



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 20, 2026 – 09:51 am BST

PDB ID : 6I0M / pdb_00006i0m
Title : Structure of human IMP dehydrogenase, isoform 2, bound to GDP
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Deposited on : 2018-10-26
Resolution : 2.57 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

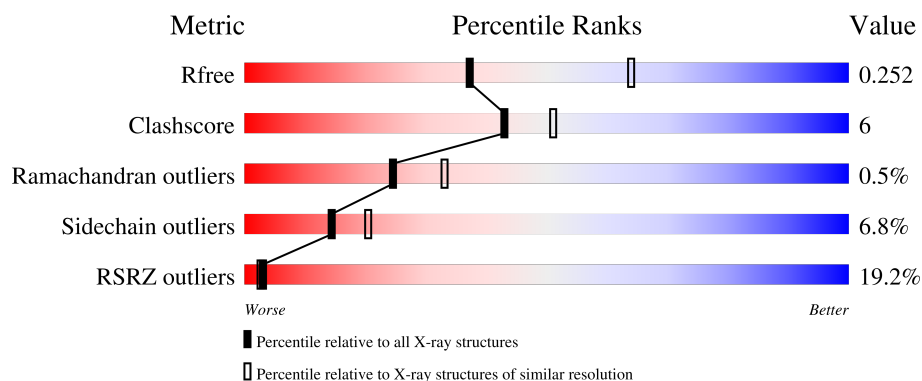
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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

Mol	Chain	Length	Quality of chain
1	A	517	12% 75% 11% • 13%
1	B	517	21% 76% 9% • 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	5GP	A	601	-	-	X	-
3	GDP	A	602	-	-	X	-
4	SO4	A	611	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13153 atoms, of which 6315 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.

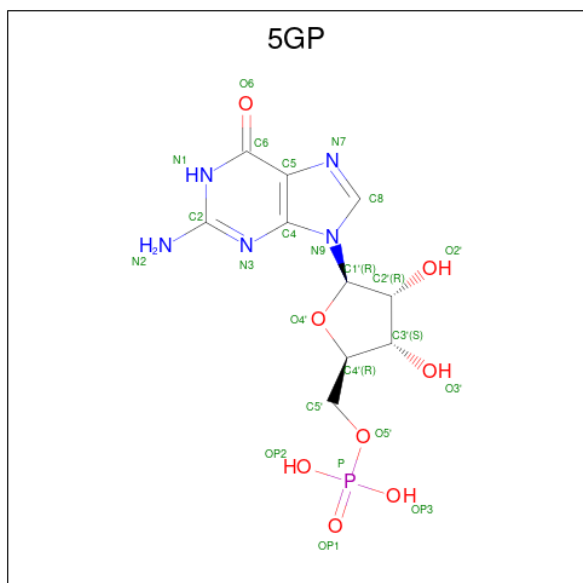
- Molecule 1 is a protein called Inosine-5'-monophosphate dehydrogenase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	450	Total	C	H	N	O	S	0	1	0
			6518	2091	3223	565	620	19			
1	B	444	Total	C	H	N	O	S	0	1	0
			6125	1995	2978	546	589	17			

There are 6 discrepancies between the modelled and reference sequences:

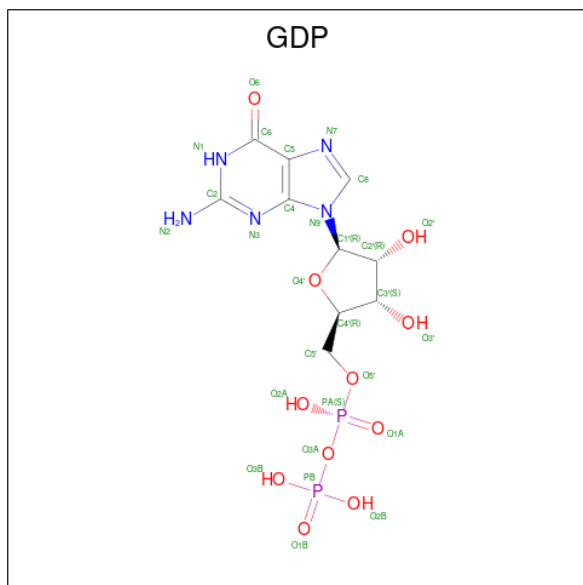
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P12268
A	-1	SER	-	expression tag	UNP P12268
A	0	HIS	-	expression tag	UNP P12268
B	-2	GLY	-	expression tag	UNP P12268
B	-1	SER	-	expression tag	UNP P12268
B	0	HIS	-	expression tag	UNP P12268

- Molecule 2 is GUANOSINE-5'-MONOPHOSPHATE (CCD ID: 5GP) (formula: $C_{10}H_{14}N_5O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	A	1	Total 35	C 10	H 11	N 5	O 8	P 1	0	0
2	B	1	Total 35	C 10	H 11	N 5	O 8	P 1	0	0

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 39	C 10	H 11	N 5	O 11	P 2	0	0
3	A	1	Total 39	C 10	H 11	N 5	O 11	P 2	0	0
3	A	1	Total 80	C 20	H 24	N 10	O 22	P 4	0	1
3	B	1	Total 39	C 10	H 11	N 5	O 11	P 2	0	0
3	B	1	Total 39	C 10	H 11	N 5	O 11	P 2	0	0
3	B	1	Total 80	C 20	H 24	N 10	O 22	P 4	0	1

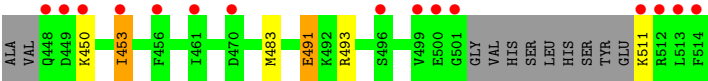
- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	53	Total	O	0	0
			53	53		
5	B	21	Total	O	0	0
			21	21		



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	134.73Å 134.73Å 324.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	162.00 – 2.57 162.00 – 2.57	Depositor EDS
% Data completeness (in resolution range)	81.2 (162.00-2.57) 81.2 (162.00-2.57)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.58Å)	Xtriage
Refinement program	PHENIX (1.12rc1_2801: ???)	Depositor
R, R_{free}	0.219 , 0.249 0.228 , 0.252	Depositor DCC
R_{free} test set	1967 reflections (4.09%)	wwPDB-VP
Wilson B-factor (Å ²)	70.1	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 91.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13153	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5GP, SO4, GDP

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	0.21	0/3346	0.41	0/4528
1	B	0.18	0/3191	0.39	0/4320
All	All	0.20	0/6537	0.40	0/8848

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	3295	3223	3248	57	0
1	B	3147	2978	2985	21	1
2	A	24	11	12	7	0
2	B	24	11	12	1	0
3	A	112	46	48	18	0
3	B	112	46	48	5	0
4	A	35	0	0	6	0
4	B	15	0	0	0	0
5	A	53	0	0	2	0
5	B	21	0	0	0	0
All	All	6838	6315	6353	81	1

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 6.

All (81) 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:A:166:LEU:C	1:A:170:GLU:HA	1.61	1.24
1:A:166:LEU:C	1:A:170:GLU:CA	2.16	1.18
1:A:364:ASP:OD1	2:A:601:5GP:O3'	1.64	1.13
1:A:166:LEU:C	1:A:170:GLU:N	2.05	1.12
1:A:166:LEU:O	1:A:170:GLU:HA	1.55	1.06
1:A:166:LEU:O	1:A:170:GLU:CA	2.13	0.95
1:A:185:LEU:HA	3:A:602:GDP:N2	1.85	0.91
1:B:261:ASP:OD1	1:B:294:TYR:OH	1.94	0.85
3:A:602:GDP:O3B	1:B:161:ARG:NH2	2.16	0.79
1:B:208:LYS:NZ	3:B:603:GDP:O1B	2.13	0.78
4:A:611:SO4:O2	5:A:701:HOH:O	2.02	0.76
1:A:180:THR:CG2	3:A:602:GDP:O2'	2.34	0.75
1:A:185:LEU:HA	3:A:602:GDP:C2	2.24	0.72
1:A:185:LEU:C	1:A:185:LEU:HD12	2.15	0.72
1:B:155:VAL:O	1:B:182:ARG:HG2	1.89	0.71
1:A:242:LYS:NZ	3:A:604[B]:GDP:O1B	2.23	0.71
1:A:180:THR:HG21	3:A:602:GDP:O2'	1.89	0.71
1:B:139:PHE:HB2	3:B:603:GDP:O2B	1.91	0.71
1:B:207:GLY:N	3:B:602:GDP:O1A	2.23	0.69
1:B:146:ASP:O	1:B:148:GLY:N	2.27	0.68
1:A:185:LEU:HA	3:A:602:GDP:HN21	1.56	0.67
1:A:332:ILE:O	1:A:334:GLN:N	2.28	0.66
3:A:604[A]:GDP:O1B	3:A:604[A]:GDP:H5'	1.96	0.65
1:A:322:ARG:NH2	2:A:601:5GP:O2'	2.31	0.63
1:A:364:ASP:CG	2:A:601:5GP:O3'	2.42	0.62
2:A:601:5GP:H1'	4:A:611:SO4:O1	2.00	0.60
2:A:601:5GP:C1'	4:A:611:SO4:O1	2.49	0.60
1:A:166:LEU:O	1:A:170:GLU:CB	2.49	0.59
1:A:186:VAL:H	3:A:602:GDP:HN1	1.51	0.59
1:A:185:LEU:HD12	1:A:185:LEU:O	2.04	0.57
1:A:159:SER:HB3	3:A:602:GDP:H3'	1.87	0.56
1:B:78:MET:HE1	1:B:453:ILE:HG21	1.88	0.56
1:A:180:THR:HG23	3:A:602:GDP:O2'	2.06	0.56
1:A:254:GLU:HB2	4:A:609:SO4:O4	2.06	0.55
1:B:296[B]:ASN:OD1	1:B:297:LEU:N	2.40	0.55
1:A:296:ASN:OD1	1:A:296:ASN:N	2.41	0.54
1:A:154:LEU:HD22	1:A:155:VAL:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:GLU:OE2	1:A:356:ARG:NH1	2.41	0.53
1:A:261:ASP:OD1	1:A:294:TYR:OH	2.27	0.52
1:A:63:THR:HG21	1:A:461:ILE:HD11	1.90	0.52
1:A:187:VAL:CG2	1:A:188:ALA:N	2.72	0.52
1:A:238:LYS:CE	3:A:604[B]:GDP:O3B	2.58	0.52
1:A:75:GLU:HG3	1:A:397:PRO:HB3	1.92	0.51
2:A:601:5GP:O4'	4:A:611:SO4:O1	2.29	0.51
1:B:275:SER:O	1:B:303:ASN:ND2	2.45	0.50
1:B:395:GLU:N	1:B:395:GLU:OE1	2.42	0.50
1:A:154:LEU:O	1:A:182:ARG:HG2	2.11	0.50
1:A:226:ASP:HB3	3:A:604[A]:GDP:HN1	1.76	0.50
1:A:390:LEU:HD22	1:A:453:ILE:HD11	1.94	0.49
1:B:139:PHE:CZ	3:B:603:GDP:C6	3.01	0.49
1:A:226:ASP:OD2	3:A:603:GDP:O2'	2.33	0.47
1:A:303:ASN:HA	1:A:322:ARG:O	2.15	0.47
1:B:145:THR:CB	1:B:153:ARG:O	2.62	0.47
1:A:395:GLU:OE1	1:A:395:GLU:N	2.44	0.47
1:A:185:LEU:C	1:A:185:LEU:CD1	2.85	0.47
1:A:226:ASP:HB3	3:A:604[B]:GDP:HN1	1.80	0.46
1:A:401:PHE:O	1:B:511:LYS:HA	2.17	0.45
1:A:49:VAL:HA	1:A:474:LYS:O	2.17	0.45
1:A:78:MET:HA	1:A:78:MET:HE3	1.99	0.43
1:A:187:VAL:HG22	1:A:188:ALA:N	2.33	0.43
1:A:415:GLY:O	2:A:601:5GP:O6	2.36	0.43
1:B:318:VAL:CG1	1:B:320:ALA:O	2.66	0.43
1:B:153:ARG:HA	1:B:217:GLU:HA	2.01	0.43
1:A:182:ARG:NH2	1:A:216:ASP:OD2	2.52	0.43
1:B:33:ASN:O	1:B:493:ARG:NH1	2.52	0.43
1:A:324:GLY:C	4:A:611:SO4:O4	2.62	0.42
1:A:121:LEU:HG	1:A:142:ILE:HG21	2.01	0.42
1:A:78:MET:HE1	1:A:453:ILE:HG13	2.01	0.42
1:B:388:SER:N	2:B:601:5GP:OP2	2.48	0.42
1:A:185:LEU:HA	3:A:602:GDP:N1	2.34	0.42
1:A:356:ARG:NH1	5:A:705:HOH:O	2.52	0.42
1:A:126:ARG:HD2	1:A:128:ARG:NH1	2.35	0.41
1:A:182:ARG:HA	1:A:182:ARG:HD2	1.86	0.41
1:A:238:LYS:NZ	3:A:604[B]:GDP:O3B	2.52	0.41
1:A:144:ILE:HD11	1:A:158:ILE:CD1	2.51	0.41
1:A:164:ASP:CB	1:B:224:ARG:HH21	2.34	0.41
1:A:182:ARG:NH2	1:A:216:ASP:OD1	2.46	0.41
1:B:242:LYS:NZ	3:B:604[B]:GDP:O2A	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ASN:O	1:A:493:ARG:NH1	2.54	0.40
1:B:212:VAL:HA	1:B:217:GLU:O	2.22	0.40
1:A:226:ASP:HB3	3:A:604[A]:GDP:N1	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:ARG:HE	1:B:491:GLU:OE1[3_865]	1.59	0.01

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	441/517 (85%)	422 (96%)	16 (4%)	3 (1%)	18	25
1	B	425/517 (82%)	404 (95%)	20 (5%)	1 (0%)	43	54
All	All	866/1034 (84%)	826 (95%)	36 (4%)	4 (0%)	24	33

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	THR
1	B	15	ASP
1	A	164	ASP
1	A	176	GLU

5.3.2 Protein sidechains [i](#)

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	329/422 (78%)	308 (94%)	21 (6%)	16	23
1	B	292/422 (69%)	270 (92%)	22 (8%)	12	18
All	All	621/844 (74%)	578 (93%)	43 (7%)	14	20

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LEU
1	A	112	GLN
1	A	154	LEU
1	A	155	VAL
1	A	157	ILE
1	A	172	ASP
1	A	177	GLU
1	A	178	ILE
1	A	180	THR
1	A	182	ARG
1	A	187	VAL
1	A	201	LEU
1	A	231	ARG
1	A	255	ASP
1	A	261	ASP
1	A	277	GLN
1	A	318	VAL
1	A	414	MET
1	A	453	ILE
1	A	483	MET
1	A	491	GLU
1	B	15	ASP
1	B	53	SER
1	B	65	LEU
1	B	103	GLU
1	B	112	GLN
1	B	119	VAL
1	B	152	SER
1	B	154	LEU
1	B	173	CYS
1	B	186	VAL
1	B	195	LYS
1	B	201	LEU

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Mol	Chain	Res	Type
1	B	211	ILE
1	B	235	LEU
1	B	277	GLN
1	B	296[A]	ASN
1	B	296[B]	ASN
1	B	403	SER
1	B	450	LYS
1	B	453	ILE
1	B	483	MET
1	B	491	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	198	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

20 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
3	GDP	B	602	-	28,30,30	1.15	3 (10%)	44,47,47	1.84	7 (15%)
3	GDP	A	604[B]	-	28,30,30	1.17	3 (10%)	44,47,47	1.93	8 (18%)
4	SO4	A	605	-	4,4,4	0.24	0	6,6,6	0.07	0
3	GDP	B	604[A]	-	28,30,30	1.17	3 (10%)	44,47,47	1.98	11 (25%)
3	GDP	A	603	-	28,30,30	1.20	4 (14%)	44,47,47	1.85	8 (18%)
4	SO4	A	609	-	4,4,4	0.29	0	6,6,6	0.06	0
2	5GP	B	601	-	26,26,26	1.18	3 (11%)	40,40,40	1.85	7 (17%)
4	SO4	B	605	-	4,4,4	0.28	0	6,6,6	0.08	0
2	5GP	A	601	-	26,26,26	1.20	3 (11%)	40,40,40	1.92	8 (20%)
3	GDP	B	604[B]	-	28,30,30	1.16	3 (10%)	44,47,47	1.92	10 (22%)
4	SO4	B	607	-	4,4,4	0.28	0	6,6,6	0.10	0
4	SO4	A	611	-	4,4,4	0.27	0	6,6,6	0.10	0
3	GDP	B	603	-	28,30,30	1.18	3 (10%)	44,47,47	1.83	8 (18%)
4	SO4	A	607	-	4,4,4	0.23	0	6,6,6	0.11	0
4	SO4	B	606	-	4,4,4	0.27	0	6,6,6	0.09	0
3	GDP	A	602	-	28,30,30	1.16	3 (10%)	44,47,47	1.88	7 (15%)
4	SO4	A	610	-	4,4,4	0.26	0	6,6,6	0.10	0
4	SO4	A	608	-	4,4,4	0.26	0	6,6,6	0.08	0
3	GDP	A	604[A]	-	28,30,30	1.16	3 (10%)	44,47,47	1.90	8 (18%)
4	SO4	A	606	-	4,4,4	0.27	0	6,6,6	0.12	0

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
3	GDP	B	602	-	-	4/16/32/32	0/3/3/3
2	5GP	A	601	-	-	0/10/26/26	0/3/3/3
3	GDP	B	604[B]	-	-	5/16/32/32	0/3/3/3
3	GDP	A	604[A]	-	-	6/16/32/32	0/3/3/3
3	GDP	A	603	-	-	3/16/32/32	0/3/3/3
3	GDP	A	604[B]	-	-	2/16/32/32	0/3/3/3
3	GDP	B	603	-	-	6/16/32/32	0/3/3/3
2	5GP	B	601	-	-	2/10/26/26	0/3/3/3
3	GDP	B	604[A]	-	-	5/16/32/32	0/3/3/3
3	GDP	A	602	-	-	3/16/32/32	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	GDP	C5-C4	2.94	1.46	1.38
3	B	604[A]	GDP	C6-N1	-2.92	1.33	1.38
3	B	602	GDP	C5-C4	2.91	1.46	1.38
2	A	601	5GP	C5-C4	2.88	1.46	1.38
3	A	603	GDP	C6-N1	-2.87	1.33	1.38
3	B	604[B]	GDP	C6-N1	-2.87	1.33	1.38
3	B	604[A]	GDP	C5-C4	2.84	1.46	1.38
2	B	601	5GP	C5-C4	2.83	1.46	1.38
3	B	603	GDP	C5-C4	2.82	1.46	1.38
3	A	604[B]	GDP	C5-C4	2.79	1.46	1.38
3	B	604[B]	GDP	C5-C4	2.78	1.46	1.38
3	A	604[B]	GDP	C6-N1	-2.75	1.33	1.38
3	B	603	GDP	C6-N1	-2.73	1.33	1.38
3	A	604[A]	GDP	C5-C4	2.71	1.46	1.38
3	A	603	GDP	C5-C4	2.69	1.46	1.38
3	A	604[A]	GDP	C6-N1	-2.69	1.33	1.38
2	A	601	5GP	C6-N1	-2.66	1.33	1.38
3	A	602	GDP	C6-N1	-2.65	1.33	1.38
2	B	601	5GP	C6-N1	-2.58	1.34	1.38
3	B	602	GDP	C6-N1	-2.56	1.34	1.38
3	A	604[B]	GDP	C5-N7	-2.51	1.34	1.39
3	A	603	GDP	C5-N7	-2.50	1.34	1.39
2	A	601	5GP	C5-N7	-2.47	1.34	1.39
3	A	604[A]	GDP	C5-N7	-2.45	1.34	1.39
3	B	603	GDP	C5-N7	-2.44	1.34	1.39
2	B	601	5GP	C5-N7	-2.39	1.34	1.39
3	B	604[B]	GDP	C5-N7	-2.37	1.34	1.39
3	B	604[A]	GDP	C5-N7	-2.35	1.34	1.39
3	B	602	GDP	C5-N7	-2.34	1.34	1.39
3	A	602	GDP	C5-N7	-2.22	1.34	1.39
3	A	603	GDP	C4-N9	-2.02	1.32	1.38

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	604[A]	GDP	C5-C4-N3	-6.49	117.93	128.46
2	A	601	5GP	C5-C4-N3	-6.31	118.22	128.46
3	B	604[B]	GDP	C5-C4-N3	-6.30	118.23	128.46
3	A	604[B]	GDP	C5-C4-N3	-6.24	118.33	128.46
3	A	602	GDP	C5-C4-N3	-6.08	118.59	128.46
3	B	603	GDP	C5-C4-N3	-6.07	118.61	128.46
2	B	601	5GP	C5-C4-N3	-6.05	118.64	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	GDP	C5-C4-N3	-6.00	118.73	128.46
3	A	604[A]	GDP	C5-C4-N3	-5.98	118.75	128.46
3	A	603	GDP	C5-C4-N3	-5.95	118.80	128.46
3	B	604[A]	GDP	C2-N3-C4	4.95	121.12	112.30
2	A	601	5GP	C2-N3-C4	4.91	121.04	112.30
3	A	604[B]	GDP	C2-N3-C4	4.90	121.03	112.30
3	B	604[B]	GDP	C2-N3-C4	4.87	120.98	112.30
2	B	601	5GP	C2-N3-C4	4.85	120.95	112.30
3	A	604[A]	GDP	C2-N3-C4	4.83	120.91	112.30
3	B	603	GDP	C2-N3-C4	4.82	120.89	112.30
3	B	604[A]	GDP	N9-C4-N3	4.81	135.60	125.94
3	A	602	GDP	C2-N3-C4	4.79	120.83	112.30
3	B	602	GDP	C2-N3-C4	4.76	120.79	112.30
3	B	604[B]	GDP	N9-C4-N3	4.70	135.38	125.94
3	A	603	GDP	C2-N3-C4	4.70	120.67	112.30
3	A	604[B]	GDP	N9-C4-N3	4.68	135.33	125.94
2	A	601	5GP	N9-C4-N3	4.66	135.30	125.94
3	A	603	GDP	N9-C4-N3	4.59	135.16	125.94
3	B	603	GDP	N9-C4-N3	4.55	135.08	125.94
3	A	602	GDP	N9-C4-N3	4.48	134.94	125.94
3	A	604[A]	GDP	N9-C4-N3	4.46	134.89	125.94
3	B	602	GDP	N9-C4-N3	4.35	134.68	125.94
2	B	601	5GP	N9-C4-N3	4.35	134.67	125.94
3	B	604[A]	GDP	PA-O3A-PB	-4.20	118.40	132.83
3	B	604[B]	GDP	PA-O3A-PB	-4.13	118.64	132.83
3	A	604[B]	GDP	PA-O3A-PB	-3.95	119.27	132.83
3	A	604[A]	GDP	PA-O3A-PB	-3.88	119.52	132.83
3	B	602	GDP	PA-O3A-PB	-3.69	120.16	132.83
3	A	602	GDP	PA-O3A-PB	-3.52	120.74	132.83
3	A	604[A]	GDP	C6-C5-N7	3.34	136.45	130.25
3	A	602	GDP	C6-C5-N7	3.28	136.35	130.25
2	B	601	5GP	C6-C5-N7	3.24	136.27	130.25
3	B	602	GDP	C6-C5-N7	3.22	136.23	130.25
3	A	603	GDP	PA-O3A-PB	-3.19	121.89	132.83
3	B	603	GDP	C6-C5-N7	3.17	136.15	130.25
3	A	604[B]	GDP	C6-C5-N7	3.16	136.12	130.25
3	B	604[A]	GDP	C6-C5-N7	3.16	136.12	130.25
3	B	604[B]	GDP	C6-C5-N7	3.14	136.09	130.25
2	A	601	5GP	C6-C5-N7	3.13	136.08	130.25
3	A	603	GDP	C6-C5-N7	3.10	136.01	130.25
3	B	604[A]	GDP	C4-C5-N7	-2.80	106.30	110.72
3	A	604[A]	GDP	C4-C5-N7	-2.78	106.32	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	5GP	C4-C5-N7	-2.76	106.36	110.72
3	A	604[B]	GDP	C4-C5-N7	-2.75	106.37	110.72
3	B	603	GDP	PA-O3A-PB	-2.75	123.40	132.83
3	A	602	GDP	C4-C5-N7	-2.73	106.40	110.72
3	B	604[B]	GDP	C4-C5-N7	-2.72	106.42	110.72
2	B	601	5GP	C4-C5-N7	-2.70	106.45	110.72
3	B	602	GDP	C4-C5-N7	-2.65	106.52	110.72
3	B	603	GDP	C4-C5-N7	-2.61	106.59	110.72
3	A	603	GDP	C4-C5-N7	-2.45	106.84	110.72
2	A	601	5GP	C3'-C2'-C1'	2.40	105.99	101.43
3	A	603	GDP	O6-C6-C5	-2.34	120.40	126.60
3	B	603	GDP	O6-C6-C5	-2.25	120.63	126.60
3	A	604[A]	GDP	O6-C6-C5	-2.19	120.80	126.60
3	A	604[B]	GDP	O6-C6-C5	-2.14	120.92	126.60
3	B	604[B]	GDP	O6-C6-C5	-2.14	120.92	126.60
3	B	604[A]	GDP	C3'-C2'-C1'	2.13	105.47	101.43
2	A	601	5GP	O6-C6-C5	-2.11	121.00	126.60
2	B	601	5GP	O6-C6-C5	-2.11	121.01	126.60
3	B	602	GDP	O6-C6-C5	-2.10	121.03	126.60
3	B	604[B]	GDP	C3'-C2'-C1'	2.10	105.41	101.43
3	B	604[A]	GDP	C5-C6-N1	2.07	118.45	113.19
2	A	601	5GP	C8-N7-C5	2.06	107.97	104.24
2	B	601	5GP	C3'-C2'-C1'	2.06	105.33	101.43
3	B	604[A]	GDP	C8-N7-C5	2.05	107.94	104.24
3	A	604[A]	GDP	C8-N7-C5	2.04	107.92	104.24
3	B	604[A]	GDP	O6-C6-C5	-2.03	121.21	126.60
3	B	604[B]	GDP	C8-N7-C5	2.02	107.90	104.24
3	B	604[B]	GDP	C5-C6-N1	2.02	118.33	113.19
3	A	603	GDP	C3'-C2'-C1'	2.02	105.26	101.43
3	B	603	GDP	C5-C6-N1	2.01	118.30	113.19
3	B	604[A]	GDP	C2-N1-C6	-2.01	121.44	125.10
3	A	604[B]	GDP	C8-N7-C5	2.01	107.87	104.24
3	A	602	GDP	O6-C6-C5	-2.00	121.29	126.60

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	5GP	O4'-C4'-C5'-O5'
3	A	602	GDP	C5'-O5'-PA-O1A
3	A	602	GDP	C5'-O5'-PA-O2A
3	A	604[A]	GDP	PA-O3A-PB-O3B

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Mol	Chain	Res	Type	Atoms
3	A	604[A]	GDP	C5'-O5'-PA-O2A
3	A	604[B]	GDP	C5'-O5'-PA-O3A
3	A	604[B]	GDP	C5'-O5'-PA-O2A
3	B	602	GDP	C5'-O5'-PA-O1A
3	B	602	GDP	C5'-O5'-PA-O2A
3	B	603	GDP	C5'-O5'-PA-O2A
3	B	604[A]	GDP	C5'-O5'-PA-O1A
3	B	604[A]	GDP	C5'-O5'-PA-O2A
3	B	604[B]	GDP	C5'-O5'-PA-O2A
3	A	603	GDP	O4'-C4'-C5'-O5'
3	B	604[A]	GDP	O4'-C4'-C5'-O5'
2	B	601	5GP	C3'-C4'-C5'-O5'
3	A	603	GDP	C3'-C4'-C5'-O5'
3	A	604[A]	GDP	C3'-C4'-C5'-O5'
3	B	604[A]	GDP	C3'-C4'-C5'-O5'
3	B	603	GDP	O4'-C4'-C5'-O5'
3	B	603	GDP	C3'-C4'-C5'-O5'
3	A	604[A]	GDP	C5'-O5'-PA-O3A
3	B	603	GDP	C5'-O5'-PA-O3A
3	B	604[A]	GDP	C5'-O5'-PA-O3A
3	B	604[B]	GDP	C5'-O5'-PA-O3A
3	A	604[A]	GDP	O4'-C4'-C5'-O5'
3	B	603	GDP	C5'-O5'-PA-O1A
3	B	604[B]	GDP	PB-O3A-PA-O1A
3	A	603	GDP	PB-O3A-PA-O1A
3	B	604[B]	GDP	PB-O3A-PA-O2A
3	B	603	GDP	PA-O3A-PB-O2B
3	A	602	GDP	C5'-O5'-PA-O3A
3	B	602	GDP	C5'-O5'-PA-O3A
3	B	602	GDP	PB-O3A-PA-O2A
3	A	604[A]	GDP	C5'-O5'-PA-O1A
3	B	604[B]	GDP	C5'-O5'-PA-O1A

There are no ring outliers.

11 monomers are involved in 34 short contacts:

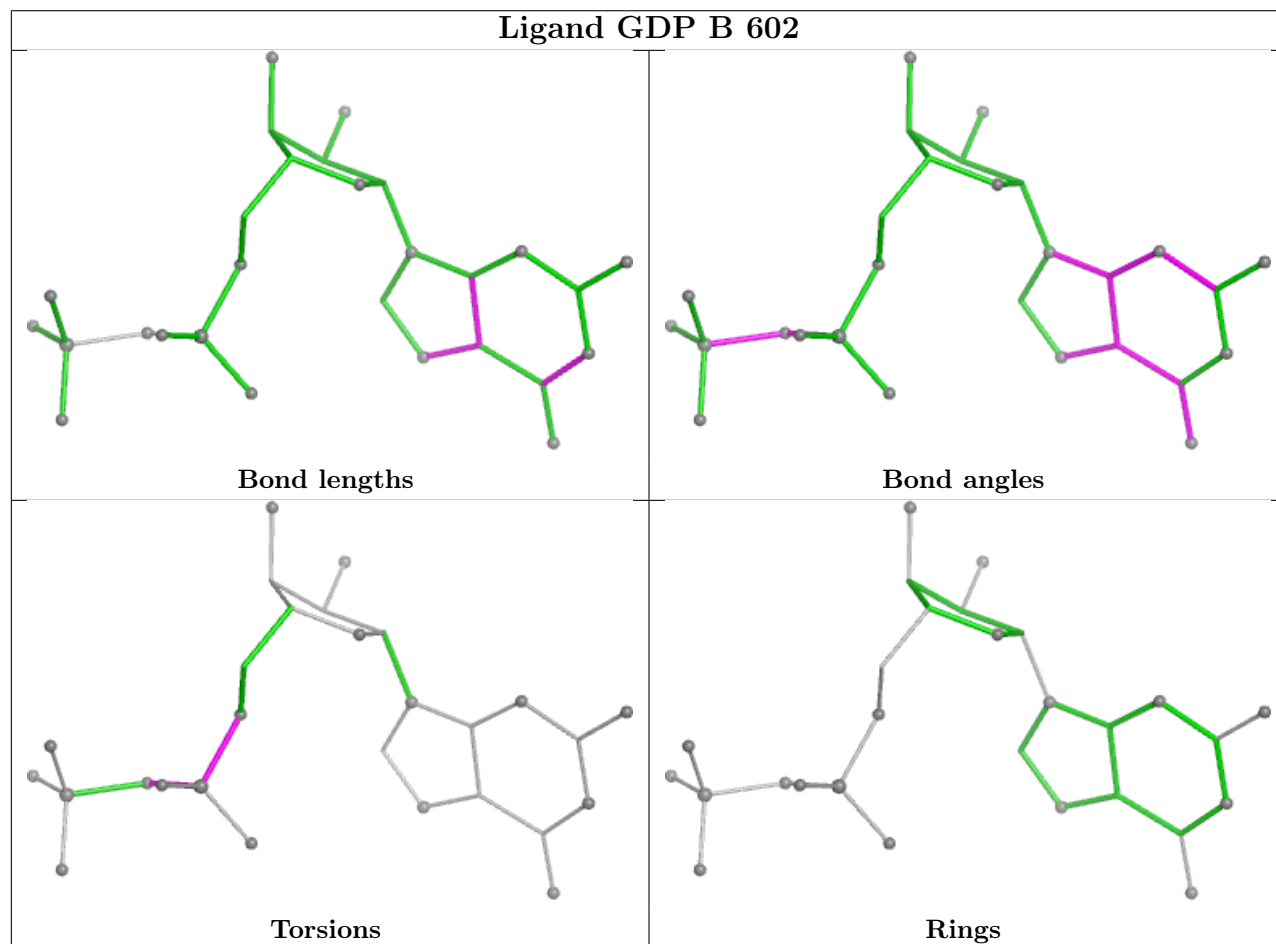
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	GDP	1	0
3	A	604[B]	GDP	4	0
3	A	603	GDP	1	0
4	A	609	SO4	1	0
2	B	601	5GP	1	0

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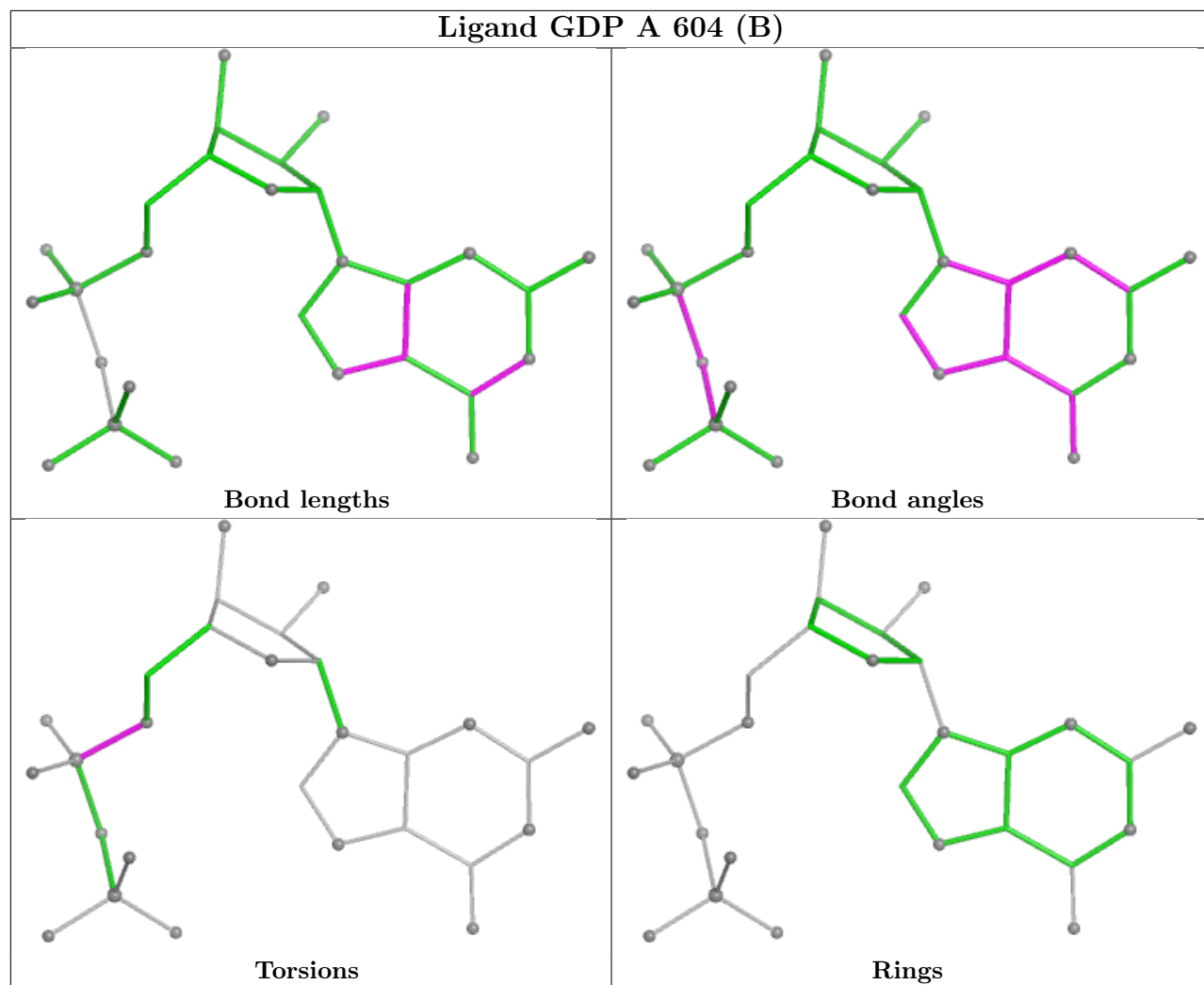
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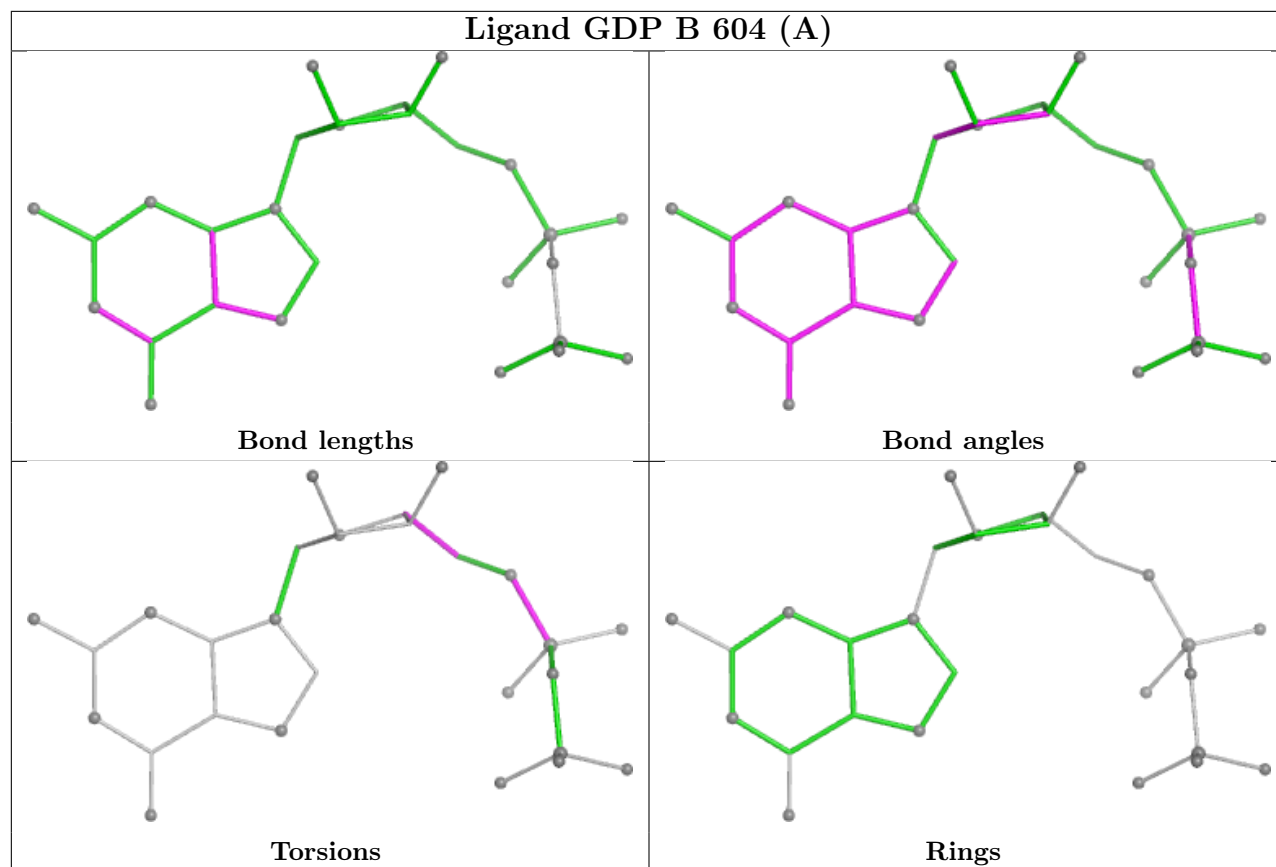
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	5GP	7	0
3	B	604[B]	GDP	1	0
4	A	611	SO4	5	0
3	B	603	GDP	3	0
3	A	602	GDP	10	0
3	A	604[A]	GDP	3	0

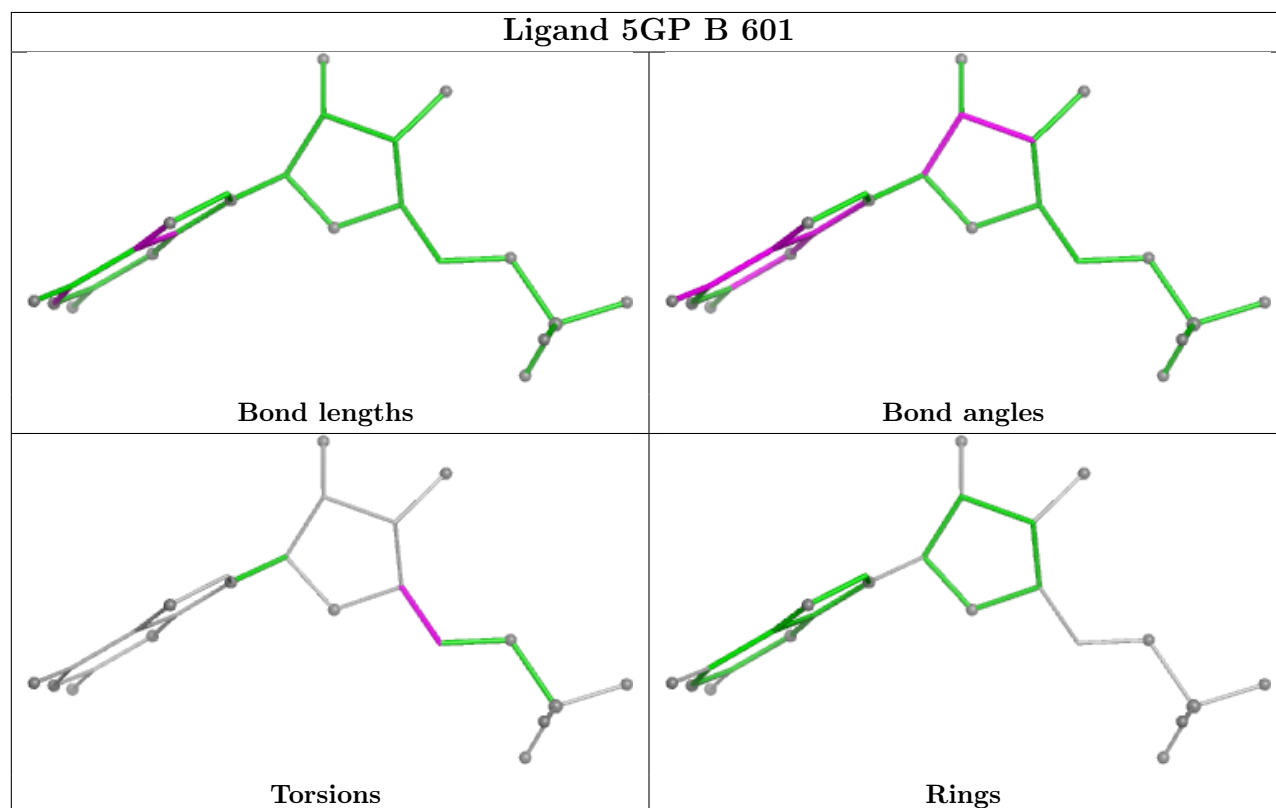
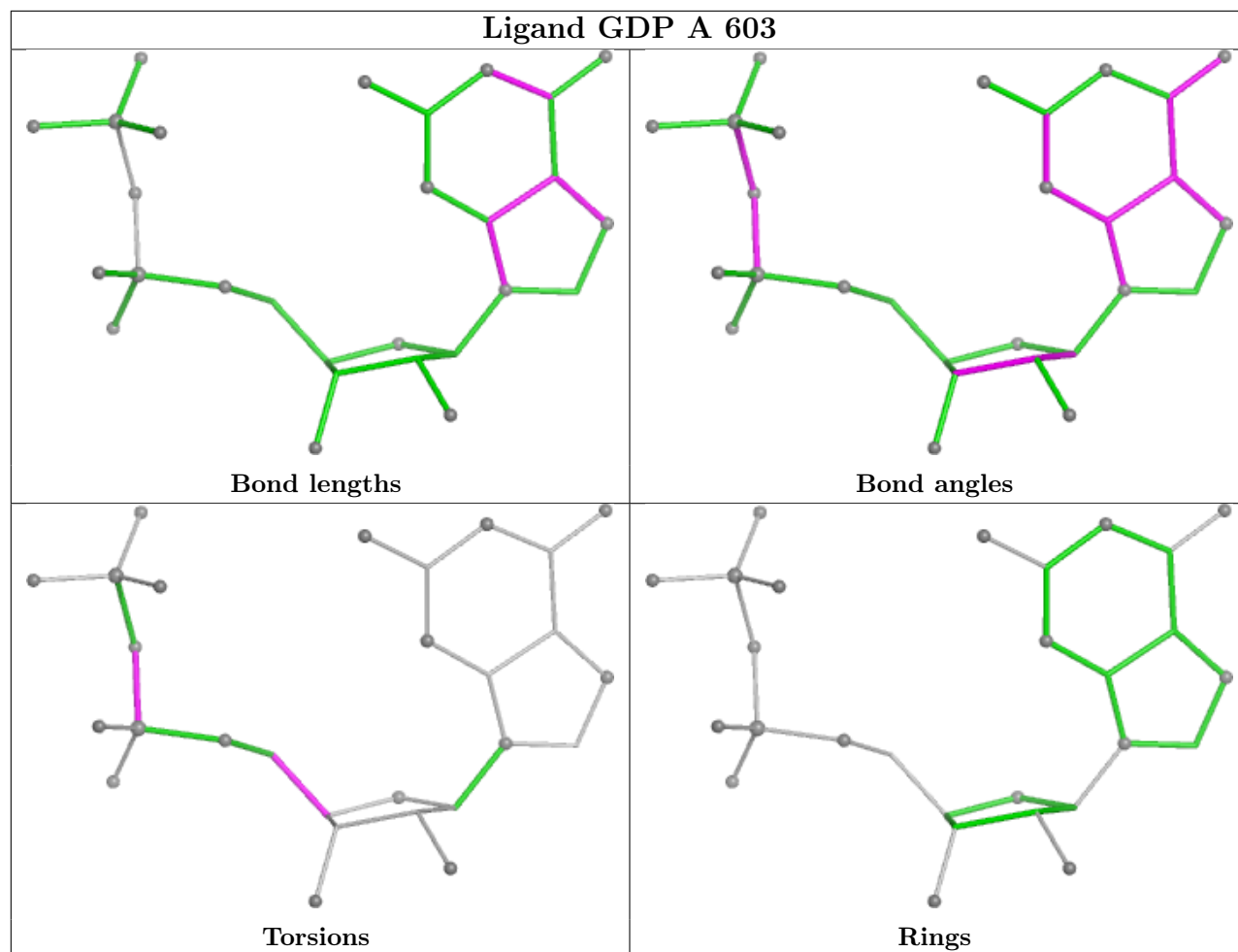
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



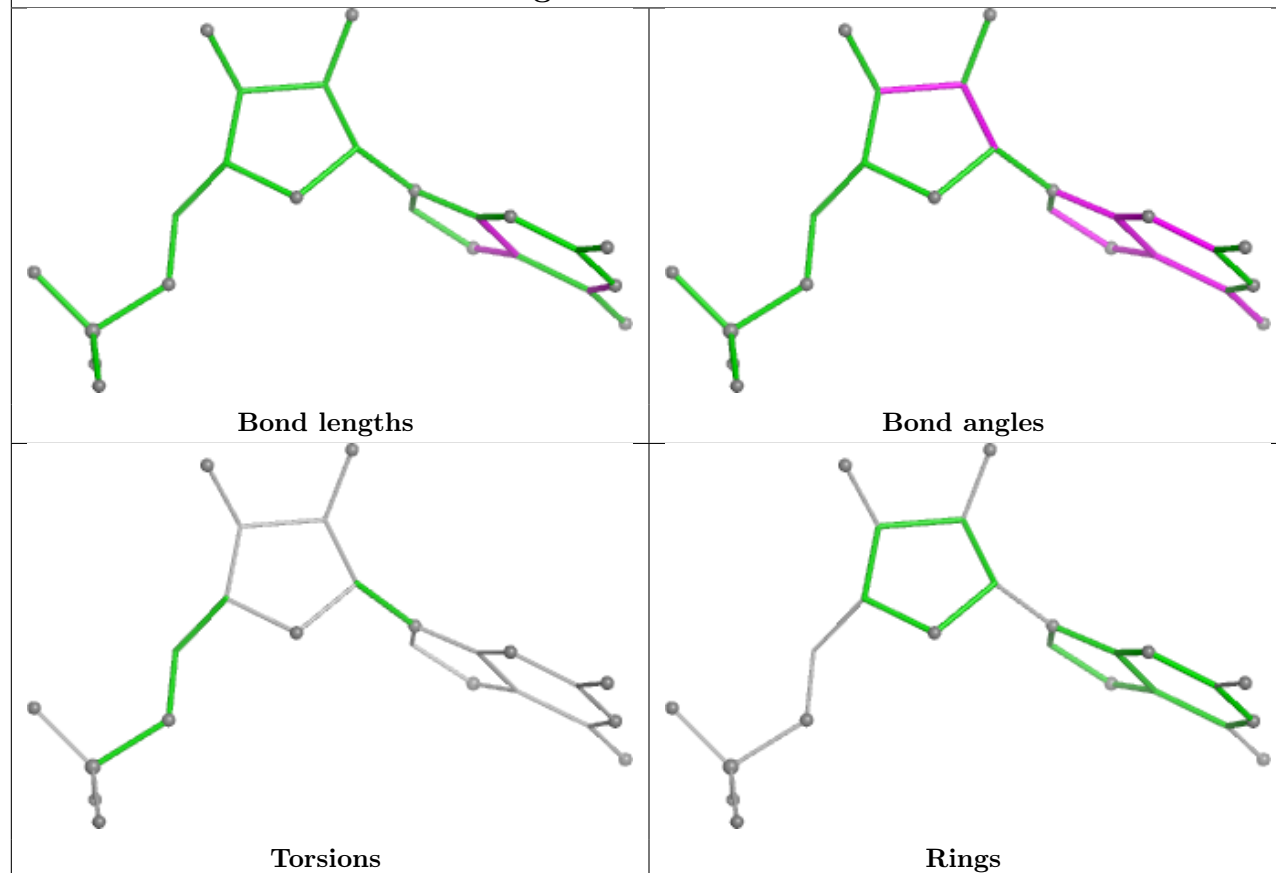
Ligand GDP A 604 (B)



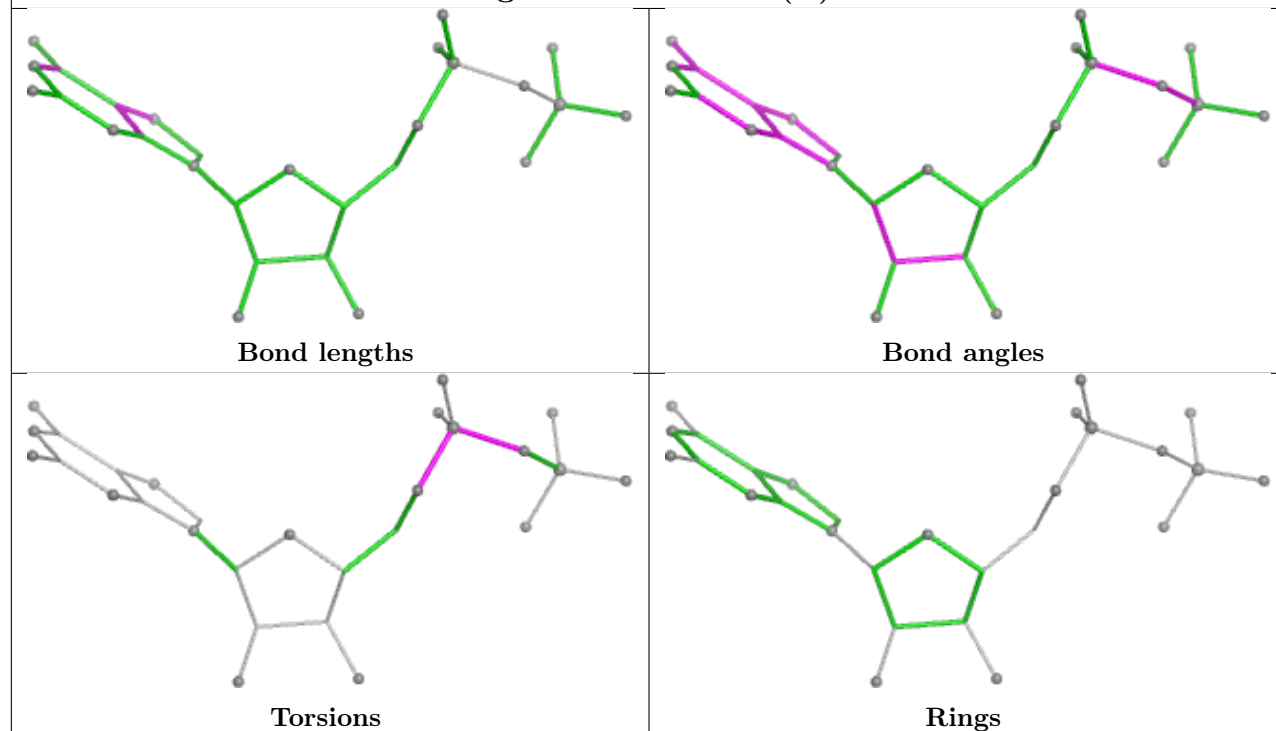


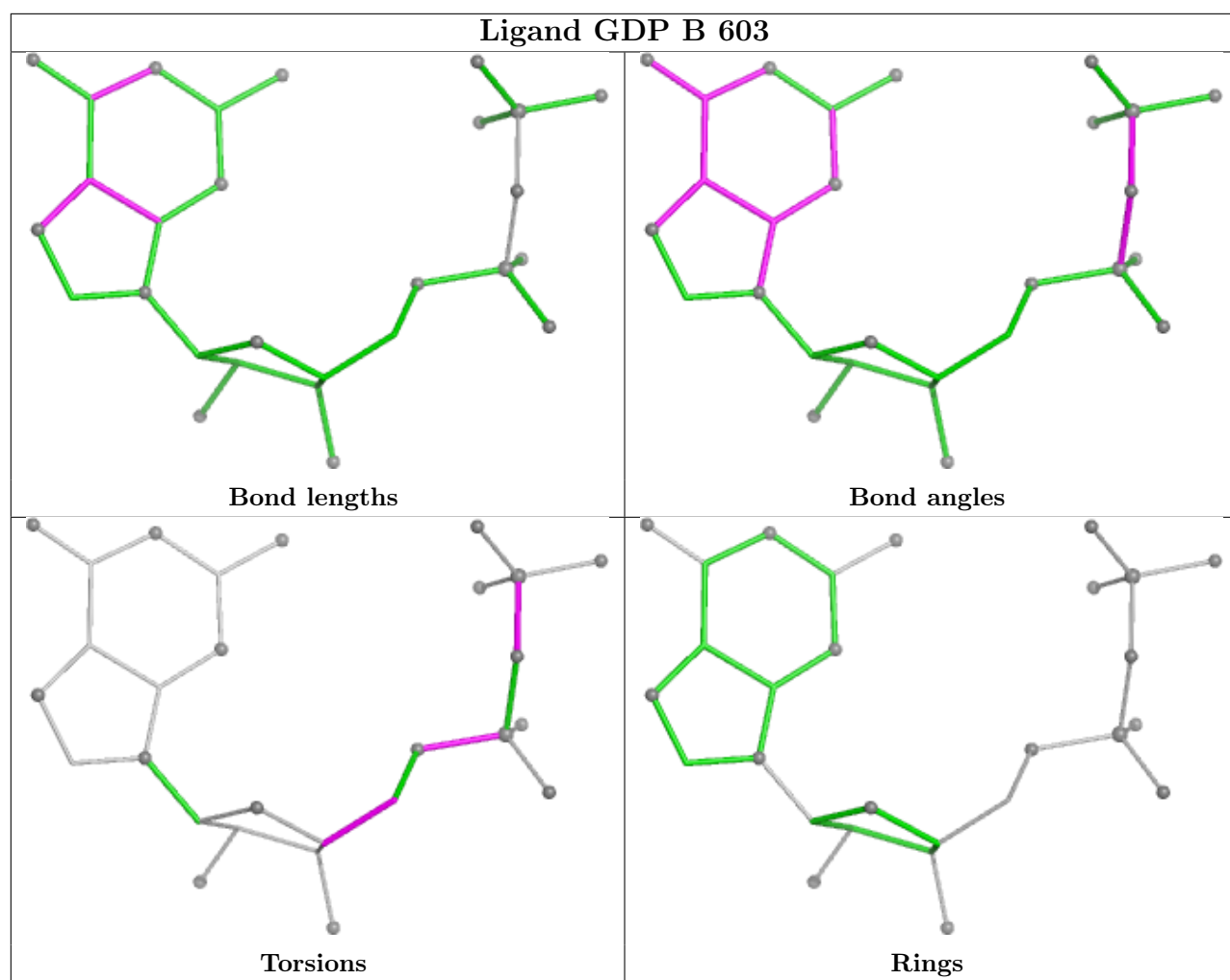


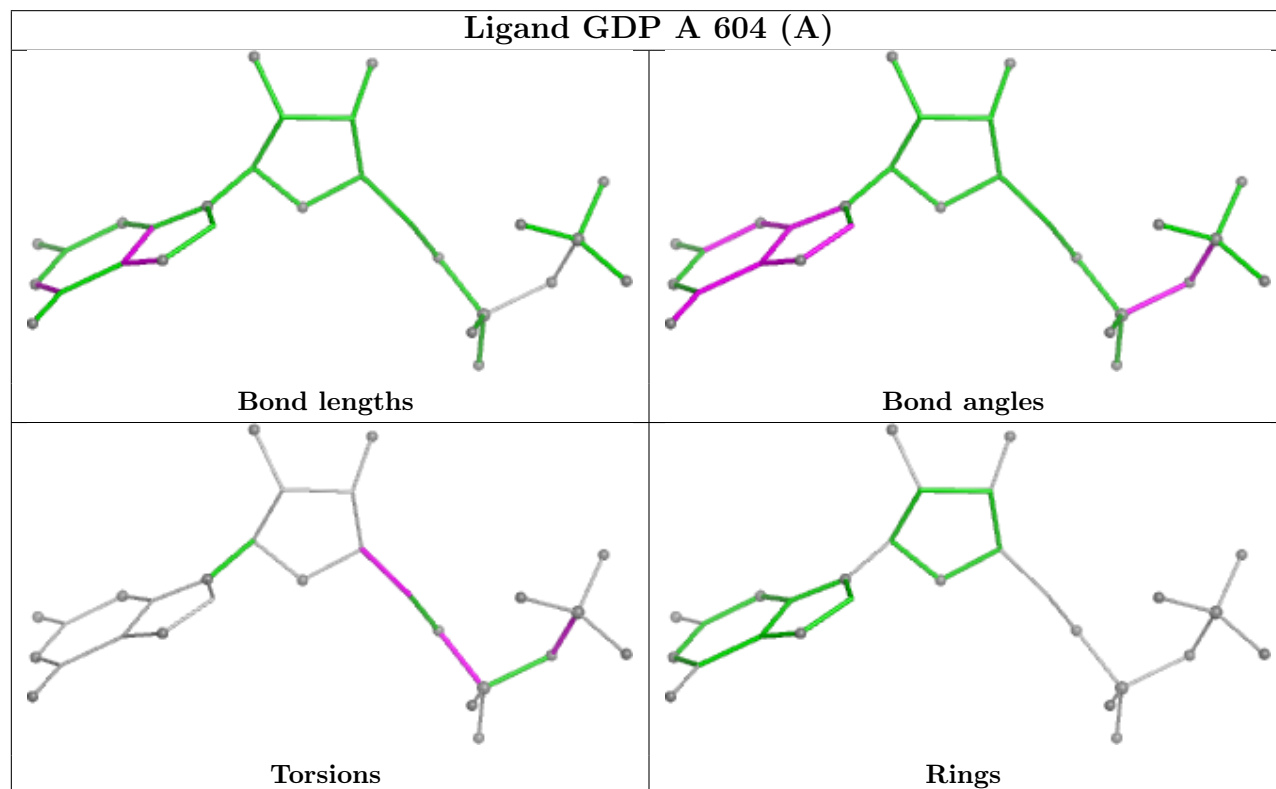
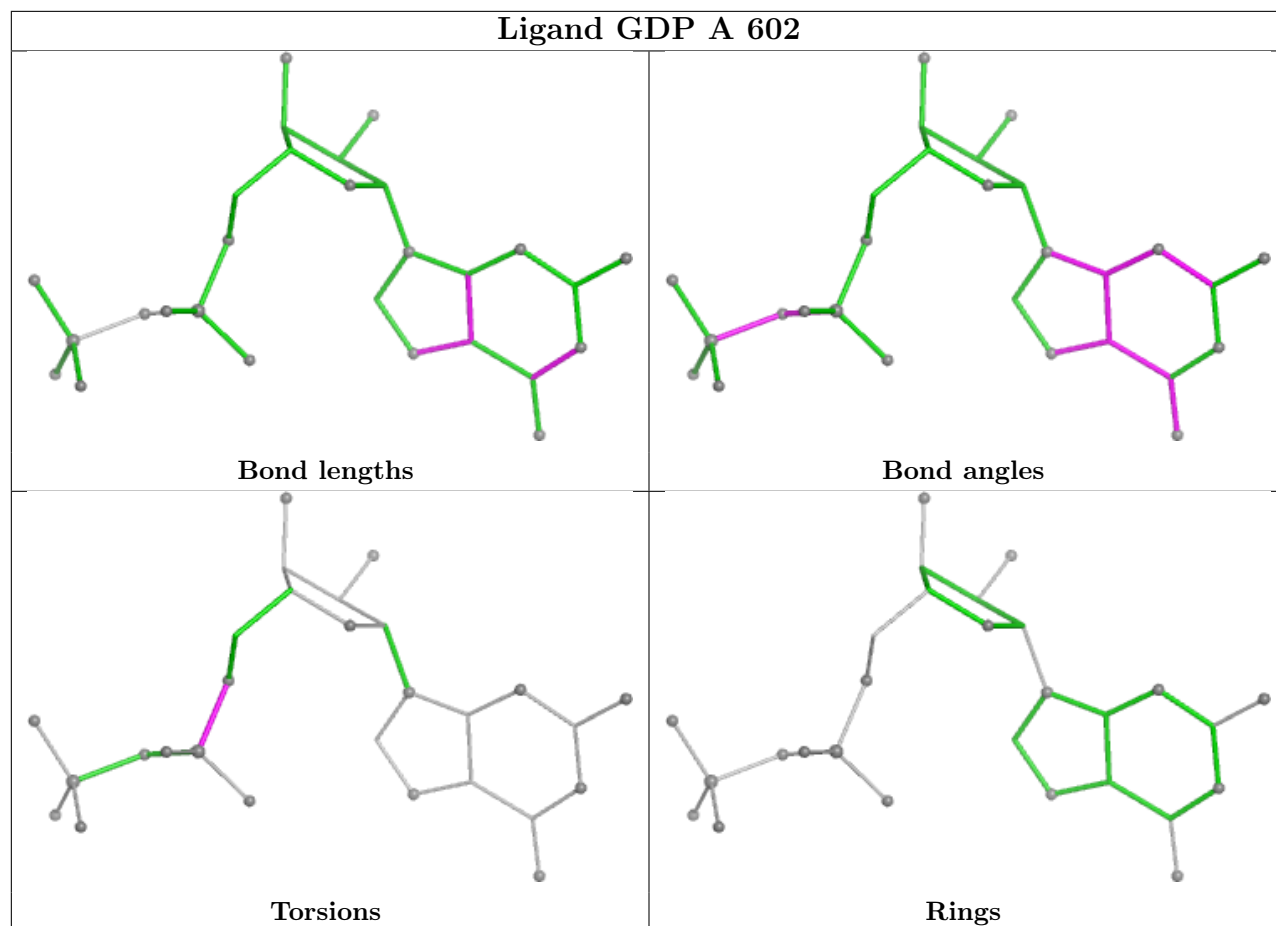
Ligand 5GP A 601



Ligand GDP B 604 (B)







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	450/517 (87%)	0.86	62 (13%) 6 6	33, 70, 137, 176	1 (0%)
1	B	444/517 (85%)	1.41	110 (24%) 2 1	56, 90, 145, 195	1 (0%)
All	All	894/1034 (86%)	1.13	172 (19%) 3 3	33, 81, 143, 195	2 (0%)

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	HIS	7.0
1	A	336	VAL	6.9
1	A	332	ILE	6.7
1	B	144	ILE	6.5
1	B	214	GLU	6.2
1	A	414	MET	6.1
1	B	178	ILE	5.9
1	B	336	VAL	5.8
1	B	12	TYR	5.7
1	A	329	SER	5.7
1	B	179	MET	5.4
1	B	449	ASP	5.4
1	B	448	GLN	5.4
1	B	335	GLU	5.3
1	A	404	ASP	5.3
1	B	403	SER	5.3
1	B	334	GLN	5.2
1	B	155	VAL	5.2
1	A	334	GLN	5.1
1	A	402	PHE	5.1
1	B	157	ILE	5.1
1	A	415	GLY	5.0
1	B	122	SER	5.0
1	A	12	TYR	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	121	LEU	4.9
1	B	16	ASP	4.9
1	B	406	ILE	4.8
1	A	413	GLY	4.7
1	A	327	SER	4.6
1	A	170	GLU	4.6
1	B	170	GLU	4.6
1	A	335	GLU	4.5
1	B	176	GLU	4.5
1	B	216	ASP	4.5
1	B	171	HIS	4.5
1	A	448	GLN	4.5
1	B	149	ARG	4.5
1	A	501	GLY	4.5
1	B	407	ARG	4.5
1	A	401	PHE	4.4
1	B	146	ASP	4.4
1	B	404	ASP	4.4
1	B	153	ARG	4.3
1	B	402	PHE	4.2
1	B	338	ALA	4.2
1	A	326	GLY	4.2
1	A	337	LEU	4.1
1	B	71	ASP	4.1
1	B	180	THR	4.1
1	B	333	THR	4.1
1	A	502	GLY	4.1
1	B	187	VAL	4.1
1	A	339	CYS	4.1
1	B	337	LEU	4.0
1	B	401	PHE	4.0
1	B	175	LEU	4.0
1	B	172	ASP	3.9
1	B	174	PHE	3.9
1	B	25	ASN	3.9
1	A	449	ASP	3.8
1	B	368	GLN	3.8
1	A	333	THR	3.8
1	A	418	ASP	3.8
1	B	329	SER	3.8
1	B	128	ARG	3.8
1	B	327	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	128	ARG	3.7
1	A	140	CYS	3.7
1	B	514	PHE	3.7
1	B	332	ILE	3.7
1	B	512	ARG	3.7
1	B	339	CYS	3.7
1	A	417	LEU	3.7
1	B	166	LEU	3.7
1	A	497	ALA	3.6
1	B	400	TYR	3.6
1	B	500	GLU	3.6
1	A	328	GLY	3.6
1	A	172	ASP	3.5
1	B	367	ILE	3.5
1	A	400	TYR	3.5
1	B	11	SER	3.5
1	B	129	ASP	3.4
1	A	416	SER	3.4
1	B	501	GLY	3.4
1	B	127	VAL	3.3
1	B	366	GLY	3.3
1	B	223	ALA	3.3
1	B	94	ASN	3.3
1	B	165	PHE	3.2
1	A	25	ASN	3.2
1	B	135	ALA	3.2
1	A	130	VAL	3.2
1	B	154	LEU	3.1
1	A	500	GLU	3.1
1	A	28	ASP	3.1
1	B	29	GLY	3.1
1	A	214	GLU	3.1
1	A	139	PHE	3.1
1	B	192	ILE	3.0
1	B	125	ASP	3.0
1	A	499	VAL	3.0
1	B	75	GLU	3.0
1	A	153	ARG	3.0
1	B	136	ARG	3.0
1	B	296[A]	ASN	3.0
1	B	145	THR	2.9
1	A	124	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	338	ALA	2.9
1	B	74	THR	2.9
1	A	166	LEU	2.9
1	A	419	ALA	2.9
1	B	405	GLY	2.9
1	B	132	GLU	2.8
1	A	181	LYS	2.8
1	B	120	VAL	2.8
1	B	513	LEU	2.8
1	B	182	ARG	2.8
1	A	302	GLY	2.8
1	A	403	SER	2.8
1	B	158	ILE	2.7
1	A	163	ILE	2.7
1	B	496	SER	2.7
1	B	15	ASP	2.6
1	B	181	LYS	2.6
1	A	399	GLU	2.6
1	B	148	GLY	2.6
1	B	173	CYS	2.6
1	B	218	LEU	2.6
1	A	27	GLY	2.6
1	A	149	ARG	2.6
1	B	227	LEU	2.6
1	B	116	THR	2.6
1	B	365	GLY	2.5
1	B	103	GLU	2.5
1	B	456	PHE	2.5
1	B	235	LEU	2.5
1	A	496	SER	2.5
1	B	189	PRO	2.5
1	A	450	LYS	2.5
1	B	79	ALA	2.4
1	B	453	ILE	2.4
1	B	499	VAL	2.4
1	A	132	GLU	2.3
1	B	196	GLU	2.3
1	B	511	LYS	2.3
1	A	137	HIS	2.3
1	B	301	GLY	2.3
1	A	313	LEU	2.3
1	B	461	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	131	PHE	2.3
1	A	471	ILE	2.2
1	B	124	LYS	2.2
1	A	301	GLY	2.2
1	B	24	PHE	2.2
1	B	268	VAL	2.2
1	B	272	VAL	2.2
1	B	450	LYS	2.2
1	B	37	ILE	2.2
1	A	85	THR	2.1
1	B	138	GLY	2.1
1	B	126	ARG	2.1
1	B	151	GLY	2.1
1	A	388	SER	2.1
1	B	470	ASP	2.0
1	B	295	PRO	2.0
1	B	150	MET	2.0
1	A	392	ALA	2.0
1	B	244	LEU	2.0
1	A	117	ASP	2.0
1	B	28	ASP	2.0
1	B	232	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	A	609	5/5	0.50	0.13	161,163,164,165	0

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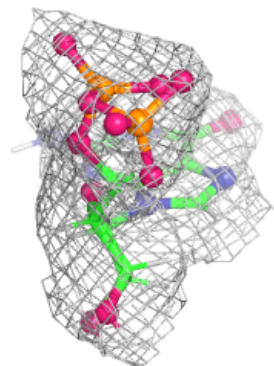
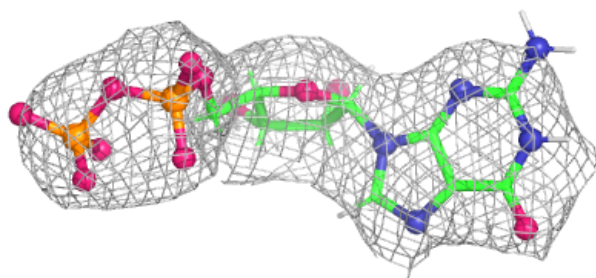
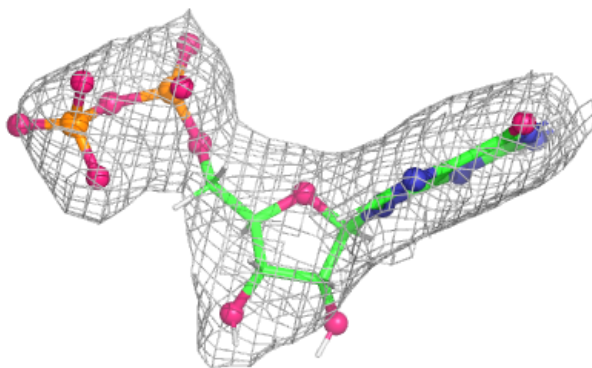
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	B	607	5/5	0.61	0.12	165,165,167,168	0
4	SO4	A	610	5/5	0.76	0.17	134,134,135,135	0
3	GDP	B	604[B]	28/28	0.77	0.16	85,94,114,115	40
3	GDP	B	604[A]	28/28	0.77	0.16	82,94,114,115	40
3	GDP	A	604[A]	28/28	0.80	0.17	64,76,91,93	40
3	GDP	A	604[B]	28/28	0.80	0.17	61,76,93,93	40
4	SO4	A	607	5/5	0.80	0.13	127,130,131,134	0
3	GDP	A	602	28/28	0.82	0.14	96,117,143,143	0
4	SO4	A	606	5/5	0.82	0.23	145,148,149,153	0
4	SO4	A	605	5/5	0.86	0.18	128,129,130,132	0
2	5GP	B	601	24/24	0.87	0.11	93,102,129,136	0
4	SO4	B	605	5/5	0.88	0.11	139,140,142,143	0
4	SO4	A	608	5/5	0.88	0.18	139,143,144,145	0
3	GDP	B	602	28/28	0.89	0.14	82,92,113,113	39
4	SO4	A	611	5/5	0.89	0.51	30,30,30,30	0
4	SO4	B	606	5/5	0.91	0.13	144,146,148,149	0
2	5GP	A	601	24/24	0.91	0.10	71,96,117,121	0
3	GDP	A	603	28/28	0.92	0.10	59,68,83,89	0
3	GDP	B	603	28/28	0.94	0.09	83,95,114,116	0

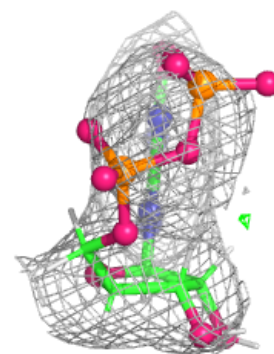
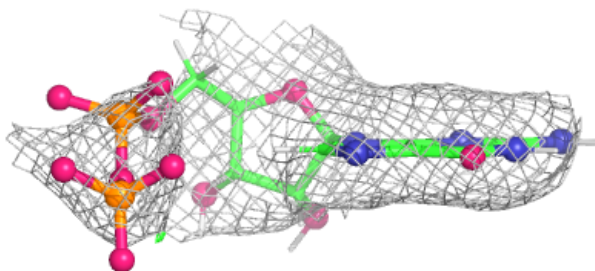
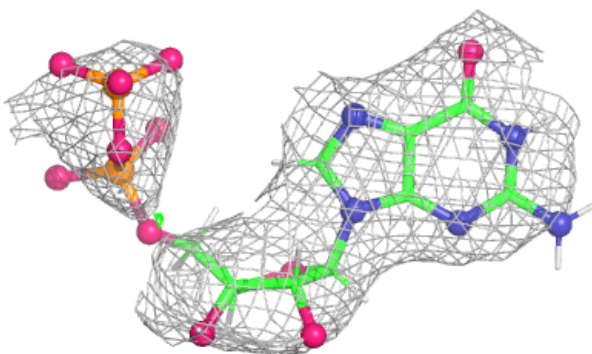
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP B 604 (B):

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

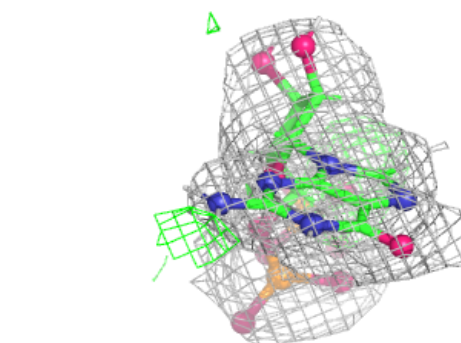
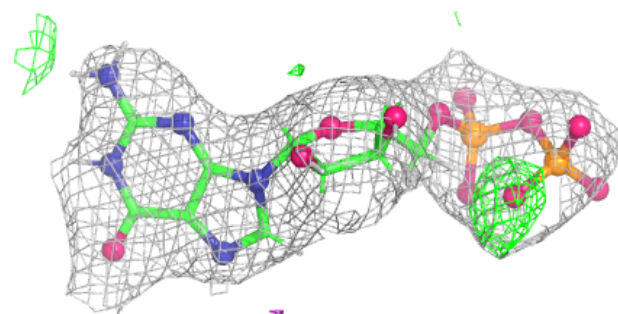
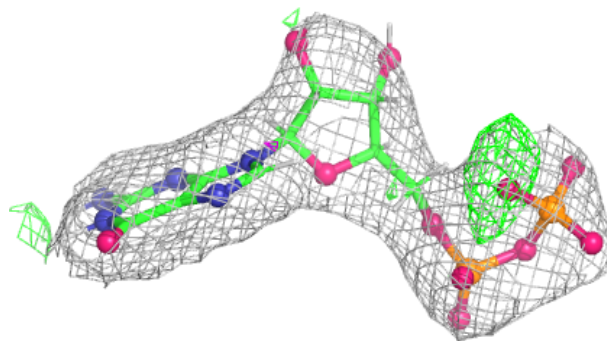
**Electron density around GDP B 604 (A):**

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

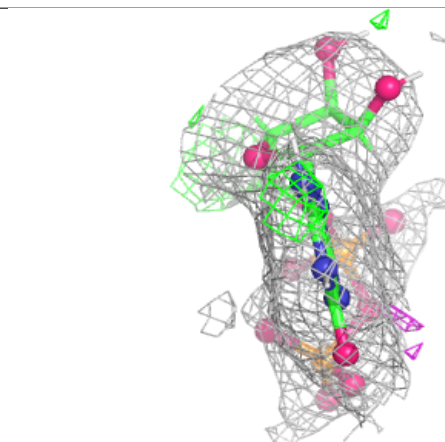
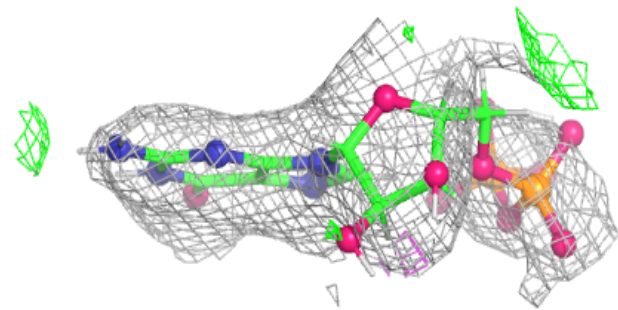
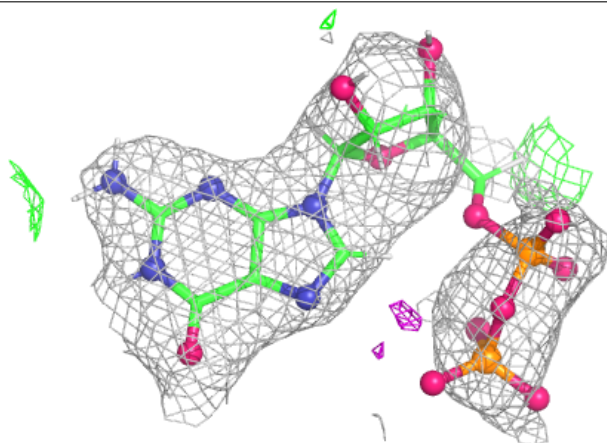


Electron density around GDP A 604 (A):

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

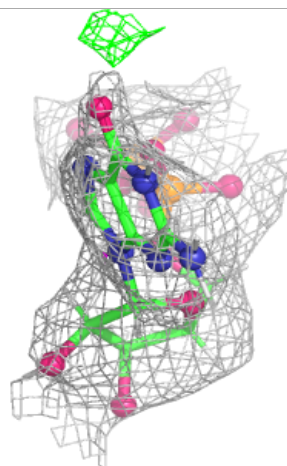
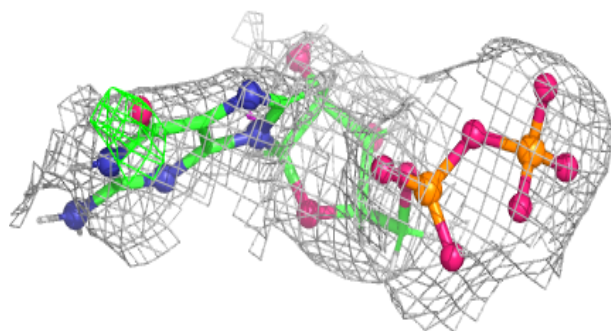
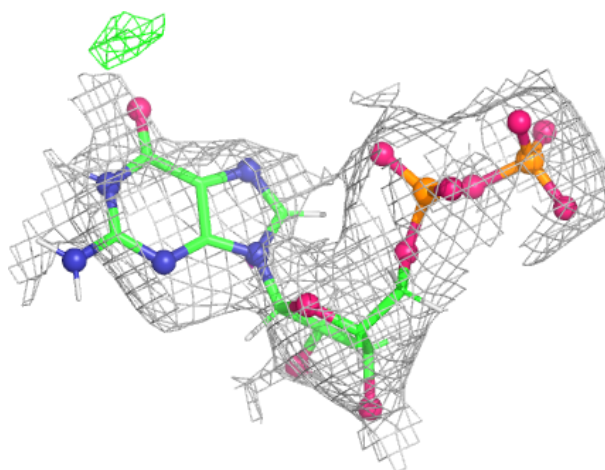
**Electron density around GDP A 604 (B):**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



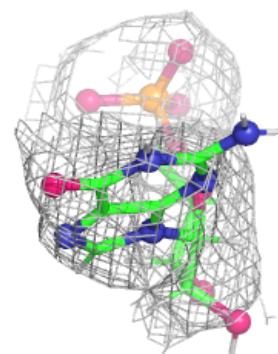
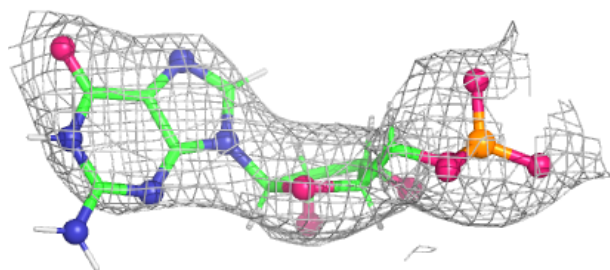
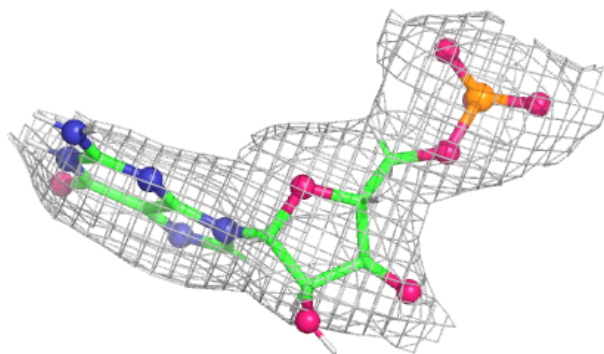
Electron density around GDP A 602:

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



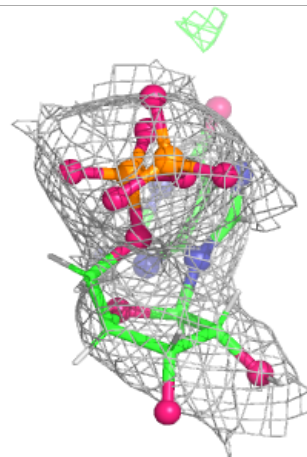
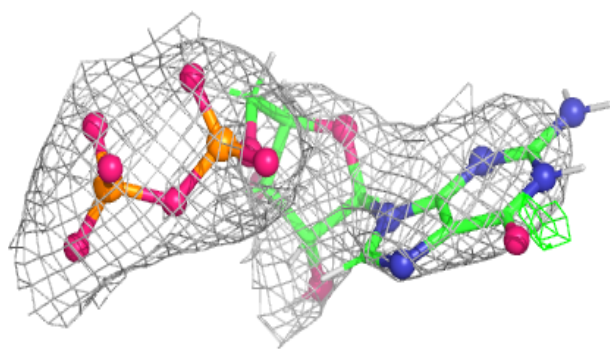
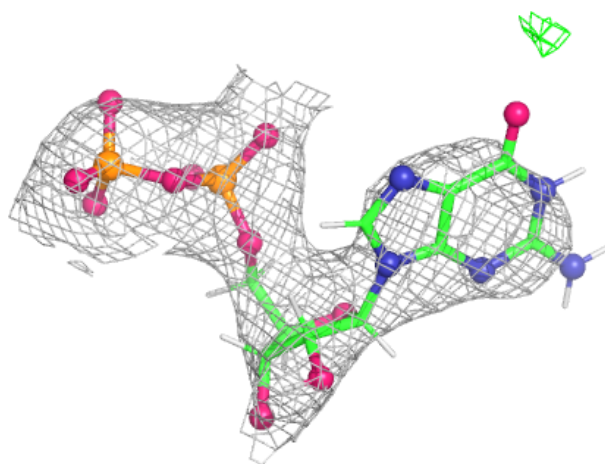
Electron density around 5GP B 601:

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and green (positive)



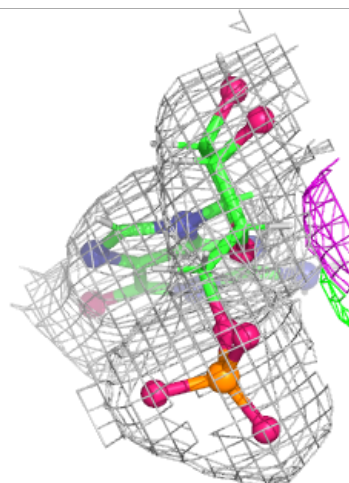
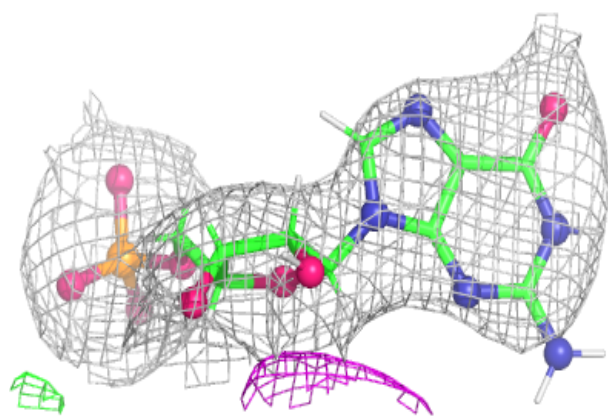
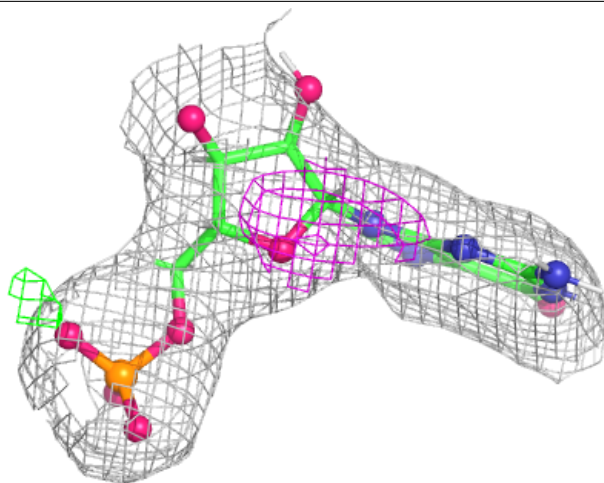
Electron density around GDP B 602:

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and green (positive)



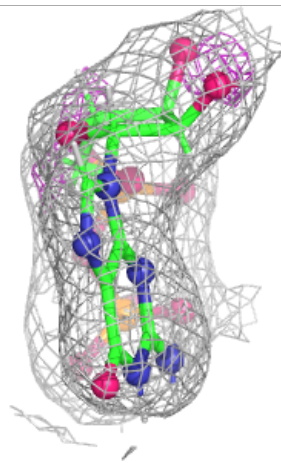
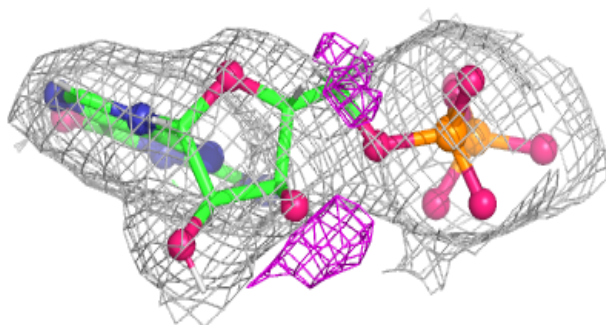
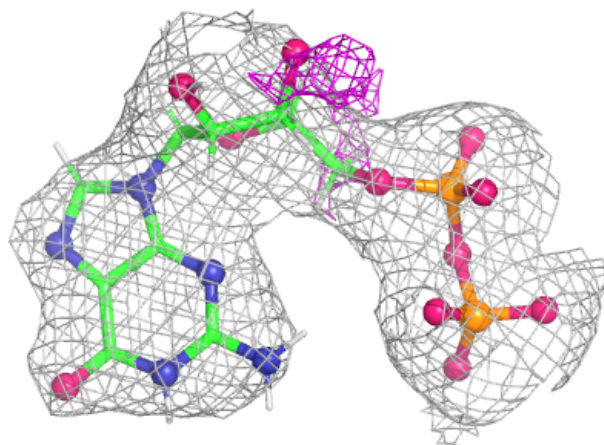
Electron density around 5GP A 601:

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and green (positive)



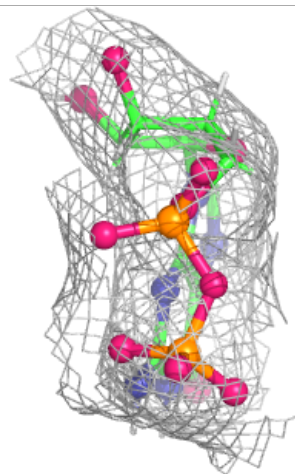
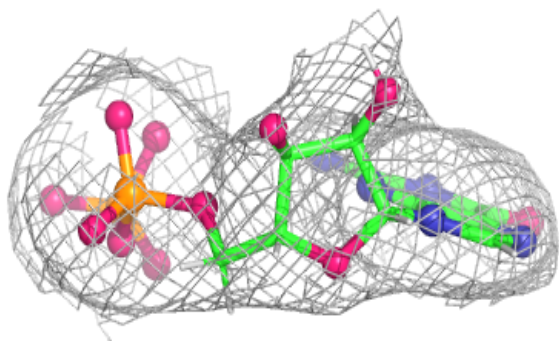
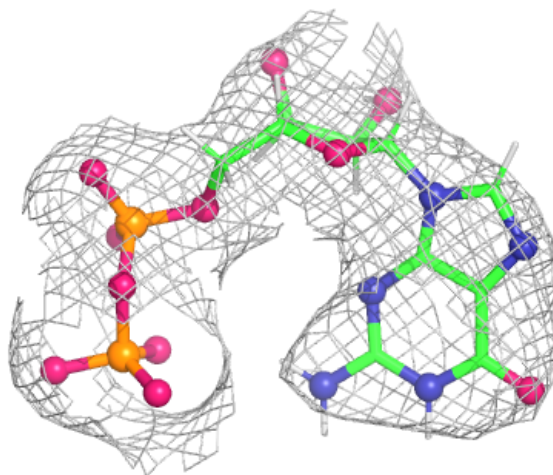
Electron density around GDP A 603:

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



Electron density around GDP B 603:

$2mF_o-DF_c$ (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.