



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:57 PM UTC

PDB ID : 6I0O / pdb_00006i0o
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
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

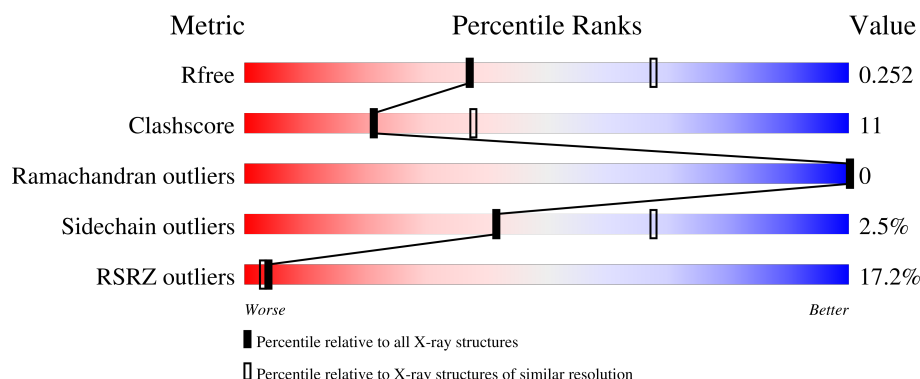
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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}	180053	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (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	16% 70% 13% • 16%
1	B	517	12% 69% 13% • 17%

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	-

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.

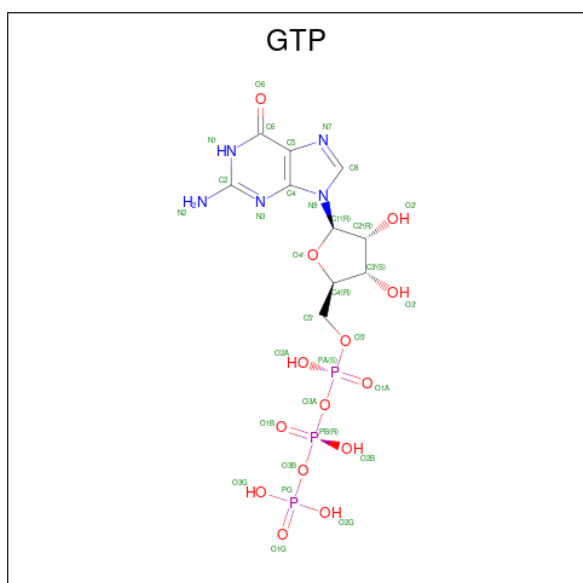
- Molecule 1 is a protein called Inosine-5'-monophosphate dehydrogenase 2.

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 (CCD ID: 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 (CCD ID: 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		

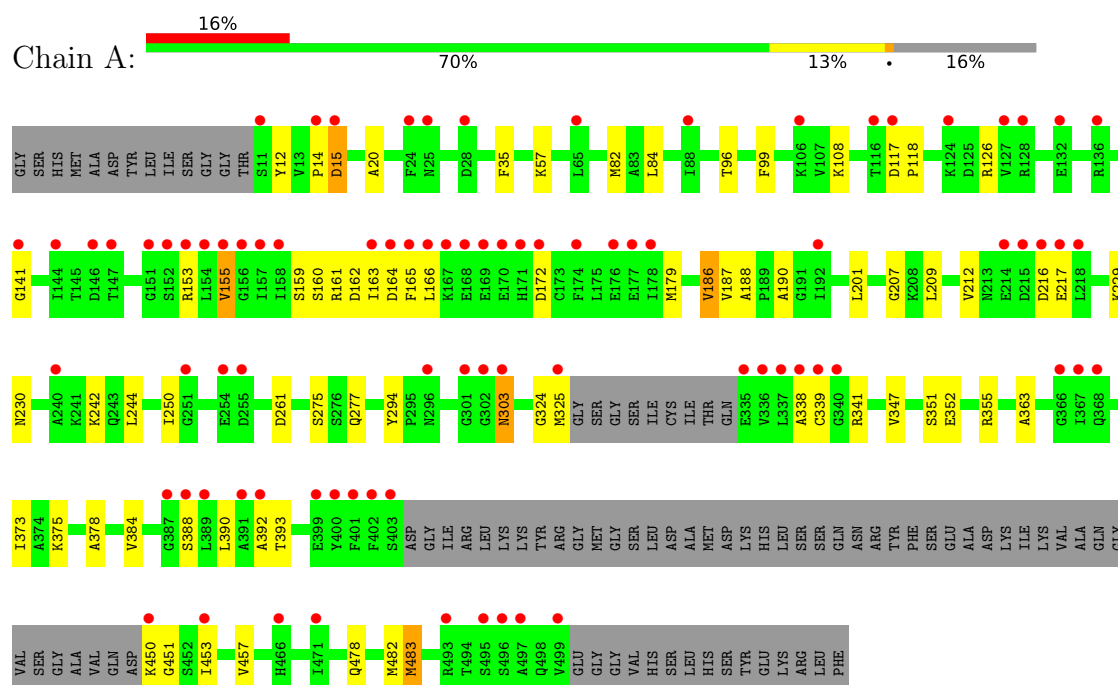
- Molecule 4 is water.

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

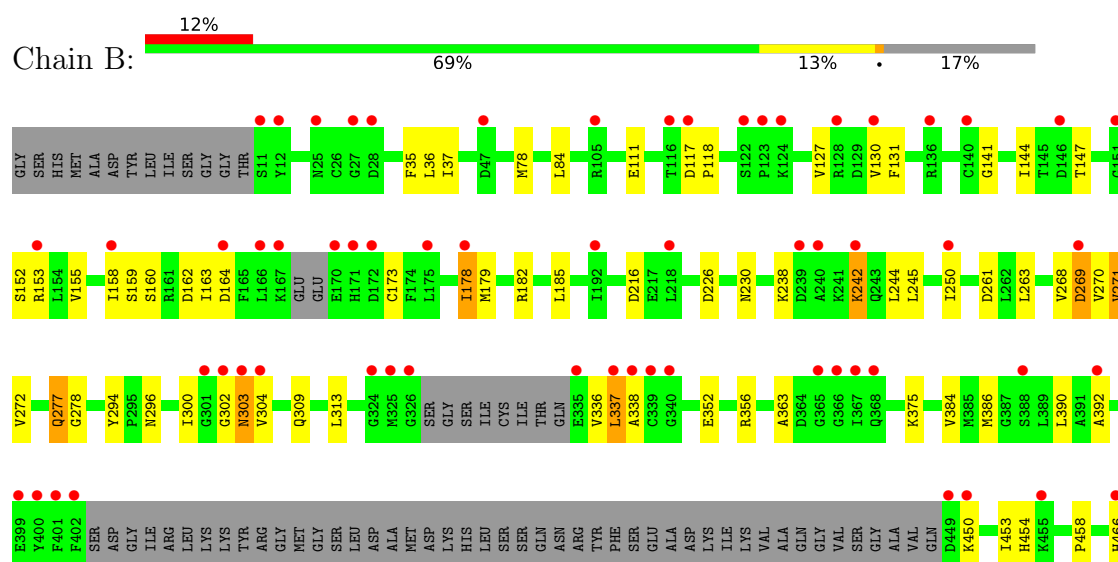
3 Residue-property plots [i](#)

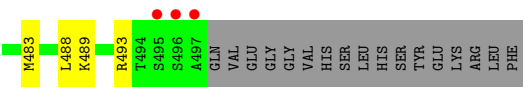
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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) 81.0 (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 (4.10%)	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 , 61.5	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	0.34	0/3205	0.54	5/4351 (0.1%)
1	B	0.32	0/3230	0.61	5/4374 (0.1%)
All	All	0.33	0/6435	0.58	10/8725 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	338	ALA	N-CA-C	9.08	123.47	108.49
1	B	337	LEU	N-CA-C	8.13	120.22	111.36
1	B	178	ILE	N-CA-C	7.68	118.48	110.72
1	B	303	ASN	N-CA-C	7.50	121.59	111.24
1	A	155	VAL	N-CA-C	7.17	117.27	110.53
1	B	269	ASP	N-CA-C	5.80	117.69	111.36
1	A	165	PHE	N-CA-C	5.80	117.40	110.44
1	A	166	LEU	N-CA-C	5.74	117.61	111.36
1	A	216	ASP	N-CA-C	5.33	119.54	113.19
1	A	390	LEU	N-CA-C	5.19	119.61	113.28

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	64	1
1	B	3183	3083	3166	76	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	142	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 (142) 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:B:230:ASN:CG	2:B:603:GTP:O3G	2.15	0.89
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:A:230:ASN:CG	2:A:603:GTP:O1G	2.16	0.88
1:B:277:GLN:NE2	1:B:309:GLN:NE2	2.23	0.86
1:B:130:VAL:HG11	1:B:163:ILE:HD11	1.57	0.84
1:B:155:VAL:CG1	1:B:179:MET:HE1	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:MET:HE1	1:B:453:ILE:HD11	1.72	0.71
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:155:VAL:HG12	1:B:179:MET:HE1	1.72	0.69
1:B:277:GLN:HE22	1:B:309:GLN:HE22	1.36	0.68
1:A:483:MET:HE2	1:A:483:MET:C	2.18	0.67
1:A:190:ALA:N	1:A:212:VAL:O	2.28	0.66
1:A:338:ALA:O	1:A:339:CYS:SG	2.53	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: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: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
1:A:20:ALA:HB3	1:A:483:MET:CE	2.30	0.62
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:B:155:VAL:HG12	1:B:179:MET:CE	2.30	0.61
1:A:392:ALA:HB3	1:A:450:LYS:CB	2.31	0.61
1:B:78:MET:HE1	1:B:453:ILE:CD1	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:20:ALA:HB3	1:A:483:MET:HE1	1.86	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:A:483:MET:HE2	1:A:483:MET:O	2.06	0.55
1:B:131:PHE:CZ	1:B:163:ILE:CG2	2.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:155:VAL:CG1	1:A:179:MET:HE1	2.38	0.52
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:A:155:VAL:HG12	1:A:179:MET:CE	2.40	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:B:277:GLN:HG3	1:B:277:GLN:O	2.09	0.51
1:A:155:VAL:HG11	1:A:179:MET:HE1	1.91	0.50
1:B:337:LEU:O	4:B:702:HOH:O	2.20	0.50
1:B:352:GLU:OE2	1:B:356:ARG:NH2	2.35	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:B:78:MET:HE1	1:B:453:ILE:CG1	2.43	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:84:LEU:HD21	1:A:244:LEU:HD11	1.96	0.47
1:A:20:ALA:CB	1:A:483:MET:HE3	2.45	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: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:386:MET:HE3	1:B:390:LEU:HD11	1.98	0.46
1:A:161:ARG:HA	1:A:164:ASP:CG	2.41	0.45
1:B:483:MET:HA	1:B:488:LEU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:20:ALA:HB3	1:A:483:MET:HE3	1.99	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:B:78:MET:HE1	1:B:453:ILE:HG13	1.99	0.44
1:B:117:ASP:N	1:B:118:PRO:CD	2.80	0.44
1:A:155:VAL:CG1	1:A:179:MET:CE	2.95	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:155:VAL:HG12	1:A:179:MET:HE3	2.01	0.43
2:A:601:GTP:H8	2:A:601:GTP:H2'	1.42	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:35:PHE:O	1:B:375:LYS:NZ	2.44	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: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

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	428/517 (83%)	418 (98%)	10 (2%)	0	100	100
1	B	423/517 (82%)	411 (97%)	12 (3%)	0	100	100
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%)	302 (97%)	9 (3%)	37	63
1	B	326/422 (77%)	319 (98%)	7 (2%)	47	72
All	All	637/844 (76%)	621 (98%)	16 (2%)	42	68

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	57	LYS
1	A	108	LYS
1	A	186	VAL
1	A	242	LYS
1	A	250	ILE
1	A	277	GLN
1	A	303	ASN

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Mol	Chain	Res	Type
1	A	483	MET
1	B	153	ARG
1	B	173	CYS
1	B	216	ASP
1	B	242	LYS
1	B	271	VAL
1	B	277	GLN
1	B	303	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	B	309	GLN
1	B	454	HIS
1	B	466	HIS

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](#)

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
3	SO4	A	612	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	A	608	-	4,4,4	0.24	0	6,6,6	0.06	0
3	SO4	B	614	-	4,4,4	0.24	0	6,6,6	0.10	0
3	SO4	B	619	-	4,4,4	0.23	0	6,6,6	0.14	0
3	SO4	A	606	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	A	609	-	4,4,4	0.24	0	6,6,6	0.07	0
2	GTP	B	602	-	33,34,34	3.66	16 (48%)	50,54,54	2.60	12 (24%)
3	SO4	B	605	-	4,4,4	0.24	0	6,6,6	0.06	0
3	SO4	A	607	-	4,4,4	0.23	0	6,6,6	0.09	0
2	GTP	A	602	-	33,34,34	3.67	16 (48%)	50,54,54	2.66	11 (22%)
2	GTP	A	601	-	33,34,34	3.68	16 (48%)	50,54,54	2.34	11 (22%)
3	SO4	B	607	-	4,4,4	0.24	0	6,6,6	0.20	0
3	SO4	B	604	-	4,4,4	0.28	0	6,6,6	0.27	0
3	SO4	B	616	-	4,4,4	0.22	0	6,6,6	0.08	0
3	SO4	A	613	-	4,4,4	0.35	0	6,6,6	0.18	0
2	GTP	B	601	-	33,34,34	3.67	16 (48%)	50,54,54	2.32	13 (26%)
2	GTP	B	603	-	33,34,34	1.23	4 (12%)	50,54,54	1.77	8 (16%)
3	SO4	B	613	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	B	610	-	4,4,4	0.24	0	6,6,6	0.06	0
3	SO4	B	615	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	B	611	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	B	606	-	4,4,4	0.40	0	6,6,6	0.22	0
2	GTP	A	603	-	33,34,34	1.17	4 (12%)	50,54,54	1.73	5 (10%)
3	SO4	A	605	-	4,4,4	0.23	0	6,6,6	0.09	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	617	-	4,4,4	0.24	0	6,6,6	0.10	0
3	SO4	B	612	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	B	608	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	A	604	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	B	609	-	4,4,4	0.24	0	6,6,6	0.12	0
3	SO4	A	610	-	4,4,4	0.23	0	6,6,6	0.06	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	B	601	-	-	4/22/38/38	0/3/3/3
2	GTP	B	602	-	-	6/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GTP	B	603	-	-	3/22/38/38	0/3/3/3
2	GTP	A	602	-	-	7/22/38/38	0/3/3/3
2	GTP	A	601	-	-	7/22/38/38	0/3/3/3
2	GTP	A	603	-	-	6/22/38/38	0/3/3/3

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	GTP	O4'-C1'	9.17	1.63	1.42
2	A	601	GTP	O4'-C1'	8.93	1.62	1.42
2	A	602	GTP	O4'-C1'	8.88	1.62	1.42
2	B	602	GTP	O4'-C1'	8.74	1.62	1.42
2	A	602	GTP	C2'-C1'	-7.26	1.30	1.53
2	B	602	GTP	C2'-C1'	-7.19	1.30	1.53
2	A	601	GTP	C2'-C1'	-6.82	1.32	1.53
2	A	601	GTP	C4-N3	6.80	1.49	1.34
2	B	601	GTP	C2'-C1'	-6.80	1.32	1.53
2	B	601	GTP	C4-N3	6.76	1.49	1.34
2	B	602	GTP	C4-N3	6.67	1.49	1.34
2	A	602	GTP	C4-N3	6.65	1.49	1.34
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
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	5.63	1.46	1.33
2	B	601	GTP	C2-N3	5.61	1.46	1.33
2	A	602	GTP	C2-N3	5.56	1.46	1.33
2	B	601	GTP	PB-O3B	5.49	1.65	1.59
2	B	602	GTP	C2-N3	5.43	1.46	1.33
2	B	601	GTP	C2-N2	5.34	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	602	GTP	C2-N2	5.20	1.46	1.34
2	B	603	GTP	C6-N1	-3.22	1.32	1.38
2	B	601	GTP	O2'-C2'	3.12	1.50	1.43
2	A	603	GTP	C6-N1	-3.10	1.33	1.38
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
2	B	603	GTP	C5-N7	-2.94	1.33	1.39
2	A	601	GTP	C5-N7	-2.92	1.33	1.39
2	B	601	GTP	C5-N7	-2.92	1.33	1.39
2	B	602	GTP	C6-N1	2.80	1.44	1.38
2	A	603	GTP	C5-C4	2.75	1.46	1.38
2	B	602	GTP	O3'-C3'	-2.68	1.36	1.43
2	A	602	GTP	C6-N1	2.65	1.43	1.38
2	B	601	GTP	C6-N1	2.64	1.43	1.38
2	A	602	GTP	C5-C6	2.64	1.54	1.44
2	A	602	GTP	O3'-C3'	-2.64	1.36	1.43
2	A	602	GTP	C5-N7	-2.64	1.33	1.39
2	B	602	GTP	C5-C6	2.62	1.54	1.44
2	B	601	GTP	C5-C6	2.60	1.54	1.44
2	B	601	GTP	O3'-C3'	-2.58	1.36	1.43
2	B	603	GTP	C5-C4	2.57	1.45	1.38
2	A	601	GTP	C5-C6	2.56	1.54	1.44
2	B	602	GTP	C5-N7	-2.54	1.34	1.39
2	A	601	GTP	O3'-C3'	-2.53	1.36	1.43
2	A	601	GTP	C6-N1	2.44	1.43	1.38
2	A	603	GTP	C5-N7	-2.39	1.34	1.39
2	A	601	GTP	O6-C6	-2.35	1.19	1.23
2	A	602	GTP	O6-C6	-2.35	1.19	1.23
2	B	602	GTP	O6-C6	-2.33	1.19	1.23
2	B	601	GTP	O6-C6	-2.29	1.19	1.23
2	A	603	GTP	C4-N9	-2.10	1.32	1.38
2	B	603	GTP	C4-N9	-2.02	1.32	1.38

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	602	GTP	C1'-N9-C8	-11.08	95.26	126.73
2	B	602	GTP	C1'-N9-C8	-10.75	96.19	126.73
2	A	602	GTP	C1'-N9-C4	10.29	156.88	126.49
2	B	602	GTP	C1'-N9-C4	9.87	155.64	126.49
2	A	601	GTP	C1'-N9-C8	-8.89	101.48	126.73
2	A	601	GTP	C1'-N9-C4	8.72	152.26	126.49
2	B	601	GTP	C1'-N9-C8	-8.56	102.42	126.73
2	B	601	GTP	C1'-N9-C4	8.46	151.48	126.49
2	B	603	GTP	C5-C4-N3	-6.77	117.61	128.39
2	A	603	GTP	C5-C4-N3	-6.10	118.69	128.39
2	A	601	GTP	C5-C4-N3	-5.27	120.00	128.39
2	B	601	GTP	C5-C4-N3	-5.21	120.10	128.39
2	B	603	GTP	N9-C4-N3	5.11	136.17	125.95
2	B	603	GTP	C2-N3-C4	5.05	120.99	112.30
2	A	602	GTP	C5-C4-N3	-4.90	120.59	128.39
2	A	603	GTP	C2-N3-C4	4.81	120.59	112.30
2	B	601	GTP	C2-N3-C4	4.59	120.20	112.30
2	B	602	GTP	C5-C4-N3	-4.56	121.14	128.39
2	A	601	GTP	C2-N3-C4	4.50	120.05	112.30
2	A	603	GTP	N9-C4-N3	4.40	134.75	125.95
2	A	602	GTP	C2-N3-C4	4.36	119.81	112.30
2	B	602	GTP	C2-N3-C4	4.34	119.78	112.30
2	A	603	GTP	C6-C5-N7	3.32	136.34	130.29
2	A	602	GTP	C2-N1-C6	-3.04	119.60	125.11
2	B	602	GTP	N9-C8-N7	-3.01	107.82	113.40
2	B	602	GTP	C2-N1-C6	-2.91	119.84	125.11
2	B	601	GTP	C2-N1-C6	-2.86	119.93	125.11
2	A	602	GTP	N9-C8-N7	-2.85	108.12	113.40
2	A	603	GTP	C4-C5-N7	-2.78	106.26	110.67
2	B	601	GTP	C2'-C1'-N9	2.78	120.99	113.25
2	A	602	GTP	C3'-C2'-C1'	2.77	106.71	101.46
2	B	602	GTP	C3'-C2'-C1'	2.75	106.67	101.46
2	B	603	GTP	C6-C5-N7	2.74	135.27	130.29
2	A	601	GTP	C2-N1-C6	-2.74	120.15	125.11
2	B	603	GTP	C4-C5-N7	-2.72	106.36	110.67
2	B	602	GTP	C5-C6-N1	2.61	119.89	113.25
2	A	601	GTP	C2'-C1'-N9	2.59	120.45	113.25
2	A	602	GTP	C5-C6-N1	2.57	119.80	113.25
2	A	602	GTP	N9-C4-N3	2.53	131.02	125.95
2	B	601	GTP	C5-C6-N1	2.49	119.58	113.25
2	B	602	GTP	O6-C6-C5	-2.44	120.08	126.53
2	B	601	GTP	O6-C6-C5	-2.44	120.10	126.53
2	A	601	GTP	C5-C6-N1	2.43	119.44	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	GTP	O6-C6-C5	-2.41	120.18	126.53
2	A	601	GTP	N9-C4-N3	2.40	130.74	125.95
2	A	602	GTP	O6-C6-C5	-2.38	120.25	126.53
2	B	601	GTP	N9-C8-N7	-2.35	109.04	113.40
2	B	602	GTP	C2'-C1'-N9	-2.30	106.86	113.25
2	B	602	GTP	N9-C4-N3	2.28	130.52	125.95
2	A	601	GTP	N9-C8-N7	-2.28	109.18	113.40
2	B	603	GTP	O6-C6-C5	-2.23	120.65	126.53
2	B	601	GTP	N9-C4-N3	2.20	130.36	125.95
2	B	601	GTP	C5-C4-N9	2.17	109.54	105.66
2	B	603	GTP	C8-N7-C5	2.10	107.99	104.26
2	B	602	GTP	C8-N7-C5	2.09	107.98	104.26
2	A	602	GTP	C8-N7-C5	2.05	107.92	104.26
2	B	603	GTP	C2-N1-C6	-2.03	121.42	125.11
2	B	601	GTP	C4-C5-N7	-2.01	107.48	110.67
2	A	601	GTP	C5-C4-N9	2.01	109.25	105.66
2	B	601	GTP	C8-N7-C5	2.01	107.83	104.26

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
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

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Mol	Chain	Res	Type	Atoms
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

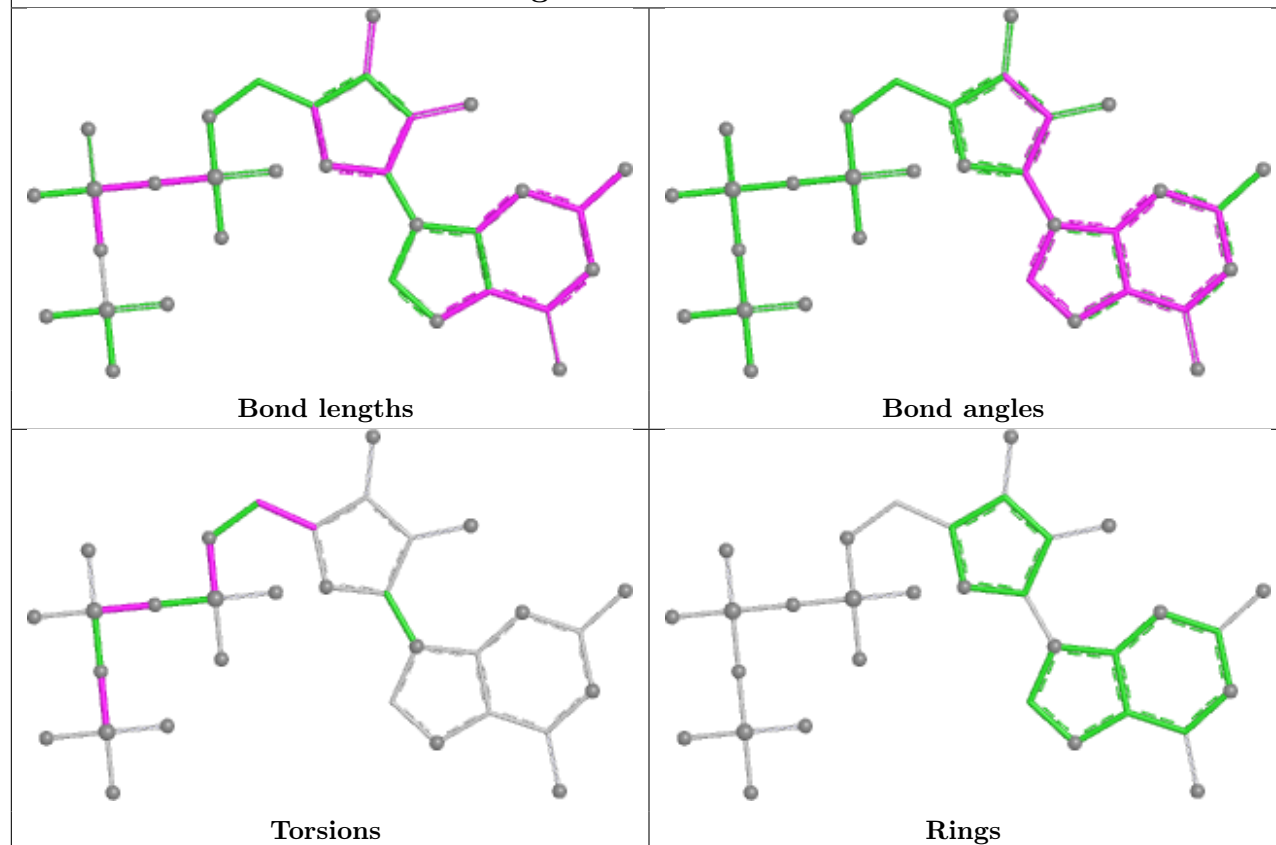
There are no ring outliers.

9 monomers are involved in 28 short contacts:

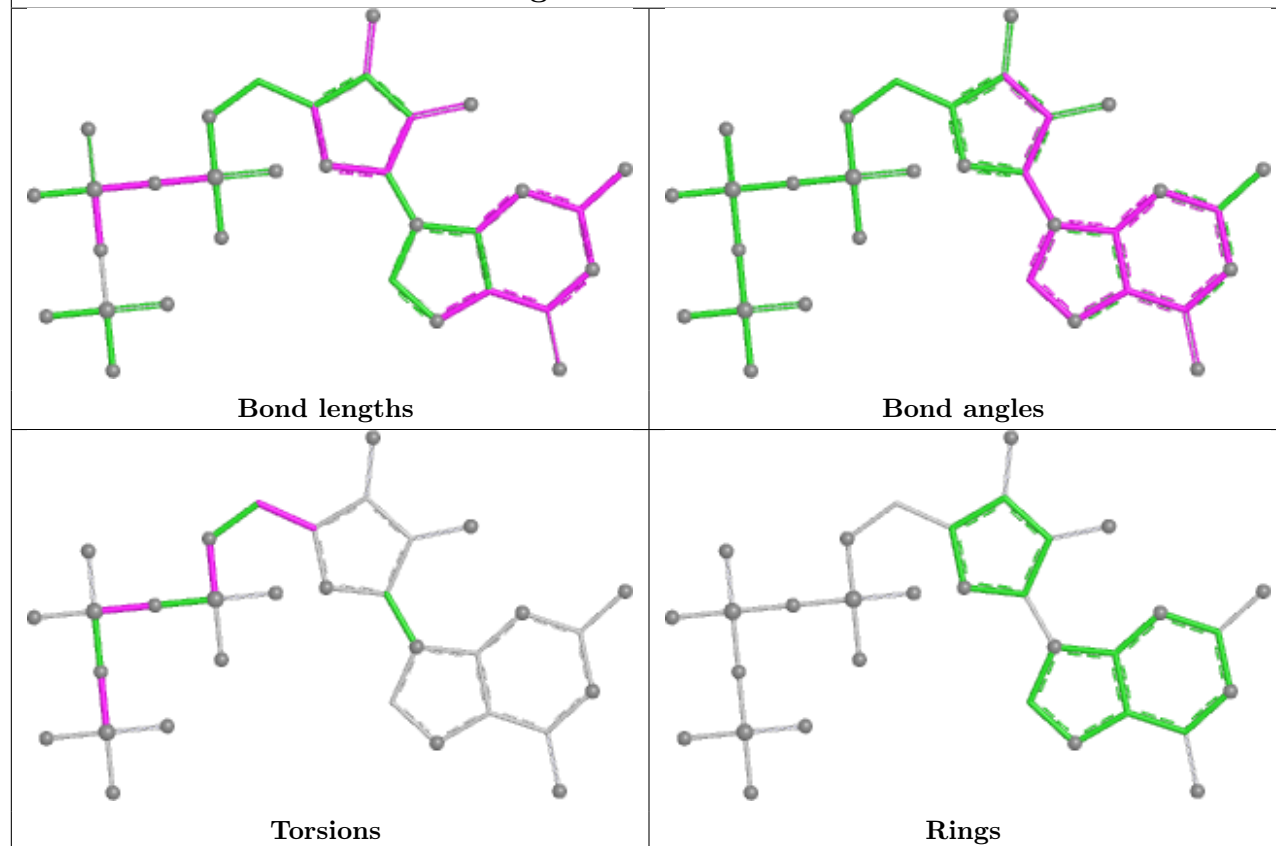
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	612	SO4	1	0
2	B	602	GTP	2	0
3	B	605	SO4	1	0
2	A	602	GTP	2	0
2	A	601	GTP	5	0
2	B	601	GTP	2	0
2	B	603	GTP	9	0
2	A	603	GTP	5	0
3	B	609	SO4	1	0

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.

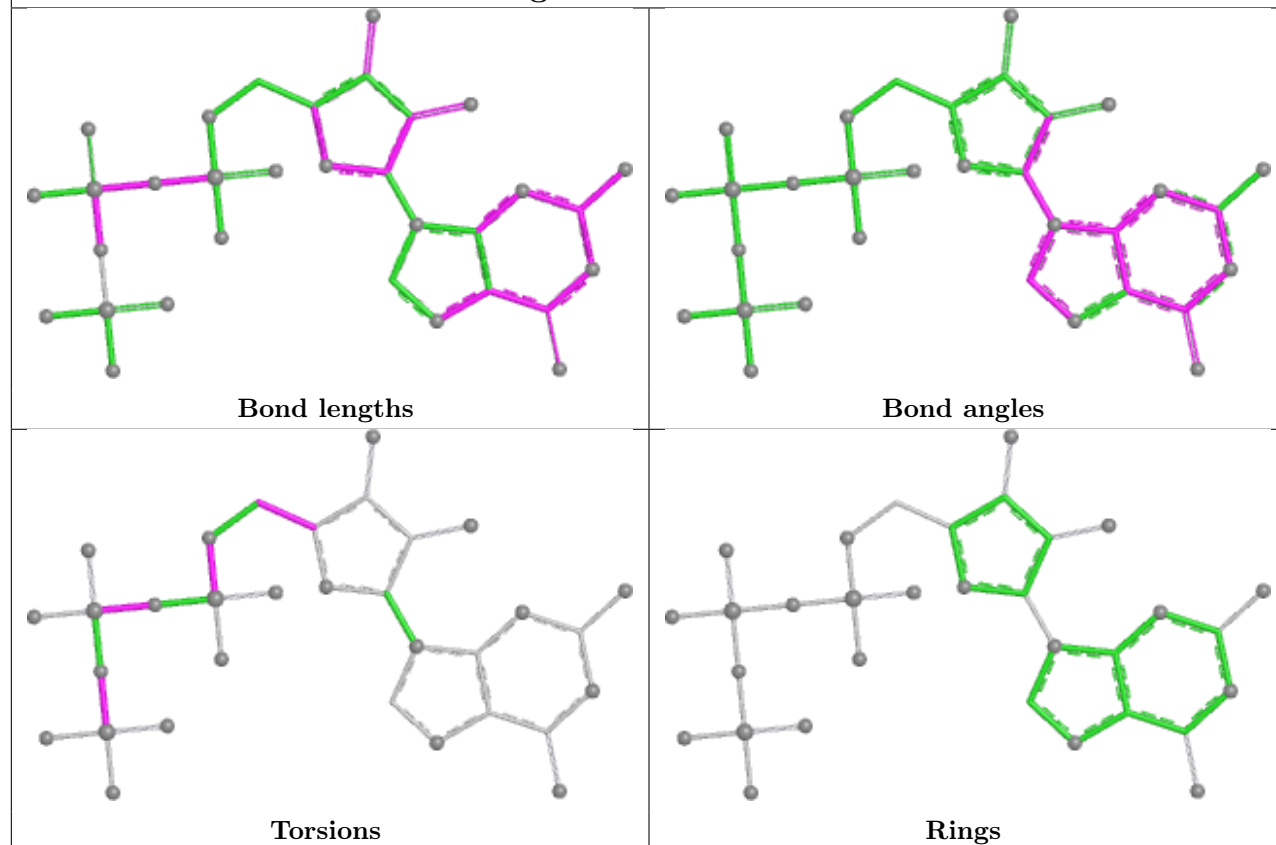
Ligand GTP B 602



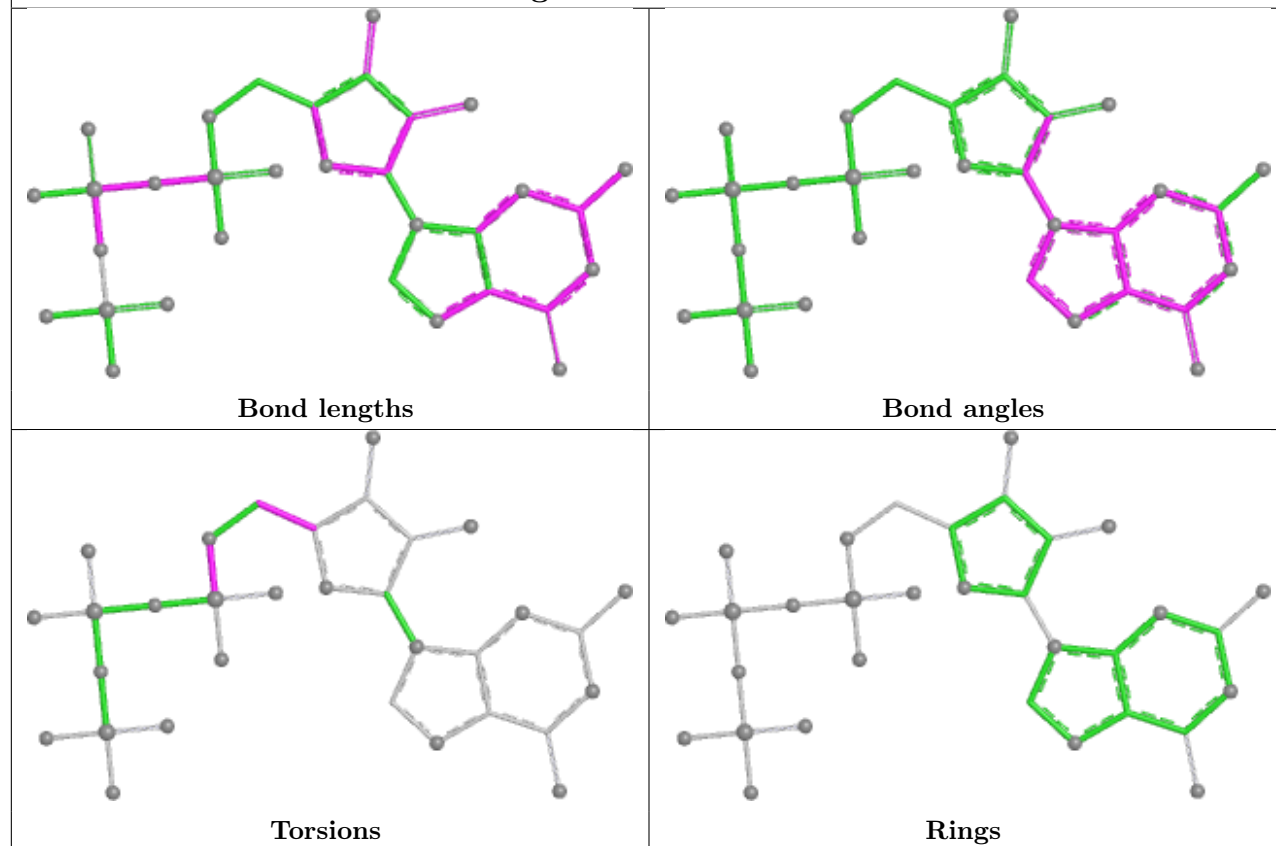
Ligand GTP A 602



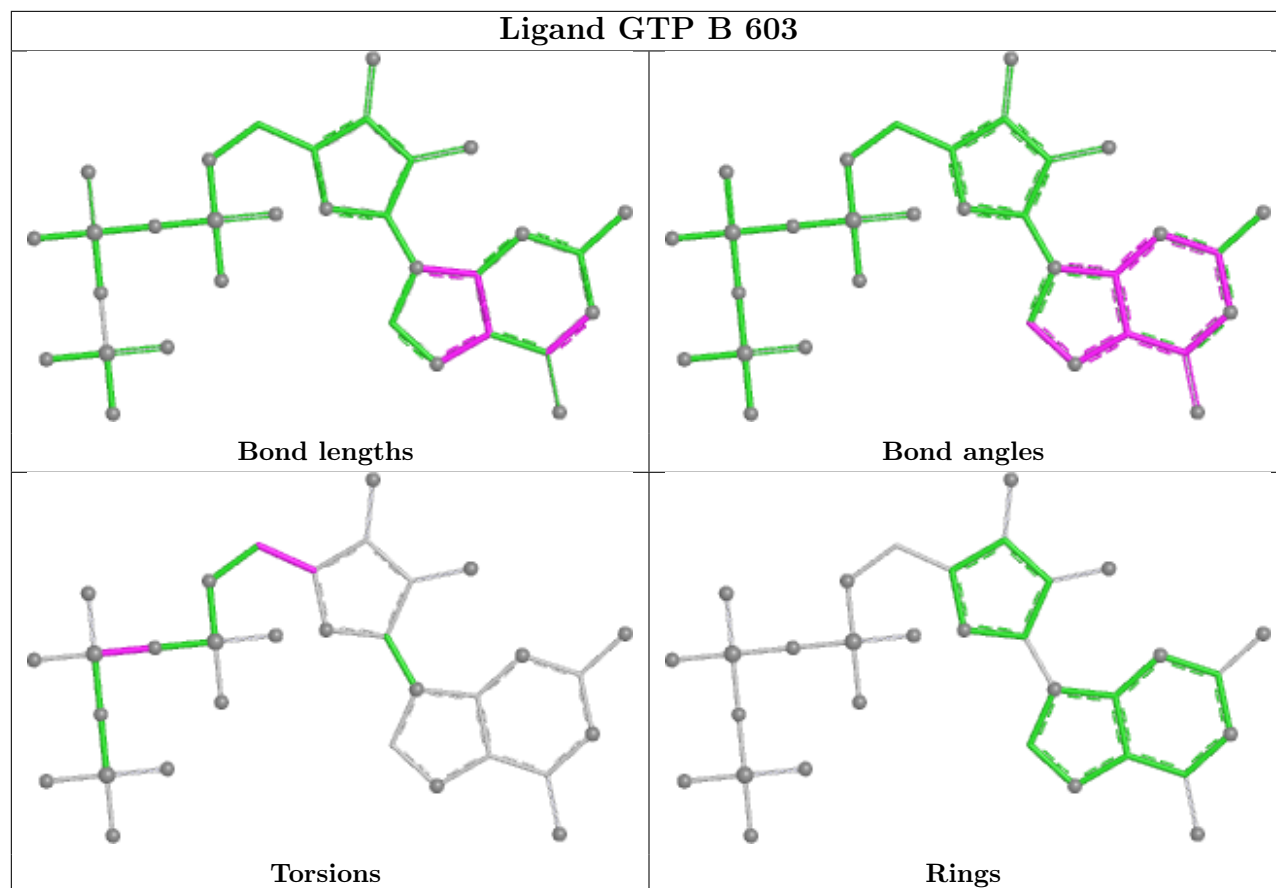
Ligand GTP A 601



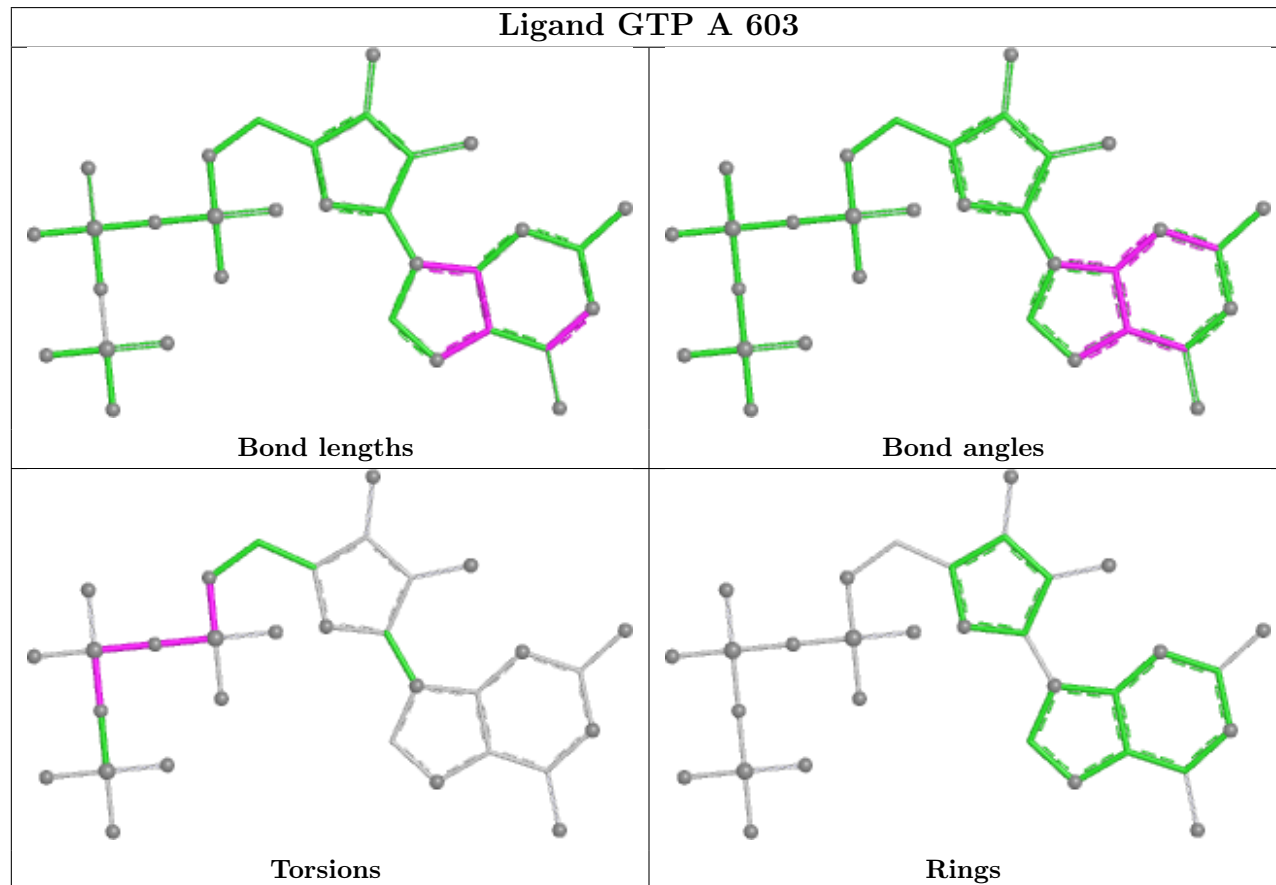
Ligand GTP B 601



Ligand GTP B 603



Ligand GTP A 603



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%)	1.22	85 (19%) 3 2	57, 87, 127, 170	0
1	B	431/517 (83%)	0.79	64 (14%) 5 4	30, 67, 107, 142	0
All	All	865/1034 (83%)	1.01	149 (17%) 4 3	30, 77, 123, 170	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	401	PHE	7.4
1	A	403	SER	6.9
1	A	339	CYS	6.7
1	A	336	VAL	6.7
1	B	172	ASP	6.4
1	B	11	SER	6.1
1	A	499	VAL	6.0
1	B	170	GLU	5.7
1	A	337	LEU	5.7
1	B	340	GLY	5.7
1	B	324	GLY	5.5
1	B	399	GLU	5.4
1	A	155	VAL	5.4
1	B	497	ALA	5.2
1	B	402	PHE	5.2
1	B	400	TYR	5.2
1	A	335	GLU	5.2
1	A	216	ASP	5.1
1	B	240	ALA	5.0
1	A	172	ASP	4.9
1	A	11	SER	4.9
1	A	296	ASN	4.8
1	B	335	GLU	4.8
1	A	401	PHE	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	368	GLN	4.7
1	A	453	ILE	4.7
1	A	168	GLU	4.6
1	A	338	ALA	4.6
1	A	167	LYS	4.6
1	B	338	ALA	4.5
1	A	174	PHE	4.4
1	A	215	ASP	4.4
1	A	496	SER	4.2
1	A	214	GLU	4.0
1	B	178	ILE	4.0
1	B	303	ASN	4.0
1	A	169	GLU	4.0
1	B	302	GLY	4.0
1	A	166	LEU	4.0
1	A	340	GLY	4.0
1	A	367	ILE	3.9
1	B	326	GLY	3.9
1	A	400	TYR	3.8
1	A	325	MET	3.7
1	B	496	SER	3.7
1	B	368	GLN	3.7
1	A	147	THR	3.7
1	B	325	MET	3.7
1	B	495	SER	3.6
1	A	124	LYS	3.6
1	A	301	GLY	3.5
1	A	495	SER	3.4
1	A	116	THR	3.4
1	A	164	ASP	3.4
1	A	144	ILE	3.3
1	A	65	LEU	3.3
1	B	136	ARG	3.3
1	B	337	LEU	3.3
1	B	164	ASP	3.3
1	A	117	ASP	3.3
1	B	392	ALA	3.3
1	A	302	GLY	3.2
1	B	450	LYS	3.2
1	B	301	GLY	3.2
1	B	365	GLY	3.2
1	A	240	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	171	HIS	3.1
1	A	152	SER	3.1
1	B	367	ILE	3.1
1	A	24	PHE	3.1
1	A	178	ILE	3.1
1	A	387	GLY	3.0
1	B	25	ASN	3.0
1	A	156	GLY	3.0
1	A	151	GLY	2.9
1	B	171	HIS	2.9
1	B	167	LYS	2.9
1	A	146	ASP	2.9
1	B	250	ILE	2.9
1	A	391	ALA	2.9
1	A	136	ARG	2.9
1	B	130	VAL	2.9
1	A	170	GLU	2.8
1	A	15	ASP	2.8
1	B	47	ASP	2.8
1	B	117	ASP	2.8
1	B	12	TYR	2.8
1	A	254	GLU	2.8
1	A	399	GLU	2.8
1	A	402	PHE	2.8
1	B	339	CYS	2.7
1	A	192	ILE	2.7
1	B	158	ILE	2.7
1	A	177	GLU	2.7
1	B	175	LEU	2.7
1	A	128	ARG	2.6
1	B	105	ARG	2.6
1	B	146	ASP	2.6
1	B	218	LEU	2.6
1	B	242	LYS	2.6
1	A	389	LEU	2.6
1	B	304	VAL	2.6
1	A	153	ARG	2.6
1	A	218	LEU	2.5
1	B	239	ASP	2.5
1	A	127	VAL	2.5
1	B	128	ARG	2.5
1	A	217	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	27	GLY	2.5
1	B	116	THR	2.5
1	B	366	GLY	2.5
1	B	166	LEU	2.4
1	B	455	LYS	2.4
1	A	163	ILE	2.4
1	A	28	ASP	2.4
1	A	176	GLU	2.4
1	A	366	GLY	2.4
1	A	466	HIS	2.4
1	A	132	GLU	2.4
1	A	450	LYS	2.3
1	A	493	ARG	2.3
1	A	25	ASN	2.3
1	B	122	SER	2.3
1	B	153	ARG	2.3
1	A	392	ALA	2.3
1	A	165	PHE	2.3
1	A	157	ILE	2.2
1	B	123	PRO	2.2
1	B	449	ASP	2.2
1	A	303	ASN	2.2
1	B	151	GLY	2.2
1	A	388	SER	2.2
1	B	388	SER	2.2
1	A	158	ILE	2.1
1	A	471	ILE	2.1
1	B	192	ILE	2.1
1	B	140	CYS	2.1
1	A	497	ALA	2.1
1	A	154	LEU	2.1
1	A	255	ASP	2.1
1	A	251	GLY	2.1
1	B	28	ASP	2.0
1	B	466	HIS	2.0
1	B	269	ASP	2.0
1	A	106	LYS	2.0
1	B	124	LYS	2.0
1	A	14	PRO	2.0
1	A	88	ILE	2.0
1	A	141	GLY	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.

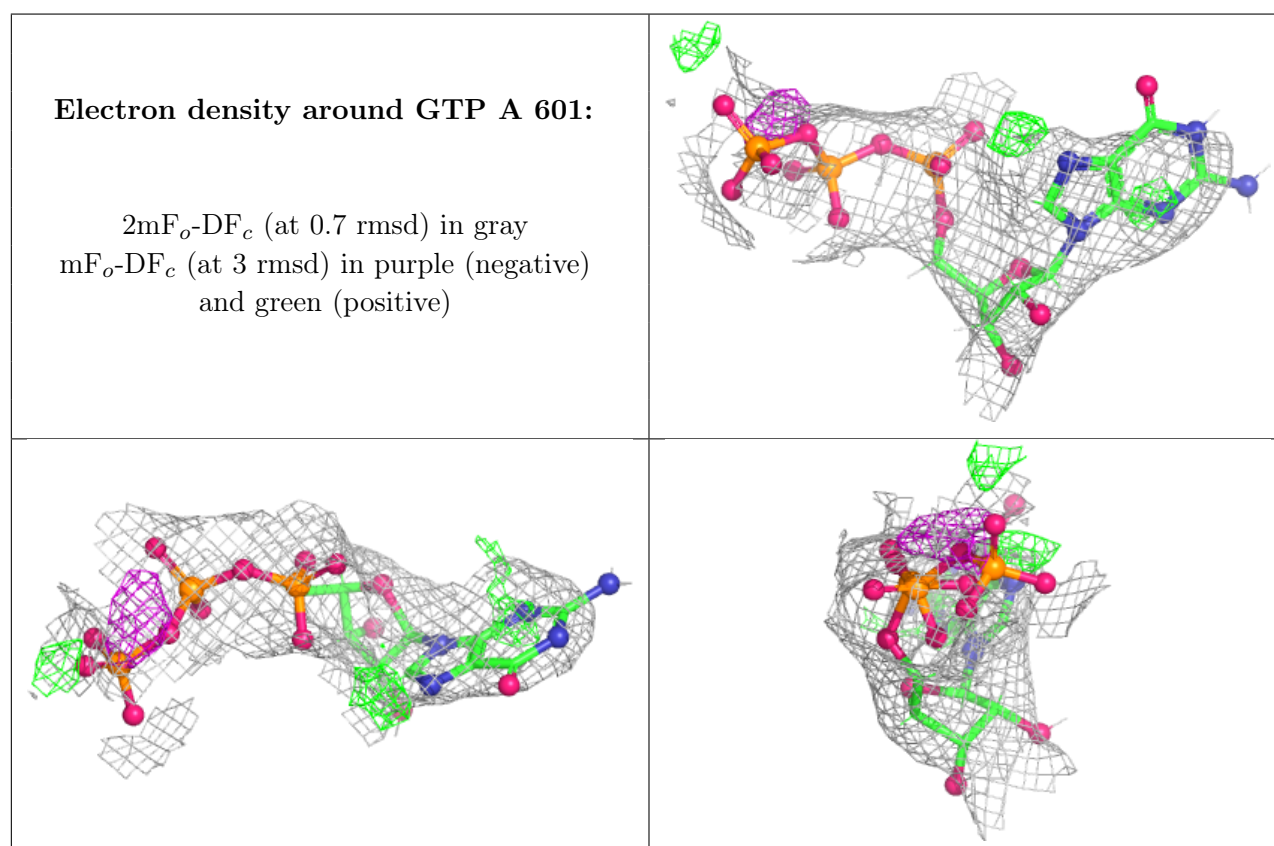
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	B	616	5/5	0.46	0.17	149,149,151,151	0
3	SO4	A	610	5/5	0.50	0.15	148,149,150,151	0
3	SO4	B	608	5/5	0.58	0.16	142,144,145,146	0
3	SO4	B	615	5/5	0.66	0.27	164,165,166,167	0
3	SO4	B	606	5/5	0.66	0.18	165,167,168,168	0
3	SO4	A	606	5/5	0.67	0.19	145,147,148,149	0
3	SO4	A	611	5/5	0.69	0.11	151,152,153,153	0
3	SO4	A	608	5/5	0.73	0.18	156,159,159,160	0
3	SO4	B	619	5/5	0.73	0.17	129,130,133,134	0
3	SO4	A	613	5/5	0.74	0.15	144,147,147,148	0
3	SO4	A	609	5/5	0.75	0.22	156,156,158,159	0
2	GTP	A	601	32/32	0.76	0.17	117,136,161,169	0
3	SO4	B	612	5/5	0.78	0.29	136,139,139,140	0
3	SO4	B	607	5/5	0.78	0.24	138,138,140,141	0
3	SO4	B	611	5/5	0.79	0.20	176,177,178,179	0
3	SO4	A	612	5/5	0.80	0.11	154,154,154,155	0
3	SO4	B	614	5/5	0.81	0.19	130,130,133,136	0
3	SO4	B	610	5/5	0.81	0.23	148,150,151,152	0
3	SO4	B	617	5/5	0.82	0.17	121,124,126,127	0
3	SO4	B	609	5/5	0.84	0.17	154,155,155,156	0
3	SO4	B	605	5/5	0.85	0.23	131,133,136,136	0
3	SO4	A	605	5/5	0.86	0.23	150,150,151,153	0
2	GTP	A	602	32/32	0.86	0.17	85,99,128,137	0
2	GTP	B	601	32/32	0.86	0.14	108,119,141,145	0
3	SO4	B	604	5/5	0.87	0.25	125,127,128,129	0
3	SO4	B	618	5/5	0.89	0.13	137,138,139,141	0
3	SO4	B	613	5/5	0.89	0.16	99,101,104,108	0

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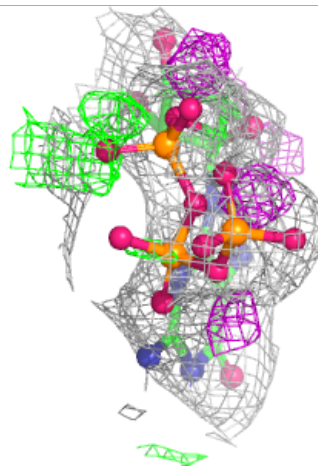
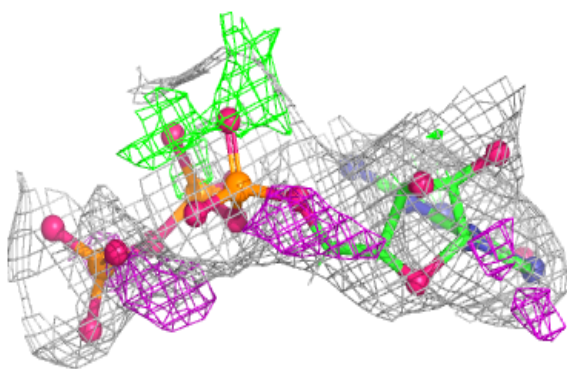
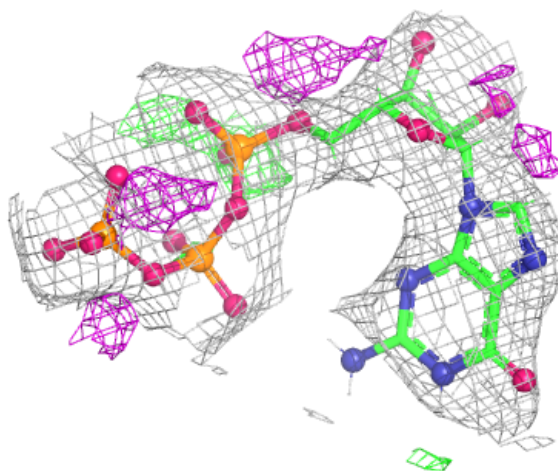
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GTP	B	602	32/32	0.90	0.11	51,74,118,122	0
3	SO4	A	607	5/5	0.90	0.13	137,137,138,138	0
2	GTP	A	603	32/32	0.91	0.12	80,94,117,125	0
2	GTP	B	603	32/32	0.93	0.11	56,72,91,105	0
3	SO4	A	604	5/5	0.95	0.15	131,132,135,136	0

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.



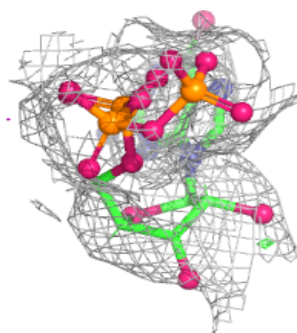
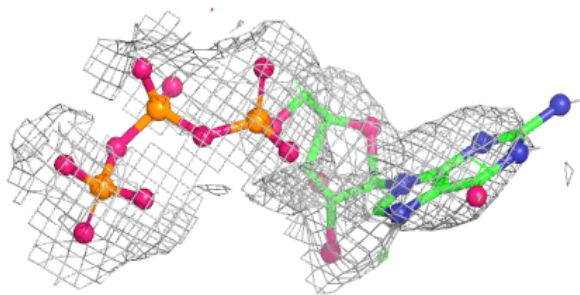
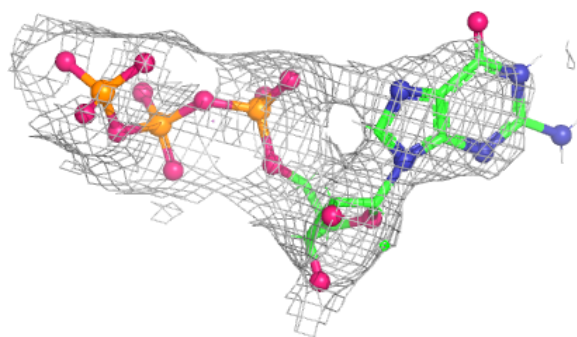
Electron density around GTP A 602:

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



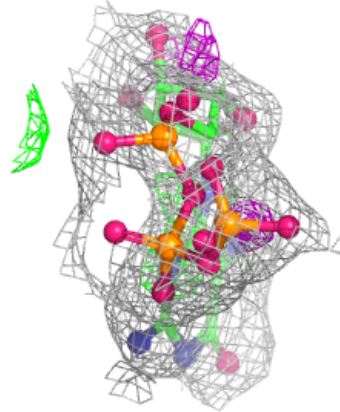
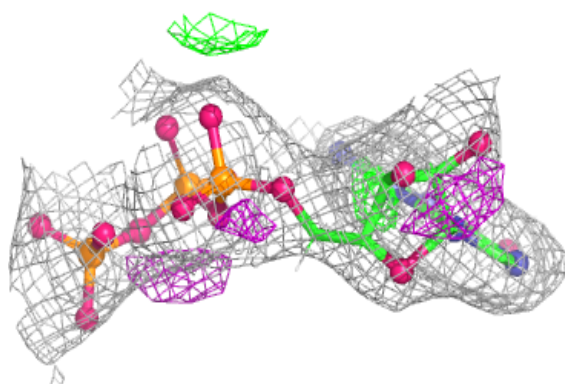
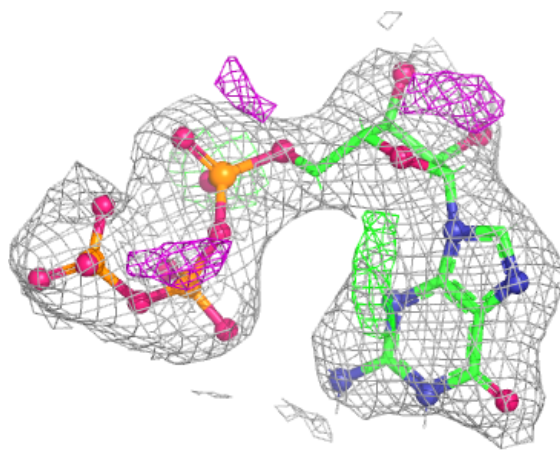
Electron density around GTP B 601:

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



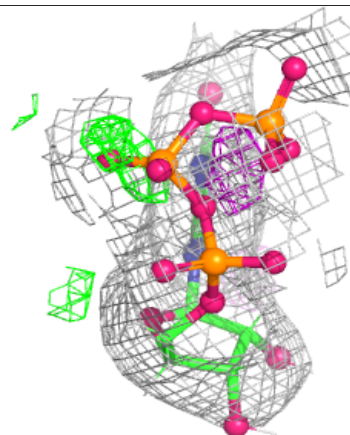
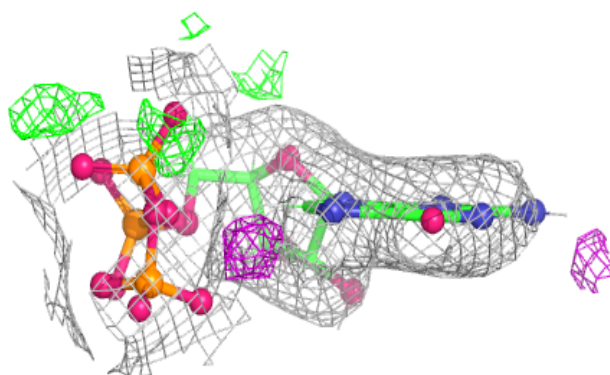
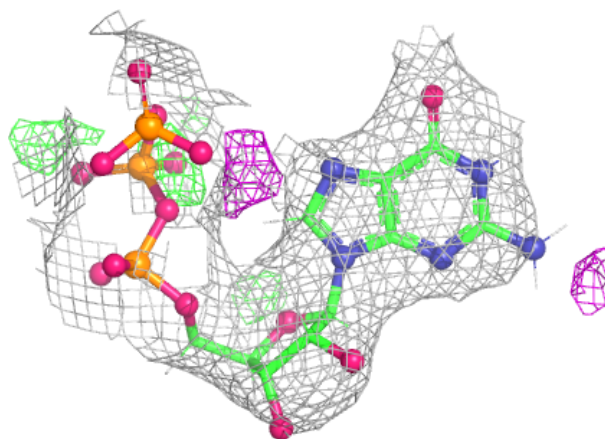
Electron density around GTP B 602:

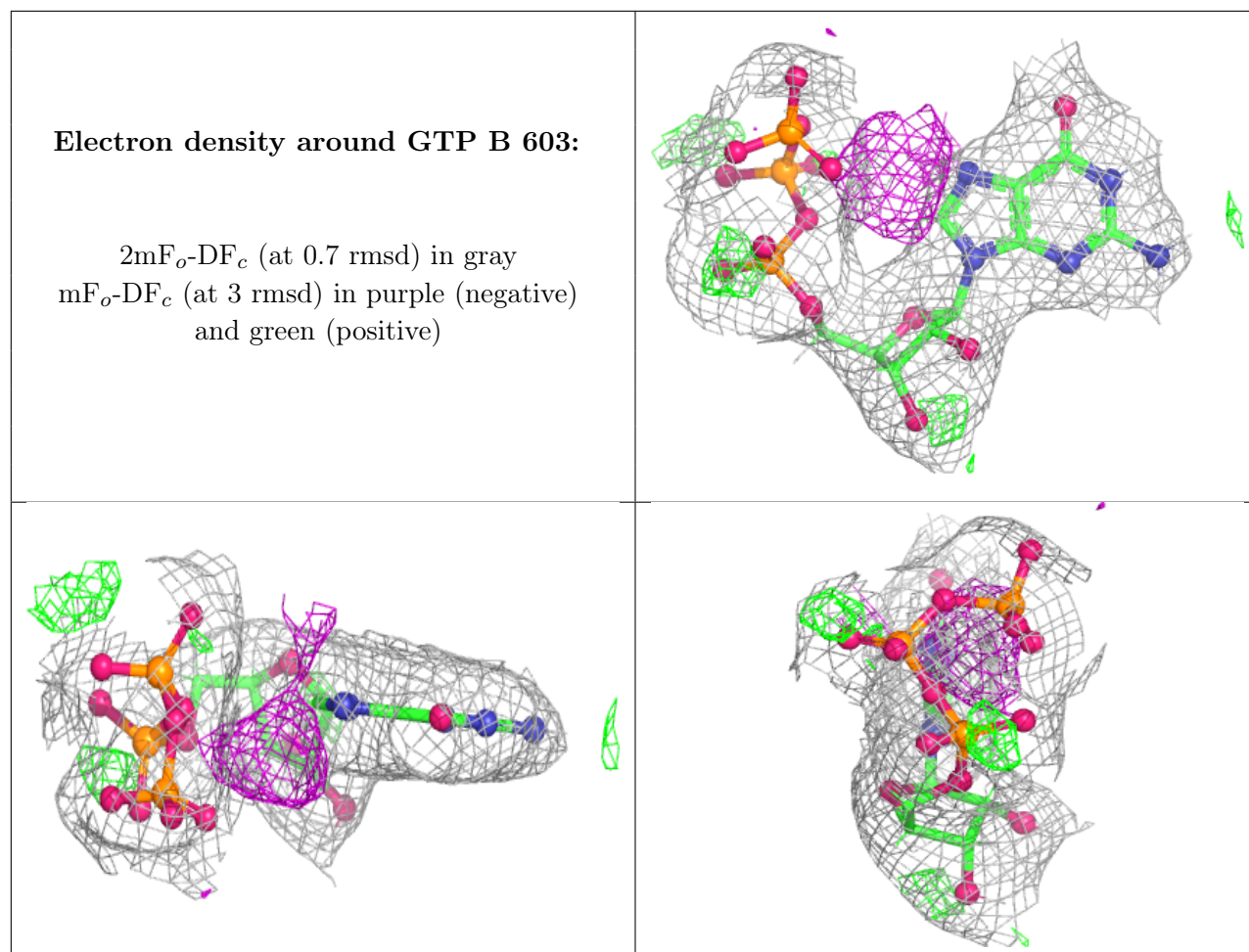
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.