



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2019 – 11:19 AM EST

PDB ID : 6S8L  
Title : Structure, Thermodynamics, and Kinetics of Plinabulin Binding to two Tubulin Isotypes  
Authors : Sharma, A.; Olieric, N.; Steinmetz, M.  
Deposited on : 2019-07-10  
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : 2.4  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

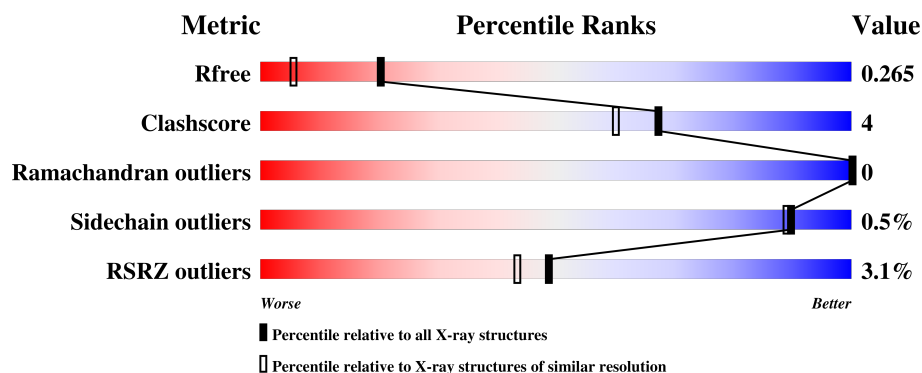
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	111664	5253 (1.80-1.80)
Clashscore	122126	6077 (1.80-1.80)
Ramachandran outliers	120053	6011 (1.80-1.80)
Sidechain outliers	120020	6010 (1.80-1.80)
RSRZ outliers	108989	5157 (1.80-1.80)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	<div> <div>3%</div> <div>86%</div> <div>8%</div> <div>6%</div> </div>
2	B	450	<div> <div>4%</div> <div>82%</div> <div>11%</div> <div>7%</div> </div>
3	F	157	<div> <div>89%</div> <div>10%</div> <div>.</div> </div>

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 8691 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	424	Total	C	N	O	S	0	1	0
			3334	2115	565	632	22			

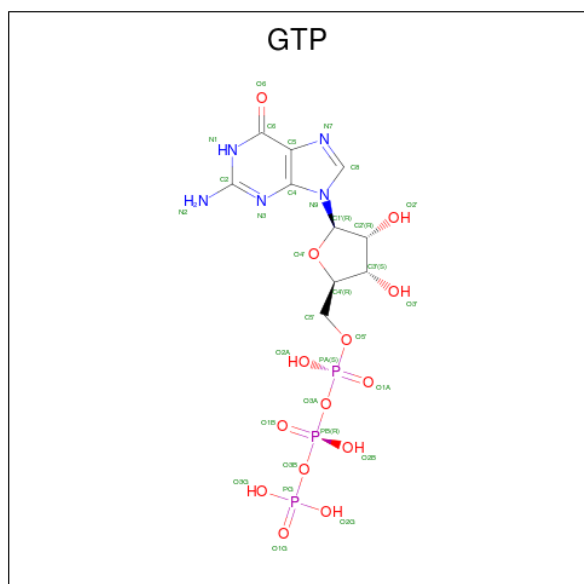
- Molecule 2 is a protein called Tubulin beta-3 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	420	Total	C	N	O	S	0	4	0
			3320	2097	563	635	25			

- Molecule 3 is a protein called Designed ankyrin repeat protein (DARPIN) D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	155	Total	C	N	O	S	0	2	0
			1163	736	198	226	3			

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).

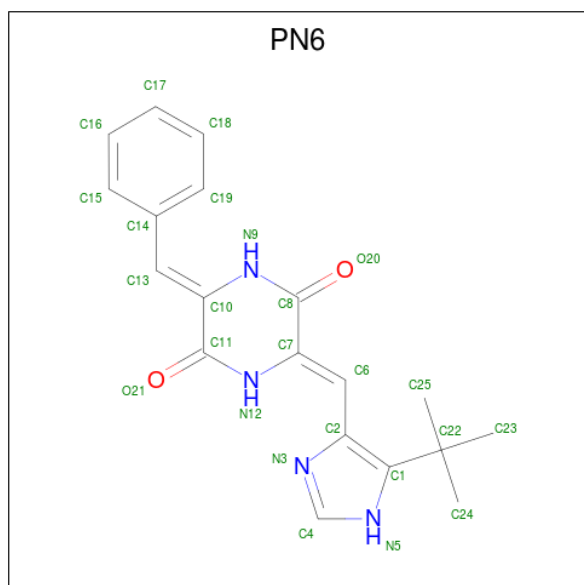


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

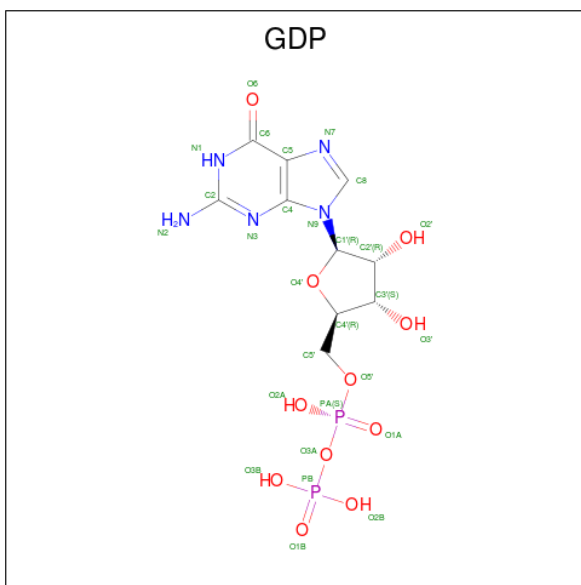
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is (3Z,6Z)-3-benzylidene-6-[(5-tert-butyl-1H-imidazol-4-yl)methylidene]piperazine-2,5-dione (three-letter code: PN6) (formula: C<sub>19</sub>H<sub>20</sub>N<sub>4</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			25	19	4	2		

- Molecule 7 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	
7	B	1	Total 28	C 10	N 5	O 11	P 2	0	0

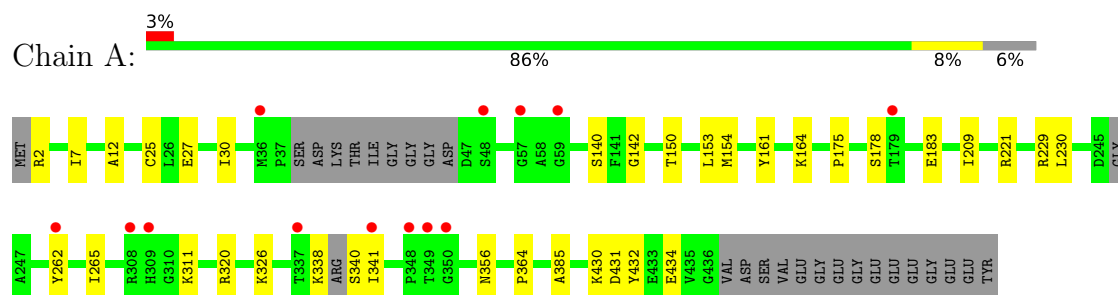
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	353	Total O 353 353	0	0
8	B	248	Total O 248 248	0	0
8	F	186	Total O 186 186	0	0

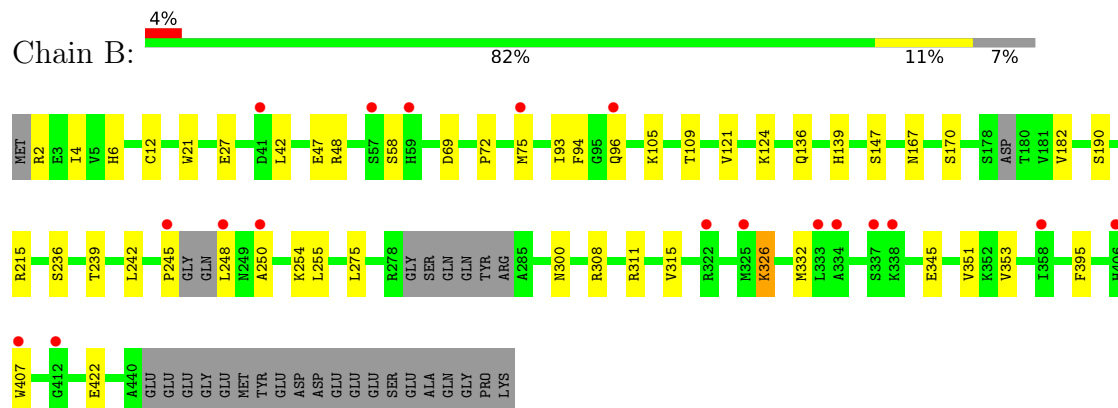
### 3 Residue-property plots [i](#)

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

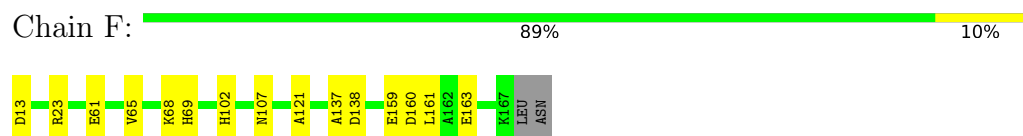
#### • Molecule 1: Tubulin alpha-1B chain



#### • Molecule 2: Tubulin beta-3 chain



#### • Molecule 3: Designed ankyrin repeat protein (DARPIN) D1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.63Å 91.20Å 82.64Å 90.00° 97.49° 90.00°	Depositor
Resolution (Å)	45.60 – 1.80 49.19 – 1.80	Depositor EDS
% Data completeness (in resolution range)	93.3 (45.60-1.80) 93.4 (49.19-1.80)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.04 (at 1.79Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, $R_{free}$	0.215 , 0.266 0.215 , 0.265	Depositor DCC
$R_{free}$ test set	4692 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.0	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 44.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8691	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GTP, MG, PN6

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	0.30	0/3409	0.47	0/4627
2	B	0.29	0/3405	0.46	0/4611
3	F	0.28	0/1185	0.47	0/1611
All	All	0.29	0/7999	0.47	0/10849

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

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	3334	0	3243	23	0
2	B	3320	0	3219	31	0
3	F	1163	0	1176	14	0
4	A	32	0	10	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	B	25	0	20	4	0
7	B	28	0	11	1	0
8	A	353	0	0	5	0
8	B	248	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	186	0	0	5	0
All	All	8691	0	7679	66	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 4.

All (66) 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:338:LYS:O	1:A:340:SER:N	2.24	0.70
3:F:13:ASP:N	8:F:203:HOH:O	2.24	0.70
1:A:326:LYS:NZ	8:A:605:HOH:O	2.29	0.66
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.79	0.64
2:B:275:LEU:HD11	2:B:300:ASN:HA	1.79	0.63
2:B:326:LYS:H	2:B:326:LYS:HD3	1.65	0.61
3:F:107:ASN:HD21	3:F:138:ASP:H	1.47	0.61
2:B:48:ARG:HG3	2:B:245:PRO:HD3	1.85	0.59
1:A:364:PRO:O	8:A:601:HOH:O	2.17	0.59
2:B:72:PRO:HG3	2:B:96:GLN:HA	1.87	0.57
2:B:4:ILE:HD11	2:B:242:LEU:HD23	1.87	0.57
3:F:107:ASN:HD21	3:F:137:ALA:HA	1.72	0.55
1:A:2:ARG:NH1	8:A:616:HOH:O	2.40	0.54
3:F:13:ASP:OD1	8:F:201:HOH:O	2.18	0.54
1:A:229:ARG:NH1	8:A:602:HOH:O	2.24	0.53
2:B:239:THR:HG22	6:B:501:PN6:C17	2.39	0.52
1:A:175:PRO:HA	1:A:178:SER:HB3	1.92	0.51
3:F:107:ASN:ND2	3:F:138:ASP:H	2.09	0.51
2:B:42:LEU:HA	2:B:47:GLU:HG2	1.94	0.50
2:B:215:ARG:NH1	3:F:160:ASP:OD1	2.45	0.49
2:B:27:GLU:OE1	2:B:236:SER:OG	2.27	0.48
1:A:311:LYS:NZ	8:A:624:HOH:O	2.46	0.47
2:B:395:PHE:CE1	2:B:422:GLU:HB2	2.49	0.47
3:F:121:ALA:HB1	3:F:161:LEU:HD21	1.96	0.47
1:A:430:LYS:NZ	1:A:434:GLU:OE2	2.43	0.47
2:B:2:ARG:N	8:B:621:HOH:O	2.48	0.47
2:B:124:LYS:HE3	2:B:124:LYS:HB2	1.61	0.45
2:B:147:SER:HB2	2:B:190:SER:OG	2.16	0.45
2:B:315:VAL:HB	2:B:351:VAL:HG22	1.98	0.45
3:F:107:ASN:HD21	3:F:138:ASP:N	2.12	0.45
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.36	0.44
2:B:93:ILE:HD11	2:B:121:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:68:LYS:NZ	8:F:205:HOH:O	2.31	0.44
1:A:265:ILE:HD11	1:A:431:ASP:HB3	1.99	0.44
3:F:102:HIS:HD2	8:F:340:HOH:O	2.00	0.44
2:B:311:ARG:NH2	2:B:345:GLU:OE1	2.42	0.44
2:B:139:HIS:HE1	2:B:170:SER:OG	2.00	0.43
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.53	0.43
2:B:182:VAL:HG21	2:B:407[B]:TRP:HZ3	1.83	0.43
2:B:255:LEU:HB3	6:B:501:PN6:C11	2.48	0.43
2:B:242:LEU:HD22	6:B:501:PN6:C16	2.49	0.43
2:B:69:ASP:O	2:B:94:PHE:HA	2.18	0.43
1:A:142:GLY:HA3	1:A:183:GLU:OE1	2.19	0.43
1:A:430:LYS:O	1:A:434:GLU:HG3	2.19	0.43
3:F:159:GLU:O	3:F:163:GLU:HG2	2.19	0.42
2:B:308:ARG:NH1	8:B:617:HOH:O	2.47	0.42
1:A:385:ALA:HB2	1:A:432:TYR:CG	2.55	0.42
1:A:341:ILE:HG13	1:A:341:ILE:O	2.20	0.42
2:B:332:MET:HG3	2:B:353:VAL:HG21	2.02	0.42
3:F:65:VAL:O	3:F:69:HIS:HD2	2.02	0.42
2:B:12:CYS:HB2	7:B:502:GDP:C8	2.54	0.42
2:B:250:ALA:HA	2:B:254:LYS:HD2	2.01	0.42
1:A:12:ALA:HB3	1:A:140:SER:HB3	2.01	0.41
1:A:7:ILE:HG21	1:A:153:LEU:HD21	2.02	0.41
2:B:255:LEU:HB3	6:B:501:PN6:N12	2.35	0.41
3:F:23:ARG:NH2	8:F:204:HOH:O	2.30	0.41
2:B:105:LYS:HA	2:B:109:THR:OG1	2.20	0.41
1:A:161:TYR:HB3	1:A:164:LYS:CG	2.50	0.40
1:A:221:ARG:CG	2:B:326:LYS:HG3	2.51	0.40
3:F:61:GLU:O	3:F:65:VAL:HG23	2.22	0.40
1:A:320:ARG:HA	1:A:356:ASN:O	2.20	0.40
1:A:25:CYS:HB3	1:A:30:ILE:O	2.21	0.40
1:A:27:GLU:CD	1:A:320:ARG:HH22	2.24	0.40
1:A:150:THR:O	1:A:154:MET:HG2	2.21	0.40
2:B:136:GLN:HA	2:B:167:ASN:O	2.22	0.40
2:B:75:MET:HG3	2:B:94:PHE:CD2	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	417/451 (92%)	409 (98%)	8 (2%)	0	100	100
2	B	416/450 (92%)	408 (98%)	8 (2%)	0	100	100
3	F	155/157 (99%)	155 (100%)	0	0	100	100
All	All	988/1058 (93%)	972 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	360/379 (95%)	359 (100%)	1 (0%)	93	92
2	B	365/386 (95%)	362 (99%)	3 (1%)	83	80
3	F	122/122 (100%)	122 (100%)	0	100	100
All	All	847/887 (96%)	843 (100%)	4 (0%)	90	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	262	TYR
2	B	58	SER
2	B	248	LEU
2	B	326	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	139	HIS
2	B	426	ASN
3	F	107	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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\# Z  > 2$
4	GTP	A	501	5	26,34,34	4.37	13 (50%)	29,54,54	3.34	11 (37%)
6	PN6	B	501	-	19,27,27	3.51	8 (42%)	19,39,39	1.61	2 (10%)
7	GDP	B	502	5	24,30,30	4.40	14 (58%)	27,47,47	2.17	7 (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
4	GTP	A	501	5	-	7/18/38/38	0/3/3/3
6	PN6	B	501	-	-	2/10/14/14	0/3/3/3
7	GDP	B	502	5	-	4/12/32/32	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	GTP	O4'-C1'	14.34	1.61	1.41
7	B	502	GDP	C2'-C3'	-10.73	1.25	1.53
4	A	501	GTP	C6-C5	7.72	1.55	1.41
7	B	502	GDP	C4-N3	7.69	1.47	1.35
6	B	501	PN6	C8-N9	7.61	1.46	1.33
7	B	502	GDP	O4'-C1'	7.35	1.51	1.41
7	B	502	GDP	C6-C5	7.29	1.54	1.41
4	A	501	GTP	C4-N3	7.27	1.47	1.35
6	B	501	PN6	C10-N9	6.89	1.46	1.35
6	B	501	PN6	C11-N12	6.76	1.44	1.33
6	B	501	PN6	C7-N12	6.28	1.45	1.35
4	A	501	GTP	C6-N1	6.16	1.43	1.33
7	B	502	GDP	O4'-C4'	-5.95	1.31	1.45
4	A	501	GTP	O4'-C4'	-5.68	1.32	1.45
4	A	501	GTP	C2-N2	5.66	1.45	1.33
7	B	502	GDP	C6-N1	5.56	1.42	1.33
7	B	502	GDP	C2-N2	5.28	1.44	1.33
4	A	501	GTP	C2-N1	5.13	1.44	1.35
7	B	502	GDP	C3'-C4'	5.02	1.65	1.53
7	B	502	GDP	C2-N1	4.79	1.43	1.35
6	B	501	PN6	C2-C6	3.57	1.55	1.41
6	B	501	PN6	C14-C13	3.47	1.54	1.47
4	A	501	GTP	PG-O3B	3.33	1.65	1.60
7	B	502	GDP	O2'-C2'	3.13	1.50	1.43
4	A	501	GTP	O2'-C2'	2.90	1.49	1.43
4	A	501	GTP	O3'-C3'	-2.77	1.36	1.43
7	B	502	GDP	PB-O3A	2.64	1.64	1.60
6	B	501	PN6	O20-C8	-2.42	1.18	1.24
6	B	501	PN6	O21-C11	-2.40	1.18	1.24
7	B	502	GDP	C2-N3	2.36	1.46	1.35
7	B	502	GDP	O6-C6	-2.22	1.19	1.24
7	B	502	GDP	O3'-C3'	2.11	1.48	1.43
4	A	501	GTP	O6-C6	-2.06	1.19	1.24
4	A	501	GTP	C2-N3	2.03	1.44	1.35
4	A	501	GTP	C8-N7	2.01	1.38	1.34

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	GTP	C1'-N9-C4	12.65	148.49	126.64
7	B	502	GDP	C1'-N9-C4	-5.92	116.41	126.64
4	A	501	GTP	N3-C2-N1	-5.61	119.66	127.25
6	B	501	PN6	C7-C6-C2	-5.55	120.99	128.66
4	A	501	GTP	C4'-O4'-C1'	-5.38	104.22	109.83
7	B	502	GDP	N3-C2-N1	-4.86	120.67	127.25
7	B	502	GDP	C2-N3-C4	4.67	120.69	115.36
4	A	501	GTP	C6-C5-C4	-3.94	117.00	120.79
4	A	501	GTP	C6-N1-C2	3.72	121.36	116.06
4	A	501	GTP	N2-C2-N1	3.60	122.89	117.25
4	A	501	GTP	C5-C6-N1	-3.22	118.99	123.47
4	A	501	GTP	C2-N3-C4	3.14	118.94	115.36
4	A	501	GTP	C4-C5-N7	-3.08	106.19	109.40
7	B	502	GDP	O3'-C3'-C4'	-2.85	102.83	111.07
4	A	501	GTP	O5'-C5'-C4'	-2.85	99.17	108.99
6	B	501	PN6	C22-C1-N5	2.60	123.73	120.50
7	B	502	GDP	C5-C6-N1	-2.44	120.07	123.47
7	B	502	GDP	PA-O3A-PB	-2.37	125.05	132.57
4	A	501	GTP	PB-O3B-PG	-2.30	125.27	132.57
7	B	502	GDP	C4-C5-N7	-2.18	107.13	109.40

There are no chirality outliers.

All (13) torsion outliers are listed below:

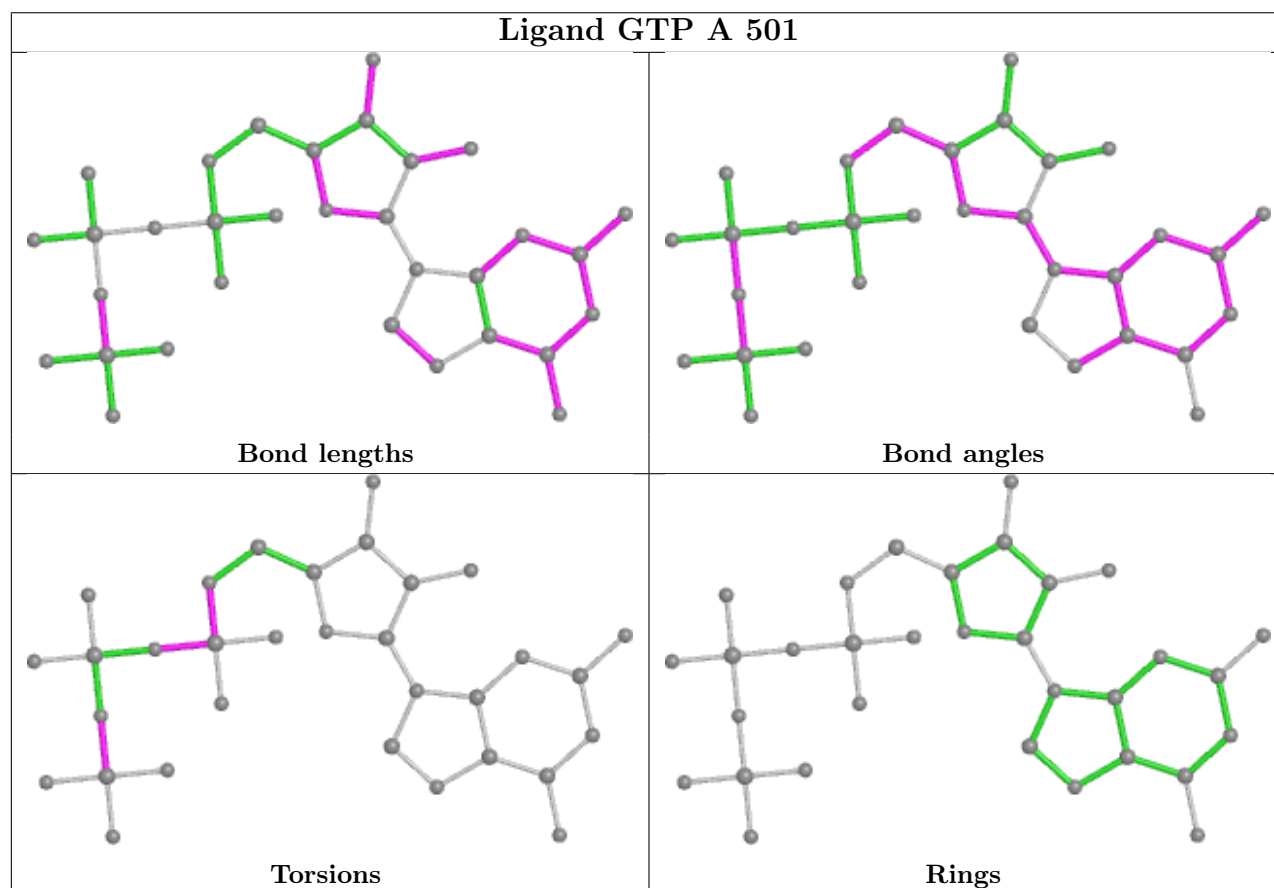
Mol	Chain	Res	Type	Atoms
4	A	501	GTP	C5'-O5'-PA-O1A
6	B	501	PN6	C1-C2-C6-C7
6	B	501	PN6	N3-C2-C6-C7
7	B	502	GDP	C5'-O5'-PA-O1A
7	B	502	GDP	C5'-O5'-PA-O2A
4	A	501	GTP	PB-O3B-PG-O1G
4	A	501	GTP	C5'-O5'-PA-O2A
7	B	502	GDP	PB-O3A-PA-O1A
4	A	501	GTP	PB-O3B-PG-O3G
4	A	501	GTP	C5'-O5'-PA-O3A
7	B	502	GDP	C5'-O5'-PA-O3A
4	A	501	GTP	PB-O3A-PA-O2A
4	A	501	GTP	PB-O3B-PG-O2G

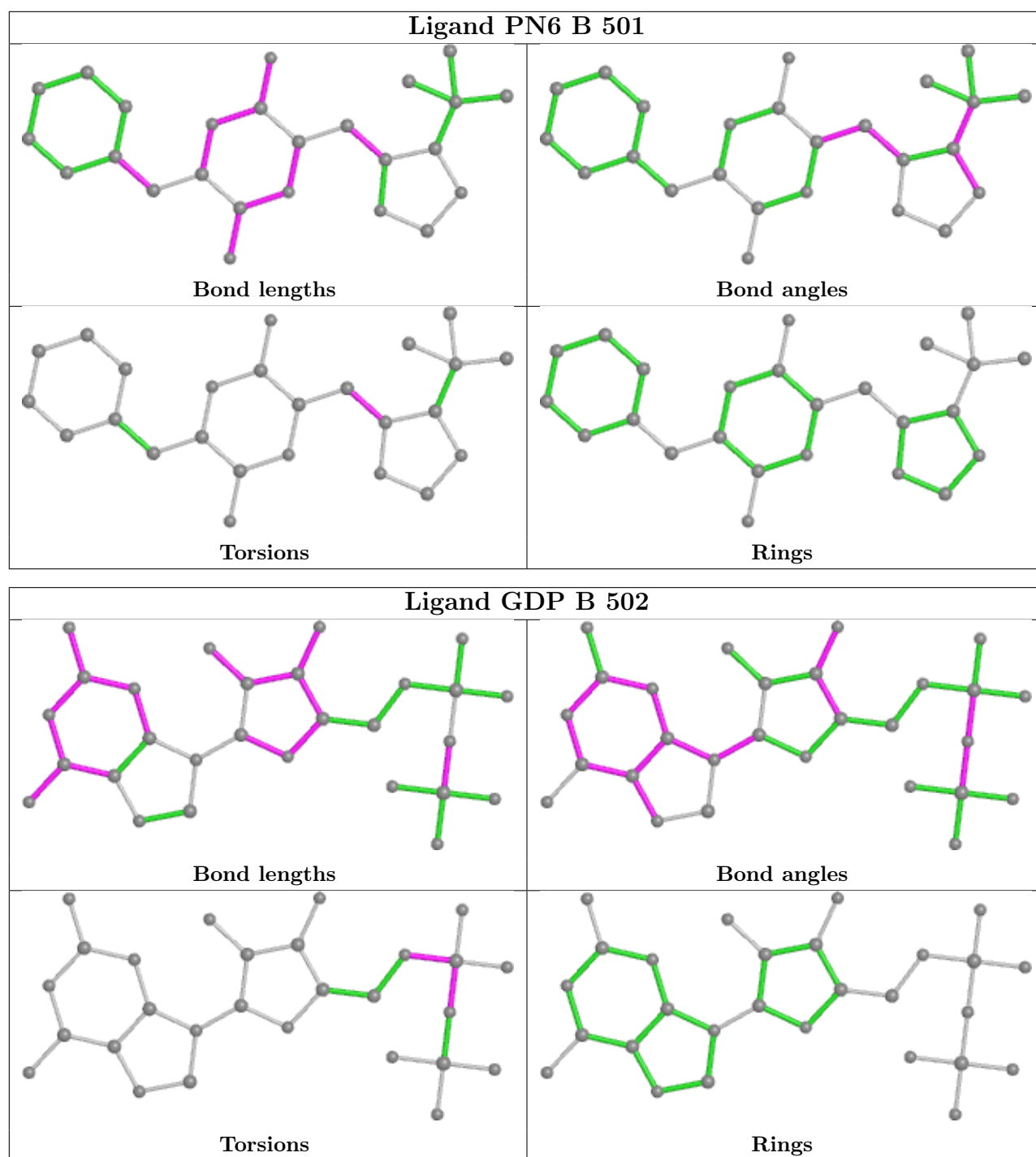
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	501	PN6	4	0
7	B	502	GDP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	424/451 (94%)	0.03	13 (3%) 49 43	10, 22, 49, 83	0
2	B	420/450 (93%)	0.10	18 (4%) 35 29	11, 27, 55, 85	0
3	F	155/157 (98%)	-0.29	0 100 100	9, 19, 41, 63	0
All	All	999/1058 (94%)	0.01	31 (3%) 49 43	9, 23, 52, 85	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	262	TYR	5.8
1	A	179	THR	4.1
2	B	57	SER	3.9
2	B	250	ALA	3.8
1	A	348	PRO	3.6
1	A	59	GLY	3.3
1	A	309	HIS	3.2
1	A	57	GLY	3.1
2	B	325	MET	2.8
2	B	338	LYS	2.8
2	B	248	LEU	2.8
1	A	349	THR	2.7
2	B	245	PRO	2.7
2	B	337	SER	2.7
2	B	333	LEU	2.4
2	B	59	HIS	2.4
2	B	412	GLY	2.3
1	A	48	SER	2.3
2	B	41	ASP	2.3
2	B	407[A]	TRP	2.2
2	B	96	GLN	2.2
1	A	341	ILE	2.2
2	B	75	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	308	ARG	2.1
2	B	334	ALA	2.1
1	A	350	GLY	2.1
1	A	36	MET	2.1
1	A	337	THR	2.1
2	B	358	ILE	2.1
2	B	322	ARG	2.0
2	B	406	HIS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

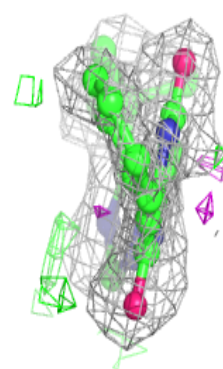
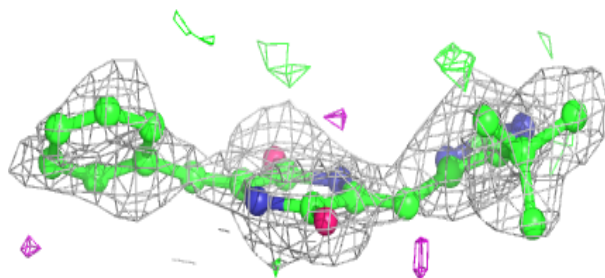
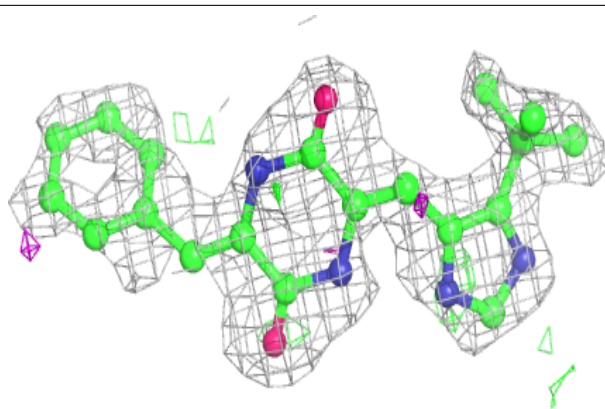
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	PN6	B	501	25/25	0.84	0.22	19,27,32,34	25
5	MG	B	503	1/1	0.95	0.07	27,27,27,27	0
5	MG	A	502	1/1	0.97	0.06	15,15,15,15	0
7	GDP	B	502	28/28	0.97	0.07	10,15,20,21	0
4	GTP	A	501	32/32	0.97	0.09	5,12,19,21	0

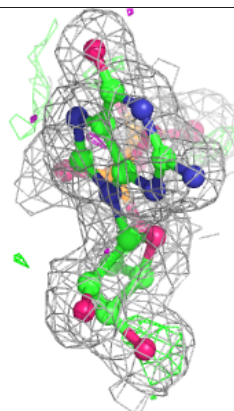
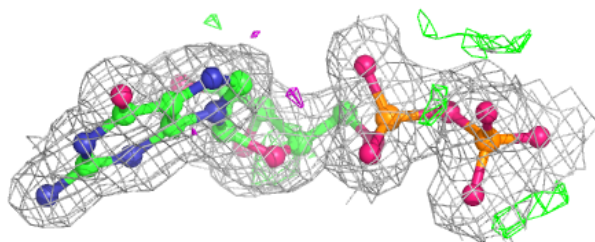
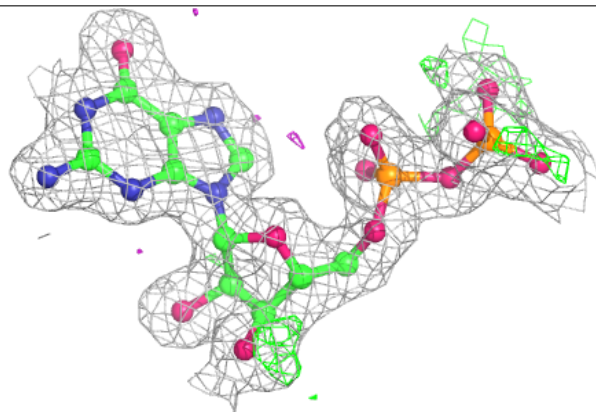
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

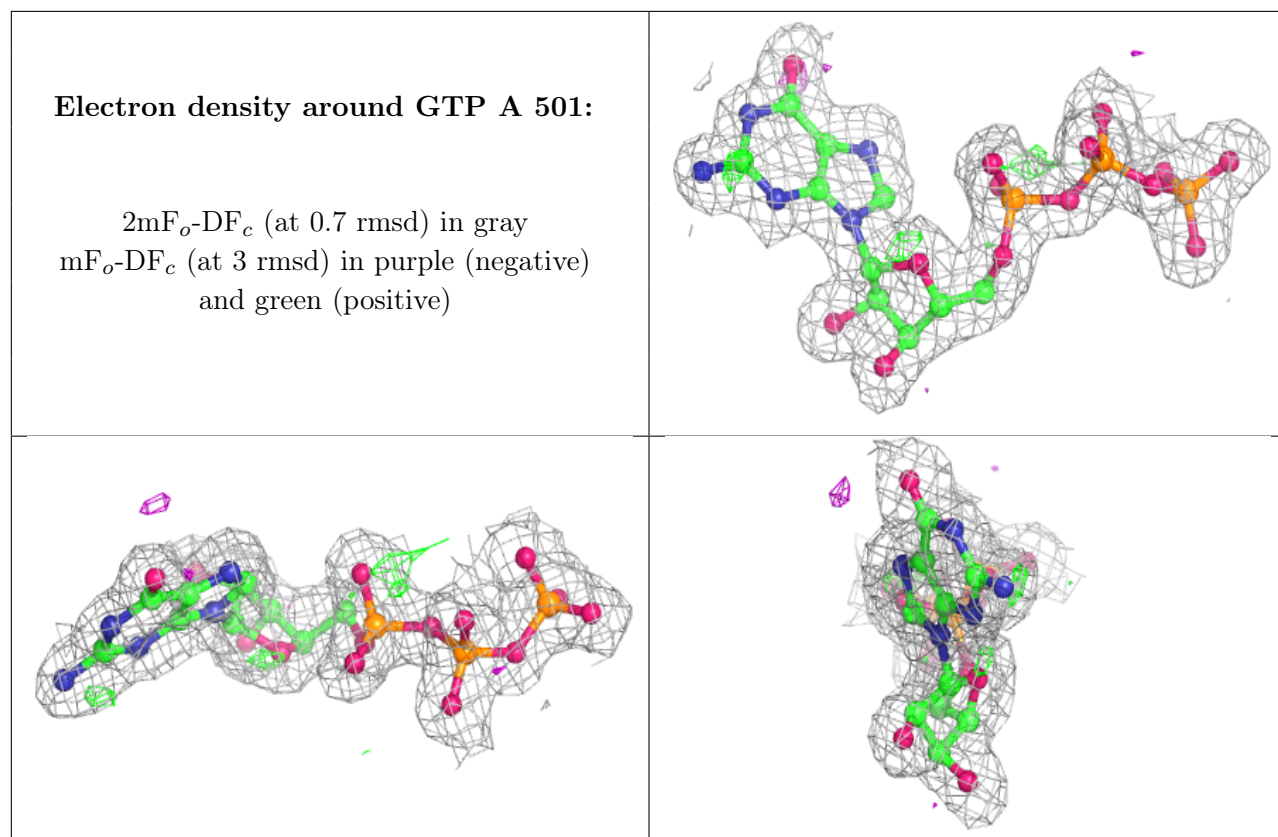
**Electron density around PN6 B 501:**

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

**Electron density around GDP B 502:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.