



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2021 – 10:46 PM JST

PDB ID : 7CPQ  
Title : crystal structure of T2R-TTL-(+)-6-Cl-JP18 complex  
Authors : Jiang, H.; Luo, C.  
Deposited on : 2020-08-07  
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 2.23.1  
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) : 2.23.1

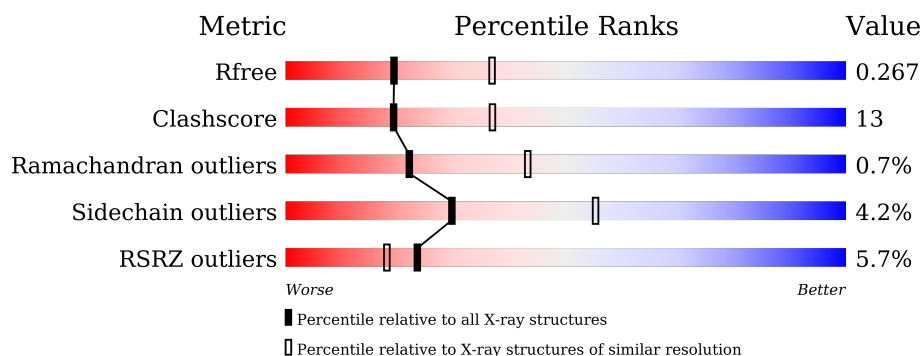
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>3%</div> <div>74%</div> <div>22%</div> <div>..</div> </div>
1	C	451	<div> <div>78%</div> <div>18%</div> <div>..</div> </div>
2	B	445	<div> <div>4%</div> <div>71%</div> <div>22%</div> <div>6%</div> </div>
2	D	445	<div> <div>8%</div> <div>64%</div> <div>29%</div> <div>6%</div> </div>
3	E	189	<div> <div>6%</div> <div>43%</div> <div>17%</div> <div>..</div> <div>36%</div> </div>
4	F	378	<div> <div>10%</div> <div>41%</div> <div>20%</div> <div>.</div> <div>36%</div> </div>

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 17035 atoms, of which 110 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	438	Total	C	N	O	S	16	13	0
			3482	2214	584	659	25			
1	C	440	Total	C	N	O	S	20	8	0
			3475	2200	586	666	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	420	Total	C	N	O	S	10	11	0
			3359	2117	566	650	26			
2	D	420	Total	C	N	O	S	9	4	0
			3317	2089	560	640	28			

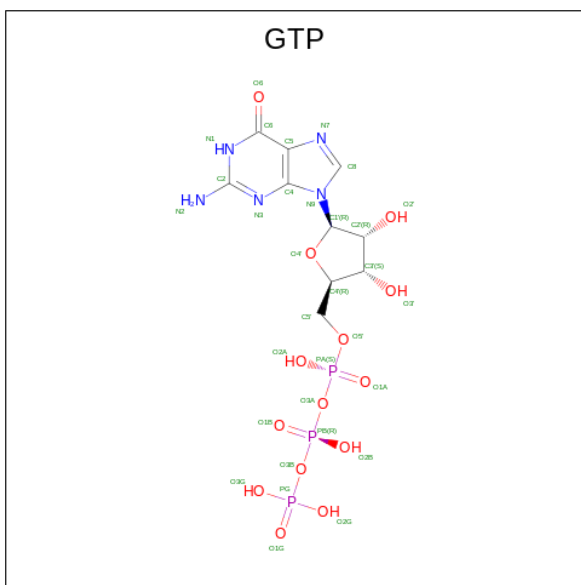
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	3	0
			1016	628	183	199	6			

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	243	Total	C	N	O	S	13	5	0
			2014	1318	333	351	12			

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	P	0	0
			44	10	12	5	14	3		
5	C	1	Total	C	H	N	O	P	0	0
			44	10	12	5	14	3		

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

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

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

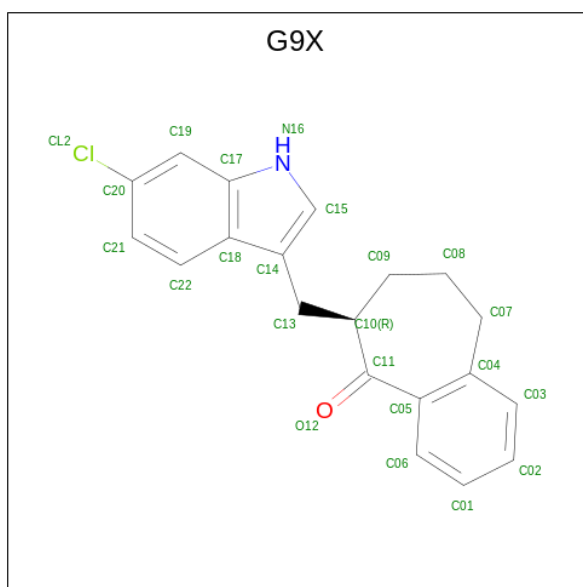
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		

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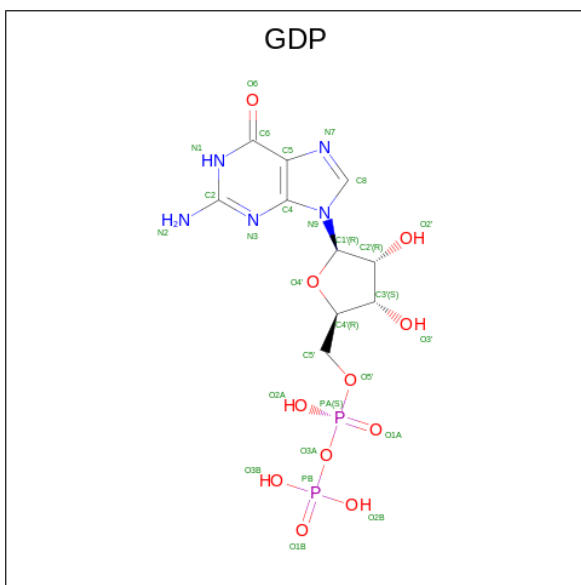
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is (6R)-6-[(6-chloranyl-1H-indol-3-yl)methyl]-6,7,8,9-tetrahydrobenzo[7]annulen-5-one (three-letter code: G9X) (formula: C<sub>20</sub>H<sub>18</sub>ClNO) (labeled as "Ligand of Interest" by depositor).



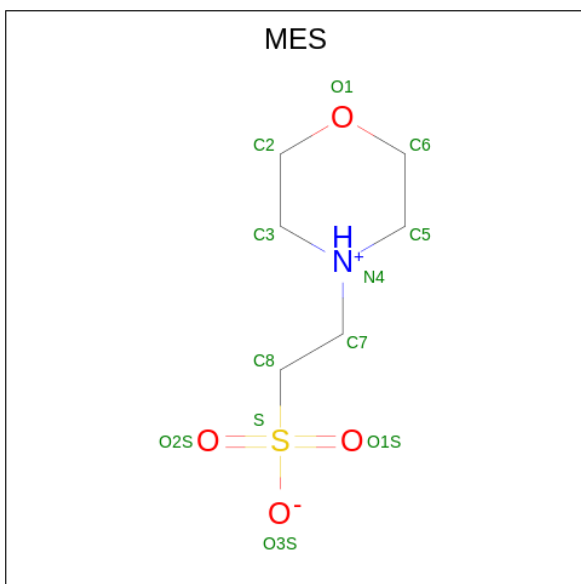
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	B	1	Total	C	Cl	H	N	O	0	0
			41	20	1	18	1	1		

- Molecule 9 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>).



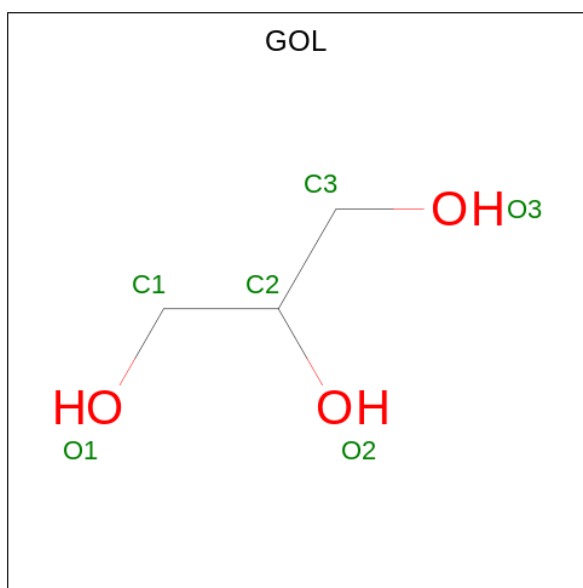
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	B	1	Total 40	C 10	H 12	N 5	O 11	P 2	0	0
9	D	1	Total 40	C 10	H 12	N 5	O 11	P 2	0	0

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $\text{C}_6\text{H}_{13}\text{NO}_4\text{S}$ ).



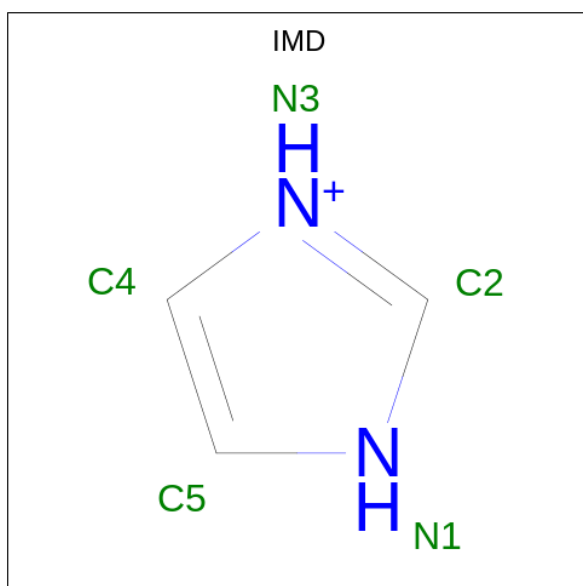
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

- Molecule 11 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	C	1	Total	C	H	O	0	0
			14	3	8	3		
11	C	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 12 is IMIDAZOLE (three-letter code: IMD) (formula:  $C_3H_5N_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	C	1	Total	C	H	N	0	0
			10	3	5	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	C	1	Total	C	H	N	0	0
			10	3	5	2		
12	E	1	Total	C	H	N	0	0
			10	3	5	2		

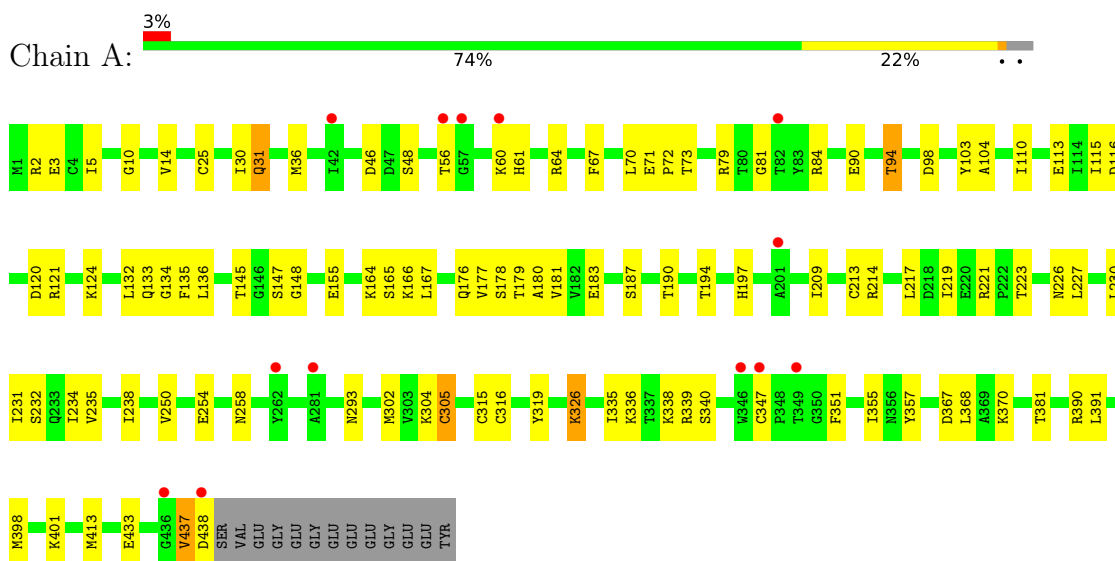
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	11	Total	O	0	0
			11	11		
13	B	15	Total	O	0	0
			15	15		
13	C	37	Total	O	0	0
			37	37		
13	D	2	Total	O	0	0
			2	2		
13	E	1	Total	O	0	0
			1	1		
13	F	6	Total	O	0	0
			6	6		

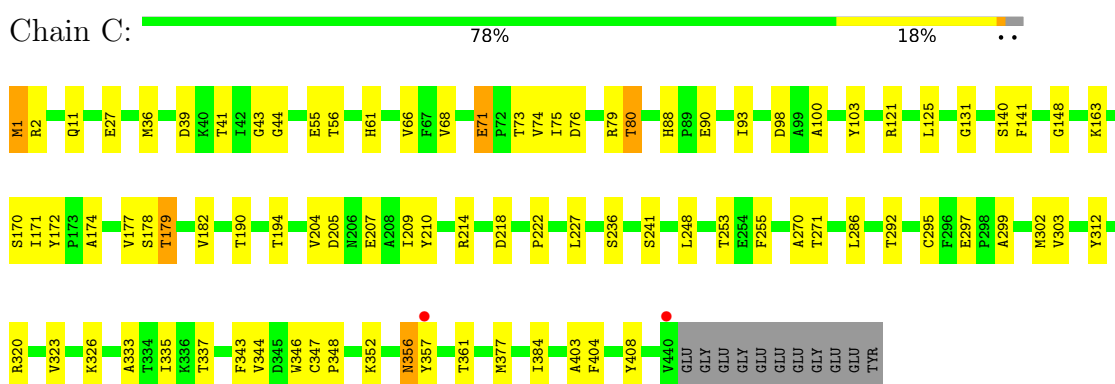
### 3 Residue-property plots [i](#)

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.

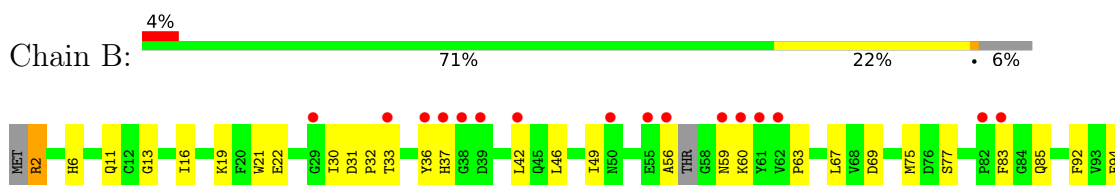
- Molecule 1: Tubulin alpha-1B chain

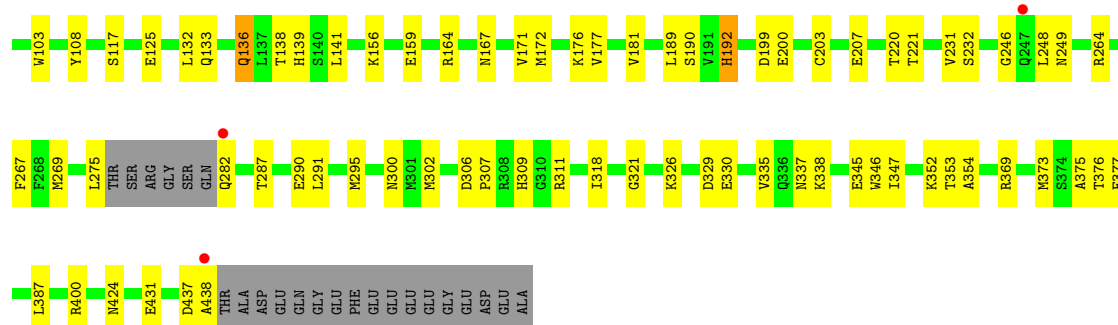


- Molecule 1: Tubulin alpha-1B chain

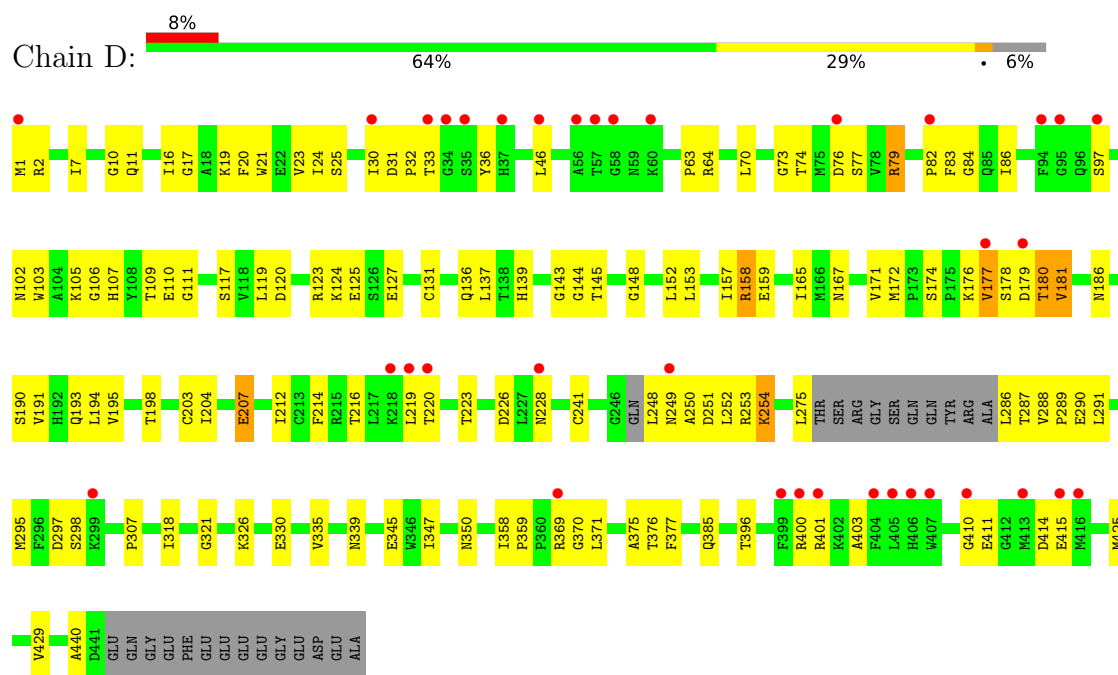


- Molecule 2: Tubulin beta-2B chain

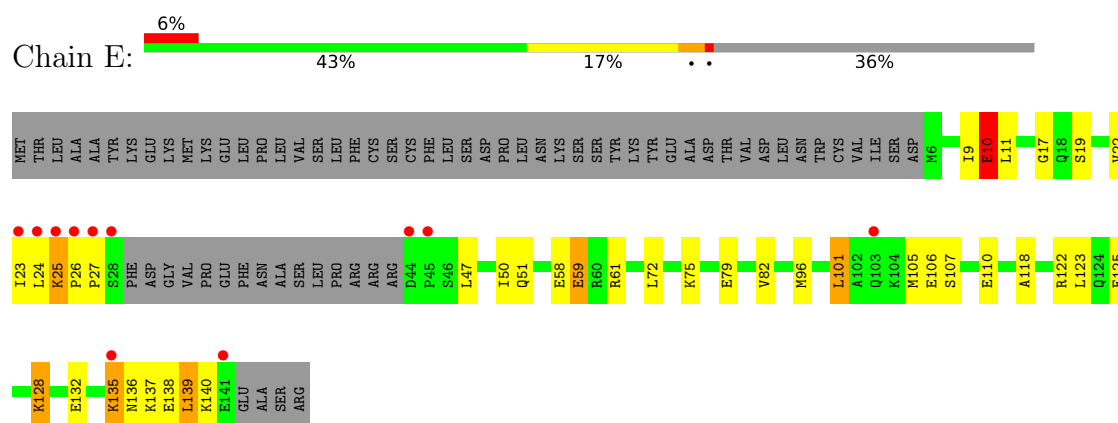




• Molecule 2: Tubulin beta-2B chain

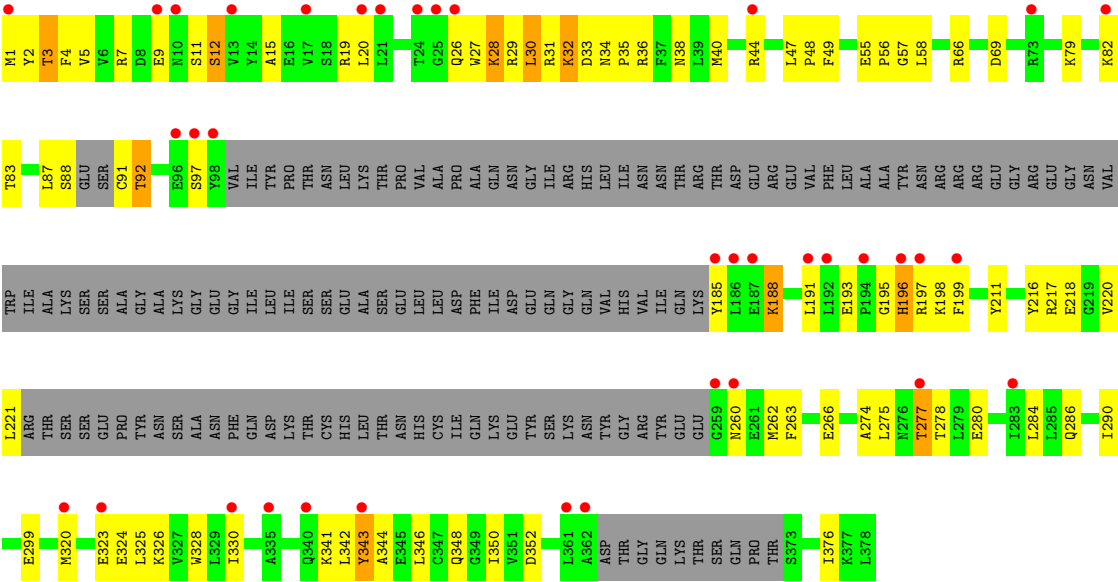


• Molecule 3: Stathmin-4



• 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, $\alpha$ , $\beta$ , $\gamma$	104.88Å 156.62Å 182.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.90 – 2.60 49.90 – 2.59	Depositor EDS
% Data completeness (in resolution range)	96.7 (49.90-2.60) 96.7 (49.90-2.59)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.92 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.220 , 0.267 0.223 , 0.267	Depositor DCC
$R_{free}$ test set	4654 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.2	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 32.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	17035	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: CA, IMD, GTP, MES, G9X, GOL, 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	0.49	0/3599	0.52	0/4887
1	C	0.61	0/3574	0.59	0/4853
2	B	0.53	1/3462 (0.0%)	0.55	0/4687
2	D	0.43	0/3401	0.51	0/4607
3	E	0.38	0/1033	0.48	0/1370
4	F	0.48	0/2073	0.55	0/2798
All	All	0.51	1/17142 (0.0%)	0.54	0/23202

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	171	VAL	C-N	-5.28	1.22	1.34

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	3482	0	3436	77	0
1	C	3475	0	3394	66	0
2	B	3359	0	3249	83	0
2	D	3317	0	3212	100	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1016	0	1041	35	0
4	F	2014	0	2054	93	0
5	A	32	12	12	0	0
5	C	32	12	12	1	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	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	23	18	0	1	0
9	B	28	12	12	1	0
9	D	28	12	12	5	0
10	B	12	13	13	1	0
11	C	12	16	16	4	0
12	C	10	10	10	0	0
12	E	5	5	5	0	0
13	A	11	0	0	1	0
13	B	15	0	0	3	0
13	C	37	0	0	1	0
13	D	2	0	0	1	0
13	E	1	0	0	0	0
13	F	6	0	0	0	0
All	All	16925	110	16478	427	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 13.

The worst 5 of 427 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:92:THR:HG22	4:F:92:THR:O	1.61	0.98
1:A:398:MET:HE3	2:B:347:ILE:HG23	1.45	0.98
1:C:1:MET:O	1:C:2:ARG:HG2	1.68	0.93
2:B:337:ASN:HD21	4:F:36:ARG:HE	0.98	0.92
1:A:71:GLU:OE2	1:A:73:THR:HG23	1.79	0.83

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	449/451 (100%)	425 (95%)	21 (5%)	3 (1%)	22	43
1	C	446/451 (99%)	434 (97%)	12 (3%)	0	100	100
2	B	425/445 (96%)	409 (96%)	14 (3%)	2 (0%)	29	52
2	D	418/445 (94%)	395 (94%)	19 (4%)	4 (1%)	15	32
3	E	120/189 (64%)	114 (95%)	3 (2%)	3 (2%)	5	9
4	F	237/378 (63%)	221 (93%)	13 (6%)	3 (1%)	12	24
All	All	2095/2359 (89%)	1998 (95%)	82 (4%)	15 (1%)	22	43

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	59	ASN
4	F	32	LYS
4	F	343	TYR
2	D	177	VAL
2	D	181	VAL

### 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	382/379 (101%)	368 (96%)	14 (4%)	34	60
1	C	379/379 (100%)	368 (97%)	11 (3%)	42	68
2	B	373/383 (97%)	357 (96%)	16 (4%)	29	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	367/383 (96%)	354 (96%)	13 (4%)	36	62
3	E	112/171 (66%)	102 (91%)	10 (9%)	9	19
4	F	224/336 (67%)	212 (95%)	12 (5%)	22	44
All	All	1837/2031 (90%)	1761 (96%)	76 (4%)	30	56

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	96	MET
4	F	188	LYS
3	E	107	SER
4	F	11	SER
4	F	277	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	301	GLN
1	C	309	HIS
4	F	34	ASN
2	D	228	ASN
2	B	337	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry

Of 19 ligands modelled in this entry, 8 are monoatomic - leaving 11 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
12	IMD	C	506	-	3,5,5	1.02	0	4,5,5	0.67	0
12	IMD	E	201	-	3,5,5	0.94	0	4,5,5	0.52	0
11	GOL	C	502	-	5,5,5	0.38	0	5,5,5	0.39	0
5	GTP	C	501	6	26,34,34	2.22	12 (46%)	33,54,54	1.97	8 (24%)
9	GDP	D	501	6	24,30,30	1.61	5 (20%)	31,47,47	2.09	11 (35%)
12	IMD	C	507	-	3,5,5	1.03	0	4,5,5	0.54	0
10	MES	B	505	-	12,12,12	1.47	1 (8%)	14,16,16	2.00	6 (42%)
5	GTP	A	501	6	26,34,34	2.05	10 (38%)	33,54,54	1.90	9 (27%)
9	GDP	B	502	6	24,30,30	2.25	13 (54%)	31,47,47	1.91	7 (22%)
11	GOL	C	503	-	5,5,5	0.46	0	5,5,5	0.33	0
8	G9X	B	501	-	24,26,26	5.08	12 (50%)	29,37,37	1.44	5 (17%)

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
12	IMD	C	506	-	-	-	0/1/1/1
12	IMD	E	201	-	-	-	0/1/1/1
11	GOL	C	502	-	-	4/4/4/4	-
5	GTP	C	501	6	-	4/18/38/38	0/3/3/3
9	GDP	D	501	6	-	4/12/32/32	0/3/3/3
12	IMD	C	507	-	-	-	0/1/1/1
10	MES	B	505	-	-	6/6/14/14	0/1/1/1
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
9	GDP	B	502	6	-	5/12/32/32	0/3/3/3
11	GOL	C	503	-	-	4/4/4/4	-
8	G9X	B	501	-	-	0/3/18/18	0/4/4/4

The worst 5 of 53 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	501	G9X	C19-C17	10.30	1.57	1.41
8	B	501	G9X	C06-C05	8.79	1.53	1.39
8	B	501	G9X	C03-C04	7.90	1.53	1.39
8	B	501	G9X	C22-C18	7.69	1.58	1.42
8	B	501	G9X	C05-C04	7.64	1.50	1.40

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	501	GDP	C2-N3-C4	5.62	121.77	115.36
5	C	501	GTP	C6-C5-C4	-5.23	115.80	120.80
5	C	501	GTP	C2-N3-C4	4.91	120.96	115.36
9	B	502	GDP	C6-C5-C4	-4.77	116.25	120.80
5	A	501	GTP	C2-N3-C4	4.72	120.75	115.36

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
9	B	502	GDP	C5'-O5'-PA-O3A

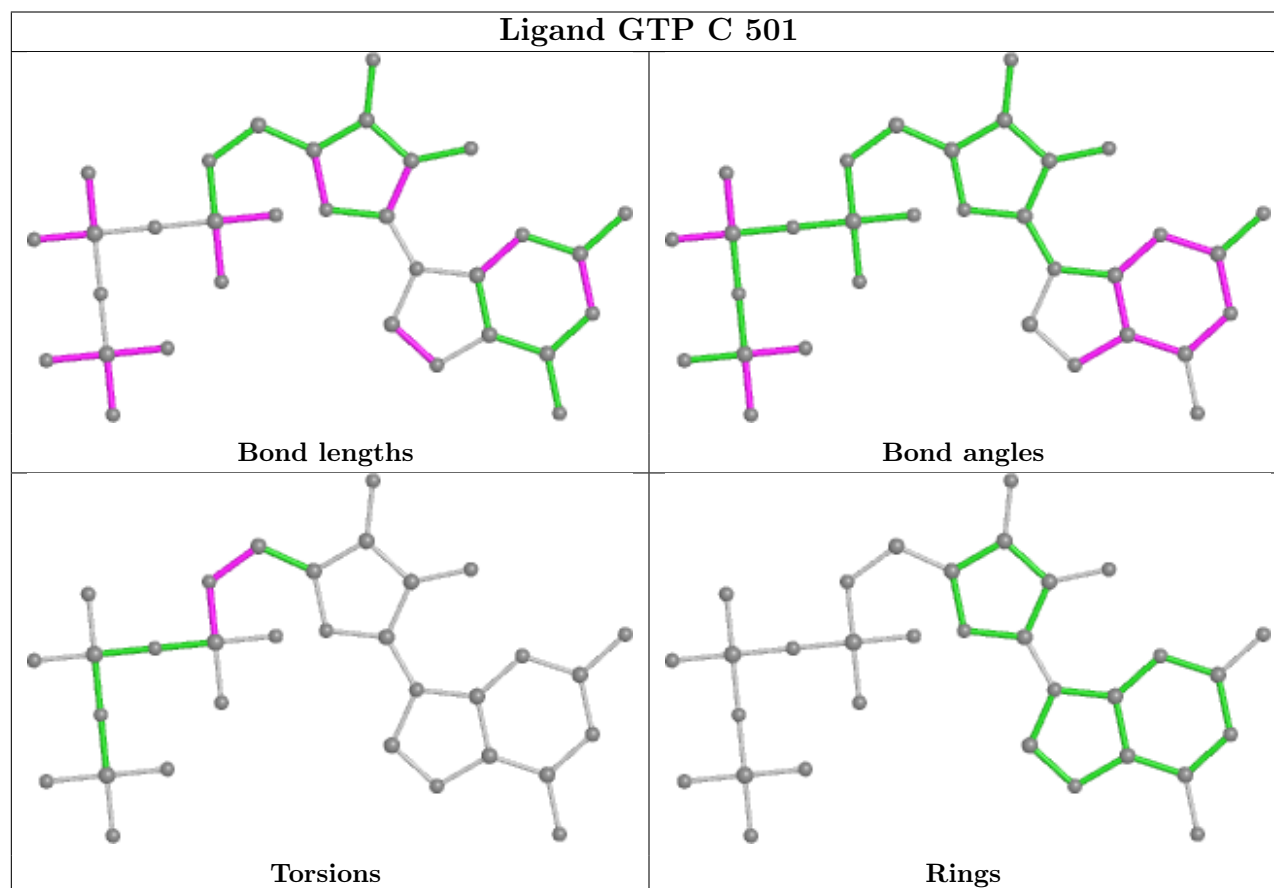
There are no ring outliers.

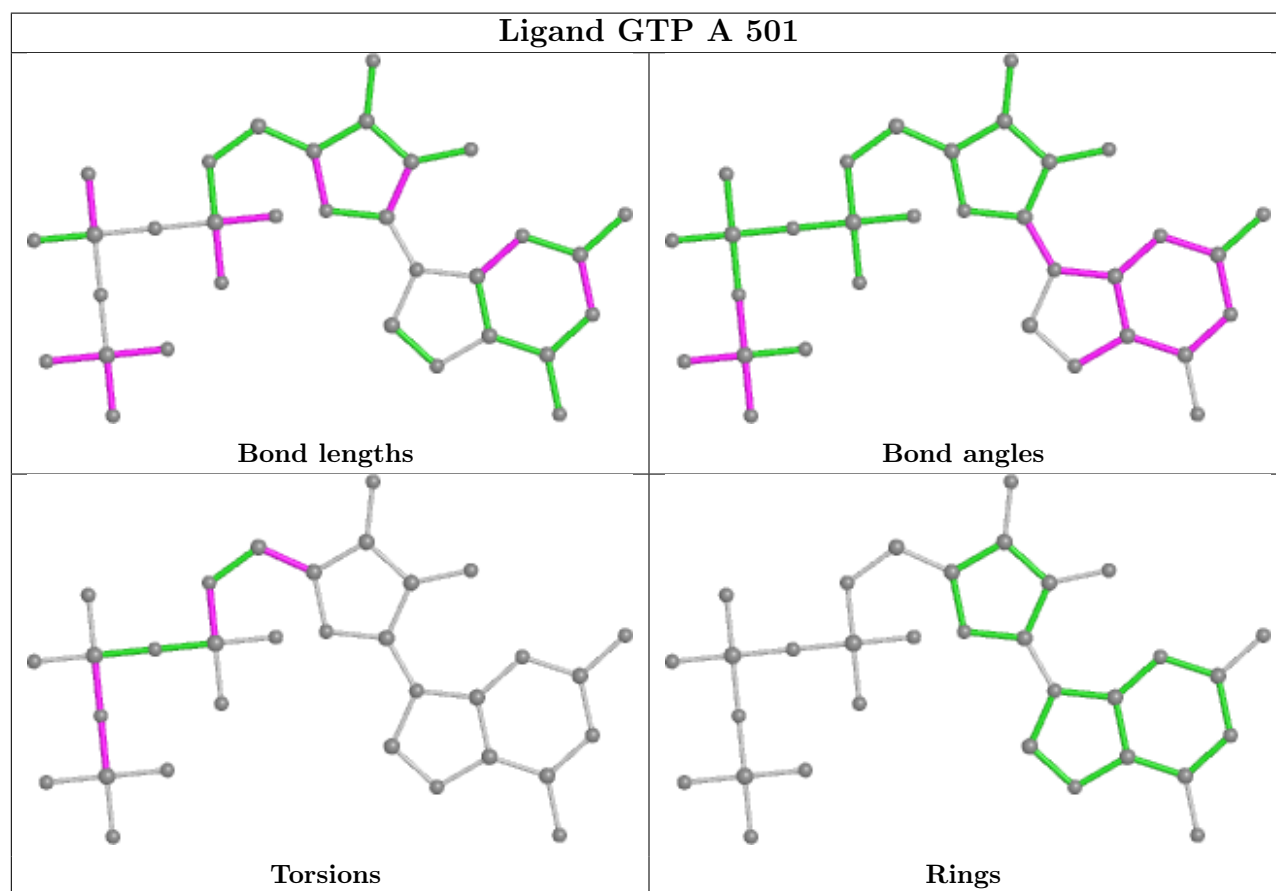
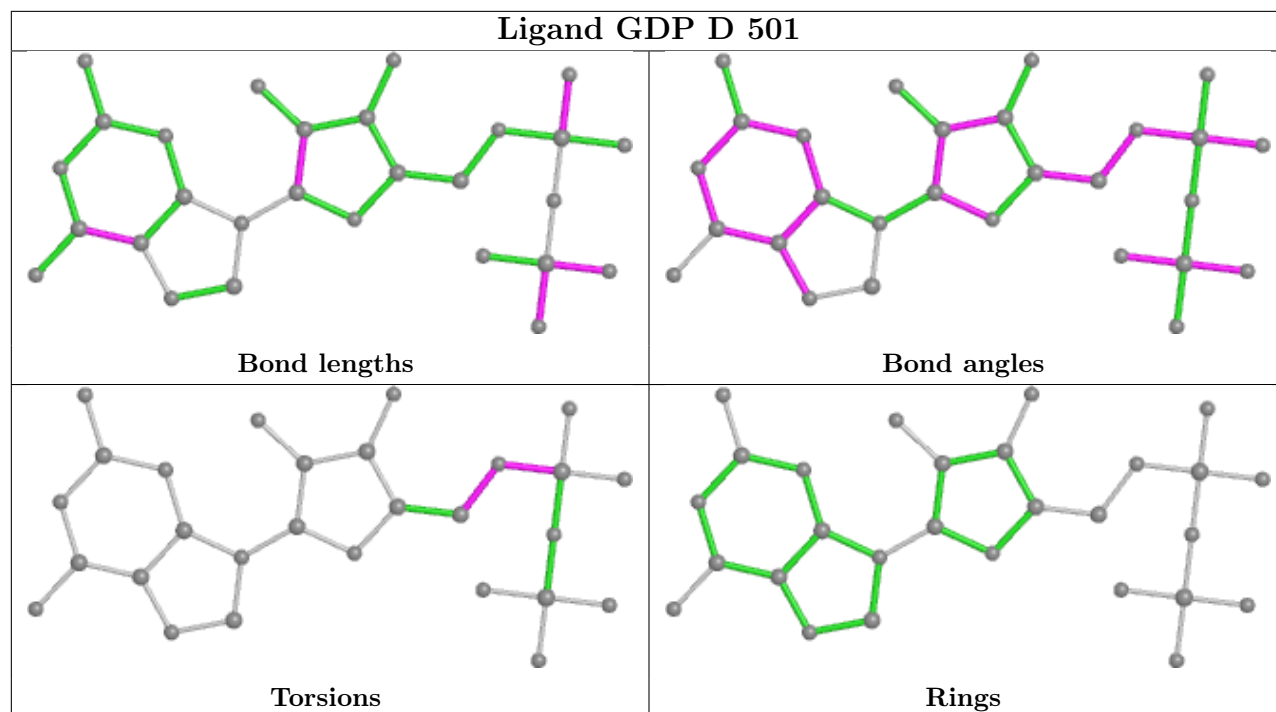
7 monomers are involved in 13 short contacts:

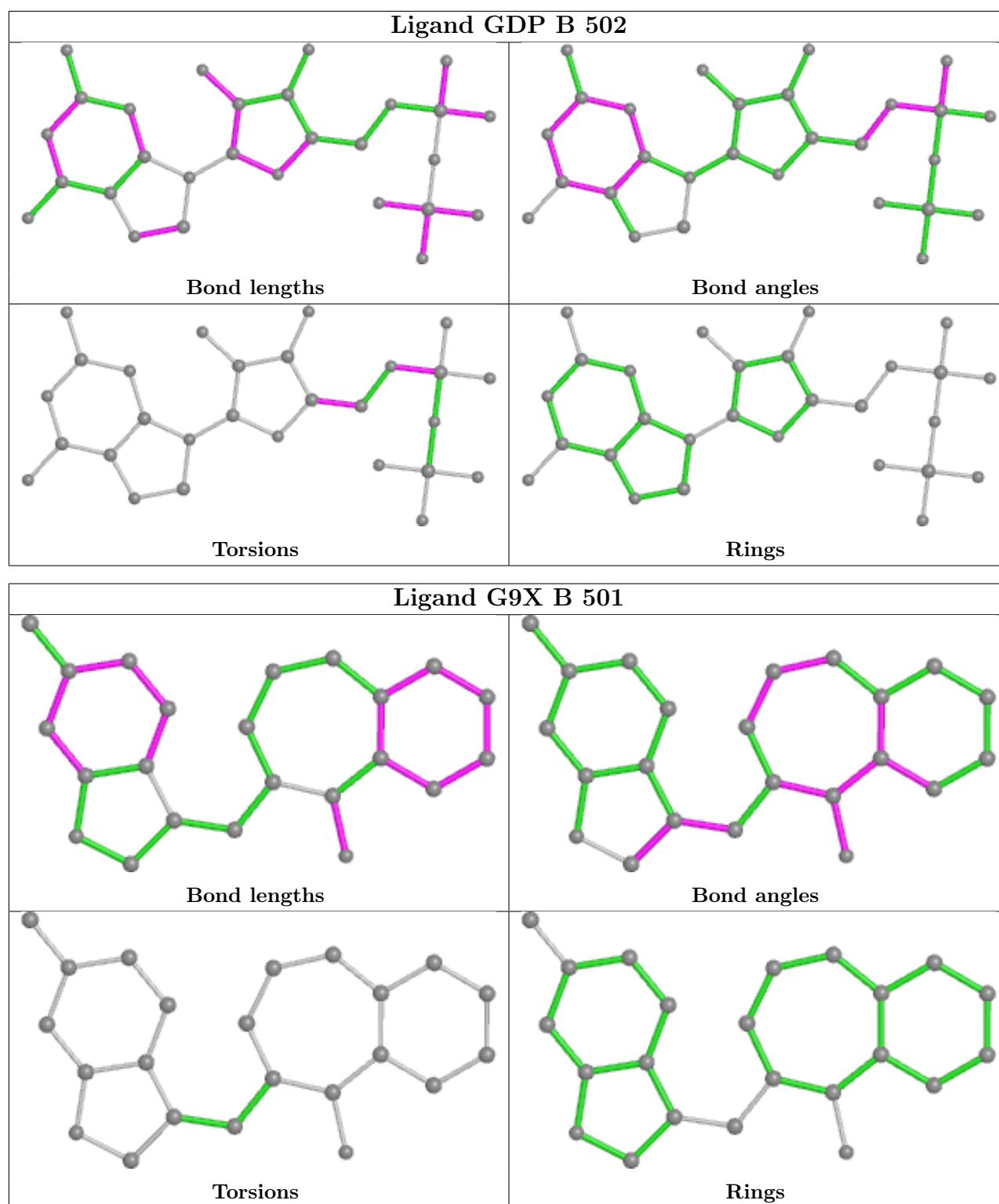
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	502	GOL	1	0
5	C	501	GTP	1	0
9	D	501	GDP	5	0
10	B	505	MES	1	0
9	B	502	GDP	1	0
11	C	503	GOL	3	0
8	B	501	G9X	1	0

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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	438/451 (97%)	0.31	13 (2%) 50 43	30, 46, 65, 78	0
1	C	440/451 (97%)	0.02	2 (0%) 91 89	25, 34, 49, 60	0
2	B	420/445 (94%)	0.10	19 (4%) 33 26	24, 32, 55, 83	2 (0%)
2	D	420/445 (94%)	0.51	36 (8%) 10 7	36, 51, 67, 82	3 (0%)
3	E	121/189 (64%)	0.43	11 (9%) 9 6	31, 50, 71, 86	0
4	F	243/378 (64%)	0.80	37 (15%) 2 1	32, 56, 90, 106	0
All	All	2082/2359 (88%)	0.31	118 (5%) 23 18	24, 43, 68, 106	5 (0%)

The worst 5 of 118 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	27	PRO	5.1
2	D	94	PHE	4.9
2	B	56	ALA	4.7
2	D	37	HIS	4.7
2	B	59	ASN	4.6

### 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 ⓘ

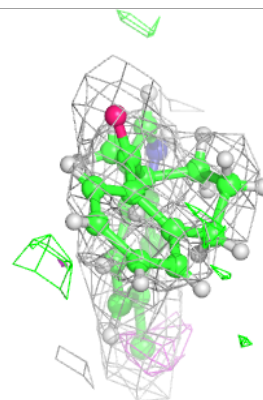
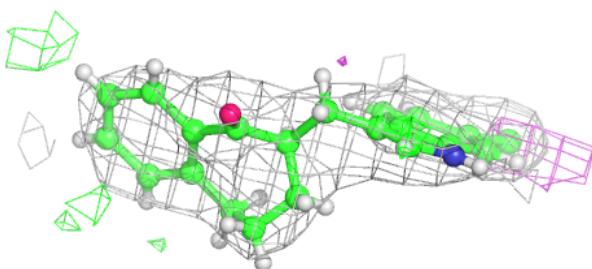
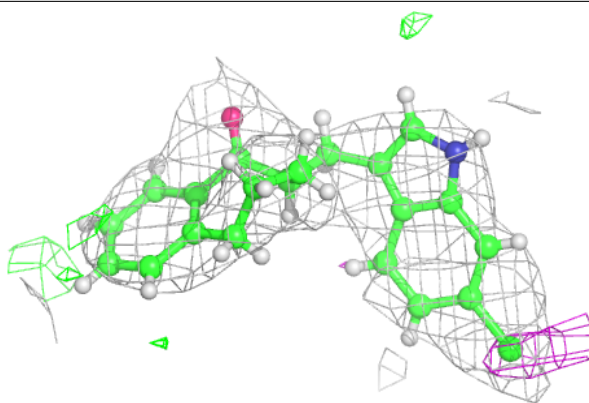
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
11	GOL	C	503	6/6	0.82	0.22	37,67,81,90	0
11	GOL	C	502	6/6	0.86	0.21	42,58,64,73	0
12	IMD	C	507	5/5	0.89	0.19	53,60,72,72	0
10	MES	B	505	12/12	0.90	0.20	29,36,48,110	0
12	IMD	C	506	5/5	0.90	0.26	47,56,62,70	0
6	MG	C	504	1/1	0.90	0.21	32,32,32,32	0
12	IMD	E	201	5/5	0.90	0.21	64,74,88,89	0
6	MG	F	401	1/1	0.91	0.16	65,65,65,65	0
6	MG	B	503	1/1	0.93	0.30	25,25,25,25	0
7	CA	C	505	1/1	0.93	0.11	92,92,92,92	0
8	G9X	B	501	23/23	0.94	0.14	28,37,51,55	0
7	CA	B	504	1/1	0.95	0.12	119,119,119,119	0
6	MG	A	502	1/1	0.96	0.35	35,35,35,35	0
7	CA	A	503	1/1	0.97	0.03	68,68,68,68	0
9	GDP	D	501	28/28	0.97	0.10	50,53,63,69	0
6	MG	D	502	1/1	0.97	0.08	54,54,54,54	0
5	GTP	A	501	32/32	0.97	0.18	32,35,41,43	0
9	GDP	B	502	28/28	0.98	0.14	24,25,31,31	0
5	GTP	C	501	32/32	0.98	0.13	30,31,38,38	0

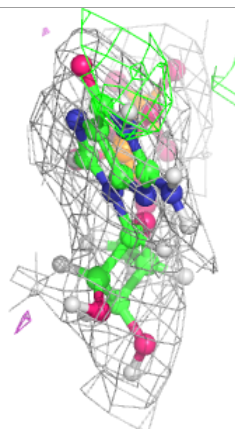
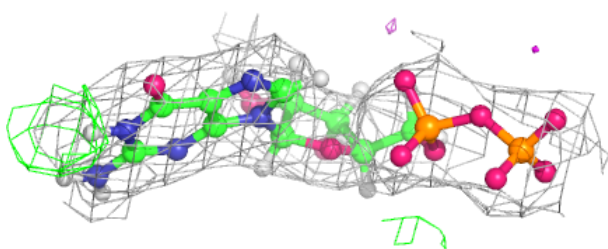
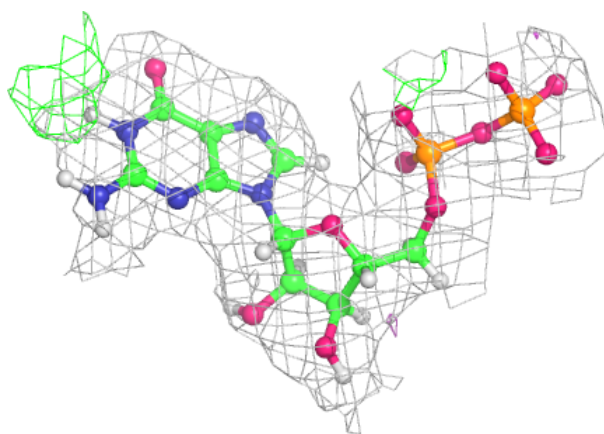
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around G9X 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)

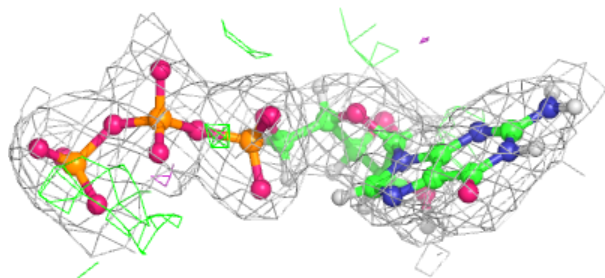
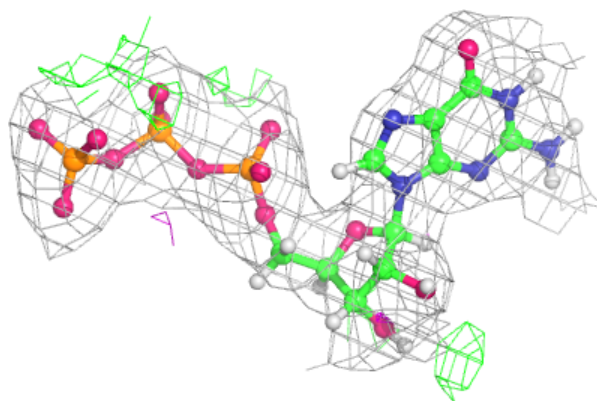
**Electron density around GDP D 501:**

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

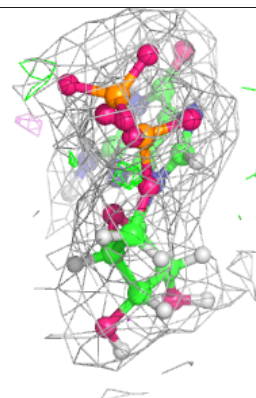
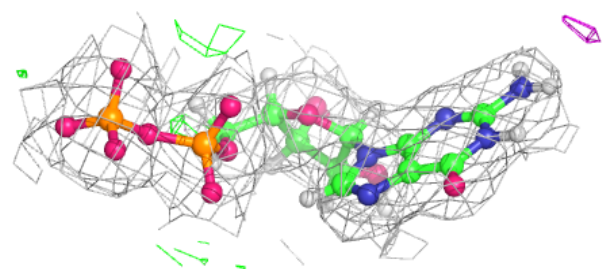
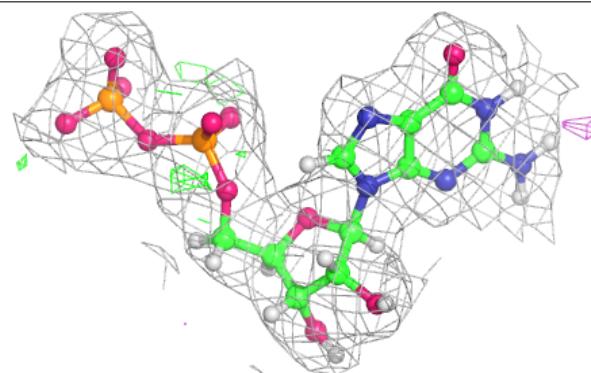


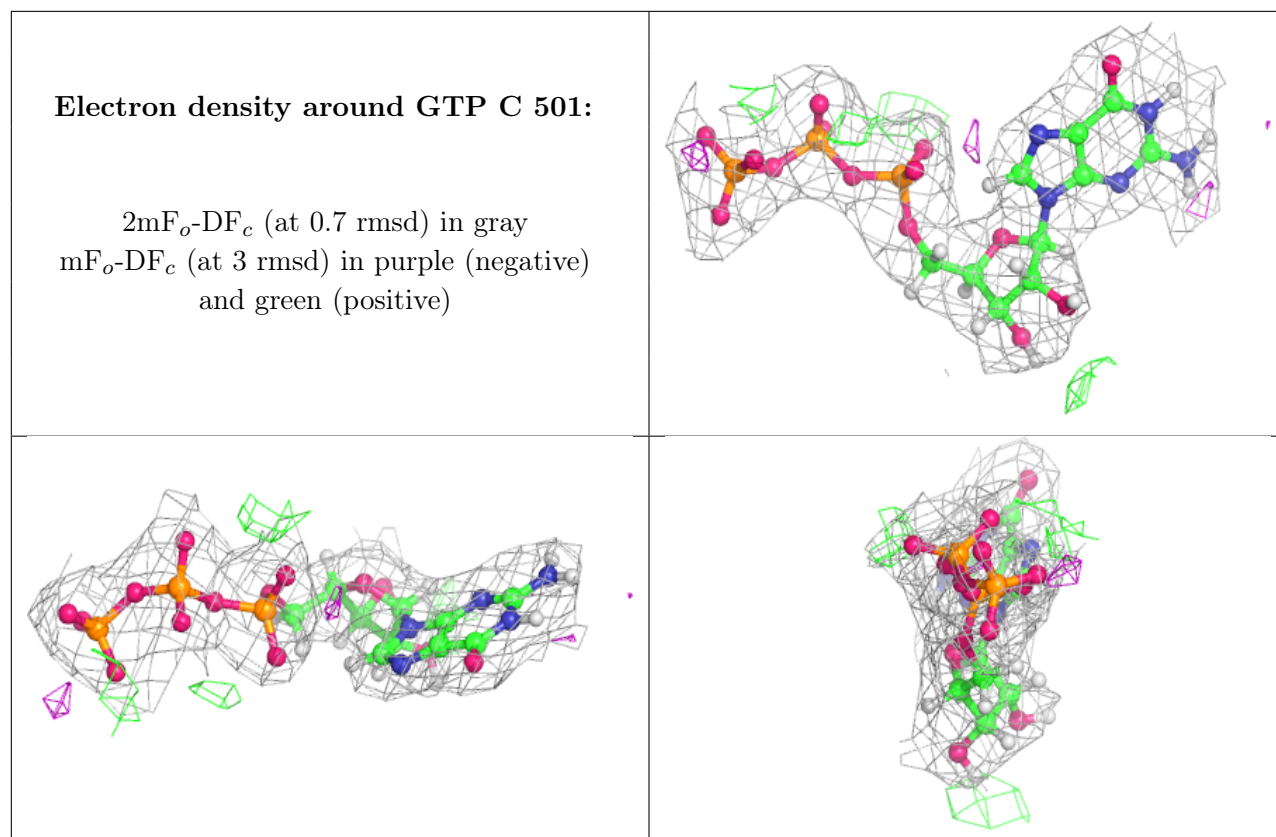
**Electron density around GTP A 501:**

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

**Electron density around GDP B 502:**

$2mF_o-DF_c$  (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.