



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 10:27 PM EDT

PDB ID : 6I0O
Title : Structure of human IMP dehydrogenase, isoform 2, bound to GTP
Authors : Buey, R.M.; Fernandez-Justel, D.; Revuelta, J.L.
Deposited on : 2018-10-26
Resolution : 2.62 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

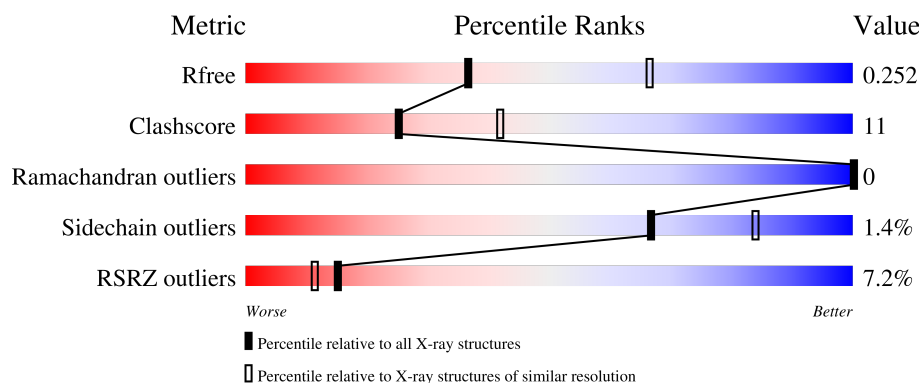
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.62 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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	
1	B	517	

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	GTP	B	603	-	-	X	-
3	SO4	A	605	-	-	-	X
3	SO4	B	606	-	-	-	X
3	SO4	B	607	-	-	-	X
3	SO4	B	609	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12957 atoms, of which 6206 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.

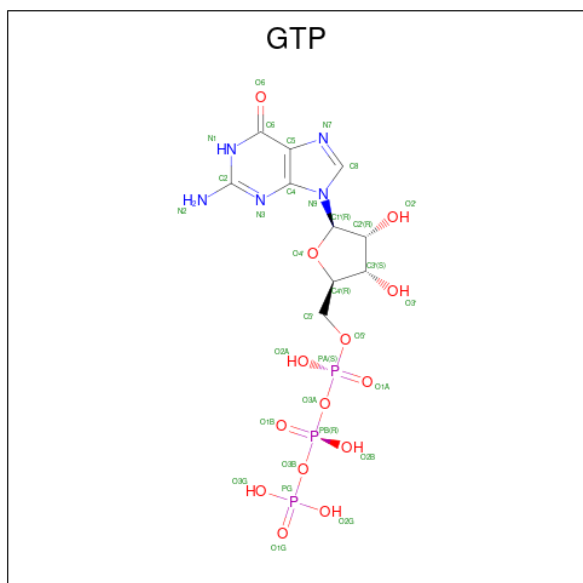
- Molecule 1 is a protein called Inosine-5'-monophosphate dehydrogenase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	434	Total	C	H	N	O	S	0	0	0
			6212	2009	3055	537	593	18			
1	B	431	Total	C	H	N	O	S	0	0	0
			6266	2019	3083	546	601	17			

There are 6 discrepancies between the modelled and reference sequences:

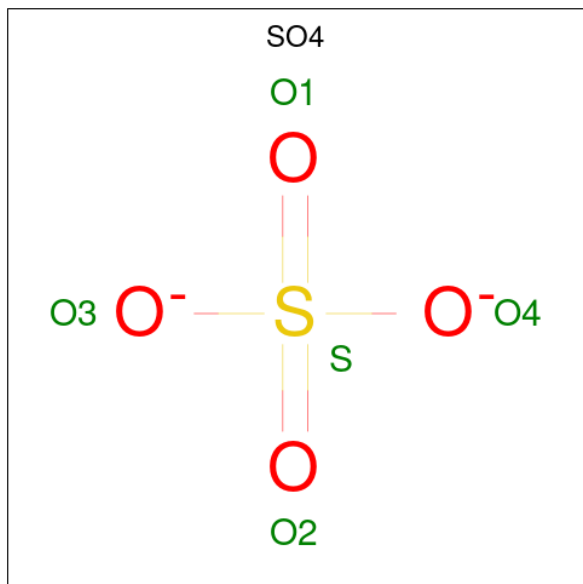
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P12268
A	-1	SER	-	expression tag	UNP P12268
A	0	HIS	-	expression tag	UNP P12268
B	-2	GLY	-	expression tag	UNP P12268
B	-1	SER	-	expression tag	UNP P12268
B	0	HIS	-	expression tag	UNP P12268

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			43	10	11	5	14	3		
2	A	1	Total	C	H	N	O	P	0	0
			43	10	11	5	14	3		
2	A	1	Total	C	H	N	O	P	0	0
			44	10	12	5	14	3		
2	B	1	Total	C	H	N	O	P	0	0
			43	10	11	5	14	3		
2	B	1	Total	C	H	N	O	P	0	0
			43	10	11	5	14	3		
2	B	1	Total	C	H	N	O	P	0	0
			44	10	12	5	14	3		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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

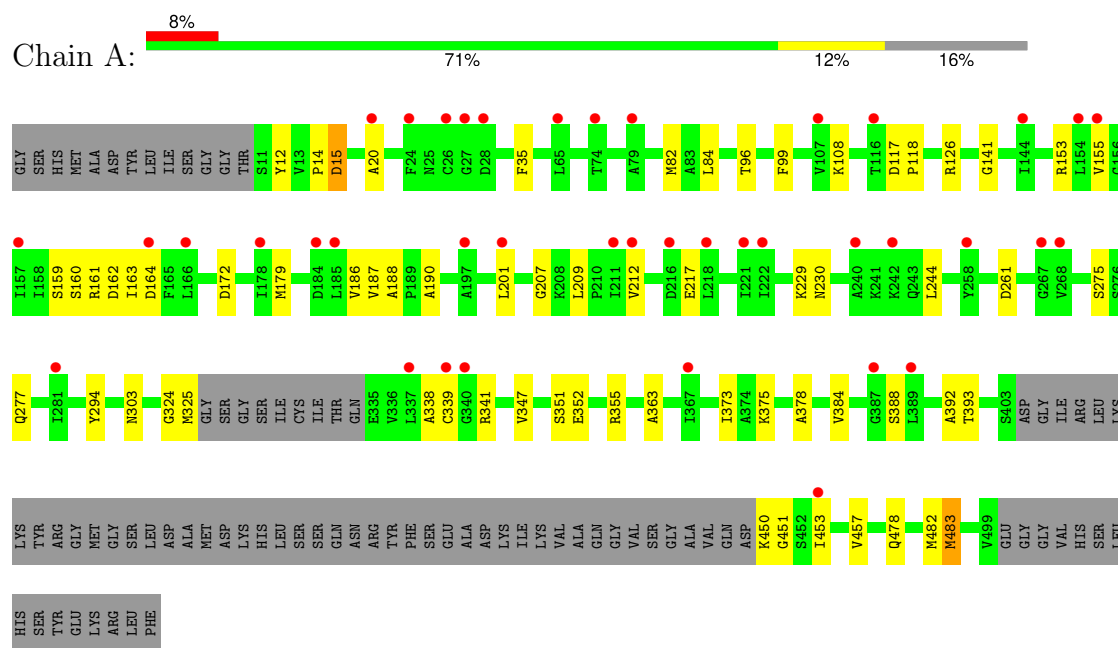
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total 30	O 30	0	0
4	B	59	Total 59	O 59	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 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	134.12Å 134.12Å 325.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.95 – 2.62 81.95 – 2.62	Depositor EDS
% Data completeness (in resolution range)	81.1 (81.95-2.62) 81.1 (81.95-2.62)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.62Å)	Xtriage
Refinement program	PHENIX (1.12rc1_2801: ???)	Depositor
R, R_{free}	0.219 , 0.244 0.233 , 0.252	Depositor DCC
R_{free} test set	1844 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	65.1	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12957	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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: SO4, GTP

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	0.33	0/3205	0.50	0/4351
1	B	0.30	0/3230	0.50	0/4374
All	All	0.31	0/6435	0.50	0/8725

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	3157	3055	3090	63	1
1	B	3183	3083	3166	74	1
2	A	96	34	33	12	0
2	B	96	34	33	13	0
3	A	50	0	0	1	0
3	B	80	0	0	2	0
4	A	30	0	0	0	0
4	B	59	0	0	2	0
All	All	6751	6206	6322	139	2

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 11.

All (139) 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:B:277:GLN:HE22	1:B:309:GLN:NE2	1.39	1.20
1:A:230:ASN:OD1	2:A:603:GTP:O1G	1.68	1.12
1:B:130:VAL:HG11	1:B:163:ILE:CD1	1.78	1.10
1:B:127:VAL:CG2	1:B:178:ILE:CD1	2.36	1.02
1:A:303:ASN:ND2	1:A:324:GLY:O	1.94	1.00
1:B:277:GLN:HE22	1:B:309:GLN:HE21	1.14	0.94
1:B:245:LEU:CD2	1:B:269:ASP:OD2	2.19	0.91
1:A:453:ILE:CG1	1:A:457:VAL:HG23	2.02	0.89
1:B:230:ASN:ND2	2:B:603:GTP:O3G	2.05	0.88
1:B:245:LEU:HD22	1:B:269:ASP:OD2	1.74	0.88
1:B:277:GLN:NE2	1:B:309:GLN:NE2	2.23	0.86
1:B:230:ASN:CG	2:B:603:GTP:O3G	2.15	0.85
1:B:130:VAL:HG11	1:B:163:ILE:HD11	1.57	0.84
1:A:230:ASN:CG	2:A:603:GTP:O1G	2.16	0.83
1:A:153:ARG:HA	1:A:217:GLU:HA	1.60	0.82
1:B:147:THR:HG1	1:B:152:SER:HG	0.82	0.80
1:B:127:VAL:HG22	1:B:178:ILE:CD1	2.11	0.80
1:B:230:ASN:OD1	2:B:603:GTP:O3G	2.00	0.80
1:B:130:VAL:CG1	1:B:163:ILE:CD1	2.60	0.79
1:B:127:VAL:HG21	1:B:178:ILE:CD1	2.15	0.77
1:A:453:ILE:HG13	1:A:457:VAL:HG23	1.67	0.76
1:A:229:LYS:NZ	2:A:602:GTP:O3'	2.21	0.74
1:A:453:ILE:HG12	1:A:457:VAL:HG23	1.69	0.74
1:B:127:VAL:CG2	1:B:178:ILE:HD12	2.17	0.72
1:B:245:LEU:HD23	1:B:269:ASP:OD2	1.88	0.72
1:A:373:ILE:HG23	1:A:384:VAL:HG21	1.73	0.70
1:B:127:VAL:CG2	1:B:178:ILE:HD11	2.22	0.70
1:B:277:GLN:HE22	1:B:309:GLN:HE22	1.36	0.68
1:A:20:ALA:HB3	1:A:483:MET:HE1	1.77	0.66
1:A:190:ALA:N	1:A:212:VAL:O	2.28	0.66
1:B:127:VAL:HG21	1:B:178:ILE:HD11	1.77	0.65
1:B:296:ASN:ND2	3:B:609:SO4:O2	2.28	0.65
1:A:338:ALA:O	1:A:339:CYS:SG	2.53	0.65
1:B:261:ASP:OD1	1:B:294:TYR:OH	2.13	0.65
1:B:226:ASP:OD1	2:B:602:GTP:O3'	2.14	0.64
1:B:155:VAL:HG12	1:B:179:MET:HE3	1.80	0.64
1:B:130:VAL:HG11	1:B:163:ILE:HD12	1.75	0.64
1:A:392:ALA:HB1	1:A:450:LYS:N	2.13	0.63
1:A:347:VAL:O	1:A:351:SER:OG	2.05	0.63
1:B:37:ILE:CG2	1:B:488:LEU:HD11	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ALA:HB3	1:A:483:MET:CE	2.30	0.62
1:B:155:VAL:HG12	1:B:179:MET:CE	2.30	0.61
1:A:161:ARG:NH2	2:B:601:GTP:O1B	2.33	0.61
1:A:161:ARG:HA	1:A:164:ASP:OD2	2.00	0.61
1:B:78:MET:CE	1:B:453:ILE:HG13	2.30	0.61
1:A:392:ALA:HB3	1:A:450:LYS:CB	2.31	0.61
2:B:603:GTP:O1B	4:B:701:HOH:O	2.16	0.61
1:A:453:ILE:HG12	1:A:457:VAL:CG2	2.30	0.60
1:A:96:THR:HG23	1:A:99:PHE:H	1.65	0.60
1:A:82:MET:SD	1:A:453:ILE:HD11	2.42	0.59
1:B:127:VAL:CG2	1:B:178:ILE:HD13	2.31	0.58
1:A:230:ASN:ND2	2:A:603:GTP:O1G	2.36	0.58
1:A:141:GLY:O	2:A:602:GTP:N2	2.36	0.57
1:B:37:ILE:HG21	1:B:488:LEU:HD11	1.86	0.57
1:A:453:ILE:CG1	1:A:457:VAL:CG2	2.79	0.57
1:B:127:VAL:HG22	1:B:178:ILE:HD12	1.78	0.57
1:B:130:VAL:CG1	1:B:163:ILE:HD13	2.34	0.57
1:A:261:ASP:OD1	1:A:294:TYR:OH	2.23	0.56
1:A:155:VAL:HG12	1:A:179:MET:HE3	1.87	0.56
1:B:111:GLU:OE2	2:B:603:GTP:O6	2.24	0.56
1:B:160:SER:O	1:B:164:ASP:N	2.38	0.56
1:B:162:ASP:OD1	2:B:601:GTP:O3'	2.24	0.55
1:B:78:MET:HE1	1:B:453:ILE:HG13	1.87	0.55
1:B:131:PHE:CZ	1:B:163:ILE:CG2	2.90	0.55
1:A:393:THR:HA	1:A:451:GLY:O	2.08	0.54
1:A:159:SER:OG	1:A:160:SER:N	2.38	0.54
1:B:277:GLN:NE2	1:B:309:GLN:HE21	1.96	0.54
1:A:483:MET:HE2	1:A:483:MET:C	2.28	0.53
1:A:82:MET:SD	1:A:453:ILE:CD1	2.96	0.53
1:B:144:ILE:HD11	1:B:158:ILE:HD12	1.89	0.53
1:A:363:ALA:HB3	1:A:384:VAL:HG12	1.89	0.53
1:A:187:VAL:HG12	1:A:188:ALA:N	2.24	0.53
1:A:352:GLU:O	1:A:355:ARG:HG2	2.09	0.53
1:B:230:ASN:OD1	1:B:238:LYS:NZ	2.41	0.53
1:B:127:VAL:HG22	1:B:178:ILE:HD13	1.89	0.52
1:B:141:GLY:O	2:B:602:GTP:N2	2.35	0.52
1:B:277:GLN:NE2	1:B:309:GLN:HE22	2.01	0.52
1:A:160:SER:O	1:A:164:ASP:OD1	2.28	0.52
1:A:155:VAL:HG12	1:A:179:MET:CE	2.40	0.51
1:B:277:GLN:HG3	1:B:277:GLN:O	2.09	0.51
1:B:337:LEU:O	4:B:702:HOH:O	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:GLU:OE2	1:B:356:ARG:NH2	2.35	0.50
1:B:155:VAL:CG1	1:B:179:MET:CE	2.90	0.50
1:B:392:ALA:HB1	1:B:450:LYS:H	1.76	0.50
1:A:126:ARG:HB3	1:A:172:ASP:HA	1.94	0.49
1:A:230:ASN:OD1	2:A:603:GTP:C8	2.65	0.49
1:A:35:PHE:O	1:A:375:LYS:NZ	2.41	0.48
1:B:270:VAL:HG22	1:B:271:VAL:N	2.27	0.48
1:A:12:TYR:O	1:A:14:PRO:HD3	2.15	0.47
1:B:263:LEU:O	1:B:268:VAL:HG12	2.13	0.47
1:A:160:SER:OG	2:A:601:GTP:O1G	2.16	0.47
1:B:242:LYS:NZ	2:B:603:GTP:O2B	2.47	0.47
1:A:162:ASP:OD1	2:A:601:GTP:O3'	2.32	0.47
1:A:230:ASN:OD1	2:A:603:GTP:N7	2.48	0.47
1:A:483:MET:HE2	1:A:483:MET:O	2.14	0.47
1:A:84:LEU:HD21	1:A:244:LEU:HD11	1.96	0.47
1:B:272:VAL:HG22	1:B:300:ILE:HD12	1.97	0.47
1:A:201:LEU:HD13	1:A:209:LEU:HB2	1.95	0.47
1:B:78:MET:HE1	1:B:453:ILE:CG1	2.44	0.47
1:B:182:ARG:HD2	1:B:185:LEU:HD11	1.97	0.47
1:B:454:HIS:O	1:B:458:PRO:HG2	2.15	0.46
1:A:388:SER:N	3:A:612:SO4:O2	2.41	0.46
1:B:483:MET:HA	1:B:488:LEU:HB3	1.98	0.45
1:A:478:GLN:O	1:A:482:MET:HG3	2.16	0.45
1:B:250:ILE:HG22	1:B:272:VAL:O	2.17	0.45
1:B:386:MET:HE3	1:B:390:LEU:HD11	1.99	0.45
1:B:35:PHE:O	1:B:375:LYS:NZ	2.44	0.45
1:A:378:ALA:O	1:A:483:MET:HG2	2.16	0.44
1:A:187:VAL:CG1	1:A:188:ALA:N	2.81	0.44
1:B:36:LEU:HD23	1:B:493:ARG:HD3	1.98	0.44
1:A:155:VAL:CG1	1:A:179:MET:CE	2.95	0.44
1:B:117:ASP:N	1:B:118:PRO:CD	2.80	0.44
1:B:230:ASN:OD1	2:B:603:GTP:C8	2.71	0.44
1:B:392:ALA:HB3	1:B:450:LYS:CG	2.48	0.44
1:B:363:ALA:HB3	1:B:384:VAL:HG12	1.98	0.43
1:B:230:ASN:OD1	2:B:603:GTP:N7	2.51	0.43
1:B:454:HIS:O	1:B:458:PRO:HD2	2.18	0.43
1:A:20:ALA:CB	1:A:483:MET:CE	2.95	0.43
1:B:304:VAL:HG11	1:B:313:LEU:HD12	2.00	0.43
1:A:84:LEU:HD23	1:A:244:LEU:HD21	2.01	0.43
1:A:483:MET:HE3	1:A:483:MET:HB2	1.81	0.43
1:A:155:VAL:HG11	1:A:179:MET:HE1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:601:GTP:H8	2:A:601:GTP:H2'	1.42	0.42
1:A:20:ALA:CB	1:A:483:MET:HE1	2.48	0.42
1:A:186:VAL:HG12	2:A:601:GTP:HN1	1.84	0.42
1:A:207:GLY:N	2:A:601:GTP:O2A	2.47	0.42
1:B:278:GLY:HA3	1:B:302:GLY:O	2.20	0.41
1:A:275:SER:O	1:A:303:ASN:HB2	2.20	0.41
1:B:84:LEU:HD23	1:B:244:LEU:HD21	2.02	0.41
1:A:117:ASP:N	1:A:118:PRO:CD	2.84	0.41
1:A:161:ARG:HA	1:A:164:ASP:CG	2.41	0.41
1:A:163:ILE:O	1:A:163:ILE:HG22	2.19	0.41
1:A:325:MET:O	1:A:341:ARG:N	2.42	0.41
1:B:242:LYS:HG3	2:B:603:GTP:N7	2.35	0.40
1:B:159:SER:OG	1:B:160:SER:N	2.54	0.40
1:B:489:LYS:N	3:B:605:SO4:O3	2.55	0.40
1:A:15:ASP:OD1	1:A:15:ASP:N	2.52	0.40
1:B:270:VAL:CG2	1:B:271:VAL:N	2.84	0.40
1:B:163:ILE:O	1:B:163:ILE:HG22	2.21	0.40

All (2) 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:336:VAL:CG2	1:B:466:HIS:HD2[3_455]	1.51	0.09
1:A:15:ASP:OD2	1:A:15:ASP:OD2[5_455]	2.18	0.02

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	428/517 (83%)	418 (98%)	10 (2%)	0	100	100
1	B	423/517 (82%)	411 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	851/1034 (82%)	829 (97%)	22 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	311/422 (74%)	307 (99%)	4 (1%)	69	85
1	B	326/422 (77%)	321 (98%)	5 (2%)	65	82
All	All	637/844 (76%)	628 (99%)	9 (1%)	67	84

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	108	LYS
1	A	277	GLN
1	A	483	MET
1	B	112	GLN
1	B	216	ASP
1	B	242	LYS
1	B	277	GLN
1	B	303	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	B	277	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

32 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	GTP	A	602	-	29,34,34	4.45	14 (48%)	35,54,54	1.25	4 (11%)
3	SO4	A	606	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	B	605	-	4,4,4	0.24	0	6,6,6	0.06	0
3	SO4	B	606	-	4,4,4	0.40	0	6,6,6	0.22	0
2	GTP	A	603	-	29,34,34	0.98	1 (3%)	35,54,54	1.15	2 (5%)
3	SO4	A	605	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	B	610	-	4,4,4	0.24	0	6,6,6	0.06	0
3	SO4	B	607	-	4,4,4	0.24	0	6,6,6	0.20	0
2	GTP	A	601	-	29,34,34	4.47	14 (48%)	35,54,54	1.29	5 (14%)
3	SO4	B	617	-	4,4,4	0.24	0	6,6,6	0.10	0
3	SO4	A	607	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	B	611	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	B	615	-	4,4,4	0.23	0	6,6,6	0.08	0
2	GTP	B	602	-	29,34,34	4.43	14 (48%)	35,54,54	1.28	4 (11%)
2	GTP	B	601	-	29,34,34	4.51	14 (48%)	35,54,54	1.30	6 (17%)
3	SO4	B	612	-	4,4,4	0.23	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	B	609	-	4,4,4	0.24	0	6,6,6	0.12	0
3	SO4	A	608	-	4,4,4	0.24	0	6,6,6	0.06	0
3	SO4	B	619	-	4,4,4	0.23	0	6,6,6	0.14	0
3	SO4	A	604	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	B	614	-	4,4,4	0.24	0	6,6,6	0.10	0
3	SO4	A	609	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	A	612	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	B	616	-	4,4,4	0.22	0	6,6,6	0.08	0
3	SO4	A	611	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	B	618	-	4,4,4	0.23	0	6,6,6	0.18	0
3	SO4	B	604	-	4,4,4	0.28	0	6,6,6	0.27	0
3	SO4	A	613	-	4,4,4	0.35	0	6,6,6	0.18	0
3	SO4	B	608	-	4,4,4	0.24	0	6,6,6	0.07	0
2	GTP	B	603	-	29,34,34	1.03	1 (3%)	35,54,54	1.10	3 (8%)
3	SO4	A	610	-	4,4,4	0.23	0	6,6,6	0.06	0
3	SO4	B	613	-	4,4,4	0.23	0	6,6,6	0.08	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	GTP	A	602	-	-	7/18/38/38	0/3/3/3
2	GTP	A	603	-	-	6/18/38/38	0/3/3/3
2	GTP	B	602	-	-	6/18/38/38	0/3/3/3
2	GTP	B	601	-	-	4/18/38/38	0/3/3/3
2	GTP	B	603	-	-	3/18/38/38	0/3/3/3
2	GTP	A	601	-	-	7/18/38/38	0/3/3/3

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	GTP	O4'-C1'	17.00	1.63	1.40
2	A	601	GTP	O4'-C1'	16.57	1.62	1.40
2	A	602	GTP	O4'-C1'	16.47	1.62	1.40
2	B	602	GTP	O4'-C1'	16.24	1.62	1.40
2	B	601	GTP	O4'-C4'	-6.36	1.30	1.45
2	A	602	GTP	O4'-C4'	-6.27	1.31	1.45
2	A	601	GTP	O4'-C4'	-6.23	1.31	1.45
2	B	602	GTP	O4'-C4'	-6.21	1.31	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	GTP	PA-O3A	6.18	1.66	1.59
2	A	601	GTP	PB-O3A	6.15	1.66	1.59
2	A	602	GTP	PB-O3B	6.07	1.66	1.59
2	B	602	GTP	PB-O3B	5.99	1.66	1.59
2	B	602	GTP	PA-O3A	5.98	1.66	1.59
2	B	601	GTP	PB-O3A	5.95	1.65	1.59
2	B	601	GTP	PA-O3A	5.89	1.65	1.59
2	A	602	GTP	PA-O3A	5.80	1.65	1.59
2	B	602	GTP	PB-O3A	5.77	1.65	1.59
2	A	601	GTP	PB-O3B	5.72	1.65	1.59
2	A	602	GTP	PB-O3A	5.71	1.65	1.59
2	A	601	GTP	C2-N3	5.58	1.46	1.33
2	B	601	GTP	C2-N3	5.57	1.46	1.33
2	A	602	GTP	C2-N3	5.52	1.46	1.33
2	B	601	GTP	PB-O3B	5.49	1.65	1.59
2	B	602	GTP	C2-N3	5.39	1.46	1.33
2	B	601	GTP	C2-N2	5.34	1.46	1.34
2	A	601	GTP	C2-N2	5.29	1.46	1.34
2	B	602	GTP	C2-N2	5.25	1.46	1.34
2	A	601	GTP	C4-N3	5.22	1.49	1.37
2	A	602	GTP	C2-N2	5.20	1.46	1.34
2	B	601	GTP	C4-N3	5.18	1.49	1.37
2	B	602	GTP	C4-N3	5.10	1.49	1.37
2	A	602	GTP	C4-N3	5.07	1.49	1.37
2	B	602	GTP	C6-N1	4.11	1.44	1.37
2	A	602	GTP	C6-N1	3.93	1.43	1.37
2	B	601	GTP	C6-N1	3.92	1.43	1.37
2	A	601	GTP	C6-N1	3.67	1.43	1.37
2	A	602	GTP	C5-C6	3.46	1.54	1.47
2	B	602	GTP	C5-C6	3.42	1.54	1.47
2	B	601	GTP	C5-C6	3.38	1.54	1.47
2	A	601	GTP	C5-C6	3.31	1.54	1.47
2	B	603	GTP	C6-N1	-3.25	1.32	1.37
2	B	601	GTP	O2'-C2'	3.12	1.50	1.43
2	A	603	GTP	C6-N1	-3.10	1.33	1.37
2	B	602	GTP	C2-N1	3.05	1.45	1.37
2	A	602	GTP	C2-N1	3.05	1.45	1.37
2	B	601	GTP	C2-N1	3.05	1.45	1.37
2	A	602	GTP	O2'-C2'	3.04	1.50	1.43
2	A	601	GTP	C2-N1	3.02	1.45	1.37
2	B	602	GTP	O2'-C2'	3.01	1.50	1.43
2	A	601	GTP	O2'-C2'	3.00	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	GTP	O3'-C3'	-2.68	1.36	1.43
2	A	602	GTP	O3'-C3'	-2.64	1.36	1.43
2	B	601	GTP	O3'-C3'	-2.58	1.36	1.43
2	A	601	GTP	O3'-C3'	-2.53	1.36	1.43
2	A	602	GTP	C5-C4	-2.47	1.37	1.43
2	B	602	GTP	C5-C4	-2.47	1.37	1.43
2	B	601	GTP	C5-C4	-2.47	1.37	1.43
2	A	601	GTP	C5-C4	-2.42	1.37	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	GTP	C4'-O4'-C1'	-3.43	106.78	109.92
2	B	603	GTP	C8-N7-C5	3.20	107.99	102.55
2	B	602	GTP	C8-N7-C5	3.19	107.98	102.55
2	A	602	GTP	C8-N7-C5	3.15	107.92	102.55
2	B	601	GTP	C8-N7-C5	3.10	107.83	102.55
2	A	603	GTP	C8-N7-C5	3.09	107.81	102.55
2	B	602	GTP	C5-C6-N1	3.05	119.89	114.07
2	A	602	GTP	C2-N1-C6	-3.01	119.60	125.11
2	A	601	GTP	C8-N7-C5	3.01	107.67	102.55
2	A	602	GTP	C5-C6-N1	3.01	119.80	114.07
2	B	601	GTP	C5-C6-N1	2.89	119.58	114.07
2	B	602	GTP	C2-N1-C6	-2.88	119.84	125.11
2	B	601	GTP	C2-N1-C6	-2.83	119.93	125.11
2	A	601	GTP	C5-C6-N1	2.81	119.44	114.07
2	A	601	GTP	C2-N1-C6	-2.71	120.15	125.11
2	B	601	GTP	C4'-O4'-C1'	-2.27	107.84	109.92
2	B	601	GTP	O4'-C1'-N9	-2.17	105.86	108.75
2	B	602	GTP	O6-C6-C5	-2.14	120.08	124.32
2	B	601	GTP	O6-C6-C5	-2.13	120.10	124.32
2	A	601	GTP	O6-C6-C5	-2.09	120.18	124.32
2	A	602	GTP	O6-C6-C5	-2.06	120.25	124.32
2	A	603	GTP	C5-C6-N1	2.04	117.97	114.07
2	B	603	GTP	C5-C6-N1	2.04	117.96	114.07
2	B	603	GTP	C2-N1-C6	-2.02	121.42	125.11

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GTP	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
2	A	601	GTP	C5'-O5'-PA-O1A
2	A	603	GTP	C5'-O5'-PA-O3A
2	A	603	GTP	C5'-O5'-PA-O1A
2	A	603	GTP	C5'-O5'-PA-O2A
2	B	601	GTP	C5'-O5'-PA-O3A
2	B	602	GTP	C5'-O5'-PA-O2A
2	B	601	GTP	C3'-C4'-C5'-O5'
2	A	601	GTP	C3'-C4'-C5'-O5'
2	B	601	GTP	O4'-C4'-C5'-O5'
2	A	601	GTP	O4'-C4'-C5'-O5'
2	B	603	GTP	O4'-C4'-C5'-O5'
2	A	602	GTP	PB-O3B-PG-O1G
2	A	602	GTP	O4'-C4'-C5'-O5'
2	B	603	GTP	C3'-C4'-C5'-O5'
2	B	602	GTP	PA-O3A-PB-O2B
2	A	601	GTP	C5'-O5'-PA-O3A
2	A	601	GTP	C5'-O5'-PA-O2A
2	A	602	GTP	C5'-O5'-PA-O3A
2	A	602	GTP	C5'-O5'-PA-O1A
2	A	602	GTP	C5'-O5'-PA-O2A
2	B	601	GTP	C5'-O5'-PA-O1A
2	B	602	GTP	C5'-O5'-PA-O3A
2	B	602	GTP	C5'-O5'-PA-O1A
2	A	602	GTP	PA-O3A-PB-O1B
2	B	602	GTP	PB-O3B-PG-O2G
2	B	602	GTP	O4'-C4'-C5'-O5'
2	A	603	GTP	PA-O3A-PB-O1B
2	A	603	GTP	PB-O3A-PA-O1A
2	A	601	GTP	PA-O3A-PB-O2B
2	A	602	GTP	PA-O3A-PB-O2B
2	A	603	GTP	PG-O3B-PB-O1B
2	B	603	GTP	PA-O3A-PB-O2B

There are no ring outliers.

9 monomers are involved in 28 short contacts:

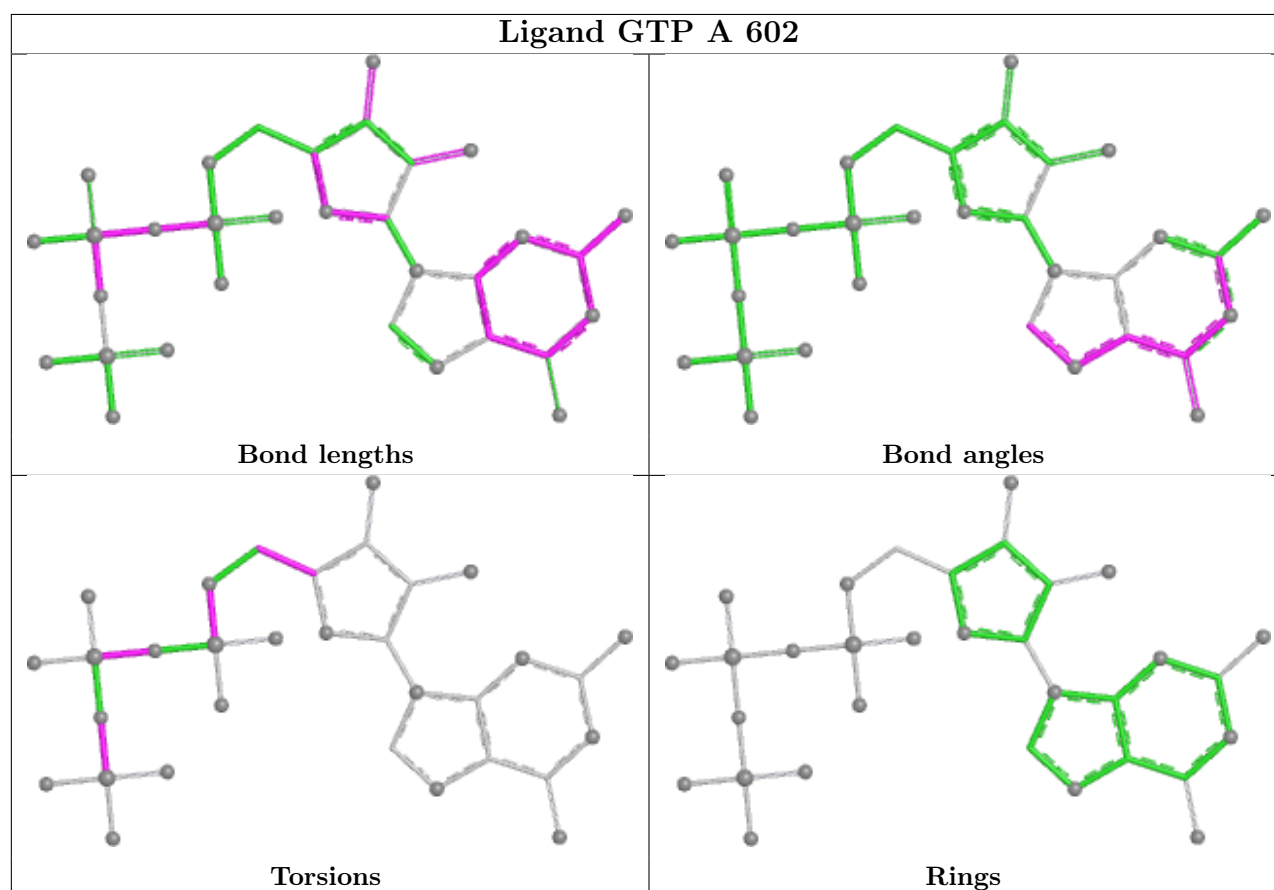
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	602	GTP	2	0
3	B	605	SO4	1	0
2	A	603	GTP	5	0
2	A	601	GTP	5	0
2	B	602	GTP	2	0

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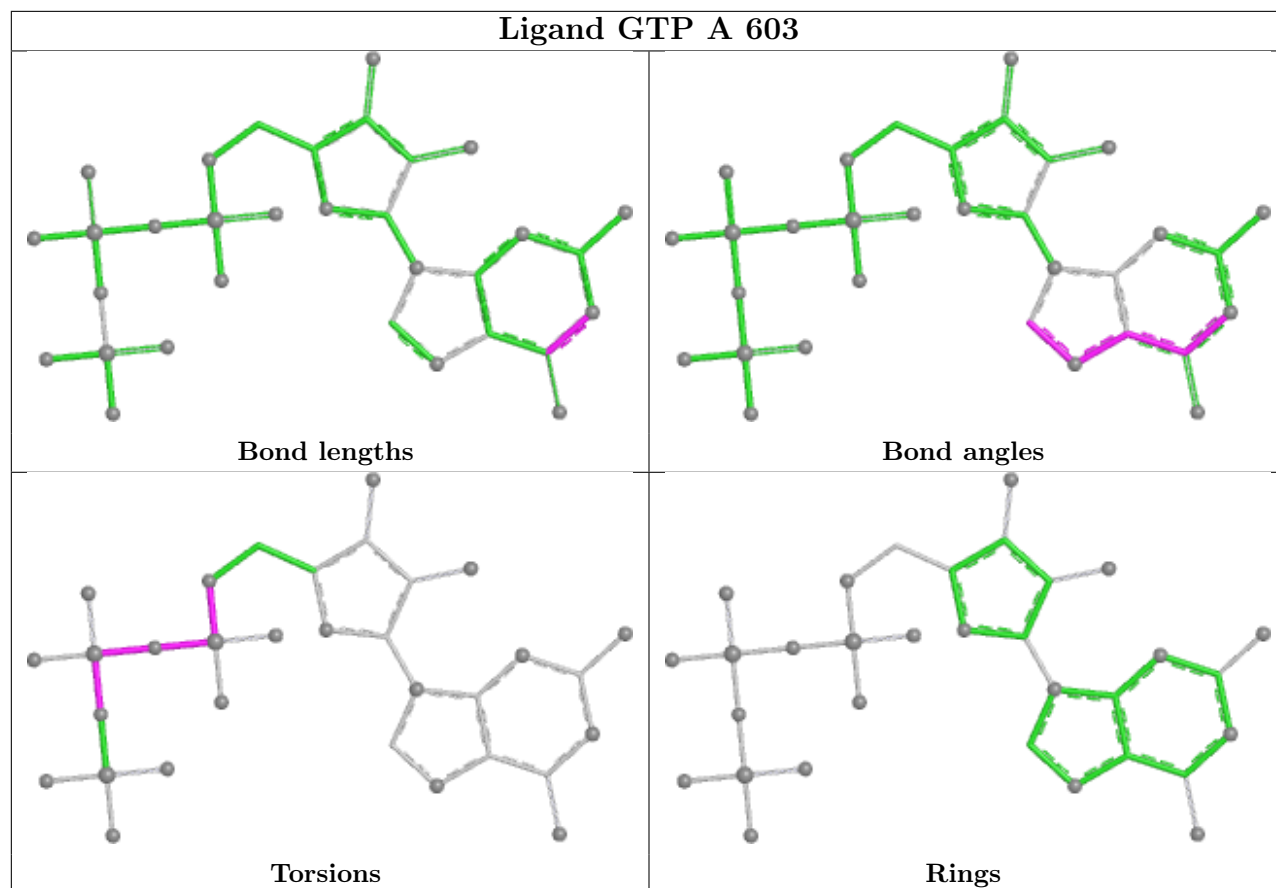
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	GTP	2	0
3	B	609	SO4	1	0
3	A	612	SO4	1	0
2	B	603	GTP	9	0

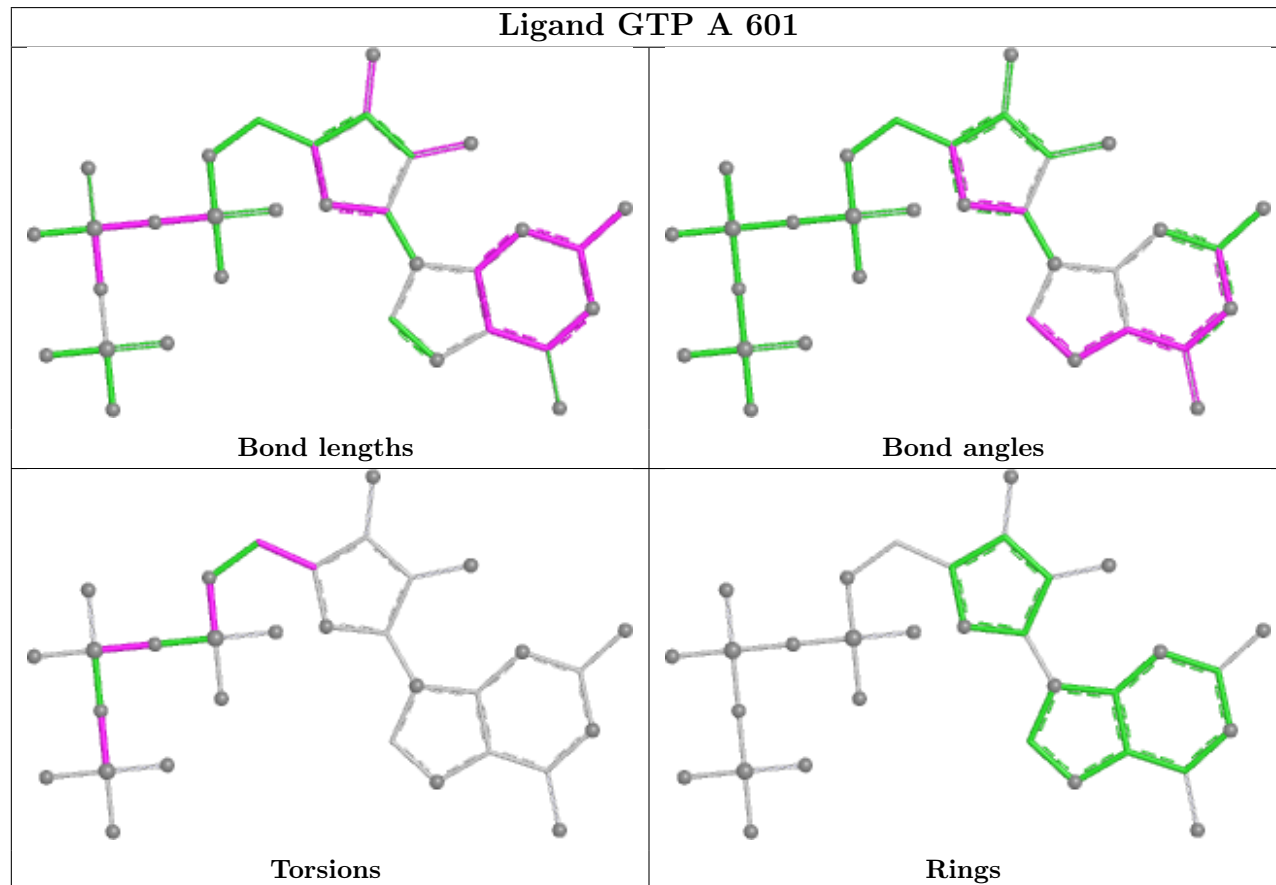
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

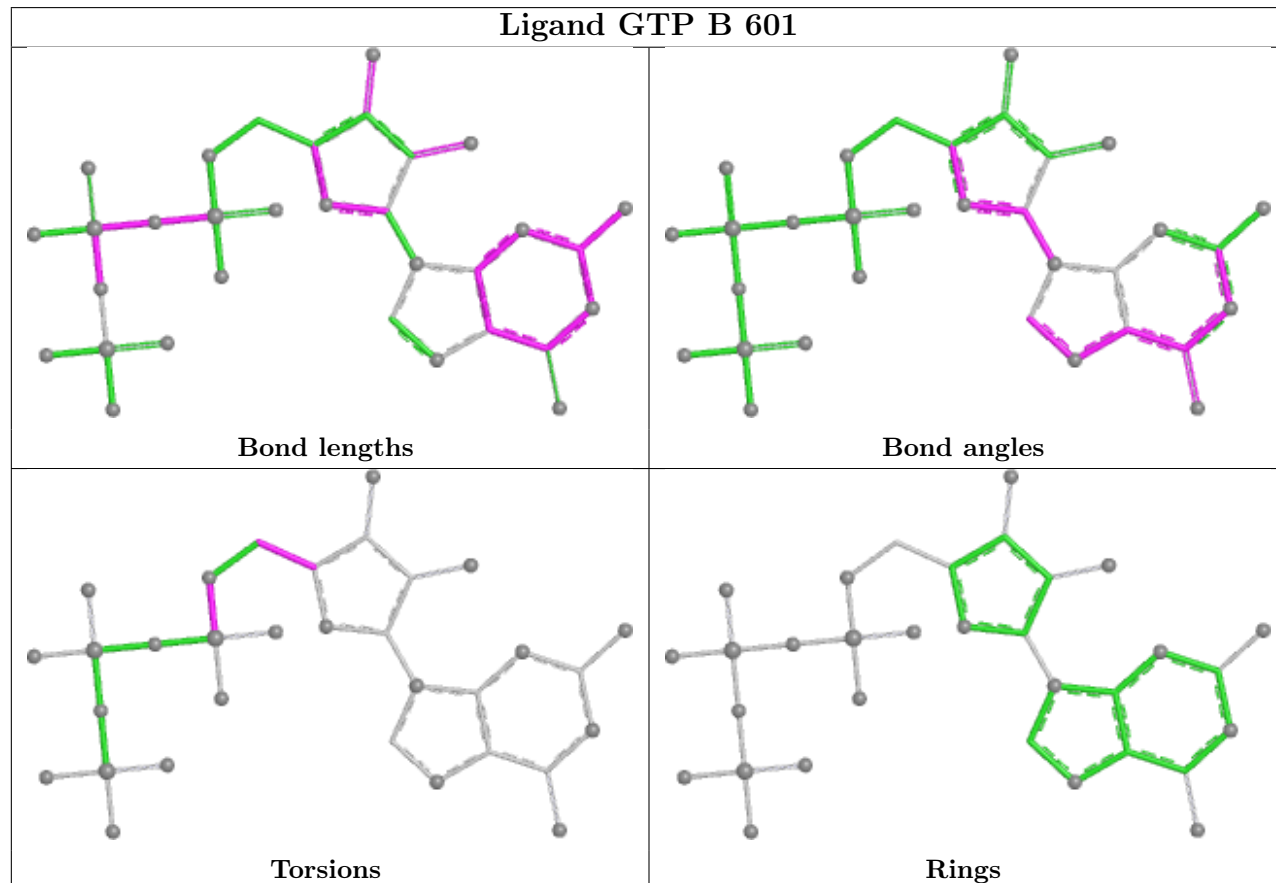
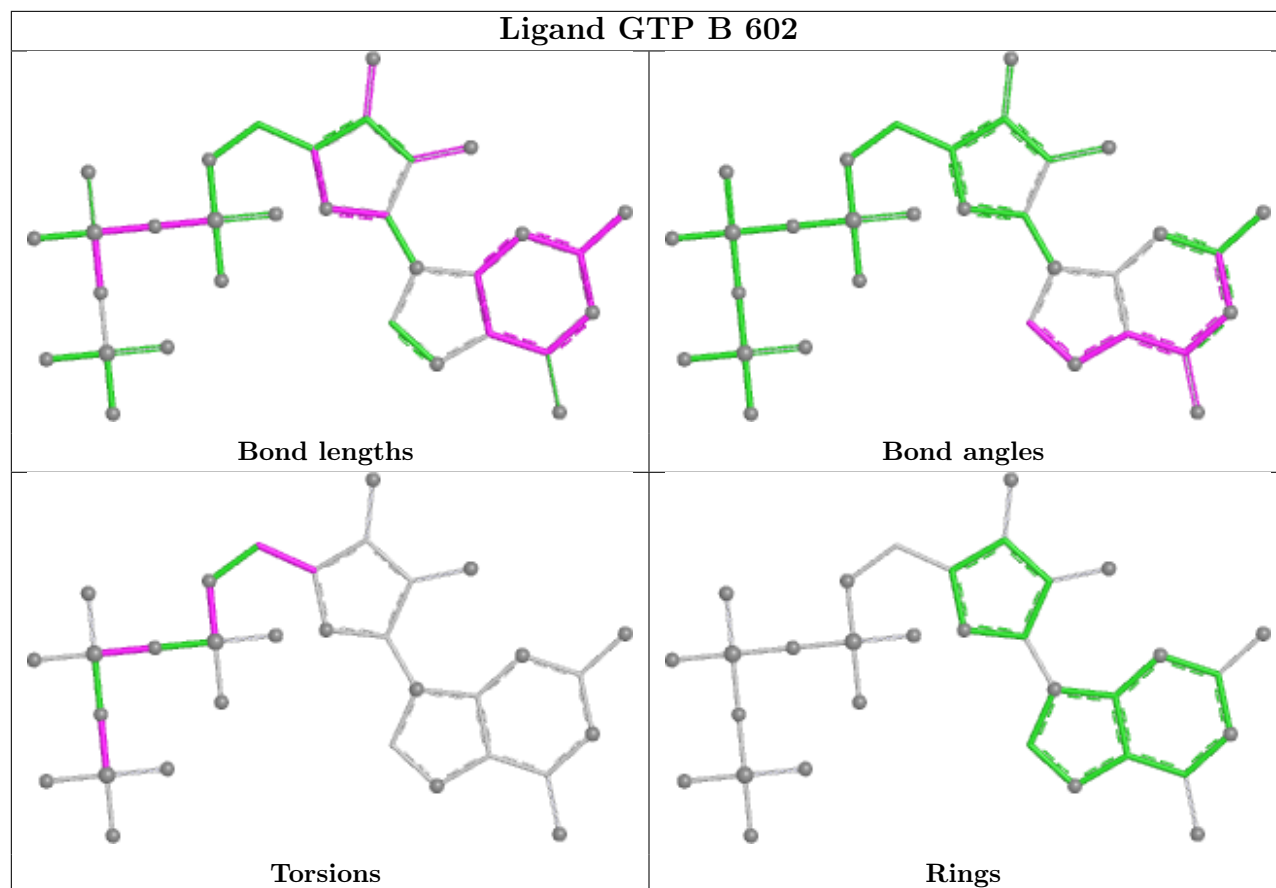


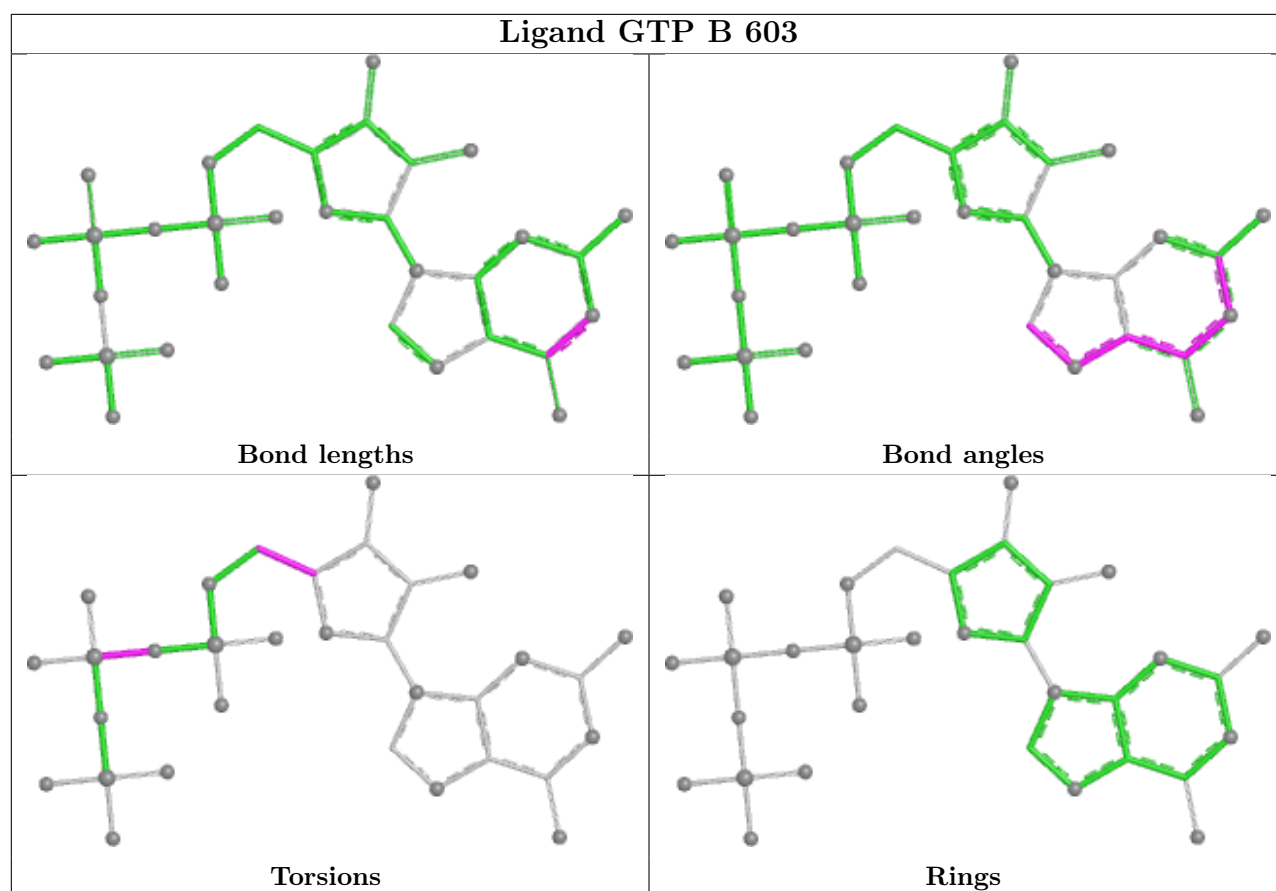
Ligand GTP A 603



Ligand GTP A 601







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	434/517 (83%)	0.89	40 (9%) 9 6	52, 79, 119, 153	0
1	B	431/517 (83%)	0.68	22 (5%) 28 22	30, 60, 101, 135	0
All	All	865/1034 (83%)	0.79	62 (7%) 15 11	30, 70, 113, 153	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	216	ASP	5.3
1	A	367	ILE	4.7
1	A	387	GLY	3.8
1	B	174	PHE	3.7
1	A	218	LEU	3.6
1	B	175	LEU	3.5
1	A	337	LEU	3.4
1	B	340	GLY	3.4
1	A	240	ALA	3.3
1	B	339	CYS	3.2
1	A	339	CYS	3.2
1	B	165	PHE	3.2
1	B	402	PHE	3.1
1	A	212	VAL	3.1
1	A	453	ILE	3.0
1	A	27	GLY	3.0
1	B	218	LEU	3.0
1	B	140	CYS	2.9
1	A	157	ILE	2.8
1	B	166	LEU	2.8
1	A	116	THR	2.7
1	B	178	ILE	2.7
1	A	20	ALA	2.6
1	A	166	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	24	PHE	2.6
1	B	73	VAL	2.6
1	B	163	ILE	2.6
1	B	250	ILE	2.6
1	B	158	ILE	2.6
1	A	178	ILE	2.5
1	A	65	LEU	2.5
1	B	338	ALA	2.5
1	A	154	LEU	2.5
1	A	268	VAL	2.4
1	B	105	ARG	2.4
1	B	303	ASN	2.4
1	B	324	GLY	2.4
1	A	164	ASP	2.4
1	A	155	VAL	2.4
1	A	211	ILE	2.4
1	A	144	ILE	2.3
1	B	304	VAL	2.3
1	A	26	CYS	2.3
1	B	130	VAL	2.3
1	A	107	VAL	2.3
1	A	267	GLY	2.3
1	A	185	LEU	2.3
1	A	201	LEU	2.3
1	A	242	LYS	2.2
1	A	221	ILE	2.2
1	A	340	GLY	2.2
1	A	222	ILE	2.2
1	A	197	ALA	2.2
1	A	258	TYR	2.2
1	B	256	ASP	2.1
1	A	79	ALA	2.1
1	B	155	VAL	2.1
1	A	184	ASP	2.1
1	A	28	ASP	2.1
1	A	281	ILE	2.0
1	A	74	THR	2.0
1	A	389	LEU	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 ⓘ

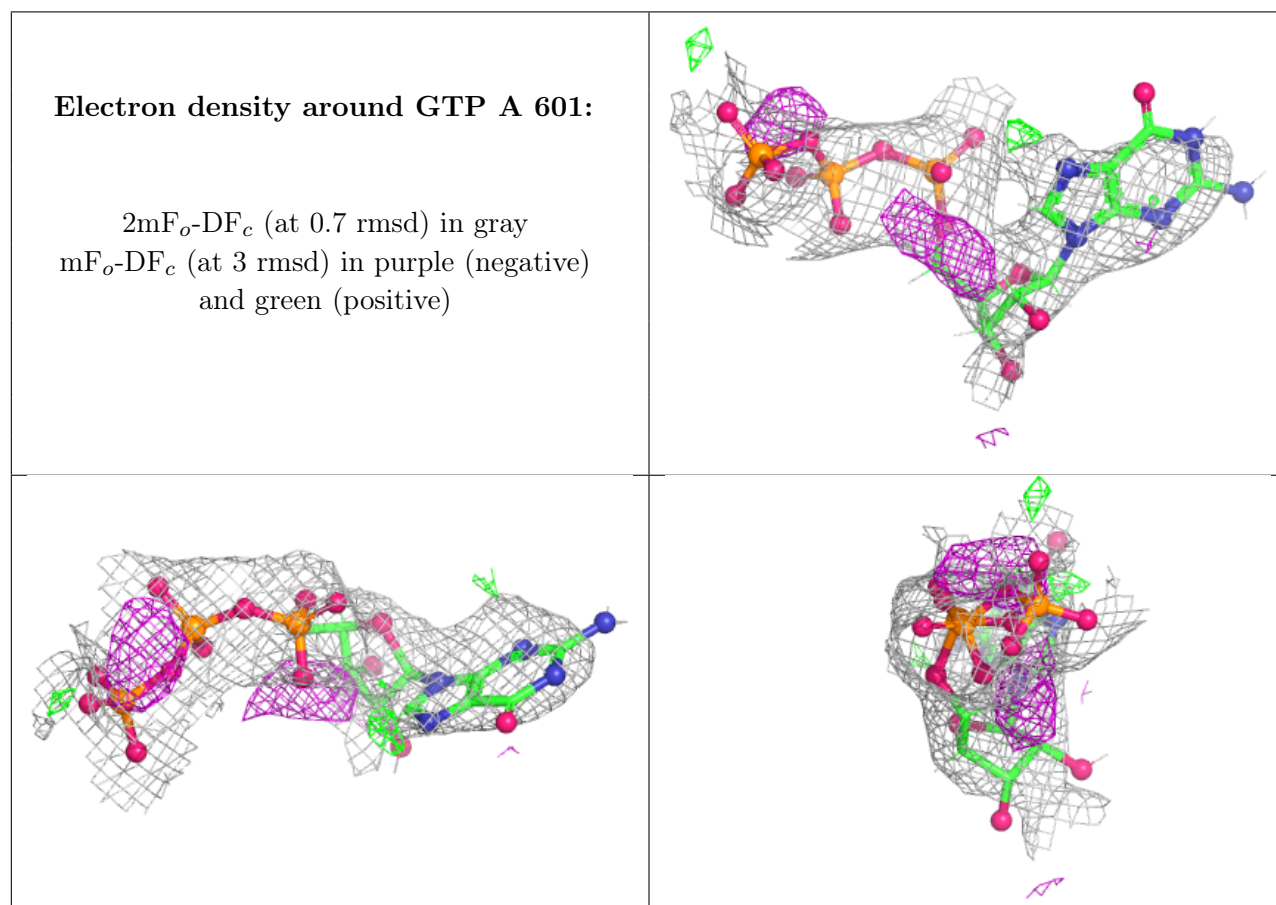
There are no monosaccharides in this entry.

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.

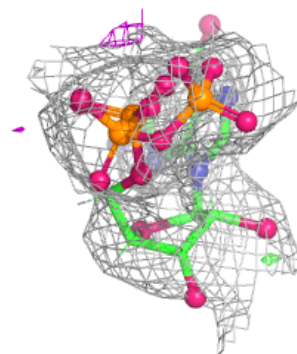
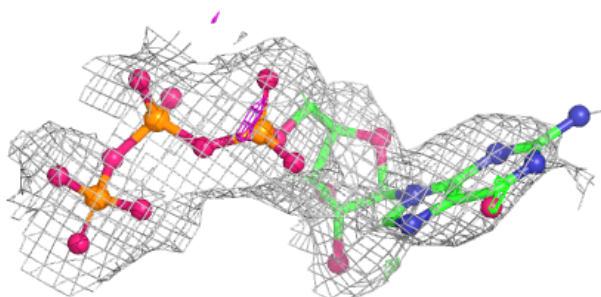
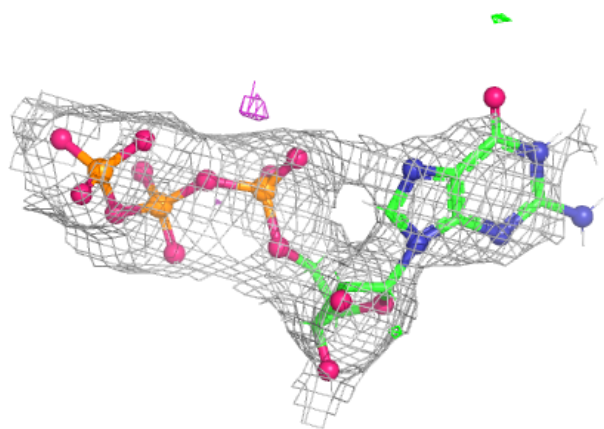
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	B	606	5/5	0.29	0.40	165,167,168,168	0
3	SO4	A	609	5/5	0.55	0.36	156,156,158,159	0
3	SO4	A	610	5/5	0.56	0.23	148,149,150,151	0
3	SO4	B	611	5/5	0.58	0.34	176,177,178,179	0
3	SO4	B	609	5/5	0.63	0.55	154,155,155,156	0
3	SO4	B	618	5/5	0.66	0.26	137,138,139,141	0
3	SO4	B	604	5/5	0.67	0.35	125,127,128,129	0
3	SO4	B	610	5/5	0.69	0.34	148,150,151,152	0
3	SO4	B	607	5/5	0.70	0.42	138,138,140,141	0
3	SO4	A	612	5/5	0.71	0.31	154,154,154,155	0
3	SO4	A	606	5/5	0.73	0.39	145,147,148,149	0
3	SO4	A	605	5/5	0.74	0.45	150,150,151,153	0
3	SO4	B	619	5/5	0.74	0.29	129,130,133,134	0
3	SO4	B	614	5/5	0.75	0.19	130,130,133,136	0
3	SO4	B	616	5/5	0.75	0.22	149,149,151,151	0
3	SO4	B	608	5/5	0.75	0.25	142,144,145,146	0
3	SO4	B	605	5/5	0.75	0.40	131,133,136,136	0
3	SO4	A	608	5/5	0.77	0.39	156,159,159,160	0
2	GTP	A	601	32/32	0.77	0.31	117,136,161,169	0
3	SO4	A	611	5/5	0.78	0.16	151,152,153,153	0
3	SO4	B	615	5/5	0.79	0.32	164,165,166,167	0
3	SO4	B	612	5/5	0.82	0.42	136,139,139,140	0
3	SO4	B	613	5/5	0.83	0.33	99,101,104,108	0
3	SO4	A	613	5/5	0.84	0.43	144,147,147,148	0
3	SO4	A	604	5/5	0.86	0.36	131,132,135,136	0
2	GTP	B	601	32/32	0.87	0.23	108,119,141,145	0
2	GTP	A	602	32/32	0.89	0.23	85,99,128,137	0
3	SO4	B	617	5/5	0.90	0.23	121,124,126,127	0
2	GTP	A	603	32/32	0.90	0.21	80,94,117,125	0
2	GTP	B	602	32/32	0.90	0.21	51,74,118,122	0
2	GTP	B	603	32/32	0.91	0.20	56,72,91,105	0
3	SO4	A	607	5/5	0.92	0.51	137,137,138,138	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.



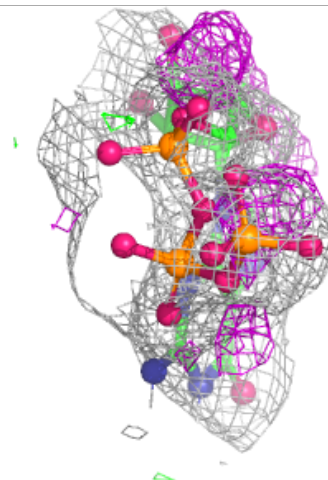
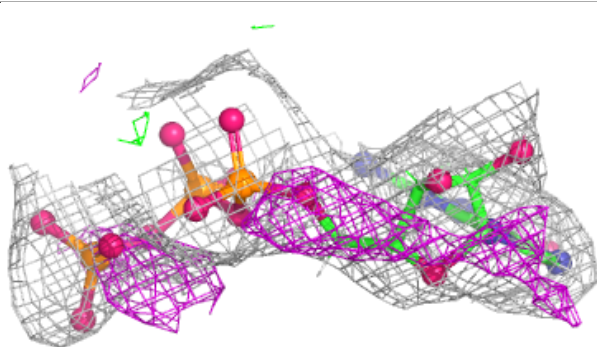
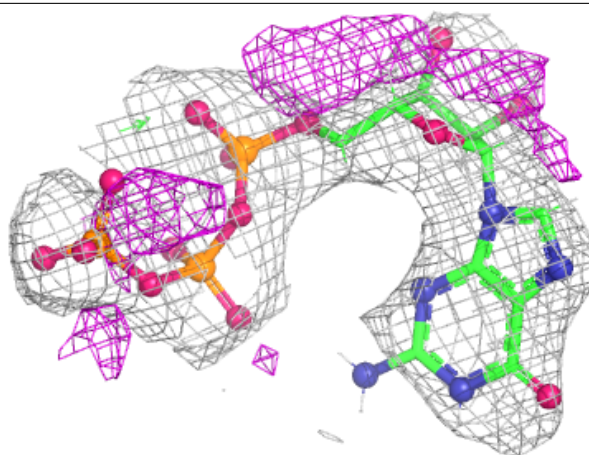
Electron density around GTP B 601:

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



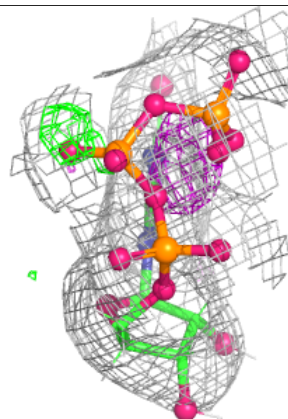
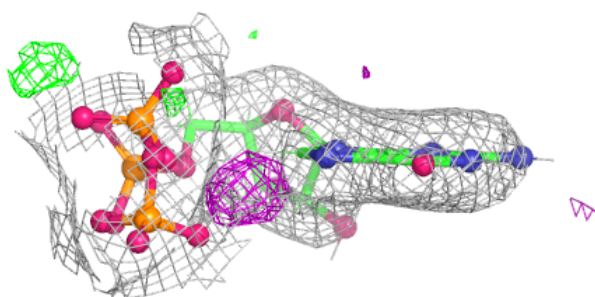
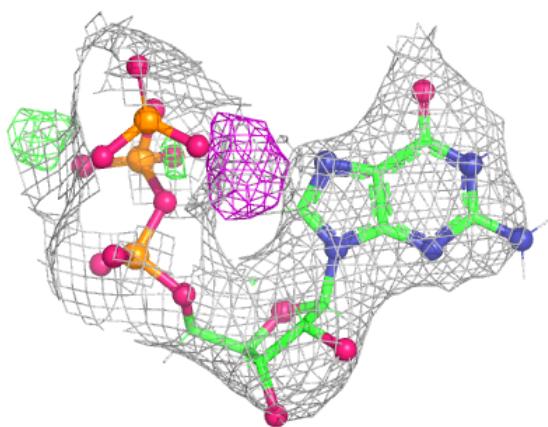
Electron density around GTP A 602:

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



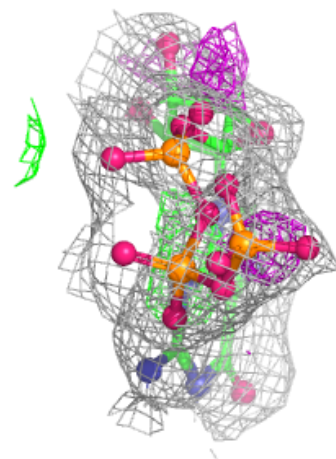
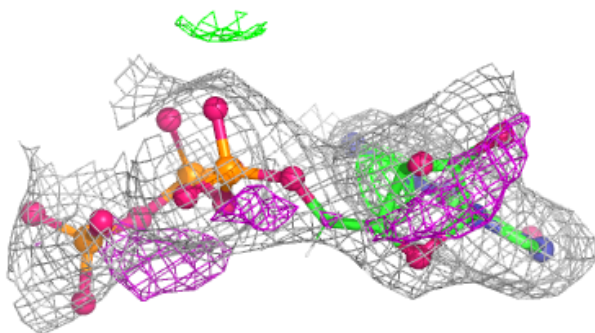
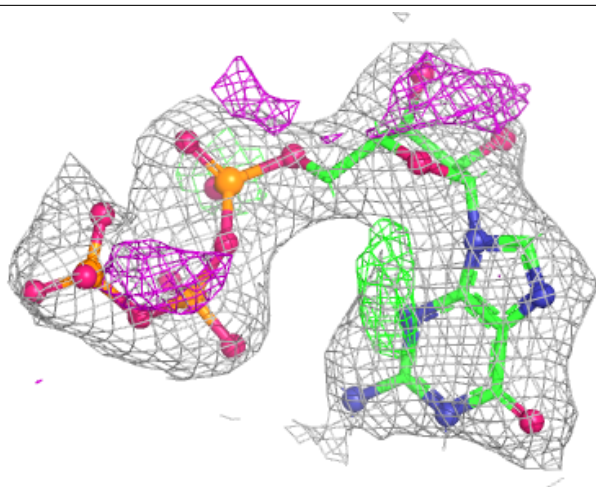
Electron density around GTP A 603:

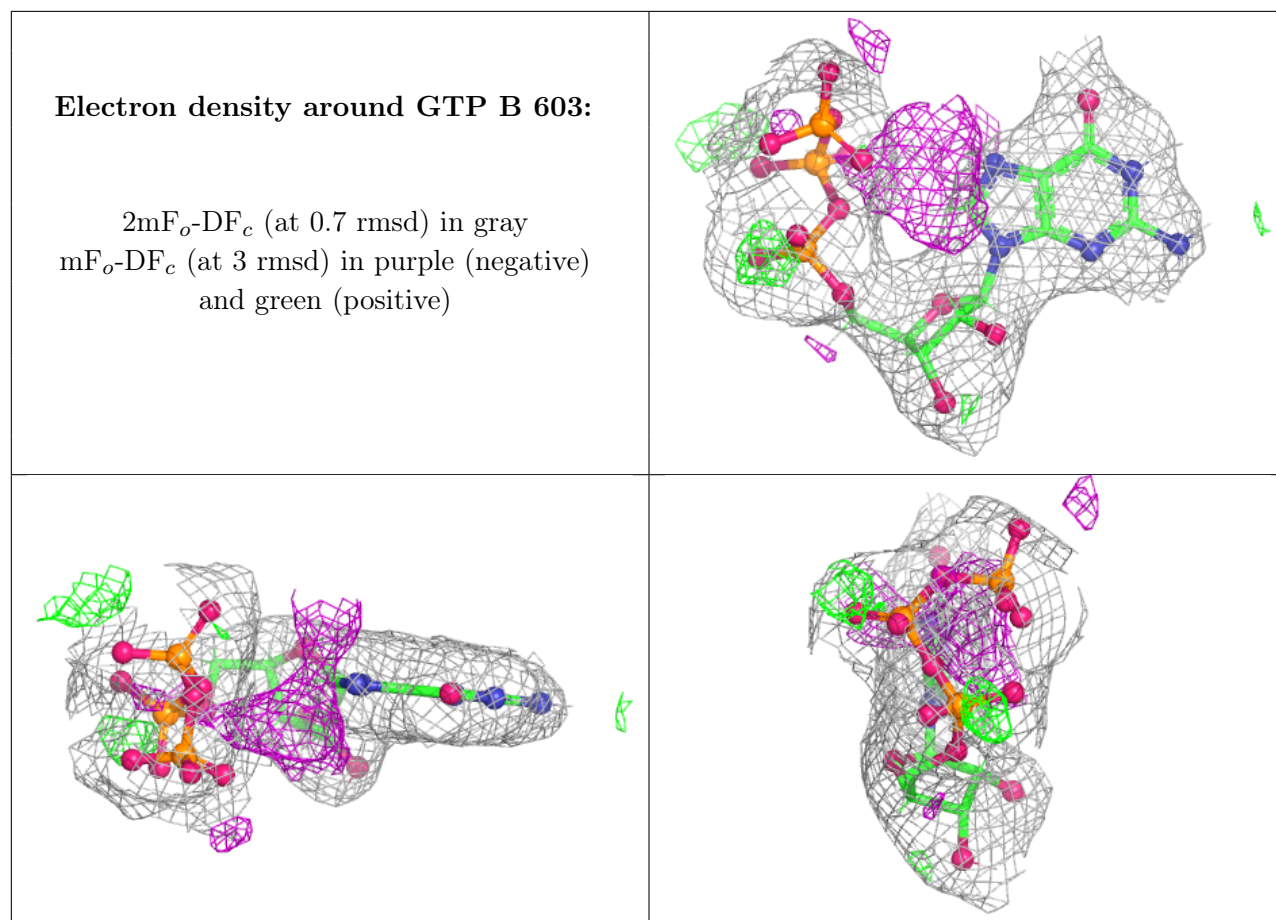
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GTP 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.