



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:48 PM UTC

PDB ID : 9GNU / pdb\_00009gnu  
Title : Tubulin in complex with a dioxane analog of zampanolide  
Authors : Oliva, M.A.; Diaz, J.F.; Altmann, K.H.  
Deposited on : 2024-09-04  
Resolution : 2.20 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

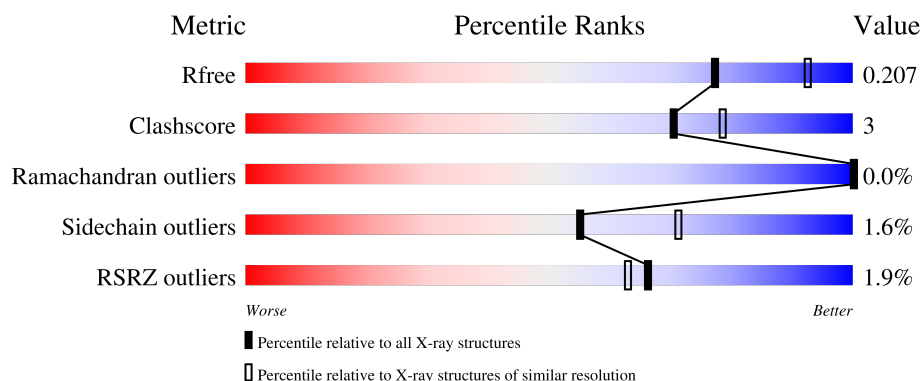
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>2%</div> <div>86%</div> <div>9%</div> <div>• •</div> </div>
1	C	451	<div> <div>2%</div> <div>81%</div> <div>16%</div> <div>•</div> </div>
2	B	445	<div> <div>0%</div> <div>80%</div> <div>12%</div> <div>• 6%</div> </div>
2	D	445	<div> <div>0%</div> <div>84%</div> <div>12%</div> <div>• •</div> </div>
3	E	189	<div> <div>2%</div> <div>50%</div> <div>11%</div> <div>40%</div> </div>

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Mol	Chain	Length	Quality of chain
4	F	384	<div><div></div><div>3%</div><div>73%</div><div>8%</div><div>17%</div></div>

## 2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 35660 atoms, of which 17150 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	434	Total	C	H	N	O	S	108	7	0
			6803	2173	3365	583	658	24			
1	C	439	Total	C	H	N	O	S	115	14	0
			6966	2225	3436	600	680	25			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	417	Total	C	H	N	O	S	102	10	0
			6605	2108	3241	572	657	27			
2	D	429	Total	C	H	N	O	S	105	5	0
			6701	2137	3292	583	661	28			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	114	Total	C	H	N	O	S	18	4	0
			1986	604	1008	181	189	4			

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	319	Total	C	H	N	O	S	77	3	0
			5283	1702	2637	449	482	13			

There are 39 discrepancies between the modelled and reference sequences:

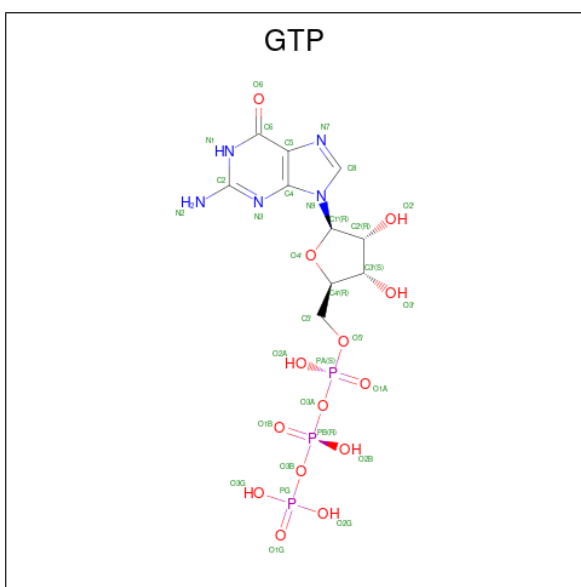
Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	MET	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	PRO	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	LYS	deletion	UNP A0A8V0Z8P0
F	?	-	ASN	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	PHE	deletion	UNP A0A8V0Z8P0
F	379	HIS	-	expression tag	UNP A0A8V0Z8P0
F	380	HIS	-	expression tag	UNP A0A8V0Z8P0
F	381	HIS	-	expression tag	UNP A0A8V0Z8P0
F	382	HIS	-	expression tag	UNP A0A8V0Z8P0
F	383	HIS	-	expression tag	UNP A0A8V0Z8P0
F	384	HIS	-	expression tag	UNP A0A8V0Z8P0

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: 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	
			44	10	12	5	14	3	2
5	C	1	Total	C	H	N	O	P	
			44	10	12	5	14	3	2
5	D	1	Total	C	H	N	O	P	
			44	10	12	5	14	3	2

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

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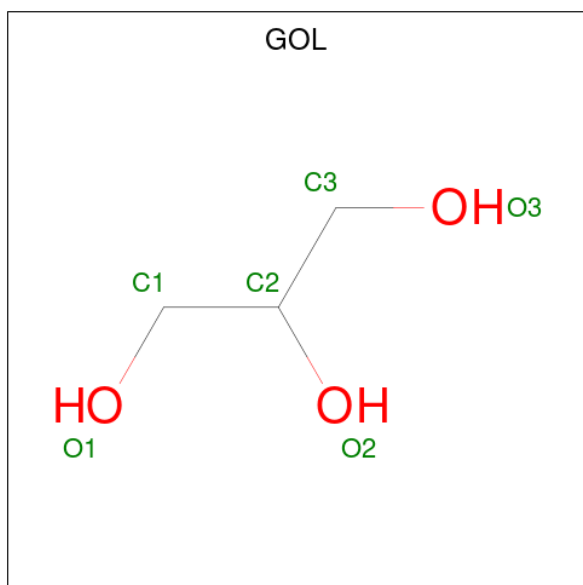
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

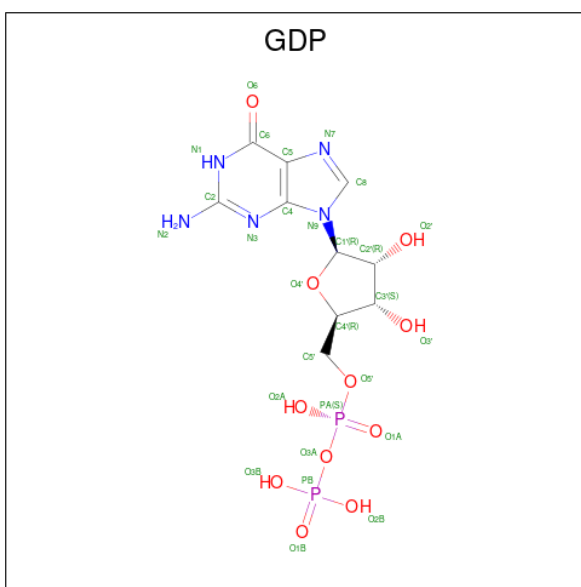
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



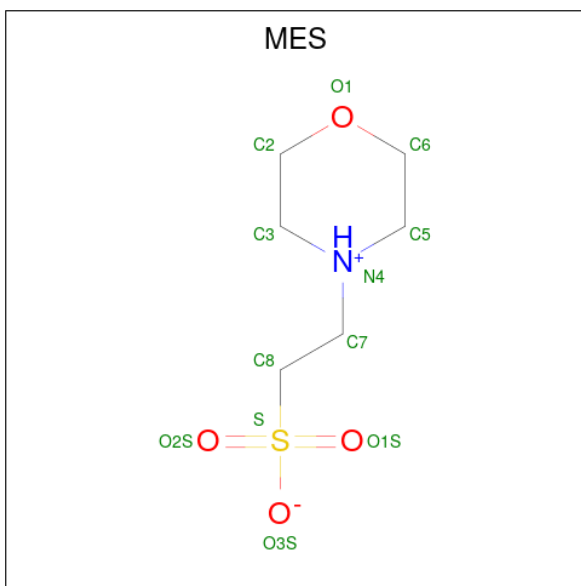
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	H	O	3	0
			14	3	8	3		
9	B	1	Total	C	H	O	3	0
			14	3	8	3		
9	C	1	Total	C	H	O	3	0
			14	3	8	3		

- Molecule 10 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: 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
10	B	1	Total	C	H	N	O	P	
			40	10	12	5	11	2	

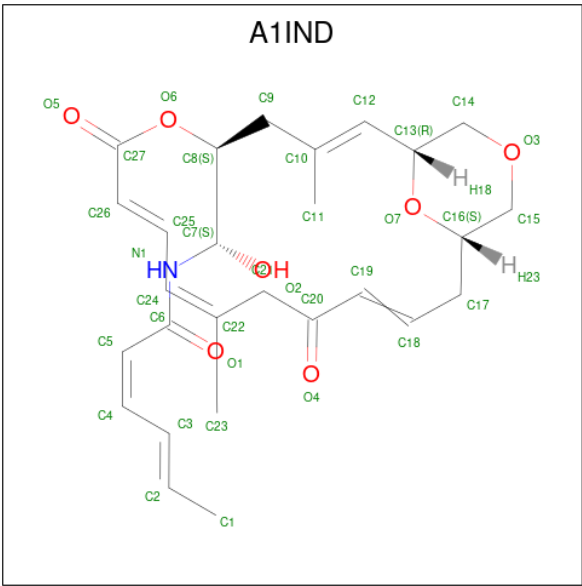
- Molecule 11 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula:  $C_6H_{13}NO_4S$ ).



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

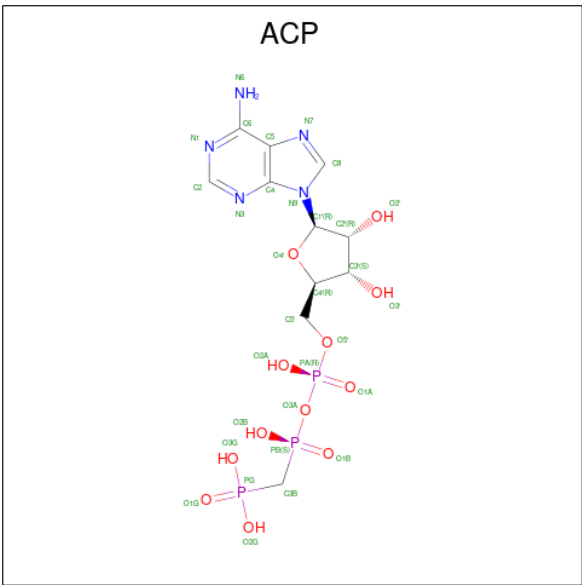
- Molecule 12 is (2Z,4E)-N-((S)-((1R,2E,5S,8E,10Z,14E,17S)-3,11-dimethyl-7,13-dioxo-6,19,21-trioxabicyclo[15.3.1]henicosa-2,8,10,14-tetraen-5-yl)(hydroxy)methyl)hexa-2,4-dienamide

(CCD ID: A1IND) (formula: C<sub>27</sub>H<sub>35</sub>NO<sub>7</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	B	1	Total	C	H	N	O	10	0
			71	27	36	1	7		
12	D	1	Total	C	H	N	O	10	0
			71	27	36	1	7		

- Molecule 13 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: 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
13	F	1	Total	C	H	N	O	P	2	0
			45	11	14	5	12	3		

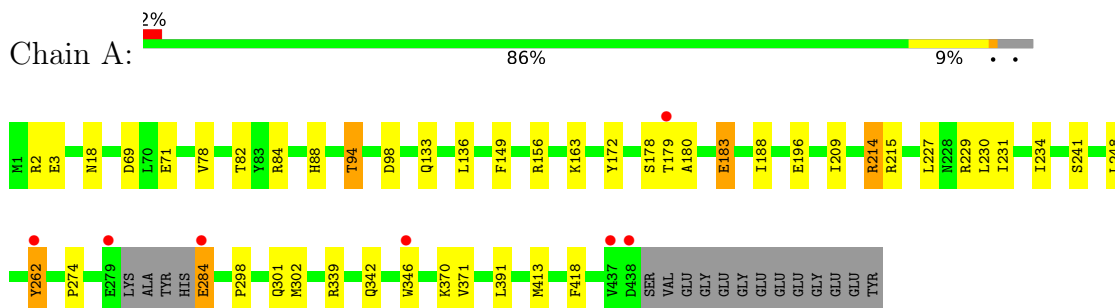
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	169	Total	O	0	0
			169	169		
14	B	149	Total	O	0	0
			149	149		
14	C	296	Total	O	0	0
			296	296		
14	D	141	Total	O	0	0
			141	141		
14	E	43	Total	O	0	0
			43	43		
14	F	82	Total	O	0	0
			82	82		

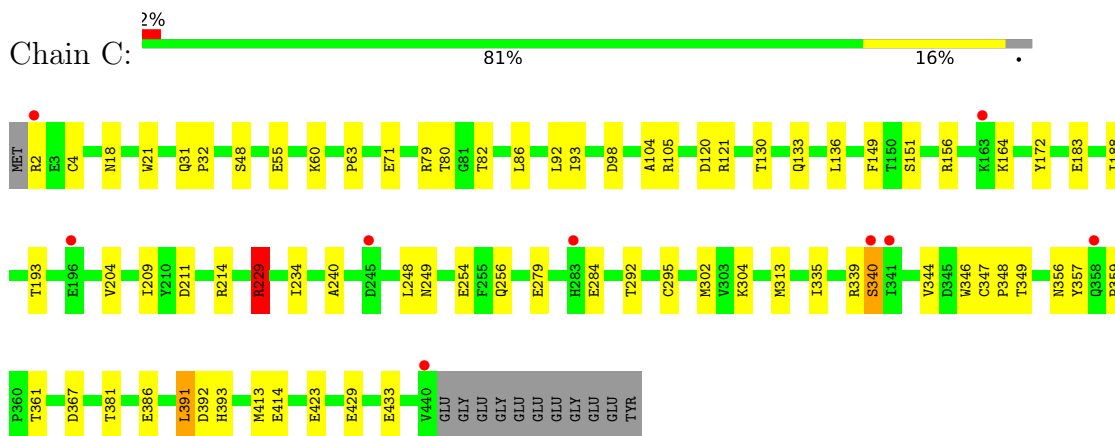
### 3 Residue-property plots [i](#)

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.

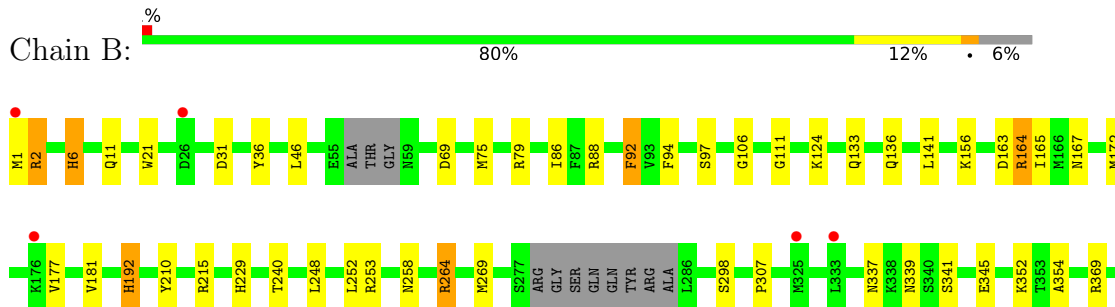
- Molecule 1: Tubulin alpha-1B chain

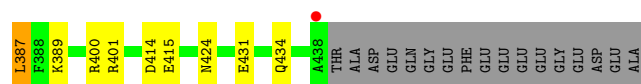


- Molecule 1: Tubulin alpha-1B chain

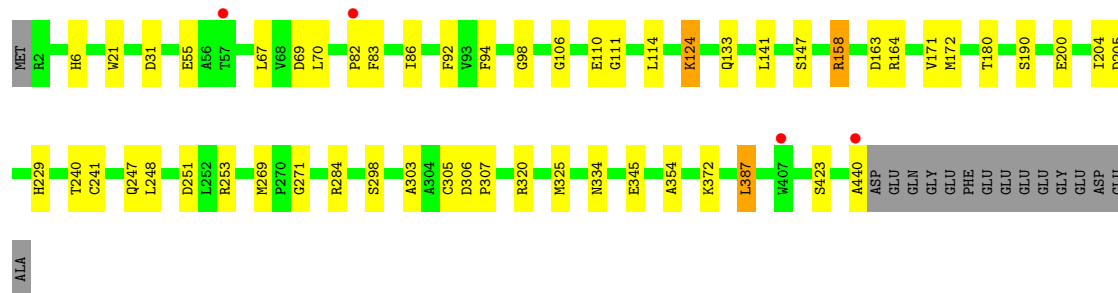
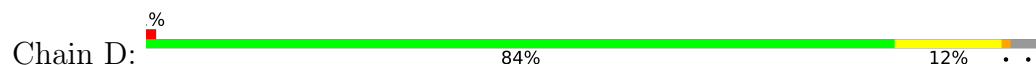


- Molecule 2: Tubulin beta-2B chain

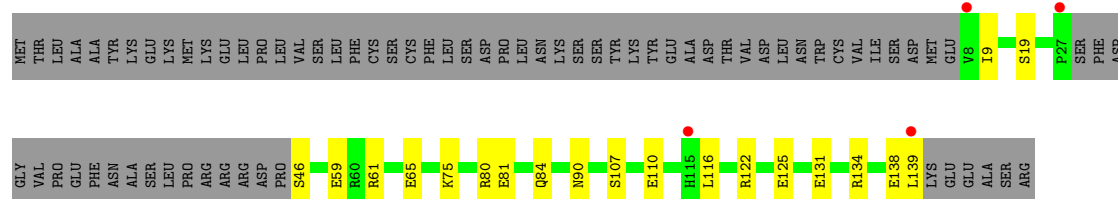




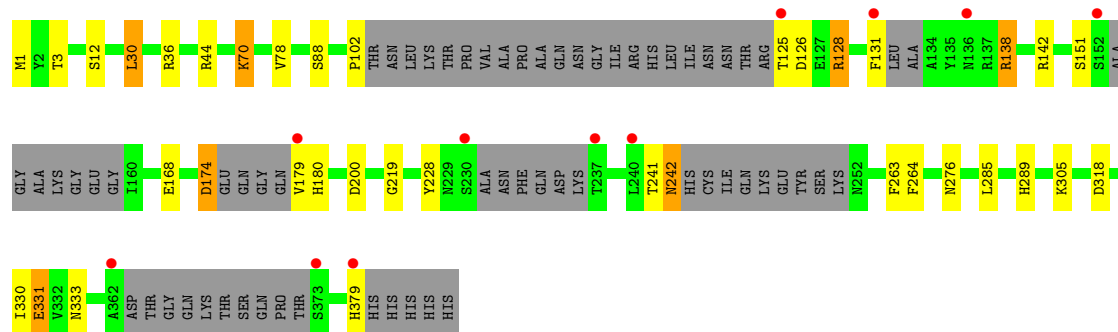
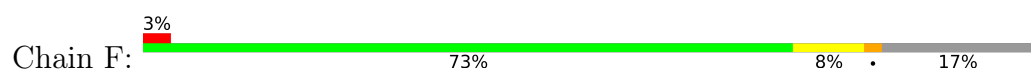
• Molecule 2: Tubulin beta-2B chain



• 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, $\alpha$ , $\beta$ , $\gamma$	105.20Å 159.17Å 178.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.14 – 2.20 48.14 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.14-2.20) 99.9 (48.14-2.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.164 , 0.206 0.165 , 0.207	Depositor DCC
$R_{free}$ test set	7610 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.5	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 39.3	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	0.97	EDS
Total number of atoms	35660	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACP, MES, GTP, MG, CL, GOL, A1IND, CA, GDP

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	0.96	1/3513 (0.0%)	1.37	19/4769 (0.4%)
1	C	1.08	6/3609 (0.2%)	1.46	24/4902 (0.5%)
2	B	0.98	5/3436 (0.1%)	1.43	19/4651 (0.4%)
2	D	0.94	2/3484 (0.1%)	1.36	15/4720 (0.3%)
3	E	1.04	0/986	1.74	10/1307 (0.8%)
4	F	0.83	1/2702 (0.0%)	1.43	21/3646 (0.6%)
All	All	0.97	15/17730 (0.1%)	1.43	108/23995 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	C	0	4
2	B	0	5
2	D	0	3
4	F	0	3
All	All	0	19

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	229	HIS	CE1-NE2	9.08	1.41	1.32
1	C	367	ASP	CG-OD2	7.57	1.39	1.25
2	D	229	HIS	ND1-CE1	7.17	1.39	1.32
2	B	229	HIS	ND1-CE1	6.06	1.38	1.32
4	F	289	HIS	CE1-NE2	5.95	1.38	1.32

The worst 5 of 108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	131	PHE	CA-C-O	-10.99	102.12	120.80
4	F	174	ASP	CA-CB-CG	9.72	122.33	112.60
1	C	130	THR	OG1-CB-CG2	-9.45	90.41	109.30
2	B	269	MET	CG-SD-CE	-9.08	80.93	100.90
4	F	305	LYS	CA-C-N	-8.78	109.42	122.86

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	214	ARG	Sidechain
1	A	229	ARG	Sidechain
1	A	339	ARG	Sidechain
1	A	84	ARG	Sidechain
2	B	2	ARG	Sidechain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3438	3365	3345	17	0
1	C	3530	3436	3410	34	0
2	B	3364	3241	3221	33	0
2	D	3409	3292	3279	23	0
3	E	978	1008	997	3	0
4	F	2646	2637	2618	11	0
5	A	32	12	12	0	0
5	C	32	12	12	0	0
5	D	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	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	6	8	8	0	0
9	B	6	8	8	0	0
9	C	6	8	8	0	0
10	B	28	12	12	0	0
11	B	12	13	13	3	0
12	B	35	36	0	0	0
12	D	35	36	0	0	0
13	F	31	14	14	3	0
14	A	169	0	0	1	0
14	B	149	0	0	10	0
14	C	296	0	0	9	0
14	D	141	0	0	7	0
14	E	43	0	0	1	0
14	F	82	0	0	0	0
All	All	18510	17150	16969	119	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 3.

The worst 5 of 119 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193[A]:THR:HG22	14:C:646:HOH:O	1.38	1.20
14:C:840:HOH:O	2:D:325:MET:HE2	1.54	1.05
1:C:4[B]:CYS:SG	1:C:136:LEU:HG	2.15	0.87
2:B:414[A]:ASP:OD1	14:B:601:HOH:O	1.95	0.85
1:C:234:ILE:HD13	1:C:302[A]:MET:SD	2.21	0.81

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	437/451 (97%)	433 (99%)	4 (1%)	0	100	100
1	C	451/451 (100%)	443 (98%)	8 (2%)	0	100	100
2	B	421/445 (95%)	415 (99%)	6 (1%)	0	100	100
2	D	432/445 (97%)	424 (98%)	8 (2%)	0	100	100
3	E	114/189 (60%)	113 (99%)	1 (1%)	0	100	100
4	F	306/384 (80%)	299 (98%)	6 (2%)	1 (0%)	36	42
All	All	2161/2365 (91%)	2127 (98%)	33 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	88	SER

### 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	373/379 (98%)	368 (99%)	5 (1%)	61	76
1	C	384/379 (101%)	378 (98%)	6 (2%)	55	71
2	B	373/383 (97%)	369 (99%)	4 (1%)	65	79
2	D	375/383 (98%)	370 (99%)	5 (1%)	61	76
3	E	106/171 (62%)	100 (94%)	6 (6%)	18	23
4	F	292/342 (85%)	288 (99%)	4 (1%)	59	75
All	All	1903/2037 (93%)	1873 (98%)	30 (2%)	55	71

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	414	GLU
4	F	30	LEU
2	D	372	LYS
4	F	331	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	E	107	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	436	GLN
3	E	90	ASN
4	F	281	ASN
3	E	92	ASN
2	B	385	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 10 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
5	GTP	D	501	6	33,34,34	1.54	3 (9%)	50,54,54	0.85	2 (4%)
5	GTP	C	501	6	33,34,34	1.40	2 (6%)	50,54,54	1.05	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	GOL	A	506	-	5,5,5	0.47	0	5,5,5	0.94	0
10	GDP	B	501	6	29,30,30	0.77	1 (3%)	45,47,47	0.61	0
9	GOL	C	504	-	5,5,5	0.16	0	5,5,5	0.50	0
12	A1IND	B	506	2	34,36,36	1.33	1 (2%)	32,46,46	2.44	8 (25%)
11	MES	B	502	-	12,12,12	0.91	0	15,16,16	0.98	1 (6%)
12	A1IND	D	503	2	34,36,36	1.68	3 (8%)	32,46,46	2.10	6 (18%)
9	GOL	B	503	-	5,5,5	0.33	0	5,5,5	0.77	0
5	GTP	A	501	6	33,34,34	0.95	1 (3%)	50,54,54	1.04	5 (10%)
13	ACP	F	401	6	31,33,33	0.98	2 (6%)	47,52,52	0.95	3 (6%)

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	D	501	6	-	7/22/38/38	0/3/3/3
5	GTP	C	501	6	-	6/22/38/38	0/3/3/3
9	GOL	A	506	-	-	1/4/4/4	-
10	GDP	B	501	6	-	4/16/32/32	0/3/3/3
9	GOL	C	504	-	-	2/4/4/4	-
12	A1IND	B	506	2	-	7/41/51/51	0/0/2/2
11	MES	B	502	-	-	3/6/14/14	0/1/1/1
12	A1IND	D	503	2	-	7/41/51/51	0/0/2/2
9	GOL	B	503	-	-	0/4/4/4	-
5	GTP	A	501	6	-	7/22/38/38	0/3/3/3
13	ACP	F	401	6	-	3/19/38/38	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	503	A1IND	C19-C18	7.39	1.52	1.32
5	D	501	GTP	PA-O3A	7.13	1.67	1.59
12	B	506	A1IND	C19-C18	7.07	1.51	1.32
5	C	501	GTP	PA-O3A	6.24	1.66	1.59
12	D	503	A1IND	O7-C13	-3.43	1.35	1.44

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	506	A1IND	O1-C6-N1	-9.32	110.28	122.44
12	D	503	A1IND	C17-C18-C19	-6.31	112.28	125.93
12	B	506	A1IND	C25-C24-C22	5.08	134.83	127.69
12	D	503	A1IND	O7-C16-C15	4.96	113.71	109.63
12	D	503	A1IND	O3-C15-C16	-4.27	102.92	111.38

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

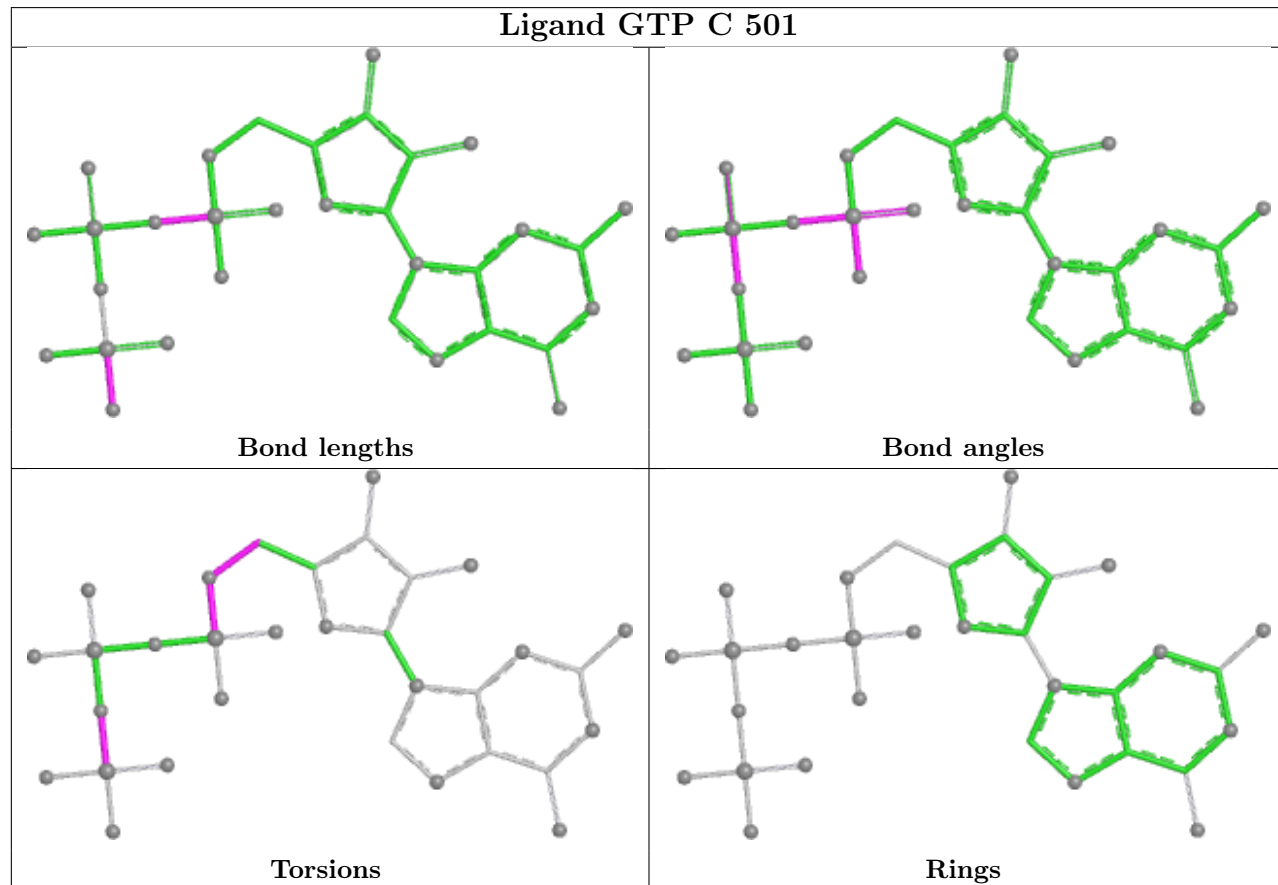
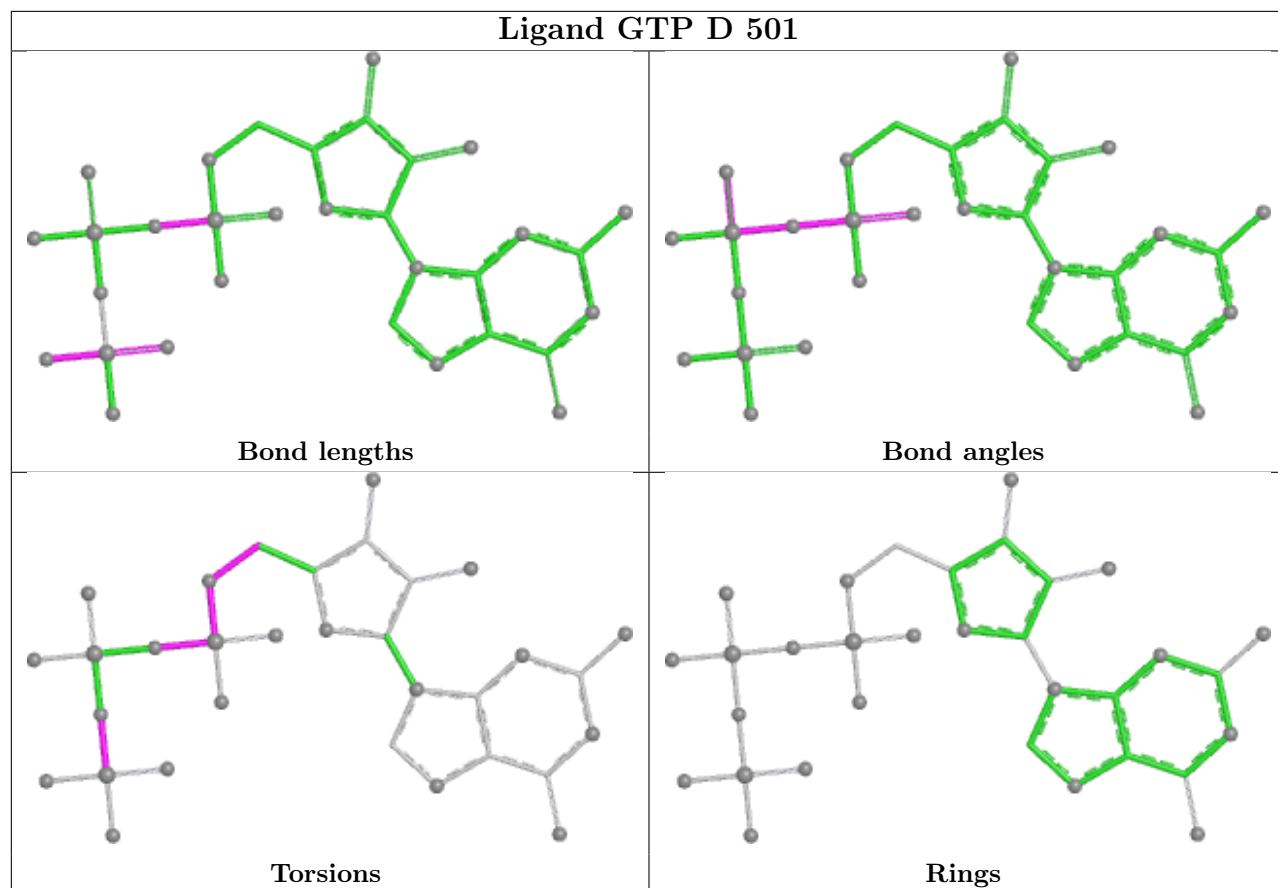
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G

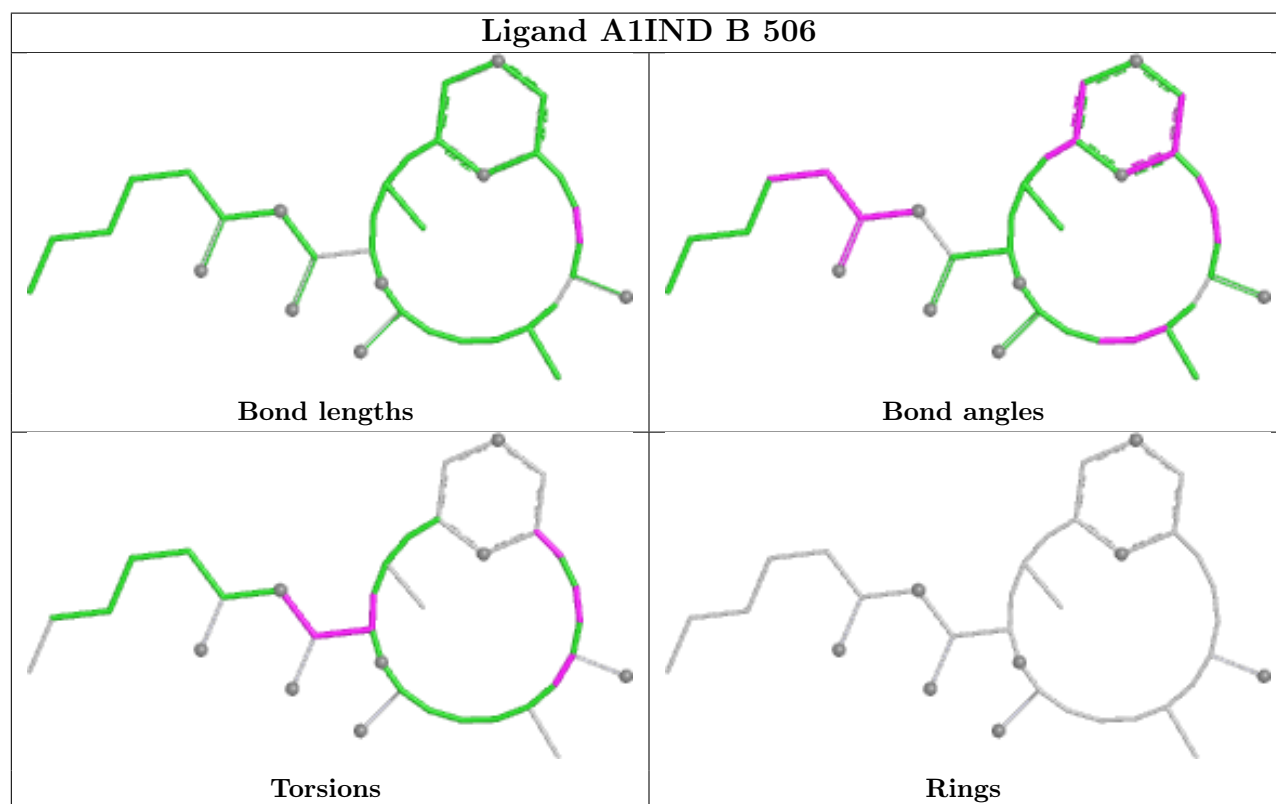
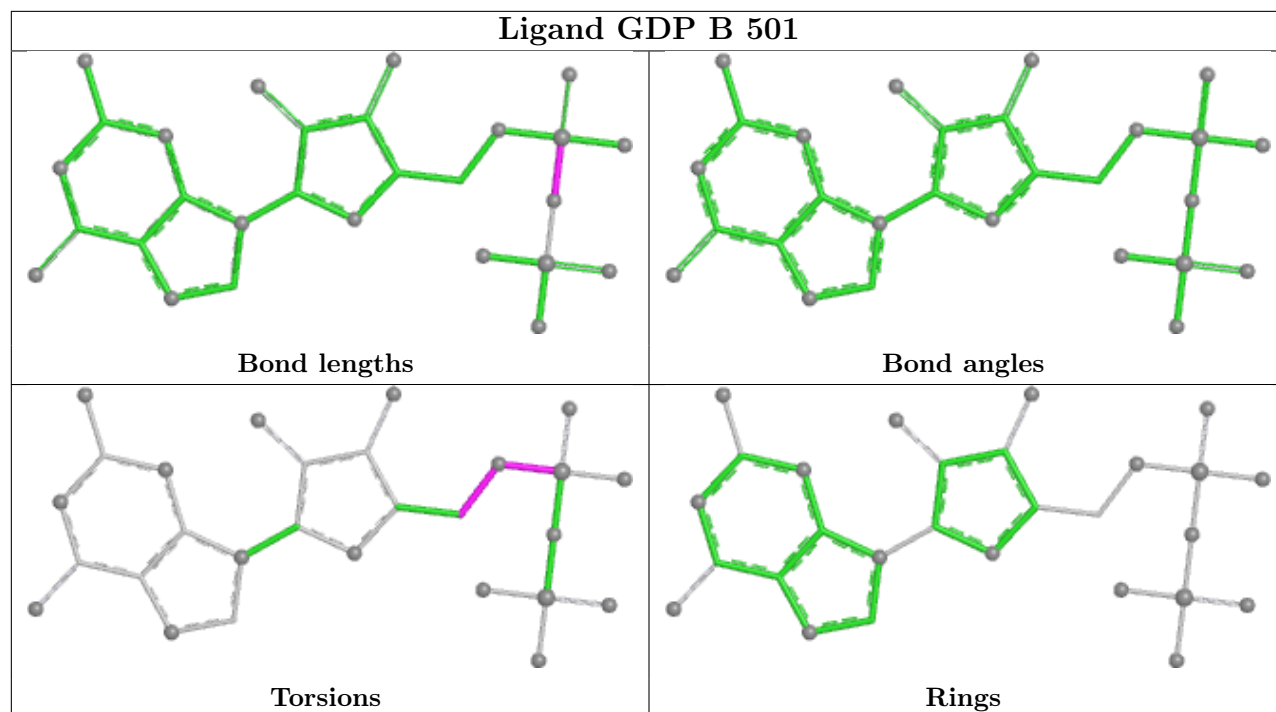
There are no ring outliers.

3 monomers are involved in 7 short contacts:

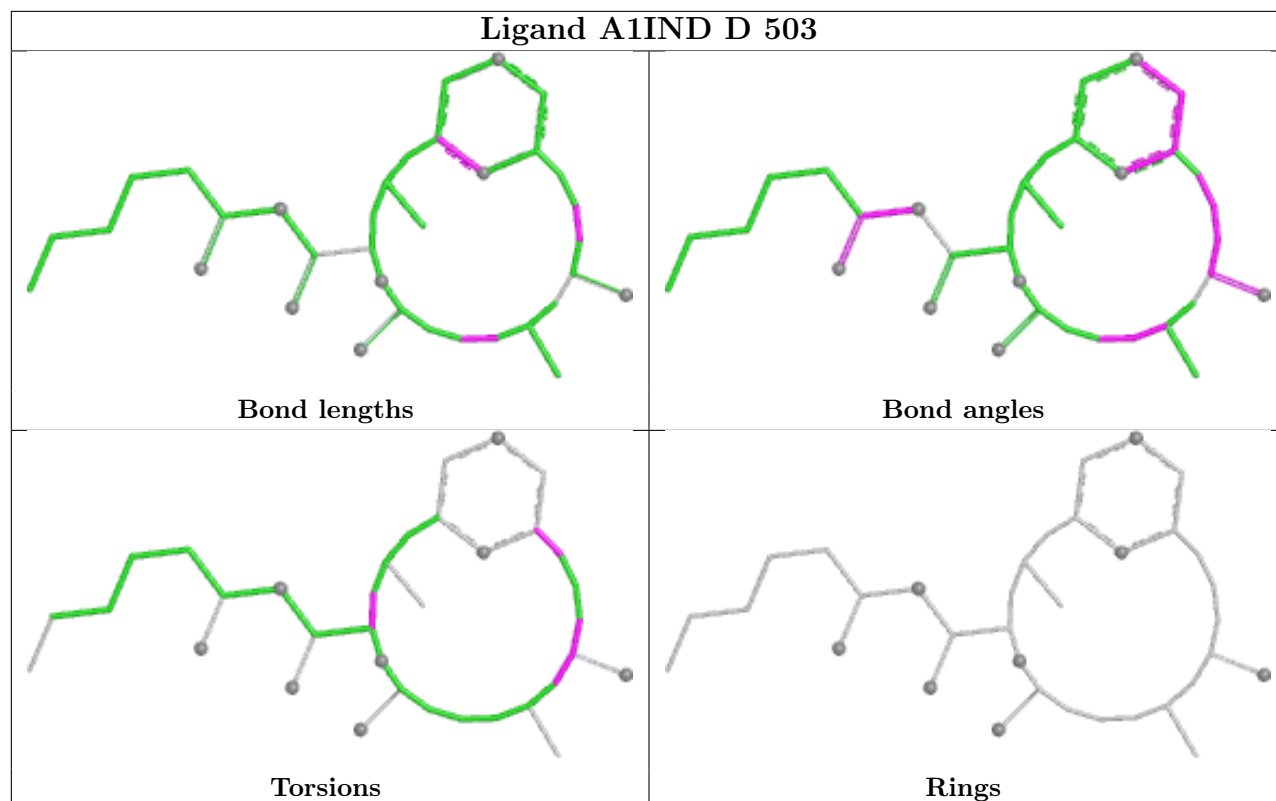
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	501	GTP	1	0
11	B	502	MES	3	0
13	F	401	ACP	3	0

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.

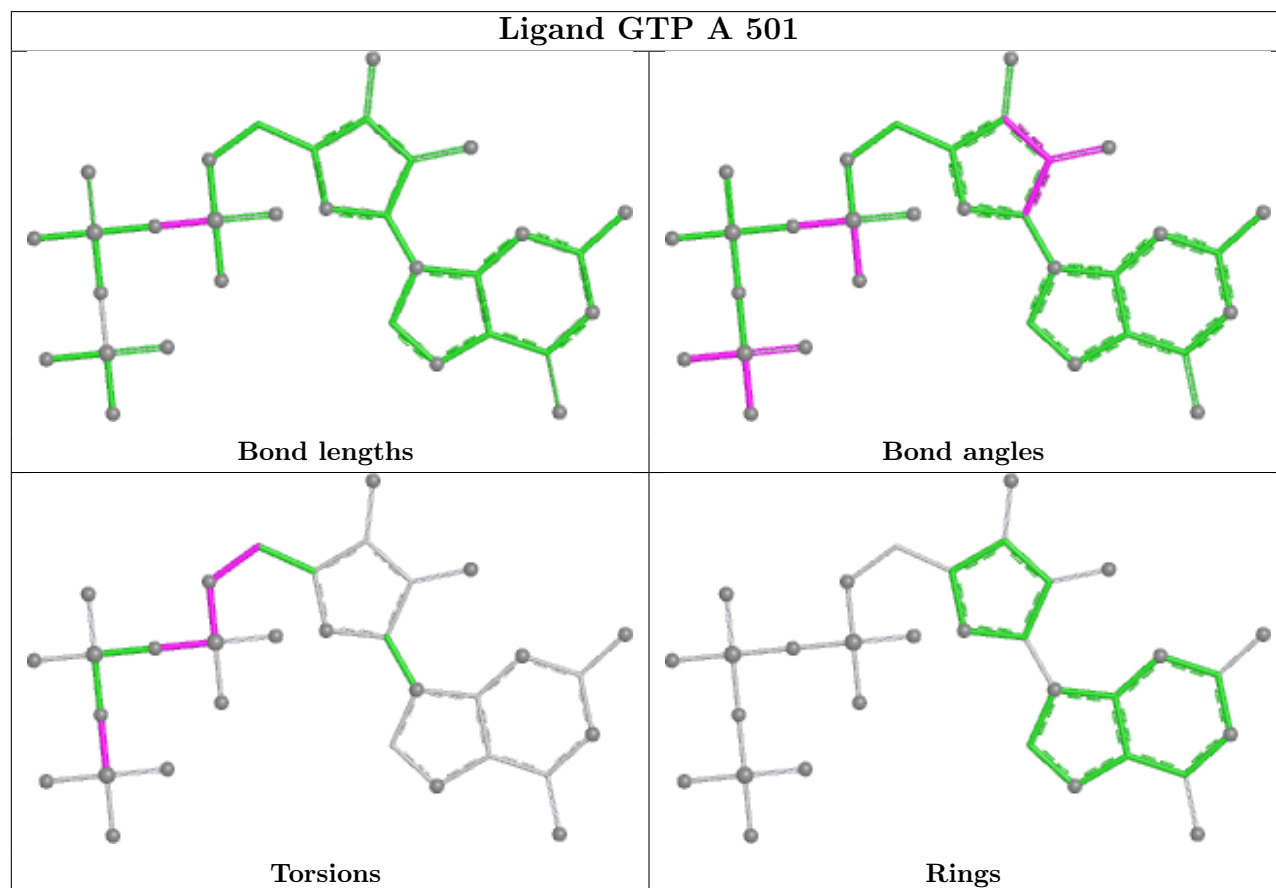


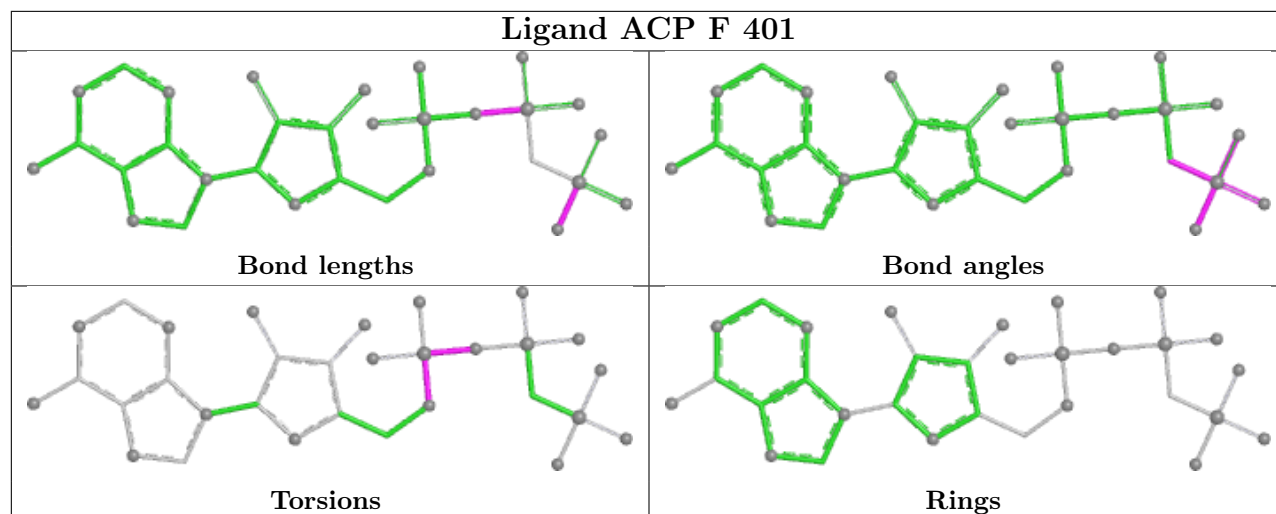


## Ligand A1IND D 503



## Ligand GTP A 501





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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	434/451 (96%)	-0.47	7 (1%) 70 67	19, 47, 78, 108	7 (1%)
1	C	439/451 (97%)	-0.58	9 (2%) 63 60	14, 38, 66, 103	14 (3%)
2	B	417/445 (93%)	-0.33	6 (1%) 73 71	16, 48, 87, 125	12 (2%)
2	D	429/445 (96%)	-0.34	4 (0%) 81 79	18, 50, 84, 112	9 (2%)
3	E	114/189 (60%)	0.04	4 (3%) 47 44	19, 59, 97, 118	4 (3%)
4	F	319/384 (83%)	-0.20	11 (3%) 48 45	21, 60, 95, 122	3 (0%)
All	All	2152/2365 (90%)	-0.37	41 (1%) 66 63	14, 48, 87, 125	49 (2%)

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	237	THR	4.8
3	E	27	PRO	4.5
3	E	139	LEU	4.3
1	C	163	LYS	4.1
1	C	340	SER	4.0

### 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 oligosaccharides in this entry.

## 6.4 Ligands ⓘ

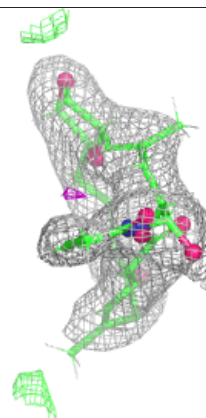
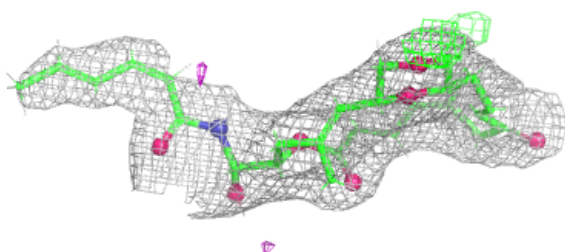
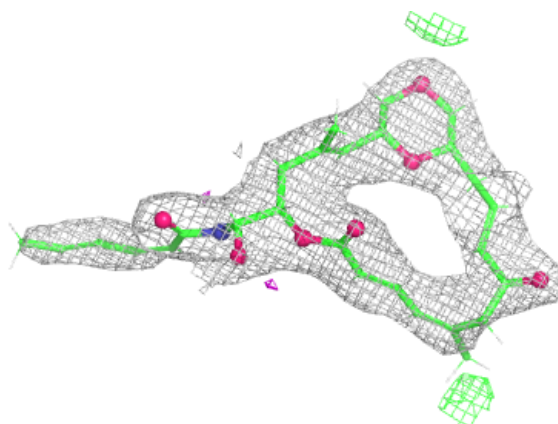
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
6	MG	D	502	1/1	0.78	0.29	74,74,74,74	0
9	GOL	A	506	6/6	0.90	0.14	30,72,78,78	3
6	MG	F	402	1/1	0.91	0.17	59,59,59,59	0
7	CA	B	505	1/1	0.94	0.07	82,82,82,82	0
9	GOL	B	503	6/6	0.94	0.12	30,70,74,75	3
9	GOL	C	504	6/6	0.94	0.14	30,75,80,94	3
12	A1IND	B	506	35/35	0.94	0.10	30,63,76,77	10
13	ACP	F	401	31/31	0.95	0.06	30,64,85,99	2
7	CA	A	505	1/1	0.96	0.08	92,92,92,92	0
11	MES	B	502	12/12	0.97	0.07	44,52,59,81	0
5	GTP	D	501	32/32	0.98	0.05	30,48,69,88	2
12	A1IND	D	503	35/35	0.98	0.06	30,47,60,66	10
8	CL	A	504	1/1	0.98	0.06	67,67,67,67	0
10	GDP	B	501	28/28	0.99	0.04	30,35,41,42	2
5	GTP	C	501	32/32	0.99	0.04	26,30,33,35	2
5	GTP	A	501	32/32	0.99	0.03	30,34,38,39	2
6	MG	A	502	1/1	0.99	0.07	36,36,36,36	0
6	MG	C	502	1/1	0.99	0.08	31,31,31,31	0
6	MG	B	504	1/1	1.00	0.06	29,29,29,29	0
7	CA	A	503	1/1	1.00	0.04	60,60,60,60	0
7	CA	C	503	1/1	1.00	0.01	50,50,50,50	0

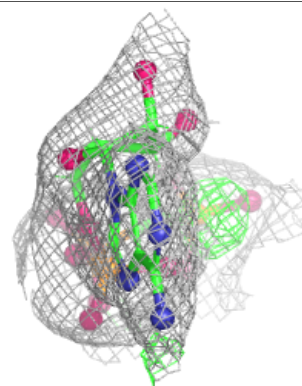
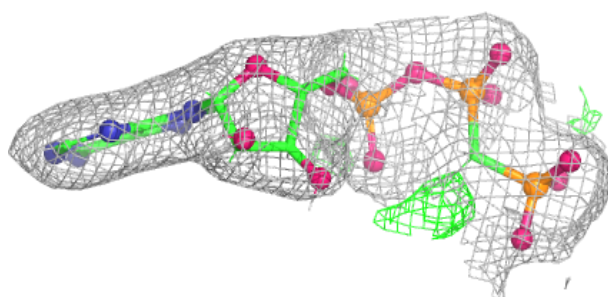
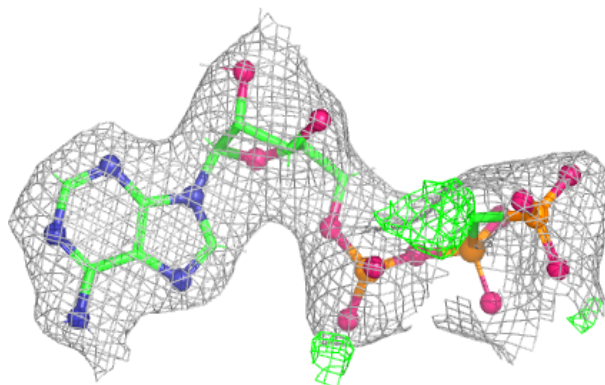
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around A1IND 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)

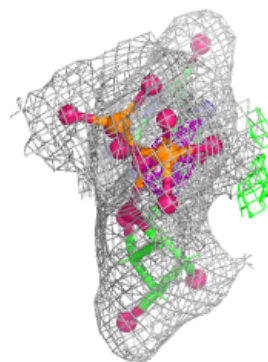
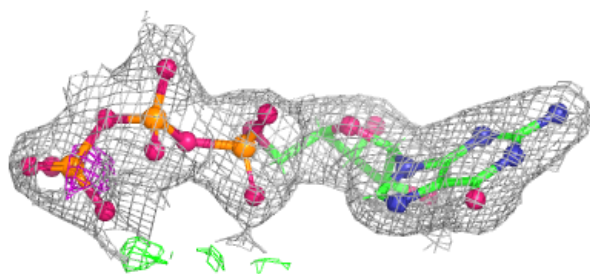
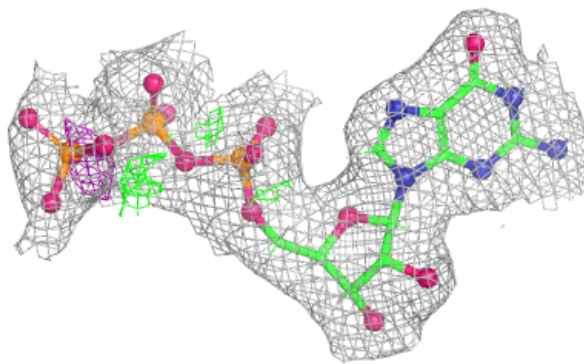
**Electron density around ACP F 401:**

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

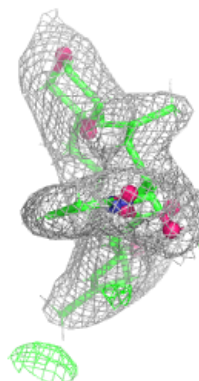
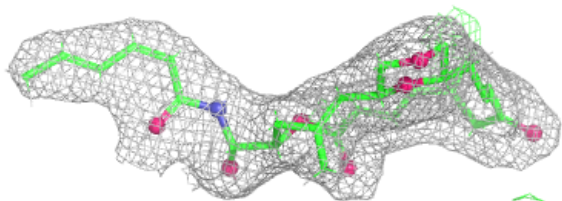
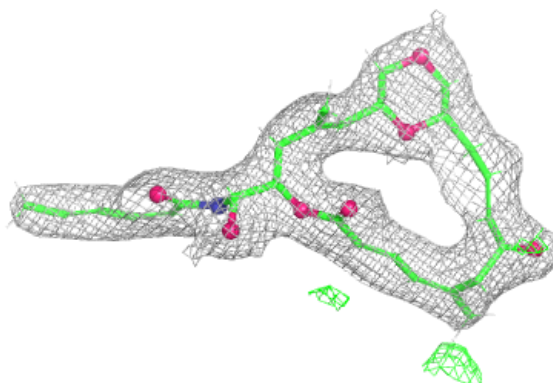


**Electron density around GTP D 501:**

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

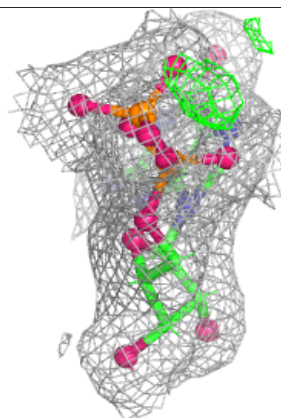
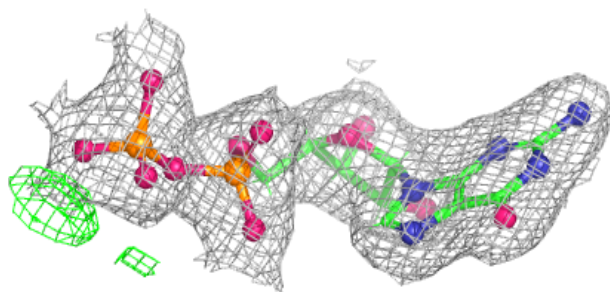
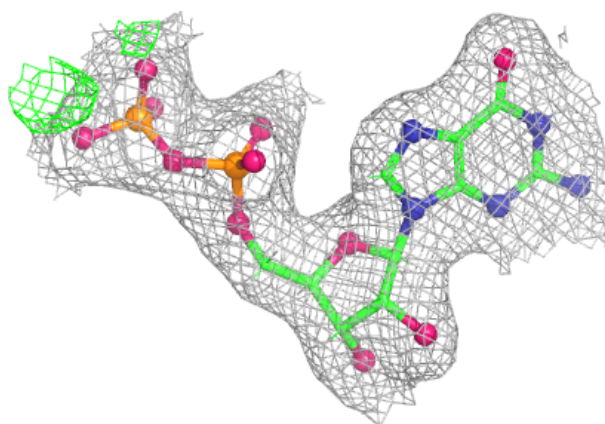
**Electron density around A1IND D 503:**

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

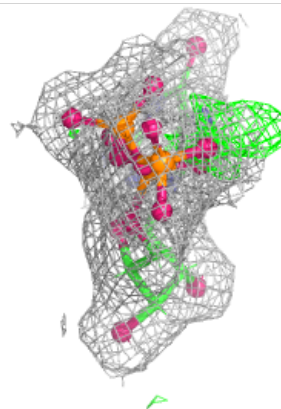
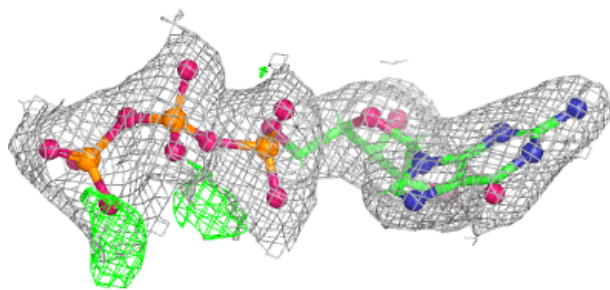
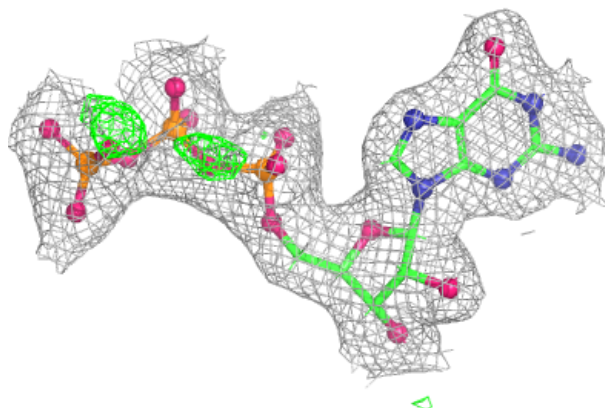


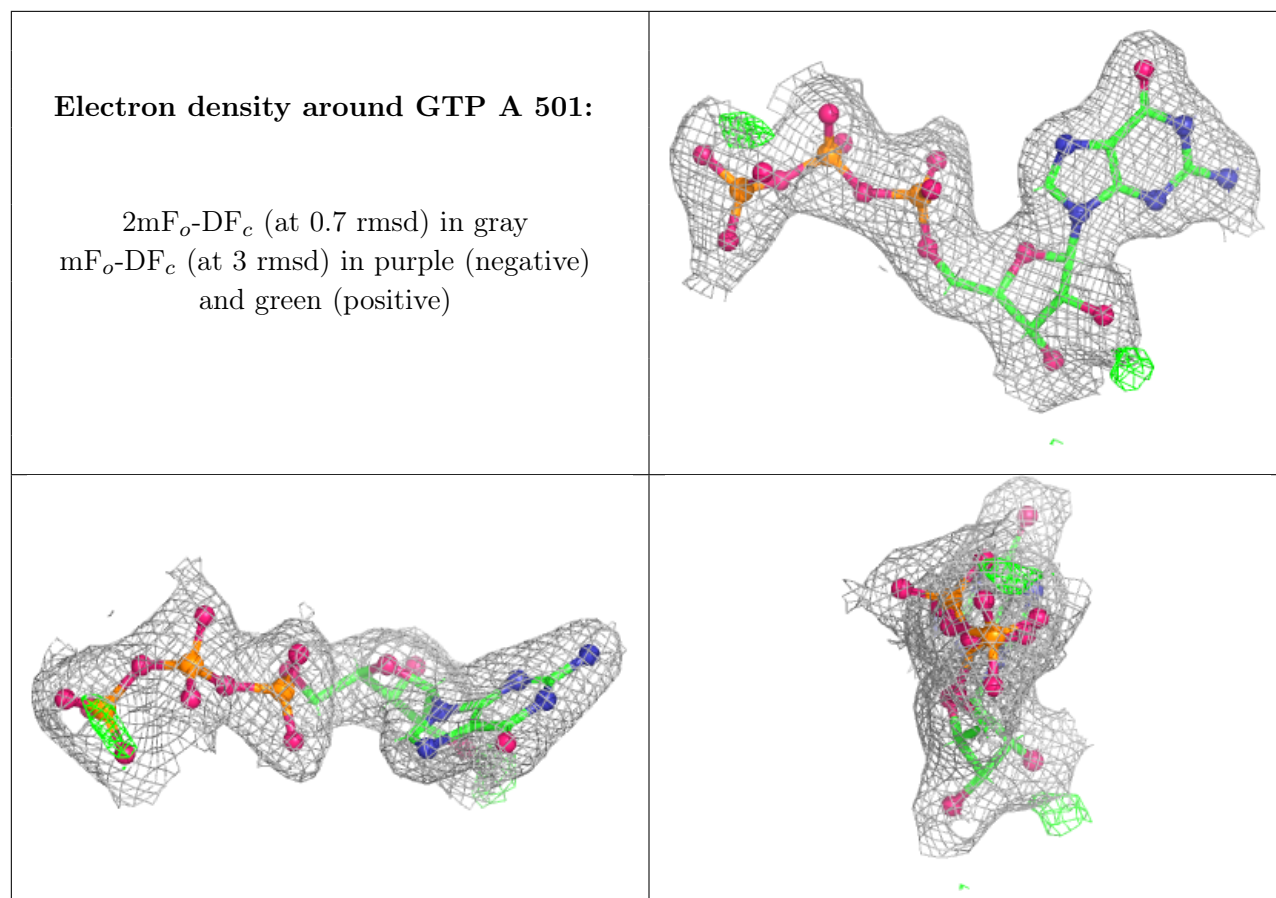
**Electron density around GDP B 501:**

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

**Electron density around GTP 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 ⓘ

There are no such residues in this entry.