Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2023 – 12:30 pm GMT

PDB ID	:	7YZ2
Title	:	Molecular snapshots of drug release from tubulin: 10 milliseconds after photoactivation.
Authors	:	Wranik, M.; Weinert, T.; Standfuss, J.
Deposited on	:	2022-02-18
Resolution	:	2.20 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:

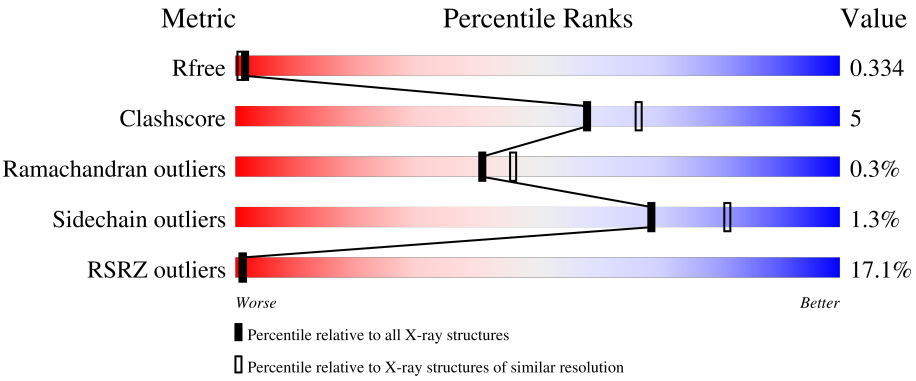
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	451	9% 86% 9%
2	B	445	28% 85% 12%
3	F	169	7% 77% 15% 8%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8210 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 Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	431	3406	2162	579	640	25	2	8	0

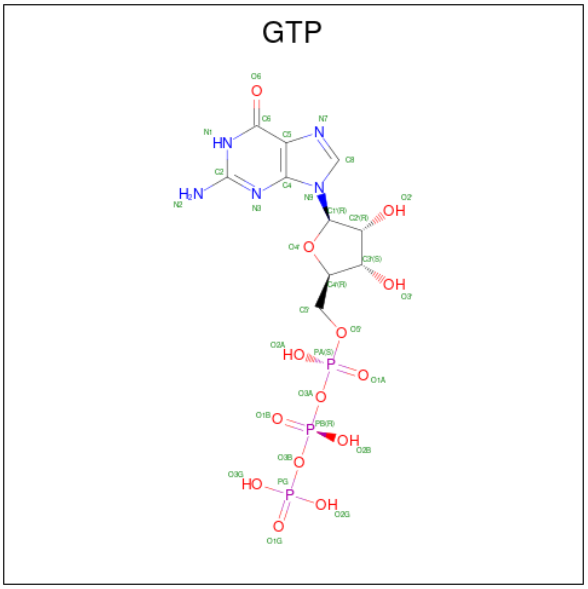
- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	431	3371	2117	573	654	27	5	3	0

- Molecule 3 is a protein called Designed Ankyrin Repeat Protein (DARPIN) D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	F	155	1154	728	195	228	3	0	1	0

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

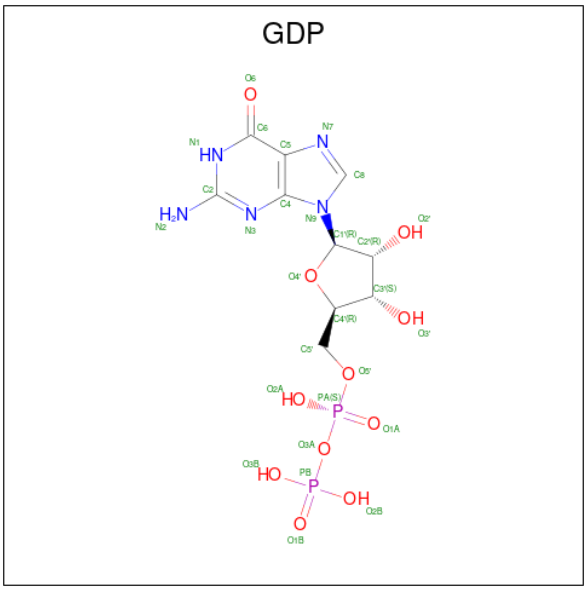


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 7 is water.

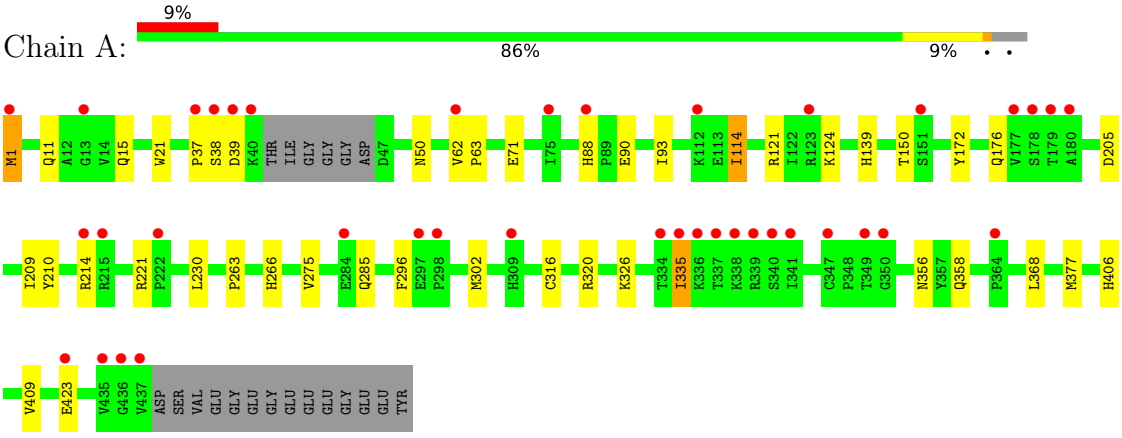
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	106	Total	O	0	0
			106	106		
7	B	67	Total	O	0	0
			67	67		
7	F	45	Total	O	0	0
			45	45		

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.

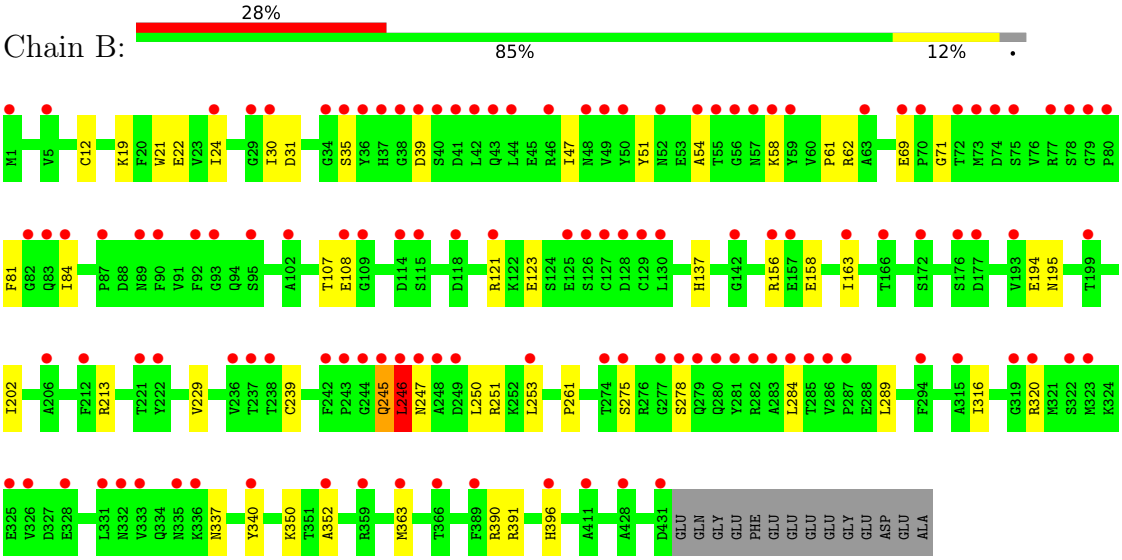
• Molecule 1: Tubulin alpha-1B chain

Chain A:



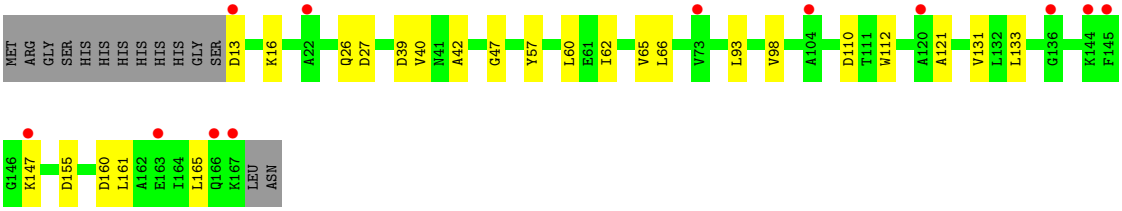
• Molecule 2: Tubulin beta-2B chain

Chain B:



• Molecule 3: Designed Ankyrin Repeat Protein (DARPIN) D1

Chain F:


MET ARG GLY SER HIS HIS HIS HIS HIS HIS GLY SER D13 K16 A22 Q26 D27 D39 V40 N41 A42 G47 Y57 L60 E61 I62 V65 L66 V73 L93 V98 A104 D110 T111 W112 A120 A121 V131 L132 L133 G136 K144 F145
G146 K147 D155 D160 L161 A162 E163 I164 L165 Q166 K167 LEU ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.53Å 92.58Å 83.99Å 90.00° 96.71° 90.00°	Depositor
Resolution (Å)	9.49 – 2.20 9.49 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.5 (9.49-2.20) 93.5 (9.49-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.86 (at 2.21Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.285 , 0.334 0.285 , 0.334	Depositor DCC
R_{free} test set	1854 reflections (3.49%)	wwPDB-VP
Wilson B-factor (Å^2)	36.8	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 69.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	8210	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, GDP, MG

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	0.24	0/3504	0.45	0/4756
2	B	0.24	0/3451	0.45	0/4677
3	F	0.22	0/1173	0.40	0/1595
All	All	0.24	0/8128	0.44	0/11028

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	3406	0	3326	26	0
2	B	3371	0	3226	36	0
3	F	1154	0	1151	17	0
4	A	32	0	12	1	0
5	A	1	0	0	0	0
6	B	28	0	12	1	0
7	A	106	0	0	7	0
7	B	67	0	0	4	0
7	F	45	0	0	3	0
All	All	8210	0	7727	75	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 5.

All (75) 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)
3:F:47:GLY:O	7:F:201:HOH:O	2.05	0.73
3:F:26:GLN:NE2	7:F:202:HOH:O	2.23	0.70
1:A:316[A]:CYS:SG	7:A:674:HOH:O	2.53	0.67
1:A:316[B]:CYS:SG	7:A:674:HOH:O	2.53	0.67
2:B:213:ARG:NH2	3:F:160:ASP:OD1	2.29	0.66
1:A:358:GLN:NE2	7:A:602:HOH:O	2.28	0.66
2:B:246:LEU:HG	2:B:247:ASN:H	1.60	0.65
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.76	0.65
2:B:289:LEU:HD11	2:B:363:MET:HB3	1.77	0.65
1:A:90:GLU:O	1:A:121:ARG:NH1	2.31	0.63
2:B:30:ILE:HD11	2:B:47:ILE:HD11	1.84	0.59
2:B:316:ILE:HA	2:B:352:ALA:HB3	1.84	0.59
2:B:245:GLN:O	2:B:247:ASN:N	2.36	0.58
2:B:31:ASP:OD1	2:B:35:SER:N	2.39	0.56
2:B:246:LEU:HD13	2:B:352:ALA:HB2	1.87	0.56
2:B:396:HIS:NE2	3:F:57:TYR:OH	2.32	0.55
1:A:37:PRO:O	1:A:39:ASP:N	2.39	0.55
3:F:13:ASP:OD2	3:F:16:LYS:NZ	2.37	0.55
3:F:40:VAL:HG13	3:F:66:LEU:HD22	1.90	0.53
1:A:209:ILE:HD11	1:A:302[A]:MET:HG3	1.91	0.53
3:F:133:LEU:HD11	3:F:165:LEU:HD23	1.91	0.53
2:B:123:GLU:O	7:B:602:HOH:O	2.19	0.53
3:F:147:LYS:NZ	3:F:155:ASP:OD2	2.36	0.53
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.91	0.52
2:B:69:GLU:HG2	2:B:71:GLY:H	1.74	0.51
2:B:163:ILE:HG21	2:B:250:LEU:HB3	1.91	0.51
2:B:239:CYS:SG	2:B:246:LEU:HD11	2.50	0.51
3:F:160:ASP:HB2	7:F:208:HOH:O	2.10	0.50
3:F:121:ALA:HB1	3:F:161:LEU:HD21	1.94	0.49
2:B:54:ALA:HB3	2:B:58:LYS:HB3	1.95	0.49
2:B:61:PRO:HD3	2:B:84:ILE:HG13	1.94	0.49
1:A:263:PRO:HA	7:A:681:HOH:O	2.11	0.49
1:A:263:PRO:O	1:A:266:HIS:ND1	2.37	0.48
2:B:337:ASN:HB3	2:B:340:TYR:HD2	1.79	0.48
1:A:406:HIS:HA	1:A:409:VAL:HG22	1.95	0.48
2:B:202:ILE:HD13	2:B:229:VAL:HG13	1.94	0.48
1:A:15:GLN:NE2	4:A:501:GTP:O6	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:156[A]:ARG:NH1	2:B:194:GLU:O	2.47	0.47
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.50	0.46
2:B:51:TYR:O	2:B:62:ARG:NH2	2.49	0.46
2:B:39:ASP:N	2:B:39:ASP:OD1	2.50	0.45
2:B:245:GLN:HB2	2:B:246:LEU:H	1.53	0.45
2:B:12:CYS:HB2	6:B:501:GDP:C8	2.52	0.44
3:F:60:LEU:HD11	3:F:98:VAL:HG21	1.99	0.44
2:B:247:ASN:ND2	2:B:253:LEU:HD13	2.33	0.44
2:B:261:PRO:HB2	7:B:641:HOH:O	2.18	0.44
1:A:124:LYS:NZ	7:A:605:HOH:O	2.31	0.43
1:A:62:VAL:HG11	1:A:88:HIS:CD2	2.53	0.43
1:A:93:ILE:HG22	1:A:114:ILE:HD11	1.99	0.43
2:B:22:GLU:HG2	2:B:81:PHE:CD1	2.54	0.43
3:F:27:ASP:N	3:F:27:ASP:OD1	2.50	0.43
3:F:93:LEU:HD11	3:F:131:VAL:HG21	2.01	0.42
2:B:247:ASN:ND2	7:B:601:HOH:O	2.16	0.42
2:B:275:SER:HB2	2:B:278:SER:HB3	2.01	0.42
2:B:19:LYS:HD3	2:B:19:LYS:HA	1.91	0.42
1:A:296:PHE:CZ	1:A:377:MET:HE1	2.54	0.42
2:B:390:ARG:HD2	3:F:112:TRP:NE1	2.35	0.42
2:B:391:ARG:NH2	3:F:110:ASP:OD2	2.50	0.42
2:B:121:ARG:NH2	2:B:158:GLU:OE2	2.53	0.42
1:A:210:TYR:CE2	1:A:214[B]:ARG:HD2	2.55	0.42
1:A:139:HIS:CD2	1:A:150:THR:HG21	2.55	0.41
1:A:176:GLN:OE1	1:A:176:GLN:N	2.47	0.41
1:A:320:ARG:HA	1:A:356:ASN:O	2.20	0.41
3:F:39:ASP:HB3	3:F:42:ALA:HB2	2.01	0.41
1:A:11:GLN:HB2	7:A:626:HOH:O	2.21	0.41
1:A:335:ILE:HD13	1:A:335:ILE:HA	1.92	0.41
1:A:1:MET:HG2	1:A:50:ASN:HB2	2.02	0.41
3:F:62:ILE:HA	3:F:65:VAL:HG22	2.03	0.40
1:A:285:GLN:NE2	7:A:609:HOH:O	2.36	0.40
2:B:21:TRP:CE3	2:B:24:ILE:HD11	2.56	0.40
2:B:107:THR:OG1	2:B:108:GLU:N	2.54	0.40
1:A:275:VAL:HG13	1:A:368:LEU:HD21	2.04	0.40
2:B:156[A]:ARG:NH1	2:B:195:ASN:HA	2.37	0.40
2:B:320:ARG:HG3	7:B:612:HOH:O	2.21	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	435/451 (96%)	420 (97%)	13 (3%)	2 (0%)	29	31
2	B	432/445 (97%)	410 (95%)	21 (5%)	1 (0%)	47	55
3	F	154/169 (91%)	151 (98%)	3 (2%)	0	100	100
All	All	1021/1065 (96%)	981 (96%)	37 (4%)	3 (0%)	41	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	SER
2	B	246	LEU
1	A	114	ILE

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	367/379 (97%)	360 (98%)	7 (2%)	57	71
2	B	366/383 (96%)	361 (99%)	5 (1%)	67	80
3	F	120/132 (91%)	120 (100%)	0	100	100
All	All	853/894 (95%)	841 (99%)	12 (1%)	69	80

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	71	GLU
1	A	221	ARG
1	A	326	LYS
1	A	335	ILE
1	A	423[A]	GLU
1	A	423[B]	GLU
2	B	137	HIS
2	B	245	GLN
2	B	246	LEU
2	B	284	LEU
2	B	350	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
2	B	195	ASN
2	B	247	ASN
2	B	337	ASN
2	B	426	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)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
4	GTP	A	501	5	26,34,34	1.11	2 (7%)	32,54,54	1.52	7 (21%)
6	GDP	B	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.27	4 (13%)

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
4	GTP	A	501	5	-	6/18/38/38	0/3/3/3
6	GDP	B	501	-	-	4/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	GTP	C5-C6	-3.93	1.39	1.47
6	B	501	GDP	C6-N1	-2.36	1.34	1.37
4	A	501	GTP	C2-N3	2.16	1.38	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	501	GTP	PB-O3B-PG	-3.24	121.70	132.83
4	A	501	GTP	C5-C6-N1	3.20	119.61	113.95
4	A	501	GTP	PA-O3A-PB	-3.08	122.25	132.83
6	B	501	GDP	PA-O3A-PB	-3.06	122.32	132.83
4	A	501	GTP	C8-N7-C5	3.06	108.82	102.99
4	A	501	GTP	C2-N1-C6	-2.81	119.92	125.10
6	B	501	GDP	C3'-C2'-C1'	2.78	105.16	100.98
6	B	501	GDP	C8-N7-C5	2.35	107.46	102.99
6	B	501	GDP	C5-C6-N1	2.29	118.00	113.95
4	A	501	GTP	C3'-C2'-C1'	2.28	104.41	100.98
4	A	501	GTP	O6-C6-C5	-2.10	120.27	124.37

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	GTP	PB-O3B-PG-O2G
4	A	501	GTP	C5'-O5'-PA-O1A
4	A	501	GTP	C5'-O5'-PA-O2A
6	B	501	GDP	C5'-O5'-PA-O1A
6	B	501	GDP	C5'-O5'-PA-O2A
4	A	501	GTP	C5'-O5'-PA-O3A
4	A	501	GTP	C4'-C5'-O5'-PA
6	B	501	GDP	PB-O3A-PA-O2A
6	B	501	GDP	C5'-O5'-PA-O3A
4	A	501	GTP	C3'-C4'-C5'-O5'

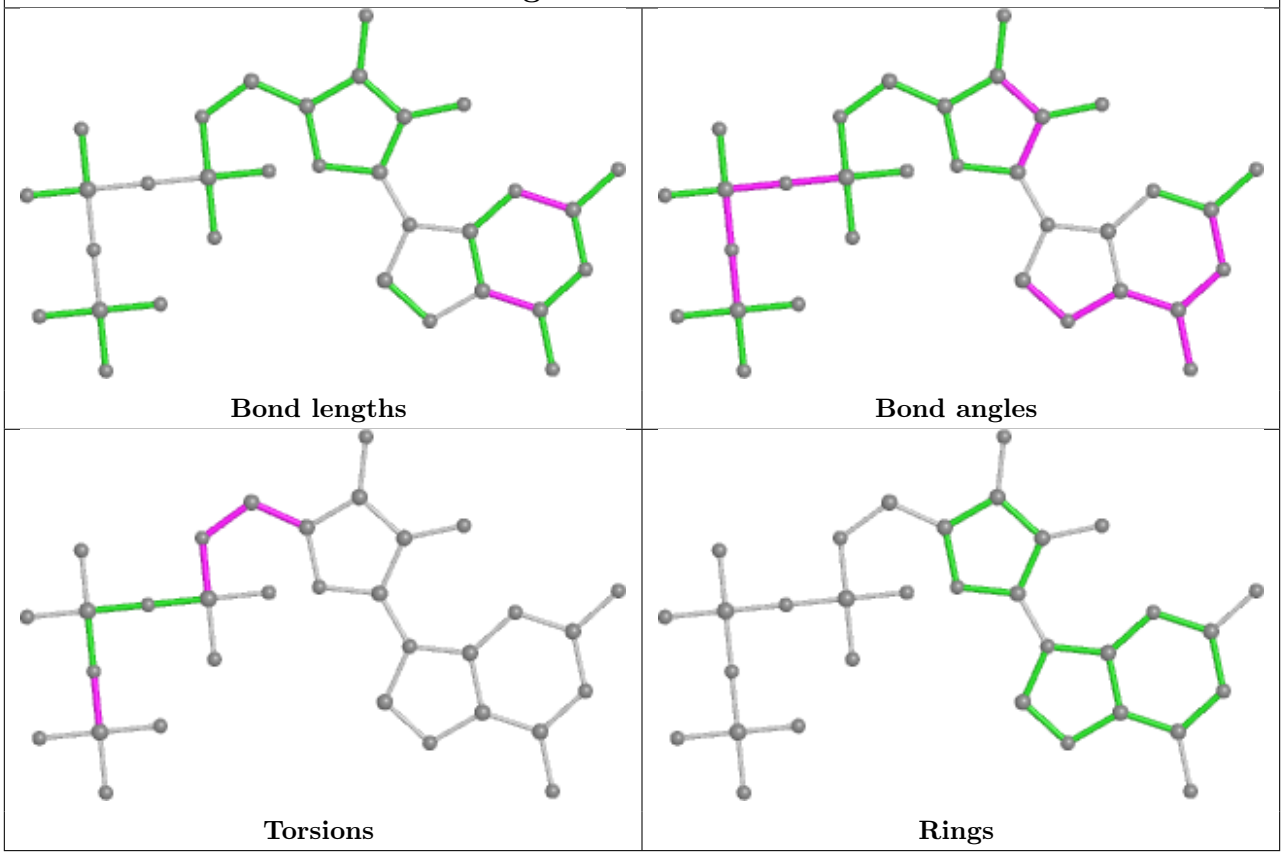
There are no ring outliers.

2 monomers are involved in 2 short contacts:

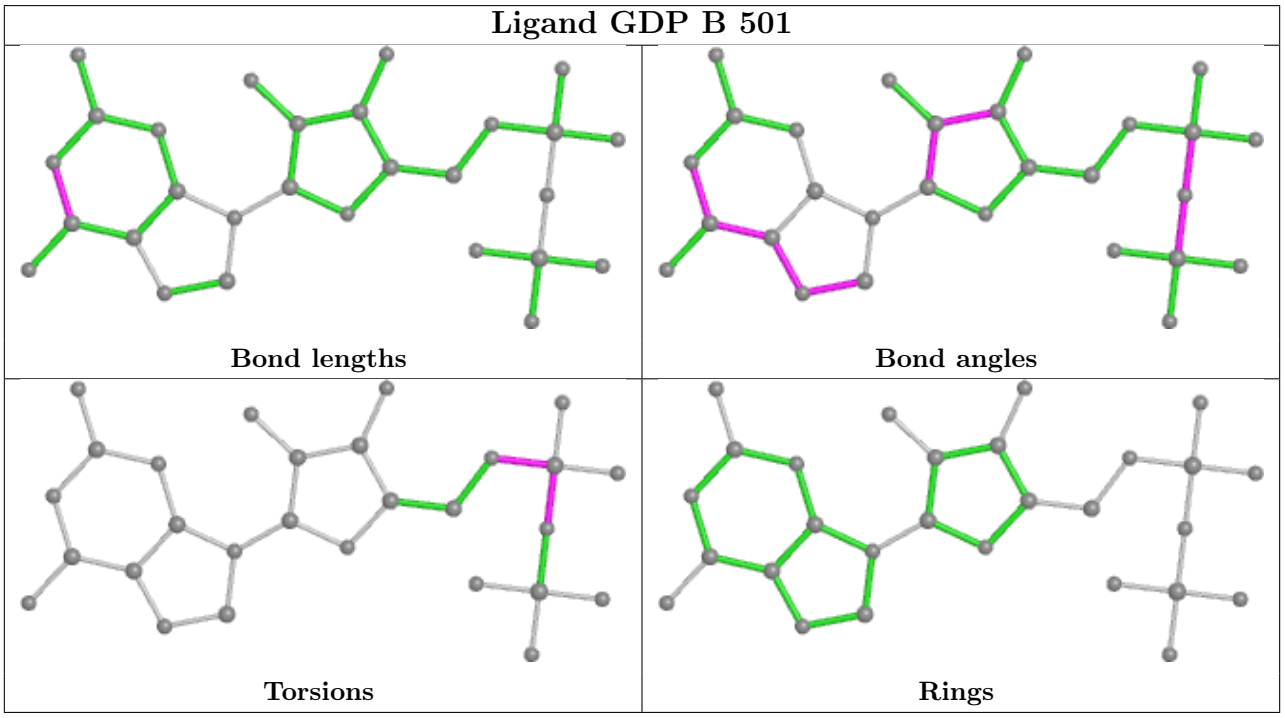
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	GTP	1	0
6	B	501	GDP	1	0

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 A 501



Ligand GDP B 501



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, 95^{th} 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	431/451 (95%)	0.81	39 (9%) 9 8	24, 35, 54, 85	2 (0%)
2	B	431/445 (96%)	1.54	123 (28%) 0 0	29, 45, 73, 124	0
3	F	155/169 (91%)	0.82	12 (7%) 13 12	25, 35, 48, 73	0
All	All	1017/1065 (95%)	1.12	174 (17%) 1 1	24, 38, 67, 124	2 (0%)

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	283	ALA	17.6
2	B	280	GLN	11.5
2	B	282	ARG	11.3
1	A	437	VAL	10.0
2	B	248	ALA	8.5
2	B	42	LEU	7.4
2	B	281	TYR	6.9
1	A	436	GLY	6.6
1	A	38	SER	5.9
2	B	279	GLN	5.8
2	B	431	ASP	5.8
2	B	39	ASP	5.7
2	B	95	SER	5.5
1	A	39	ASP	5.4
2	B	247	ASN	5.2
1	A	339	ARG	5.0
2	B	57	ASN	4.8
2	B	73	MET	4.8
1	A	335	ILE	4.8
2	B	246	LEU	4.7
2	B	41	ASP	4.7
1	A	338	LYS	4.6
2	B	275	SER	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	178	SER	4.4
2	B	127	CYS	4.4
2	B	93	GLY	4.4
1	A	349	THR	4.4
1	A	350	GLY	4.3
2	B	80	PRO	4.2
2	B	56	GLY	4.1
2	B	328	GLU	4.0
2	B	157	GLU	4.0
2	B	92	PHE	3.9
2	B	130	LEU	3.9
2	B	322	SER	3.9
3	F	167	LYS	3.8
2	B	72	THR	3.8
2	B	335	ASN	3.8
2	B	245	GLN	3.7
2	B	333	VAL	3.7
2	B	244	GLY	3.7
2	B	38	GLY	3.7
2	B	331	LEU	3.7
2	B	43	GLN	3.7
2	B	34	GLY	3.6
1	A	40	LYS	3.6
1	A	177	VAL	3.6
2	B	74	ASP	3.5
2	B	284	LEU	3.5
2	B	243	PRO	3.5
2	B	54	ALA	3.4
3	F	163	GLU	3.4
2	B	36	TYR	3.4
2	B	89	ASN	3.4
2	B	46	ARG	3.4
2	B	75	SER	3.4
2	B	285	THR	3.4
2	B	87	PRO	3.3
2	B	277	GLY	3.3
2	B	121	ARG	3.3
2	B	249	ASP	3.3
2	B	172	SER	3.3
2	B	69	GLU	3.3
2	B	323	MET	3.3
3	F	145	PHE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	212	PHE	3.2
2	B	58	LYS	3.2
2	B	55	THR	3.1
2	B	221	THR	3.1
2	B	37	HIS	3.0
2	B	129	CYS	3.0
3	F	22	ALA	3.0
2	B	237	THR	3.0
3	F	166	GLN	3.0
2	B	332	ASN	3.0
2	B	70	PRO	3.0
2	B	82	GLY	3.0
2	B	242	PHE	2.9
2	B	193	VAL	2.9
2	B	278	SER	2.9
2	B	126	SER	2.8
2	B	49	VAL	2.8
1	A	1	MET	2.8
2	B	286	VAL	2.8
2	B	128	ASP	2.8
1	A	37	PRO	2.8
2	B	326	VAL	2.8
1	A	179	THR	2.7
3	F	73	VAL	2.7
1	A	336	LYS	2.7
2	B	44	LEU	2.7
1	A	75	ILE	2.7
2	B	79	GLY	2.7
1	A	337	THR	2.7
2	B	325	GLU	2.6
1	A	423[A]	GLU	2.6
2	B	118	ASP	2.6
2	B	84	ILE	2.6
2	B	102	ALA	2.6
1	A	88	HIS	2.6
3	F	147	LYS	2.6
2	B	63	ALA	2.6
2	B	78	SER	2.6
2	B	109	GLY	2.6
2	B	236	VAL	2.5
3	F	13	ASP	2.5
2	B	274	THR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	1	MET	2.5
2	B	363	MET	2.5
2	B	294	PHE	2.5
2	B	30	ILE	2.5
2	B	40	SER	2.4
2	B	352	ALA	2.4
2	B	5	VAL	2.4
2	B	125	GLU	2.4
2	B	83	GLN	2.4
2	B	315	ALA	2.4
2	B	115	SER	2.4
2	B	176	SER	2.4
1	A	180	ALA	2.4
2	B	222	TYR	2.3
3	F	104	ALA	2.3
1	A	284	GLU	2.3
2	B	52	ASN	2.3
1	A	309	HIS	2.3
2	B	142	GLY	2.3
2	B	336	LYS	2.3
3	F	144	LYS	2.3
2	B	253	LEU	2.3
1	A	151	SER	2.3
2	B	320	ARG	2.3
1	A	112	LYS	2.3
1	A	222	PRO	2.3
2	B	114	ASP	2.2
2	B	177[A]	ASP	2.2
1	A	123[A]	ARG	2.2
2	B	206	ALA	2.2
2	B	396	HIS	2.2
2	B	156[A]	ARG	2.2
1	A	214[A]	ARG	2.2
1	A	215	ARG	2.2
2	B	389	PHE	2.2
3	F	136	GLY	2.2
2	B	428	ALA	2.2
2	B	48	ASN	2.2
2	B	411	ALA	2.2
1	A	297	GLU	2.2
2	B	59	TYR	2.2
2	B	108	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	238	THR	2.2
2	B	29	GLY	2.2
2	B	163	ILE	2.1
2	B	199	THR	2.1
1	A	340	SER	2.1
1	A	364	PRO	2.1
2	B	166	THR	2.1
2	B	90	PHE	2.1
1	A	62	VAL	2.1
1	A	435	VAL	2.1
3	F	120	ALA	2.1
2	B	319	GLY	2.1
2	B	35	SER	2.1
2	B	287	PRO	2.1
2	B	366	THR	2.1
1	A	13	GLY	2.1
2	B	50	TYR	2.1
2	B	340	TYR	2.1
2	B	24	ILE	2.0
1	A	298	PRO	2.0
2	B	77	ARG	2.0
2	B	359	ARG	2.0
1	A	347	CYS	2.0
1	A	341	ILE	2.0
1	A	334	THR	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)

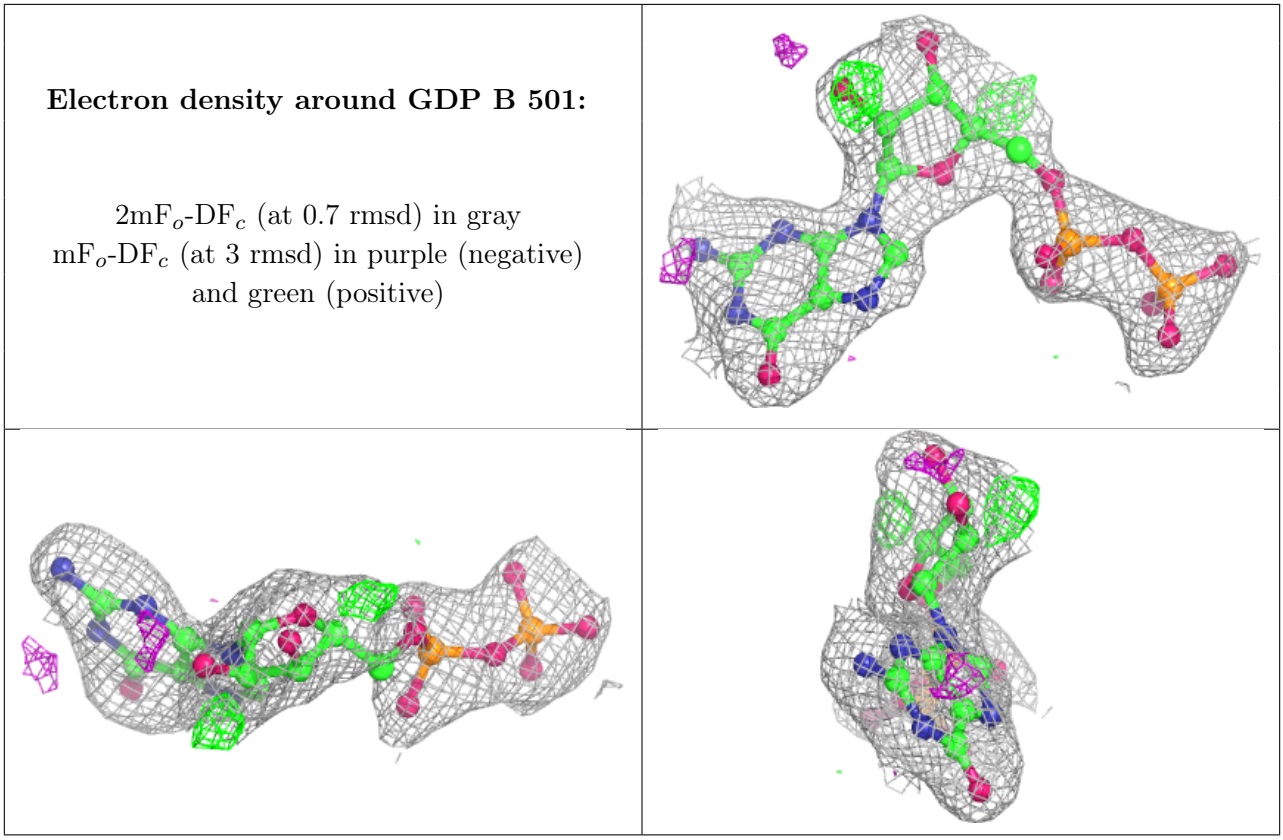
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
5	MG	A	502	1/1	0.69	0.26	33,33,33,33	0
6	GDP	B	501	28/28	0.88	0.18	33,39,46,54	0
4	GTP	A	501	32/32	0.89	0.18	22,27,32,36	0

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

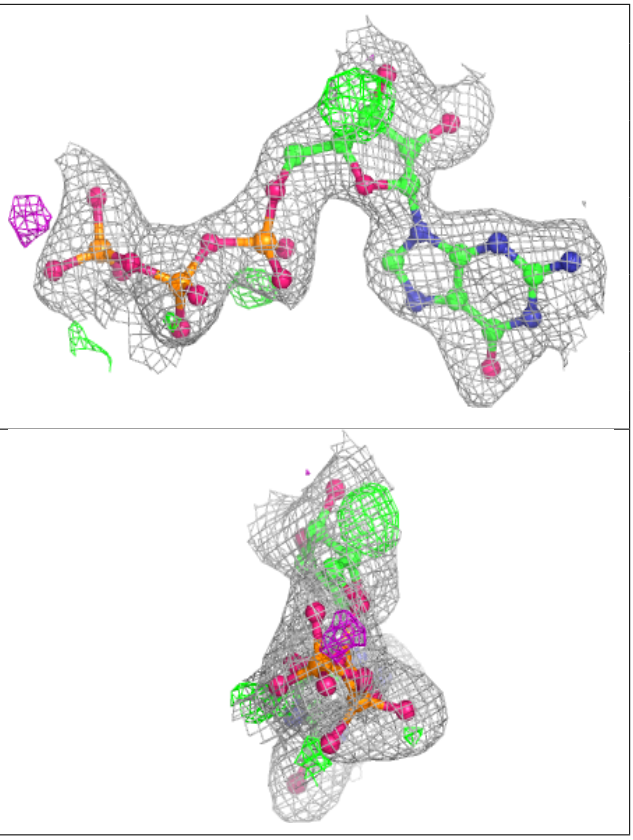
Electron density around GDP B 501:

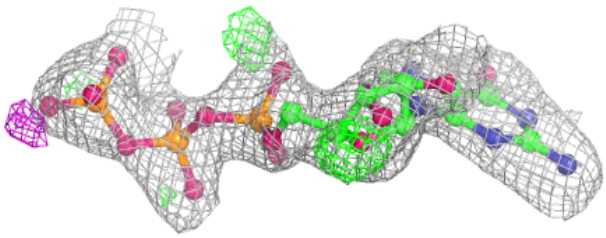
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around GTP A 501:

$2mF_o$-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.