



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 03:21 am BST

PDB ID : 6I0M
Title : Structure of human IMP dehydrogenase, isoform 2, bound to GDP
Authors : Buey, R.M.; Fernandez-Justel, D.; Revuelta, J.L.
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 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 : 2.11
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) : 2.11

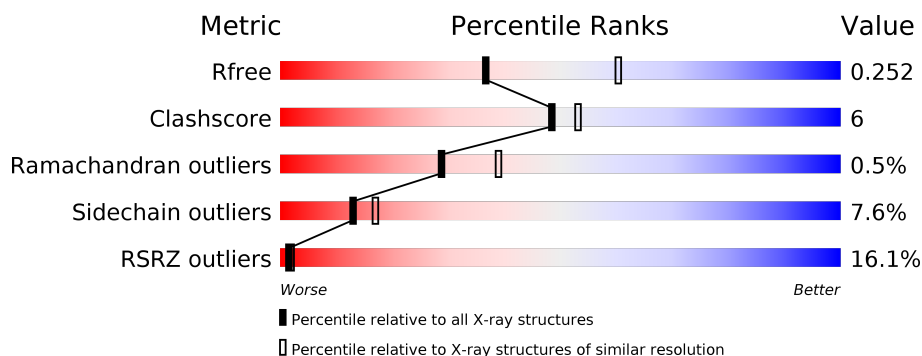
1 Overall quality at a glance

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}	130704	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (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 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	517	<div> <div>12%</div> <div>74%</div> <div>11%</div> <div>•</div> <div>13%</div> </div>
1	B	517	<div> <div>15%</div> <div>77%</div> <div>9%</div> <div>•</div> <div>14%</div> </div>

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	-
4	SO4	B	606	-	-	-	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.

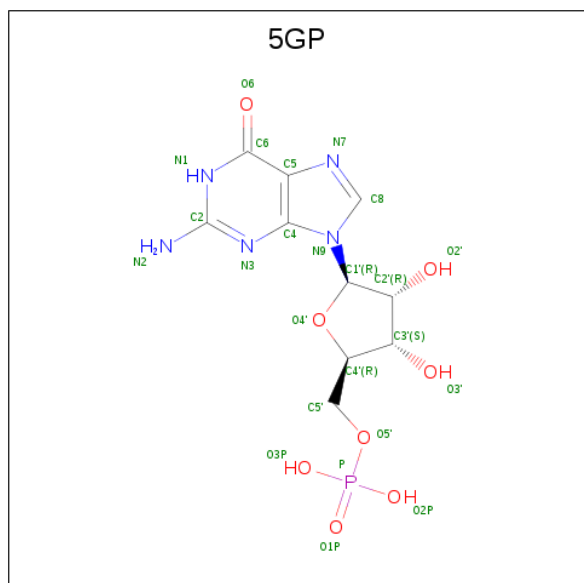
- Molecule 1 is a protein called Inosine-5'-monophosphate dehydrogenase 2.

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:

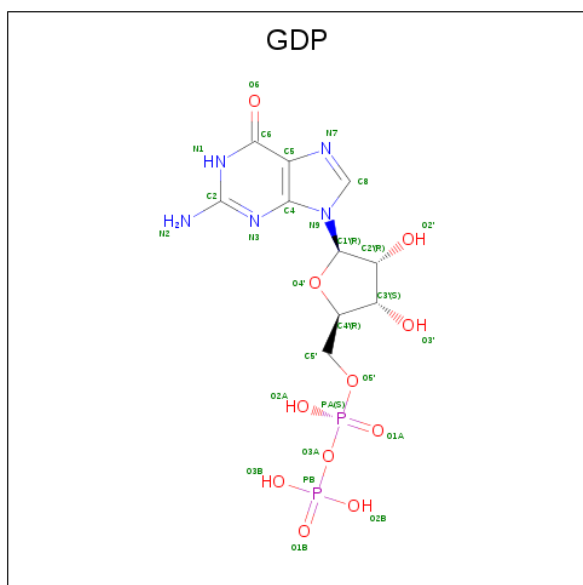
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P12268
A	-1	SER	-	expression tag	UNP P12268
A	0	HIS	-	expression tag	UNP P12268
B	-2	GLY	-	expression tag	UNP P12268
B	-1	SER	-	expression tag	UNP P12268
B	0	HIS	-	expression tag	UNP P12268

- Molecule 2 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula: C₁₀H₁₄N₅O₈P).



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

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



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

- Molecule 4 is SULFATE ION (three-letter code: SO_4) (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		

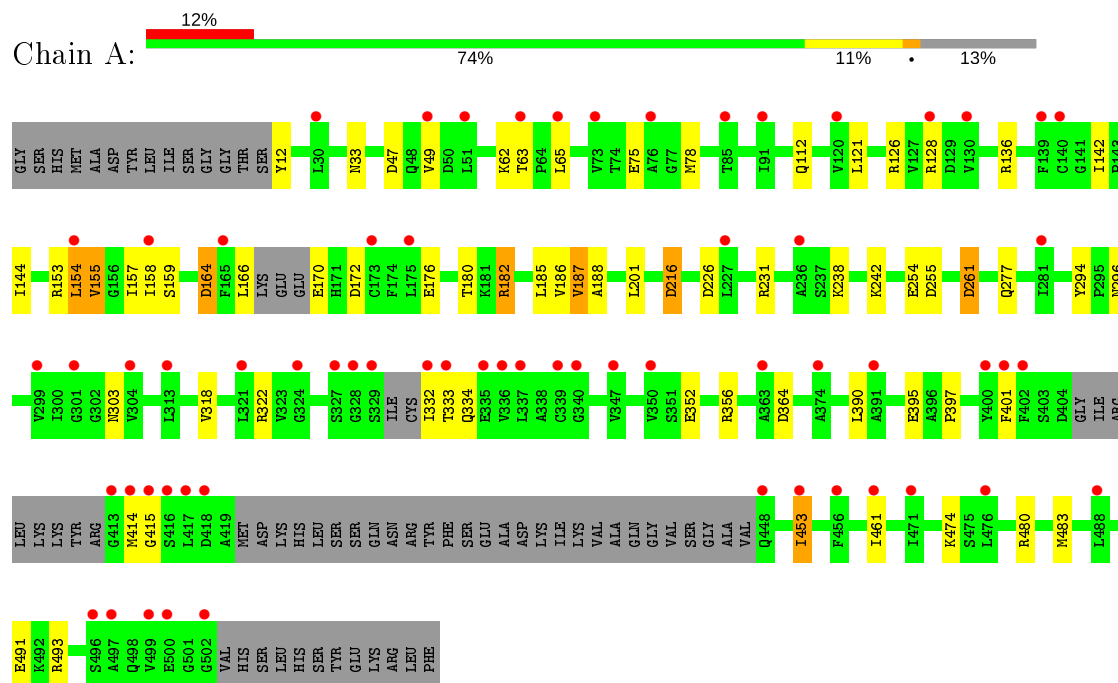
- Molecule 5 is water.

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

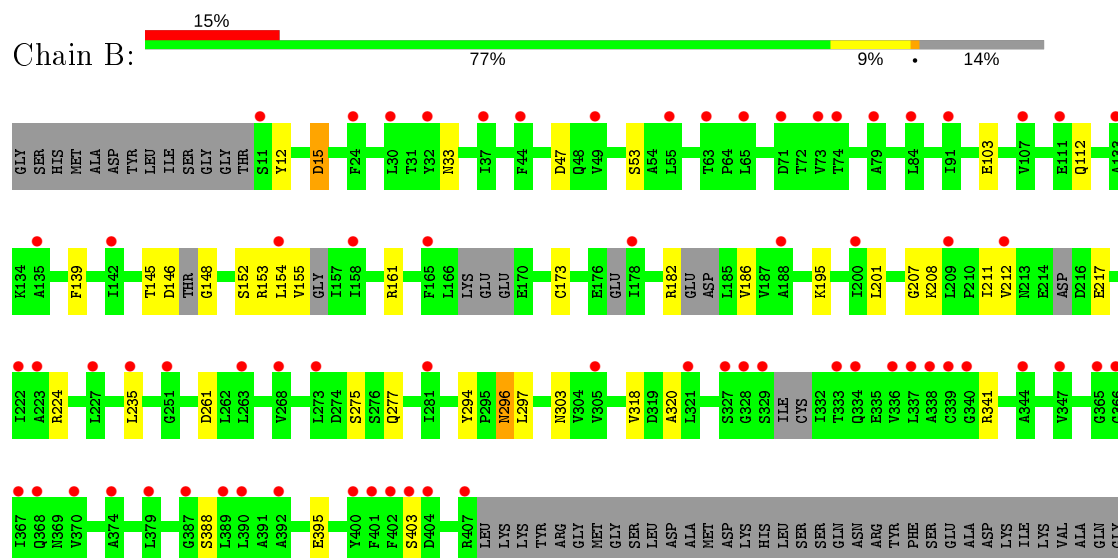
3 Residue-property plots [i](#)

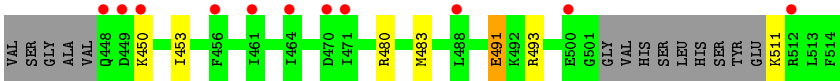
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Inosine-5'-monophosphate dehydrogenase 2



• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2





4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	134.73 Å 134.73 Å 324.08 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	162.00 – 2.57 162.04 – 2.57	Depositor EDS
% Data completeness (in resolution range)	81.2 (162.00-2.57) 81.2 (162.04-2.57)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.58 Å)	Xtriage
Refinement program	PHENIX (1.12rc1_2801: ???)	Depositor
R, R_{free}	0.219 , 0.249 0.229 , 0.252	Depositor DCC
R_{free} test set	1967 reflections (5.04%)	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)	0.38 , 62.5	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	0.92	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: GDP, 5GP, SO4

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	0.27	0/3346	0.47	0/4528
1	B	0.27	0/3191	0.47	0/4320
All	All	0.27	0/6537	0.47	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	56	0
1	B	3147	2978	2985	19	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	4	0
4	A	35	0	0	5	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	78	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 (78) 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	1.19
1:A:166:LEU:C	1:A:170:GLU:CA	2.16	1.14
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	1.08
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	0.96
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: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:HD12	1:A:185:LEU:C	2.15	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
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:O	1:A:185:LEU:HD12	2.04	0.57
1:A:364:ASP:CG	2:A:601:5GP:O3'	2.42	0.57
1:A:159:SER:HB3	3:A:602:GDP:H3'	1.87	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:N	1:A:296:ASN:OD1	2.41	0.54
1:A:154:LEU:HD22	1:A:155:VAL:N	2.24	0.53
1:A:352:GLU:OE2	1:A:356:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:601:5GP:O4'	4:A:611:SO4:O1	2.29	0.51
1:A:75:GLU:HG3	1:A:397:PRO:HB3	1.92	0.51
1:B:275:SER:O	1:B:303:ASN:ND2	2.45	0.50
1:B:395:GLU:OE1	1:B:395:GLU:N	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:78:MET:HE3	1:A:78:MET:HA	1.94	0.49
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: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: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:78:MET:HE1	1:A:453:ILE:HG13	2.02	0.42
1:A:121:LEU:HG	1:A:142:ILE:HG21	2.01	0.42
1:B:388:SER:N	2:B:601:5GP:O3P	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:HD2	1:A:182:ARG:HA	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:182:ARG:NH2	1:A:216:ASP:OD1	2.46	0.41
1:A:164:ASP:CB	1:B:224:ARG:HH21	2.34	0.41
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:185:LEU:CD1	1:A:185:LEU:C	2.85	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

5.3.1 Protein backbone

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%)	22	29
1	B	425/517 (82%)	404 (95%)	20 (5%)	1 (0%)	47	58
All	All	866/1034 (84%)	826 (95%)	36 (4%)	4 (0%)	29	39

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

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%)	304 (92%)	25 (8%)	13	17
1	B	292/422 (69%)	269 (92%)	23 (8%)	12	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	621/844 (74%)	573 (92%)	48 (8%)	13	16

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	TYR
1	A	47	ASP
1	A	62	LYS
1	A	65	LEU
1	A	112	GLN
1	A	136	ARG
1	A	153	ARG
1	A	154	LEU
1	A	155	VAL
1	A	157	ILE
1	A	172	ASP
1	A	182	ARG
1	A	187	VAL
1	A	201	LEU
1	A	216	ASP
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	480	ARG
1	A	483	MET
1	A	491	GLU
1	B	12	TYR
1	B	15	ASP
1	B	47	ASP
1	B	53	SER
1	B	103	GLU
1	B	112	GLN
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	480	ARG
1	B	483	MET
1	B	491	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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
2	5GP	A	601	-	22,26,26	1.16	2 (9%)	27,40,40	2.01	7 (25%)
4	SO4	A	611	-	4,4,4	0.27	0	6,6,6	0.10	0
3	GDP	A	602	-	24,30,30	1.16	2 (8%)	31,47,47	1.99	8 (25%)
3	GDP	A	604[B]	-	24,30,30	1.10	2 (8%)	31,47,47	2.00	8 (25%)
3	GDP	B	602	-	24,30,30	1.12	2 (8%)	31,47,47	1.97	8 (25%)
3	GDP	A	603	-	24,30,30	1.08	2 (8%)	31,47,47	1.93	8 (25%)
4	SO4	A	606	-	4,4,4	0.27	0	6,6,6	0.12	0
3	GDP	B	603	-	24,30,30	1.11	2 (8%)	31,47,47	1.90	8 (25%)
4	SO4	B	605	-	4,4,4	0.28	0	6,6,6	0.08	0
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
4	SO4	A	609	-	4,4,4	0.29	0	6,6,6	0.06	0
4	SO4	B	607	-	4,4,4	0.28	0	6,6,6	0.10	0
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	604[A]	-	24,30,30	1.07	2 (8%)	31,47,47	2.01	8 (25%)
3	GDP	B	604[A]	-	24,30,30	1.10	2 (8%)	31,47,47	1.98	8 (25%)
2	5GP	B	601	-	22,26,26	1.15	2 (9%)	27,40,40	1.98	7 (25%)
3	GDP	B	604[B]	-	24,30,30	1.08	2 (8%)	31,47,47	1.96	8 (25%)
4	SO4	A	605	-	4,4,4	0.24	0	6,6,6	0.07	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
2	5GP	A	601	-	-	0/6/26/26	0/3/3/3
3	GDP	A	602	-	-	3/12/32/32	0/3/3/3
3	GDP	B	602	-	-	4/12/32/32	0/3/3/3
3	GDP	A	603	-	-	3/12/32/32	0/3/3/3
3	GDP	B	603	-	-	6/12/32/32	0/3/3/3
3	GDP	A	604[B]	-	-	2/12/32/32	0/3/3/3
3	GDP	A	604[A]	-	-	6/12/32/32	0/3/3/3
3	GDP	B	604[A]	-	-	5/12/32/32	0/3/3/3
2	5GP	B	601	-	-	2/6/26/26	0/3/3/3
3	GDP	B	604[B]	-	-	5/12/32/32	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	GDP	C6-C5	4.20	1.48	1.41
3	B	602	GDP	C6-C5	4.00	1.48	1.41
2	A	601	5GP	C6-C5	3.98	1.48	1.41
2	B	601	5GP	C6-C5	3.93	1.48	1.41
3	B	604[A]	GDP	C6-C5	3.90	1.48	1.41
3	A	604[B]	GDP	C6-C5	3.88	1.48	1.41
3	B	604[B]	GDP	C6-C5	3.82	1.47	1.41
3	A	604[A]	GDP	C6-C5	3.80	1.47	1.41
3	B	603	GDP	C6-C5	3.74	1.47	1.41
3	A	603	GDP	C6-C5	3.51	1.47	1.41
3	A	602	GDP	C5-C4	2.27	1.46	1.40
3	B	602	GDP	C5-C4	2.23	1.46	1.40
2	A	601	5GP	C5-C4	2.20	1.46	1.40
3	B	604[A]	GDP	C5-C4	2.16	1.46	1.40
2	B	601	5GP	C5-C4	2.15	1.46	1.40
3	B	603	GDP	C5-C4	2.14	1.46	1.40
3	A	604[B]	GDP	C5-C4	2.11	1.46	1.40
3	B	604[B]	GDP	C5-C4	2.09	1.46	1.40
3	A	604[A]	GDP	C5-C4	2.02	1.46	1.40
3	A	603	GDP	C5-C4	2.00	1.46	1.40

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	604[A]	GDP	C2-N3-C4	5.05	121.12	115.36
2	A	601	5GP	C2-N3-C4	4.98	121.04	115.36
3	A	604[B]	GDP	C2-N3-C4	4.97	121.03	115.36
3	B	604[B]	GDP	C2-N3-C4	4.92	120.98	115.36
2	B	601	5GP	C2-N3-C4	4.90	120.95	115.36
3	A	604[A]	GDP	C2-N3-C4	4.87	120.91	115.36
3	B	603	GDP	C2-N3-C4	4.85	120.89	115.36
3	A	602	GDP	C2-N3-C4	4.79	120.83	115.36
3	B	602	GDP	C2-N3-C4	4.75	120.79	115.36
3	A	603	GDP	C2-N3-C4	4.65	120.67	115.36
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	B	602	GDP	C5-C6-N1	-3.91	118.09	123.43
3	A	604[B]	GDP	C5-C6-N1	-3.89	118.12	123.43
3	A	602	GDP	C5-C6-N1	-3.88	118.12	123.43
3	A	604[A]	GDP	PA-O3A-PB	-3.88	119.52	132.83
2	A	601	5GP	C5-C6-N1	-3.85	118.17	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	604[A]	GDP	C5-C6-N1	-3.85	118.17	123.43
2	B	601	5GP	C5-C6-N1	-3.84	118.18	123.43
3	A	603	GDP	C6-C5-C4	-3.82	117.16	120.80
3	A	603	GDP	C5-C6-N1	-3.81	118.22	123.43
3	A	602	GDP	C6-N1-C2	3.77	121.92	115.93
3	B	602	GDP	C6-N1-C2	3.77	121.92	115.93
3	B	603	GDP	C5-C6-N1	-3.75	118.30	123.43
3	A	604[A]	GDP	C6-C5-C4	-3.74	117.23	120.80
3	B	604[B]	GDP	C5-C6-N1	-3.73	118.33	123.43
3	A	603	GDP	C6-N1-C2	3.72	121.84	115.93
3	A	604[A]	GDP	C6-N1-C2	3.72	121.84	115.93
3	B	602	GDP	C6-C5-C4	-3.72	117.25	120.80
3	A	602	GDP	C6-C5-C4	-3.72	117.25	120.80
3	B	603	GDP	C6-C5-C4	-3.71	117.26	120.80
3	B	602	GDP	PA-O3A-PB	-3.69	120.16	132.83
2	B	601	5GP	C6-N1-C2	3.69	121.80	115.93
2	B	601	5GP	C6-C5-C4	-3.68	117.28	120.80
3	A	604[B]	GDP	C6-N1-C2	3.68	121.78	115.93
3	B	604[A]	GDP	C5-C6-N1	-3.64	118.45	123.43
3	B	603	GDP	C6-N1-C2	3.64	121.70	115.93
2	A	601	5GP	C6-N1-C2	3.63	121.69	115.93
3	B	604[B]	GDP	C6-N1-C2	3.57	121.60	115.93
3	A	602	GDP	PA-O3A-PB	-3.52	120.74	132.83
3	B	604[A]	GDP	C6-N1-C2	3.47	121.44	115.93
3	B	604[B]	GDP	C6-C5-C4	-3.46	117.49	120.80
3	A	604[B]	GDP	C6-C5-C4	-3.44	117.51	120.80
2	A	601	5GP	C6-C5-C4	-3.39	117.56	120.80
3	B	604[A]	GDP	C6-C5-C4	-3.37	117.58	120.80
2	A	601	5GP	C3'-C2'-C1'	3.33	105.99	100.98
3	A	603	GDP	PA-O3A-PB	-3.19	121.89	132.83
3	A	604[A]	GDP	N3-C2-N1	-3.10	123.09	127.22
2	B	601	5GP	N3-C2-N1	-3.05	123.15	127.22
3	B	602	GDP	N3-C2-N1	-3.00	123.22	127.22
3	B	603	GDP	N3-C2-N1	-3.00	123.23	127.22
3	A	604[B]	GDP	N3-C2-N1	-2.99	123.23	127.22
3	B	604[A]	GDP	C3'-C2'-C1'	2.98	105.47	100.98
3	B	604[A]	GDP	C4-C5-N7	-2.98	106.30	109.40
3	A	604[A]	GDP	C4-C5-N7	-2.96	106.32	109.40
3	B	604[B]	GDP	C3'-C2'-C1'	2.95	105.41	100.98
3	A	602	GDP	N3-C2-N1	-2.94	123.30	127.22
3	A	603	GDP	N3-C2-N1	-2.94	123.30	127.22
2	A	601	5GP	N3-C2-N1	-2.93	123.32	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	5GP	C4-C5-N7	-2.92	106.36	109.40
3	A	604[B]	GDP	C4-C5-N7	-2.91	106.37	109.40
2	B	601	5GP	C3'-C2'-C1'	2.89	105.33	100.98
3	B	604[B]	GDP	N3-C2-N1	-2.88	123.38	127.22
3	A	602	GDP	C4-C5-N7	-2.88	106.40	109.40
3	B	604[B]	GDP	C4-C5-N7	-2.86	106.42	109.40
3	A	603	GDP	C3'-C2'-C1'	2.84	105.26	100.98
2	B	601	5GP	C4-C5-N7	-2.83	106.45	109.40
3	B	604[A]	GDP	N3-C2-N1	-2.81	123.47	127.22
3	B	602	GDP	C4-C5-N7	-2.76	106.52	109.40
3	B	603	GDP	PA-O3A-PB	-2.75	123.40	132.83
3	A	602	GDP	C3'-C2'-C1'	2.73	105.09	100.98
3	B	603	GDP	C4-C5-N7	-2.69	106.59	109.40
3	B	603	GDP	C3'-C2'-C1'	2.63	104.93	100.98
3	A	604[B]	GDP	C3'-C2'-C1'	2.61	104.91	100.98
3	A	603	GDP	C4-C5-N7	-2.46	106.84	109.40
3	A	604[A]	GDP	C3'-C2'-C1'	2.44	104.65	100.98
3	B	602	GDP	C3'-C2'-C1'	2.36	104.53	100.98

There are no chirality outliers.

All (36) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
3	B	603	GDP	O4'-C4'-C5'-O5'
3	B	603	GDP	C3'-C4'-C5'-O5'
3	B	603	GDP	C5'-O5'-PA-O3A
3	A	604[A]	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

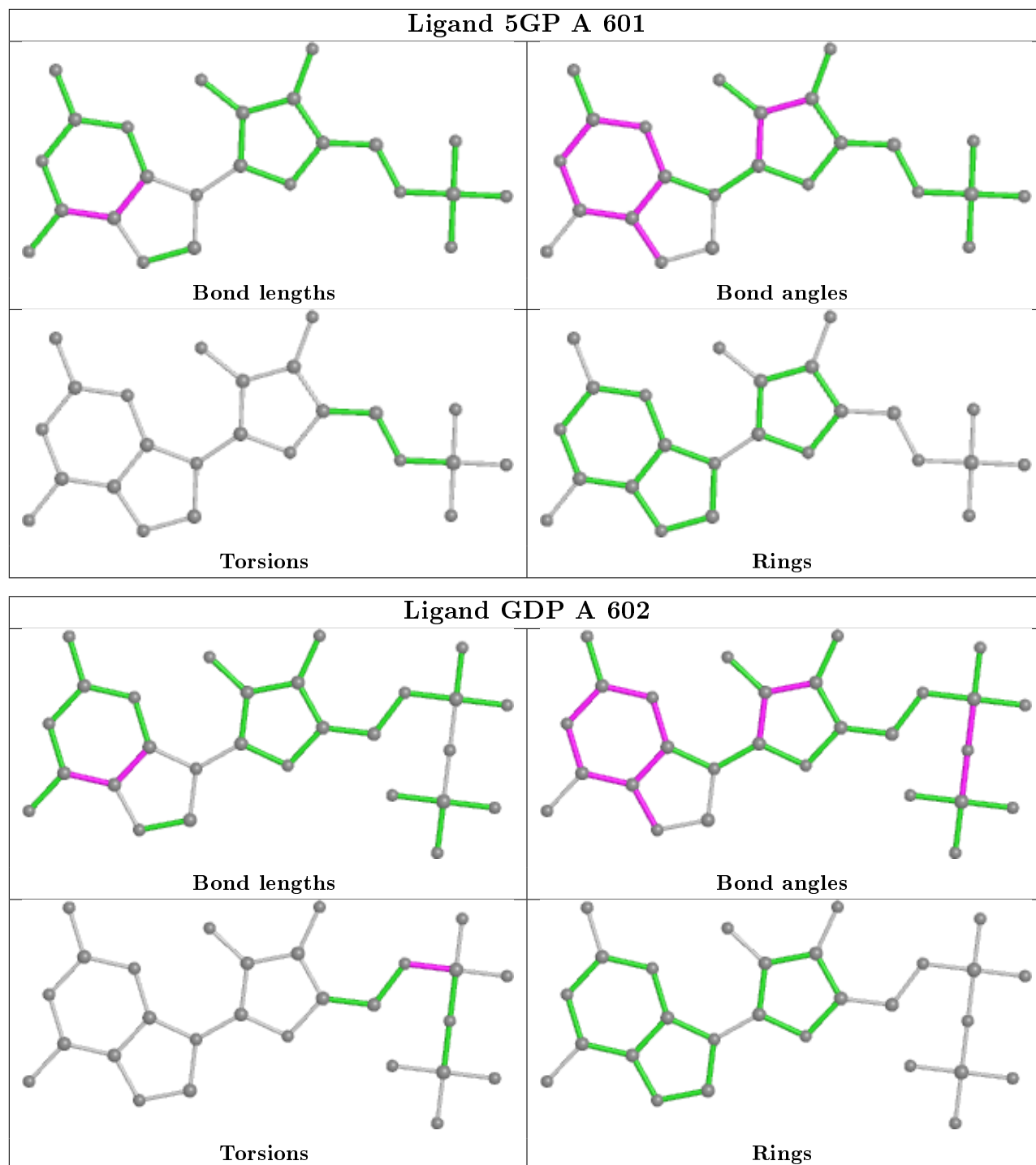
There are no ring outliers.

10 monomers are involved in 32 short contacts:

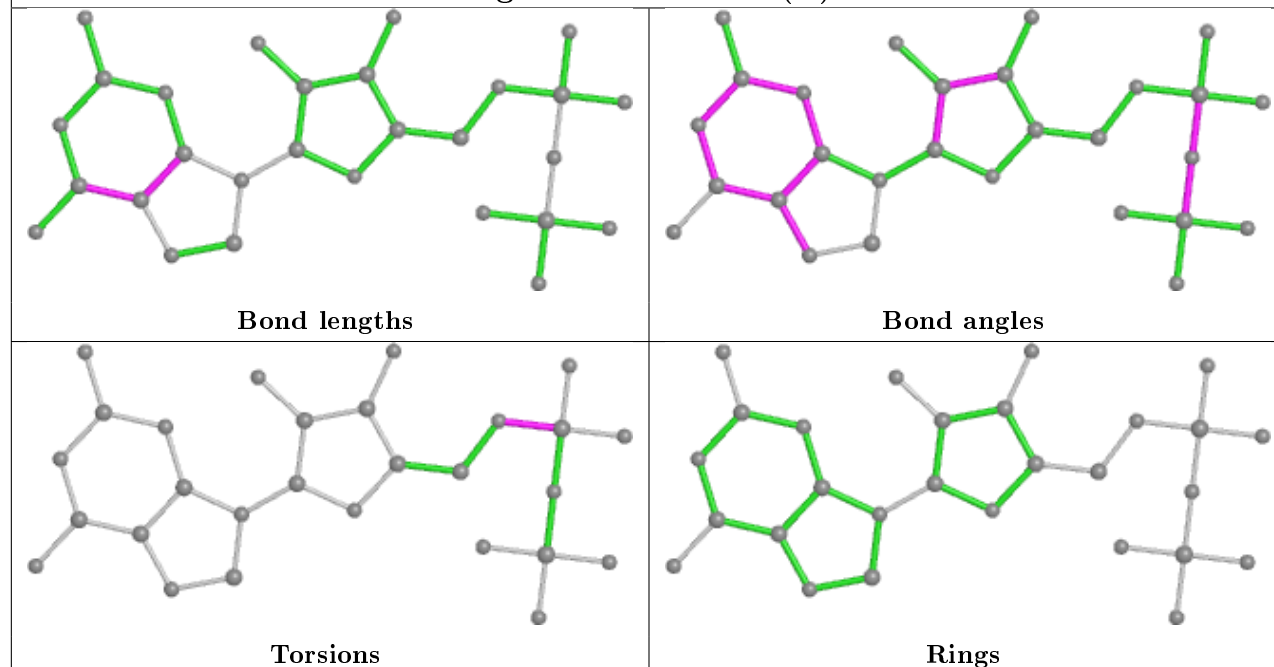
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	5GP	7	0
4	A	611	SO4	4	0
3	A	602	GDP	10	0
3	A	604[B]	GDP	4	0
3	B	602	GDP	1	0
3	A	603	GDP	1	0
3	B	603	GDP	3	0
4	A	609	SO4	1	0
3	A	604[A]	GDP	3	0
2	B	601	5GP	1	0

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

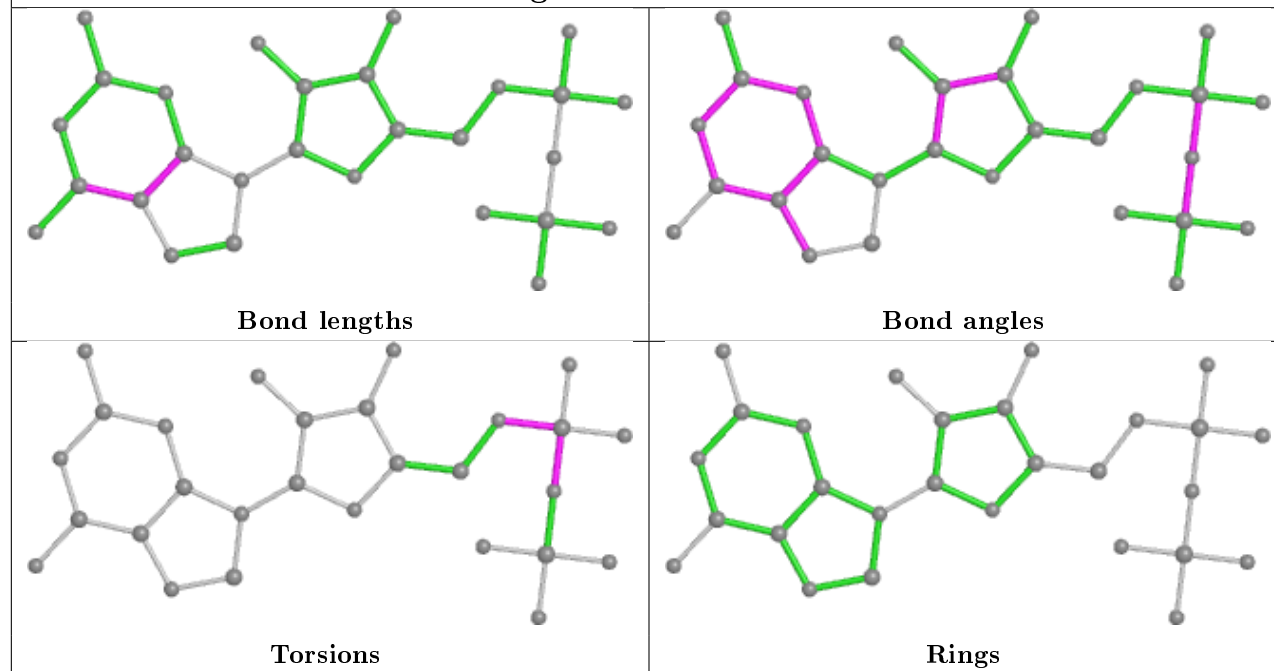
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

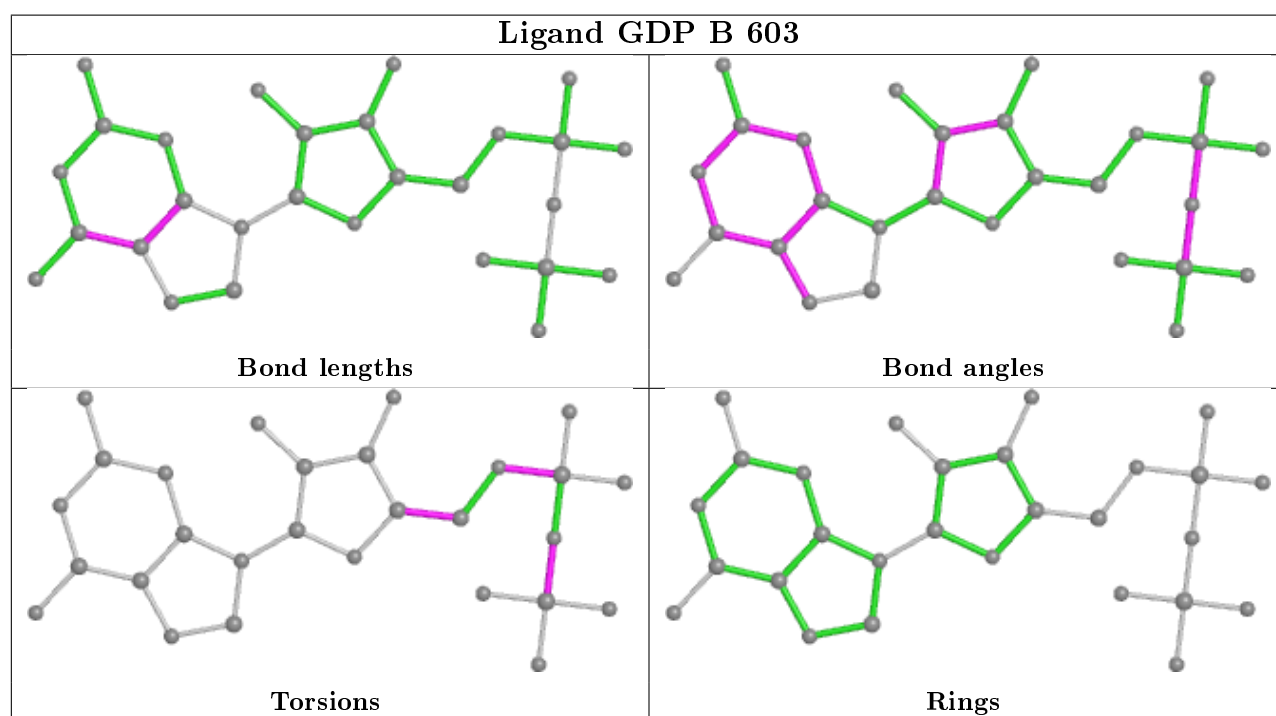
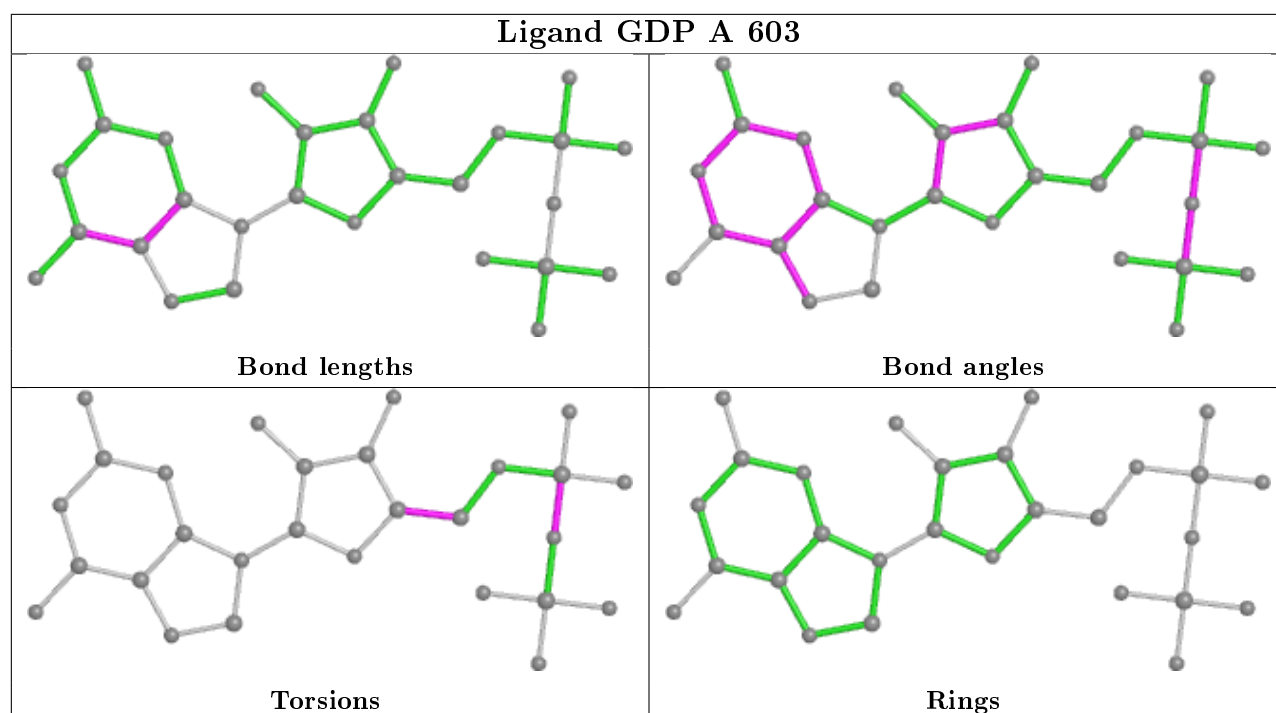


Ligand GDP A 604 (B)

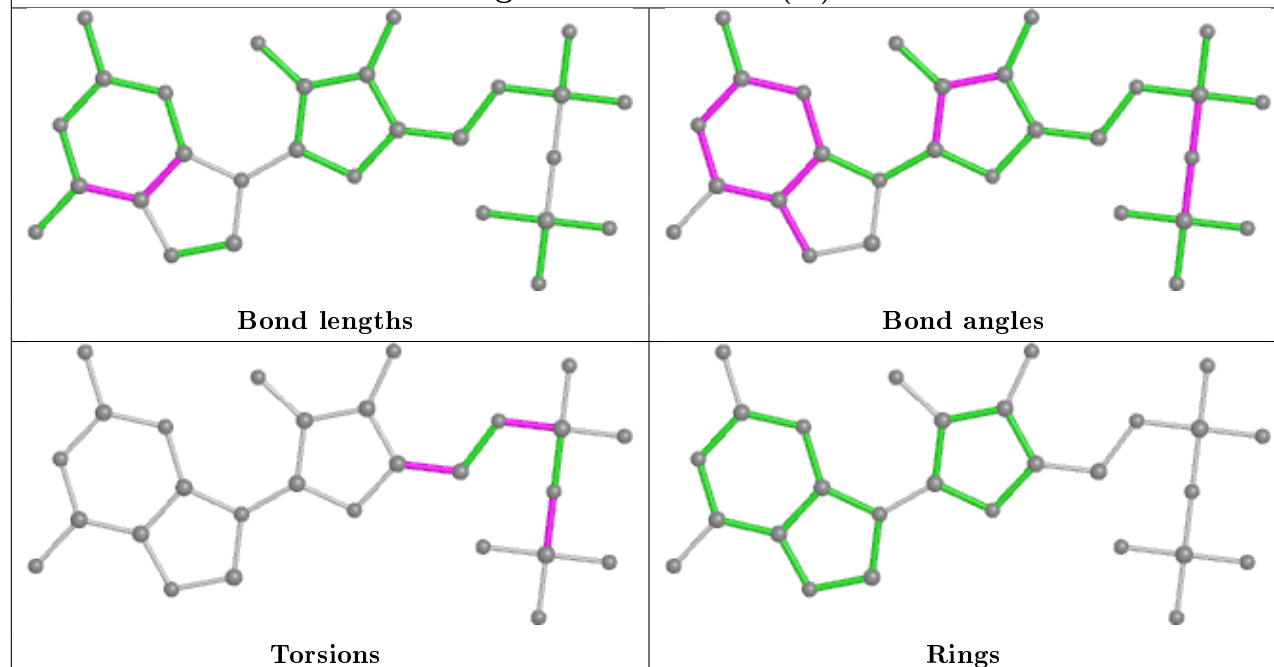


Ligand GDP B 602

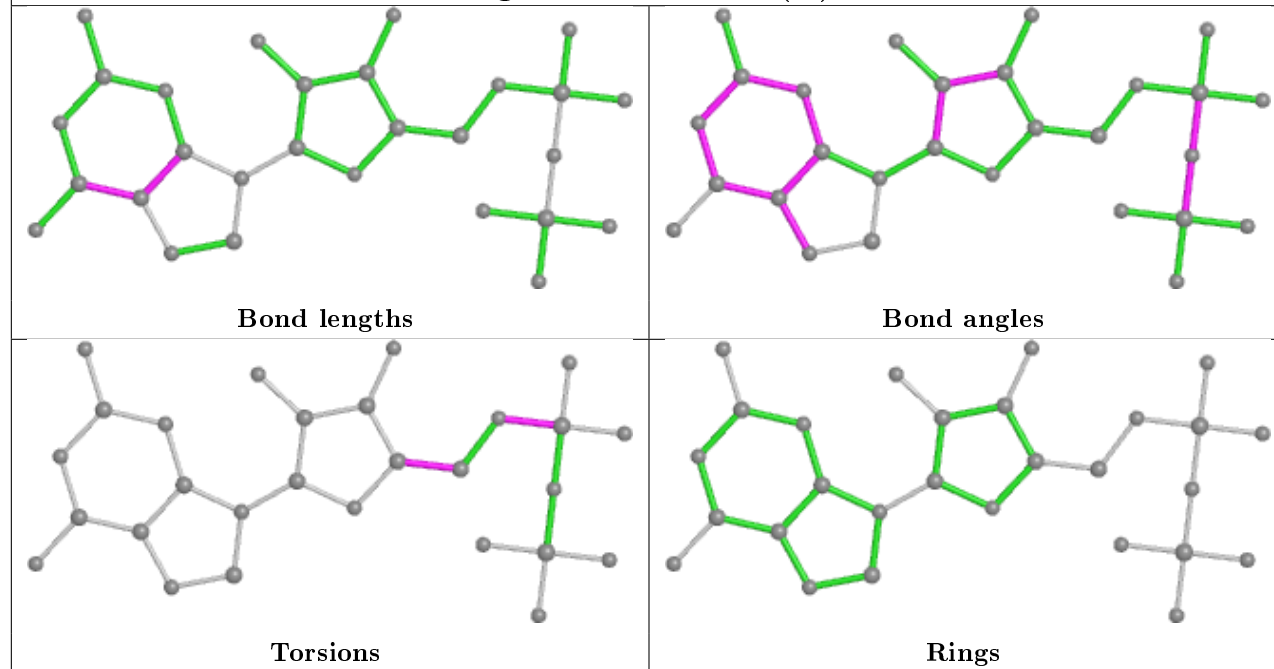


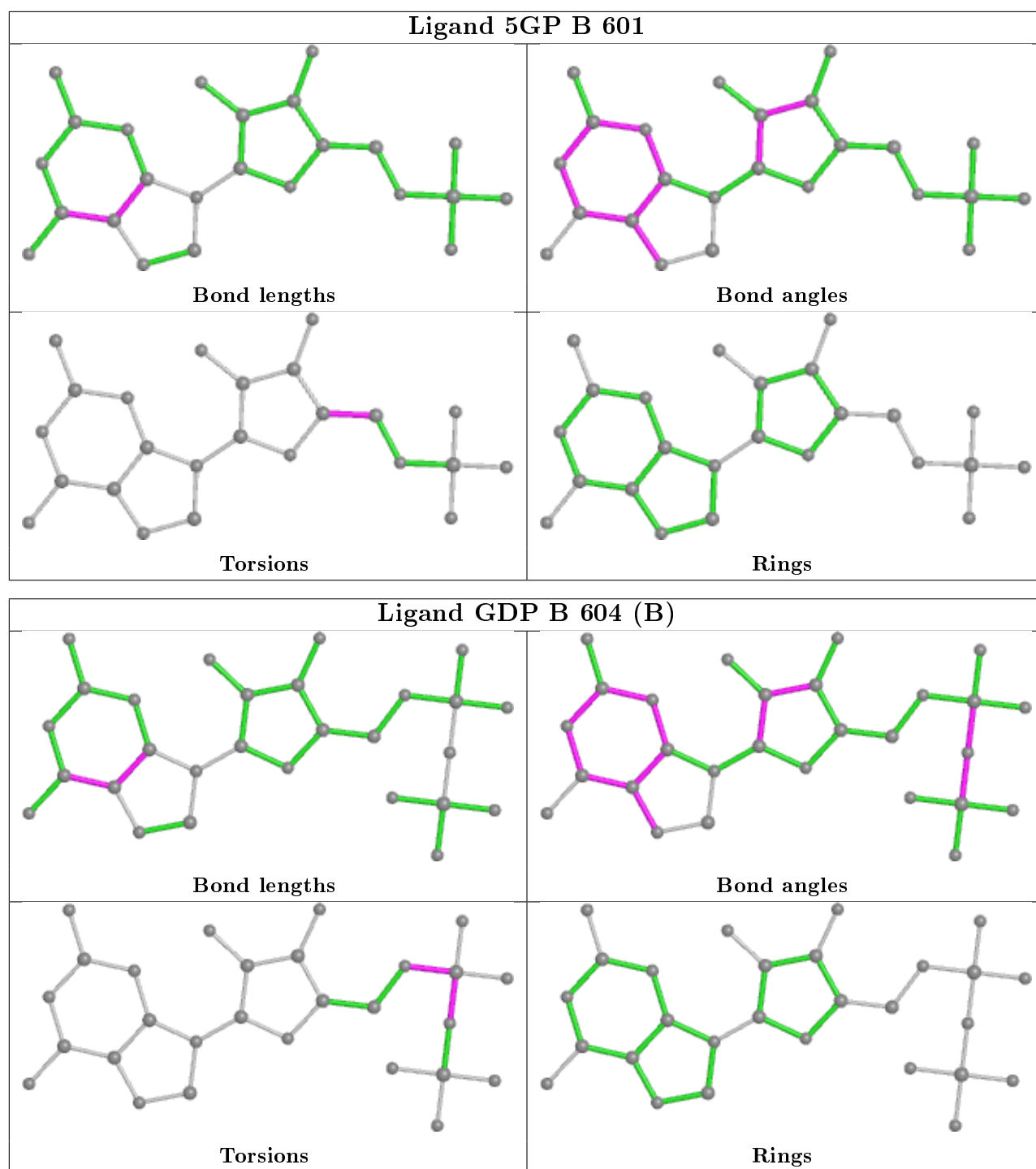


Ligand GDP A 604 (A)



Ligand GDP B 604 (A)





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	450/517 (87%)	1.13	64 (14%) 2 3	39, 63, 127, 161	0
1	B	444/517 (85%)	1.05	80 (18%) 1 1	51, 82, 134, 185	0
All	All	894/1034 (86%)	1.09	144 (16%) 1 2	39, 73, 133, 185	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	448	GLN	7.0
1	A	402	PHE	6.6
1	A	414	MET	6.3
1	A	329	SER	5.9
1	A	401	PHE	5.8
1	A	497	ALA	5.6
1	A	336	VAL	5.4
1	A	413	GLY	5.3
1	B	337	LEU	5.1
1	B	449	ASP	5.0
1	B	338	ALA	4.7
1	A	415	GLY	4.6
1	B	402	PHE	4.4
1	B	327	SER	4.4
1	A	416	SER	4.4
1	B	227	LEU	4.1
1	A	337	LEU	4.1
1	B	367	ILE	3.7
1	A	502	GLY	3.6
1	B	404	ASP	3.6
1	A	400	TYR	3.6
1	A	448	GLN	3.6
1	A	313	LEU	3.6
1	A	496	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	499	VAL	3.5
1	B	223	ALA	3.4
1	B	333	THR	3.4
1	B	74	THR	3.4
1	B	401	PHE	3.3
1	B	461	ILE	3.3
1	B	135	ALA	3.2
1	B	334	GLN	3.2
1	B	403	SER	3.2
1	A	328	GLY	3.2
1	B	340	GLY	3.1
1	A	304	VAL	3.0
1	A	500	GLU	2.9
1	A	471	ILE	2.9
1	A	85	THR	2.9
1	A	30	LEU	2.9
1	B	390	LEU	2.9
1	B	73	VAL	2.9
1	B	142	ILE	2.9
1	B	158	ILE	2.9
1	B	235	LEU	2.9
1	A	301	GLY	2.8
1	A	281	ILE	2.8
1	A	324	GLY	2.8
1	A	130	VAL	2.8
1	A	453	ILE	2.8
1	B	65	LEU	2.8
1	B	49	VAL	2.8
1	B	44	PHE	2.8
1	A	154	LEU	2.8
1	B	321	LEU	2.8
1	A	128	ARG	2.7
1	A	456	PHE	2.7
1	A	140	CYS	2.7
1	B	328	GLY	2.7
1	A	418	ASP	2.7
1	B	71	ASP	2.7
1	B	471	ILE	2.7
1	B	133	ALA	2.7
1	B	154	LEU	2.7
1	B	251	GLY	2.7
1	B	30	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	51	LEU	2.6
1	B	339	CYS	2.6
1	B	336	VAL	2.6
1	B	387	GLY	2.6
1	B	281	ILE	2.6
1	B	11	SER	2.6
1	A	158	ILE	2.6
1	B	165	PHE	2.6
1	B	222	ILE	2.6
1	B	209	LEU	2.6
1	A	332	ILE	2.6
1	B	407	ARG	2.6
1	B	91	ILE	2.5
1	B	188	ALA	2.5
1	B	212	VAL	2.5
1	A	91	ILE	2.5
1	A	139	PHE	2.5
1	B	79	ALA	2.5
1	B	365	GLY	2.5
1	B	400	TYR	2.4
1	A	327	SER	2.4
1	A	333	THR	2.4
1	B	368	GLN	2.4
1	A	63	THR	2.4
1	B	24	PHE	2.4
1	B	512	ARG	2.4
1	A	65	LEU	2.4
1	A	391	ALA	2.4
1	B	379	LEU	2.4
1	B	389	LEU	2.4
1	B	450	LYS	2.3
1	B	329	SER	2.3
1	A	335	GLU	2.3
1	B	200	ILE	2.3
1	A	461	ILE	2.3
1	B	37	ILE	2.3
1	A	488	LEU	2.3
1	B	273	LEU	2.3
1	B	268	VAL	2.3
1	A	374	ALA	2.3
1	B	32	TYR	2.3
1	B	464	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	84	LEU	2.3
1	B	107	VAL	2.3
1	A	476	LEU	2.3
1	B	178	ILE	2.2
1	B	374	ALA	2.2
1	B	63	THR	2.2
1	B	263	LEU	2.2
1	A	339	CYS	2.2
1	A	321	LEU	2.2
1	B	500	GLU	2.2
1	A	347	VAL	2.2
1	A	175	LEU	2.2
1	B	488	LEU	2.2
1	B	347	VAL	2.2
1	B	392	ALA	2.2
1	A	73	VAL	2.2
1	A	299	VAL	2.2
1	A	417	LEU	2.2
1	A	350	VAL	2.1
1	B	470	ASP	2.1
1	A	340	GLY	2.1
1	B	366	GLY	2.1
1	A	227	LEU	2.1
1	A	236	ALA	2.1
1	B	55	LEU	2.1
1	A	173	CYS	2.1
1	A	363	ALA	2.0
1	A	120	VAL	2.0
1	B	305	VAL	2.0
1	B	456	PHE	2.0
1	B	344	ALA	2.0
1	A	49	VAL	2.0
1	B	370	VAL	2.0
1	A	165	PHE	2.0
1	A	76	ALA	2.0
1	B	111	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

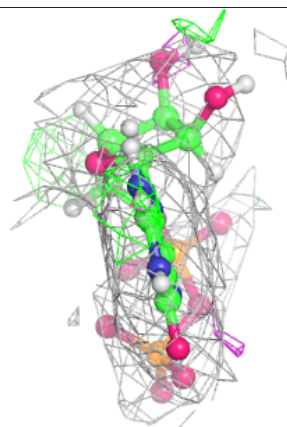
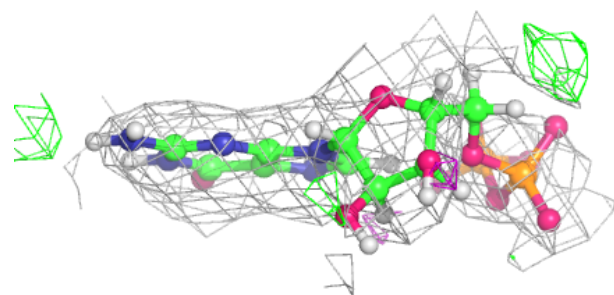
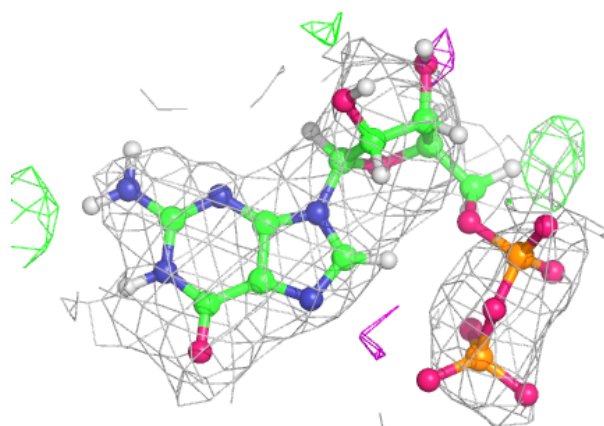
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	A	609	5/5	0.64	0.22	161,163,164,165	0
4	SO4	A	606	5/5	0.75	0.25	145,148,149,153	0
4	SO4	B	606	5/5	0.77	0.55	144,146,148,149	0
4	SO4	B	605	5/5	0.78	0.20	139,140,142,143	0
4	SO4	B	607	5/5	0.81	0.16	165,165,167,168	0
4	SO4	A	608	5/5	0.83	0.35	139,143,144,145	0
3	GDP	A	604[B]	28/28	0.83	0.26	61,76,93,93	40
4	SO4	A	607	5/5	0.83	0.27	127,130,131,134	0
3	GDP	A	604[A]	28/28	0.83	0.26	64,76,91,93	40
3	GDP	B	604[A]	28/28	0.83	0.22	82,94,114,115	40
3	GDP	B	604[B]	28/28	0.83	0.22	85,94,114,115	40
4	SO4	A	610	5/5	0.86	0.59	134,134,135,135	0
4	SO4	A	605	5/5	0.88	0.23	128,129,130,132	0
3	GDP	A	602	28/28	0.90	0.23	96,117,143,143	0
2	5GP	B	601	24/24	0.91	0.23	93,102,129,136	0
2	5GP	A	601	24/24	0.93	0.21	71,96,117,121	0
3	GDP	B	602	28/28	0.93	0.28	82,92,113,113	39
4	SO4	A	611	5/5	0.93	0.61	30,30,30,30	0
3	GDP	A	603	28/28	0.94	0.23	59,68,83,89	0
3	GDP	B	603	28/28	0.95	0.17	83,95,114,116	0

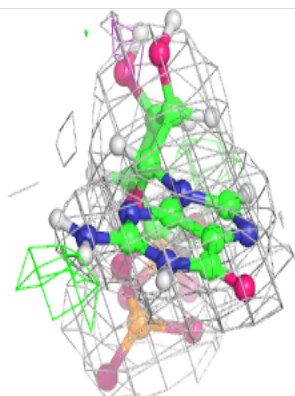
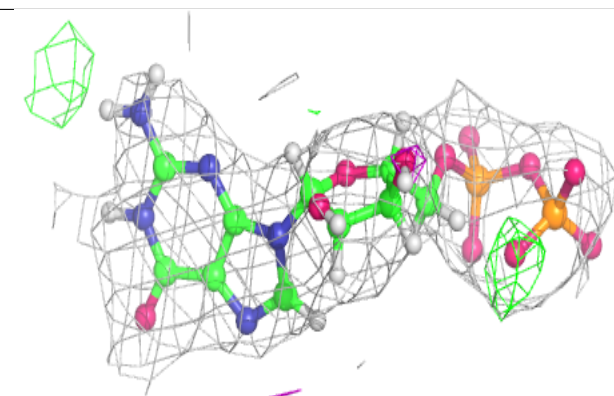
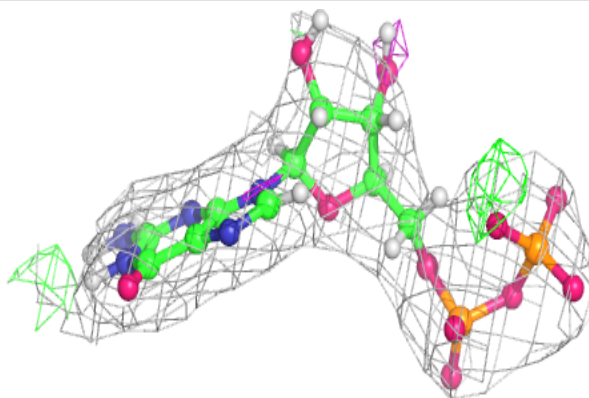
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP A 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)

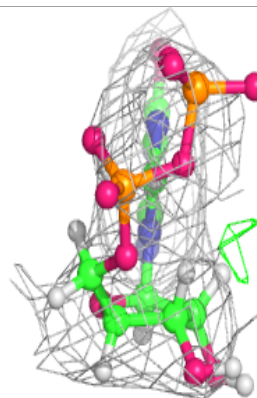
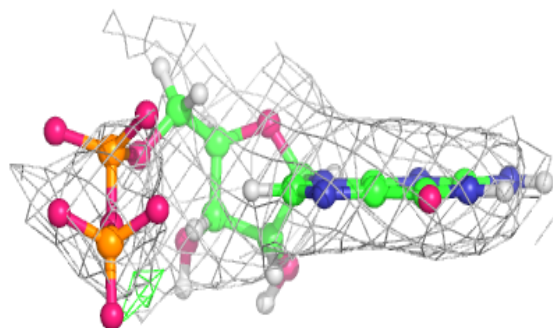
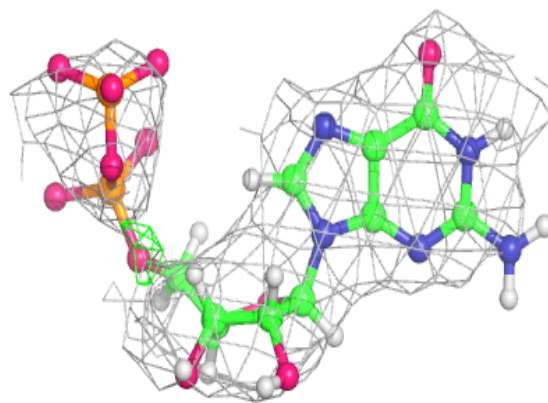
**Electron density around GDP A 604 (A):**

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

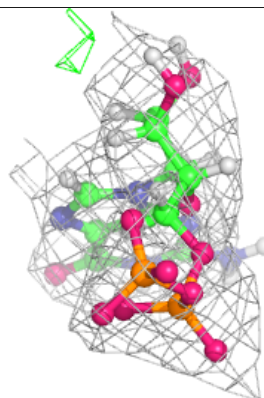
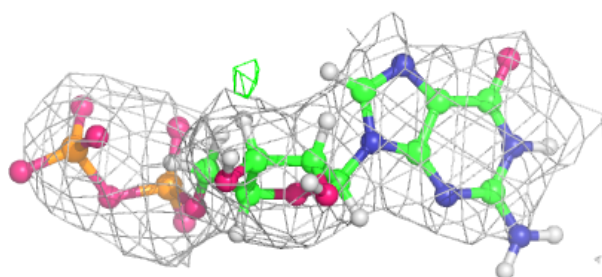
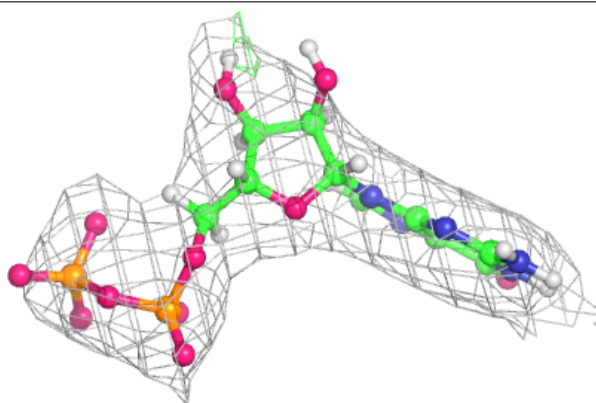


Electron density around GDP B 604 (A):

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

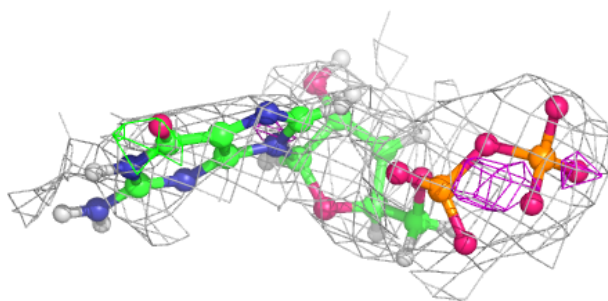
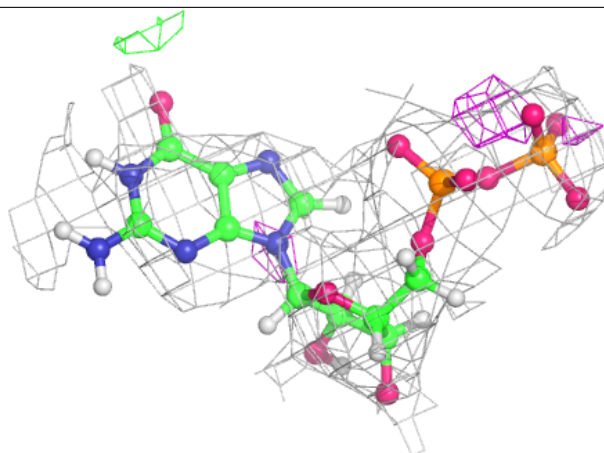
**Electron density around GDP B 604 (B):**

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

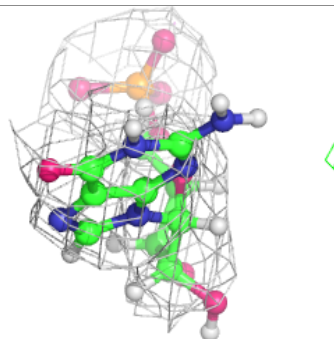
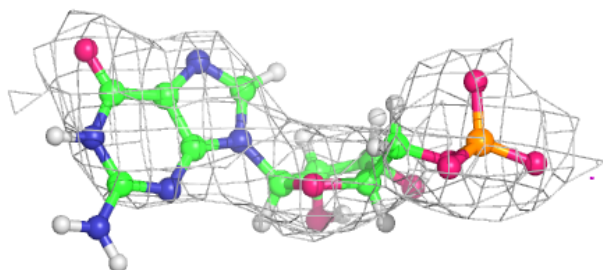
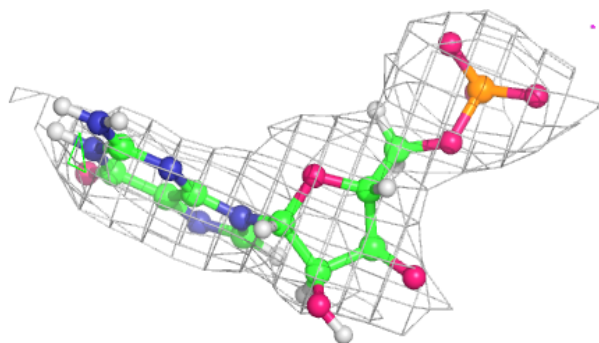


Electron density around GDP A 602:

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

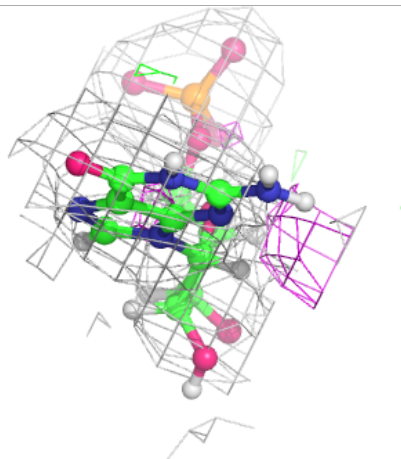
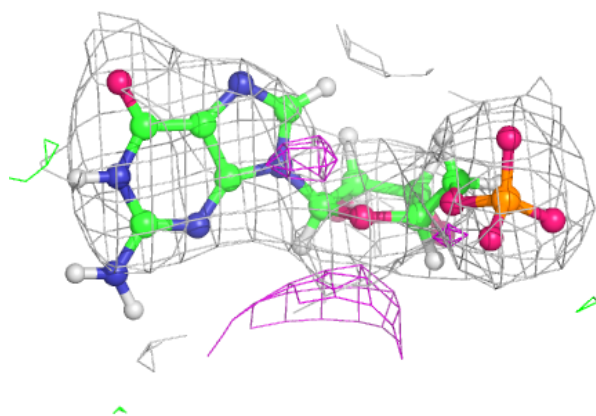
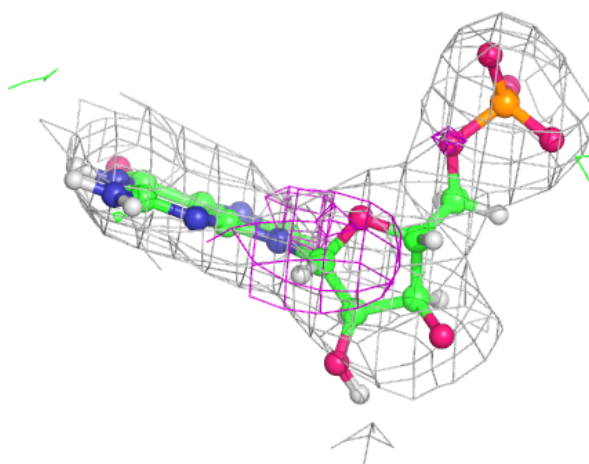
**Electron density around 5GP B 601:**

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



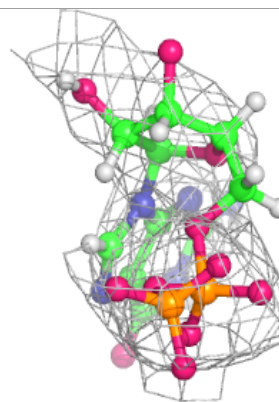
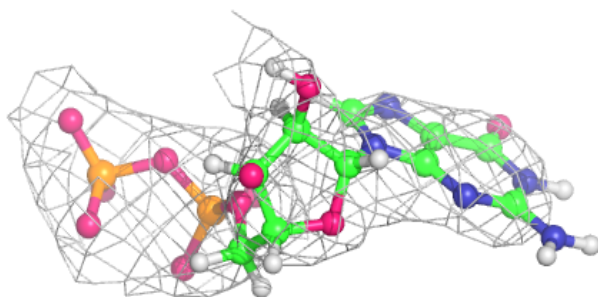
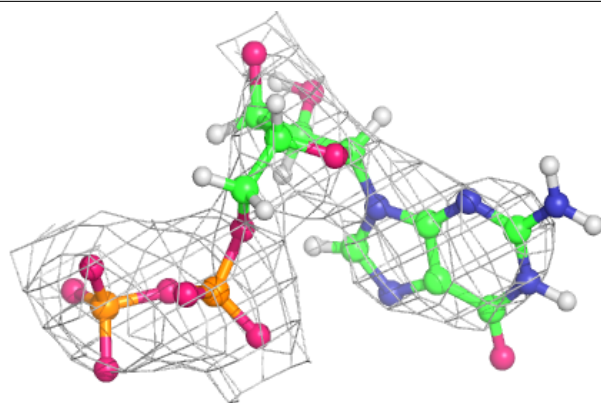
Electron density around 5GP A 601:

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



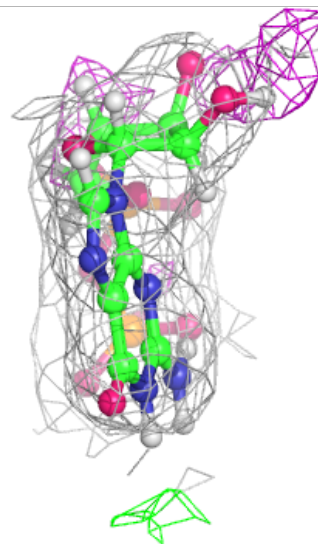
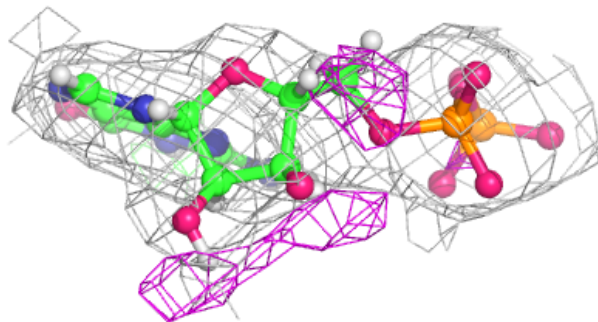
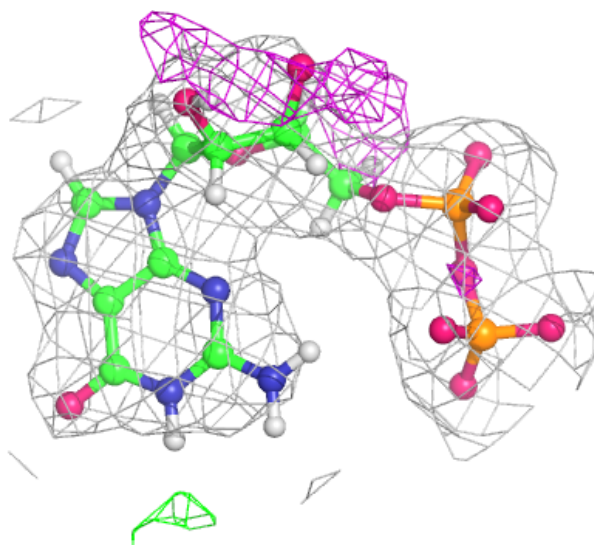
Electron density around GDP B 602:

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



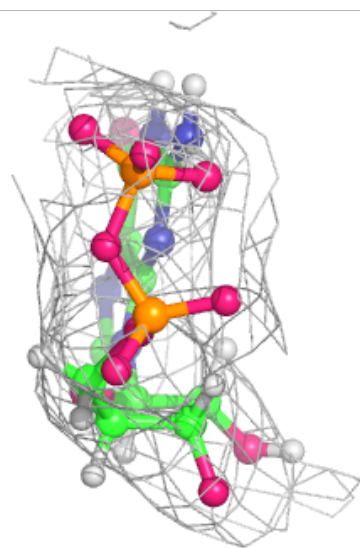
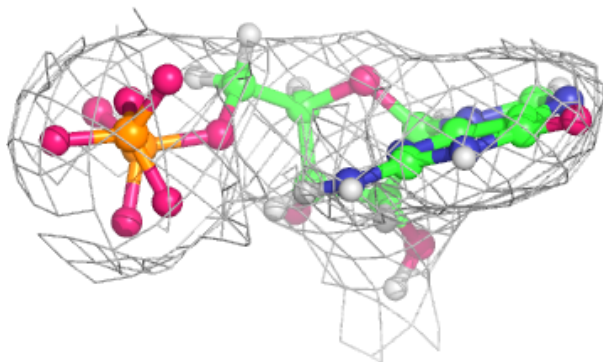
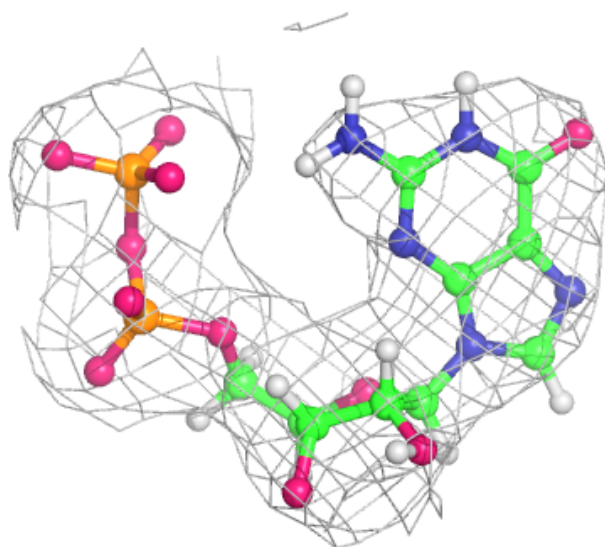
Electron density around GDP A 603:

$2mF_o-DF_c$ (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.