



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 09:07 pm BST

PDB ID : 6F7C  
Title : TUBULIN-Compound 12 complex  
Authors : Muehlethaler, T.; Protá, A.E.; Steinmetz, M.O.  
Deposited on : 2017-12-08  
Resolution : 2.00 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

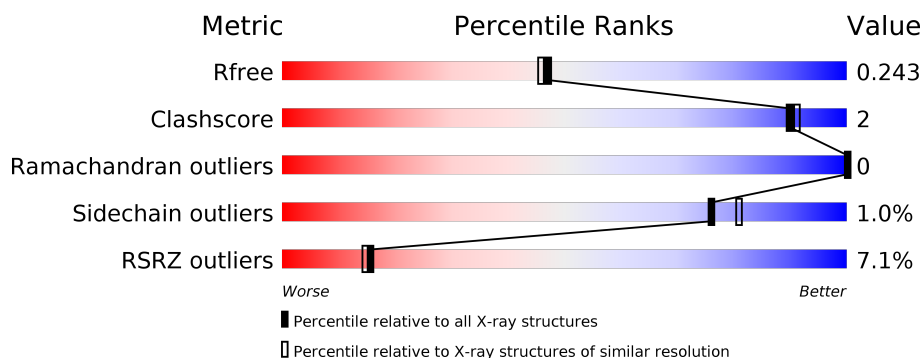
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	451	<div> <div>0%</div> <div>92%</div> <div>5%</div> <div>5%</div> </div>
1	C	451	<div> <div>2%</div> <div>92%</div> <div>5%</div> <div>5%</div> </div>
2	B	445	<div> <div>2%</div> <div>90%</div> <div>5%</div> <div>5%</div> </div>
2	D	445	<div> <div>10%</div> <div>88%</div> <div>6%</div> <div>6%</div> </div>
3	E	143	<div> <div>10%</div> <div>78%</div> <div>17%</div> </div>
4	F	384	<div> <div>18%</div> <div>70%</div> <div>27%</div> </div>

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 34179 atoms, of which 16500 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	431	Total	C	H	N	O	S	0	3	0
			6665	2133	3295	572	641	24			
1	C	440	Total	C	H	N	O	S	0	4	0
			6831	2188	3379	584	658	22			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	424	Total	C	H	N	O	S	0	2	0
			6596	2108	3240	576	646	26			
2	D	420	Total	C	H	N	O	S	0	2	0
			6500	2081	3191	561	640	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	118	Total	C	H	N	O	S	0	1	0
			1984	605	1006	178	191	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	ILE	cloning artifact	UNP P63043
E	4	ALA	SER	cloning artifact	UNP P63043

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	281	Total	C	H	N	O	S	0	0	0
			4609	1492	2306	388	411	12			

There are 6 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
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

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



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	P	0	0	
			41	10	9	5	14	3			
5	C	1	Total	C	H	N	O	P	0	0	
			41	10	9	5	14	3			

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

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

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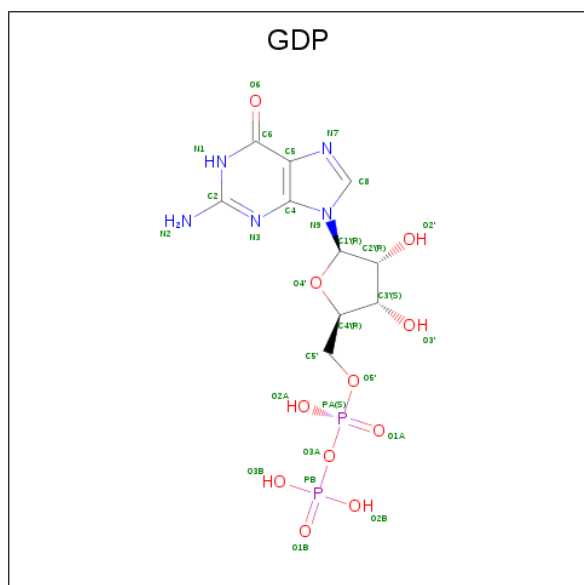
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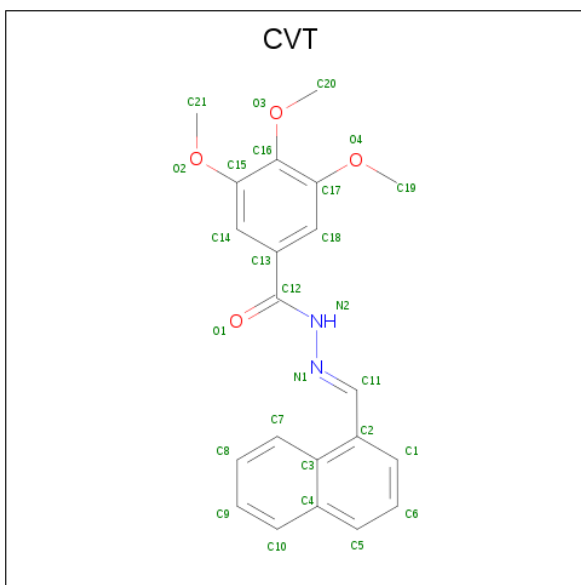
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	2	Total	Ca	0	0
			2	2		

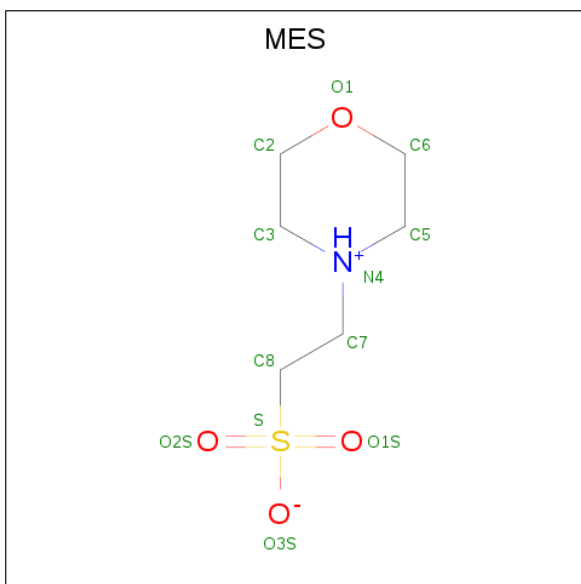
- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).





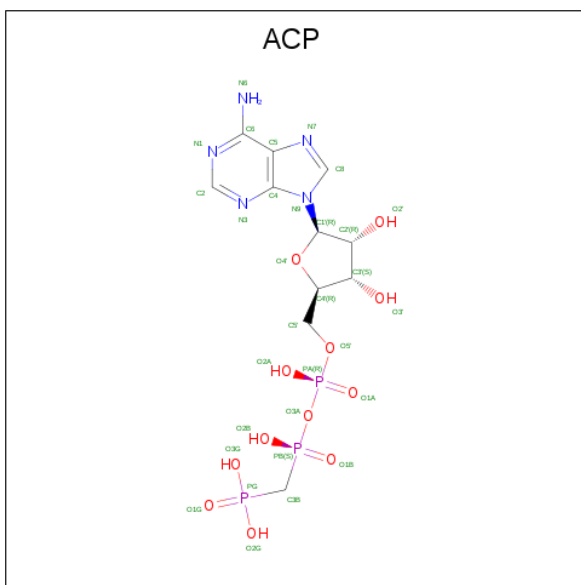
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	0	0
			47	21	20	2	4		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



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

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula:  $C_{11}H_{18}N_5O_{12}P_3$ ).



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

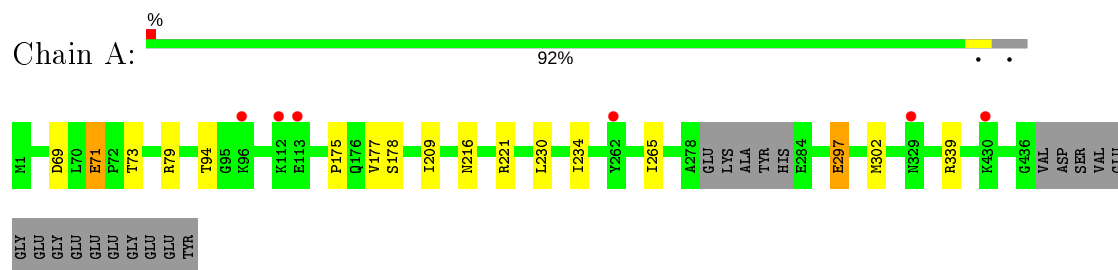
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	127	Total O 127 127	0	0
12	B	161	Total O 161 161	0	0
12	C	293	Total O 293 293	0	0
12	D	63	Total O 63 63	0	0
12	E	29	Total O 29 29	0	0
12	F	40	Total O 40 40	0	0

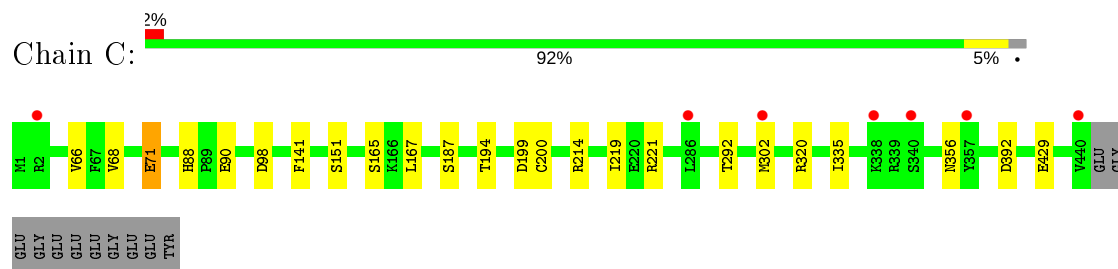
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

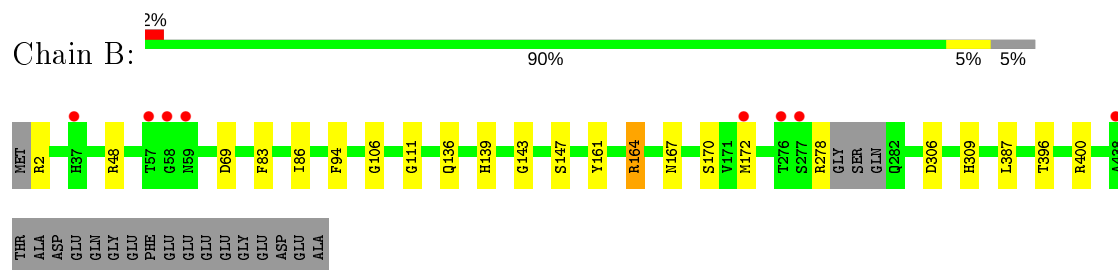
- Molecule 1: Tubulin alpha-1B chain



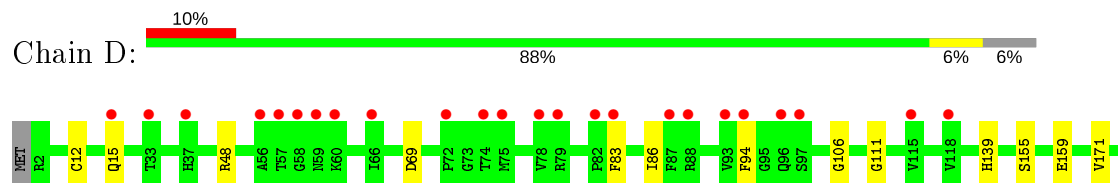
- Molecule 1: Tubulin alpha-1B chain



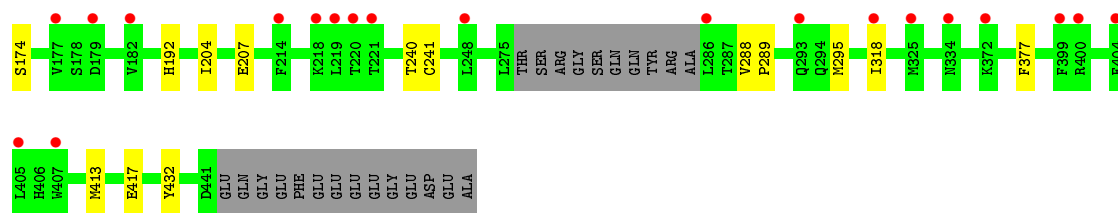
- Molecule 2: Tubulin beta-2B chain



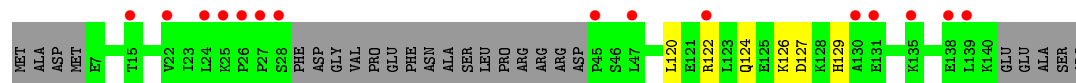
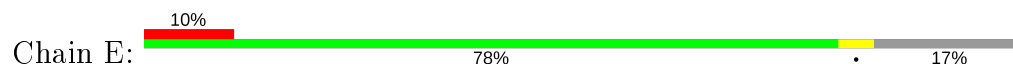
- Molecule 2: Tubulin beta-2B chain



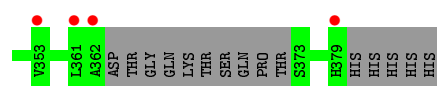
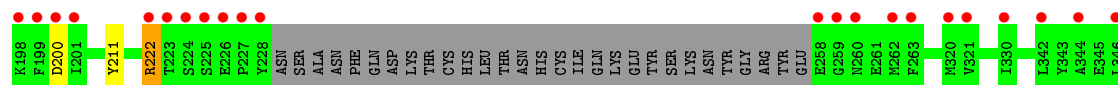
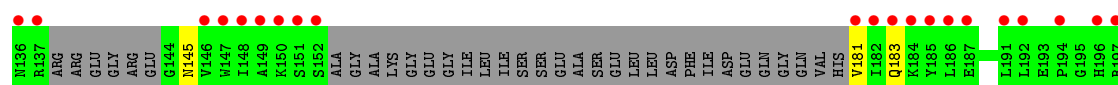
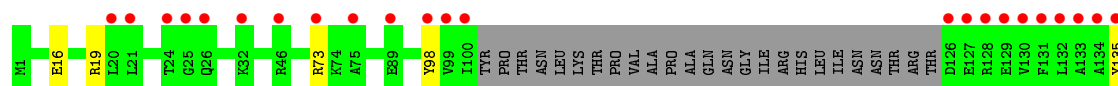




● Molecule 3: Stathmin-4



● 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, $\alpha$ , $\beta$ , $\gamma$	104.81Å 157.90Å 180.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.54 – 2.00 59.54 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (59.54-2.00) 99.2 (59.54-2.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.01 (at 2.00Å)	Xtriage
Refinement program	PHENIX (dev_2863: ???)	Depositor
R, $R_{free}$	0.212 , 0.243 0.211 , 0.243	Depositor DCC
$R_{free}$ test set	10120 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.1	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 50.1	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	0.96	EDS
Total number of atoms	34179	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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, CVT, GTP, ACP, MES, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.33	0/3456	0.50	0/4690
1	C	0.42	0/3542	0.56	0/4811
2	B	0.38	0/3433	0.52	0/4648
2	D	0.32	0/3388	0.48	0/4590
3	E	0.36	0/989	0.43	0/1311
4	F	0.30	0/2354	0.45	0/3178
All	All	0.36	0/17162	0.50	0/23228

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	3370	3295	3286	14	0
1	C	3452	3379	3378	11	0
2	B	3356	3240	3238	11	0
2	D	3309	3191	3191	17	0
3	E	978	1006	1005	4	0
4	F	2303	2306	2306	5	0
5	A	32	9	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	9	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	C	2	0	0	0	0
8	B	28	9	12	0	0
8	D	28	9	12	2	0
9	B	27	20	0	0	0
10	B	12	13	13	0	0
11	F	31	14	14	0	0
12	A	127	0	0	0	0
12	B	161	0	0	1	0
12	C	293	0	0	0	0
12	D	63	0	0	2	0
12	E	29	0	0	0	0
12	F	40	0	0	1	0
All	All	17679	16500	16479	59	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 (59) 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)
4:F:200:ASP:OD1	4:F:222:ARG:HB2	1.81	0.80
2:D:15:GLN:NE2	8:D:501:GDP:O6	2.34	0.58
1:A:297:GLU:OE1	1:A:339:ARG:NH2	2.37	0.57
2:D:417:GLU:OE2	3:E:129:HIS:NE2	2.40	0.54
4:F:16:GLU:OE2	4:F:19:ARG:NH2	2.41	0.53
1:A:175:PRO:HA	1:A:178:SER:HB3	1.89	0.53
2:B:143:GLY:O	2:B:147:SER:OG	2.28	0.52
2:B:170:SER:O	2:B:172:MET:HE3	2.09	0.52
2:D:106:GLY:O	2:D:111:GLY:HA3	2.09	0.52
2:D:295:MET:CG	2:D:377:PHE:HB2	2.39	0.52
1:A:234:ILE:HD13	1:A:302:MET:SD	2.52	0.50
1:C:392:ASP:OD2	1:C:429:GLU:OE2	2.29	0.50
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.93	0.49
2:D:288:VAL:HB	2:D:289:PRO:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:GLN:HA	2:B:167:ASN:O	2.13	0.49
1:C:320:ARG:HA	1:C:356:ASN:O	2.13	0.48
2:D:171:VAL:HA	2:D:204:ILE:O	2.14	0.47
1:A:297:GLU:HG3	12:F:524:HOH:O	2.15	0.47
1:A:297:GLU:CD	1:A:339:ARG:HH22	2.19	0.46
1:C:88:HIS:HB3	1:C:90:GLU:OE1	2.16	0.45
2:D:48:ARG:NH2	12:D:603:HOH:O	2.49	0.45
2:D:155[B]:SER:OG	3:E:126:LYS:HE2	2.17	0.45
2:B:161:TYR:HB3	2:B:164:ARG:HG3	1.98	0.45
1:A:297:GLU:CA	1:A:297:GLU:OE1	2.65	0.45
1:A:71:GLU:OE1	1:A:73:THR:OG1	2.24	0.45
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.32	0.44
2:D:413:MET:CE	2:D:417:GLU:OE1	2.66	0.44
2:D:240:THR:HB	2:D:318:ILE:HD13	2.00	0.44
2:D:69:ASP:O	2:D:94:PHE:HA	2.18	0.44
2:B:69:ASP:O	2:B:94:PHE:HA	2.18	0.43
4:F:98:TYR:O	4:F:181:VAL:N	2.51	0.43
2:B:396:THR:O	2:B:400:ARG:HG2	2.18	0.43
2:B:83:PHE:O	2:B:86:ILE:HG22	2.18	0.43
1:C:151[B]:SER:HA	1:C:194[B]:THR:HG22	2.01	0.43
1:C:165:SER:HA	1:C:199:ASP:OD2	2.18	0.43
2:D:241:CYS:SG	2:D:318:ILE:HD12	2.59	0.43
2:D:432:TYR:OH	12:D:601:HOH:O	2.21	0.43
2:B:48:ARG:NH2	12:B:615:HOH:O	2.49	0.42
1:A:209:ILE:HD11	1:A:302:MET:SD	2.59	0.42
2:B:106:GLY:O	2:B:111:GLY:HA3	2.19	0.42
3:E:120:LEU:O	3:E:124:GLN:HG2	2.20	0.42
2:D:159:GLU:OE2	3:E:127:ASP:OD2	2.38	0.42
1:A:177:VAL:HG23	1:A:177:VAL:O	2.19	0.41
1:A:297:GLU:HA	1:A:297:GLU:OE1	2.20	0.41
2:D:174:SER:OG	2:D:207:GLU:OE1	2.23	0.41
1:A:69:ASP:O	1:A:94:THR:HA	2.21	0.41
1:C:66:VAL:HG12	1:C:68[A]:VAL:HG23	2.03	0.41
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.56	0.41
1:C:167:LEU:HG	1:C:200:CYS:HB3	2.01	0.41
2:D:83:PHE:O	2:D:86:ILE:HG22	2.21	0.41
1:C:71:GLU:HG2	1:C:98:ASP:HB3	2.03	0.41
1:C:214:ARG:HG2	1:C:219:ILE:O	2.21	0.41
1:A:216:ASN:OD1	1:A:216:ASN:N	2.54	0.40
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.52	0.40
1:A:265:ILE:HG22	1:A:265:ILE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:200:ASP:OD2	4:F:222:ARG:NH1	2.54	0.40
1:C:141:PHE:HB3	1:C:187:SER:OG	2.21	0.40
1:A:209:ILE:HG23	1:A:230:LEU:HD23	2.02	0.40
4:F:135:TYR:O	4:F:145:ASN:ND2	2.54	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	430/451 (95%)	418 (97%)	12 (3%)	0	100	100
1	C	442/451 (98%)	433 (98%)	9 (2%)	0	100	100
2	B	422/445 (95%)	413 (98%)	9 (2%)	0	100	100
2	D	418/445 (94%)	408 (98%)	10 (2%)	0	100	100
3	E	115/143 (80%)	114 (99%)	1 (1%)	0	100	100
4	F	269/384 (70%)	257 (96%)	12 (4%)	0	100	100
All	All	2096/2319 (90%)	2043 (98%)	53 (2%)	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	365/379 (96%)	361 (99%)	4 (1%)	73	78
1	C	375/379 (99%)	372 (99%)	3 (1%)	81	86
2	B	369/383 (96%)	365 (99%)	4 (1%)	73	78
2	D	365/383 (95%)	363 (100%)	2 (0%)	88	92
3	E	107/127 (84%)	106 (99%)	1 (1%)	78	83
4	F	253/342 (74%)	249 (98%)	4 (2%)	62	67
All	All	1834/1993 (92%)	1816 (99%)	18 (1%)	76	81

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	79	ARG
1	A	221	ARG
1	A	297	GLU
2	B	2	ARG
2	B	139	HIS
2	B	164	ARG
2	B	278	ARG
1	C	71	GLU
1	C	221	ARG
1	C	302	MET
2	D	139	HIS
2	D	192	HIS
3	E	122	ARG
4	F	73	ARG
4	F	183	GLN
4	F	211	TYR
4	F	222	ARG

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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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
5	GTP	C	501	6	26,34,34	0.95	1 (3%)	33,54,54	1.58	4 (12%)
8	GDP	B	501	6	24,30,30	1.13	3 (12%)	31,47,47	1.99	7 (22%)
8	GDP	D	501	6	24,30,30	1.11	2 (8%)	31,47,47	1.94	7 (22%)
9	CVT	B	503	-	29,29,29	1.29	1 (3%)	39,39,39	1.35	5 (12%)
10	MES	B	504	-	12,12,12	2.05	1 (8%)	14,16,16	1.48	2 (14%)
11	ACP	F	401	6	27,33,33	1.25	4 (14%)	32,52,52	1.36	3 (9%)
5	GTP	A	501	6	26,34,34	0.94	1 (3%)	33,54,54	1.72	6 (18%)

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
5	GTP	C	501	6	-	8/18/38/38	0/3/3/3
8	GDP	B	501	6	-	5/12/32/32	0/3/3/3
8	GDP	D	501	6	-	5/12/32/32	0/3/3/3
9	CVT	B	503	-	-	4/16/16/16	0/3/3/3
10	MES	B	504	-	-	1/6/14/14	0/1/1/1
11	ACP	F	401	6	-	3/15/38/38	0/3/3/3
5	GTP	A	501	6	-	8/18/38/38	0/3/3/3

All (13) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	504	MES	C8-S	-6.85	1.67	1.77
9	B	503	CVT	C12-N2	5.76	1.43	1.35
8	D	501	GDP	C6-C5	3.71	1.47	1.41
11	F	401	ACP	PB-O2B	-3.39	1.48	1.56
8	B	501	GDP	C6-C5	3.19	1.46	1.41
5	C	501	GTP	C6-N1	2.98	1.38	1.33
11	F	401	ACP	PG-O2G	2.95	1.61	1.54
11	F	401	ACP	PG-O3G	-2.74	1.48	1.54
5	A	501	GTP	C6-N1	2.58	1.37	1.33
8	D	501	GDP	C5-C4	2.46	1.47	1.40
8	B	501	GDP	C5-C4	2.42	1.47	1.40
8	B	501	GDP	O4'-C1'	2.36	1.44	1.41
11	F	401	ACP	O4'-C1'	2.26	1.44	1.41

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	501	GDP	C6-N1-C2	5.33	124.39	115.93
8	B	501	GDP	C6-C5-C4	-5.23	115.81	120.80
5	C	501	GTP	N3-C2-N1	-4.93	120.65	127.22
8	D	501	GDP	C6-N1-C2	4.86	123.66	115.93
5	A	501	GTP	N3-C2-N1	-4.86	120.74	127.22
8	D	501	GDP	C6-C5-C4	-4.75	116.26	120.80
11	F	401	ACP	N3-C2-N1	-4.72	121.31	128.68
9	B	503	CVT	C13-C12-N2	4.33	122.06	115.97
8	D	501	GDP	C5-C6-N1	-4.31	117.53	123.43
5	A	501	GTP	C5-C6-N1	-4.30	117.56	123.43
8	B	501	GDP	C5-C6-N1	-4.16	117.74	123.43
8	B	501	GDP	N3-C2-N1	-3.97	121.93	127.22
8	D	501	GDP	C2-N3-C4	3.95	119.87	115.36
5	C	501	GTP	C5-C6-N1	-3.81	118.22	123.43
8	B	501	GDP	C2-N3-C4	3.50	119.35	115.36
8	D	501	GDP	N3-C2-N1	-3.47	122.59	127.22
10	B	504	MES	O1S-S-C8	3.44	111.05	106.92
5	A	501	GTP	C6-N1-C2	3.42	121.36	115.93
5	C	501	GTP	C6-N1-C2	3.22	121.05	115.93
10	B	504	MES	C5-N4-C3	3.09	115.80	108.83
9	B	503	CVT	C21-O2-C15	2.99	122.04	117.53
5	C	501	GTP	C2-N3-C4	2.93	118.70	115.36
5	A	501	GTP	C2-N3-C4	2.89	118.66	115.36
8	D	501	GDP	PA-O3A-PB	-2.65	123.73	132.83
5	A	501	GTP	PA-O3A-PB	-2.54	124.12	132.83
11	F	401	ACP	C3'-C2'-C1'	2.48	104.71	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	PB-O3B-PG	-2.45	124.43	132.83
9	B	503	CVT	C12-N2-N1	2.42	122.45	118.91
9	B	503	CVT	O4-C17-C16	2.32	119.25	115.16
11	F	401	ACP	C4-C5-N7	-2.31	106.99	109.40
8	B	501	GDP	C1'-N9-C4	-2.09	122.97	126.64
8	D	501	GDP	C4-C5-N7	-2.08	107.23	109.40
8	B	501	GDP	PA-O3A-PB	-2.03	125.86	132.83
9	B	503	CVT	C19-O4-C17	2.00	120.55	117.53

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
11	F	401	ACP	O4'-C4'-C5'-O5'
11	F	401	ACP	C3'-C4'-C5'-O5'
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
9	B	503	CVT	C16-C17-O4-C19
9	B	503	CVT	C18-C17-O4-C19
9	B	503	CVT	O1-C12-N2-N1
9	B	503	CVT	C13-C12-N2-N1
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3B-PG-O1G
11	F	401	ACP	PB-O3A-PA-O1A
8	B	501	GDP	PB-O3A-PA-O2A
8	D	501	GDP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O3A

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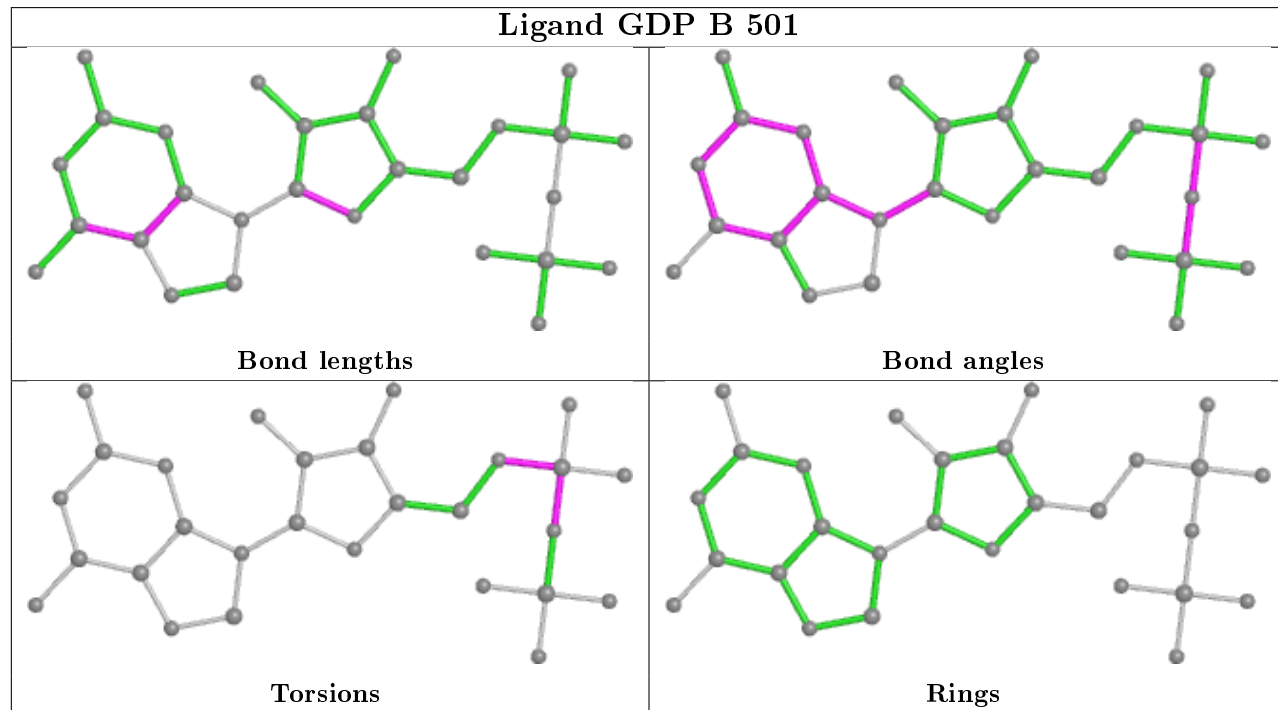
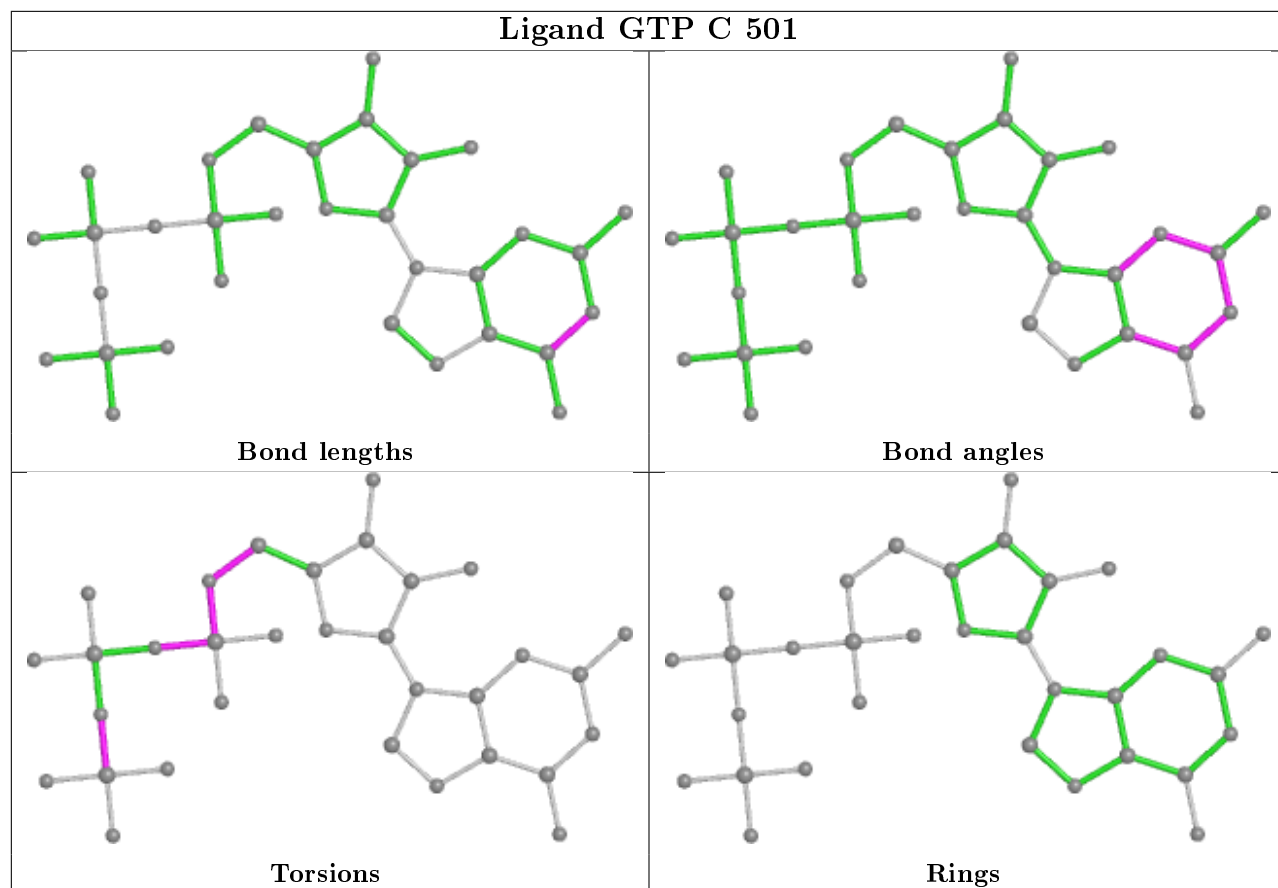
Mol	Chain	Res	Type	Atoms
5	C	501	GTP	PB-O3A-PA-O1A
8	B	501	GDP	PB-O3A-PA-O1A
8	D	501	GDP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3A-PA-O1A
10	B	504	MES	C8-C7-N4-C3

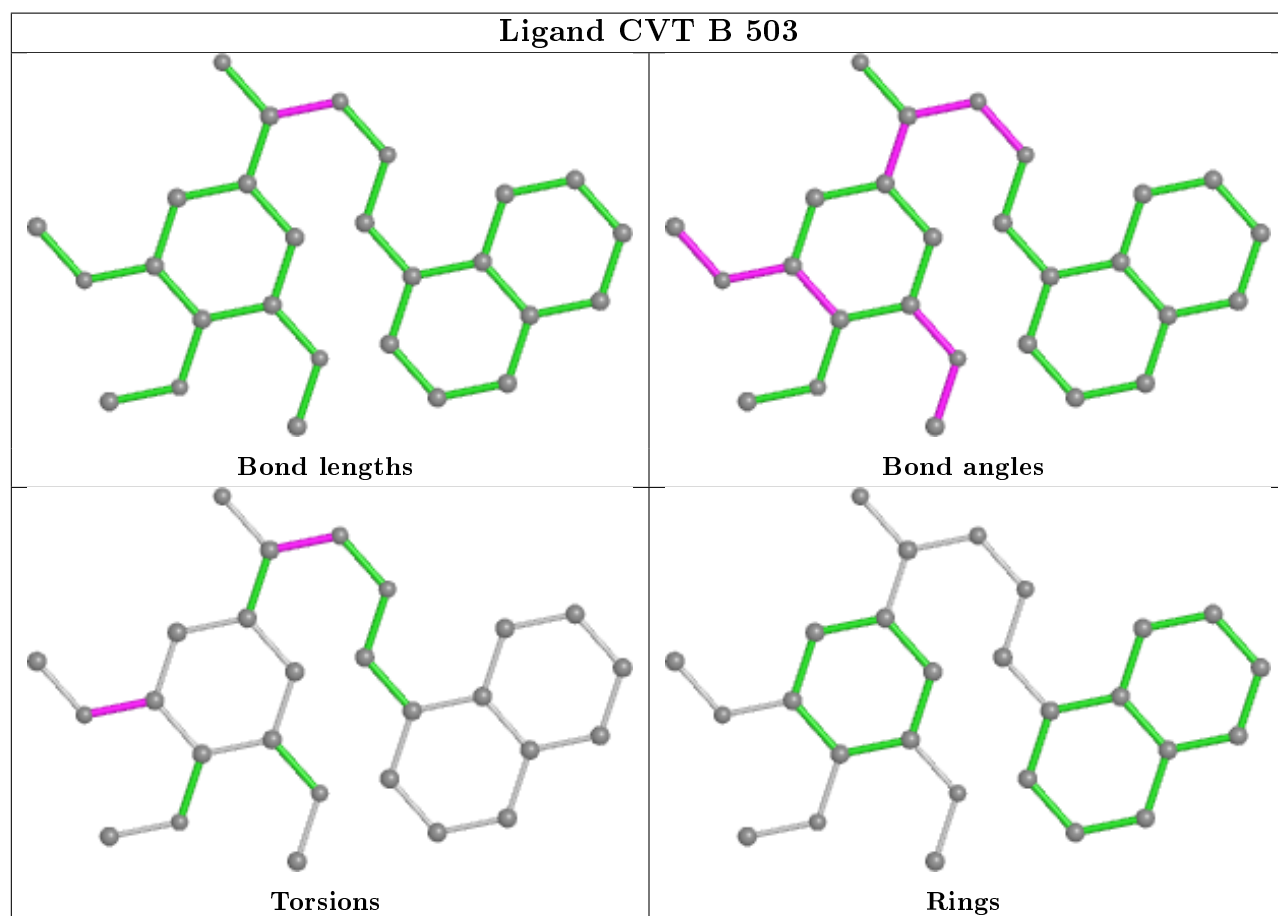
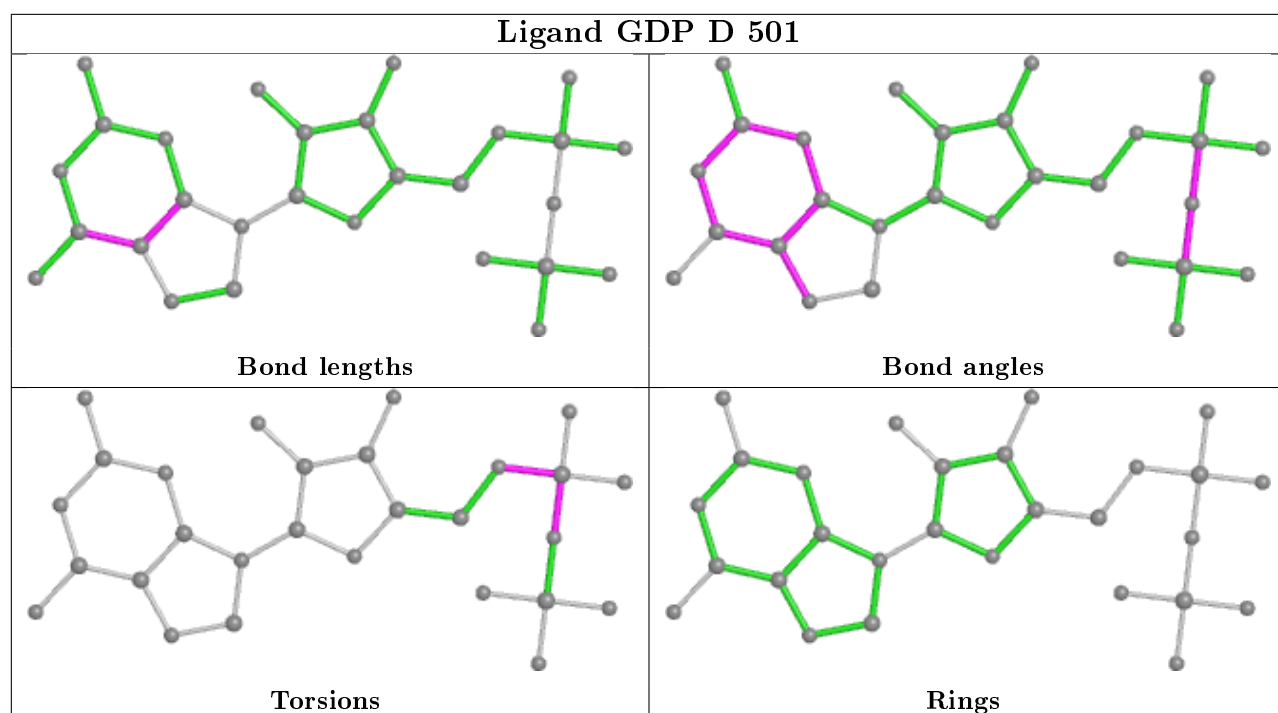
There are no ring outliers.

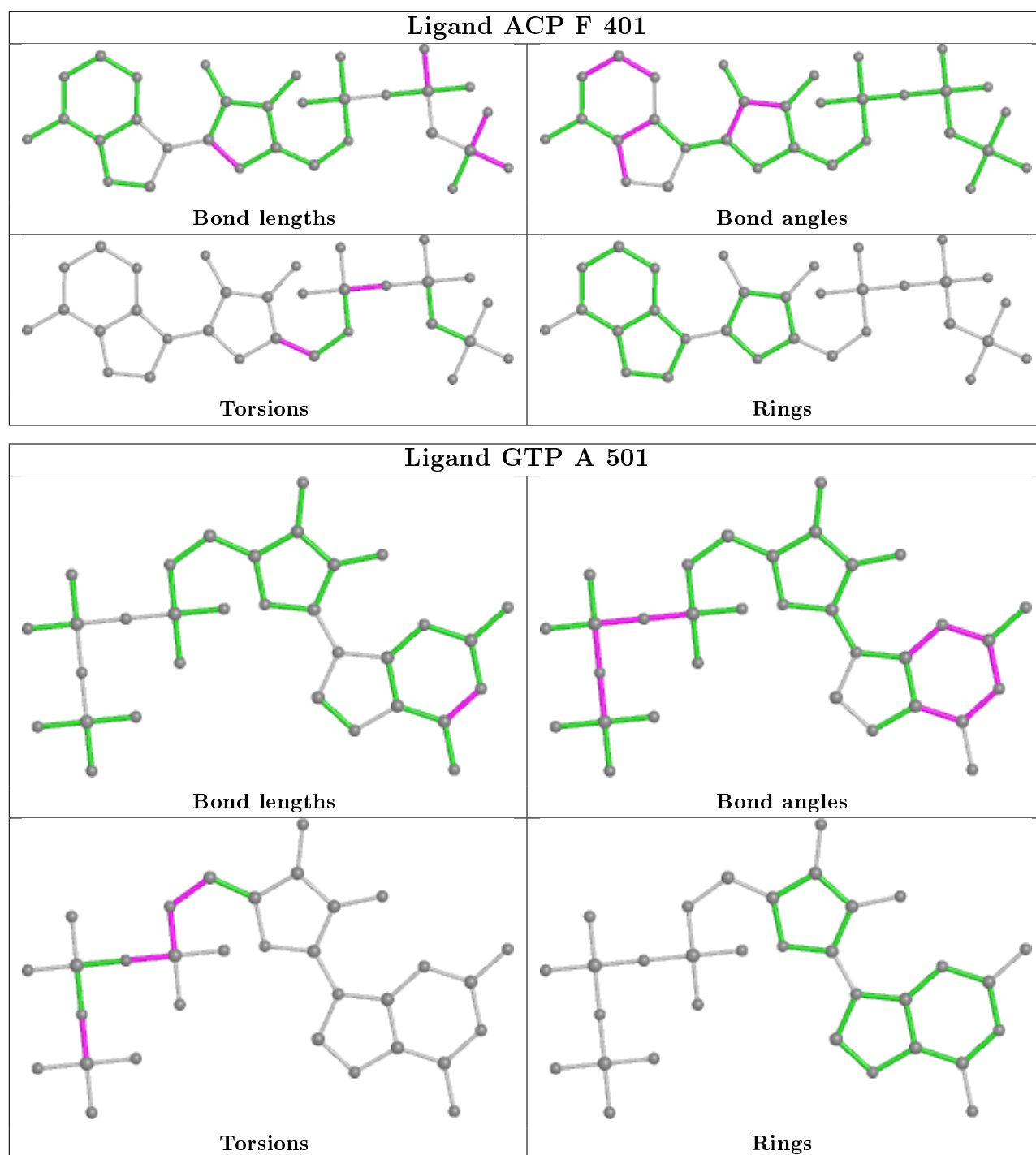
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	501	GDP	2	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	431/451 (95%)	0.28	6 (1%) 75 74	38, 59, 92, 114	0
1	C	440/451 (97%)	0.27	7 (1%) 72 70	31, 45, 72, 125	0
2	B	424/445 (95%)	0.41	8 (1%) 66 65	32, 53, 95, 137	0
2	D	420/445 (94%)	0.67	44 (10%) 6 5	41, 69, 105, 141	0
3	E	118/143 (82%)	0.81	15 (12%) 3 3	45, 73, 115, 152	0
4	F	281/384 (73%)	1.26	70 (24%) 0 0	49, 77, 124, 153	0
All	All	2114/2319 (91%)	0.54	150 (7%) 16 15	31, 60, 103, 153	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	132	LEU	8.0
4	F	130	VAL	7.8
4	F	182	ILE	7.6
4	F	99	VAL	7.4
4	F	131	PHE	7.4
4	F	186	LEU	6.9
4	F	147	TRP	5.6
4	F	100	ILE	5.6
4	F	133	ALA	5.4
4	F	199	PHE	5.3
2	D	57	THR	5.3
4	F	135	TYR	5.1
1	A	262	TYR	4.9
4	F	361	LEU	4.8
4	F	134	ALA	4.8
1	C	340	SER	4.8
4	F	75	ALA	4.7
4	F	129	GLU	4.7
4	F	181	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
4	F	148	ILE	4.4
4	F	228	TYR	4.4
4	F	225	SER	4.3
4	F	98	TYR	4.3
4	F	259	GLY	4.2
2	D	82	PRO	4.1
4	F	149	ALA	4.1
4	F	320	MET	4.1
2	D	94	PHE	4.1
4	F	192	LEU	4.1
4	F	227	PRO	4.0
4	F	146	VAL	4.0
4	F	20	LEU	4.0
4	F	263	PHE	4.0
4	F	330	ILE	3.9
2	B	57	THR	3.9
2	D	58	GLY	3.8
4	F	183	GLN	3.7
2	D	400	ARG	3.7
4	F	150	LYS	3.7
4	F	136	ASN	3.7
2	D	248	LEU	3.6
4	F	379	HIS	3.6
4	F	128	ARG	3.6
3	E	26	PRO	3.6
2	D	118	VAL	3.5
4	F	185	TYR	3.4
1	C	357	TYR	3.4
3	E	138	GLU	3.4
2	D	405	LEU	3.3
4	F	223	THR	3.3
4	F	126	ASP	3.3
4	F	224	SER	3.3
2	D	372	LYS	3.3
2	B	59	ASN	3.3
2	D	325	MET	3.2
4	F	226	GLU	3.2
2	D	179	ASP	3.2
2	D	37	HIS	3.2
2	D	221	THR	3.2
4	F	346	LEU	3.1
3	E	131	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	219	LEU	3.1
4	F	196	HIS	3.1
4	F	184	LYS	3.1
4	F	152	SER	2.9
2	D	182	VAL	2.9
1	A	96	LYS	2.9
3	E	135	LYS	2.9
2	D	33	THR	2.9
3	E	139	LEU	2.8
2	D	74	THR	2.8
2	D	177	VAL	2.8
3	E	24	LEU	2.8
2	B	58	GLY	2.8
3	E	27	PRO	2.7
2	D	404	PHE	2.7
4	F	194	PRO	2.7
2	B	438	ALA	2.6
4	F	32	LYS	2.6
2	D	93	VAL	2.6
2	D	56	ALA	2.6
2	D	59	ASN	2.6
4	F	151	SER	2.6
4	F	46	ARG	2.6
3	E	15	THR	2.6
4	F	26	GLN	2.6
4	F	362	ALA	2.5
2	D	407	TRP	2.5
3	E	28	SER	2.5
2	D	220	THR	2.5
4	F	137	ARG	2.5
3	E	130	ALA	2.5
2	D	75	MET	2.5
4	F	24	THR	2.5
2	D	286	LEU	2.5
4	F	198	LYS	2.5
2	D	79	ARG	2.5
4	F	73	ARG	2.5
2	D	66	ILE	2.5
2	D	318	ILE	2.5
2	D	78	VAL	2.4
1	A	113	GLU	2.4
2	D	60	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	88	ARG	2.4
2	D	72	PRO	2.4
2	D	87	PHE	2.4
1	C	338	LYS	2.4
2	B	37	HIS	2.4
3	E	45	PRO	2.3
2	D	97	SER	2.3
4	F	25	GLY	2.3
4	F	200	ASP	2.3
4	F	344	ALA	2.3
4	F	89	GLU	2.3
2	D	15	GLN	2.3
4	F	201	ILE	2.3
2	B	172	MET	2.2
1	A	329	ASN	2.2
4	F	258	GLU	2.2
2	D	334	ASN	2.2
1	C	302	MET	2.2
3	E	25	LYS	2.2
4	F	353	VAL	2.2
1	C	2	ARG	2.2
3	E	47	LEU	2.1
4	F	127	GLU	2.1
1	A	430	LYS	2.1
4	F	260	ASN	2.1
1	A	112	LYS	2.1
2	D	115	VAL	2.1
2	B	277	SER	2.1
4	F	262	MET	2.1
4	F	197	ARG	2.1
4	F	191	LEU	2.1
4	F	342	LEU	2.1
2	D	218	LYS	2.1
1	C	286	LEU	2.1
4	F	21	LEU	2.1
4	F	187	GLU	2.1
2	B	276	THR	2.1
2	D	83	PHE	2.1
3	E	122	ARG	2.0
2	D	293	GLN	2.0
3	E	22	VAL	2.0
2	D	214	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	399	PHE	2.0
4	F	222	ARG	2.0
2	D	96	GLN	2.0
1	C	440	VAL	2.0
4	F	321	VAL	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.

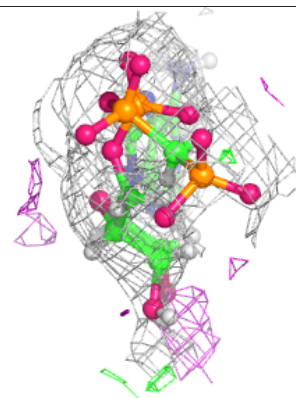
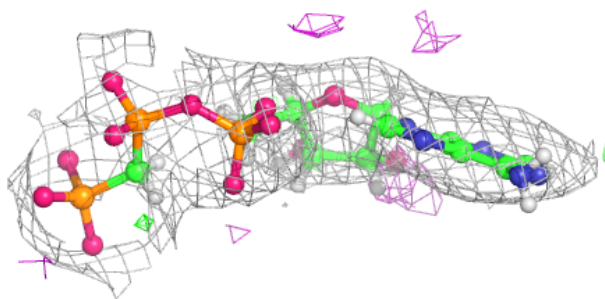
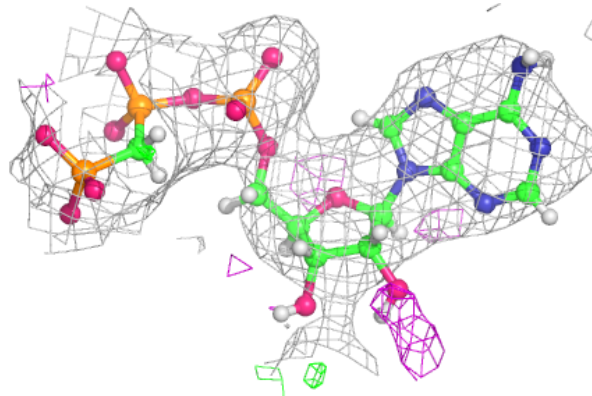
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	MG	F	402	1/1	0.85	0.06	102,102,102,102	0
6	MG	D	502	1/1	0.86	0.09	68,68,68,68	0
7	CA	C	504	1/1	0.87	0.19	38,38,38,38	0
11	ACP	F	401	31/31	0.88	0.18	85,110,130,151	0
9	CVT	B	503	27/27	0.89	0.21	49,74,90,91	0
7	CA	A	503	1/1	0.92	0.12	80,80,80,80	0
6	MG	C	502	1/1	0.95	0.22	43,43,43,43	0
10	MES	B	504	12/12	0.95	0.19	49,65,79,89	0
8	GDP	D	501	28/28	0.95	0.14	63,76,93,105	0
6	MG	A	502	1/1	0.96	0.21	47,47,47,47	0
7	CA	C	503	1/1	0.97	0.14	64,64,64,64	0
5	GTP	A	501	32/32	0.97	0.19	36,48,56,60	0
5	GTP	C	501	32/32	0.98	0.22	38,42,48,50	0
6	MG	B	502	1/1	0.98	0.26	41,41,41,41	0
8	GDP	B	501	28/28	0.98	0.18	39,46,59,60	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.

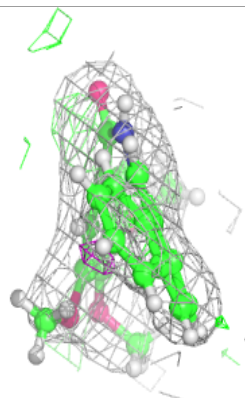
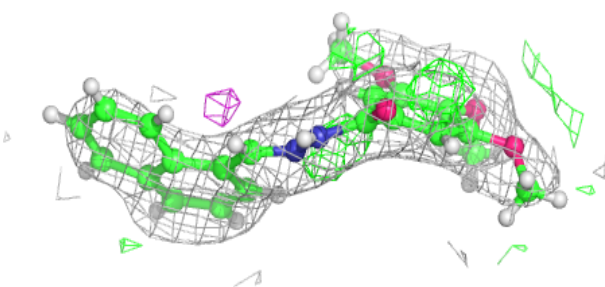
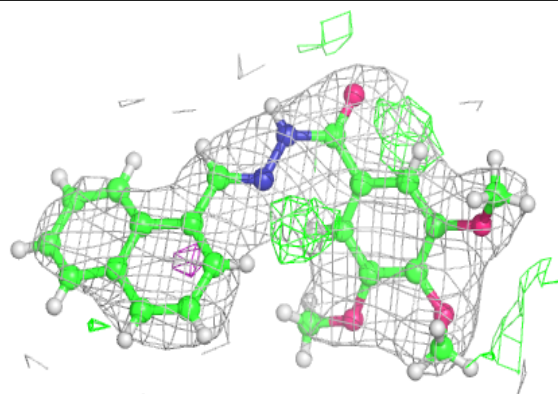
**Electron density around ACP F 401:**

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



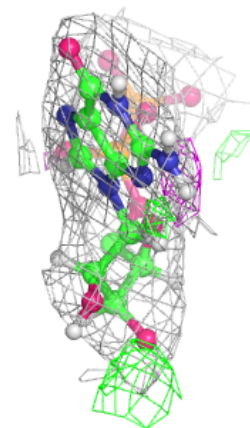
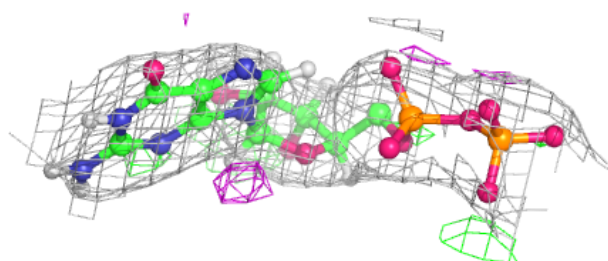
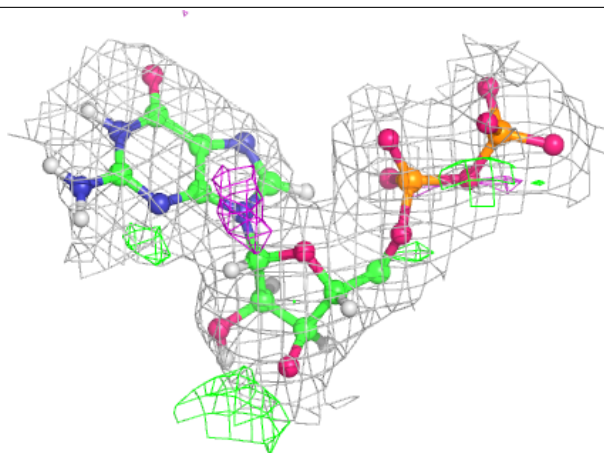
**Electron density around CVT B 503:**

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

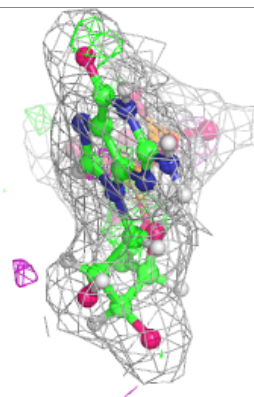
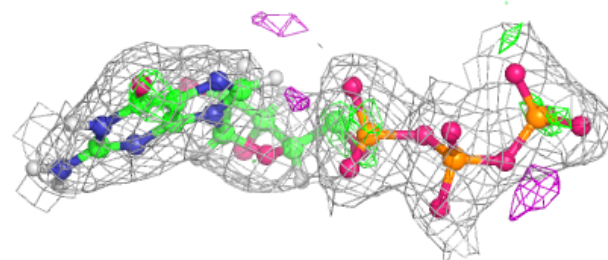
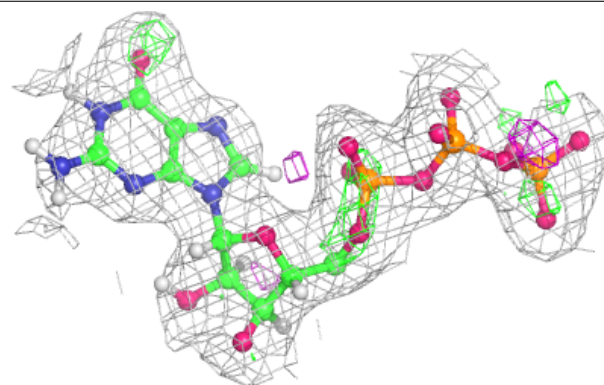


**Electron density around GDP D 501:**

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

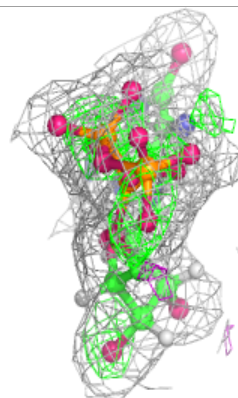
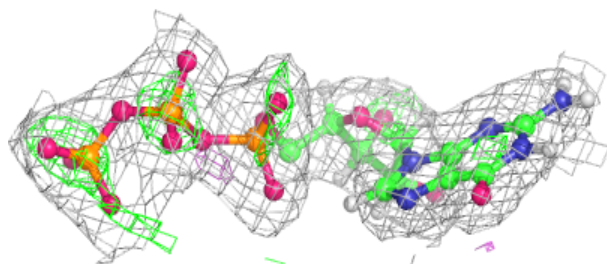
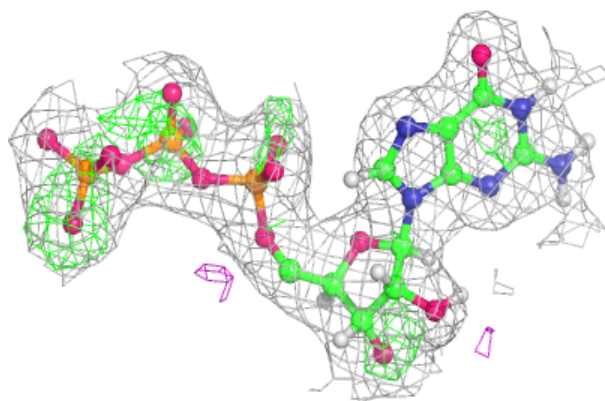
**Electron density around GTP A 501:**

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

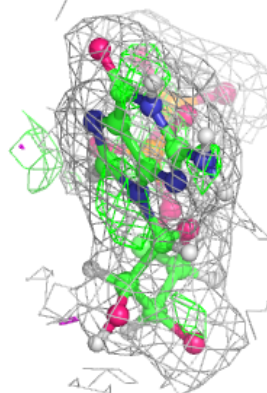
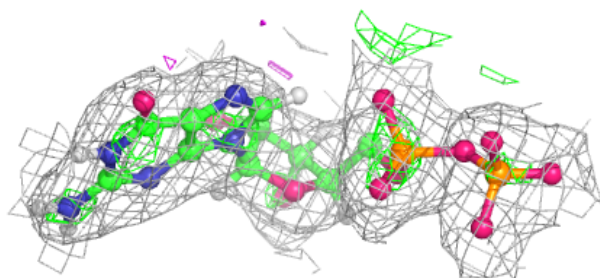
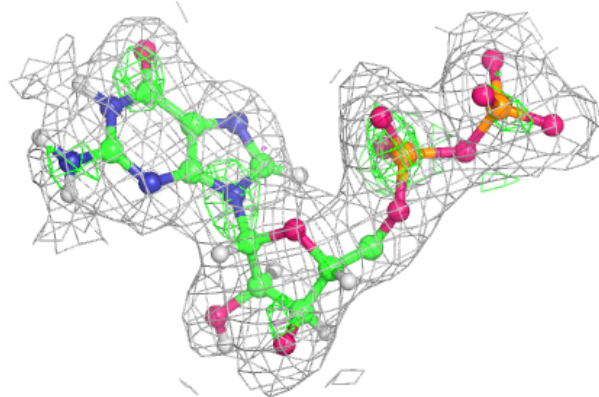


**Electron density around GTP C 501:**

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

**Electron density around 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)



## 6.5 Other polymers

There are no such residues in this entry.