



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 02:31 am BST

PDB ID : 6GZE  
Title : Tubulin-GDP.BeF complex  
Authors : Oliva, M.A.; Diaz, J.F.  
Deposited on : 2018-07-04  
Resolution : 2.49 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

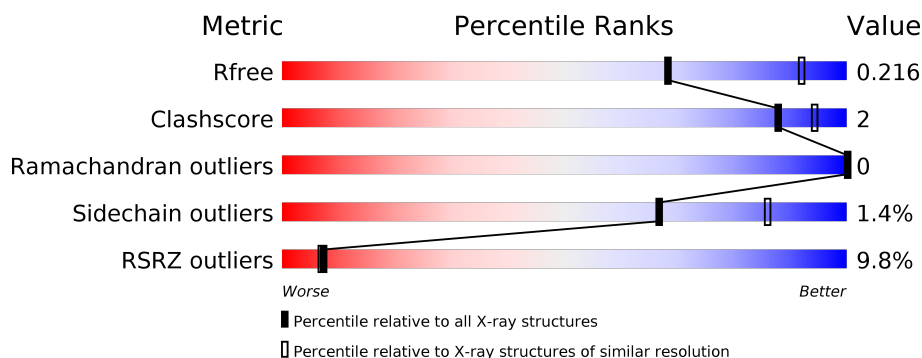
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	440	<div> <div>9%</div> <div>93%</div> <div>5%</div> </div>
1	C	440	<div> <div>2%</div> <div>96%</div> <div></div> </div>
2	B	445	<div> <div>5%</div> <div>89%</div> <div>6%</div> <div>5%</div> </div>
2	D	445	<div> <div>15%</div> <div>84%</div> <div>10%</div> <div>6%</div> </div>
3	E	189	<div> <div>5%</div> <div>60%</div> <div>39%</div> </div>
4	F	380	<div> <div>15%</div> <div>63%</div> <div>5%</div> <div>33%</div> </div>

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 33075 atoms, of which 16278 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
1	A	435	Total	C	H	N	O	S	0	3	0
			6748	2160	3338	579	648	23			
1	C	440	Total	C	H	N	O	S	0	2	0
			6805	2180	3360	584	658	23			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	423	Total	C	H	N	O	S	1	2	0
			6560	2099	3222	568	644	27			
2	D	420	Total	C	H	N	O	S	6	0	0
			6486	2076	3185	561	637	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	116	Total	C	H	N	O	S	0	1	0
			1949	596	985	176	188	4			

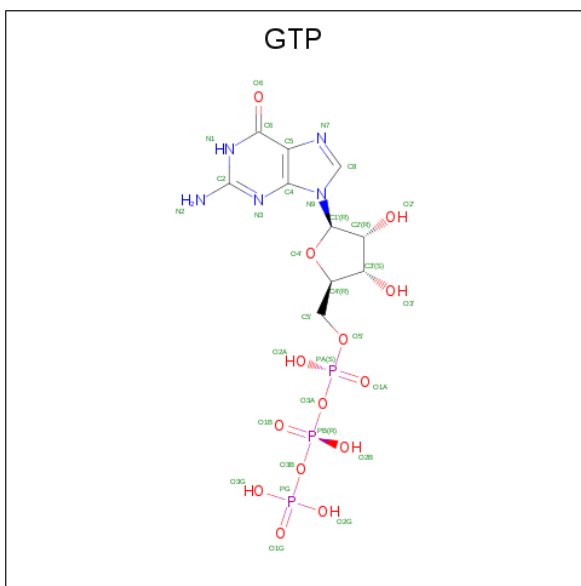
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	256	Total	C	H	N	O	S	0	0	0
			4235	1376	2121	357	369	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:

$$\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{14}\text{P}_3).$$


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total 42	C 10	H 10	N 5	O 14	P 3	0	0
5	C	1	Total 42	C 10	H 10	N 5	O 14	P 3	0	0

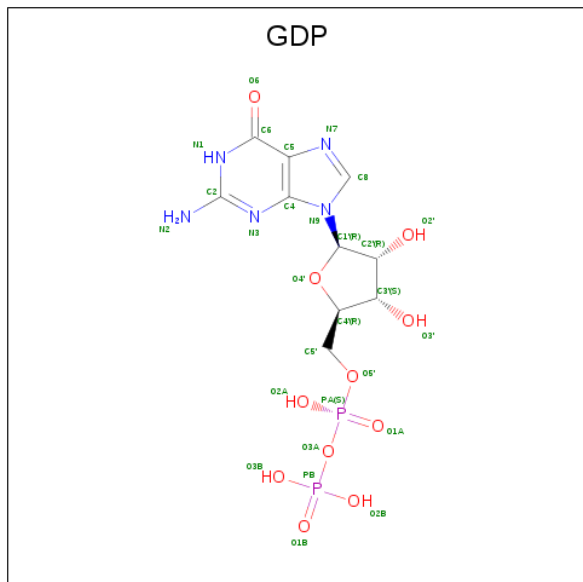
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	2	Total Mg 2 2	0	0
6	A	1	Total Mg 1 1	0	0
6	D	1	Total Mg 1 1	0	0
6	C	1	Total Mg 1 1	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

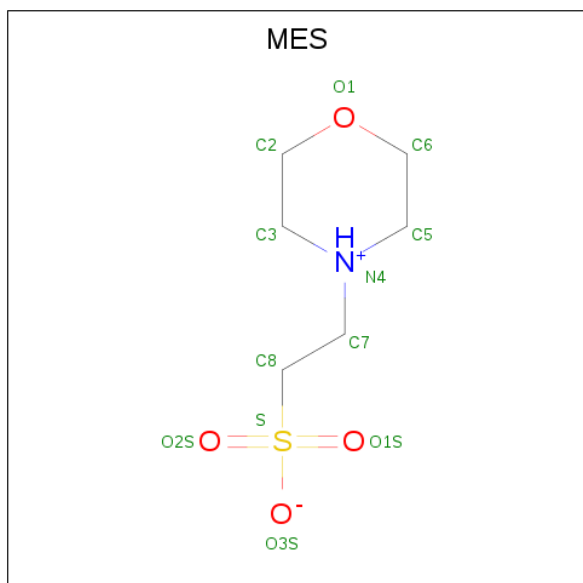
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Ca 1 1	0	0
7	A	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



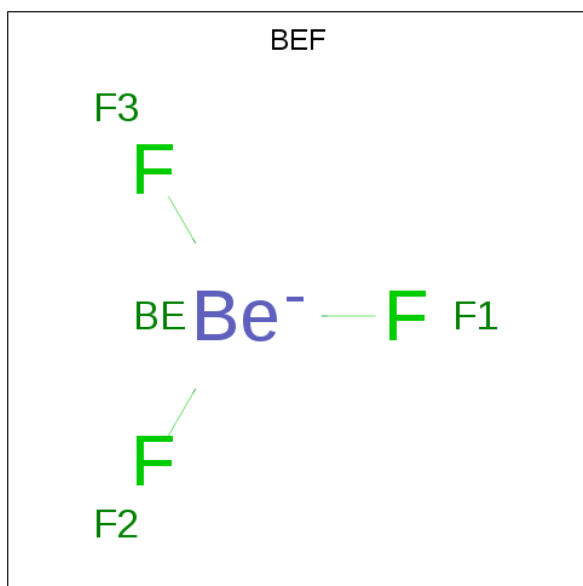
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
8	B	1	Total	C	H	N	O	P	0	0
			38	10	10	5	11	2		
8	D	1	Total	C	H	N	O	P	0	0
			38	10	10	5	11	2		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



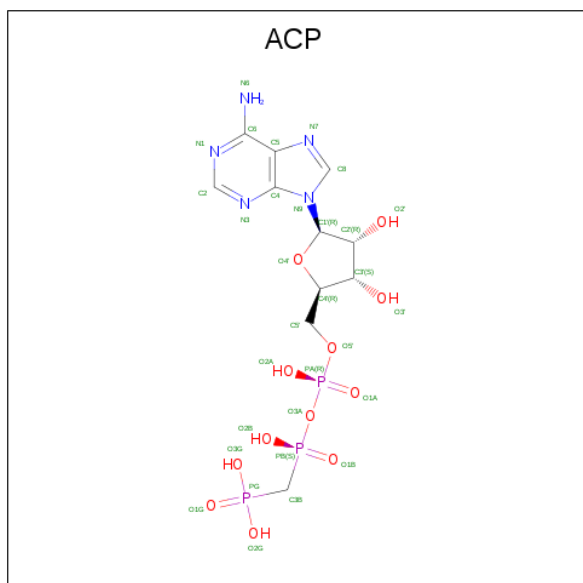
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	S	
			25	6	13	1	4	1	
								0	0

- Molecule 10 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula:  $\text{BeF}_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	D	1	Total	Be	F		
			4	1	3		
						0	0

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula:  $\text{C}_{11}\text{H}_{18}\text{N}_5\text{O}_{12}\text{P}_3$ ).



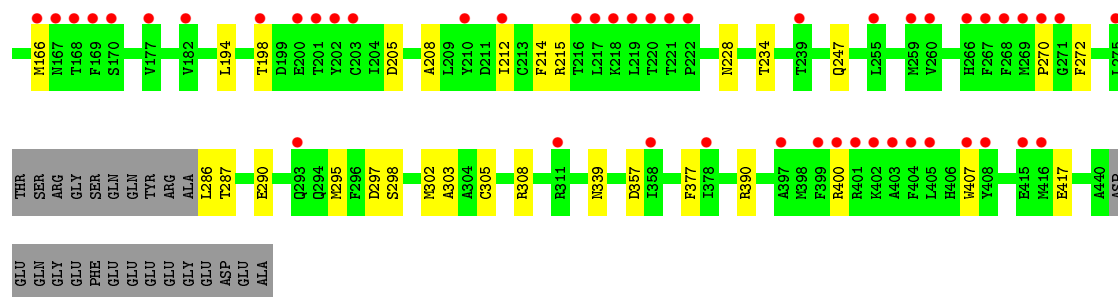
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
11	F	1	Total	C	H	N	O	P	0	0
			45	11	14	5	12	3		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	6	Total	O	0	0
			6	6		
12	B	10	Total	O	0	0
			10	10		
12	C	25	Total	O	0	0
			25	25		
12	D	3	Total	O	0	0
			3	3		
12	E	2	Total	O	0	0
			2	2		
12	F	4	Total	O	0	0
			4	4		



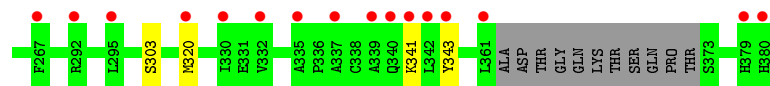
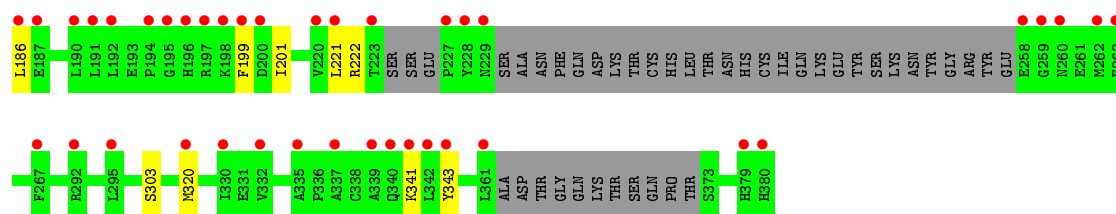
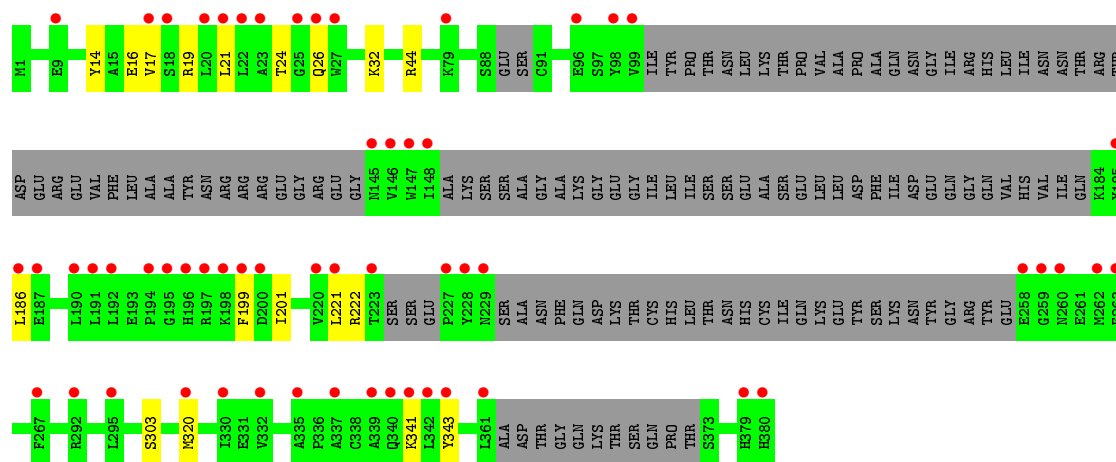




- Molecule 3: Stathmin-4



- Molecule 4: Tubulin tyrosine ligase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.18Å 156.74Å 180.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.46 – 2.49 49.46 – 2.49	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.46-2.49) 100.0 (49.46-2.49)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 2.48Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.212 , 0.257 0.214 , 0.216	Depositor DCC
$R_{free}$ test set	5257 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.2	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 47.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	33075	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.25	0/3495	0.43	0/4743
1	C	0.26	0/3529	0.43	0/4791
2	B	0.26	0/3417	0.44	0/4625
2	D	0.25	0/3374	0.42	0/4570
3	E	0.25	0/975	0.37	0/1295
4	F	0.25	0/2163	0.41	0/2919
All	All	0.25	0/16953	0.42	0/22943

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 [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	3410	3338	3337	11	0
1	C	3445	3360	3357	9	0
2	B	3338	3222	3222	14	0
2	D	3301	3185	3185	23	0
3	E	964	985	985	2	0
4	F	2114	2121	2121	8	0
5	A	32	10	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	10	12	0	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	10	12	1	0
8	D	28	10	12	0	0
9	B	12	13	13	0	0
10	D	4	0	0	0	0
11	F	31	14	12	3	0
12	A	6	0	0	0	0
12	B	10	0	0	0	0
12	C	25	0	0	0	0
12	D	3	0	0	0	0
12	E	2	0	0	0	0
12	F	4	0	0	2	0
All	All	16797	16278	16280	66	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 2.

All (66) 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:211:ASP:OD2	1:C:304:LYS:NZ	2.21	0.73
11:F:401:ACP:O3G	12:F:501:HOH:O	2.10	0.70
2:D:75:MET:SD	2:D:76:ASP:N	2.66	0.69
1:A:239:THR:OG1	1:A:243:ARG:NH1	2.31	0.63
2:B:172:MET:SD	2:B:387:LEU:HD11	2.41	0.60
11:F:401:ACP:O1B	12:F:501:HOH:O	2.17	0.59
1:A:27:GLU:OE2	1:A:243:ARG:NH2	2.37	0.57
2:B:2:ARG:NH1	2:B:3:GLU:OE2	2.41	0.54
2:B:1:MET:SD	2:B:253:ARG:NH1	2.82	0.53
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.40	0.52
3:E:138:GLU:OE1	3:E:138:GLU:N	2.44	0.51
2:B:284:ARG:H	2:B:284:ARG:CD	2.24	0.50
2:D:102:ASN:ND2	2:D:407:TRP:O	2.44	0.49
1:C:221:ARG:NH2	1:C:222:PRO:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:63:PRO:HD3	2:D:86:ILE:HG13	1.95	0.49
4:F:14:TYR:HA	4:F:17:VAL:HG12	1.95	0.48
2:D:108:TYR:OH	2:D:417:GLU:OE2	2.21	0.48
2:D:308:ARG:NH1	2:D:339:ASN:OD1	2.46	0.48
2:D:205:ASP:OD2	2:D:390:ARG:NH2	2.42	0.48
2:B:284:ARG:H	2:B:284:ARG:HD3	1.78	0.47
2:B:303:ALA:O	2:B:305:CYS:N	2.47	0.47
2:D:194:LEU:O	2:D:198:THR:HG22	2.14	0.47
2:D:214:PHE:HD1	2:D:215:ARG:HG2	1.80	0.46
2:D:70:LEU:HB3	2:D:98:GLY:HA2	1.98	0.46
4:F:199:PHE:CD1	4:F:221:LEU:HD11	2.49	0.46
1:C:274:PRO:HG2	1:C:371:VAL:HG11	1.97	0.46
1:C:11:GLN:OE1	2:D:247:GLN:NE2	2.49	0.45
1:A:158:SER:OG	1:A:166:LYS:NZ	2.24	0.45
4:F:186:LEU:HD12	4:F:320:MET:HG2	1.99	0.45
2:D:234:THR:HG21	2:D:302:MET:HG3	1.99	0.44
1:A:229:ARG:HD3	1:A:363:VAL:HG11	2.00	0.44
4:F:201:ILE:HG12	4:F:221:LEU:HD13	1.99	0.44
4:F:24:THR:HG23	4:F:26:GLN:H	1.81	0.44
2:D:297:ASP:OD1	2:D:298:SER:N	2.52	0.43
1:C:341:ILE:HG23	1:C:341:ILE:O	2.19	0.43
1:A:11:GLN:HG3	1:A:74:VAL:HG21	2.01	0.42
1:A:200:CYS:HA	1:A:266:HIS:HB2	2.00	0.42
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.01	0.42
2:D:158:ARG:HG2	3:E:123:LEU:HD11	2.02	0.42
2:B:83:PHE:O	2:B:86:ILE:HG22	2.18	0.42
1:C:4[A]:CYS:SG	1:C:136:LEU:HD13	2.60	0.42
2:B:15:GLN:NE2	8:B:501:GDP:O6	2.52	0.42
2:B:221:THR:HG21	1:C:326:LYS:HA	2.02	0.42
2:D:295:MET:CG	2:D:377:PHE:HB2	2.49	0.42
2:D:208:ALA:O	2:D:212:ILE:HG13	2.19	0.42
2:D:303:ALA:O	2:D:305:CYS:N	2.53	0.41
1:A:167:LEU:HD12	1:A:252:LEU:HD22	2.01	0.41
4:F:222:ARG:NH1	11:F:401:ACP:O2G	2.42	0.41
4:F:21:LEU:O	4:F:24:THR:HG22	2.20	0.41
2:B:158:ARG:NH1	2:B:196:GLU:O	2.54	0.41
2:D:234:THR:HG22	2:D:272:PHE:HB2	2.03	0.41
1:A:427:ALA:O	1:A:430:LYS:HG3	2.21	0.41
2:D:16:ILE:HG22	2:D:228:ASN:OD1	2.21	0.41
2:B:265:LEU:HD21	2:B:431:GLU:HB3	2.03	0.40
1:C:105:ARG:NH1	1:C:411:GLU:OE1	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:270:PRO:HG2	2:D:302:MET:HB2	2.02	0.40
2:B:165:ILE:HG21	2:B:252:LEU:HB3	2.03	0.40
4:F:16:GLU:O	4:F:19:ARG:N	2.54	0.40
1:A:188:ILE:HD12	1:A:425:MET:HG3	2.03	0.40
2:B:48:ARG:NH2	2:B:241:CYS:O	2.55	0.40
1:C:71:GLU:HB2	1:C:98:ASP:HB3	2.02	0.40
2:D:287:THR:OG1	2:D:290:GLU:HG3	2.21	0.40
2:D:83:PHE:O	2:D:86:ILE:HG22	2.22	0.40
2:D:50:ASN:ND2	2:D:55:GLU:OE2	2.52	0.40
2:B:42:LEU:HB2	2:B:358:ILE:HD11	2.02	0.40
2:D:154:ILE:HG23	2:D:166:MET:HG2	2.03	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	434/440 (99%)	422 (97%)	12 (3%)	0	100	100
1	C	440/440 (100%)	433 (98%)	7 (2%)	0	100	100
2	B	419/445 (94%)	407 (97%)	12 (3%)	0	100	100
2	D	416/445 (94%)	402 (97%)	14 (3%)	0	100	100
3	E	113/189 (60%)	113 (100%)	0	0	100	100
4	F	242/380 (64%)	238 (98%)	4 (2%)	0	100	100
All	All	2064/2339 (88%)	2015 (98%)	49 (2%)	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	370/371 (100%)	365 (99%)	5 (1%)	67	86
1	C	373/371 (100%)	371 (100%)	2 (0%)	88	96
2	B	368/383 (96%)	362 (98%)	6 (2%)	62	84
2	D	363/383 (95%)	356 (98%)	7 (2%)	57	80
3	E	105/171 (61%)	105 (100%)	0	100	100
4	F	233/338 (69%)	228 (98%)	5 (2%)	53	78
All	All	1812/2017 (90%)	1787 (99%)	25 (1%)	67	86

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	120	ASP
1	A	232	SER
1	A	420	GLU
1	A	430	LYS
2	B	90	ASP
2	B	124	LYS
2	B	139	HIS
2	B	283	TYR
2	B	284	ARG
2	B	385	GLN
1	C	284	GLU
1	C	302	MET
2	D	74	THR
2	D	75	MET
2	D	77	SER
2	D	139	HIS
2	D	286	LEU
2	D	357	ASP
2	D	400	ARG
4	F	32	LYS
4	F	44	ARG

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Mol	Chain	Res	Type
4	F	303	SER
4	F	341	LYS
4	F	343	TYR

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 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	$\# Z  > 2$
11	ACP	F	401	-	27,33,33	3.76	13 (48%)	32,52,52	1.80	6 (18%)
5	GTP	A	501	6	26,34,34	0.97	1 (3%)	33,54,54	1.71	6 (18%)
5	GTP	C	501	6	26,34,34	1.00	1 (3%)	33,54,54	1.69	6 (18%)
8	GDP	B	501	6	24,30,30	1.11	2 (8%)	31,47,47	1.85	7 (22%)
8	GDP	D	501	10,6	24,30,30	1.15	2 (8%)	31,47,47	1.91	8 (25%)
9	MES	B	505	-	12,12,12	2.16	1 (8%)	14,16,16	1.94	6 (42%)
10	BEF	D	503	8	0,3,3	0.00	-	-	-	-



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
11	ACP	F	401	-	-	6/15/38/38	0/3/3/3
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3
8	GDP	B	501	6	-	4/12/32/32	0/3/3/3
8	GDP	D	501	10,6	-	2/12/32/32	0/3/3/3
9	MES	B	505	-	-	1/6/14/14	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	401	ACP	C2'-C3'	-10.71	1.24	1.53
11	F	401	ACP	C2'-C1'	9.20	1.67	1.53
9	B	505	MES	C8-S	-7.20	1.67	1.77
11	F	401	ACP	O4'-C1'	-6.79	1.31	1.41
11	F	401	ACP	C2-N3	4.54	1.39	1.32
11	F	401	ACP	PB-O3A	4.32	1.63	1.58
8	D	501	GDP	C6-C5	3.96	1.48	1.41
11	F	401	ACP	C5'-C4'	-3.88	1.39	1.51
11	F	401	ACP	O3'-C3'	3.87	1.52	1.43
8	B	501	GDP	C6-C5	3.76	1.47	1.41
11	F	401	ACP	C3'-C4'	3.66	1.62	1.53
11	F	401	ACP	C6-N6	3.36	1.46	1.34
5	C	501	GTP	C6-N1	3.19	1.38	1.33
5	A	501	GTP	C6-N1	3.02	1.38	1.33
11	F	401	ACP	PA-O5'	2.62	1.69	1.59
8	D	501	GDP	C5-C4	2.42	1.47	1.40
11	F	401	ACP	O2'-C2'	2.39	1.48	1.43
8	B	501	GDP	C5-C4	2.37	1.47	1.40
11	F	401	ACP	O4'-C4'	2.36	1.50	1.45
11	F	401	ACP	PG-O1G	2.31	1.55	1.50

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	N3-C2-N1	-5.48	120.11	128.68
5	C	501	GTP	N3-C2-N1	-5.31	120.14	127.22
5	A	501	GTP	N3-C2-N1	-5.29	120.16	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	C3'-C2'-C1'	4.99	108.48	100.98
8	D	501	GDP	C2-N3-C4	4.35	120.32	115.36
8	B	501	GDP	C6-N1-C2	4.34	122.83	115.93
8	D	501	GDP	C6-N1-C2	4.33	122.81	115.93
8	B	501	GDP	C2-N3-C4	4.23	120.19	115.36
8	D	501	GDP	C6-C5-C4	-4.19	116.80	120.80
8	B	501	GDP	C6-C5-C4	-4.10	116.88	120.80
8	B	501	GDP	C5-C6-N1	-4.09	117.83	123.43
5	A	501	GTP	C2-N3-C4	4.09	120.03	115.36
8	D	501	GDP	C5-C6-N1	-4.07	117.86	123.43
5	C	501	GTP	C2-N3-C4	4.04	119.97	115.36
11	F	401	ACP	C1'-N9-C4	-3.89	119.80	126.64
9	B	505	MES	C2-C3-N4	-3.70	104.50	110.10
8	D	501	GDP	N3-C2-N1	-3.28	122.85	127.22
8	B	501	GDP	N3-C2-N1	-3.27	122.86	127.22
5	C	501	GTP	PB-O3B-PG	-3.11	122.16	132.83
5	A	501	GTP	C5-C6-N1	-3.09	119.21	123.43
5	C	501	GTP	C5-C6-N1	-2.97	119.37	123.43
5	A	501	GTP	PA-O3A-PB	-2.95	122.71	132.83
8	D	501	GDP	PA-O3A-PB	-2.95	122.72	132.83
9	B	505	MES	C5-N4-C3	2.92	115.41	108.83
5	A	501	GTP	PB-O3B-PG	-2.90	122.89	132.83
5	A	501	GTP	C6-N1-C2	2.68	120.19	115.93
5	C	501	GTP	C6-N1-C2	2.65	120.14	115.93
11	F	401	ACP	C5-C6-N6	2.60	124.30	120.35
5	C	501	GTP	PA-O3A-PB	-2.52	124.16	132.83
11	F	401	ACP	PA-O3A-PB	-2.52	124.56	132.56
9	B	505	MES	O3S-S-C8	2.48	109.79	105.77
8	B	501	GDP	PA-O3A-PB	-2.39	124.61	132.83
9	B	505	MES	C7-N4-C5	2.35	117.24	111.23
8	D	501	GDP	C4-C5-N7	-2.33	106.97	109.40
8	B	501	GDP	C4-C5-N7	-2.24	107.06	109.40
11	F	401	ACP	C2'-C3'-C4'	2.24	107.00	102.64
9	B	505	MES	C6-C5-N4	-2.18	106.80	110.10
8	D	501	GDP	C3'-C2'-C1'	2.18	104.25	100.98
9	B	505	MES	O2S-S-C8	2.08	109.42	106.92

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	F	401	ACP	PG-C3B-PB-O3A

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Mol	Chain	Res	Type	Atoms
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	C5'-O5'-PA-O2A
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
11	F	401	ACP	C3'-C4'-C5'-O5'
11	F	401	ACP	O4'-C4'-C5'-O5'
11	F	401	ACP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3A-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
9	B	505	MES	C8-C7-N4-C3
5	C	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	PB-O3A-PA-O2A

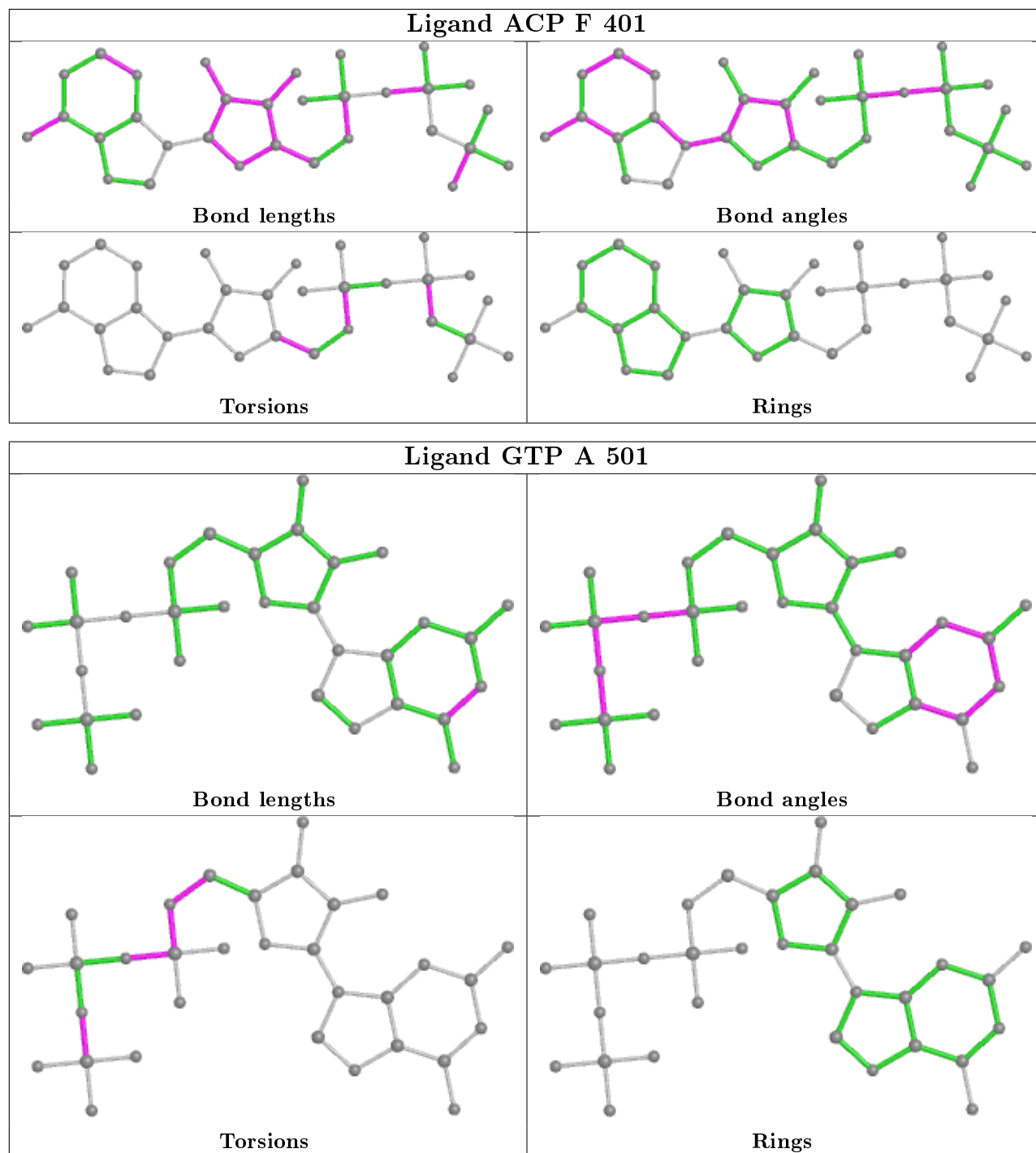
There are no ring outliers.

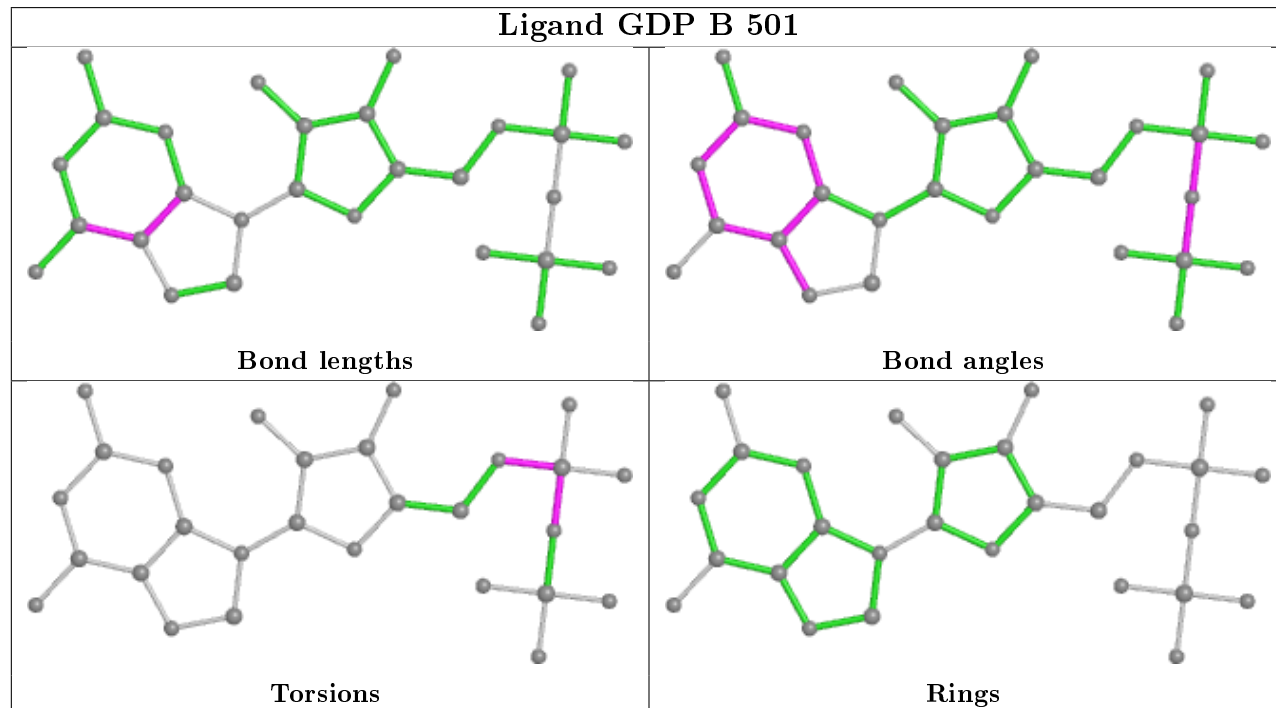
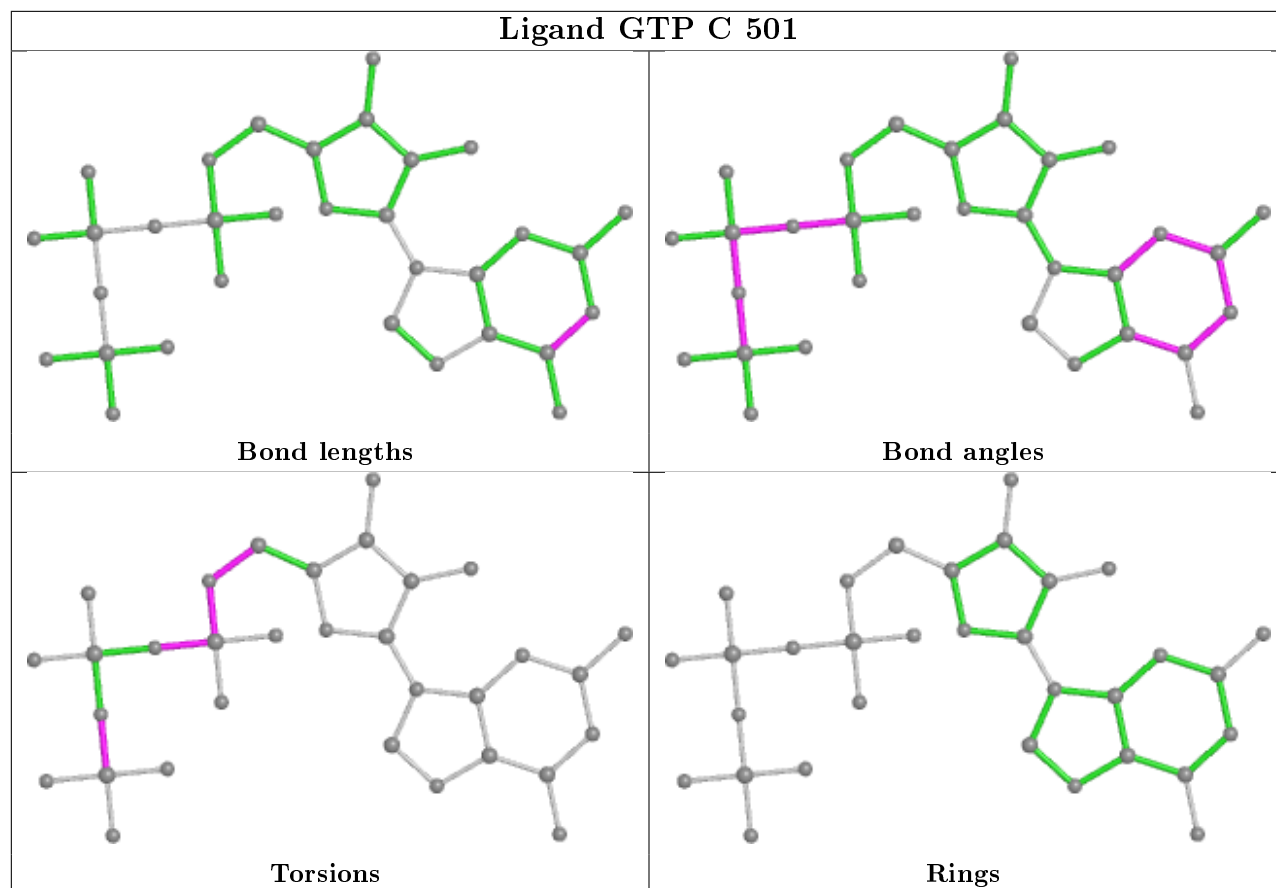
2 monomers are involved in 4 short contacts:

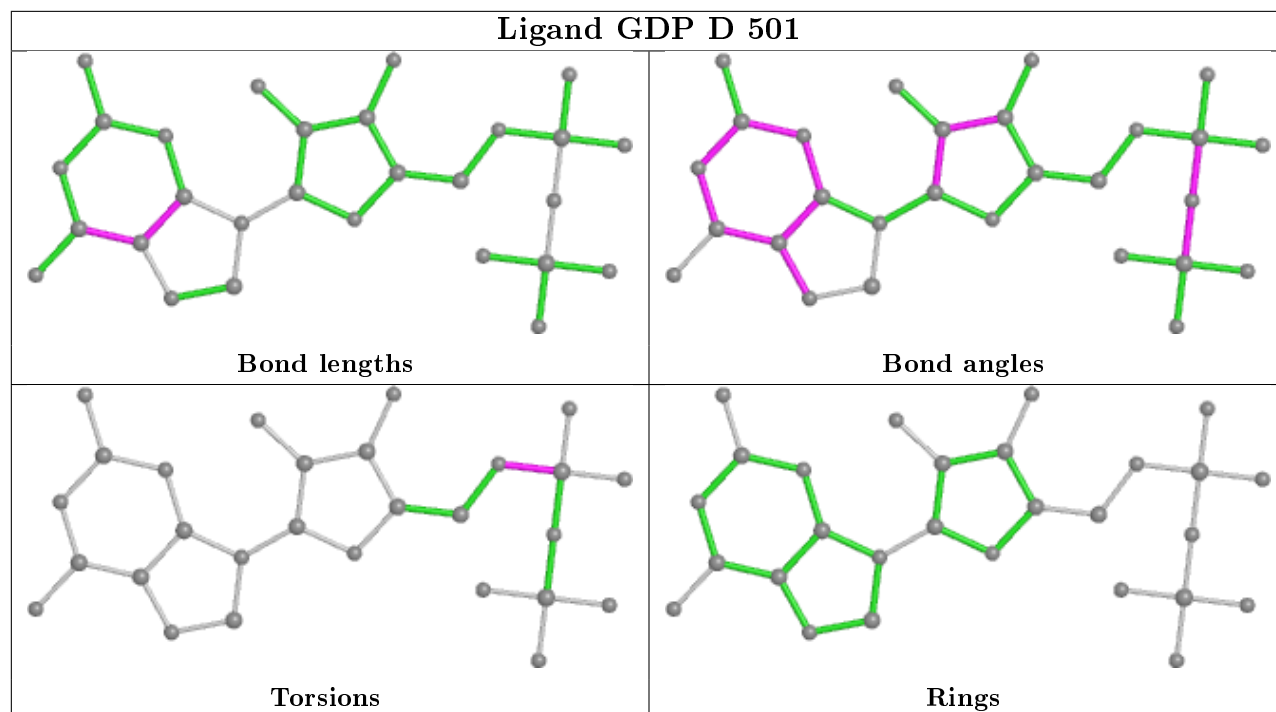
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	401	ACP	3	0
8	B	501	GDP	1	0

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 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.







## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	435/440 (98%)	0.73	38 (8%)	10 10	51, 75, 109, 149	0
1	C	440/440 (100%)	0.32	10 (2%)	60 63	45, 60, 94, 125	0
2	B	423/445 (95%)	0.55	21 (4%)	28 30	46, 69, 106, 142	3 (0%)
2	D	420/445 (94%)	0.92	68 (16%)	1 1	54, 87, 125, 170	3 (0%)
3	E	116/189 (61%)	0.71	9 (7%)	13 13	60, 86, 122, 135	0
4	F	256/380 (67%)	1.12	58 (22%)	0 0	67, 98, 132, 156	0
All	All	2090/2339 (89%)	0.69	204 (9%)	7 7	45, 77, 118, 170	6 (0%)

All (204) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	186	LEU	8.0
4	F	147	TRP	7.1
3	E	27	PRO	7.1
2	B	438	ALA	6.5
4	F	259	GLY	6.3
4	F	330	ILE	6.0
4	F	199	PHE	5.8
4	F	145	ASN	5.7
2	D	401	ARG	5.6
4	F	192	LEU	5.3
2	D	96	GLN	5.3
2	D	400	ARG	5.2
2	B	59	ASN	5.2
2	D	182	VAL	5.2
3	E	26	PRO	5.0
4	F	26	GLN	5.0
4	F	98	TYR	4.9
4	F	320	MET	4.8
4	F	99	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	364	PRO	4.7
4	F	191	LEU	4.5
4	F	198	LYS	4.5
4	F	21	LEU	4.5
4	F	223	THR	4.5
2	D	203	CYS	4.5
4	F	335	ALA	4.4
3	E	25	LYS	4.3
4	F	17	VAL	4.2
4	F	332	VAL	4.2
1	A	262	TYR	4.1
4	F	228	TYR	4.1
2	D	37	HIS	4.0
4	F	227	PRO	3.9
2	D	99	ALA	3.9
4	F	9	GLU	3.9
2	B	37	HIS	3.8
2	D	402	LYS	3.8
2	D	399	PHE	3.8
4	F	146	VAL	3.8
2	D	275	LEU	3.7
3	E	45	PRO	3.7
4	F	25	GLY	3.7
2	B	85	GLN	3.7
2	B	276	THR	3.6
2	D	404	PHE	3.6
2	D	198	THR	3.5
4	F	262	MET	3.5
4	F	22	LEU	3.5
4	F	361	LEU	3.4
1	C	340	SER	3.3
2	D	167	ASN	3.3
2	B	82	PRO	3.3
2	D	405	LEU	3.3
1	A	179	THR	3.3
2	B	36	TYR	3.2
3	E	139	LEU	3.2
2	D	75	MET	3.2
4	F	197	ARG	3.2
2	D	202	TYR	3.2
1	C	368	LEU	3.2
2	D	46	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
4	F	267	PHE	3.1
4	F	341	LYS	3.1
2	D	57	THR	3.1
4	F	20	LEU	3.1
3	E	23	ILE	3.1
2	D	403	ALA	3.0
2	B	282	GLN	3.0
4	F	190	LEU	3.0
1	A	344	VAL	3.0
4	F	200	ASP	3.0
4	F	220	VAL	3.0
4	F	260	ASN	3.0
1	C	357	TYR	3.0
2	B	61	TYR	3.0
1	A	348	PRO	2.9
1	A	170	SER	2.9
4	F	148	ILE	2.9
1	A	180	ALA	2.9
4	F	342	LEU	2.9
2	D	407	TRP	2.8
2	D	200	GLU	2.8
1	C	440	VAL	2.8
2	D	222	PRO	2.8
2	B	248	LEU	2.8
2	B	98	GLY	2.8
2	D	124	LYS	2.8
2	D	170	SER	2.8
2	D	293	GLN	2.8
1	A	172	TYR	2.8
4	F	258	GLU	2.8
1	C	341	ILE	2.7
1	A	85	GLN	2.7
2	B	62	VAL	2.7
2	D	168	THR	2.7
2	B	97	SER	2.7
1	A	124	LYS	2.7
1	A	178	SER	2.7
1	A	141	PHE	2.7
4	F	337	ALA	2.7
2	D	416	MET	2.6
4	F	187	GLU	2.6
1	A	365	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	351	PHE	2.6
2	D	210	TYR	2.6
1	C	1	MET	2.6
1	A	99	ALA	2.5
1	A	142	GLY	2.5
2	B	34	GLY	2.5
3	E	46	SER	2.5
2	D	219	LEU	2.5
4	F	340	GLN	2.5
1	A	346	TRP	2.5
4	F	263	PHE	2.5
1	C	85	GLN	2.5
2	D	415	GLU	2.5
2	D	267	PHE	2.5
2	B	60	LYS	2.4
2	D	397	ALA	2.4
2	D	177	VAL	2.4
4	F	380	HIS	2.4
1	A	42	ILE	2.4
1	A	209	ILE	2.4
3	E	122	ARG	2.4
2	D	166	MET	2.4
2	D	201	THR	2.4
2	D	221	THR	2.4
1	A	177	VAL	2.4
2	D	95	GLY	2.4
2	D	408	TYR	2.4
1	A	201	ALA	2.4
4	F	339	ALA	2.4
4	F	185	TYR	2.4
1	A	173	PRO	2.3
2	B	358	ILE	2.3
2	D	127	GLU	2.3
2	B	16	ILE	2.3
1	A	18	ASN	2.3
1	A	59	GLY	2.3
2	D	59	ASN	2.3
1	A	316[A]	CYS	2.3
2	D	169	PHE	2.3
2	B	49	ILE	2.3
1	C	4[A]	CYS	2.3
2	D	35	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	239	THR	2.3
4	F	221	LEU	2.3
4	F	295	LEU	2.3
2	D	82	PRO	2.3
1	A	146	GLY	2.3
1	A	100	ALA	2.3
1	A	88	HIS	2.2
4	F	96	GLU	2.2
2	B	56	ALA	2.2
1	A	82	THR	2.2
2	D	216	THR	2.2
1	A	9	VAL	2.2
2	D	269	MET	2.2
2	D	212	ILE	2.2
4	F	196	HIS	2.2
2	D	220	THR	2.2
4	F	194	PRO	2.2
4	F	229	ASN	2.2
2	D	93	VAL	2.2
4	F	379	HIS	2.2
2	D	70	LEU	2.2
2	D	76	ASP	2.2
3	E	24	LEU	2.2
2	D	259	MET	2.2
1	A	93	ILE	2.2
1	A	171	ILE	2.2
2	D	358	ILE	2.2
2	D	217	LEU	2.2
1	C	2	ARG	2.2
4	F	18	SER	2.2
2	D	56	ALA	2.2
2	D	33	THR	2.2
2	D	218	LYS	2.1
2	D	260	VAL	2.1
2	D	311	ARG	2.1
4	F	27	TRP	2.1
2	D	268	PHE	2.1
1	A	123	ARG	2.1
1	A	96	LYS	2.1
2	B	9	ALA	2.1
2	D	270	PRO	2.1
2	B	55	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	39	ASP	2.1
2	D	378	ILE	2.1
1	A	347	CYS	2.1
2	D	137	LEU	2.1
2	D	255	LEU	2.1
4	F	79	LYS	2.1
1	C	276	ILE	2.0
2	D	266	HIS	2.0
2	D	60	LYS	2.0
1	A	167	LEU	2.0
4	F	195	GLY	2.0
1	A	280	LYS	2.0
4	F	23	ALA	2.0
1	A	68	VAL	2.0
2	D	271	GLY	2.0
4	F	292	ARG	2.0
4	F	343	TYR	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 carbohydrates 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<sup>th</sup> 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
6	MG	B	502	1/1	0.39	0.28	64,64,64,64	0
6	MG	B	504	1/1	0.73	0.11	88,88,88,88	0
7	CA	B	503	1/1	0.73	0.23	104,104,104,104	0
10	BEF	D	503	4/4	0.86	0.12	80,81,82,84	0
11	ACP	F	401	31/31	0.90	0.20	106,110,128,131	0
6	MG	D	502	1/1	0.92	0.11	110,110,110,110	0

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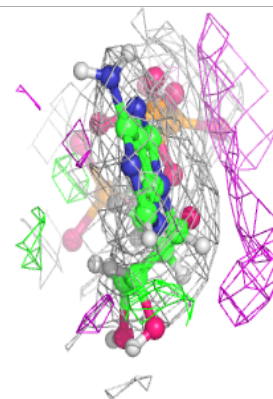
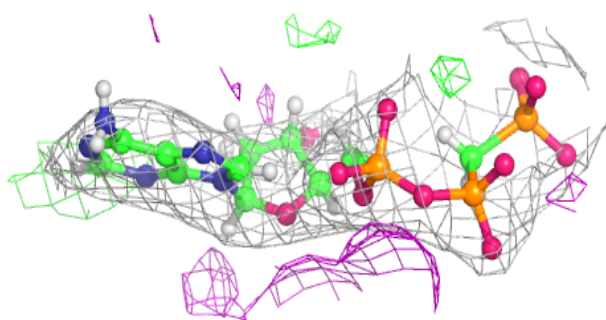
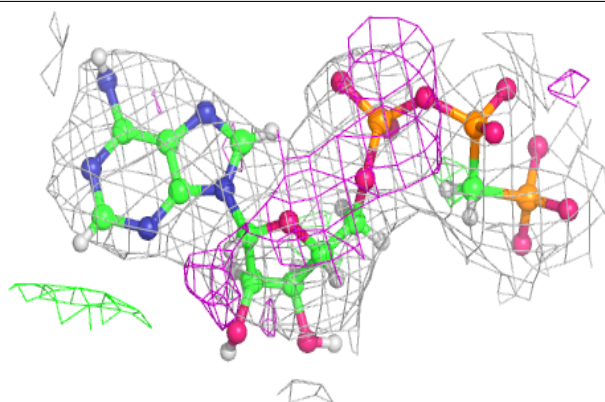
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	CA	A	503	1/1	0.93	0.03	95,95,95,95	0
7	CA	C	503	1/1	0.94	0.15	85,85,85,85	0
6	MG	C	502	1/1	0.94	0.20	51,51,51,51	0
9	MES	B	505	12/12	0.94	0.16	63,68,86,91	0
8	GDP	B	501	28/28	0.95	0.26	40,53,63,71	0
8	GDP	D	501	28/28	0.95	0.15	66,76,93,102	0
5	GTP	C	501	32/32	0.95	0.22	37,47,76,88	0
5	GTP	A	501	32/32	0.97	0.31	43,54,65,83	0
6	MG	A	502	1/1	0.98	0.27	52,52,52,52	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.

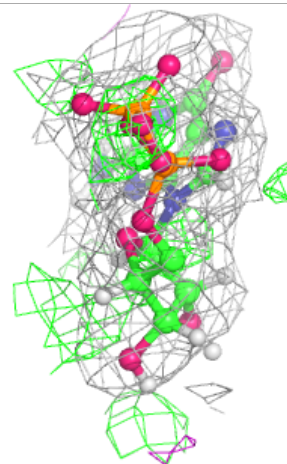
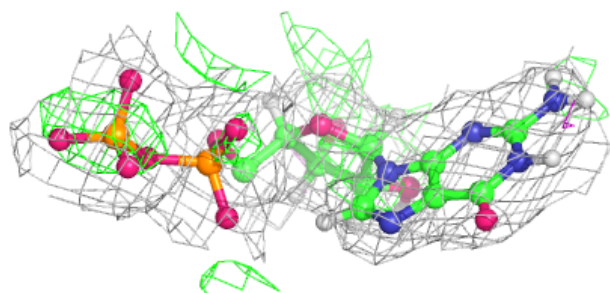
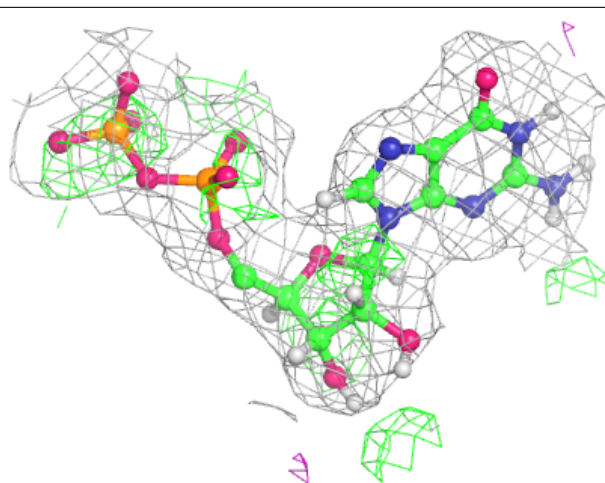
**Electron density around ACP F 401:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



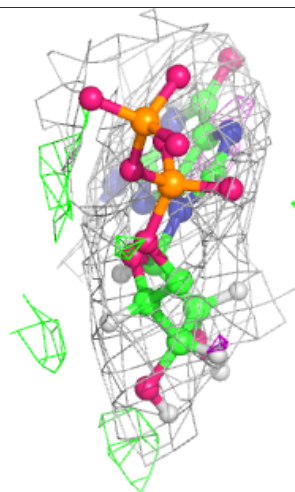
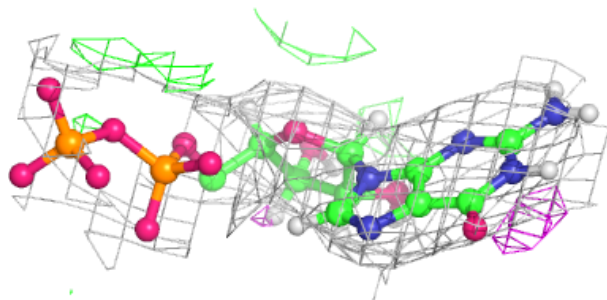
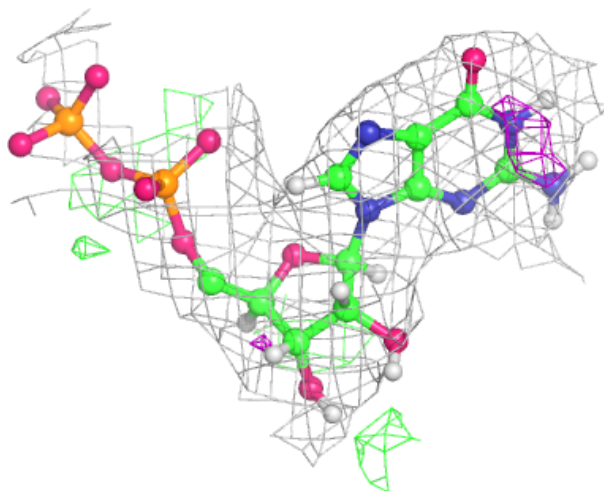
**Electron density around GDP B 501:**

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



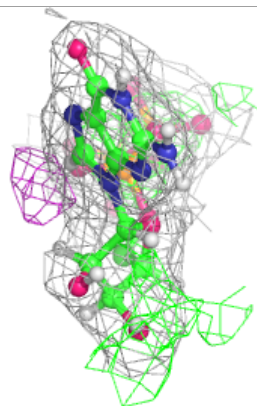
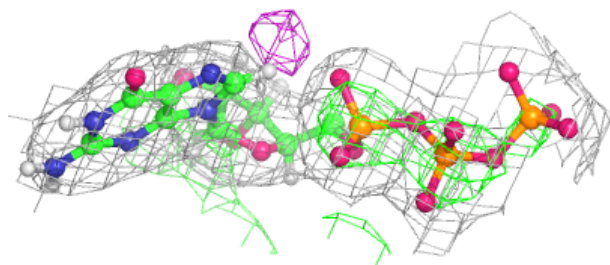
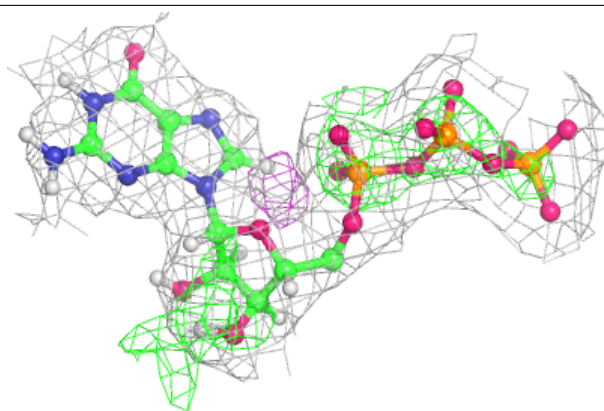
**Electron density around GDP D 501:**

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

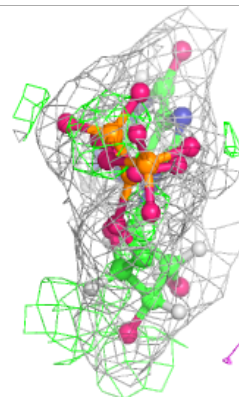
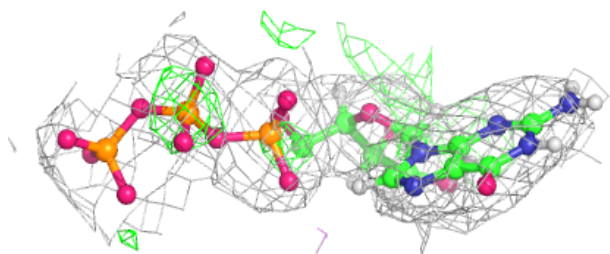
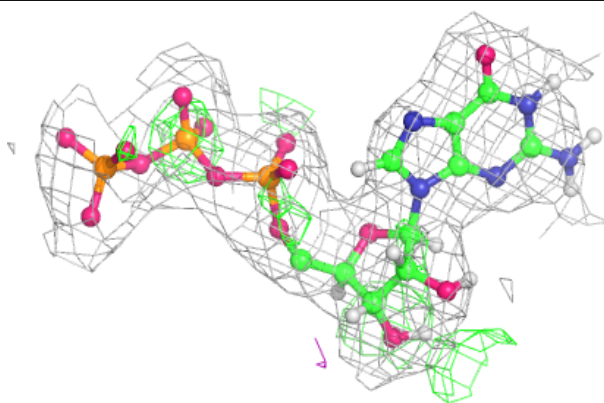


**Electron density around GTP C 501:**

$2mF_o-DF_c$  (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 [i](#)

There are no such residues in this entry.