



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 21, 2021 – 02:34 PM EDT

PDB ID : 5S52  
Title : Tubulin-Z50145861-complex  
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Deposited on : 2020-11-08  
Resolution : 2.83 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	:	2.20
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)	:	2.20

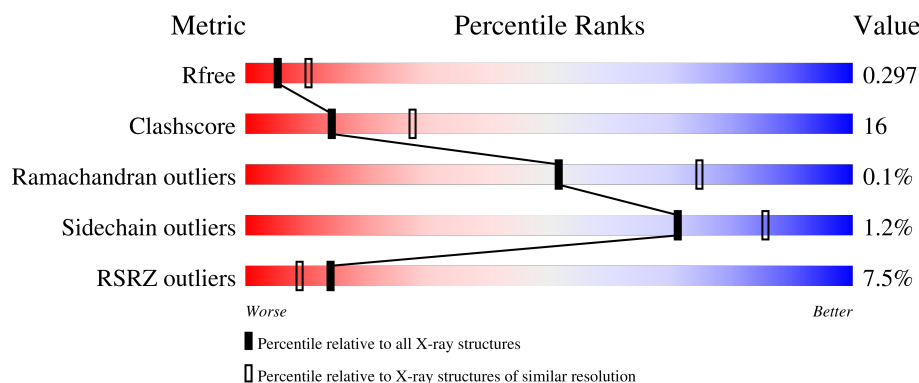
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.83 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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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>9%</div> <div>68%</div> <div>29%</div> <div>.</div> </div>
1	C	451	<div> <div>5%</div> <div>65%</div> <div>32%</div> <div>..</div> </div>
2	B	445	<div> <div>7%</div> <div>62%</div> <div>33%</div> <div>..</div> </div>
2	D	445	<div> <div>7%</div> <div>60%</div> <div>36%</div> <div>.</div> </div>
3	E	143	<div> <div>8%</div> <div>69%</div> <div>17%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
4	F	384	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: a small red segment at the beginning labeled '7%', a large green segment labeled '62%', a yellow segment labeled '29%', and a small grey segment at the end labeled '8%'. The segments are separated by thin white lines.

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17803 atoms, of which 20 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	0	0	0
			3424	2167	582	653	22			
1	C	440	Total	C	N	O	S	0	1	0
			3443	2178	585	657	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	425	Total	C	N	O	S	3	0	0
			3348	2103	573	645	27			
2	D	429	Total	C	N	O	S	6	0	0
			3358	2107	573	651	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	0	0
			1014	625	183	201	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

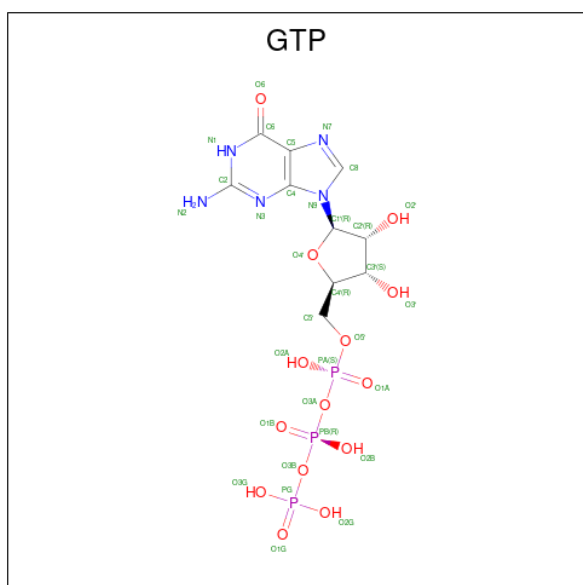
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	352	Total	C	N	O	S	0	0	0
			2877	1843	495	525	14			

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

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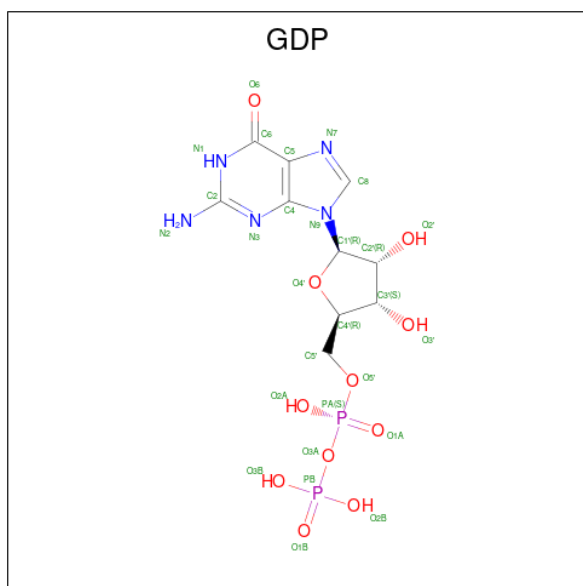
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

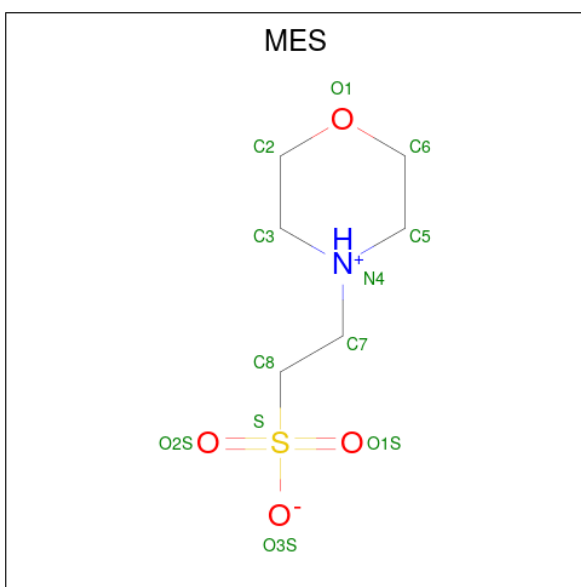
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Ca	0	0
			2	2		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- 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>).



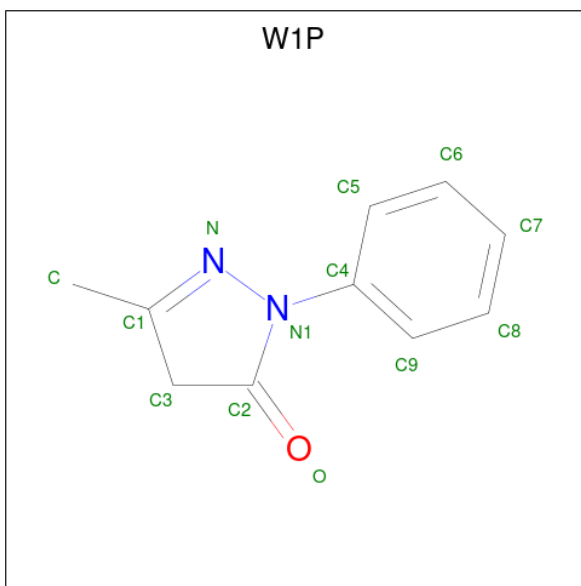
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
8	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



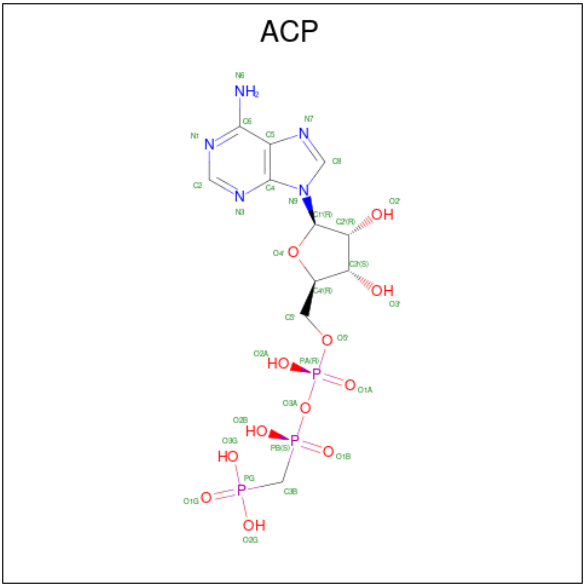
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is 5-methyl-2-phenyl-2,4-dihydro-3H-pyrazol-3-one (three-letter code: W1P) (formula:  $C_{10}H_{10}N_2O$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	0	0
			23	10	10	2	1		
10	B	1	Total	C	H	N	O	0	0
			23	10	10	2	1		

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

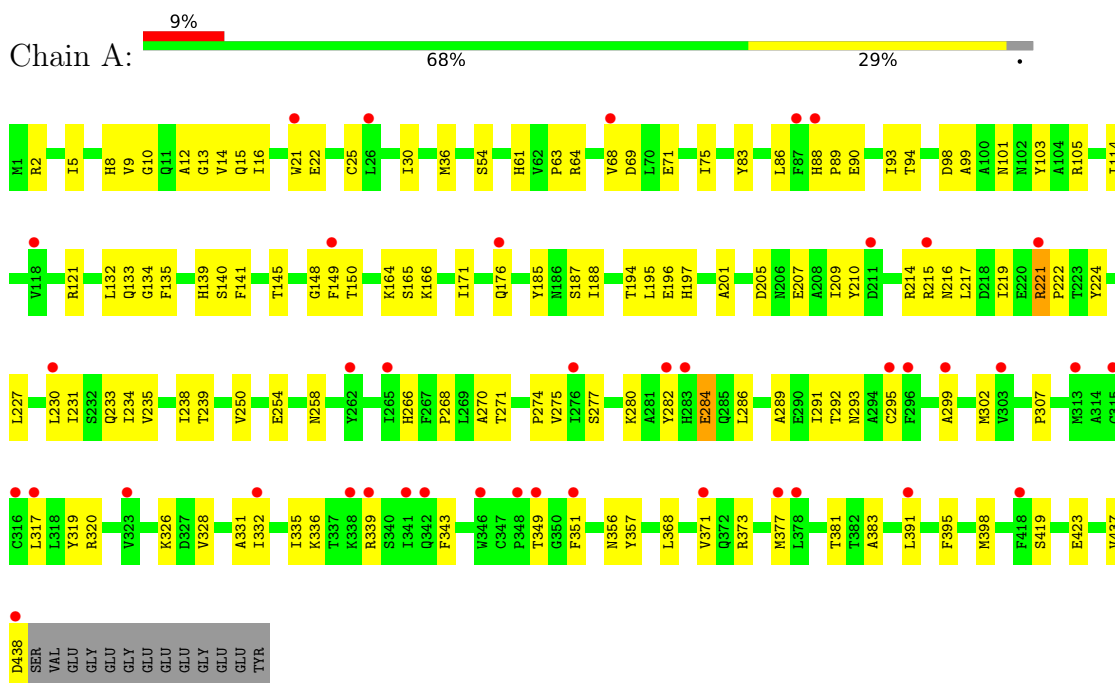
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	16	Total	O	0	0
			16	16		
12	B	36	Total	O	0	0
			36	36		
12	C	56	Total	O	0	0
			56	56		
12	D	4	Total	O	0	0
			4	4		
12	E	5	Total	O	0	0
			5	5		
12	F	4	Total	O	0	0
			4	4		

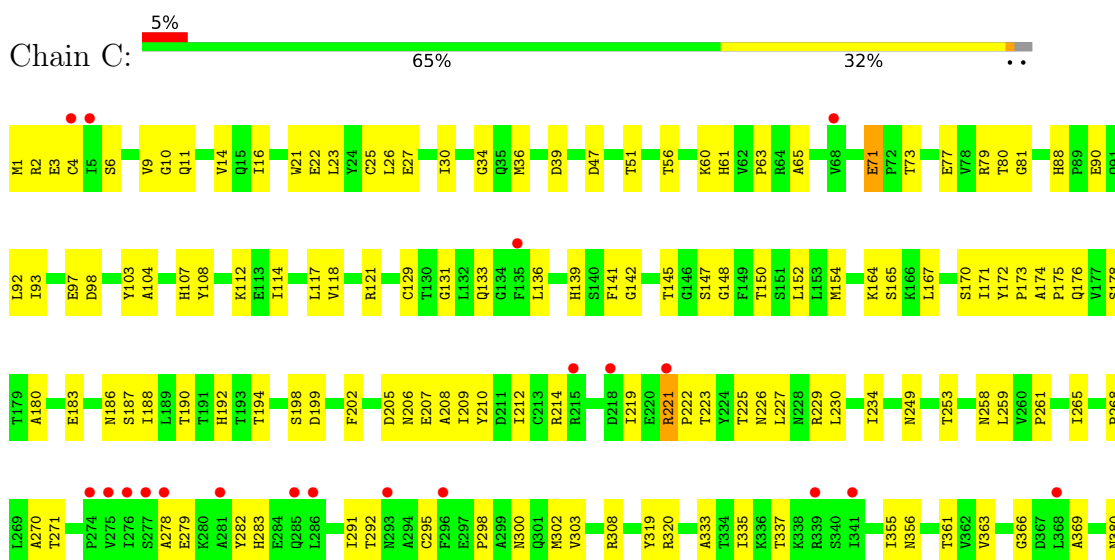
### 3 Residue-property plots [i](#)

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

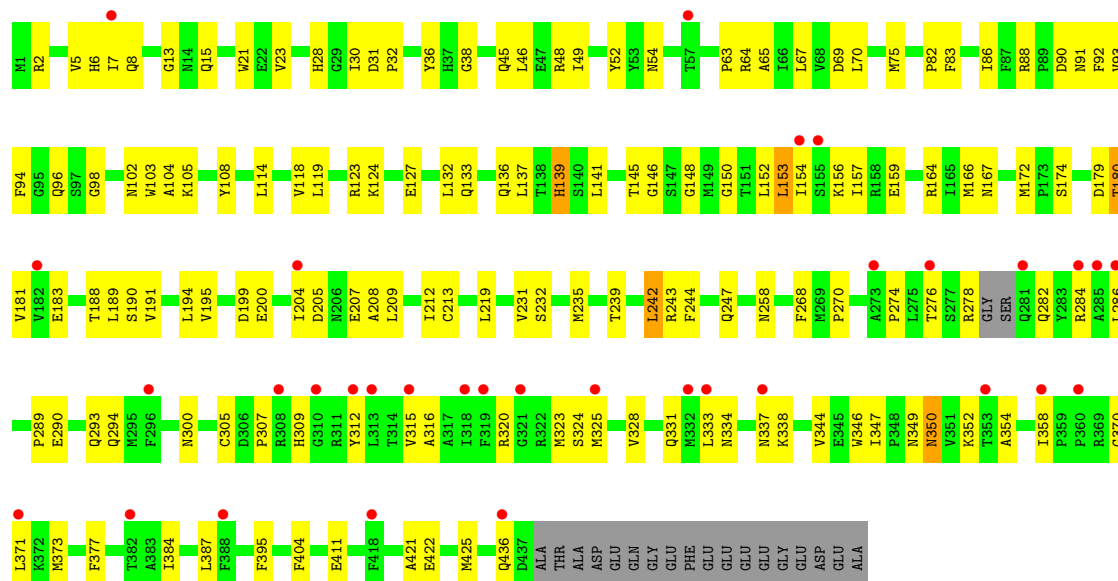


#### • Molecule 1: Tubulin alpha-1B chain

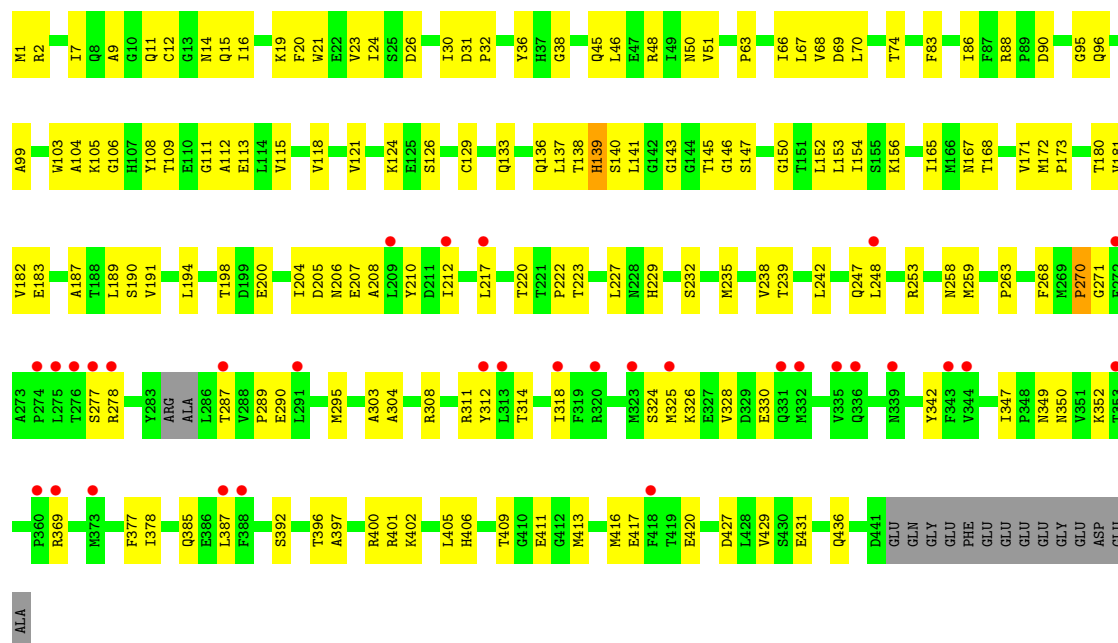




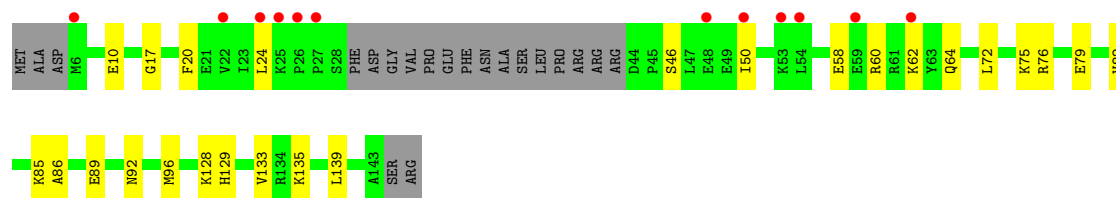
• Molecule 2: Tubulin beta-2B chain



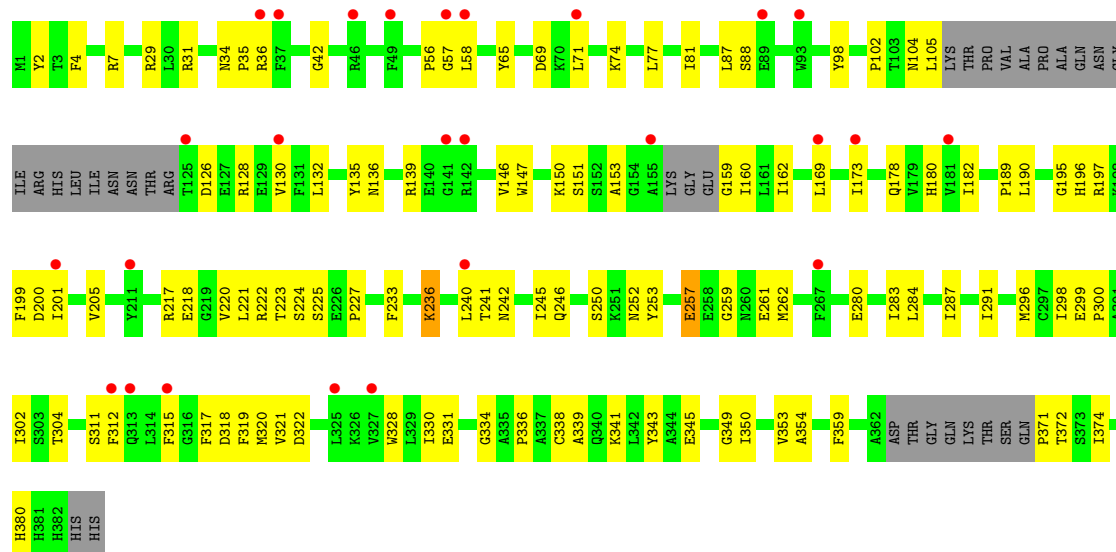
• Molecule 2: Tubulin beta-2B chain



• 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, $\alpha$ , $\beta$ , $\gamma$	105.09Å 161.57Å 174.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	118.67 – 2.83 118.67 – 2.83	Depositor EDS
% Data completeness (in resolution range)	97.3 (118.67-2.83) 97.3 (118.67-2.83)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.238 , 0.297 0.238 , 0.297	Depositor DCC
$R_{free}$ test set	3562 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.4	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 41.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	17803	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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: W1P, CA, GDP, MG, MES, ACP, GTP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.24	0/3502	0.40	0/4754
1	C	0.24	0/3521	0.40	0/4780
2	B	0.24	0/3422	0.40	0/4633
2	D	0.24	0/3431	0.39	0/4647
3	E	0.23	0/1022	0.33	0/1356
4	F	0.23	0/2944	0.39	0/3978
All	All	0.24	0/17842	0.39	0/24148

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	3424	0	3334	106	0
1	C	3443	0	3352	110	0
2	B	3348	0	3223	120	0
2	D	3358	0	3228	117	0
3	E	1014	0	1029	20	0
4	F	2877	0	2839	92	0
5	A	32	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	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	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	2	0
8	D	28	0	12	5	0
9	B	12	0	12	3	0
10	B	26	20	0	3	0
11	F	31	0	14	4	0
12	A	16	0	0	0	1
12	B	36	0	0	4	0
12	C	56	0	0	1	1
12	D	4	0	0	0	0
12	E	5	0	0	0	0
12	F	4	0	0	0	0
All	All	17783	20	17079	542	1

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 16.

The worst 5 of 542 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:A:381:THR:HG22	1:A:383:ALA:H	1.24	1.00
1:C:147:SER:HB2	1:C:190:THR:HB	1.61	0.83
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.63	0.80
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.63	0.79
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.63	0.78

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:610:HOH:O	12:C:605:HOH:O[3_555]	1.92	0.28

## 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	436/451 (97%)	415 (95%)	21 (5%)	0	100	100
1	C	439/451 (97%)	425 (97%)	14 (3%)	0	100	100
2	B	421/445 (95%)	395 (94%)	25 (6%)	1 (0%)	47	69
2	D	425/445 (96%)	403 (95%)	21 (5%)	1 (0%)	47	69
3	E	119/143 (83%)	117 (98%)	2 (2%)	0	100	100
4	F	344/384 (90%)	321 (93%)	22 (6%)	1 (0%)	41	61
All	All	2184/2319 (94%)	2076 (95%)	105 (5%)	3 (0%)	51	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	82	PRO
4	F	236	LYS
2	D	278	ARG

### 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	369/379 (97%)	365 (99%)	4 (1%)	73	86
1	C	372/379 (98%)	365 (98%)	7 (2%)	57	77
2	B	367/383 (96%)	361 (98%)	6 (2%)	62	81
2	D	368/383 (96%)	365 (99%)	3 (1%)	81	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	110/127 (87%)	110 (100%)	0	100	100
4	F	315/342 (92%)	313 (99%)	2 (1%)	86	93
All	All	1901/1993 (95%)	1879 (99%)	22 (1%)	71	85

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	279	GLU
2	D	139	HIS
1	C	406	HIS
2	D	229	HIS
2	B	180	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	96	GLN
4	F	136	ASN
4	F	242	ASN
4	F	180	HIS
2	D	294	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 9 are monoatomic - leaving 8 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	0.97	1 (3%)	33,54,54	1.75	7 (21%)
9	MES	B	504	-	12,12,12	2.24	1 (8%)	14,16,16	1.99	6 (42%)
8	GDP	D	501	6	24,30,30	1.18	2 (8%)	31,47,47	1.94	8 (25%)
11	ACP	F	401	6	27,33,33	1.37	5 (18%)	32,52,52	1.51	4 (12%)
10	W1P	B	505	-	12,14,14	0.56	0	15,19,19	0.80	1 (6%)
10	W1P	B	506	-	12,14,14	0.58	0	15,19,19	0.74	0
5	GTP	A	501	6	26,34,34	0.97	1 (3%)	33,54,54	1.75	6 (18%)
8	GDP	B	501	6	24,30,30	1.19	2 (8%)	31,47,47	2.04	8 (25%)

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	-	10/18/38/38	0/3/3/3
9	MES	B	504	-	-	4/6/14/14	0/1/1/1
8	GDP	D	501	6	-	2/12/32/32	0/3/3/3
11	ACP	F	401	6	-	8/15/38/38	0/3/3/3
10	W1P	B	505	-	-	0/4/16/16	0/2/2/2
10	W1P	B	506	-	-	0/4/16/16	0/2/2/2
5	GTP	A	501	6	-	4/18/38/38	0/3/3/3
8	GDP	B	501	6	-	2/12/32/32	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-7.47	1.66	1.77
8	D	501	GDP	C6-C5	4.20	1.48	1.41
8	B	501	GDP	C6-C5	4.16	1.48	1.41
5	C	501	GTP	C6-N1	3.03	1.38	1.33
5	A	501	GTP	C6-N1	3.01	1.38	1.33

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	N3-C2-N1	-5.35	120.08	127.22
5	C	501	GTP	N3-C2-N1	-5.28	120.18	127.22
8	B	501	GDP	C2-N3-C4	5.00	121.07	115.36
8	D	501	GDP	C2-N3-C4	4.81	120.85	115.36
11	F	401	ACP	PA-O3A-PB	-4.43	118.51	132.56

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

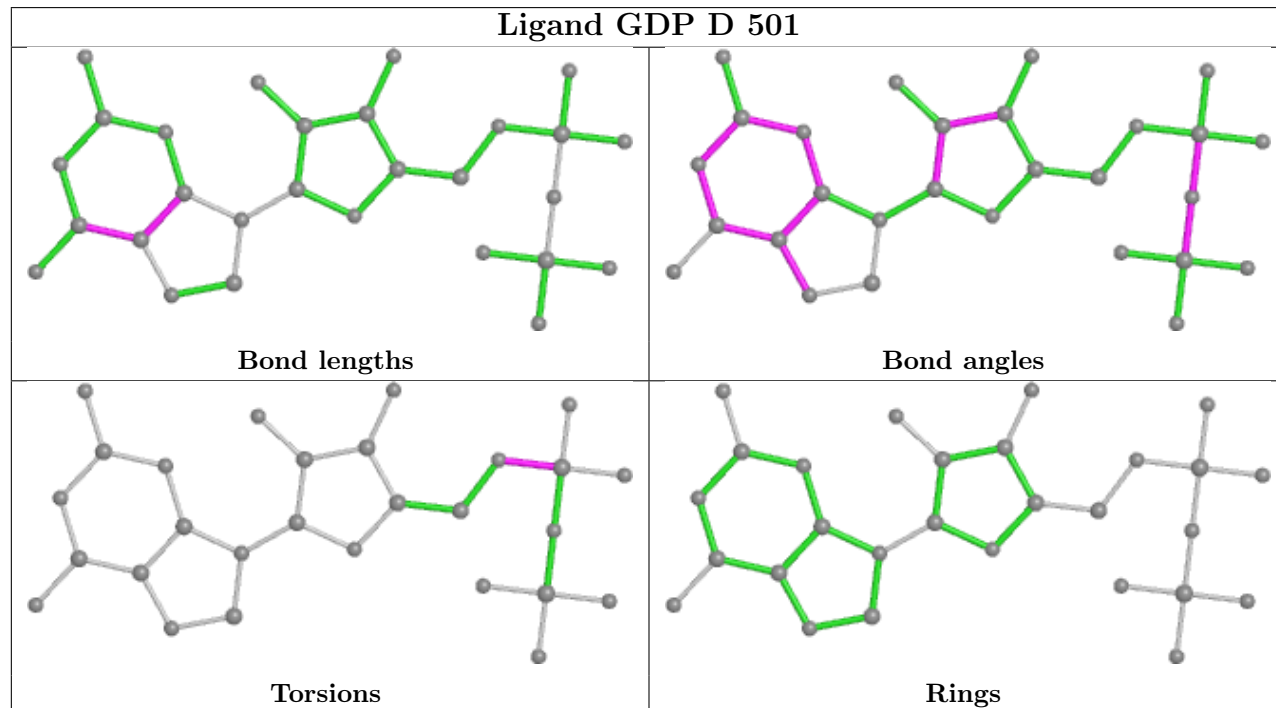
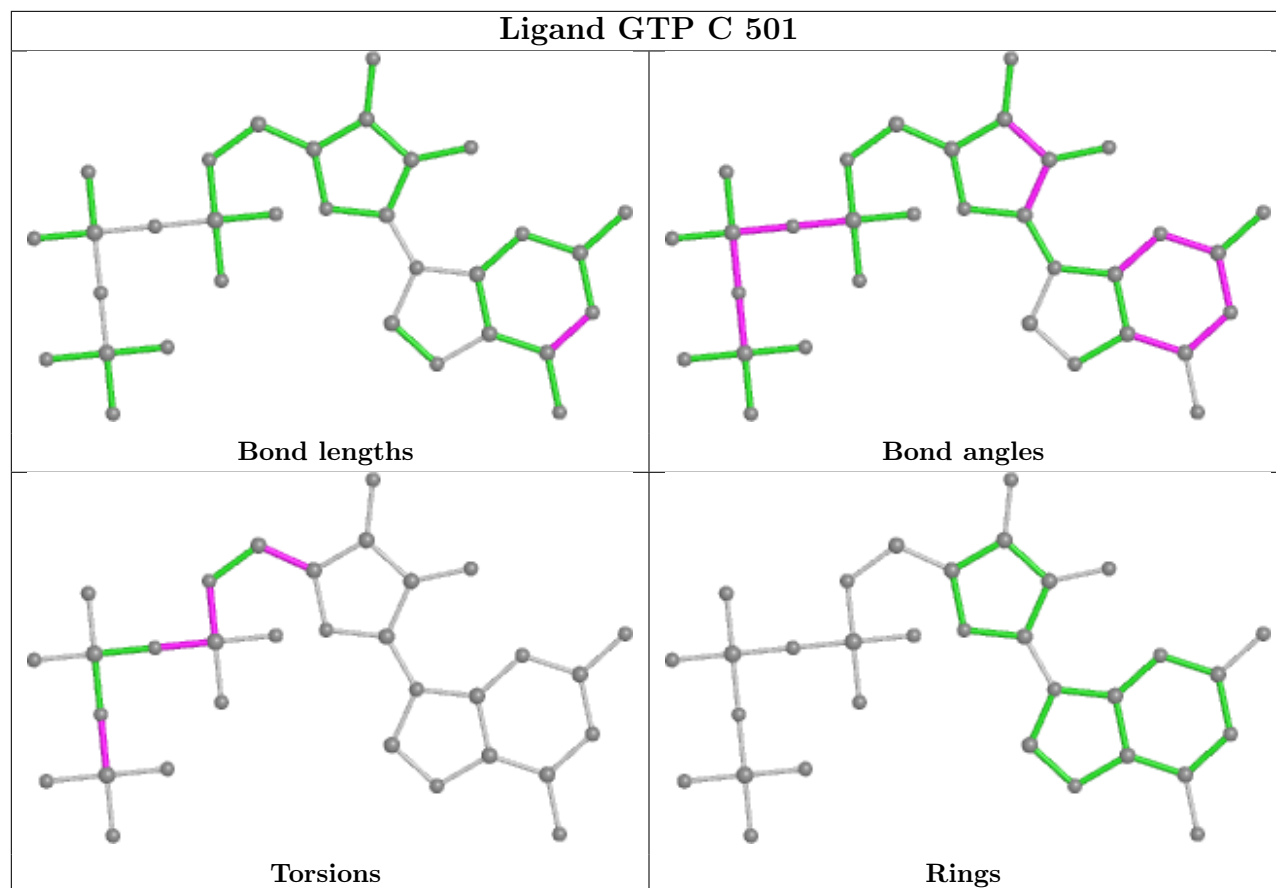
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O3A

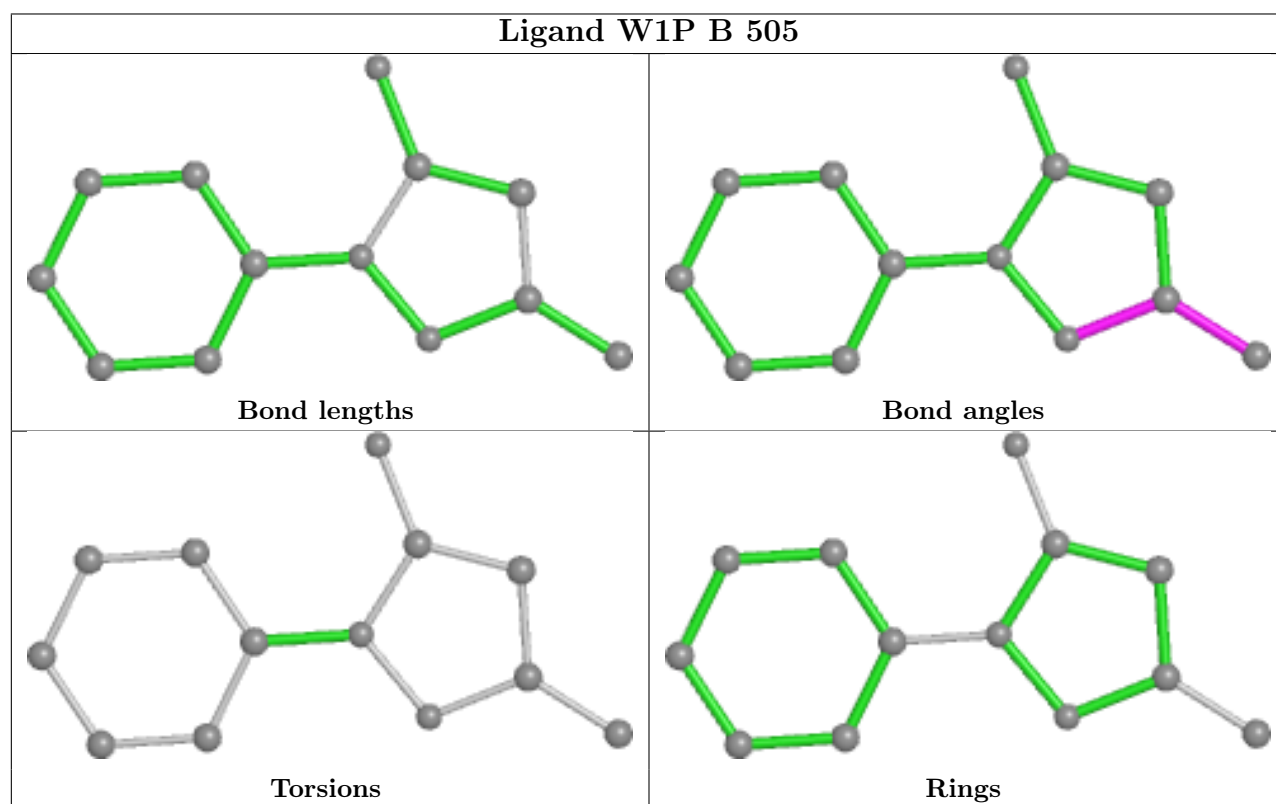
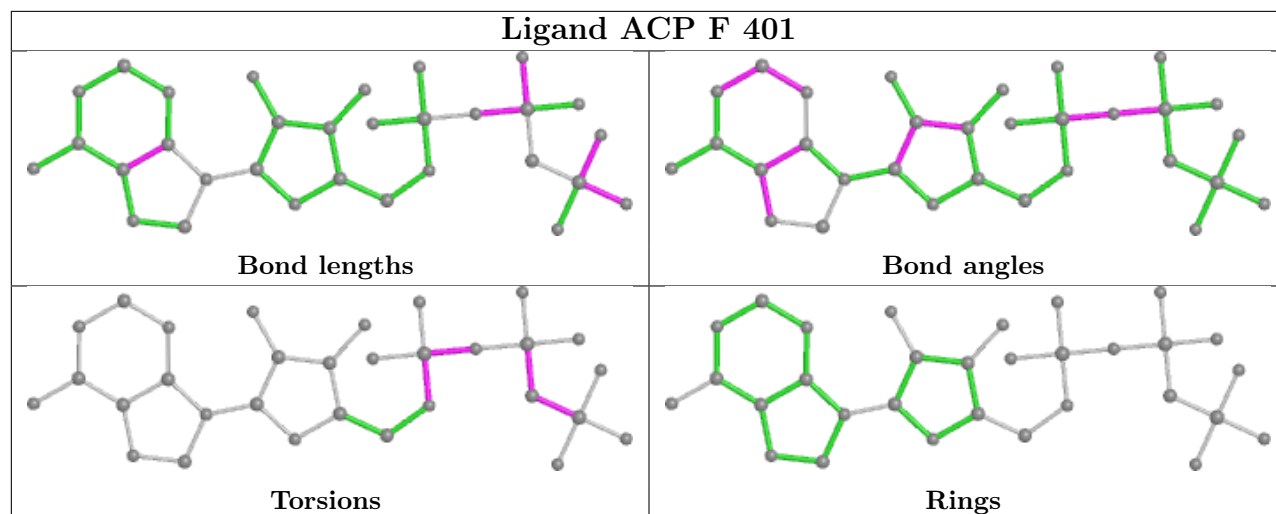
There are no ring outliers.

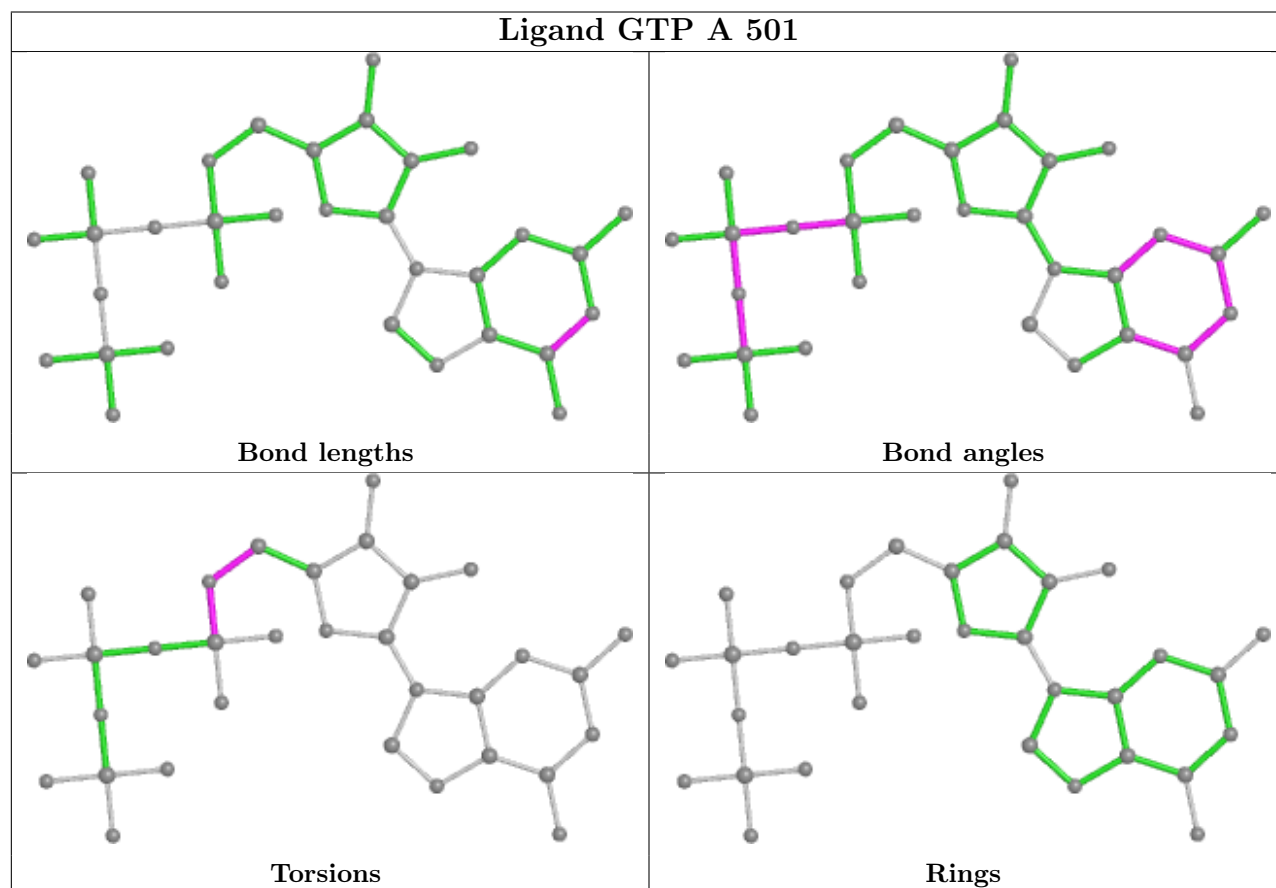
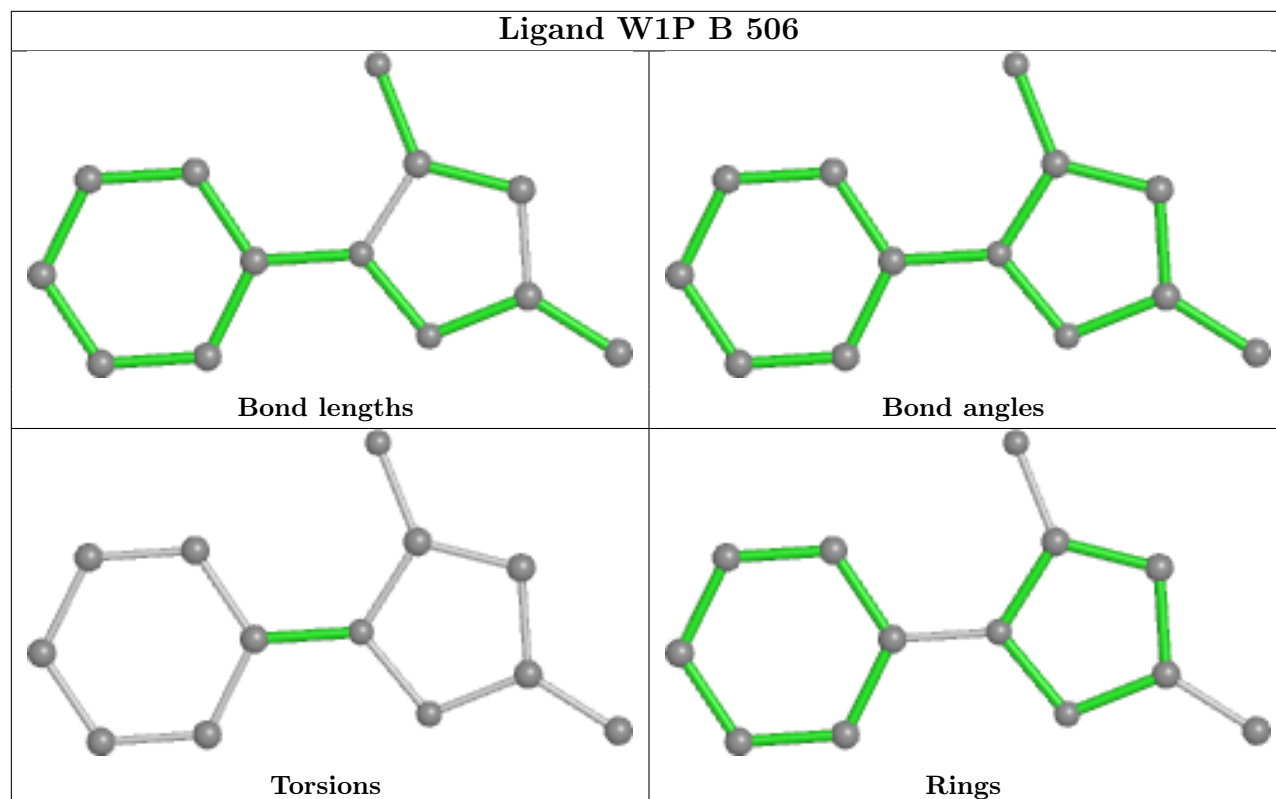
7 monomers are involved in 20 short contacts:

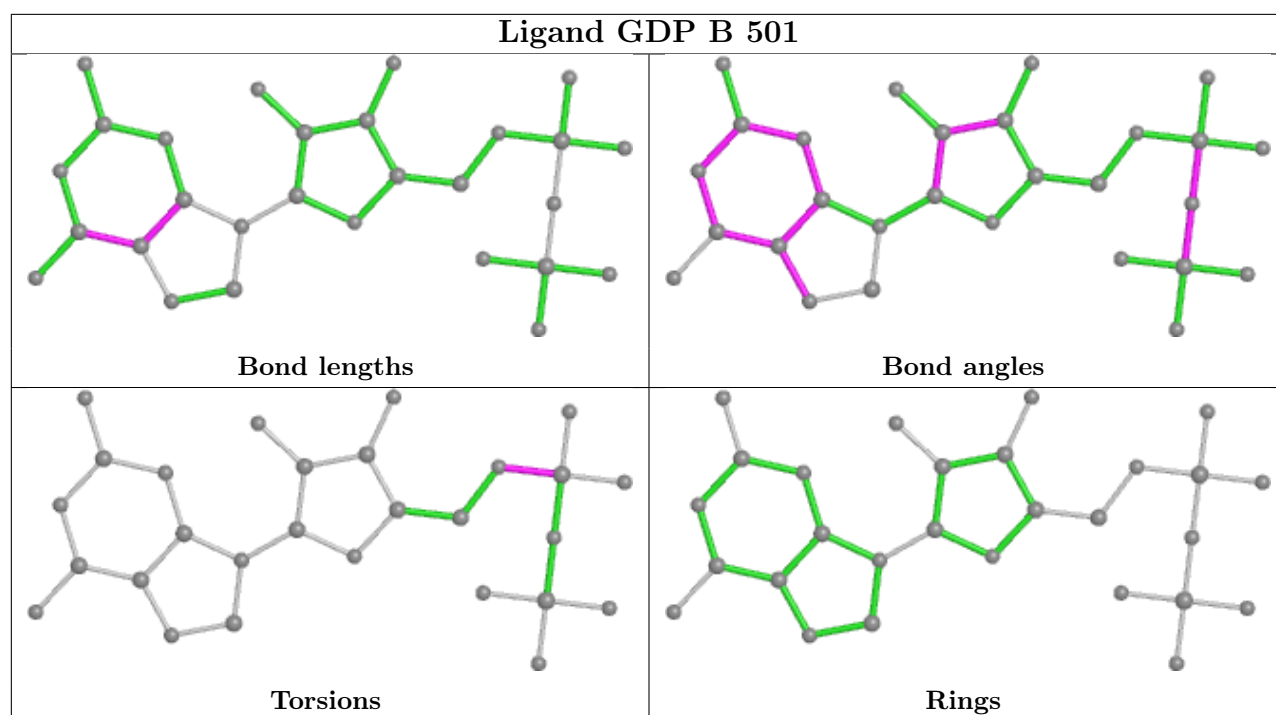
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	501	GTP	1	0
9	B	504	MES	3	0
8	D	501	GDP	5	0
11	F	401	ACP	4	0
10	B	505	W1P	3	0
5	A	501	GTP	2	0
8	B	501	GDP	2	0

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 [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%)	0.64	41 (9%) 8 4	58, 82, 130, 238	0
1	C	440/451 (97%)	0.39	21 (4%) 30 23	47, 69, 104, 154	0
2	B	425/445 (95%)	0.63	33 (7%) 13 8	52, 78, 151, 235	3 (0%)
2	D	429/445 (96%)	0.51	32 (7%) 14 9	68, 100, 138, 201	4 (0%)
3	E	123/143 (86%)	0.69	12 (9%) 7 4	72, 102, 156, 211	0
4	F	352/384 (91%)	0.46	26 (7%) 14 9	80, 116, 168, 211	0
All	All	2207/2319 (95%)	0.54	165 (7%) 14 9	47, 89, 153, 238	7 (0%)

The worst 5 of 165 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	285	ALA	11.0
2	D	278	ARG	7.4
2	B	337	ASN	6.6
2	B	333	LEU	6.5
3	E	24	LEU	6.2

### 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 ⓘ

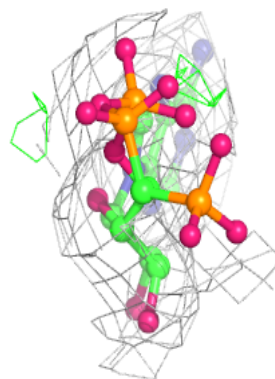
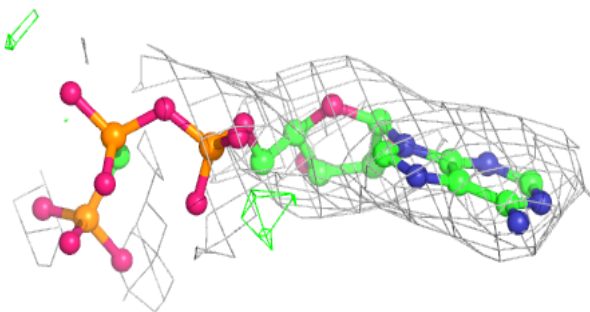
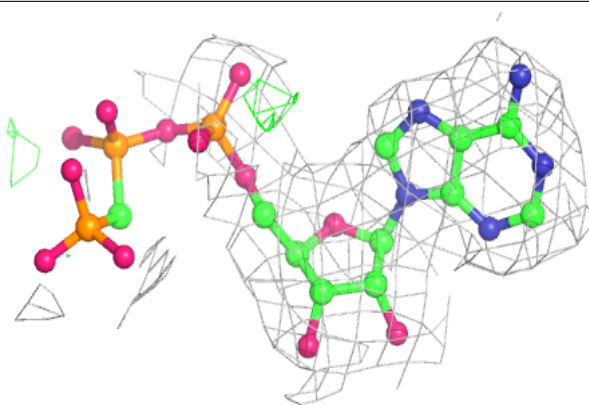
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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
7	CA	A	504	1/1	0.84	0.14	99,99,99,99	0
11	ACP	F	401	31/31	0.89	0.16	100,121,133,138	0
8	GDP	D	501	28/28	0.91	0.18	79,87,99,105	0
6	MG	D	502	1/1	0.91	0.21	83,83,83,83	0
10	W1P	B	506	13/13	0.92	0.45	61,68,84,84	23
9	MES	B	504	12/12	0.93	0.21	77,80,91,93	0
7	CA	A	503	1/1	0.95	0.18	102,102,102,102	0
10	W1P	B	505	13/13	0.95	0.45	64,71,86,86	23
5	GTP	A	501	32/32	0.96	0.17	58,63,72,77	0
5	GTP	C	501	32/32	0.96	0.17	50,59,67,69	0
8	GDP	B	501	28/28	0.97	0.17	49,56,63,64	0
6	MG	B	502	1/1	0.97	0.18	53,53,53,53	0
7	CA	B	503	1/1	0.97	0.17	112,112,112,112	0
6	MG	F	402	1/1	0.98	0.10	123,123,123,123	0
7	CA	C	503	1/1	0.98	0.20	73,73,73,73	0
6	MG	A	502	1/1	0.99	0.20	72,72,72,72	0
6	MG	C	502	1/1	0.99	0.17	58,58,58,58	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.

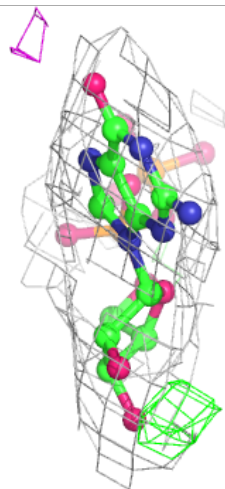
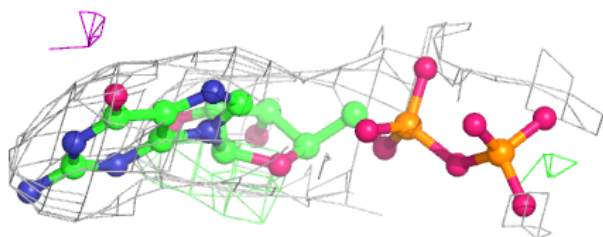
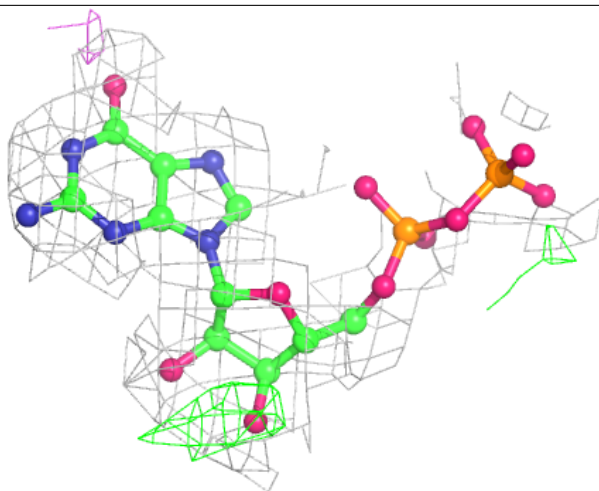
**Electron density around ACP F 401:**

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



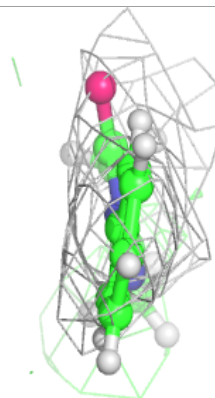
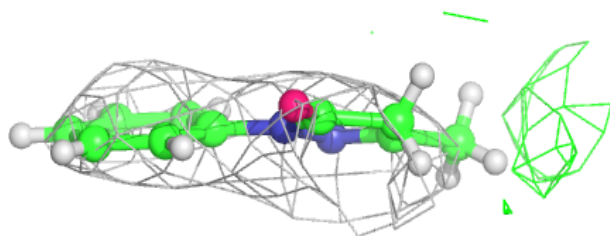
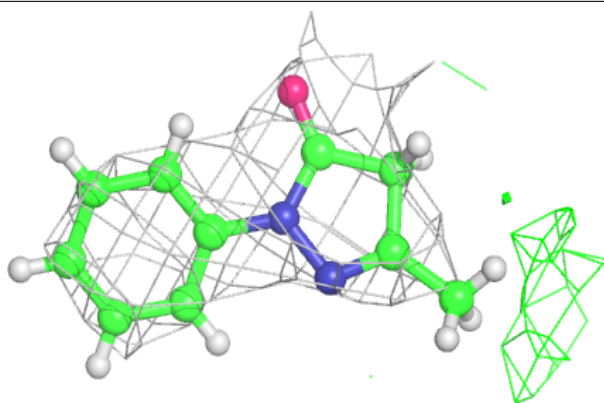
**Electron density around GDP D 501:**

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

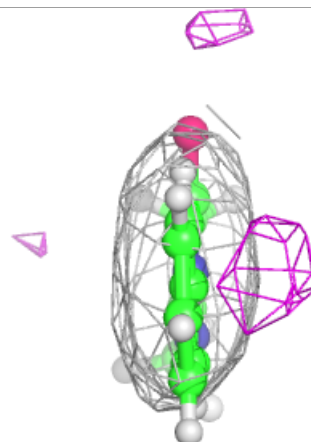
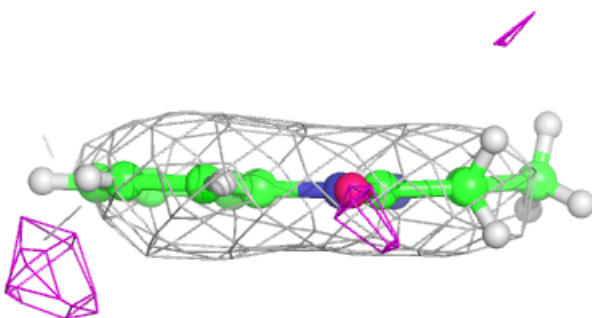
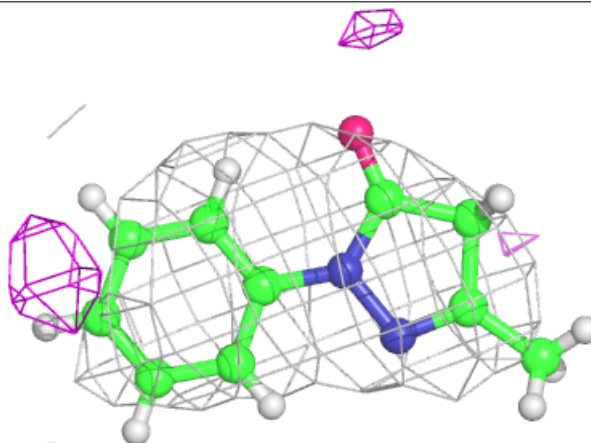


**Electron density around W1P B 506:**

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

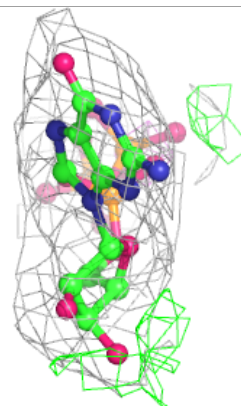
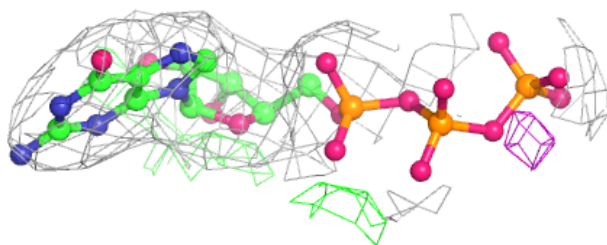
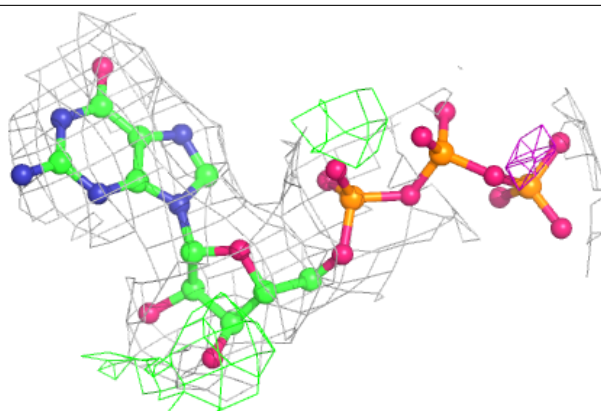
**Electron density around W1P B 505:**

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

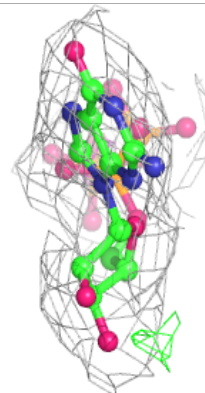
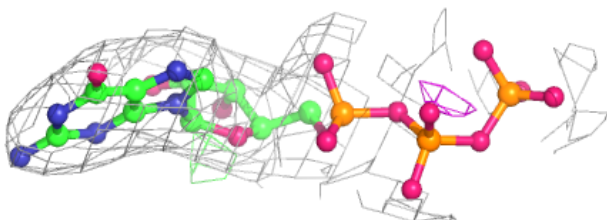
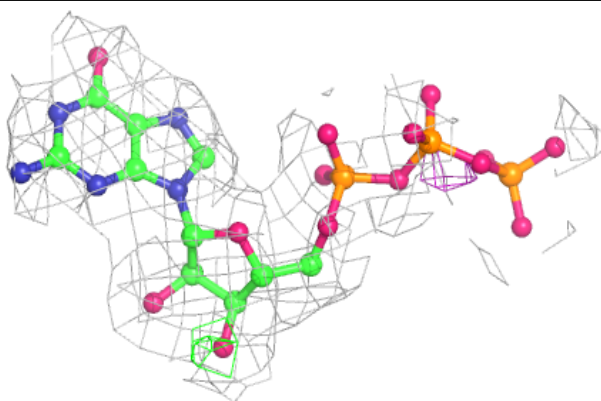


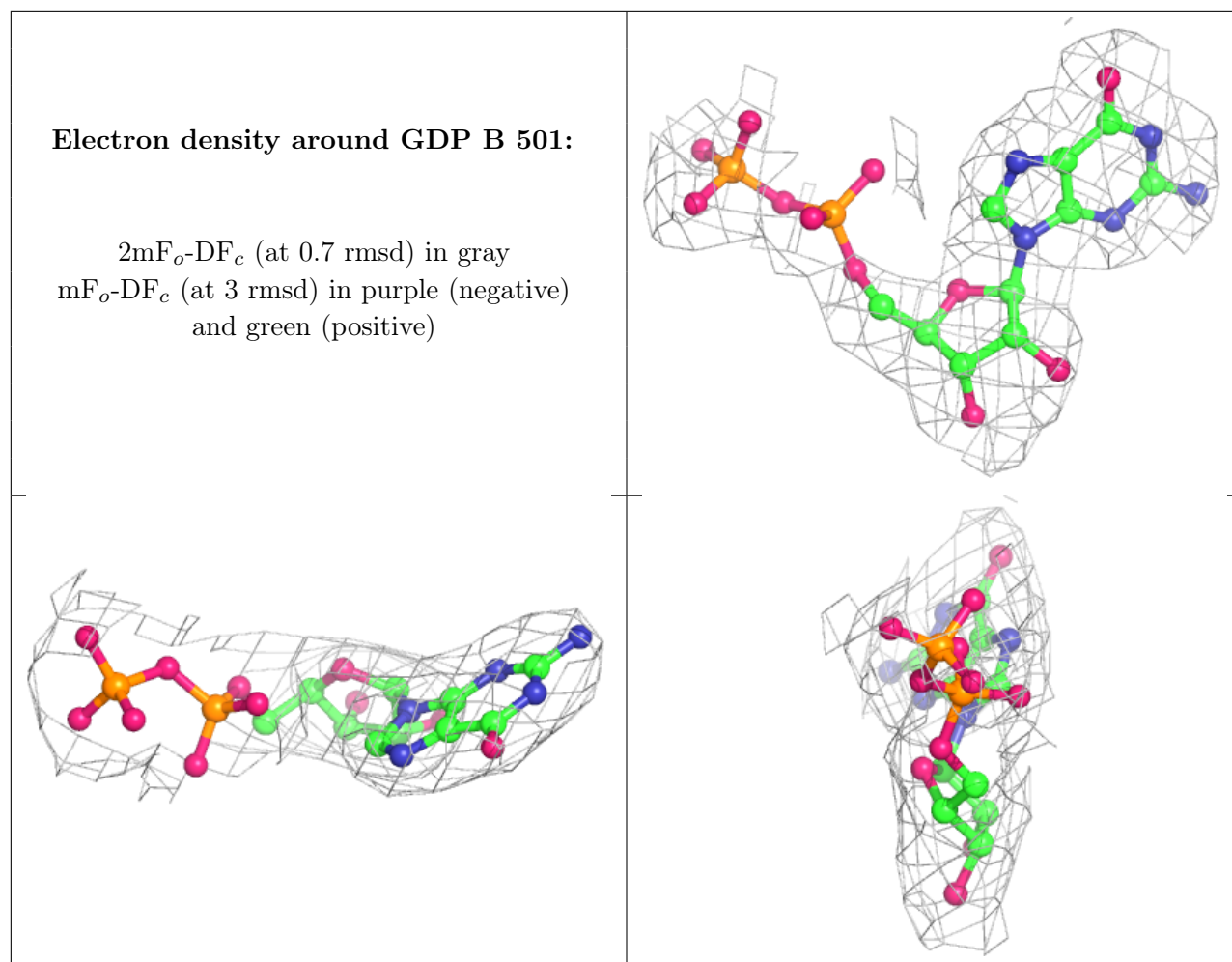
**Electron density around GTP A 501:**

$2mF_o-DF_c$  (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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.