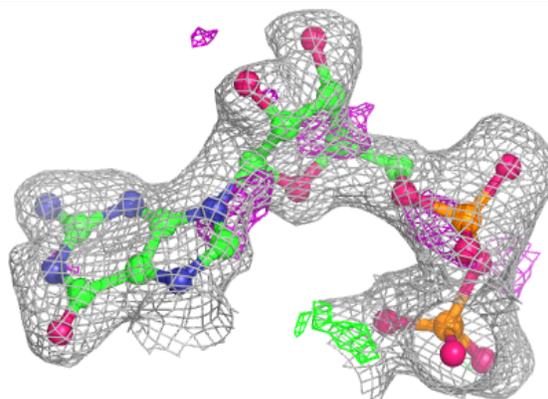


Electron density around GDP A 1182 (B):

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

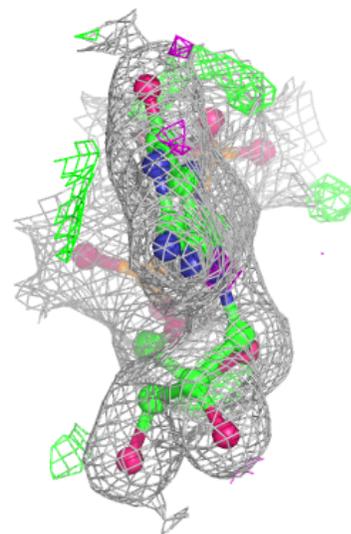
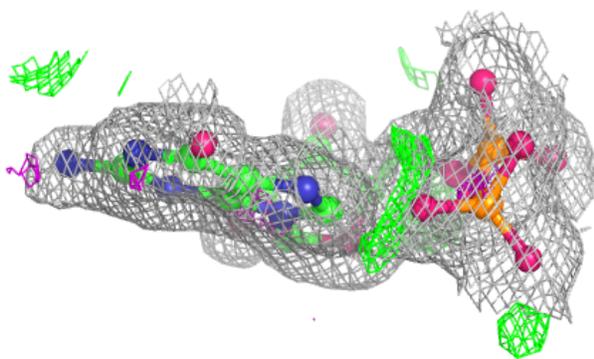
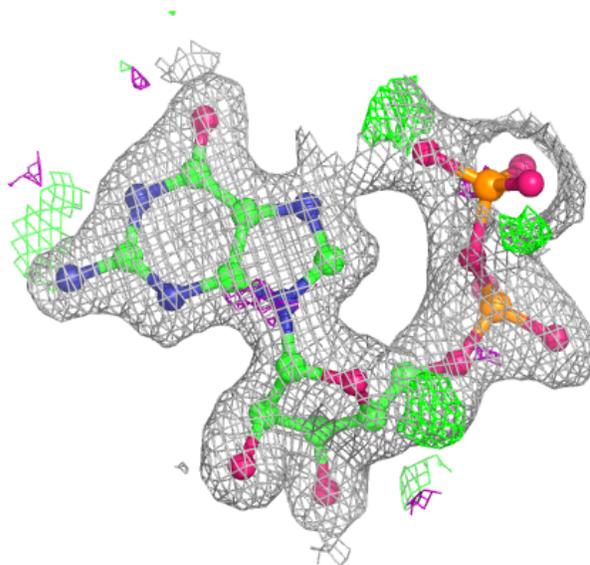
**Electron density around GDP B 1179:**

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



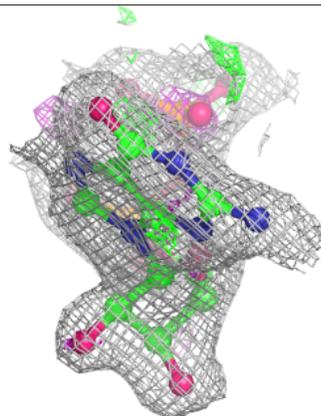
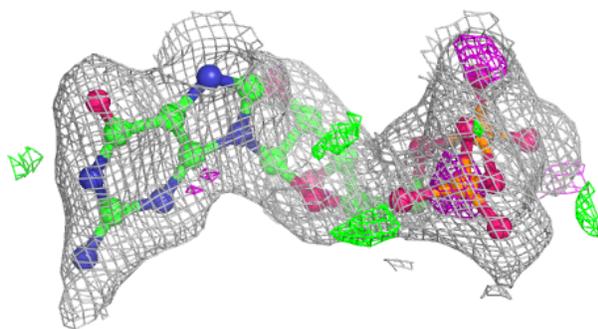
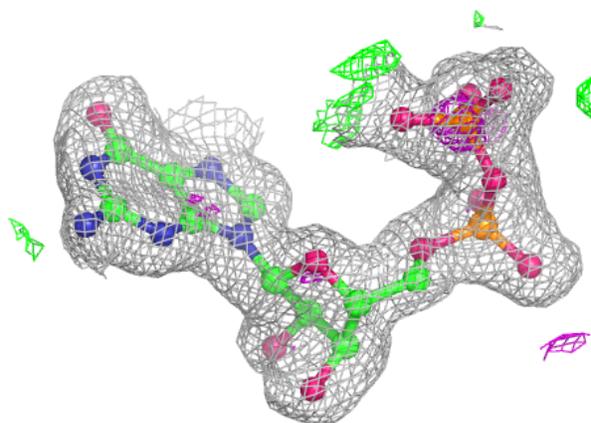
Electron density around GDP B 1180:

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



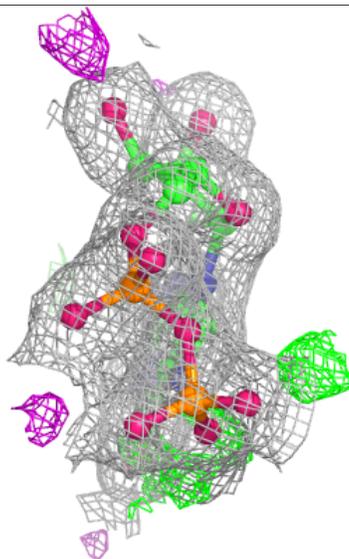
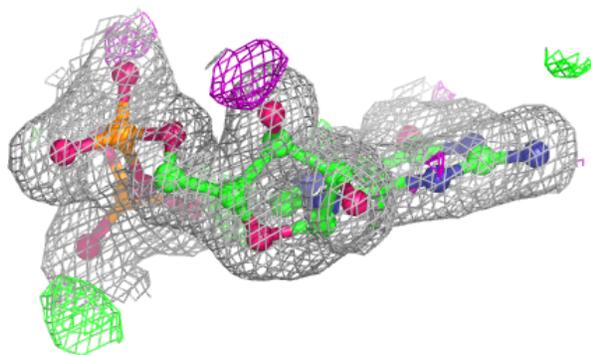
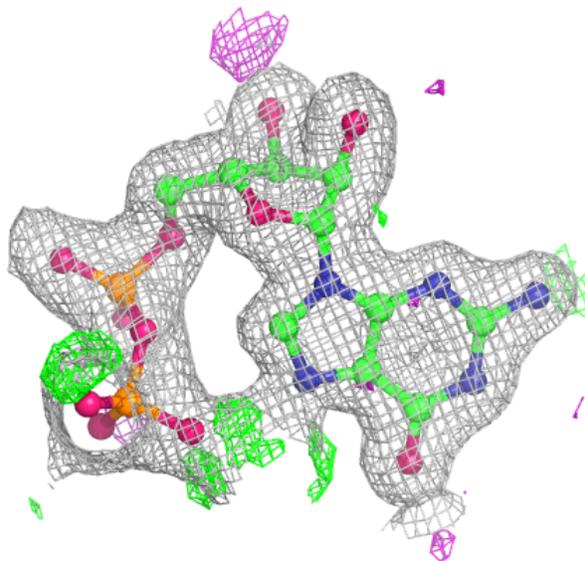
Electron density around GDP A 1179:

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



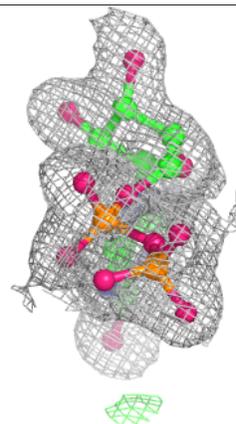
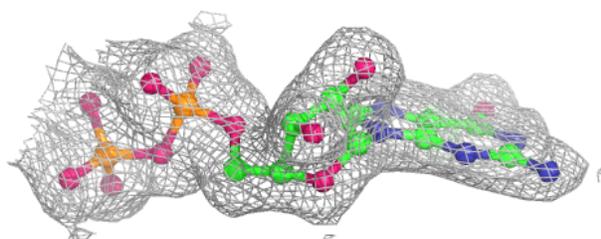
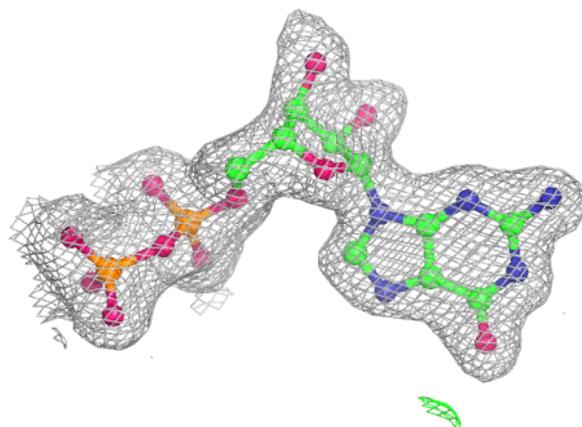
Electron density around GDP A 1180:

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

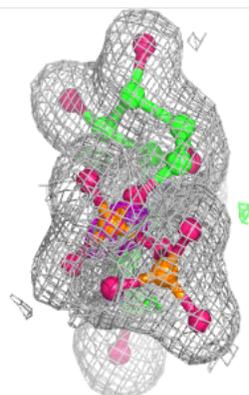
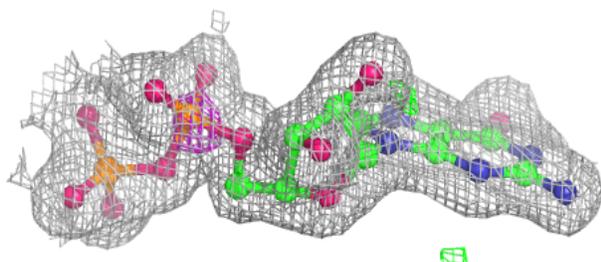
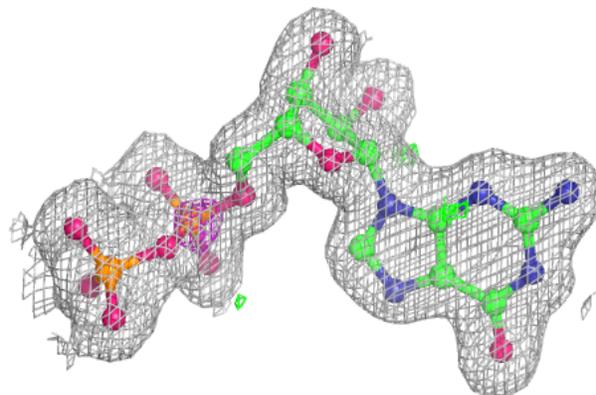


Electron density around GDP B 1178:

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

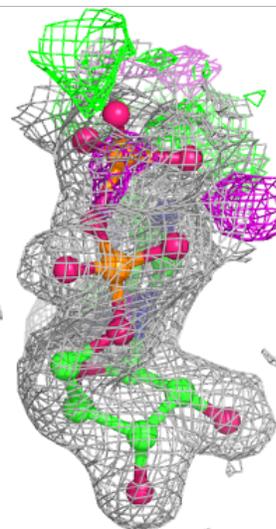
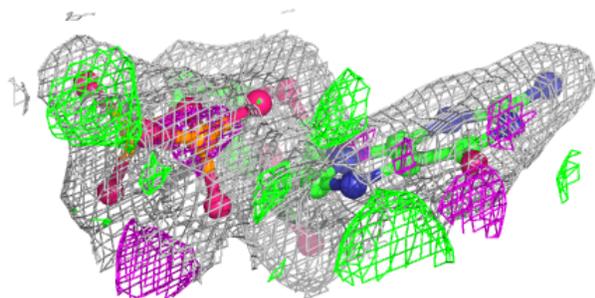
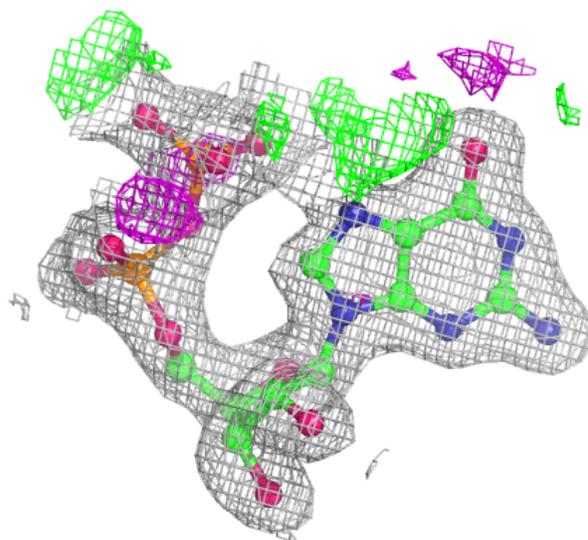
**Electron density around GDP A 1178:**

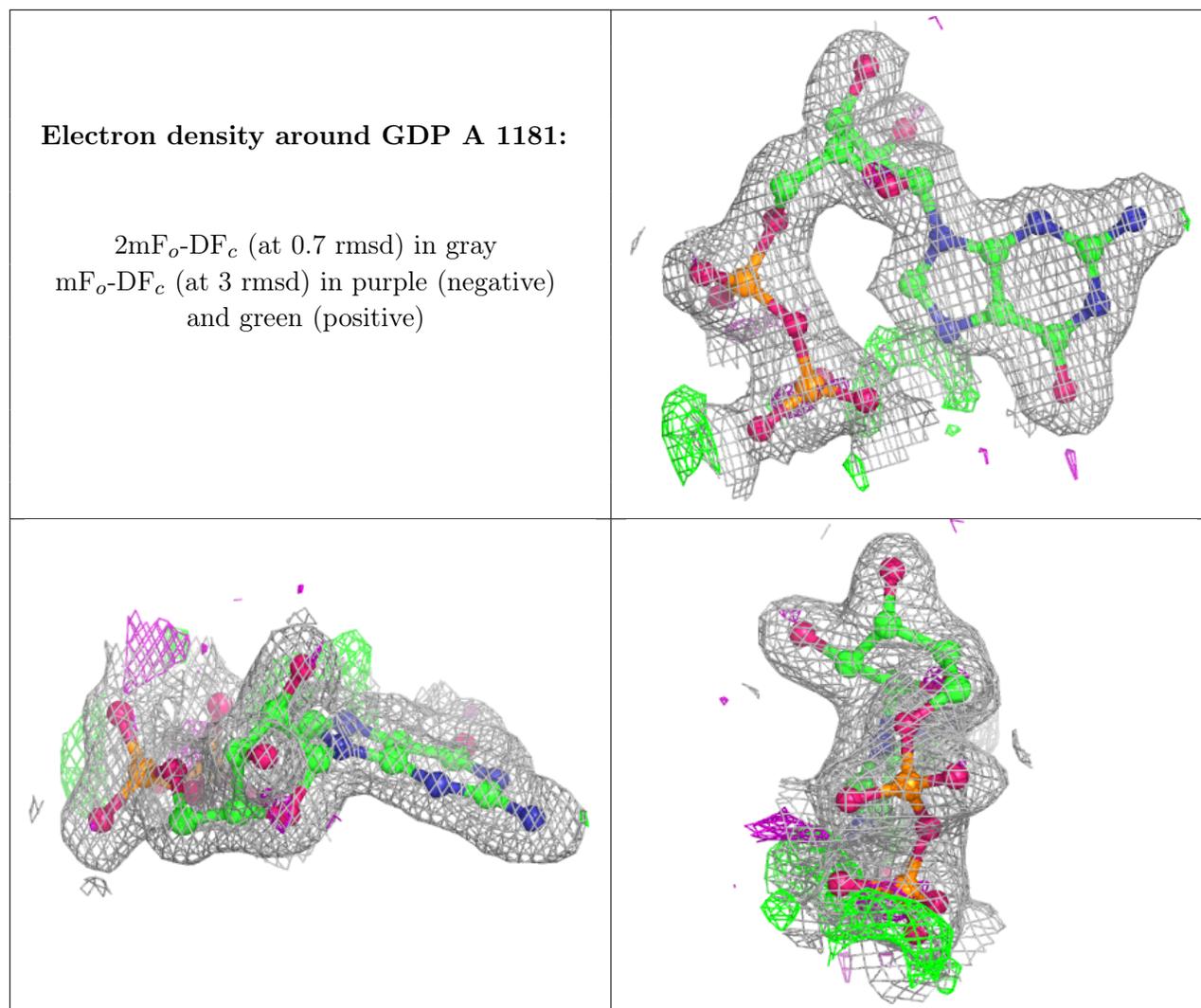
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDP B 1181:

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





5.5 Other polymers [i](#)

There are no such residues in this entry.