



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 02:57 am BST

PDB ID : 5Z4P  
Title : Crystal structure of tubulin-stathmin-TTL-Compound TCA complex  
Authors : Zhang, H.; Luo, C.  
Deposited on : 2018-01-12  
Resolution : 2.50 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 : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

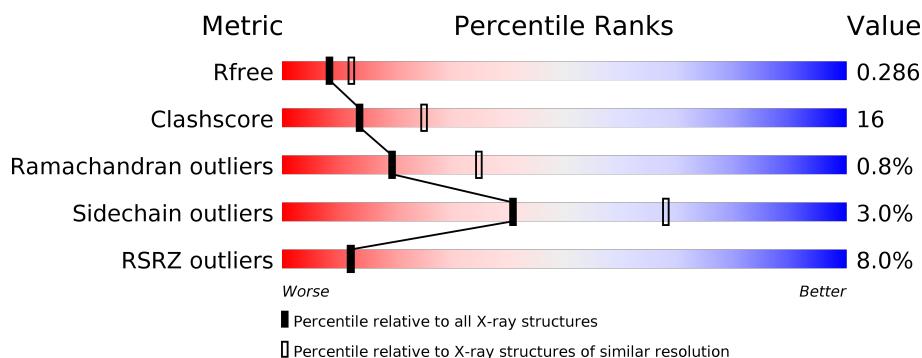
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	440	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>27%</div> <div></div> </div> </div>
1	C	440	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>23%</div> <div></div> </div> </div>
2	B	431	<div> <div>6%</div> <div> <div></div> <div>68%</div> <div>29%</div> <div></div> </div> </div>
2	D	431	<div> <div>9%</div> <div> <div></div> <div>61%</div> <div>33%</div> <div></div> </div> </div>
3	E	185	<div> <div>4%</div> <div> <div></div> <div>45%</div> <div>18%</div> <div></div> <div>35%</div> </div> </div>
4	F	378	<div> <div>22%</div> <div> <div></div> <div>48%</div> <div>35%</div> <div></div> <div>16%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	ACP	F	401	-	-	X	X
7	GOL	C	501	-	-	-	X
7	GOL	C	505	-	-	X	-
7	GOL	C	506	-	-	-	X

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 17477 atoms, of which 0 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	2	0
			3433	2175	582	653	23			
1	C	440	Total	C	N	O	S	0	3	0
			3451	2184	586	658	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	2	0
			3347	2104	568	648	27			
2	D	421	Total	C	N	O	S	0	0	0
			3309	2080	562	640	27			

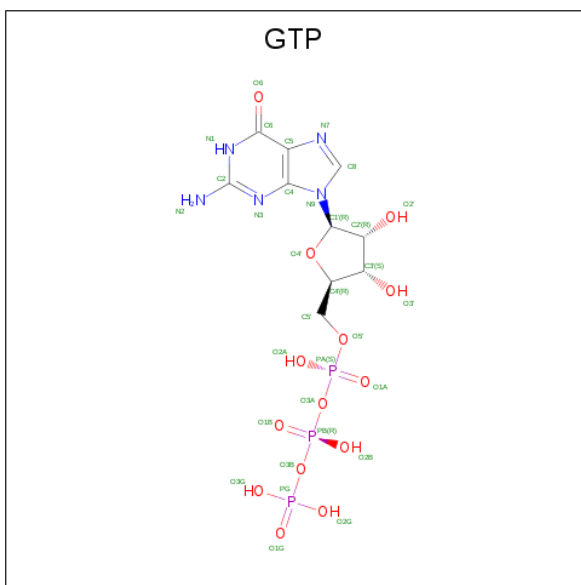
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	2	0
			1011	624	183	199	5			

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	317	Total	C	N	O	S	0	0	0
			2596	1677	434	471	14			

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

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

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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

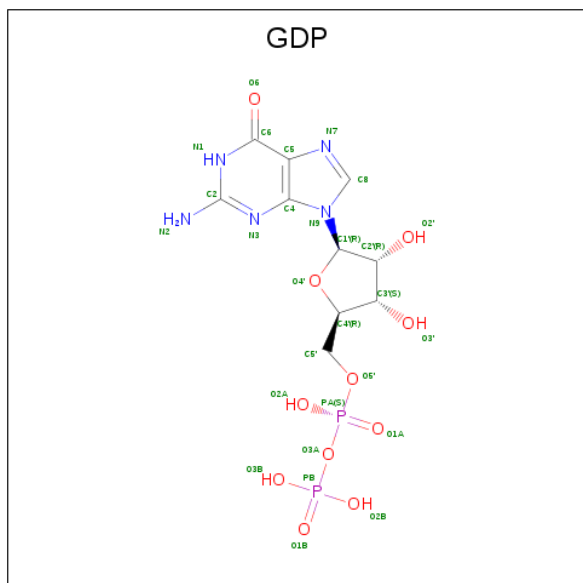
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Ca	0	0
			1	1		

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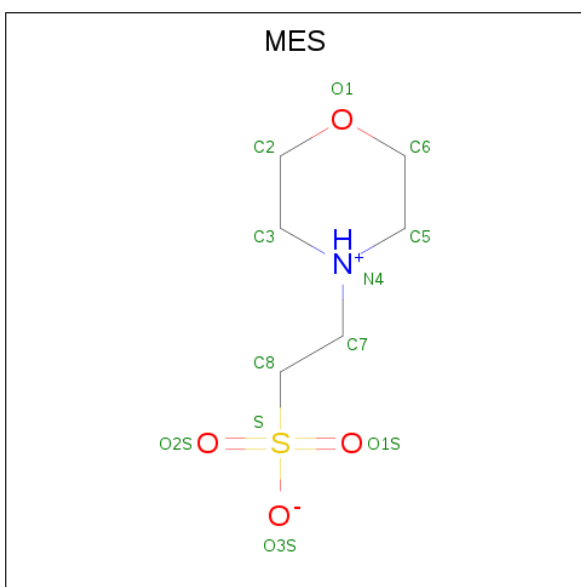
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Ca	0	0
			1	1		
8	C	1	Total	Ca	0	0
			1	1		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



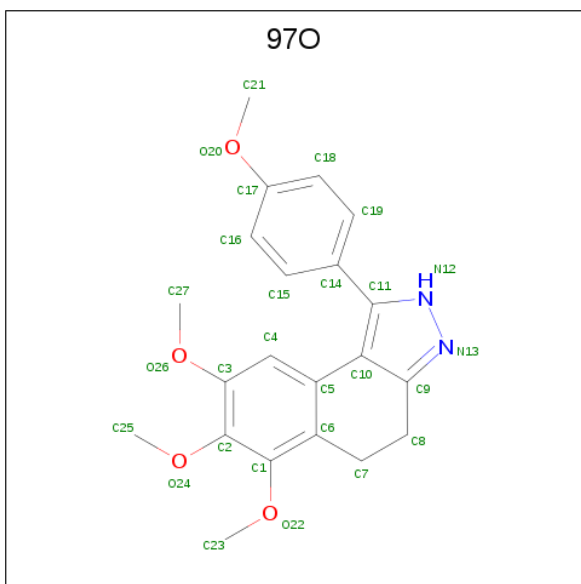
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
9	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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



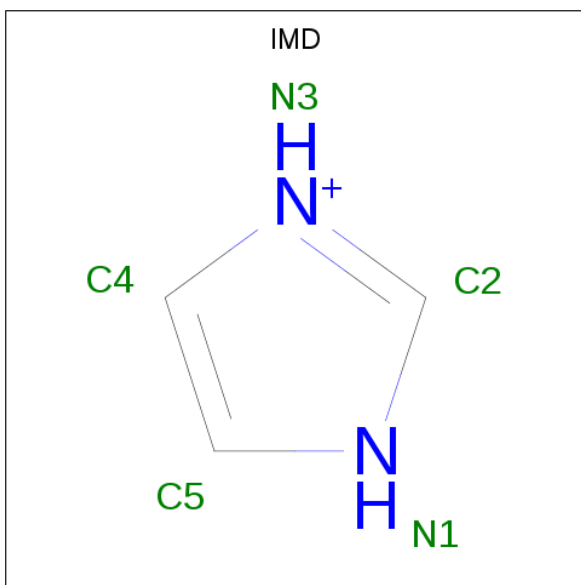
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is 6,7,8-trimethoxy-1-(4-methoxyphenyl)-4,5-dihydro-2 {H}-benzo[e]indazole (three-letter code: 97O) (formula:  $C_{21}H_{22}N_2O_4$ ).



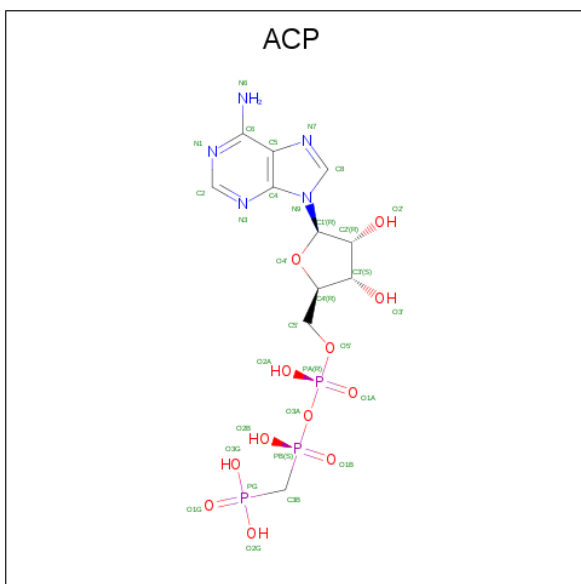
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			27	21	2	4		

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



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

- Molecule 13 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula:  $C_{11}H_{18}N_5O_{12}P_3$ ).



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

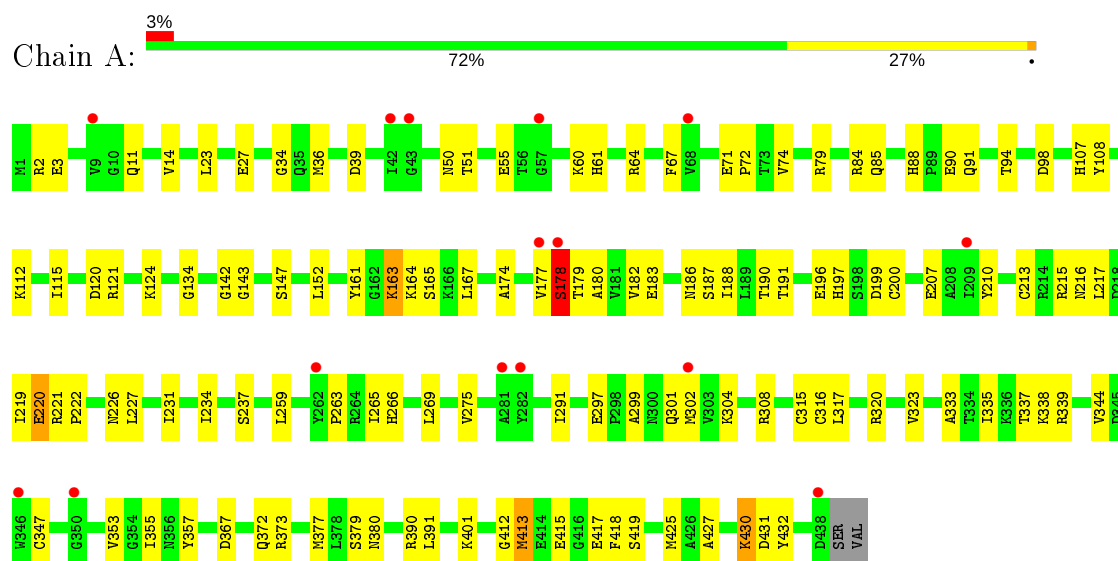
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	11	Total	O	0	0
			11	11		
14	B	13	Total	O	0	0
			13	13		
14	C	17	Total	O	0	0
			17	17		
14	D	4	Total	O	0	0
			4	4		
14	F	7	Total	O	0	0
			7	7		

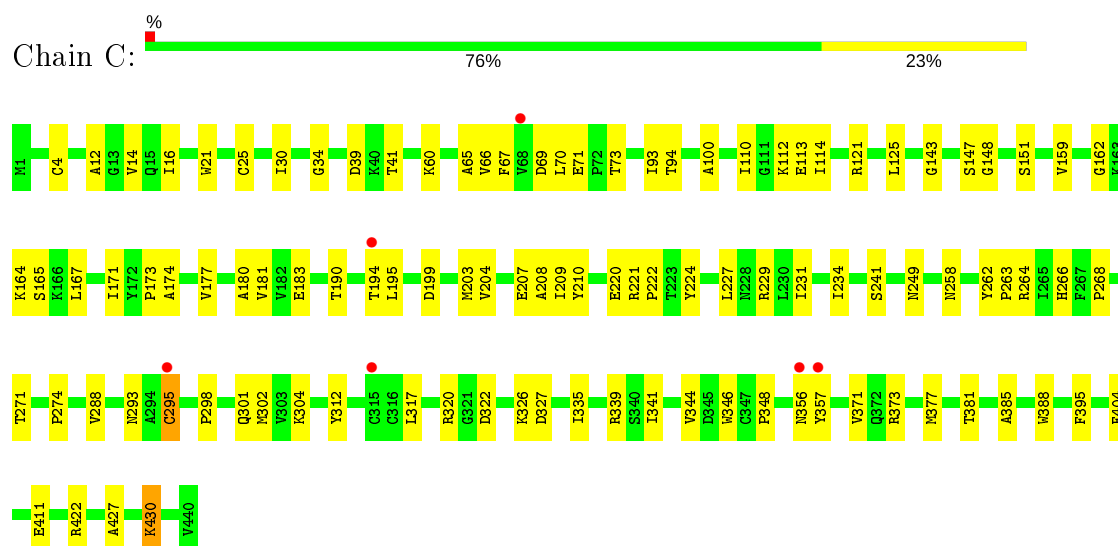
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

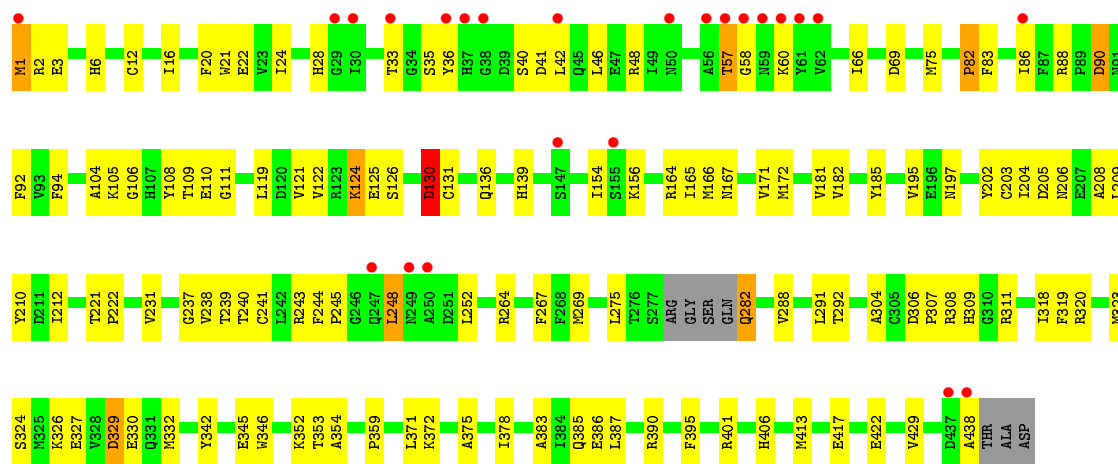


#### • Molecule 1: Tubulin alpha-1B chain

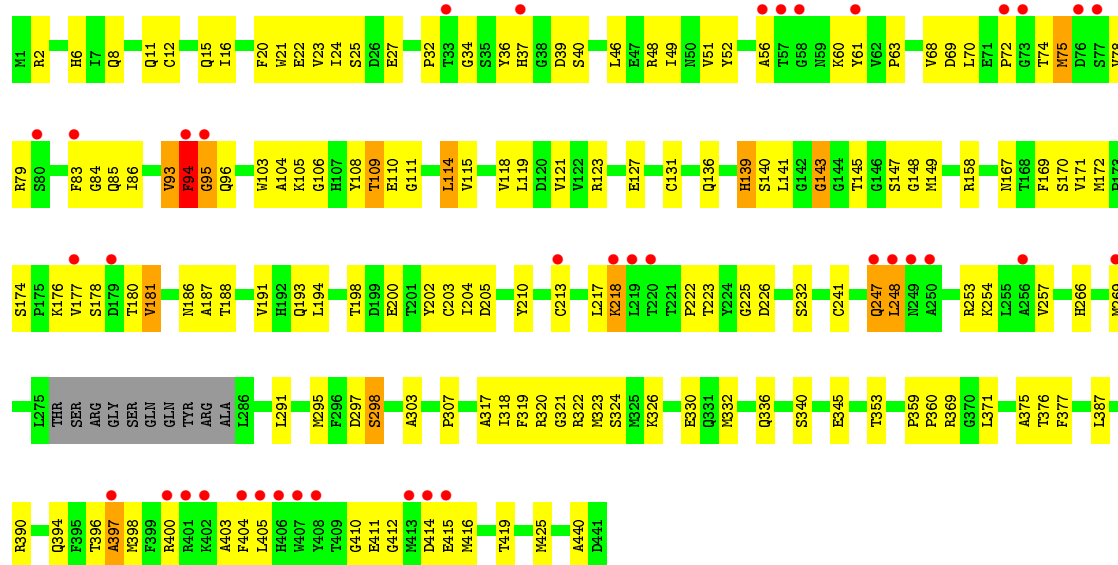


#### • Molecule 2: Tubulin beta-2B chain

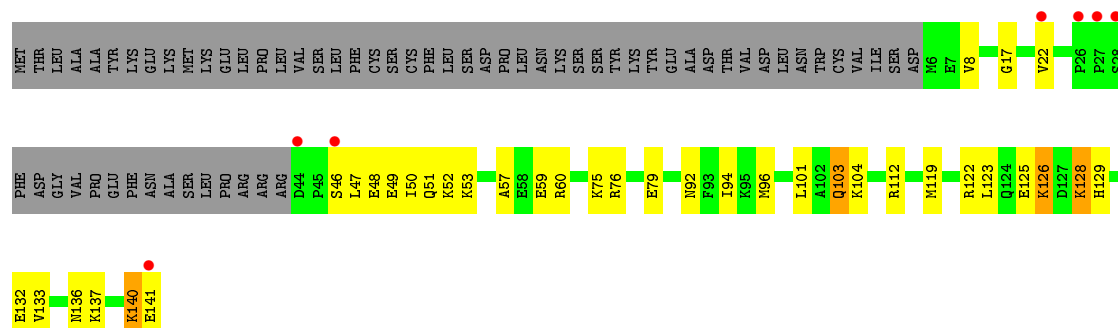




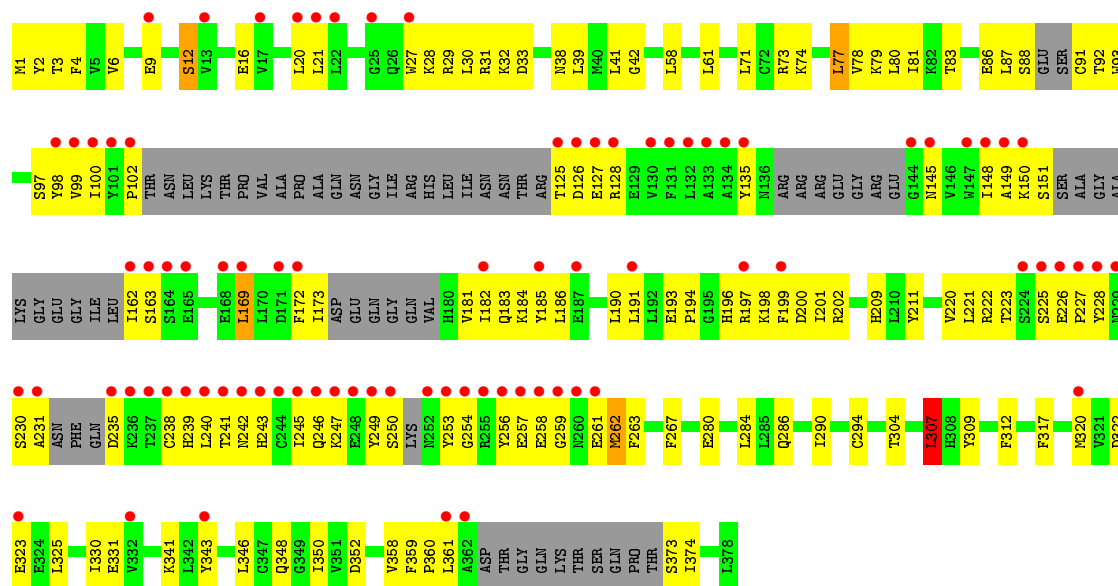
### • Molecule 2: Tubulin beta-2B chain



### • Molecule 3: Stathmin-4



### • Molecule 4: Tubulin tyrosine ligase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.83Å 154.84Å 181.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.64 – 2.50 49.64 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.64-2.50) 99.7 (49.64-2.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.05 (at 2.48Å)	Xtriage
Refinement program	PHENIX (1.13 _2998: ???)	Depositor
R, $R_{free}$	0.222 , 0.286 0.222 , 0.286	Depositor DCC
$R_{free}$ test set	813 reflections (0.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.3	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 43.1	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	0.94	EDS
Total number of atoms	17477	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: GDP, GOL, MG, IMD, CA, GTP, ACP, MES, 97O

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	0.46	0/3517	0.58	0/4774
1	C	0.54	1/3538 (0.0%)	0.64	1/4804 (0.0%)
2	B	0.50	0/3424	0.66	2/4638 (0.0%)
2	D	0.46	1/3382 (0.0%)	0.63	1/4581 (0.0%)
3	E	0.49	0/1025	0.62	0/1360
4	F	0.42	0/2652	0.62	2/3579 (0.1%)
All	All	0.48	2/17538 (0.0%)	0.63	6/23736 (0.0%)

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
2	D	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	295	CYS	CB-SG	-9.18	1.66	1.82
2	D	203	CYS	CB-SG	-5.32	1.73	1.81

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	130	ASP	CB-CG-OD1	8.52	125.97	118.30
2	B	130	ASP	CB-CG-OD2	-6.62	112.34	118.30
4	F	307	LEU	CA-CB-CG	6.52	130.29	115.30
2	D	248	LEU	CA-CB-CG	6.37	129.95	115.30
1	C	171	ILE	C-N-CA	5.83	136.28	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	247	GLN	Peptide
2	D	93	VAL	Peptide
2	D	95	GLY	Peptide

## 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	3433	0	3352	93	0
1	C	3451	0	3368	82	0
2	B	3347	0	3220	105	0
2	D	3309	0	3189	121	0
3	E	1011	0	1032	38	0
4	F	2596	0	2570	125	0
5	A	32	0	12	2	0
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
7	A	18	0	24	1	0
7	B	6	0	8	0	0
7	C	30	0	40	8	0
7	D	12	0	16	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
9	B	28	0	12	1	0
9	D	28	0	12	1	0
10	B	12	0	12	0	0
11	B	27	0	0	2	0
12	C	15	0	15	5	0
13	F	31	0	12	13	0
14	A	11	0	0	2	0
14	B	13	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	C	17	0	0	1	0
14	D	4	0	0	0	0
14	F	7	0	0	1	0
All	All	17477	0	16906	545	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 16.

The worst 5 of 545 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)
13:F:401:ACP:C3'	13:F:401:ACP:O3'	1.80	1.30
4:F:241:THR:N	13:F:401:ACP:O3'	1.73	1.21
3:E:103:GLN:OE1	3:E:104:LYS:CE	1.95	1.14
4:F:148:ILE:HA	4:F:162:ILE:HD12	1.30	1.09
4:F:241:THR:HG22	13:F:401:ACP:HO3'	1.24	1.01

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	438/440 (100%)	412 (94%)	24 (6%)	2 (0%)	29	48
1	C	441/440 (100%)	428 (97%)	13 (3%)	0	100	100
2	B	422/431 (98%)	395 (94%)	25 (6%)	2 (0%)	29	48
2	D	417/431 (97%)	387 (93%)	23 (6%)	7 (2%)	9	16
3	E	119/185 (64%)	112 (94%)	7 (6%)	0	100	100
4	F	299/378 (79%)	246 (82%)	47 (16%)	6 (2%)	7	12
All	All	2136/2305 (93%)	1980 (93%)	139 (6%)	17 (1%)	19	35

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	57	THR
2	B	82	PRO
2	D	177	VAL
4	F	254	GLY
1	A	177	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	371/371 (100%)	361 (97%)	10 (3%)	44	71
1	C	374/371 (101%)	369 (99%)	5 (1%)	69	87
2	B	368/372 (99%)	355 (96%)	13 (4%)	36	62
2	D	364/372 (98%)	350 (96%)	14 (4%)	33	58
3	E	111/168 (66%)	104 (94%)	7 (6%)	18	34
4	F	286/336 (85%)	279 (98%)	7 (2%)	49	74
All	All	1874/1990 (94%)	1818 (97%)	56 (3%)	41	68

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	357	TYR
2	D	75	MET
4	F	184	LYS
1	C	381	THR
2	D	15	GLN

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

Mol	Chain	Res	Type
2	D	85	GLN
2	D	247	GLN

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Mol	Chain	Res	Type
2	D	96	GLN
2	D	6	HIS
2	D	101	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 7 are monoatomic - leaving 21 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	$\# Z  > 2$
7	GOL	A	504	-	5,5,5	1.41	2 (40%)	5,5,5	0.88	0
11	97O	B	506	-	28,30,30	6.27	19 (67%)	35,43,43	3.52	13 (37%)
7	GOL	D	503	-	5,5,5	0.98	0	5,5,5	0.97	0
5	GTP	C	503	6	26,34,34	0.97	1 (3%)	33,54,54	1.98	9 (27%)
13	ACP	F	401	-	27,33,33	4.73	12 (44%)	32,52,52	2.90	9 (28%)
7	GOL	C	505	-	5,5,5	0.87	0	5,5,5	0.98	0
12	IMD	C	510	-	3,5,5	0.30	0	4,5,5	0.84	0
9	GDP	D	501	6	24,30,30	1.28	2 (8%)	31,47,47	1.96	7 (22%)
7	GOL	C	501	-	5,5,5	0.60	0	5,5,5	1.33	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	GOL	A	506	-	5,5,5	1.10	0	5,5,5	0.88	0
7	GOL	C	506	-	5,5,5	1.54	2 (40%)	5,5,5	0.72	0
12	IMD	C	509	-	3,5,5	0.44	0	4,5,5	0.34	0
9	GDP	B	501	6	24,30,30	1.17	2 (8%)	31,47,47	1.89	6 (19%)
12	IMD	C	511	-	3,5,5	0.45	0	4,5,5	0.18	0
10	MES	B	505	-	12,12,12	2.23	1 (8%)	14,16,16	1.99	4 (28%)
5	GTP	A	501	6	26,34,34	1.06	1 (3%)	33,54,54	1.86	9 (27%)
7	GOL	D	504	-	5,5,5	0.85	0	5,5,5	1.13	0
7	GOL	C	502	-	5,5,5	1.12	0	5,5,5	0.87	0
7	GOL	C	507	-	5,5,5	1.35	1 (20%)	5,5,5	0.76	0
7	GOL	B	503	-	5,5,5	1.19	1 (20%)	5,5,5	0.65	0
7	GOL	A	503	-	5,5,5	0.95	0	5,5,5	0.83	0

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
7	GOL	A	504	-	-	2/4/4/4	-
11	97O	B	506	-	-	4/12/21/21	0/4/4/4
7	GOL	D	503	-	-	2/4/4/4	-
5	GTP	C	503	6	-	8/18/38/38	0/3/3/3
13	ACP	F	401	-	-	4/15/38/38	0/3/3/3
7	GOL	C	505	-	-	2/4/4/4	-
12	IMD	C	509	-	-	-	0/1/1/1
7	GOL	C	501	-	-	2/4/4/4	-
7	GOL	A	506	-	-	0/4/4/4	-
7	GOL	C	506	-	-	2/4/4/4	-
9	GDP	D	501	6	-	3/12/32/32	0/3/3/3
9	GDP	B	501	6	-	4/12/32/32	0/3/3/3
7	GOL	C	502	-	-	4/4/4/4	-
10	MES	B	505	-	-	4/6/14/14	0/1/1/1
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
7	GOL	D	504	-	-	4/4/4/4	-
12	IMD	C	511	-	-	-	0/1/1/1
7	GOL	C	507	-	-	2/4/4/4	-
7	GOL	B	503	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	A	503	-	-	2/4/4/4	-
12	IMD	C	510	-	-	-	0/1/1/1

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	F	401	ACP	O3'-C3'	15.73	1.80	1.43
11	B	506	97O	C3-C2	-15.56	1.08	1.41
11	B	506	97O	C8-C9	13.66	1.72	1.50
13	F	401	ACP	C2'-C3'	-12.74	1.18	1.53
11	B	506	97O	C4-C3	-10.75	1.19	1.38

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	506	97O	C5-C6-C1	-10.38	106.49	118.41
13	F	401	ACP	O3'-C3'-C4'	7.33	132.25	111.05
11	B	506	97O	C4-C3-C2	7.29	128.47	120.22
11	B	506	97O	O26-C3-C4	-6.98	112.11	124.12
11	B	506	97O	C4-C5-C10	6.96	135.33	123.35

There are no chirality outliers.

5 of 55 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	F	401	ACP	C5'-O5'-PA-O2A
13	F	401	ACP	C5'-O5'-PA-O3A
9	D	501	GDP	C5'-O5'-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O2A
7	C	507	GOL	O1-C1-C2-C3

There are no ring outliers.

12 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	506	97O	2	0
5	C	503	GTP	1	0
13	F	401	ACP	13	0
7	C	505	GOL	5	0
12	C	510	IMD	2	0
9	D	501	GDP	1	0

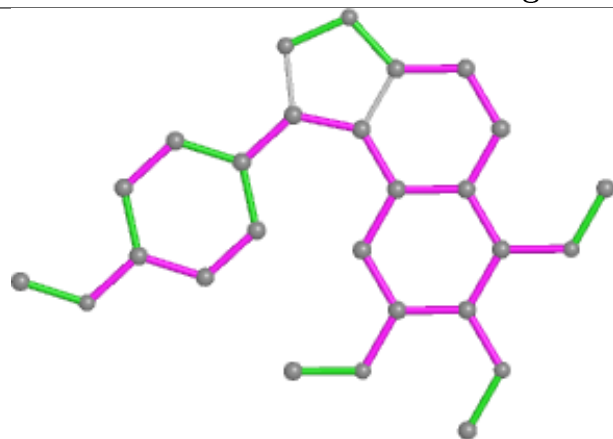
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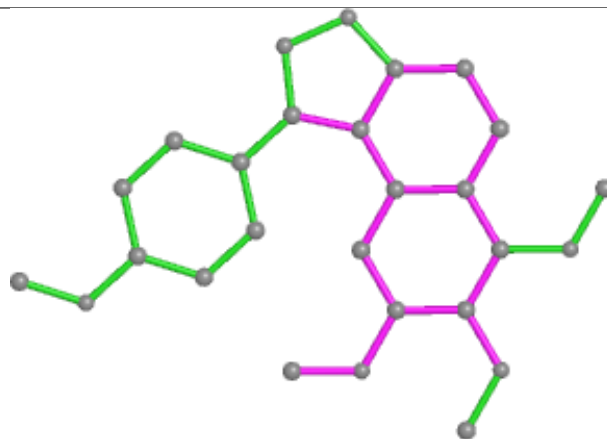
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	501	GOL	2	0
7	C	506	GOL	1	0
9	B	501	GDP	1	0
12	C	511	IMD	3	0
5	A	501	GTP	2	0
7	A	503	GOL	1	0

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.

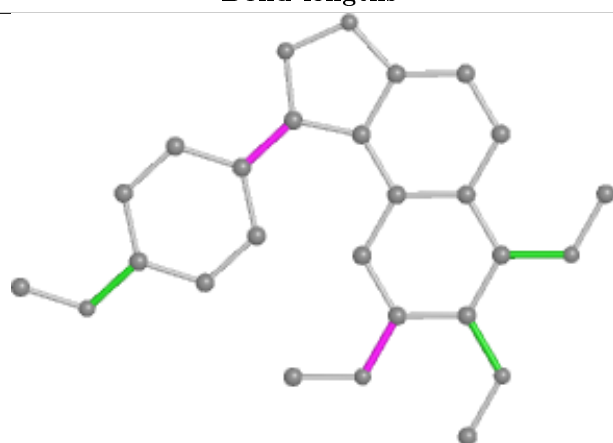
## Ligand 97O B 506



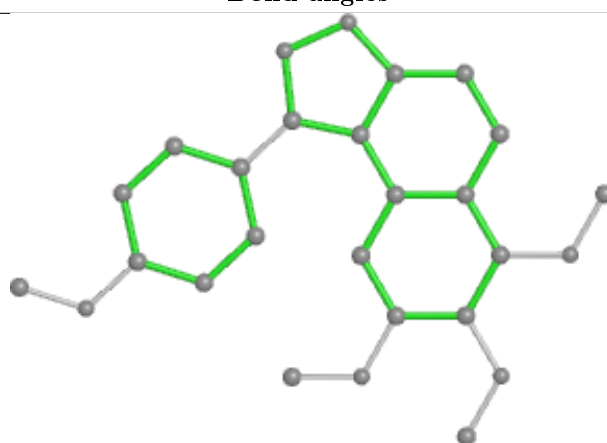
Bond lengths



Bond angles

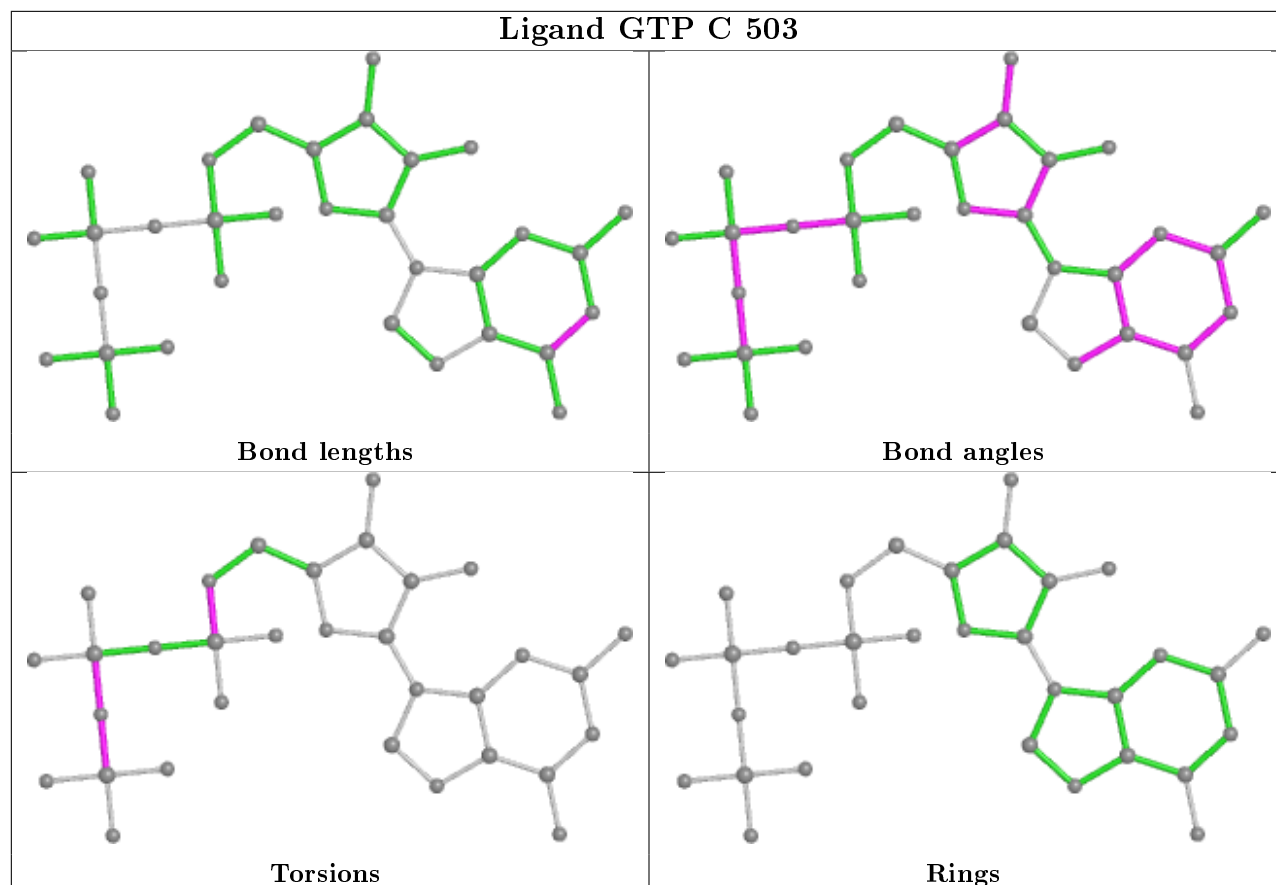


Torsions

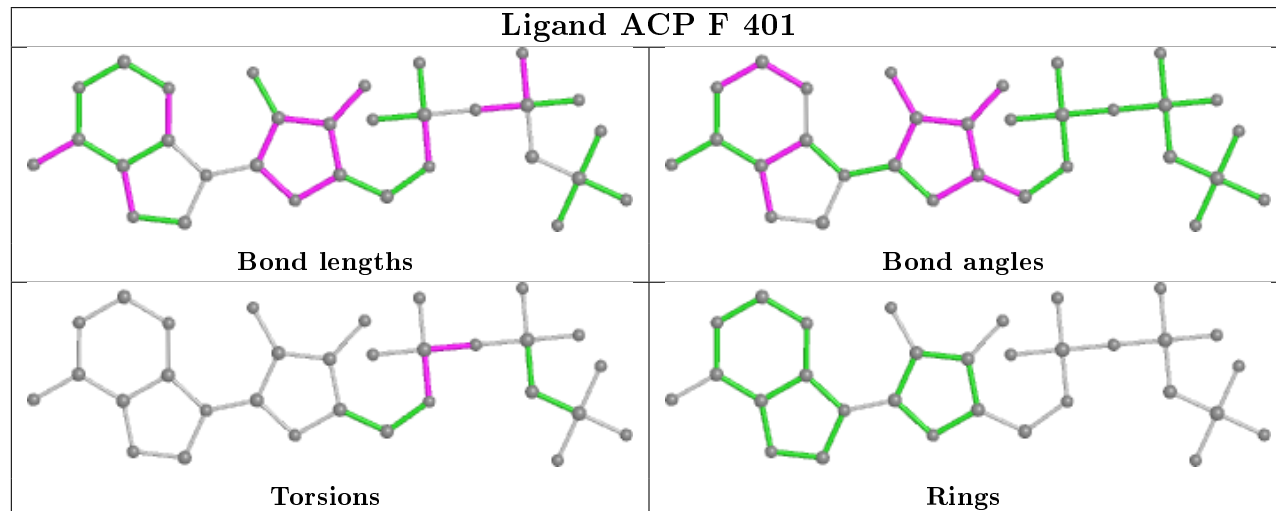


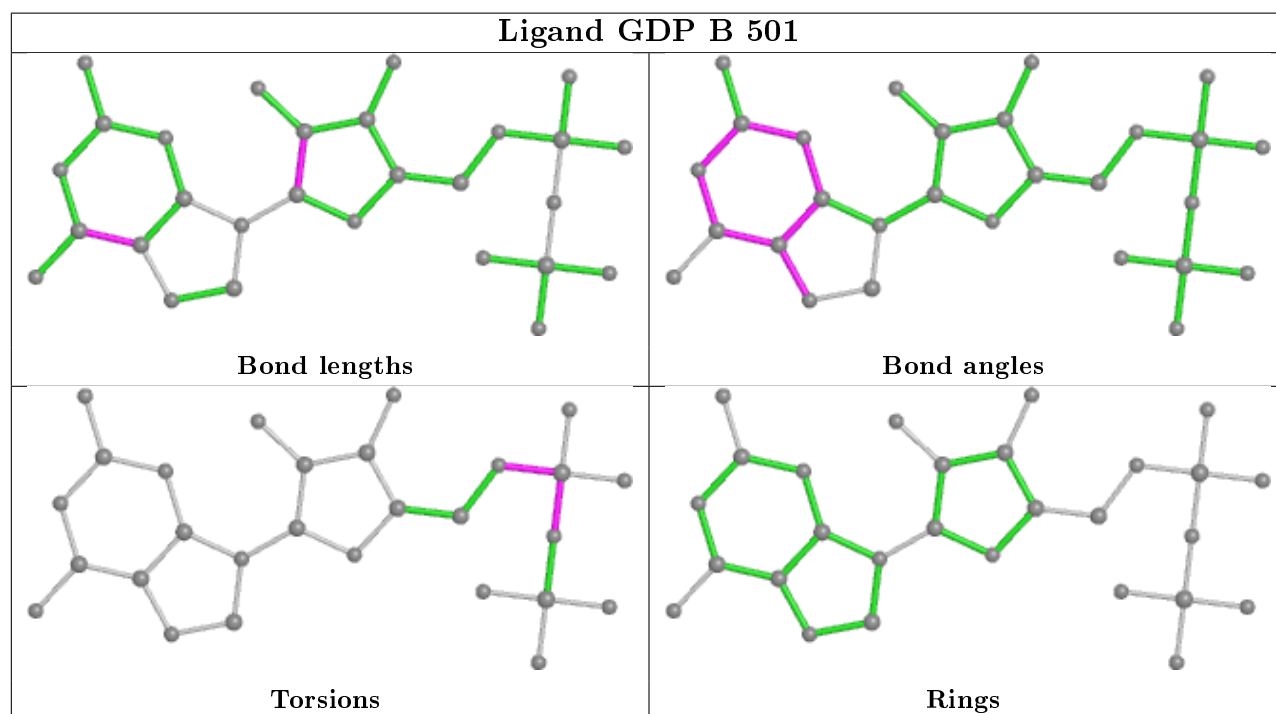
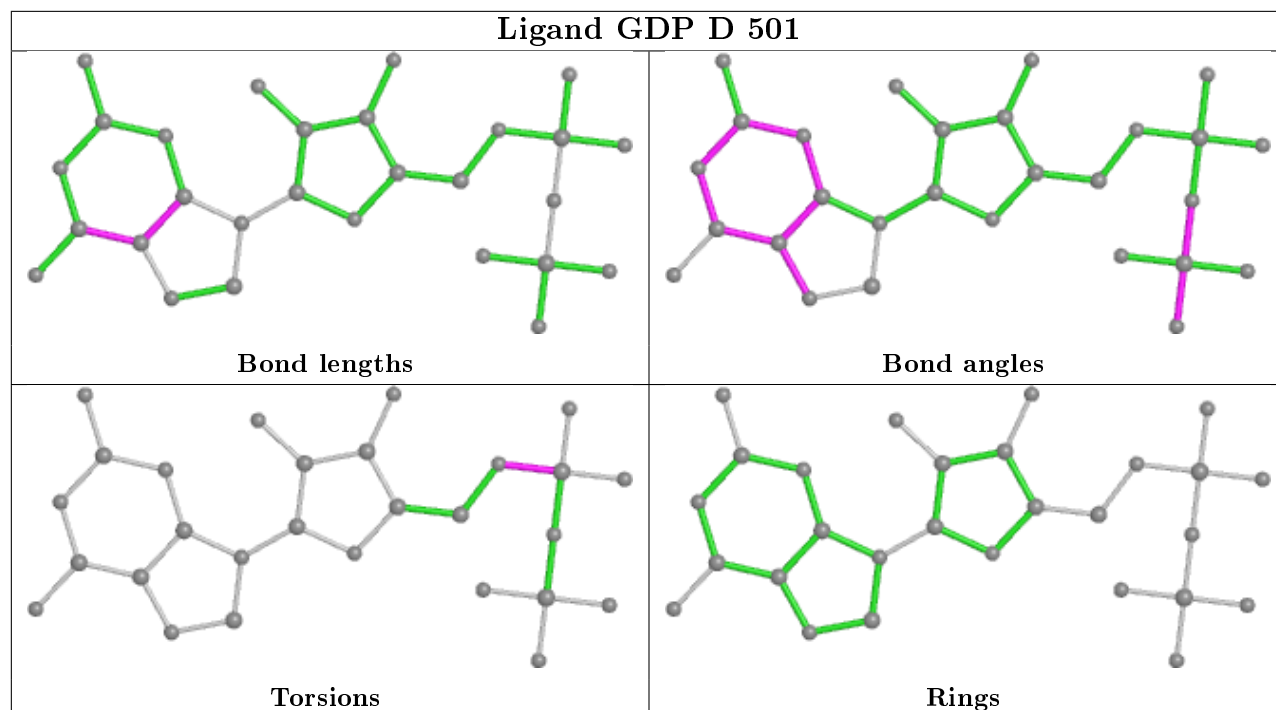
Rings

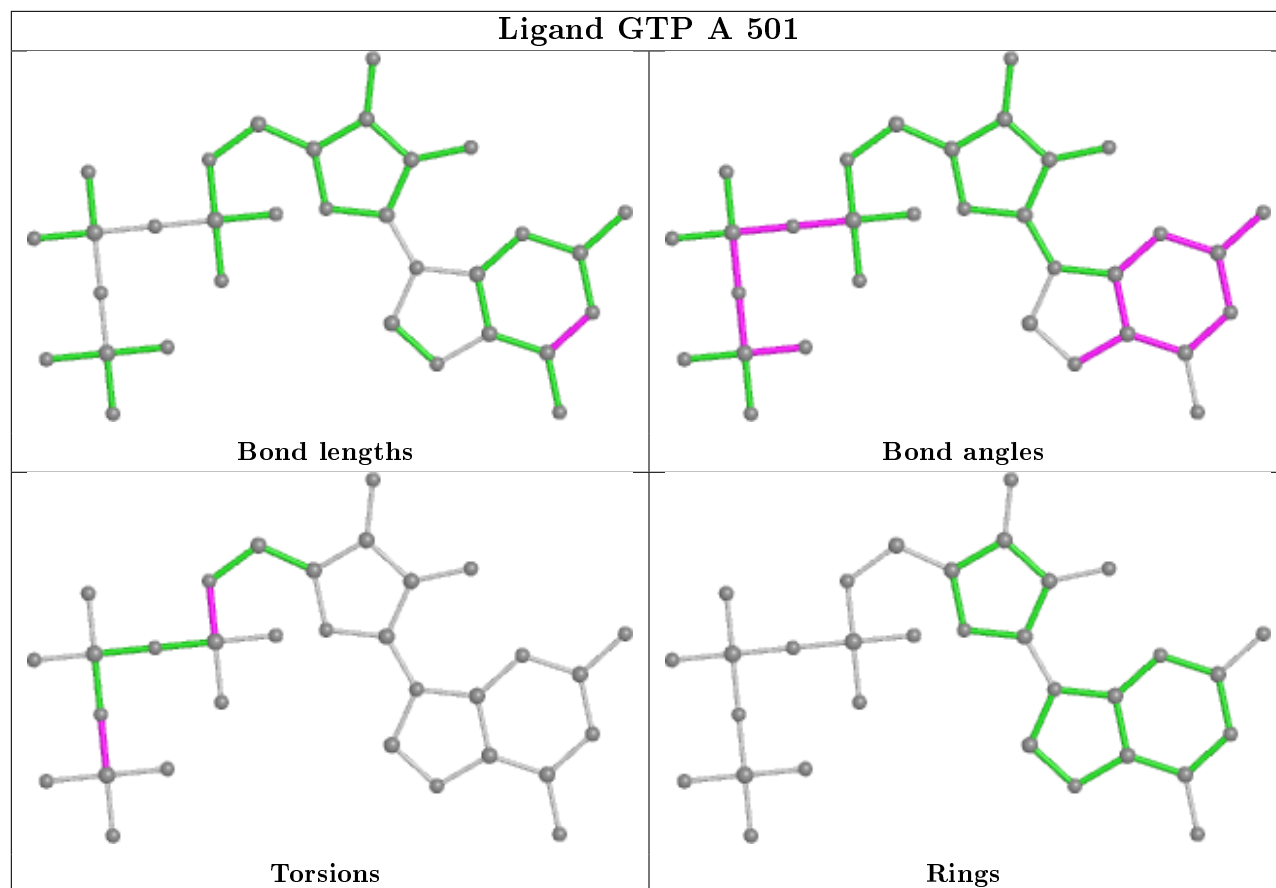
## Ligand GTP C 503



## Ligand ACP F 401







## 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	438/440 (99%)	0.36	15 (3%) 45 48	44, 63, 80, 146	0
1	C	440/440 (100%)	0.01	6 (1%) 75 77	37, 51, 71, 149	0
2	B	424/431 (98%)	0.31	24 (5%) 23 25	38, 58, 91, 135	0
2	D	421/431 (97%)	0.55	38 (9%) 9 9	46, 70, 102, 118	0
3	E	121/185 (65%)	0.39	7 (5%) 23 24	49, 71, 94, 148	0
4	F	317/378 (83%)	1.66	83 (26%) 0 0	52, 81, 247, 320	0
All	All	2161/2305 (93%)	0.51	173 (8%) 12 12	37, 64, 117, 320	0

The worst 5 of 173 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	244	CYS	24.9
4	F	249	TYR	18.6
4	F	240	LEU	14.1
4	F	235	ASP	10.9
4	F	250	SER	10.8

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

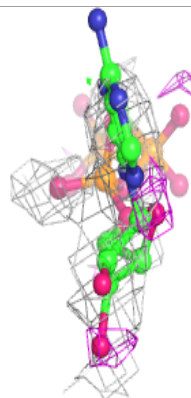
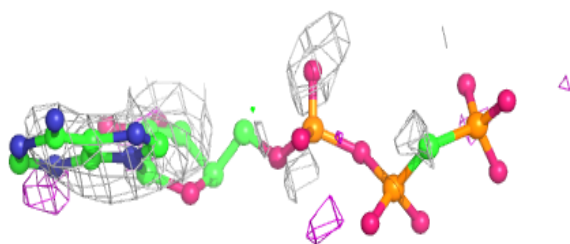
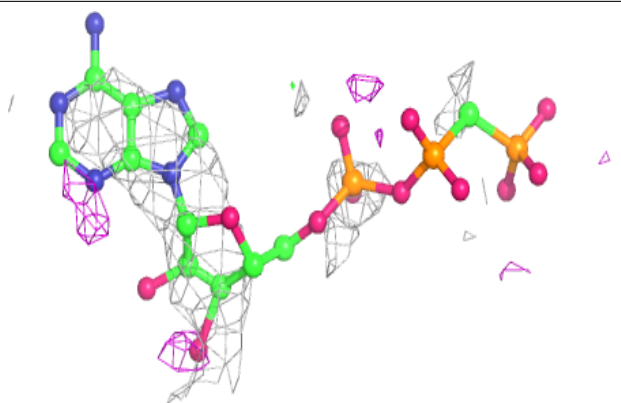
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
13	ACP	F	401	31/31	0.54	0.57	86,205,221,231	0
7	GOL	C	506	6/6	0.71	0.44	63,69,69,69	0
7	GOL	A	504	6/6	0.75	0.23	62,74,81,82	0
7	GOL	B	503	6/6	0.77	0.30	57,71,76,89	0
7	GOL	D	503	6/6	0.78	0.30	82,90,92,96	0
7	GOL	C	501	6/6	0.80	0.41	50,56,66,76	0
7	GOL	C	502	6/6	0.80	0.28	64,68,73,78	0
7	GOL	A	506	6/6	0.81	0.19	68,71,73,76	0
7	GOL	D	504	6/6	0.83	0.26	67,68,75,79	0
7	GOL	C	507	6/6	0.85	0.17	56,63,66,66	0
7	GOL	C	505	6/6	0.89	0.31	66,72,74,78	0
12	IMD	C	509	5/5	0.89	0.24	51,53,67,67	0
11	97O	B	506	27/27	0.89	0.18	58,73,78,80	0
12	IMD	C	510	5/5	0.90	0.18	61,65,71,74	0
12	IMD	C	511	5/5	0.91	0.21	65,69,75,76	0
7	GOL	A	503	6/6	0.92	0.24	67,72,75,79	0
9	GDP	D	501	28/28	0.95	0.14	66,71,81,92	0
6	MG	B	502	1/1	0.95	0.41	51,51,51,51	0
6	MG	D	502	1/1	0.95	0.14	76,76,76,76	0
6	MG	A	502	1/1	0.95	0.51	59,59,59,59	0
6	MG	C	504	1/1	0.96	0.25	50,50,50,50	0
5	GTP	C	503	32/32	0.97	0.17	35,44,50,57	0
10	MES	B	505	12/12	0.97	0.14	45,54,69,70	0
8	CA	B	504	1/1	0.97	0.09	97,97,97,97	0
8	CA	A	505	1/1	0.97	0.04	82,82,82,82	0
5	GTP	A	501	32/32	0.98	0.25	46,53,58,60	0
8	CA	C	508	1/1	0.98	0.06	85,85,85,85	0
9	GDP	B	501	28/28	0.98	0.21	38,47,50,58	0

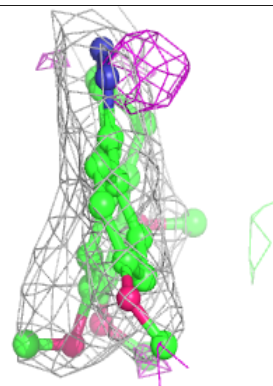
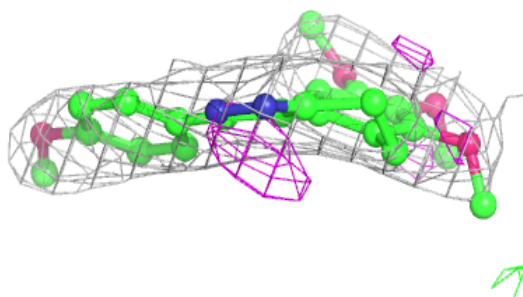
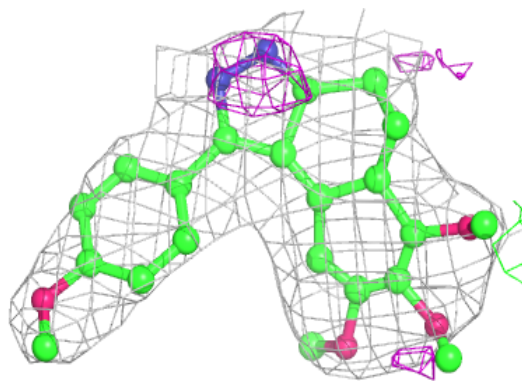
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

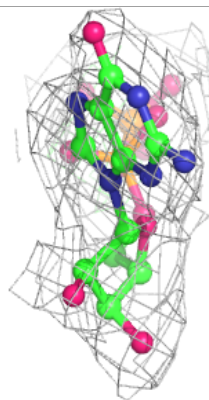
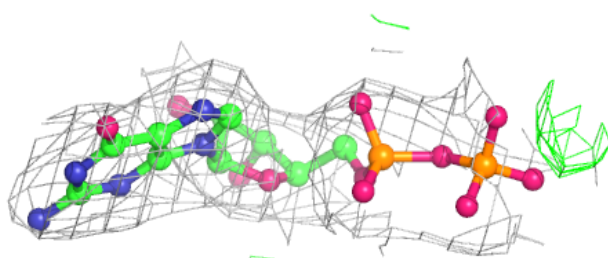
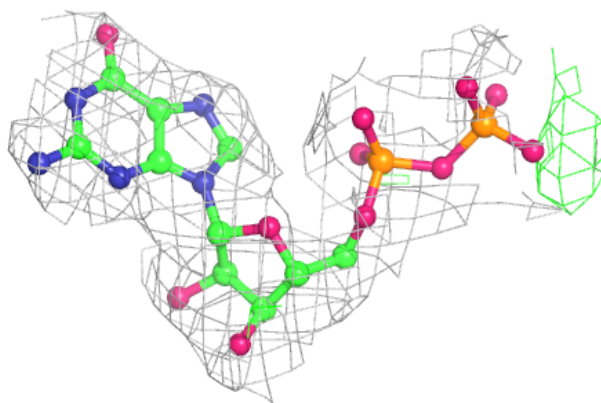
**Electron density around 97O B 506:**

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

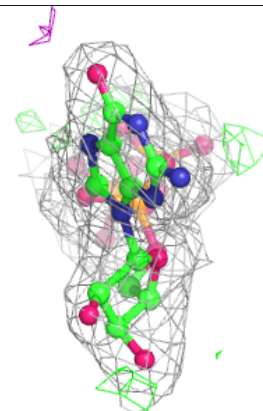
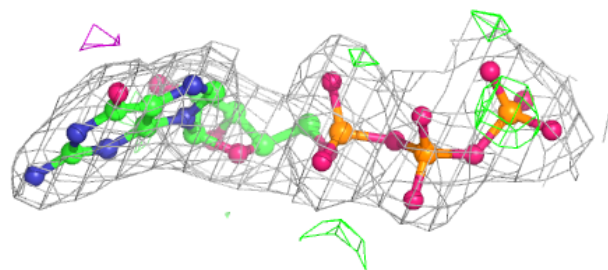
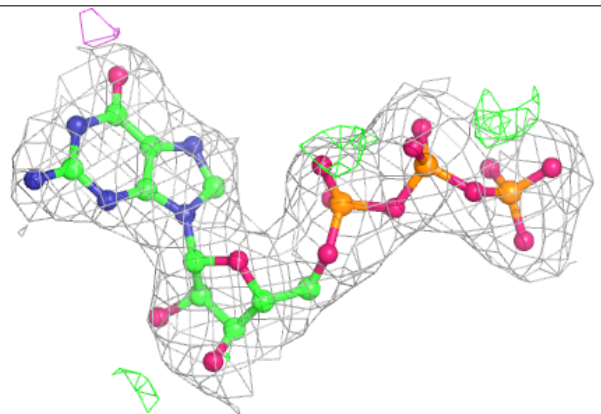


**Electron density around GDP D 501:**

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

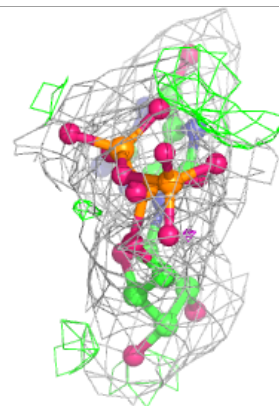
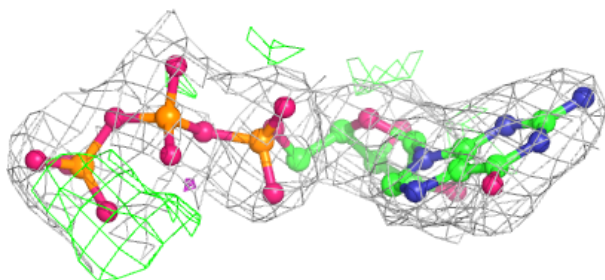
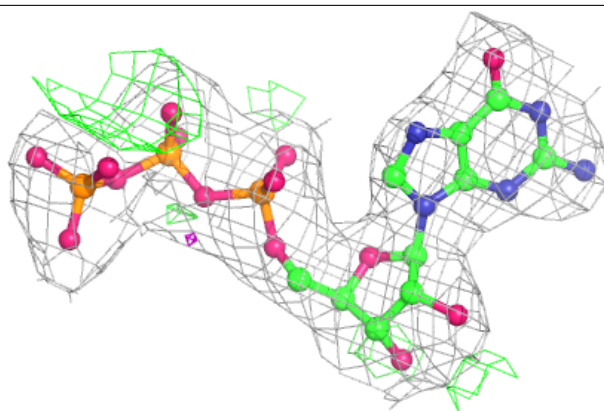
**Electron density around GTP C 503:**

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and green (positive)

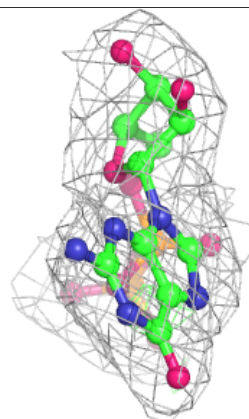
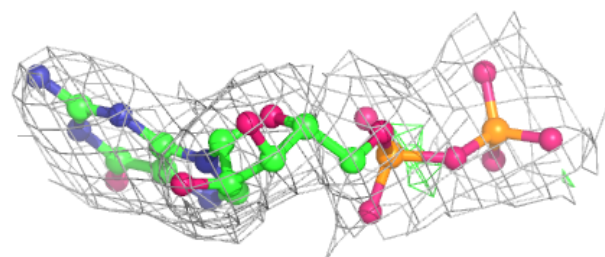
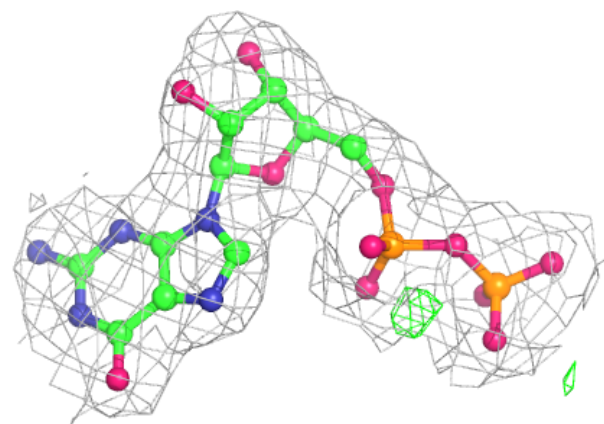


**Electron density around GTP A 501:**

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

**Electron density around GDP B 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.