Full wwPDB X-ray Structure Validation Report (i)

Nov 13, 2023 – 12:19 PM JST

PDB ID	:	5X6Z
Title	:	Crystal structure of Rice Dwarf Virus P5 in complex with GTP and GDP
Authors	:	Nakamichi, Y.; Higashiura, A.; Nakagawa, A.
Deposited on	:	2017-02-23
Resolution	:	2.10 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 (i) 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 (i)) were used in the production of this report:

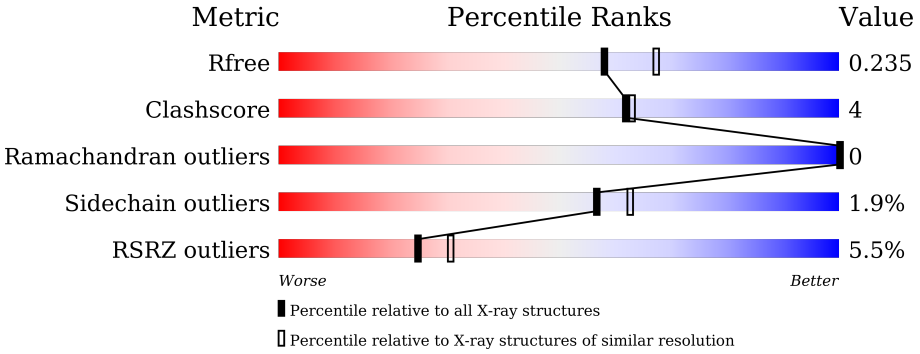
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	804	3% 87% 10% •
1	B	804	6% 83% 13% • •
1	C	804	3% 88% 8% •
1	D	804	10% 84% 14% • •

2 Entry composition (i)

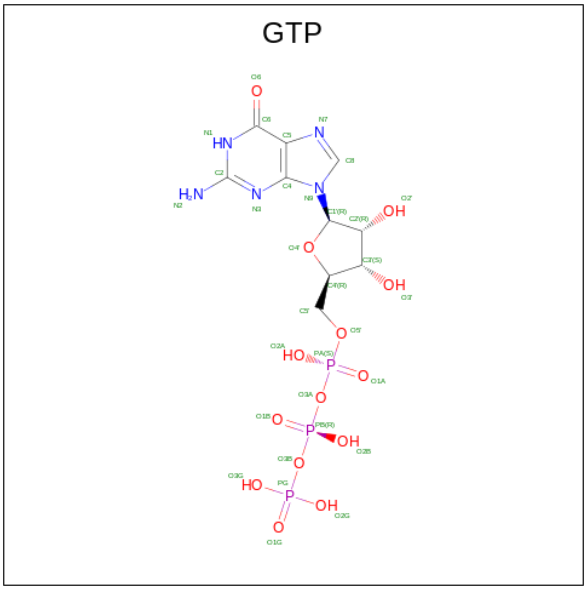
There are 4 unique types of molecules in this entry. The entry contains 26421 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called mRNA capping enzyme P5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	777	6171	3975	1022	1137	37	0	0	0
1	A	784	6233	4013	1033	1149	38	0	0	0
1	D	791	6297	4053	1047	1158	39	0	1	0
1	B	776	6180	3978	1027	1137	38	0	2	0

- 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
			Total	C	N	O	P		
2	C	1	32	10	5	14	3	0	0
2	A	1	32	10	5	14	3	0	0

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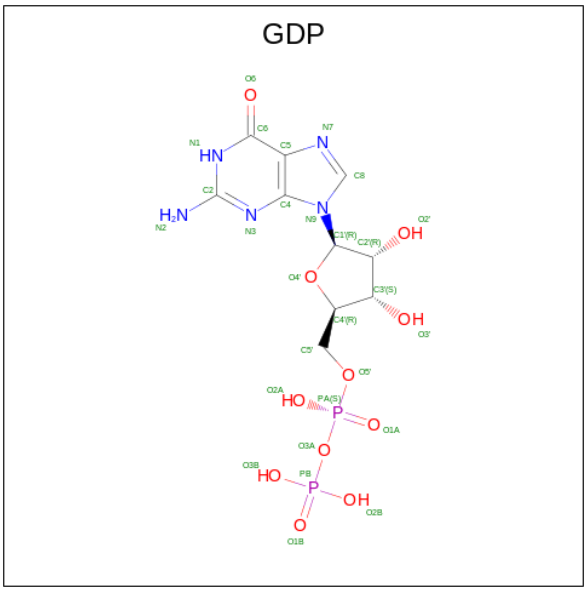
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	D	1	32	10	5	14	3	0	0
			Total	C	N	O	P		
2	B	1	32	10	5	14	3	0	0

- 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
			Total	C	N	O	P		
3	C	1	28	10	5	11	2	0	0
			Total	C	N	O	P		
3	A	1	28	10	5	11	2	0	0
			Total	C	N	O	P		
3	D	1	28	10	5	11	2	0	0
			Total	C	N	O	P		
3	B	1	28	10	5	11	2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	C	330	330	330	0	0
			Total	O		
4	A	395	395	395	0	0
			Total	O		
4	D	320	320	320	0	0

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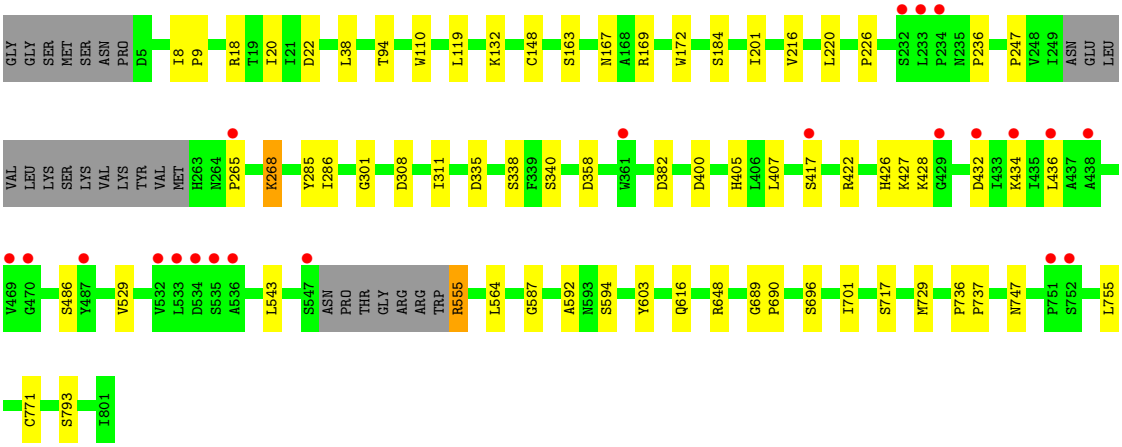
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	B	255	255	255	0	0

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.

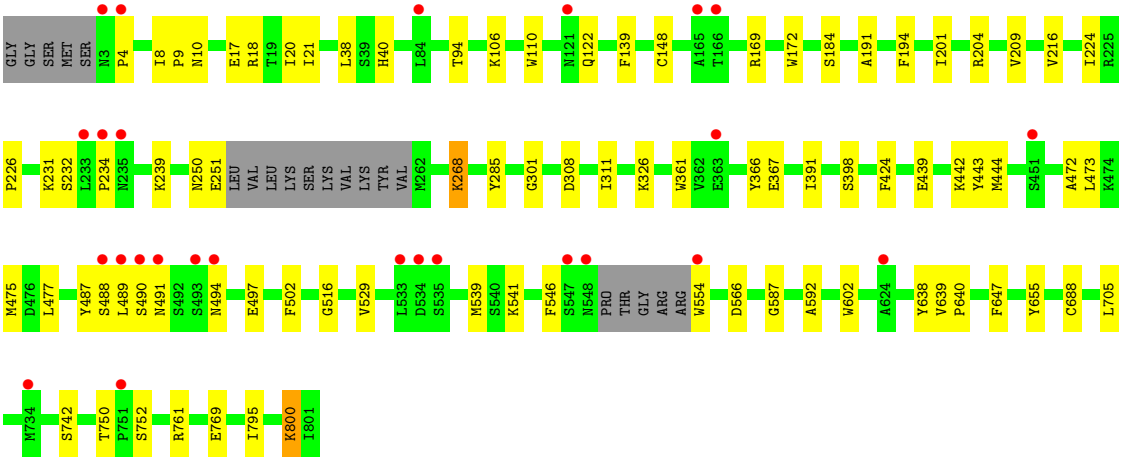
• Molecule 1: mRNA capping enzyme P5

Chain C:



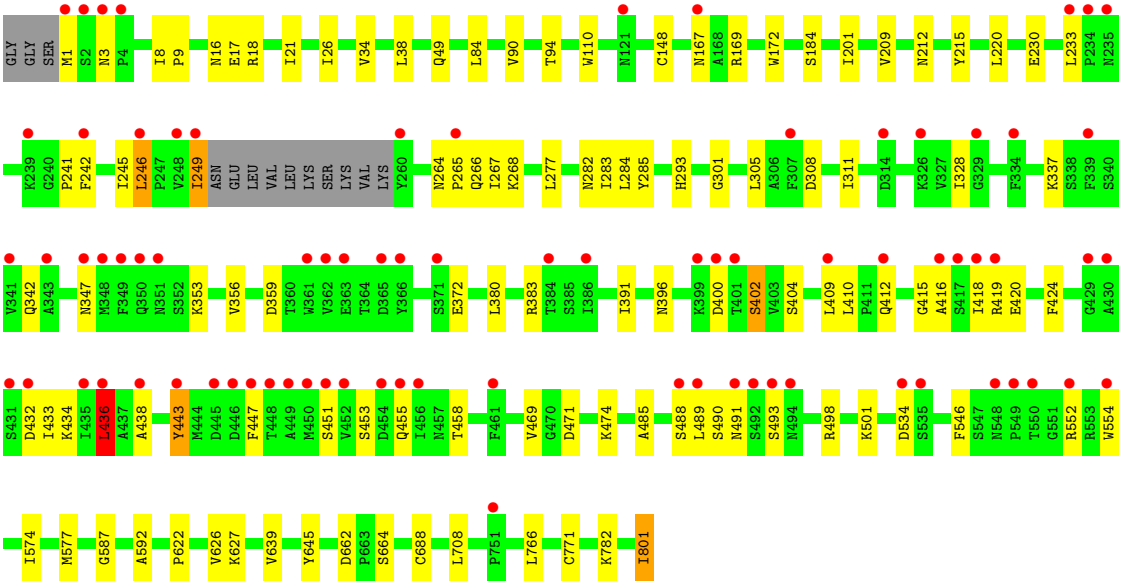
• Molecule 1: mRNA capping enzyme P5

Chain A:



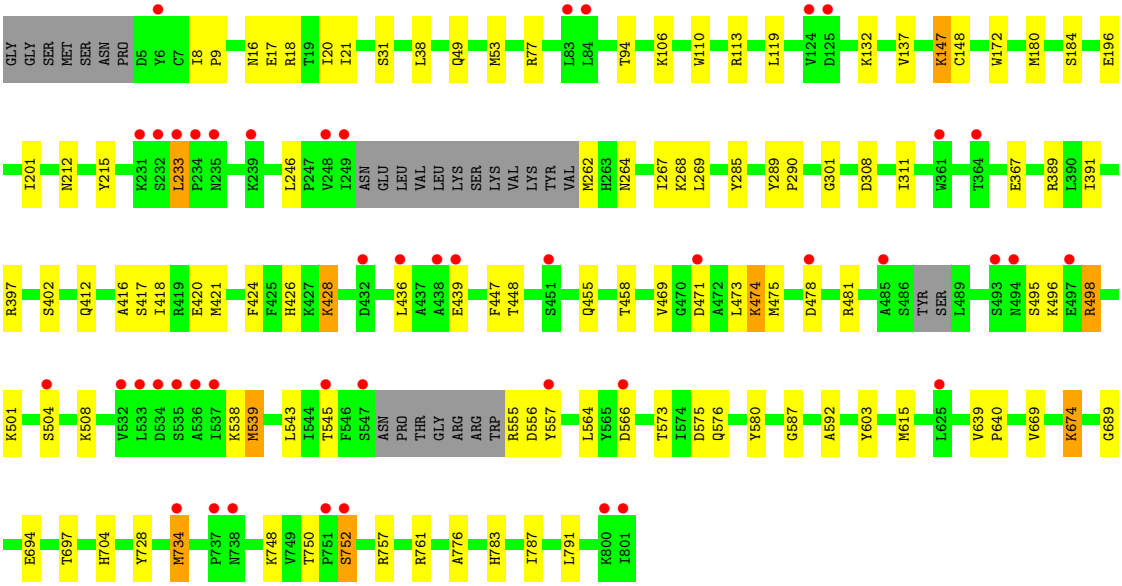
• Molecule 1: mRNA capping enzyme P5

Chain D:



- Molecule 1: mRNA capping enzyme P5

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	77.39Å 83.45Å 141.98Å 103.10° 101.98° 95.69°	Depositor
Resolution (Å)	37.66 – 2.10 37.66 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.5 (37.66-2.10) 95.5 (37.66-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.38 (at 2.10Å)	Xtriage
Refinement program	PHENIX (dev_2614: ???)	Depositor
R, R_{free}	0.184 , 0.235 0.184 , 0.235	Depositor DCC
R_{free} test set	9091 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	23.1	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 51.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	26421	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, 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	0.42	0/6384	0.53	0/8664
1	B	0.38	0/6326	0.51	0/8580
1	C	0.42	1/6319 (0.0%)	0.54	1/8574 (0.0%)
1	D	0.45	2/6451 (0.0%)	0.55	3/8756 (0.0%)
All	All	0.42	3/25480 (0.0%)	0.53	4/34574 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	443	TYR	CD1-CE1	-8.00	1.27	1.39
1	C	771	CYS	CB-SG	-5.09	1.73	1.81
1	D	771	CYS	CB-SG	-5.05	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	436	LEU	CA-CB-CG	7.34	132.19	115.30
1	D	246	LEU	CB-CG-CD1	-6.54	99.89	111.00
1	D	249	ILE	CG1-CB-CG2	-6.04	98.12	111.40
1	C	771	CYS	CA-CB-SG	-5.67	103.79	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	6233	0	6219	46	0
1	B	6180	0	6180	66	0
1	C	6171	0	6169	40	0
1	D	6297	0	6291	76	0
2	A	32	0	12	0	0
2	B	32	0	12	0	0
2	C	32	0	12	3	0
2	D	32	0	12	2	0
3	A	28	0	12	0	0
3	B	28	0	12	1	0
3	C	28	0	12	0	0
3	D	28	0	12	0	0
4	A	395	0	0	0	0
4	B	255	0	0	5	0
4	C	330	0	0	2	0
4	D	320	0	0	2	0
All	All	26421	0	24955	221	0

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 4.

All (221) 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:C:747:ASN:HB3	2:C:901:GTP:HN22	1.37	0.89
1:B:233:LEU:HD23	1:B:469:VAL:HG11	1.55	0.88
1:C:434:LYS:HE2	1:C:436:LEU:HD11	1.61	0.82
1:D:416:ALA:HA	1:D:455:GLN:HE22	1.51	0.76
1:A:18:ARG:HH12	1:B:21:ILE:HB	1.52	0.74
1:C:543:LEU:HD11	1:C:555:ARG:NH1	2.02	0.74
1:C:747:ASN:HB3	2:C:901:GTP:N2	2.03	0.74
1:B:538:LYS:HE3	1:B:539:MET:H	1.52	0.73
1:B:418:ILE:HG22	1:B:420:GLU:H	1.56	0.70
1:B:543:LEU:HD12	1:B:557:TYR:HE1	1.57	0.70
1:A:494:ASN:HB3	1:A:497:GLU:HB3	1.72	0.69
1:A:688:CYS:O	1:A:761:ARG:NH2	2.25	0.69
1:C:201:ILE:HG21	1:C:301:GLY:HA3	1.76	0.67
1:B:669:VAL:HG21	1:B:674:LYS:HD2	1.78	0.66
1:D:249:ILE:CD1	1:D:443:TYR:HE1	2.07	0.66
1:C:265:PRO:O	1:C:268:LYS:NZ	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:LEU:HD12	1:D:305:LEU:HD12	1.77	0.65
1:C:616:GLN:OE1	2:C:901:GTP:N1	2.25	0.65
1:D:418:ILE:HG12	1:D:419:ARG:H	1.61	0.65
1:B:264:ASN:HB3	1:B:267:ILE:HB	1.79	0.65
1:D:266:GLN:HG2	1:D:293:HIS:HB3	1.79	0.64
1:C:543:LEU:HD11	1:C:555:ARG:CZ	2.28	0.63
1:B:697:THR:HG21	4:B:1067:HOH:O	1.99	0.63
1:A:231:LYS:HE3	1:A:491:ASN:HB2	1.81	0.62
1:C:308:ASP:HB3	1:C:311:ILE:HG13	1.80	0.62
1:D:308:ASP:HB3	1:D:311:ILE:HG13	1.81	0.62
2:D:901:GTP:N3	2:D:901:GTP:H2'	2.14	0.61
1:D:249:ILE:CD1	1:D:443:TYR:CE1	2.84	0.60
1:D:249:ILE:HD13	1:D:443:TYR:CE1	2.36	0.60
1:A:473:LEU:HD11	1:A:490:SER:HB2	1.83	0.60
1:B:545:THR:HA	1:B:555:ARG:HD3	1.83	0.60
1:B:49:GLN:HB3	1:B:53:MET:HE2	1.85	0.59
1:C:20:ILE:HG21	1:C:529:VAL:HG11	1.83	0.59
1:D:201:ILE:HG21	1:D:301:GLY:HA3	1.84	0.59
1:D:16:ASN:HA	1:D:782:LYS:HE3	1.85	0.59
1:C:172:TRP:CZ2	1:C:592:ALA:HB2	2.37	0.58
1:D:245:ILE:HA	1:D:409:LEU:H	1.68	0.58
1:D:266:GLN:CG	1:D:293:HIS:HB3	2.32	0.58
1:D:209:VAL:HG12	1:D:488:SER:HB2	1.85	0.58
1:D:485:ALA:HB1	1:D:489:LEU:HB2	1.85	0.58
1:B:428:LYS:H	1:B:428:LYS:HD2	1.67	0.58
1:D:230:GLU:O	1:D:469:VAL:HA	2.04	0.57
1:D:284:LEU:HB3	1:D:356:VAL:HG22	1.86	0.57
1:B:184:SER:OG	1:B:587:GLY:HA3	2.05	0.57
1:B:436:LEU:HB2	1:B:439:GLU:HG3	1.86	0.57
1:B:212:ASN:HB3	1:B:215:TYR:HD2	1.70	0.57
1:D:451:SER:O	1:D:455:GLN:HG3	2.04	0.56
1:B:416:ALA:O	1:B:455:GLN:NE2	2.33	0.56
1:D:447:PHE:HE2	1:D:458:THR:HG21	1.70	0.56
1:D:337:LYS:NZ	1:D:372:GLU:OE2	2.36	0.56
1:B:475:MET:SD	1:B:481:ARG:NH2	2.78	0.56
1:D:400:ASP:OD2	1:D:436:LEU:HA	2.06	0.56
1:D:416:ALA:HA	1:D:455:GLN:NE2	2.19	0.55
1:B:17:GLU:H	1:B:17:GLU:CD	2.10	0.55
1:B:119:LEU:HD11	1:B:132:LYS:HD2	1.88	0.55
1:D:172:TRP:CZ2	1:D:592:ALA:HB2	2.42	0.54
1:A:239:LYS:NZ	1:A:439:GLU:OE2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:ARG:HG2	4:B:1083:HOH:O	2.06	0.54
1:D:284:LEU:CD1	1:D:305:LEU:HD12	2.37	0.54
1:B:9:PRO:HB3	1:B:639:VAL:HG22	1.90	0.54
1:B:106:LYS:HD2	1:B:110:TRP:CH2	2.44	0.53
1:A:18:ARG:HH12	1:B:21:ILE:CB	2.22	0.53
1:A:367:GLU:OE2	1:A:398:SER:OG	2.21	0.53
1:A:191:ALA:HA	1:A:224:ILE:HD11	1.91	0.53
1:C:382:ASP:OD2	1:C:405:HIS:NE2	2.42	0.52
1:C:38:LEU:O	1:C:94:THR:HA	2.10	0.52
1:C:335:ASP:OD2	1:C:338:SER:OG	2.27	0.52
1:C:426:HIS:CE1	1:C:428:LYS:HG2	2.44	0.52
1:D:418:ILE:HG12	1:D:419:ARG:N	2.25	0.52
1:D:305:LEU:HD23	1:D:328:ILE:HB	1.92	0.51
1:A:184:SER:OG	1:A:587:GLY:HA3	2.09	0.51
1:A:201:ILE:HG21	1:A:301:GLY:HA3	1.91	0.51
1:B:417:SER:HA	1:B:448:THR:HG22	1.93	0.51
1:B:504:SER:O	1:B:508:LYS:HG3	2.11	0.51
1:C:18:ARG:HG2	1:D:18:ARG:CZ	2.40	0.51
1:C:110:TRP:CD1	1:C:148:CYS:HA	2.46	0.51
1:C:119:LEU:HD11	1:C:132:LYS:HD2	1.93	0.51
1:D:471:ASP:HB3	1:D:474:LYS:HG3	1.93	0.50
1:B:172:TRP:CZ2	1:B:592:ALA:HB2	2.45	0.50
1:D:9:PRO:HB3	1:D:639:VAL:HG22	1.92	0.50
1:B:776:ALA:HB2	1:B:783:HIS:CE1	2.46	0.50
1:A:472:ALA:O	1:A:475:MET:HG2	2.12	0.50
1:D:246:LEU:HD11	1:D:443:TYR:CG	2.47	0.49
1:C:648:ARG:HG3	1:C:701:ILE:HD11	1.93	0.49
1:D:241:PRO:HB2	1:D:242:PHE:HD1	1.77	0.49
1:B:268:LYS:HG2	1:B:269:LEU:HD12	1.94	0.49
1:B:308:ASP:HB3	1:B:311:ILE:HG13	1.94	0.49
1:D:34:VAL:HB	1:D:90:VAL:HG22	1.94	0.49
1:B:615:MET:HE1	1:B:728:TYR:HE2	1.77	0.49
1:D:664:SER:HB3	1:B:734:MET:SD	2.53	0.48
1:B:389:ARG:O	1:B:426:HIS:ND1	2.46	0.48
1:B:689:GLY:O	1:B:761:ARG:NH2	2.41	0.48
1:D:412:GLN:CD	1:D:412:GLN:H	2.16	0.48
1:D:8:ILE:HA	1:D:9:PRO:C	2.34	0.48
1:A:705:LEU:HD11	1:A:795:ILE:HD13	1.94	0.48
1:B:694:GLU:O	1:B:697:THR:HG22	2.13	0.48
1:B:196:GLU:OE1	1:B:580:TYR:OH	2.23	0.48
1:A:172:TRP:CZ2	1:A:592:ALA:HB2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:436:LEU:HD22	1:D:438:ALA:H	1.78	0.48
1:A:139:PHE:HA	1:B:640:PRO:HB3	1.95	0.47
1:D:626:VAL:HG23	1:D:627:LYS:HG2	1.96	0.47
1:B:201:ILE:HG21	1:B:301:GLY:HA3	1.95	0.47
1:B:564:LEU:HD13	1:B:603:TYR:CZ	2.50	0.47
1:C:8:ILE:HA	1:C:9:PRO:C	2.33	0.47
1:D:249:ILE:HD11	1:D:443:TYR:CE1	2.49	0.47
1:A:750:THR:HG1	1:A:752:SER:HG	1.62	0.47
1:C:426:HIS:HE1	1:C:428:LYS:HG2	1.80	0.47
1:A:8:ILE:HA	1:A:9:PRO:C	2.35	0.47
1:A:18:ARG:CZ	1:B:18:ARG:HG2	2.44	0.47
1:D:110:TRP:CD1	1:D:148:CYS:HA	2.50	0.47
1:D:212:ASN:HB3	1:D:215:TYR:HD2	1.79	0.47
1:B:496:LYS:HG3	1:B:557:TYR:HD2	1.80	0.47
1:C:407:LEU:HB2	1:C:426:HIS:HB3	1.96	0.46
1:D:249:ILE:HD11	1:D:443:TYR:HE1	1.77	0.46
1:B:573:THR:OG1	1:B:576:GLN:HG3	2.15	0.46
1:B:787:ILE:O	1:B:791:LEU:HG	2.16	0.46
1:A:194:PHE:CG	1:A:204:ARG:HG2	2.50	0.46
1:B:38:LEU:O	1:B:94:THR:HA	2.14	0.46
1:C:236:PRO:HB2	1:C:247:PRO:HB3	1.96	0.46
1:B:501:LYS:N	1:B:501:LYS:HD2	2.31	0.46
1:B:8:ILE:HA	1:B:9:PRO:C	2.37	0.46
1:B:474:LYS:HD2	1:B:474:LYS:HA	1.81	0.46
1:B:748:LYS:HG2	4:B:1145:HOH:O	2.16	0.45
1:D:249:ILE:N	1:D:249:ILE:HD12	2.31	0.45
1:A:477:LEU:HD11	1:A:502:PHE:CE1	2.51	0.45
1:D:342:GLN:OE1	1:D:347:ASN:ND2	2.50	0.45
1:D:396:ASN:HB2	1:D:420:GLU:OE2	2.17	0.45
1:C:184:SER:OG	1:C:587:GLY:HA3	2.15	0.45
1:B:110:TRP:CD1	1:B:148:CYS:HA	2.51	0.45
1:D:49:GLN:HG2	4:D:1308:HOH:O	2.16	0.45
1:D:265:PRO:HG2	1:D:266:GLN:NE2	2.32	0.45
1:A:38:LEU:O	1:A:94:THR:HA	2.16	0.45
1:D:268:LYS:NZ	1:D:415:GLY:HA2	2.32	0.44
1:A:443:TYR:HD1	1:A:444:MET:HE2	1.82	0.44
1:D:264:ASN:HB2	1:D:267:ILE:HD13	2.00	0.44
1:D:282:ASN:HB2	1:D:353:LYS:O	2.16	0.44
1:C:747:ASN:CG	1:C:755:LEU:HD11	2.38	0.44
1:C:167:ASN:O	1:C:169:ARG:HG3	2.18	0.44
1:D:662:ASP:OD2	1:D:664:SER:OG	2.23	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:SER:OG	1:D:587:GLY:HA3	2.18	0.44
1:D:402:SER:HA	1:D:434:LYS:HA	2.00	0.44
1:B:391:ILE:O	1:B:424:PHE:HA	2.17	0.44
1:C:216:VAL:HA	1:C:226:PRO:HG3	2.00	0.44
1:A:308:ASP:HB3	1:A:311:ILE:HG13	1.99	0.44
1:B:471:ASP:OD1	1:B:498:ARG:NH2	2.51	0.44
1:C:564:LEU:HD13	1:C:603:TYR:CZ	2.53	0.43
1:D:38:LEU:O	1:D:94:THR:HA	2.18	0.43
1:D:645:TYR:OH	2:D:901:GTP:O2G	2.29	0.43
1:D:17:GLU:O	1:D:21:ILE:HG12	2.18	0.43
1:A:250:ASN:O	1:A:251:GLU:HB2	2.18	0.43
1:B:113:ARG:HD3	1:B:575:ASP:OD2	2.18	0.43
1:D:245:ILE:HD13	1:D:433:ILE:HD13	2.00	0.43
1:B:748:LYS:NZ	4:B:1002:HOH:O	2.31	0.43
1:C:729:MET:CE	1:C:755:LEU:HD23	2.48	0.43
1:D:3:ASN:OD1	1:D:3:ASN:N	2.52	0.43
1:C:22:ASP:OD2	1:D:18:ARG:NH2	2.37	0.43
1:A:110:TRP:CD1	1:A:148:CYS:HA	2.54	0.43
1:D:241:PRO:HB2	1:D:242:PHE:CD1	2.54	0.43
1:B:246:LEU:HD21	1:B:421:MET:HE1	2.01	0.43
1:A:9:PRO:HB3	1:A:639:VAL:HG22	2.01	0.43
1:D:491:ASN:HB3	1:D:493:SER:O	2.19	0.43
1:B:137:VAL:HG11	3:B:902:GDP:C2	2.54	0.43
1:B:575:ASP:HB3	4:B:1107:HOH:O	2.19	0.42
1:C:268:LYS:H	1:C:268:LYS:HD2	1.83	0.42
1:C:427:LYS:NZ	4:C:1028:HOH:O	2.52	0.42
1:A:268:LYS:H	1:A:268:LYS:HG2	1.58	0.42
1:A:638:TYR:O	1:A:640:PRO:HD3	2.19	0.42
1:B:184:SER:HG	1:B:587:GLY:HA3	1.83	0.42
1:B:31:SER:O	1:B:147:LYS:HE3	2.19	0.42
1:A:516:GLY:HA3	1:A:602:TRP:CE3	2.54	0.42
1:A:20:ILE:HG21	1:A:529:VAL:HG11	2.02	0.42
1:B:447:PHE:HE1	1:B:458:THR:HG21	1.85	0.42
1:C:696:SER:O	1:C:696:SER:OG	2.34	0.42
1:A:17:GLU:O	1:A:21:ILE:HG12	2.19	0.42
1:A:489:LEU:HD23	1:A:489:LEU:HA	1.71	0.42
1:D:220:LEU:HD13	1:D:220:LEU:HA	1.90	0.42
1:D:356:VAL:HB	1:D:391:ILE:HG12	2.00	0.42
1:D:380:LEU:O	1:D:383:ARG:HG2	2.19	0.42
1:A:9:PRO:HG2	1:A:647:PHE:CZ	2.55	0.42
1:B:750:THR:OG1	1:B:752:SER:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:ASN:O	1:D:169:ARG:HG3	2.20	0.42
1:C:422:ARG:HD2	4:C:1154:HOH:O	2.19	0.42
1:C:729:MET:SD	1:C:755:LEU:HD23	2.60	0.41
1:D:284:LEU:HD23	1:D:356:VAL:HG13	2.02	0.41
1:D:546:PHE:HB2	1:D:554:TRP:CE2	2.55	0.41
1:D:688:CYS:O	1:D:801:ILE:HG12	2.20	0.41
1:C:400:ASP:OD2	1:C:436:LEU:HD12	2.20	0.41
1:A:169:ARG:HG2	1:B:9:PRO:HD2	2.02	0.41
1:A:216:VAL:HA	1:A:226:PRO:HG3	2.03	0.41
1:D:574:ILE:HD13	1:D:577:MET:CE	2.50	0.41
1:A:391:ILE:O	1:A:424:PHE:HA	2.20	0.41
1:B:16:ASN:O	1:B:20:ILE:HG12	2.21	0.41
1:B:543:LEU:HD12	1:B:557:TYR:CE1	2.46	0.41
1:D:26:ILE:HG22	1:D:84:LEU:HD22	2.02	0.41
1:A:361:TRP:HB2	1:A:366:TYR:CZ	2.55	0.41
1:C:689:GLY:HA3	1:C:690:PRO:HA	1.95	0.41
1:A:4:PRO:O	1:A:10:ASN:ND2	2.52	0.41
1:A:232:SER:O	1:A:234:PRO:HD3	2.21	0.41
1:D:277:LEU:HD23	1:D:283:ILE:HG13	2.02	0.41
1:D:801:ILE:HD13	1:D:801:ILE:HA	1.74	0.41
1:B:262:MET:HE1	1:B:264:ASN:HD22	1.86	0.41
1:B:367:GLU:HG2	1:B:397:ARG:HD2	2.03	0.41
1:B:539:MET:HE2	1:B:539:MET:HB2	1.88	0.41
1:C:220:LEU:HD13	1:C:220:LEU:HA	1.93	0.41
1:C:286:ILE:HB	1:C:358:ASP:HA	2.02	0.41
1:D:622:PRO:HB2	1:D:626:VAL:HG13	2.04	0.41
1:C:736:PRO:HA	1:C:737:PRO:HD3	1.89	0.40
1:B:412:GLN:NE2	1:B:420:GLU:OE2	2.34	0.40
1:A:209:VAL:HG11	1:A:489:LEU:HD23	2.03	0.40
1:A:800:LYS:H	1:A:800:LYS:HG3	1.77	0.40
1:D:404:SER:HB2	4:D:1193:HOH:O	2.21	0.40
1:D:766:LEU:HD12	1:D:766:LEU:HA	1.91	0.40
1:A:487:TYR:HD2	1:A:488:SER:HB3	1.87	0.40
1:D:410:LEU:HD12	1:D:424:PHE:CE2	2.56	0.40
1:D:626:VAL:HG12	1:D:708:LEU:HG	2.04	0.40
1:B:289:TYR:HA	1:B:290:PRO:HA	1.90	0.40
1:A:40:HIS:NE2	1:A:122:GLN:O	2.52	0.40
1:A:106:LYS:HD2	1:A:110:TRP:CH2	2.57	0.40
1:A:546:PHE:HB2	1:A:554:TRP:CE2	2.56	0.40
1:A:655:TYR:CE1	1:A:769:GLU:HB3	2.56	0.40
1:D:501:LYS:HE2	1:D:501:LYS:HB2	1.83	0.40

There are no symmetry-related clashes.

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	778/804 (97%)	760 (98%)	18 (2%)	0	100	100
1	B	770/804 (96%)	748 (97%)	22 (3%)	0	100	100
1	C	771/804 (96%)	755 (98%)	16 (2%)	0	100	100
1	D	788/804 (98%)	764 (97%)	24 (3%)	0	100	100
All	All	3107/3216 (97%)	3027 (97%)	80 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	694/711 (98%)	685 (99%)	9 (1%)	69	75
1	B	688/711 (97%)	669 (97%)	19 (3%)	43	47
1	C	687/711 (97%)	676 (98%)	11 (2%)	62	69
1	D	701/711 (99%)	688 (98%)	13 (2%)	57	63
All	All	2770/2844 (97%)	2718 (98%)	52 (2%)	57	63

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	163	SER
1	C	268	LYS
1	C	285	TYR
1	C	340	SER
1	C	417	SER
1	C	432	ASP
1	C	486	SER
1	C	555	ARG
1	C	594	SER
1	C	717	SER
1	C	793	SER
1	A	268	LYS
1	A	285	TYR
1	A	326	LYS
1	A	442	LYS
1	A	539	MET
1	A	541	LYS
1	A	566	ASP
1	A	742	SER
1	A	800	LYS
1	D	1	MET
1	D	233	LEU
1	D	285	TYR
1	D	359	ASP
1	D	402	SER
1	D	432	ASP
1	D	436	LEU
1	D	453	SER
1	D	490	SER
1	D	498	ARG
1	D	534	ASP
1	D	552	ARG
1	D	801	ILE
1	B	147	LYS
1	B	180	MET
1	B	233	LEU
1	B	285	TYR
1	B	402	SER
1	B	428	LYS
1	B	473	LEU
1	B	474	LYS
1	B	478	ASP
1	B	495	SER

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Mol	Chain	Res	Type
1	B	498	ARG
1	B	539	MET
1	B	556	ASP
1	B	566	ASP
1	B	674	LYS
1	B	704	HIS
1	B	734	MET
1	B	752	SER
1	B	757	ARG

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

Mol	Chain	Res	Type
1	D	121	ASN
1	D	455	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	D	901	-	26,34,34	1.16	2 (7%)	32,54,54	1.77	7 (21%)
2	GTP	C	901	-	26,34,34	0.95	2 (7%)	32,54,54	1.51	6 (18%)
2	GTP	B	901	-	26,34,34	1.08	2 (7%)	32,54,54	1.45	6 (18%)
3	GDP	C	902	-	24,30,30	0.85	0	30,47,47	1.39	6 (20%)
3	GDP	A	902	-	24,30,30	0.87	0	30,47,47	1.32	5 (16%)
2	GTP	A	901	-	26,34,34	1.05	1 (3%)	32,54,54	1.38	6 (18%)
3	GDP	B	902	-	24,30,30	0.88	0	30,47,47	1.37	7 (23%)
3	GDP	D	902	-	24,30,30	0.83	0	30,47,47	1.43	5 (16%)

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	D	901	-	-	5/18/38/38	0/3/3/3
2	GTP	C	901	-	-	8/18/38/38	0/3/3/3
2	GTP	B	901	-	-	4/18/38/38	0/3/3/3
3	GDP	C	902	-	-	3/12/32/32	0/3/3/3
3	GDP	A	902	-	-	0/12/32/32	0/3/3/3
2	GTP	A	901	-	-	4/18/38/38	0/3/3/3
3	GDP	B	902	-	-	6/12/32/32	0/3/3/3
3	GDP	D	902	-	-	4/12/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	901	GTP	C5-C6	-4.25	1.38	1.47
2	B	901	GTP	C5-C6	-3.88	1.39	1.47
2	A	901	GTP	C5-C6	-3.80	1.39	1.47
2	C	901	GTP	C5-C6	-2.41	1.42	1.47
2	C	901	GTP	C2-N3	2.20	1.38	1.33
2	B	901	GTP	C2-N3	2.20	1.38	1.33
2	D	901	GTP	C2-N3	2.13	1.38	1.33

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	901	GTP	PB-O3B-PG	-4.16	118.55	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	901	GTP	C5-C6-N1	3.58	120.27	113.95
2	D	901	GTP	C3'-C2'-C1'	3.53	106.29	100.98
2	A	901	GTP	PB-O3B-PG	-3.38	121.22	132.83
2	B	901	GTP	C5-C6-N1	3.28	119.75	113.95
2	A	901	GTP	C5-C6-N1	3.26	119.70	113.95
2	B	901	GTP	C8-N7-C5	3.24	109.15	102.99
3	D	902	GDP	PA-O3A-PB	-3.23	121.75	132.83
2	C	901	GTP	C3'-C2'-C1'	3.19	105.78	100.98
2	D	901	GTP	C2-N1-C6	-3.17	119.27	125.10
2	D	901	GTP	O6-C6-C5	-3.12	118.28	124.37
3	C	902	GDP	C3'-C2'-C1'	3.08	105.62	100.98
3	A	902	GDP	PA-O3A-PB	-3.04	122.38	132.83
2	C	901	GTP	O6-C6-N1	-2.99	117.12	120.65
3	D	902	GDP	C3'-C2'-C1'	2.97	105.44	100.98
2	D	901	GTP	O5'-C5'-C4'	2.96	119.18	108.99
2	C	901	GTP	C8-N7-C5	2.96	108.62	102.99
2	B	901	GTP	C2-N1-C6	-2.91	119.74	125.10
2	C	901	GTP	C5-C6-N1	2.87	119.02	113.95
2	B	901	GTP	PB-O3B-PG	-2.84	123.08	132.83
3	B	902	GDP	O6-C6-C5	-2.83	118.84	124.37
3	D	902	GDP	O6-C6-C5	-2.78	118.94	124.37
2	D	901	GTP	C8-N7-C5	2.75	108.24	102.99
2	A	901	GTP	C8-N7-C5	2.75	108.22	102.99
2	C	901	GTP	PB-O3B-PG	-2.73	123.45	132.83
3	D	902	GDP	C5-C6-N1	2.73	118.78	113.95
3	B	902	GDP	C3'-C2'-C1'	2.72	105.07	100.98
2	A	901	GTP	C2-N1-C6	-2.62	120.27	125.10
2	C	901	GTP	C2-N1-C6	-2.59	120.33	125.10
3	A	902	GDP	C8-N7-C5	2.56	107.86	102.99
3	A	902	GDP	C5-C6-N1	2.55	118.45	113.95
3	C	902	GDP	PA-O3A-PB	-2.48	124.33	132.83
3	B	902	GDP	C5-C6-N1	2.44	118.26	113.95
3	D	902	GDP	C8-N7-C5	2.41	107.58	102.99
3	C	902	GDP	C5-C6-N1	2.38	118.15	113.95
3	C	902	GDP	C8-N7-C5	2.35	107.47	102.99
2	B	901	GTP	PA-O3A-PB	-2.34	124.78	132.83
3	A	902	GDP	O6-C6-C5	-2.32	119.84	124.37
3	B	902	GDP	O3B-PB-O3A	2.30	112.36	104.64
3	C	902	GDP	O6-C6-C5	-2.27	119.93	124.37
2	B	901	GTP	C3'-C2'-C1'	2.24	104.35	100.98
2	A	901	GTP	N2-C2-N1	2.22	121.43	116.71
3	B	902	GDP	C8-N7-C5	2.13	107.04	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	902	GDP	N2-C2-N1	2.11	121.22	116.71
3	B	902	GDP	PA-O3A-PB	-2.08	125.70	132.83
3	A	902	GDP	C3'-C2'-C1'	2.07	104.09	100.98
3	B	902	GDP	N2-C2-N1	2.05	121.09	116.71
2	A	901	GTP	C3'-C2'-C1'	2.03	104.03	100.98

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	901	GTP	PB-O3B-PG-O3G
2	C	901	GTP	PB-O3A-PA-O5'
2	C	901	GTP	C5'-O5'-PA-O1A
2	C	901	GTP	C5'-O5'-PA-O2A
2	D	901	GTP	C5'-O5'-PA-O3A
2	D	901	GTP	O4'-C4'-C5'-O5'
2	D	901	GTP	C3'-C4'-C5'-O5'
3	C	902	GDP	PA-O3A-PB-O2B
3	D	902	GDP	C5'-O5'-PA-O3A
3	B	902	GDP	PA-O3A-PB-O2B
3	B	902	GDP	PA-O3A-PB-O3B
3	B	902	GDP	C5'-O5'-PA-O3A
3	B	902	GDP	C5'-O5'-PA-O2A
2	B	901	GTP	PB-O3B-PG-O1G
2	B	901	GTP	PG-O3B-PB-O1B
2	C	901	GTP	C5'-O5'-PA-O3A
2	A	901	GTP	PA-O3A-PB-O1B
2	D	901	GTP	C5'-O5'-PA-O1A
2	D	901	GTP	C5'-O5'-PA-O2A
3	D	902	GDP	C5'-O5'-PA-O2A
3	B	902	GDP	C5'-O5'-PA-O1A
3	D	902	GDP	O4'-C4'-C5'-O5'
2	B	901	GTP	PA-O3A-PB-O2B
3	D	902	GDP	PB-O3A-PA-O1A
3	B	902	GDP	PA-O3A-PB-O1B
3	C	902	GDP	PA-O3A-PB-O3B
2	A	901	GTP	C5'-O5'-PA-O3A
2	C	901	GTP	PA-O3A-PB-O1B
2	C	901	GTP	PA-O3A-PB-O2B
2	A	901	GTP	PG-O3B-PB-O2B
2	B	901	GTP	PA-O3A-PB-O1B
2	A	901	GTP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	C	901	GTP	PB-O3B-PG-O1G
3	C	902	GDP	PA-O3A-PB-O1B

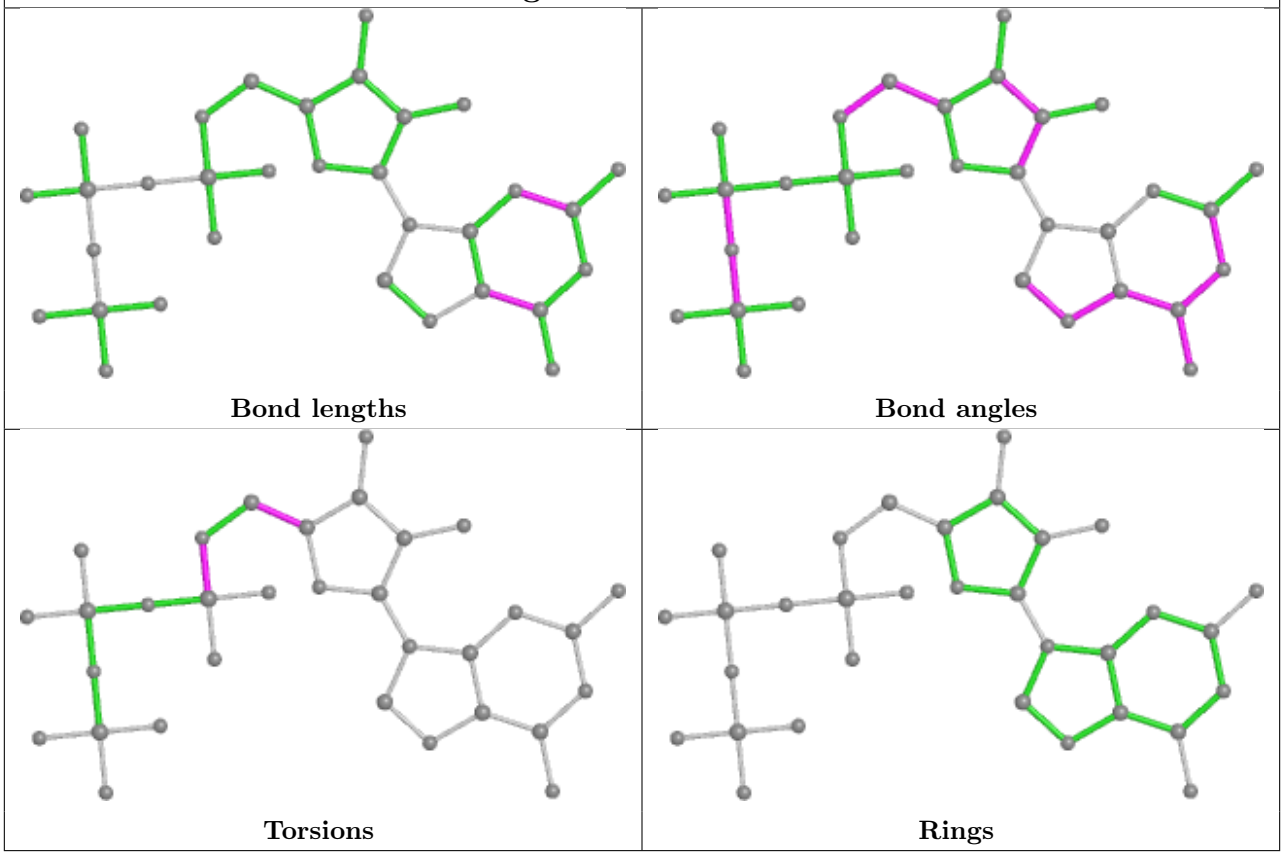
There are no ring outliers.

3 monomers are involved in 6 short contacts:

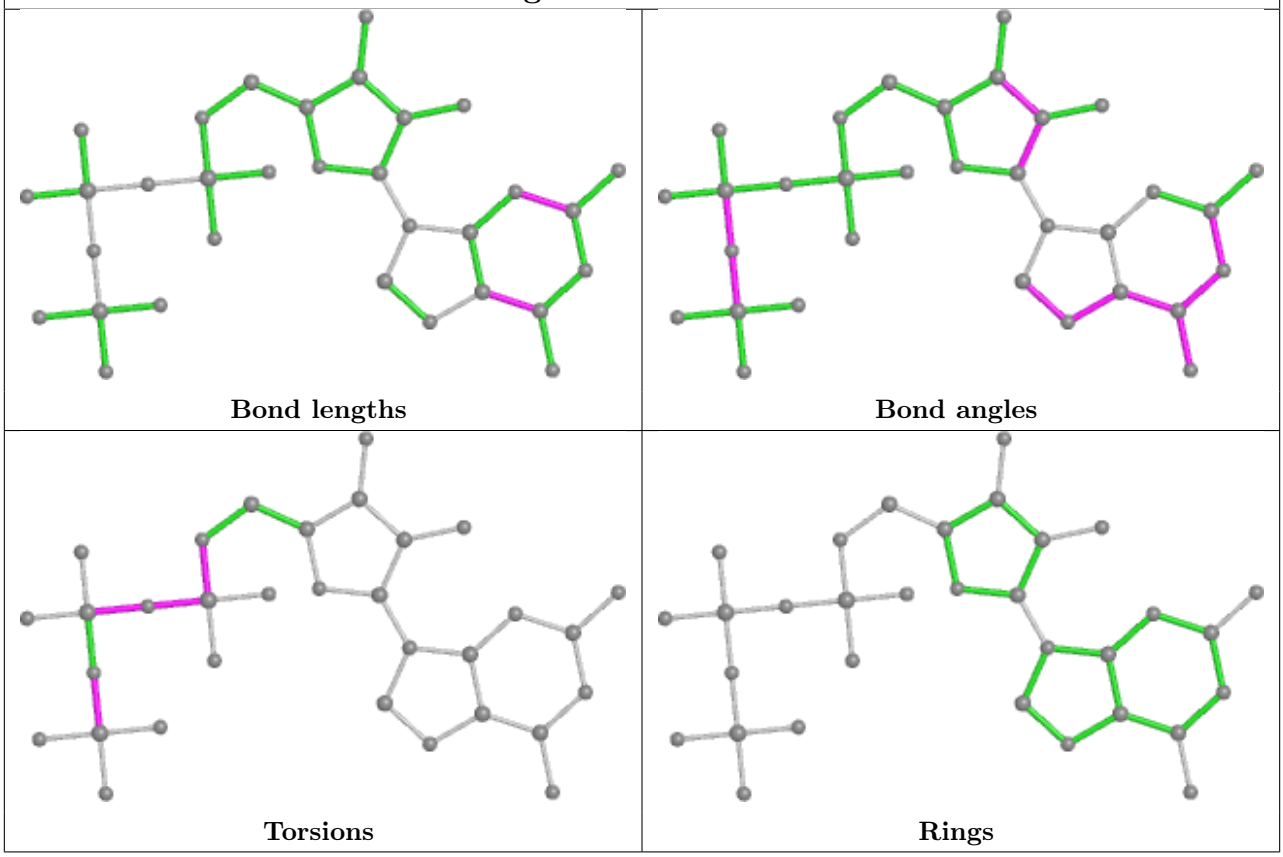
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	901	GTP	2	0
2	C	901	GTP	3	0
3	B	902	GDP	1	0

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 then 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.

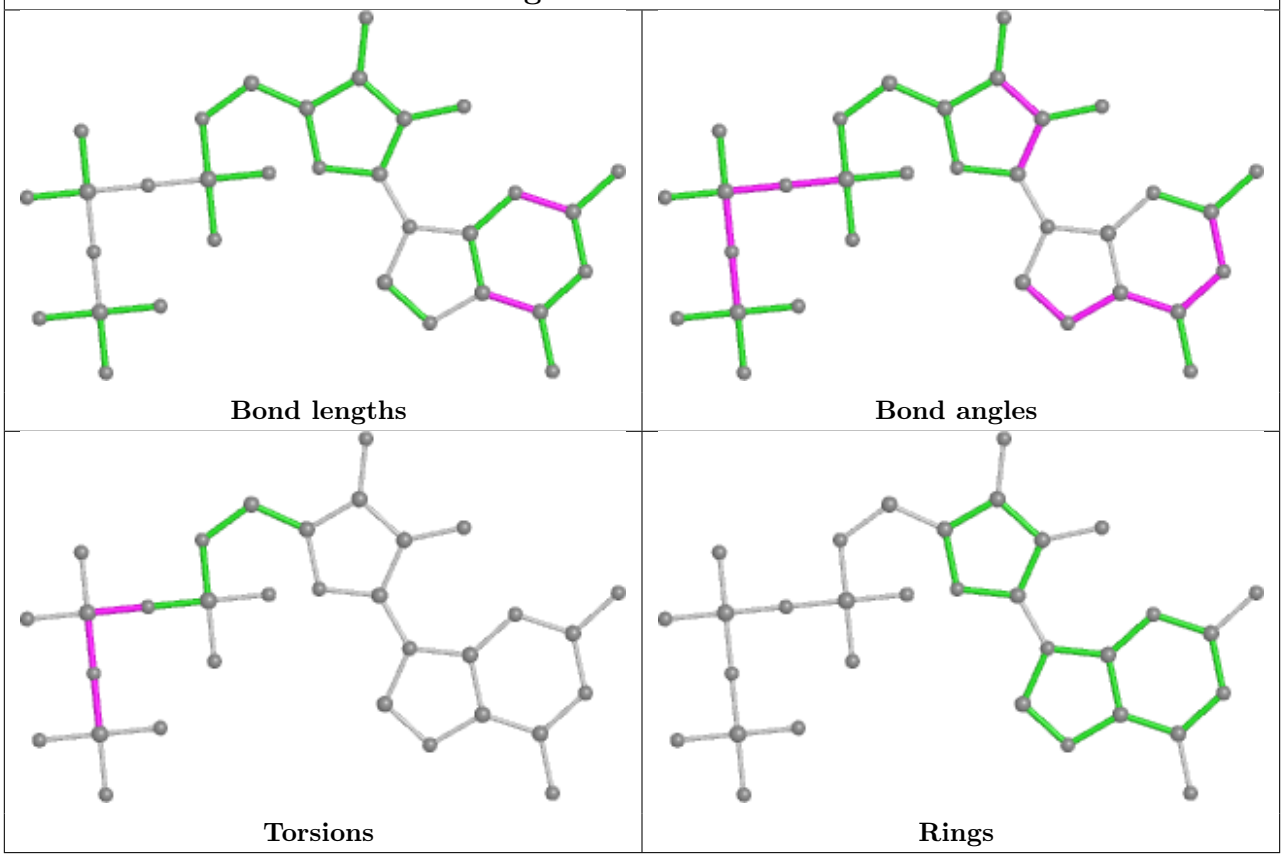
Ligand GTP D 901



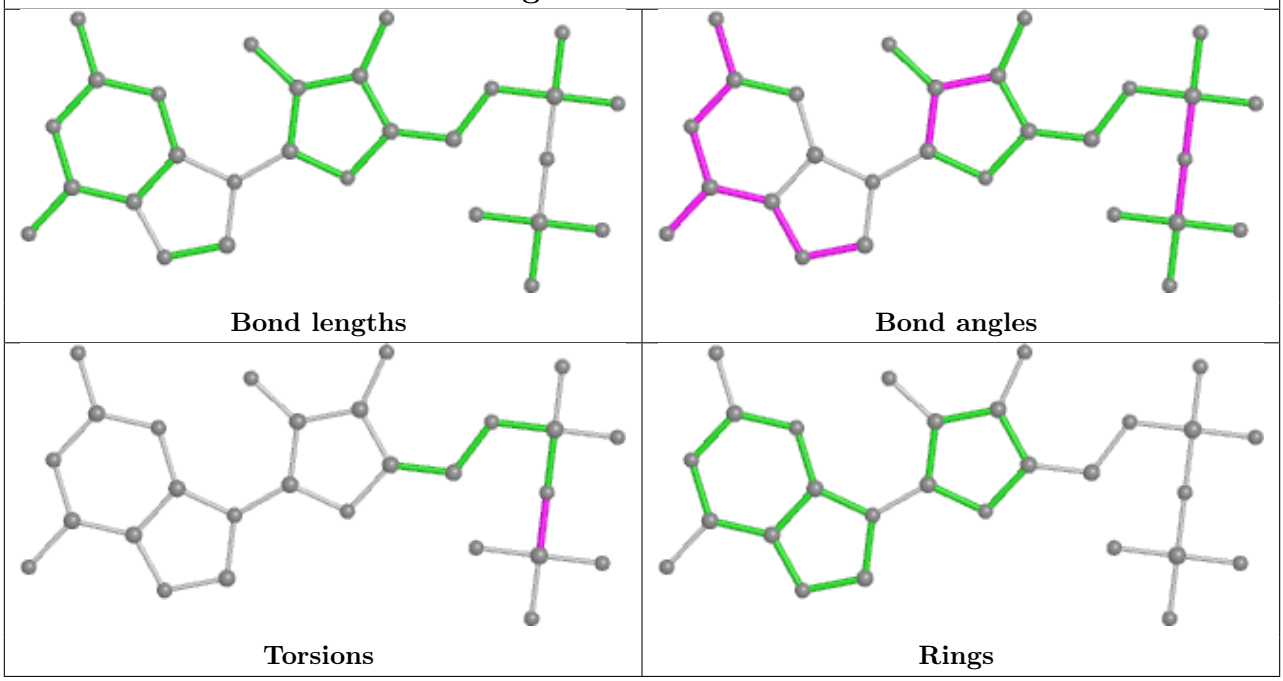
Ligand GTP C 901



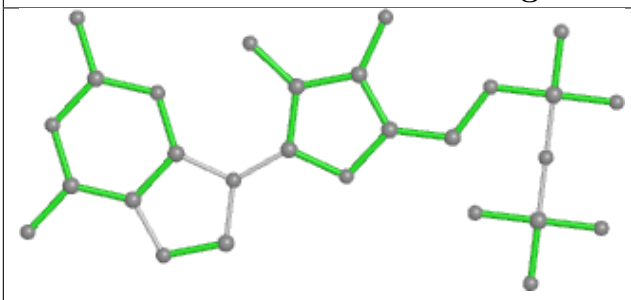
Ligand GTP B 901



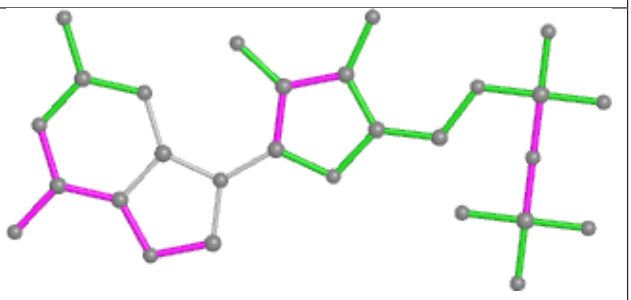
Ligand GDP C 902



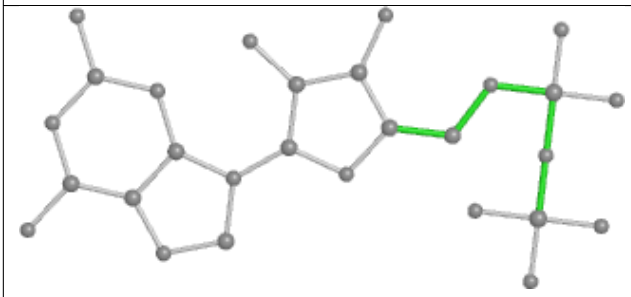
Ligand GDP A 902



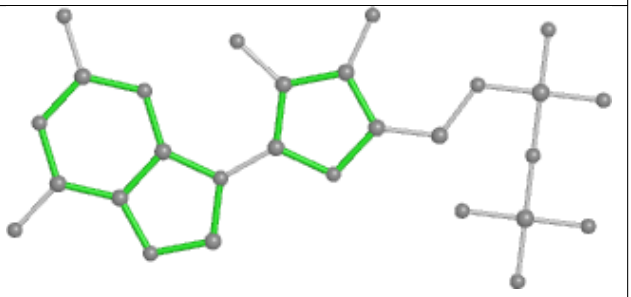
Bond lengths



Bond angles

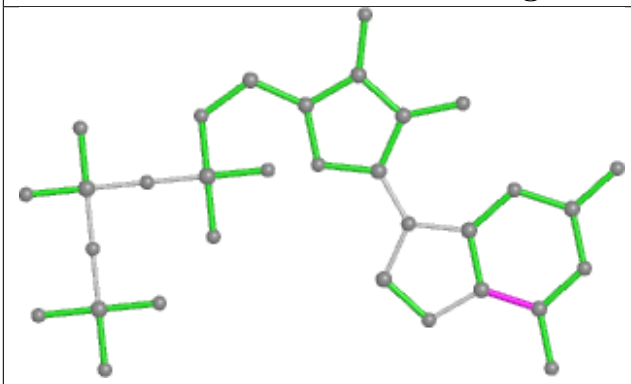


Torsions

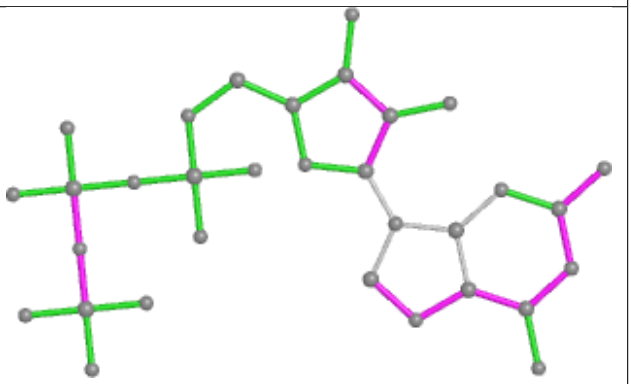


Rings

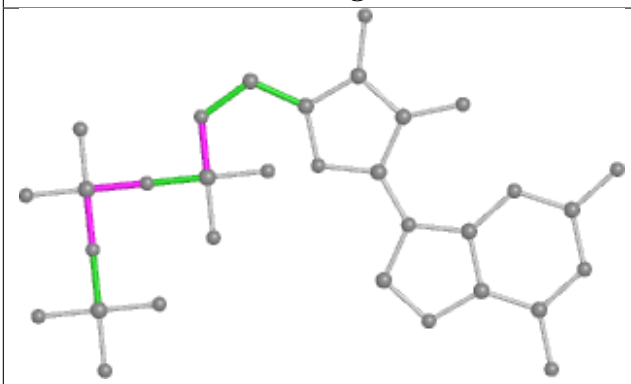
Ligand GTP A 901



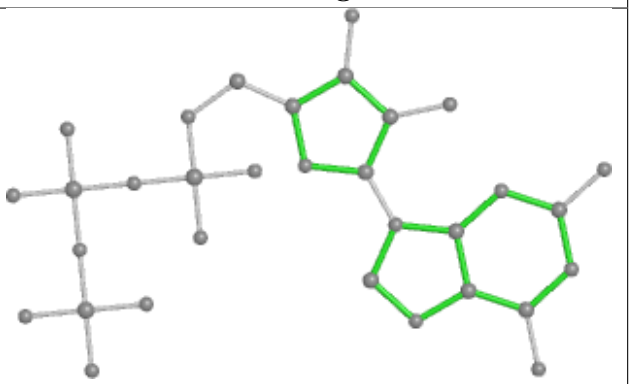
Bond lengths



Bond angles

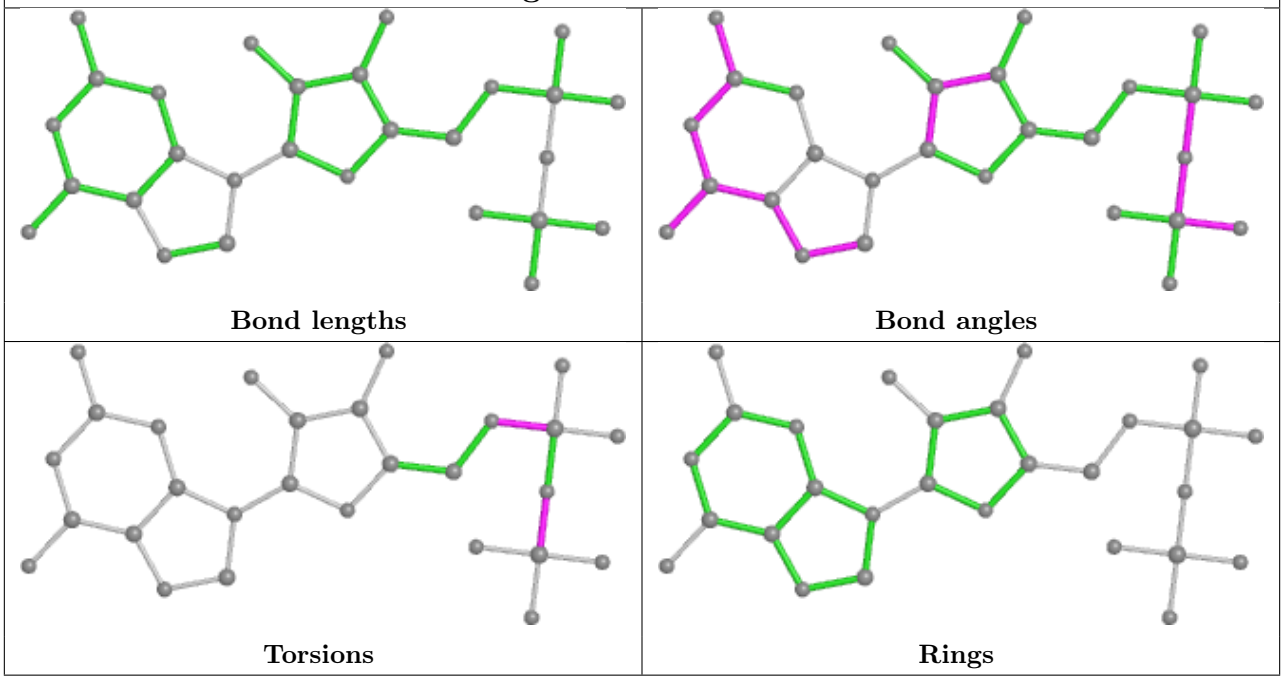


Torsions

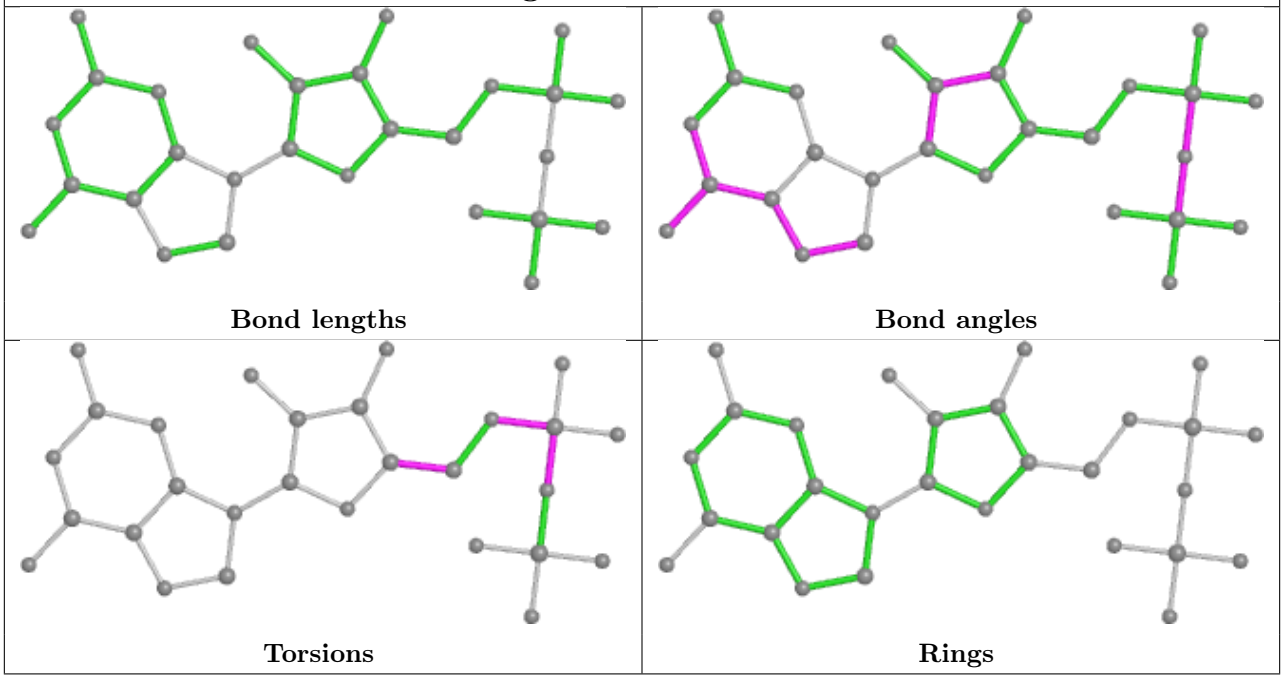


Rings

Ligand GDP B 902



Ligand GDP D 902



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	784/804 (97%)	-0.16	26 (3%) 46 53	11, 23, 47, 71	0
1	B	776/804 (96%)	0.18	45 (5%) 23 28	12, 30, 59, 83	0
1	C	777/804 (96%)	-0.04	22 (2%) 53 59	8, 26, 48, 72	0
1	D	791/804 (98%)	0.26	80 (10%) 7 9	8, 25, 70, 83	0
All	All	3128/3216 (97%)	0.06	173 (5%) 25 31	8, 26, 58, 83	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	535	SER	8.6
1	B	249	ILE	6.4
1	C	233	LEU	6.4
1	B	438	ALA	6.1
1	D	361	TRP	6.1
1	D	489	LEU	6.1
1	B	534	ASP	5.7
1	B	801	ILE	5.7
1	D	2	SER	5.6
1	D	449	ALA	5.6
1	A	494	ASN	5.3
1	D	549	PRO	5.2
1	B	233	LEU	5.1
1	D	550	THR	5.1
1	A	234	PRO	5.1
1	B	533	LEU	4.9
1	B	361	TRP	4.8
1	D	234	PRO	4.6
1	A	493	SER	4.5
1	B	232	SER	4.4
1	B	737	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	488	SER	4.4
1	D	552	ARG	4.3
1	D	362	VAL	4.3
1	B	235	ASN	4.3
1	B	234	PRO	4.1
1	B	557	TYR	4.0
1	D	443	TYR	4.0
1	C	533	LEU	4.0
1	A	535	SER	3.9
1	C	535	SER	3.8
1	D	436	LEU	3.8
1	D	412	GLN	3.8
1	D	350	GLN	3.7
1	D	416	ALA	3.6
1	D	491	ASN	3.6
1	D	239	LYS	3.5
1	D	445	ASP	3.5
1	A	533	LEU	3.5
1	D	386	ILE	3.5
1	C	232	SER	3.5
1	D	1	MET	3.4
1	B	436	LEU	3.4
1	D	246	LEU	3.4
1	D	418	ILE	3.3
1	D	242	PHE	3.3
1	B	451	SER	3.3
1	D	347	ASN	3.3
1	D	447	PHE	3.3
1	D	363	GLU	3.2
1	C	417	SER	3.2
1	C	532	VAL	3.2
1	D	430	ALA	3.2
1	B	125	ASP	3.2
1	D	438	ALA	3.1
1	C	234	PRO	3.1
1	D	249	ILE	3.1
1	D	548	ASN	3.1
1	D	265	PRO	3.1
1	D	351	ASN	3.1
1	D	349	PHE	3.0
1	D	452	VAL	3.0
1	C	470	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	438	ALA	3.0
1	D	456	ILE	3.0
1	D	341	VAL	3.0
1	C	752	SER	3.0
1	A	751	PRO	3.0
1	D	451	SER	3.0
1	A	233	LEU	3.0
1	B	536	ALA	2.9
1	B	545	THR	2.9
1	A	3	ASN	2.9
1	D	494	ASN	2.9
1	A	451	SER	2.9
1	D	492	SER	2.9
1	D	260	TYR	2.9
1	C	487	TYR	2.8
1	A	734	MET	2.8
1	D	751	PRO	2.8
1	B	124	VAL	2.8
1	B	497	GLU	2.8
1	C	534	ASP	2.8
1	D	348	MET	2.8
1	D	493	SER	2.8
1	D	365	ASP	2.7
1	D	235	ASN	2.7
1	C	361	TRP	2.7
1	A	554	TRP	2.7
1	A	491	ASN	2.7
1	D	307	PHE	2.7
1	D	343	ALA	2.6
1	D	450	MET	2.6
1	D	400	ASP	2.6
1	D	366	TYR	2.6
1	B	439	GLU	2.6
1	D	535	SER	2.6
1	D	432	ASP	2.6
1	D	326	LYS	2.6
1	A	490	SER	2.6
1	D	417	SER	2.6
1	D	534	ASP	2.6
1	C	265	PRO	2.6
1	A	4	PRO	2.6
1	D	554	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	532	VAL	2.5
1	C	547	SER	2.5
1	D	409	LEU	2.5
1	B	625	LEU	2.5
1	A	166	THR	2.5
1	D	384	THR	2.5
1	B	471	ASP	2.5
1	B	734	MET	2.5
1	A	488	SER	2.5
1	B	231	LYS	2.5
1	B	239	LYS	2.5
1	B	6	TYR	2.4
1	C	536	ALA	2.4
1	D	448	THR	2.4
1	D	3	ASN	2.4
1	B	493	SER	2.4
1	A	548	ASN	2.4
1	D	314	ASP	2.4
1	D	401	THR	2.4
1	D	446	ASP	2.4
1	B	84	LEU	2.4
1	A	235	ASN	2.4
1	C	436	LEU	2.4
1	A	489	LEU	2.4
1	B	432	ASP	2.4
1	B	751	PRO	2.4
1	D	454	ASP	2.4
1	B	752	SER	2.3
1	D	329	GLY	2.3
1	D	371	SER	2.3
1	D	431	SER	2.3
1	A	547	SER	2.3
1	A	121	ASN	2.3
1	D	435	ILE	2.3
1	D	399	LYS	2.2
1	D	461	PHE	2.2
1	D	167	ASN	2.2
1	B	83	LEU	2.2
1	B	547	SER	2.2
1	D	455	GLN	2.2
1	B	485	ALA	2.2
1	A	534	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	419	ARG	2.2
1	A	624	ALA	2.2
1	D	121	ASN	2.1
1	D	429	GLY	2.1
1	B	504	SER	2.1
1	A	84	LEU	2.1
1	C	432	ASP	2.1
1	B	248	VAL	2.1
1	B	364	THR	2.1
1	C	434	LYS	2.1
1	B	494	ASN	2.1
1	B	800	LYS	2.1
1	B	537	ILE	2.1
1	D	233	LEU	2.1
1	B	738	ASN	2.1
1	D	4	PRO	2.1
1	A	165	ALA	2.1
1	D	334	PHE	2.1
1	A	363	GLU	2.0
1	C	469	VAL	2.0
1	D	339	PHE	2.0
1	C	429	GLY	2.0
1	C	751	PRO	2.0
1	D	248	VAL	2.0
1	B	478	ASP	2.0
1	B	566	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

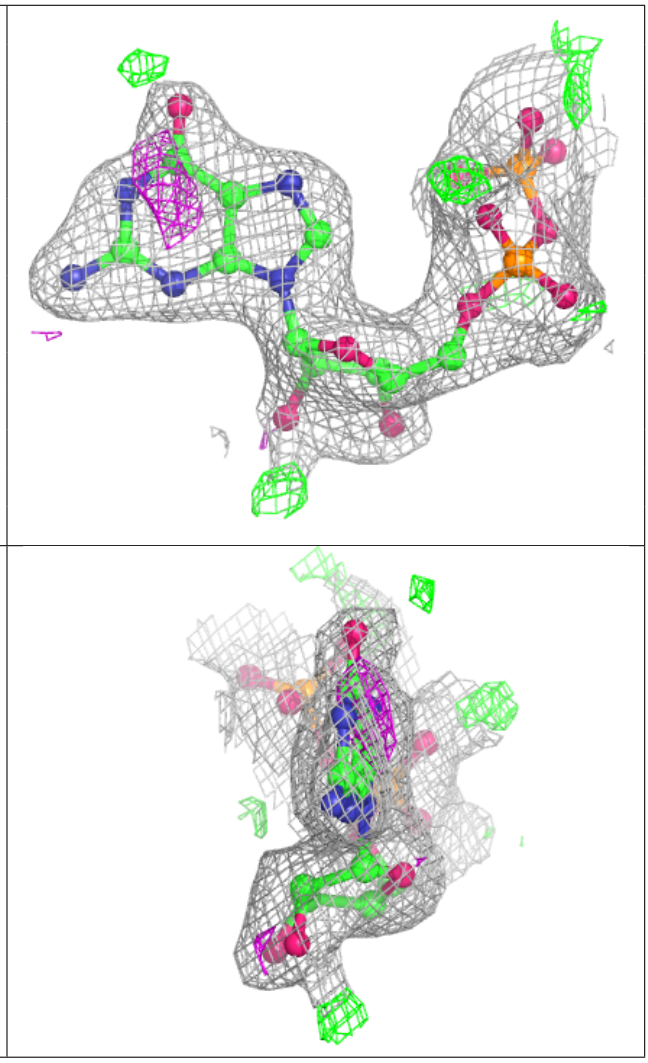
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GDP	D	902	28/28	0.85	0.15	25,37,68,84	0
2	GTP	D	901	32/32	0.87	0.14	20,41,54,62	0
2	GTP	C	901	32/32	0.88	0.13	22,37,48,50	0
3	GDP	A	902	28/28	0.89	0.14	24,36,68,77	0
3	GDP	B	902	28/28	0.89	0.11	26,37,69,78	0
3	GDP	C	902	28/28	0.91	0.14	13,35,67,79	0
2	GTP	A	901	32/32	0.93	0.11	18,27,44,47	0
2	GTP	B	901	32/32	0.93	0.11	25,36,48,55	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.

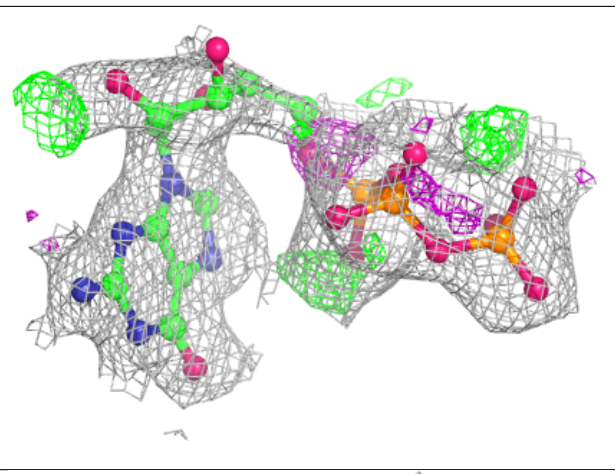
Electron density around GDP D 902:

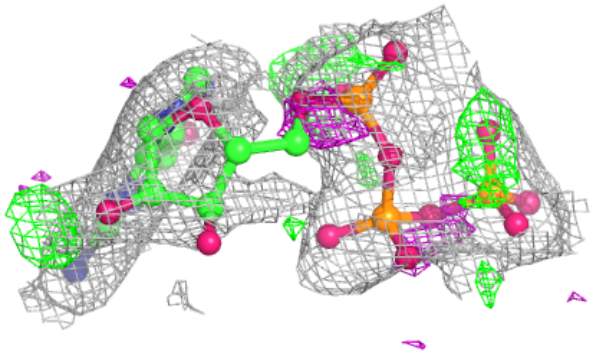
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

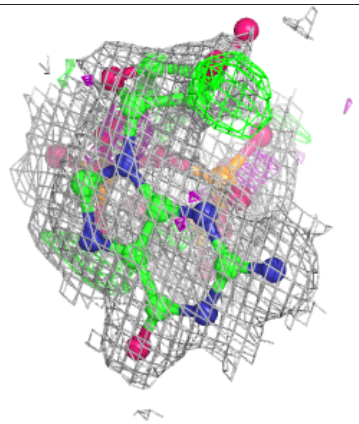


Electron density around GTP D 901:

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

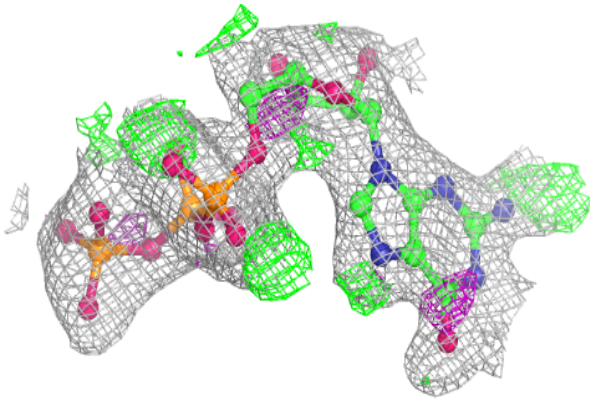


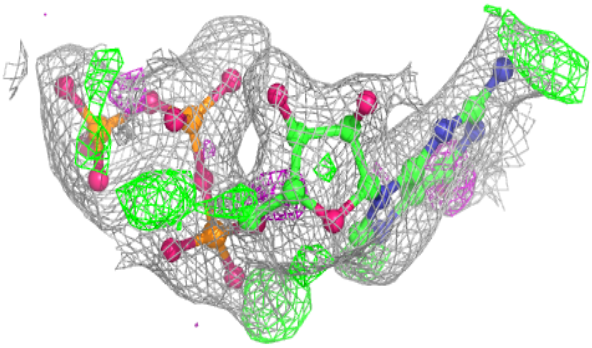


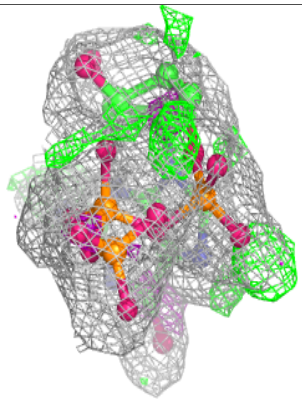


Electron density around GTP C 901:

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

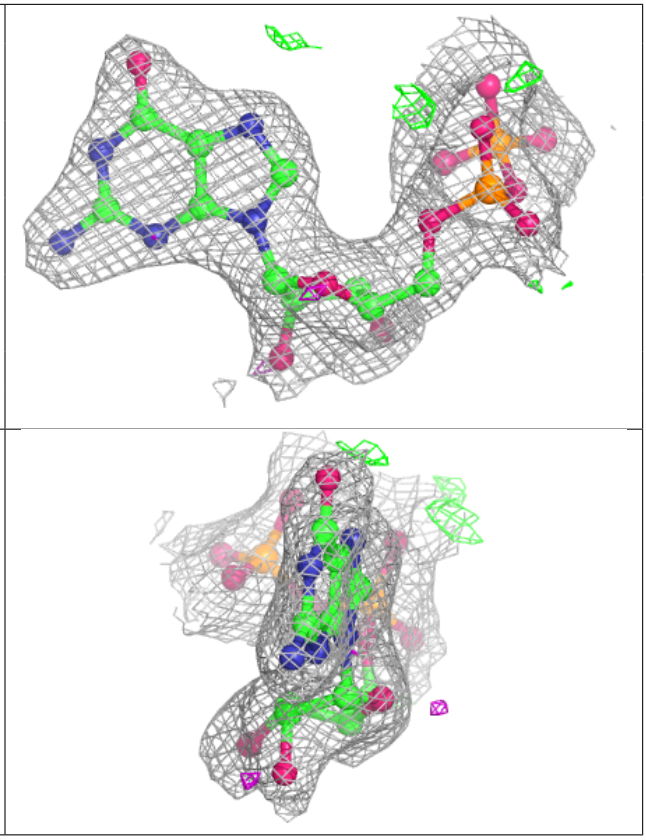






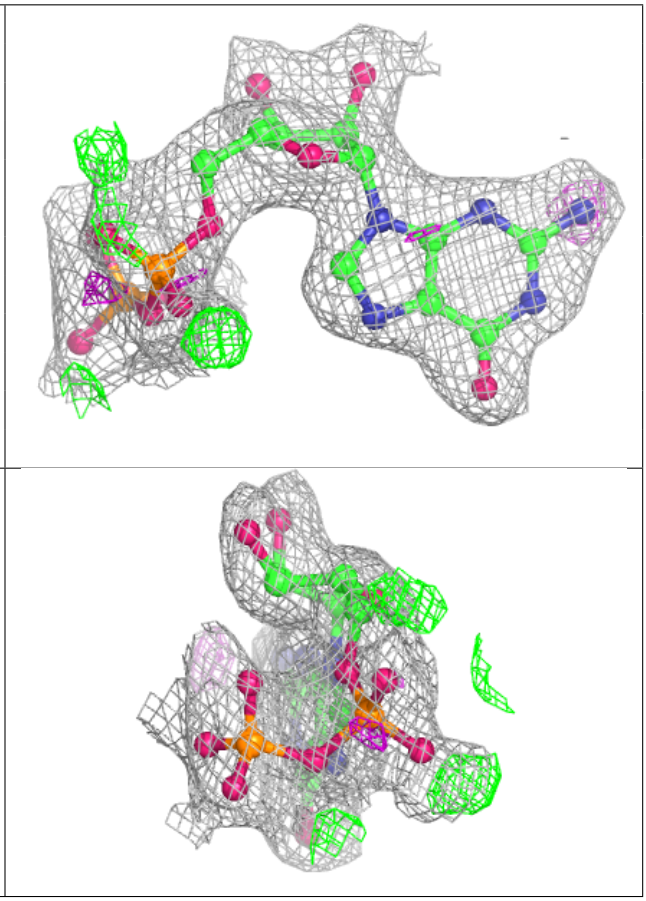
Electron density around GDP A 902:

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



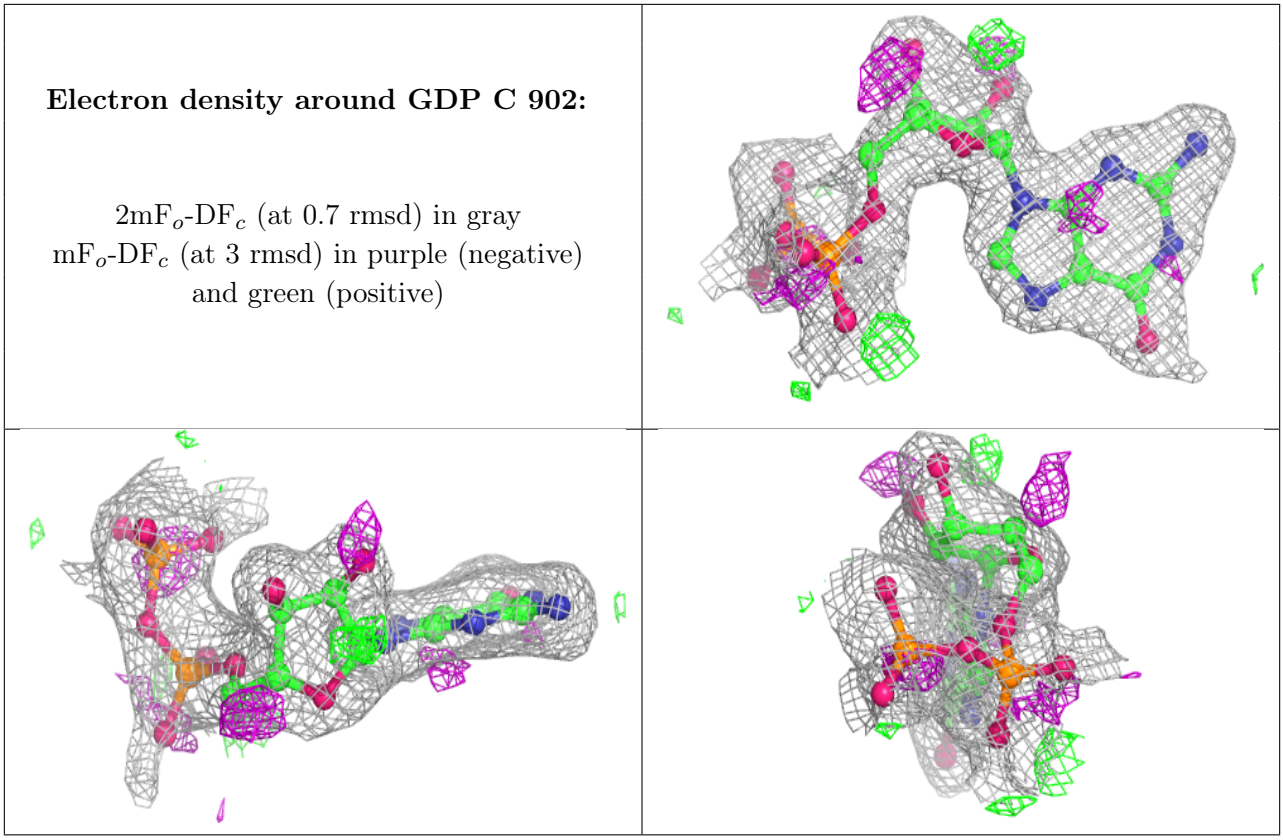
Electron density around GDP B 902:

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



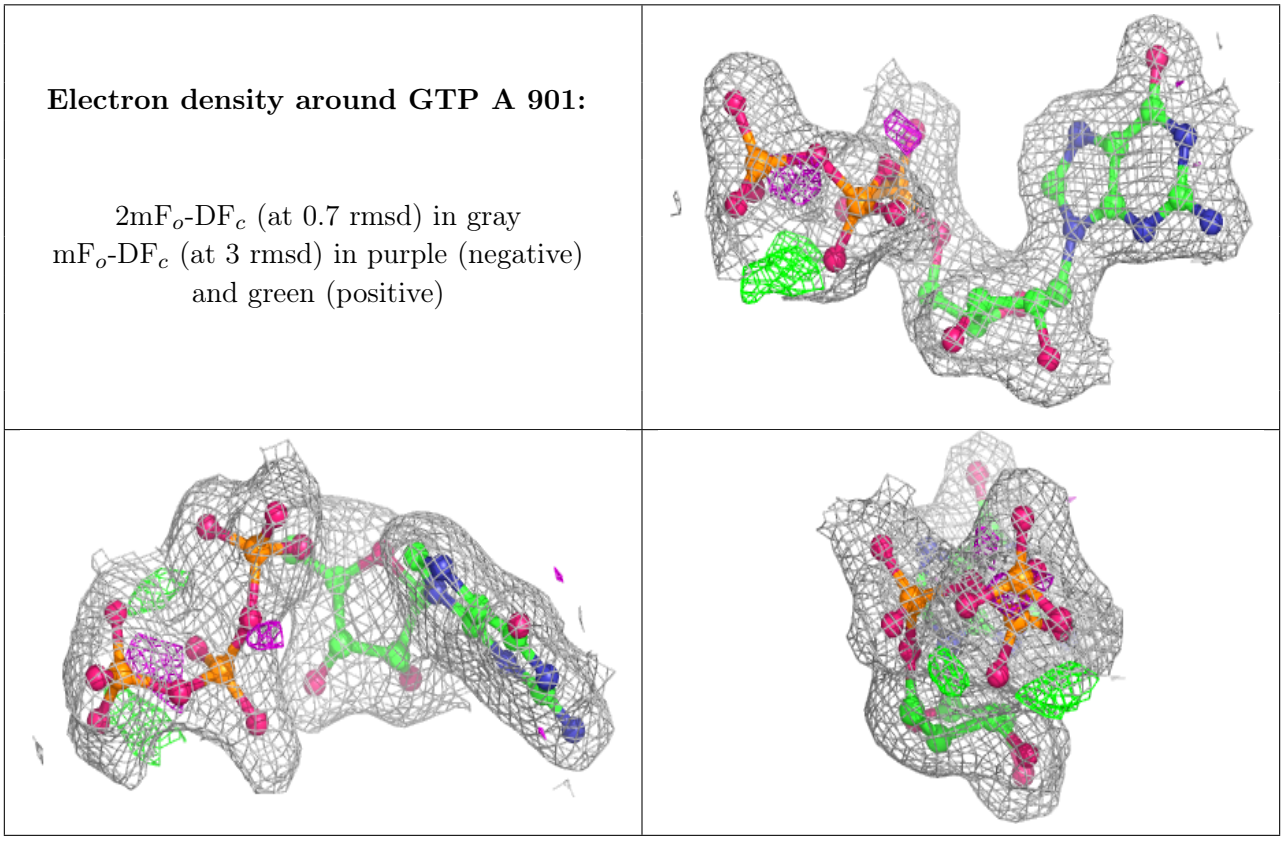
Electron density around GDP C 902:

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



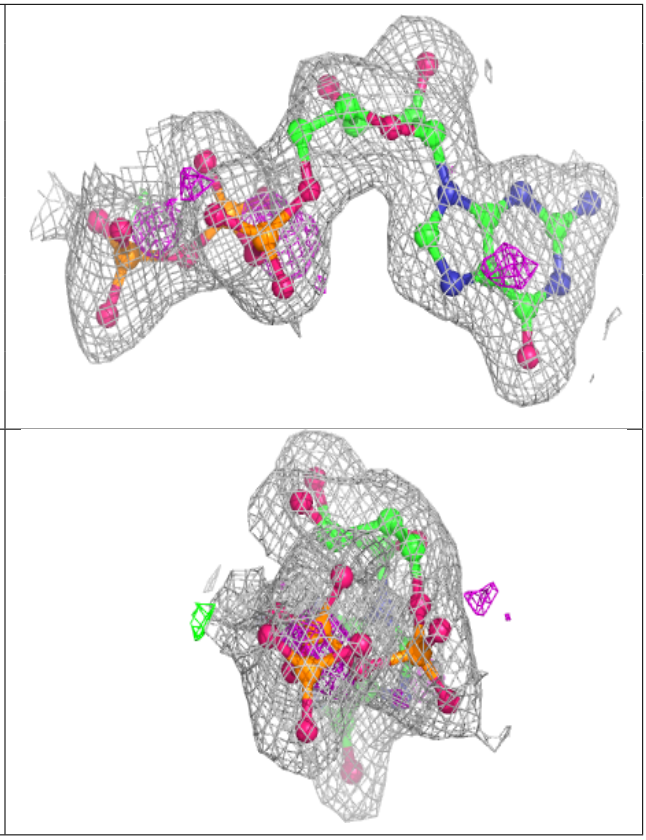
Electron density around GTP A 901:

$2mF_o$-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 901:

$2mF_o$-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.