



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 12:49 PM UTC

PDB ID : 6LSN / pdb\_00006lsn  
Title : Crystal structure of tubulin-inhibitor complex  
Authors : Gang, L.; Wang, Y.X.; Cheng, J.J.  
Deposited on : 2020-01-17  
Resolution : 2.44 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)  
Xtrriage (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

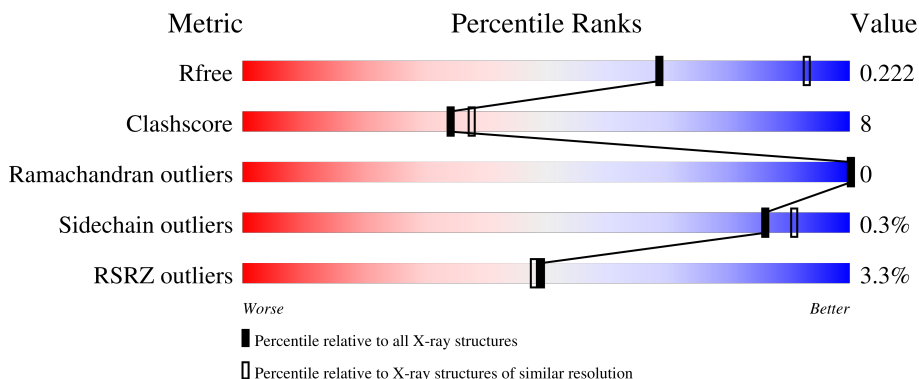
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.44 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	450	
1	C	450	
2	B	445	
2	D	445	
3	E	143	

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Mol	Chain	Length	Quality of chain
4	F	384	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment on the left labeled '10%', a large green segment labeled '67%', a yellow segment labeled '24%', and a small grey segment on the far right labeled '9%'.</p>

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 18041 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
			Total	C	N	O	S			
1	A	440	Total	C	N	O	S	0	1	0
			3435	2175	581	657	22			
1	C	440	Total	C	N	O	S	0	4	0
			3451	2184	585	660	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	424	Total	C	N	O	S	0	2	0
			3344	2104	569	645	26			
2	D	421	Total	C	N	O	S	0	3	0
			3306	2079	562	639	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	124	Total	C	N	O	S	0	1	0
			1025	631	185	204	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63042
E	4	ALA	-	expression tag	UNP P63042

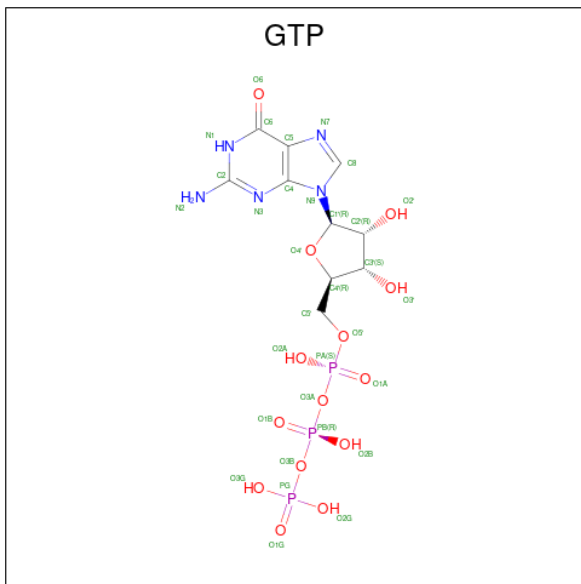
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	351	Total	C	N	O	S	0	2	0
			2887	1849	498	525	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (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	
			Total	C	N	O			P
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	2	Total	Mg	0	0
			2	2		
6	C	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		

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

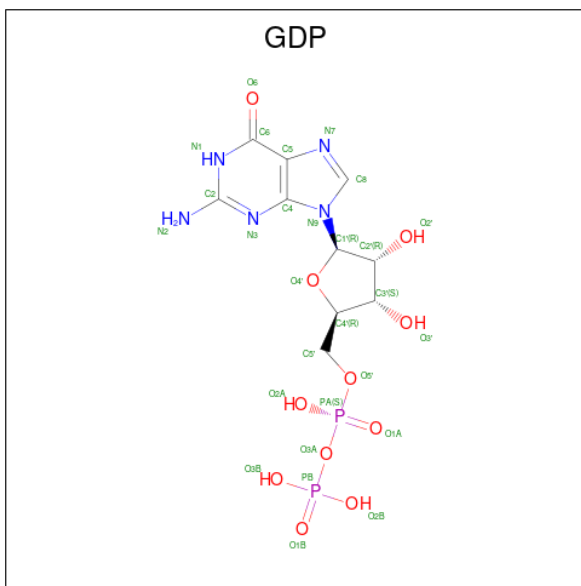
- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

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

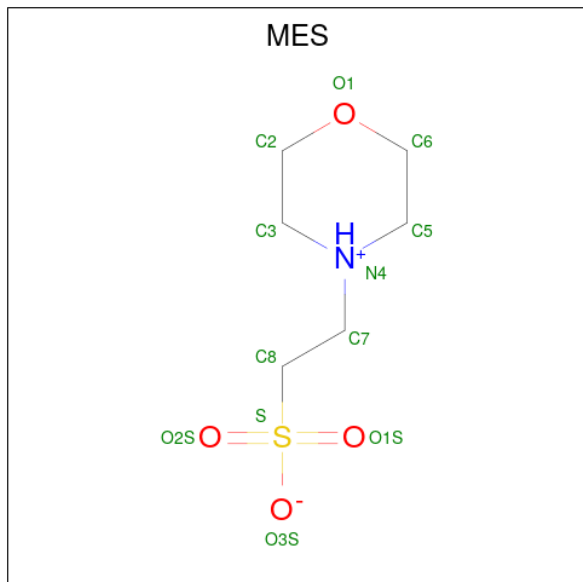
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cl 1 1	0	0

- Molecule 9 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>).



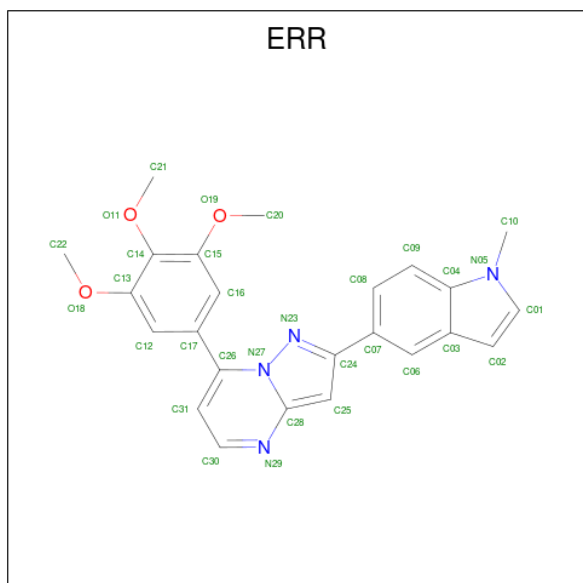
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C N O P 28 10 5 11 2	0	0
9	D	1	Total C N O P 28 10 5 11 2	0	0

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



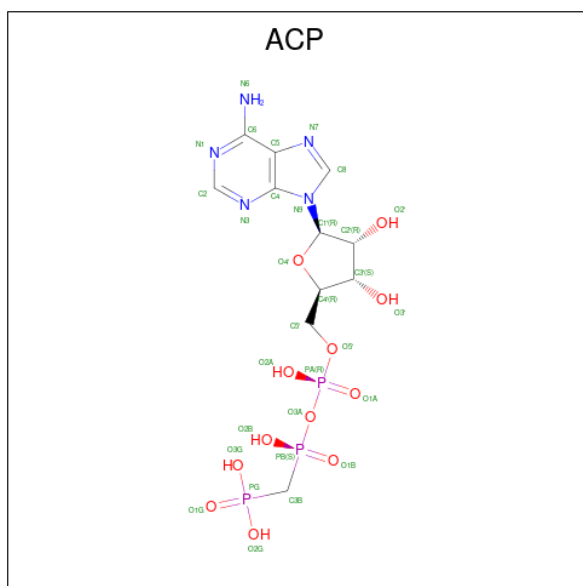
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	S			
10	B	1	Total	12	6	1	4	1	0	0
10	B	1	Total	12	6	1	4	1	0	0

- Molecule 11 is 2-(1-methylindol-5-yl)-7-(3,4,5-trimethoxyphenyl)pyrazolo[1,5-a]pyrimidine (CCD ID: ERR) (formula: C<sub>24</sub>H<sub>22</sub>N<sub>4</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
11	B	1	31	24	4	3	0	0

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula:  $C_{11}H_{18}N_5O_{12}P_3$ ).



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

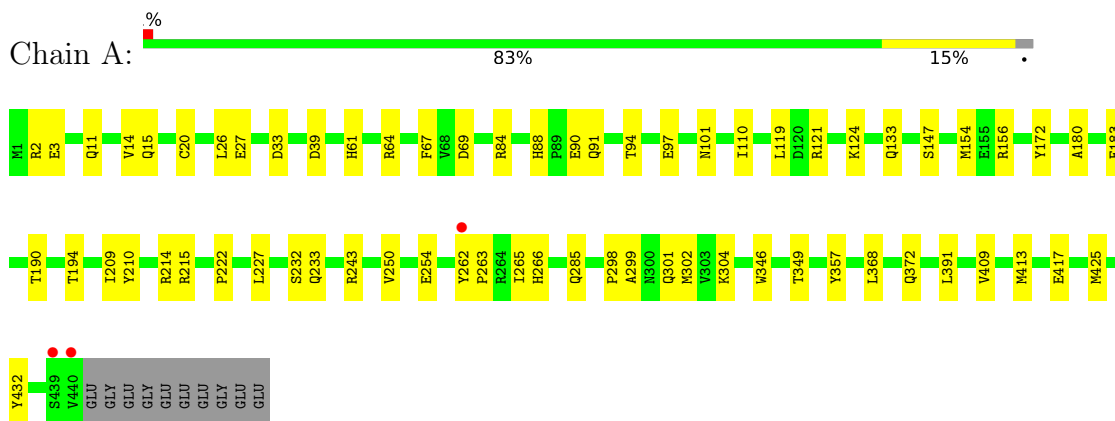
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	80	Total	O	0	0
			80	80		
13	B	68	Total	O	0	0
			68	68		
13	C	153	Total	O	0	0
			153	153		
13	D	28	Total	O	0	0
			28	28		
13	E	14	Total	O	0	0
			14	14		
13	F	33	Total	O	0	0
			33	33		

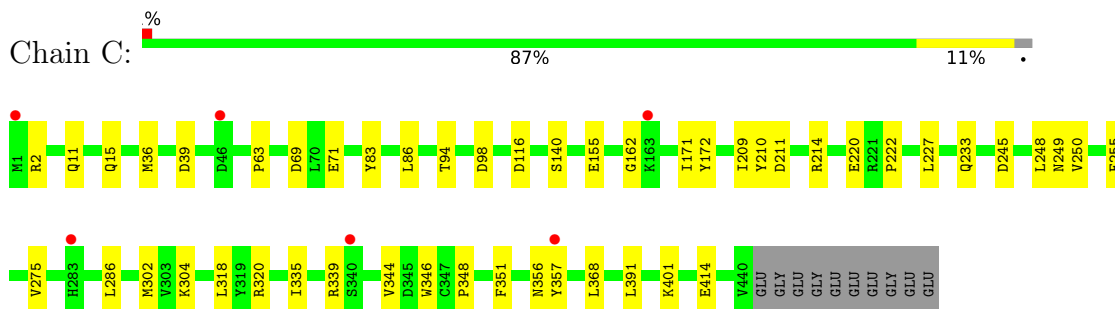
### 3 Residue-property plots [i](#)

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.

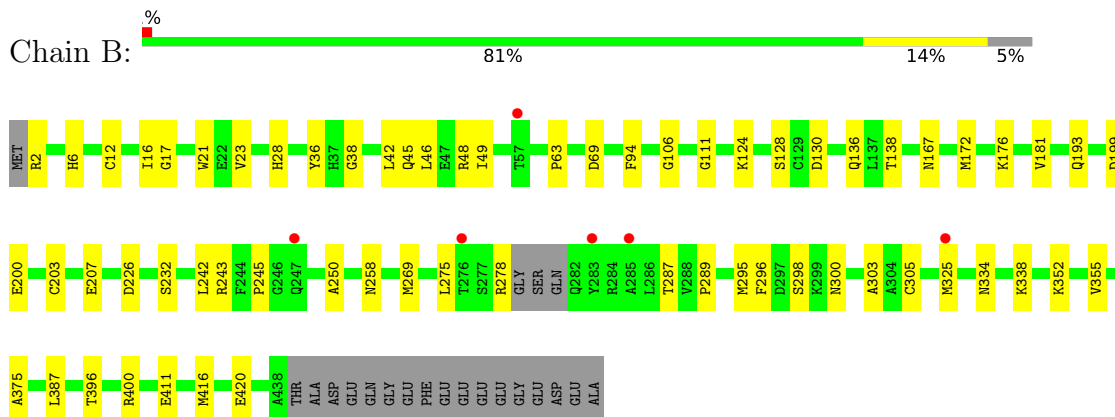
- Molecule 1: Tubulin alpha-1B chain



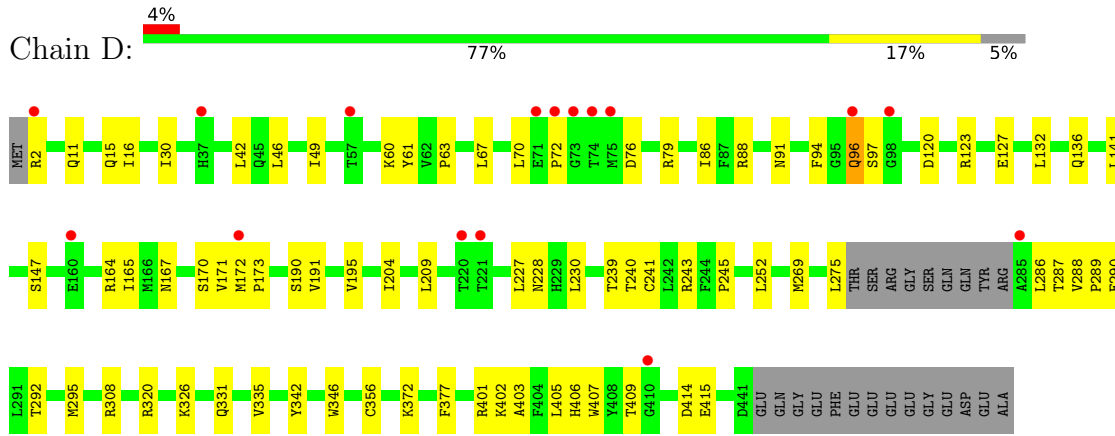
- Molecule 1: Tubulin alpha-1B chain



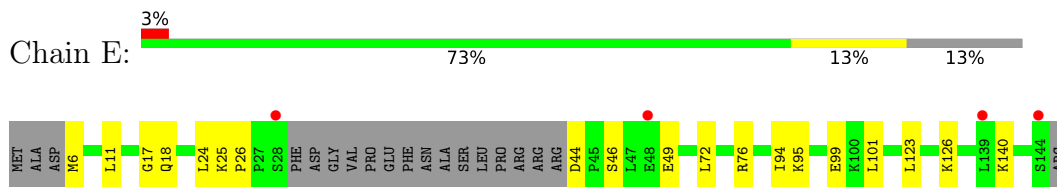
- Molecule 2: Tubulin beta chain



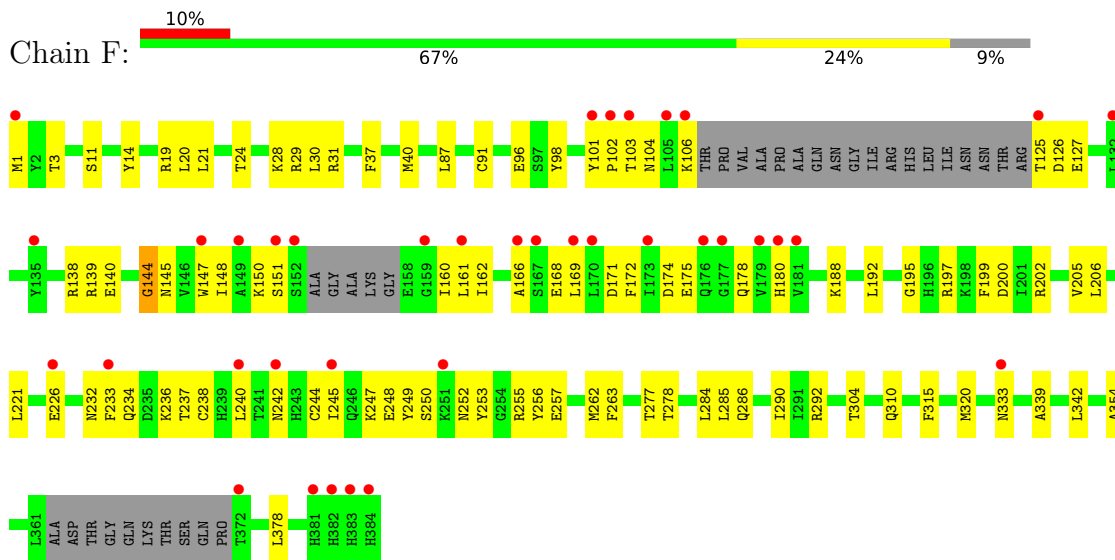
- Molecule 2: Tubulin beta chain



- 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, $\alpha$ , $\beta$ , $\gamma$	105.30Å 158.46Å 181.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.17 – 2.44 33.17 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.5 (33.17-2.44) 99.5 (33.17-2.44)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.25 (at 2.45Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.177 , 0.220 0.178 , 0.222	Depositor DCC
$R_{free}$ test set	2000 reflections (1.77%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.2	Xtrriage
Anisotropy	0.204	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 56.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	18041	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.45	0/3516	0.66	0/4775
1	C	0.56	0/3538	0.72	0/4803
2	B	0.48	0/3424	0.68	0/4638
2	D	0.45	0/3385	0.67	0/4588
3	E	0.43	0/1036	0.58	0/1375
4	F	0.35	0/2960	0.61	2/3999 (0.1%)
All	All	0.47	0/17859	0.67	2/24178 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	144	GLY	CA-C-N	-5.21	114.14	122.62
4	F	144	GLY	C-N-CA	-5.21	114.14	122.62

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3435	0	3345	49	0
1	C	3451	0	3365	32	0
2	B	3344	0	3226	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3306	0	3183	58	0
3	E	1025	0	1040	15	0
4	F	2887	0	2846	72	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	2	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
9	B	28	0	11	3	0
9	D	28	0	12	3	0
10	B	24	0	26	4	0
11	B	31	0	0	2	0
12	F	31	0	12	2	0
13	A	80	0	0	3	0
13	B	68	0	0	3	0
13	C	153	0	0	4	0
13	D	28	0	0	2	0
13	E	14	0	0	1	0
13	F	33	0	0	0	0
All	All	18041	0	17090	264	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 8.

The worst 5 of 264 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)
2:D:228:ASN:ND2	9:D:600:GDP:HN1	1.61	0.96
2:D:228:ASN:HD21	9:D:600:GDP:HN1	1.08	0.96
4:F:192:LEU:HD22	4:F:262:MET:HE1	1.61	0.82
2:B:172:MET:HG2	2:B:387:LEU:HD21	1.62	0.81
1:C:211[A]:ASP:OD2	1:C:304:LYS:NZ	2.14	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	439/450 (98%)	424 (97%)	15 (3%)	0	100	100
1	C	441/450 (98%)	429 (97%)	12 (3%)	0	100	100
2	B	422/445 (95%)	408 (97%)	14 (3%)	0	100	100
2	D	419/445 (94%)	407 (97%)	12 (3%)	0	100	100
3	E	121/143 (85%)	120 (99%)	1 (1%)	0	100	100
4	F	345/384 (90%)	330 (96%)	15 (4%)	0	100	100
All	All	2187/2317 (94%)	2118 (97%)	69 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	371/378 (98%)	371 (100%)	0	100	100
1	C	374/378 (99%)	372 (100%)	2 (0%)	81	87
2	B	368/383 (96%)	367 (100%)	1 (0%)	86	91
2	D	363/383 (95%)	361 (99%)	2 (1%)	78	85
3	E	112/127 (88%)	112 (100%)	0	100	100
4	F	318/342 (93%)	318 (100%)	0	100	100
All	All	1906/1991 (96%)	1901 (100%)	5 (0%)	86	91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	48	ARG
1	C	302	MET
1	C	318	LEU
2	D	96	GLN
2	D	97	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	128	GLN
4	F	333	ASN
2	D	11	GLN
4	F	252	ASN
1	C	393	HIS

### 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 19 ligands modelled in this entry, 11 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	ERR	B	507	-	35,35,35	3.13	15 (42%)	51,51,51	2.83	15 (29%)
9	GDP	D	600	6	29,30,30	2.16	11 (37%)	45,47,47	1.95	11 (24%)
10	MES	B	505	-	12,12,12	1.57	2 (16%)	15,16,16	2.23	5 (33%)
12	ACP	F	402	6	31,33,33	3.17	14 (45%)	47,52,52	2.15	18 (38%)
10	MES	B	504	-	12,12,12	1.31	2 (16%)	15,16,16	2.22	7 (46%)
9	GDP	B	501	6	29,30,30	3.53	11 (37%)	45,47,47	1.82	13 (28%)
5	GTP	A	501	6	33,34,34	3.40	15 (45%)	50,54,54	1.56	11 (22%)
5	GTP	C	501	6	33,34,34	3.29	14 (42%)	50,54,54	1.46	9 (18%)

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
11	ERR	B	507	-	-	2/14/14/14	0/5/5/5
9	GDP	D	600	6	-	5/16/32/32	0/3/3/3
10	MES	B	505	-	-	2/6/14/14	0/1/1/1
12	ACP	F	402	6	-	6/19/38/38	0/3/3/3
10	MES	B	504	-	-	0/6/14/14	0/1/1/1
9	GDP	B	501	6	-	3/16/32/32	0/3/3/3
5	GTP	A	501	6	-	6/22/38/38	0/3/3/3
5	GTP	C	501	6	-	4/22/38/38	0/3/3/3

The worst 5 of 84 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	507	ERR	C28-N27	-9.46	1.25	1.39
12	F	402	ACP	O4'-C1'	8.72	1.62	1.42
9	B	501	GDP	C3'-C4'	-8.70	1.30	1.53
11	B	507	ERR	C01-N05	-8.55	1.29	1.37
5	A	501	GTP	O4'-C1'	7.69	1.59	1.42

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	507	ERR	C30-N29-C28	11.00	120.81	115.82
11	B	507	ERR	C24-N23-N27	8.01	109.96	104.06
9	D	600	GDP	C5-C4-N3	-6.49	118.07	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	507	ERR	C31-C30-N29	-6.35	119.73	124.75
11	B	507	ERR	C30-C31-C26	-5.81	116.88	120.69

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

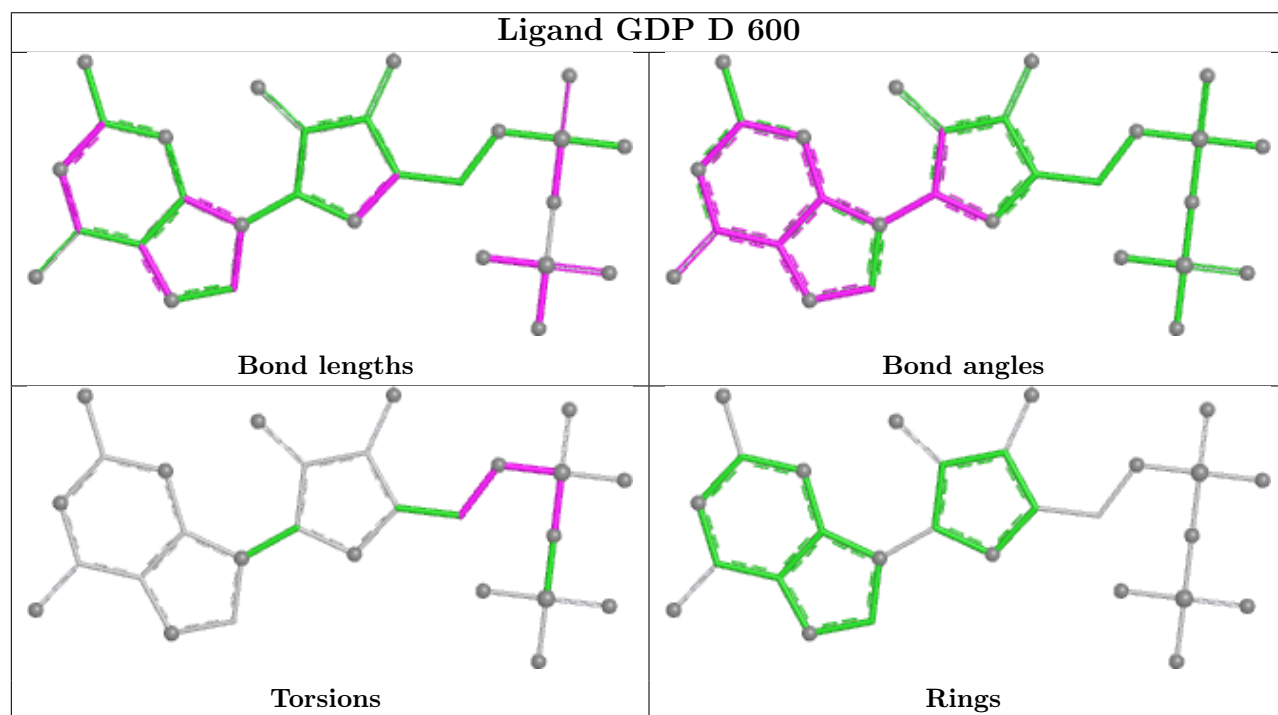
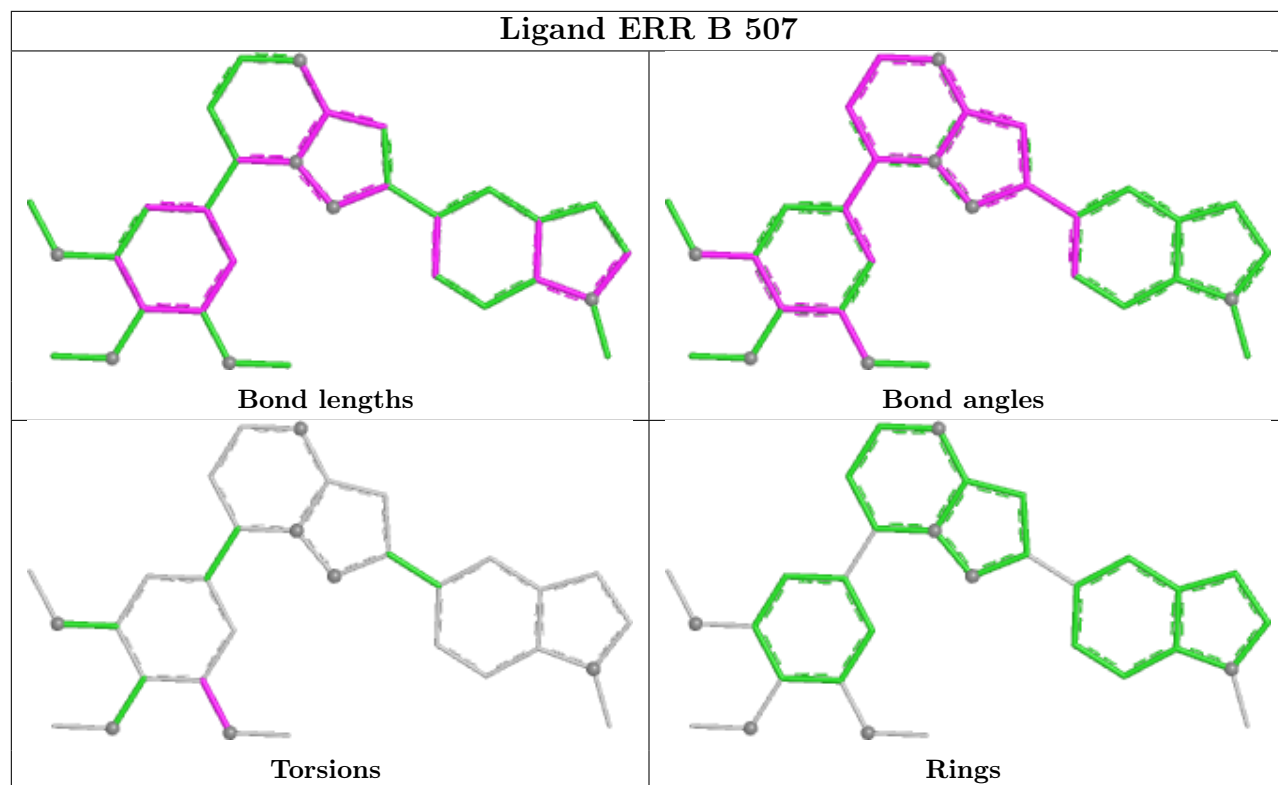
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A

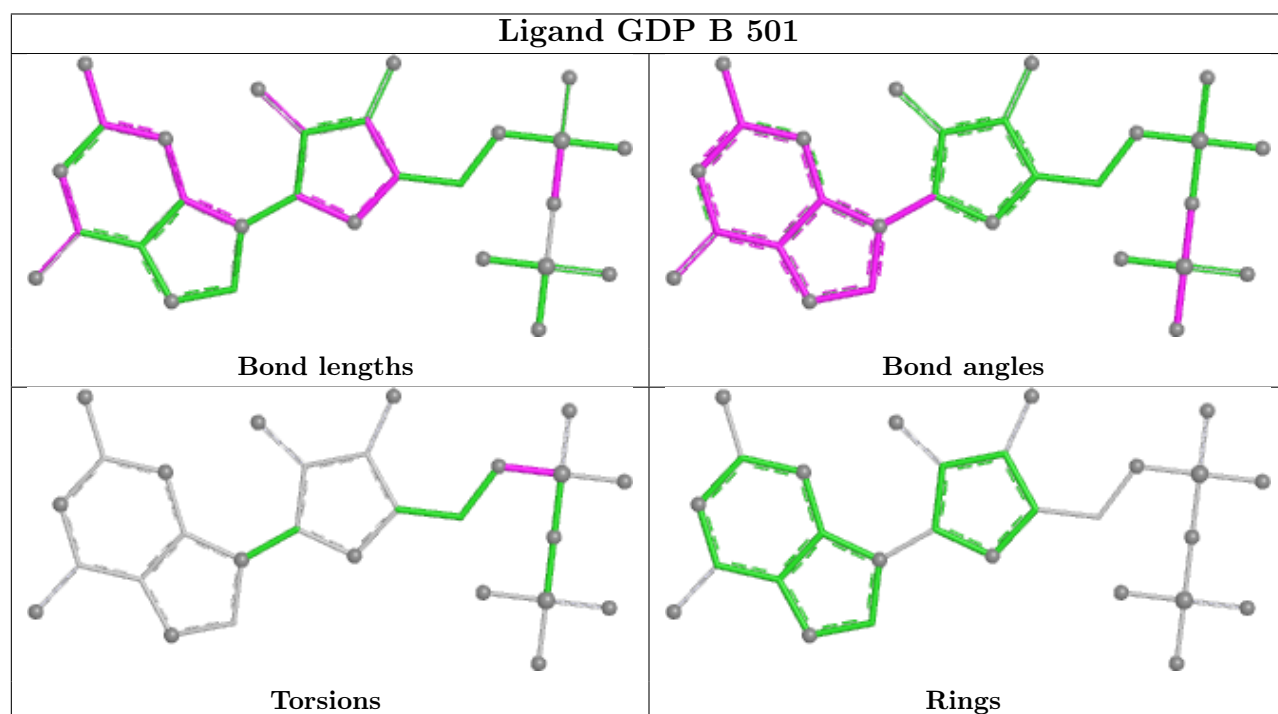
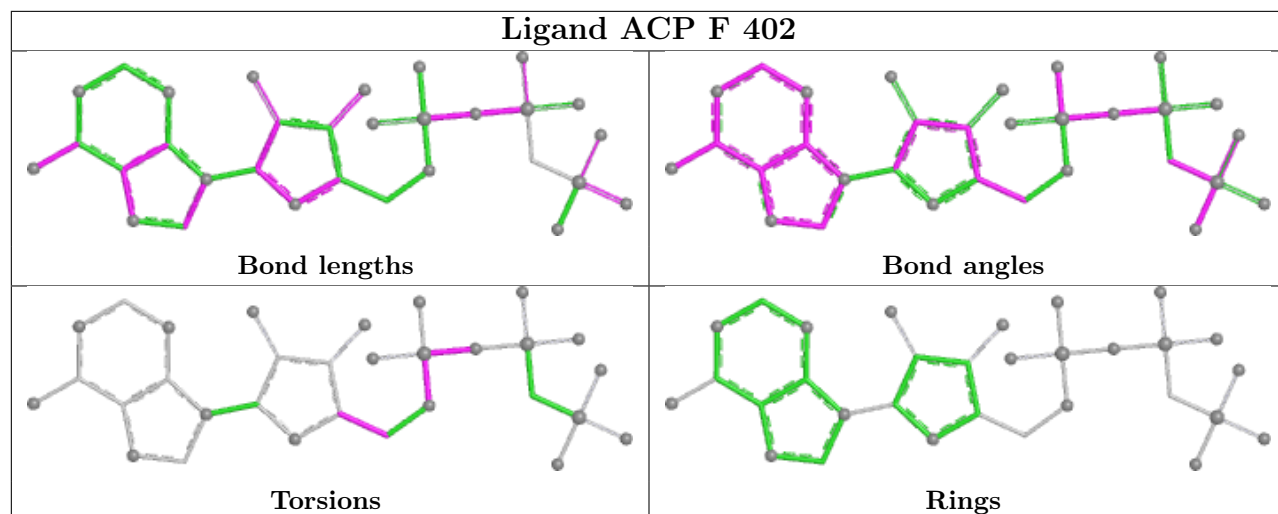
There are no ring outliers.

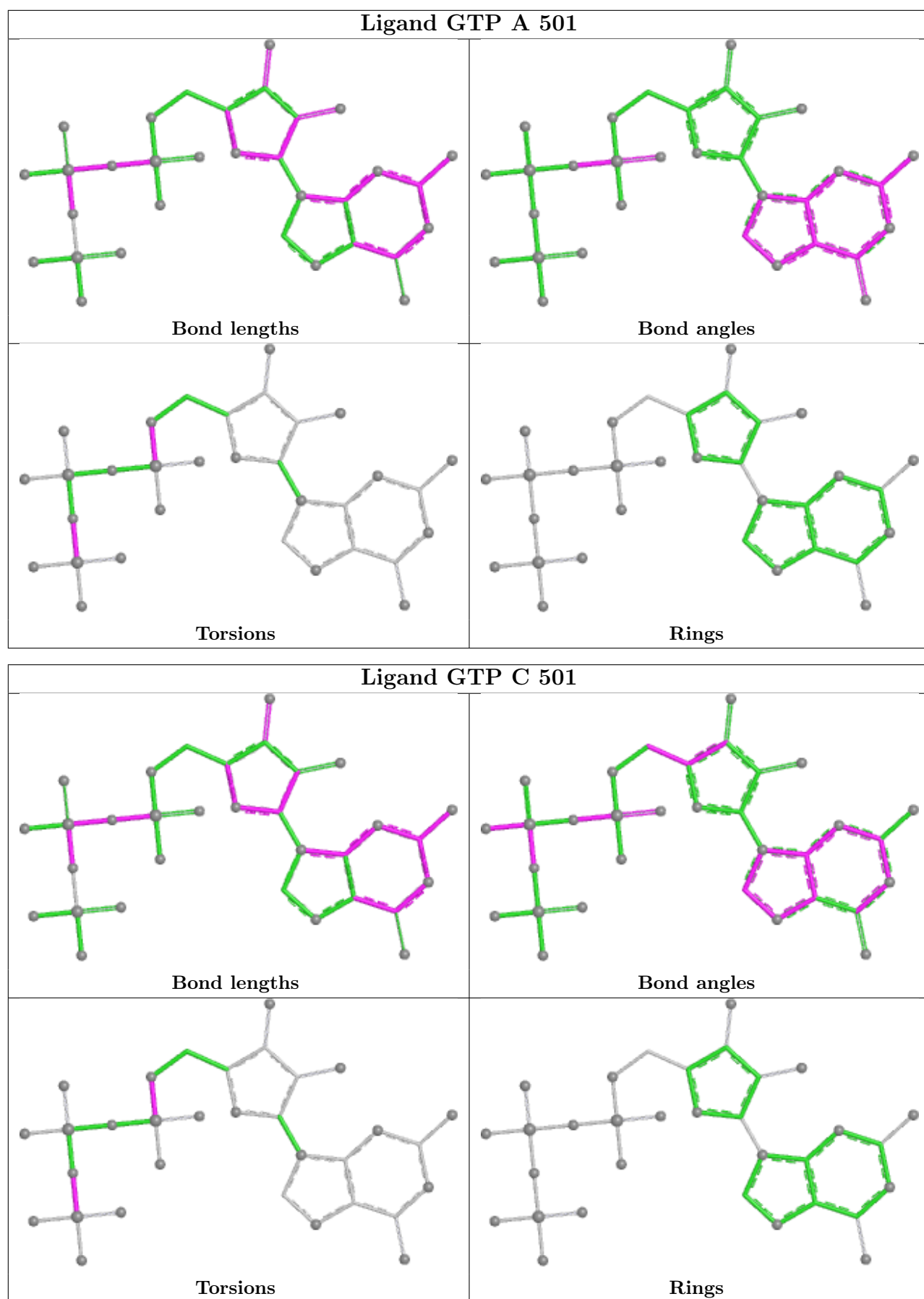
6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	507	ERR	2	0
9	D	600	GDP	3	0
10	B	505	MES	2	0
12	F	402	ACP	2	0
10	B	504	MES	2	0
9	B	501	GDP	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.







## 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	440/450 (97%)	-0.28	3 (0%) 84 85	30, 50, 82, 137	1 (0%)
1	C	440/450 (97%)	-0.50	6 (1%) 73 75	24, 40, 68, 91	3 (0%)
2	B	424/445 (95%)	-0.25	6 (1%) 73 75	24, 49, 82, 155	3 (0%)
2	D	421/445 (94%)	0.24	16 (3%) 44 42	33, 66, 110, 142	9 (2%)
3	E	124/143 (86%)	0.30	4 (3%) 50 49	27, 66, 107, 143	1 (0%)
4	F	351/384 (91%)	0.57	37 (10%) 11 9	31, 77, 154, 174	2 (0%)
All	All	2200/2317 (94%)	-0.05	72 (3%) 49 48	24, 56, 112, 174	19 (0%)

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	220	THR	5.0
2	D	75	MET	4.9
2	D	74	THR	4.9
4	F	166	ALA	4.4
2	B	276	THR	4.3

### 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

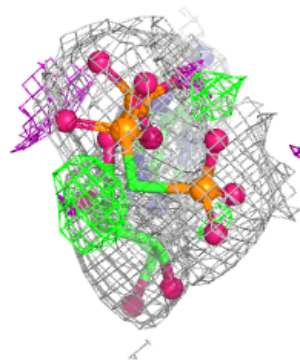
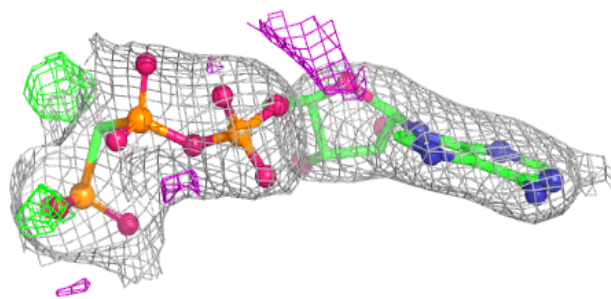
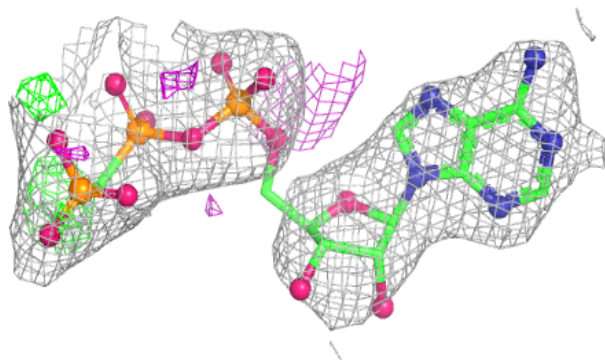
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
7	CA	B	503	1/1	0.76	0.14	97,97,97,97	0
7	CA	A	505	1/1	0.83	0.15	105,105,105,105	0
12	ACP	F	402	31/31	0.86	0.15	73,89,148,153	0
6	MG	F	401	1/1	0.87	0.09	78,78,78,78	0
6	MG	D	601	1/1	0.88	0.11	68,68,68,68	0
6	MG	C	502	1/1	0.90	0.09	39,39,39,39	0
6	MG	B	506	1/1	0.91	0.11	72,72,72,72	0
9	GDP	D	600	28/28	0.92	0.11	49,63,77,83	0
10	MES	B	505	12/12	0.93	0.10	71,80,87,96	0
6	MG	A	502	1/1	0.94	0.15	36,36,36,36	0
10	MES	B	504	12/12	0.94	0.09	40,58,79,93	0
11	ERR	B	507	31/31	0.95	0.09	41,57,72,80	0
8	CL	A	504	1/1	0.96	0.08	76,76,76,76	0
7	CA	A	503	1/1	0.97	0.07	79,79,79,79	0
9	GDP	B	501	28/28	0.98	0.06	29,38,42,43	0
5	GTP	C	501	32/32	0.98	0.07	26,36,41,48	0
5	GTP	A	501	32/32	0.98	0.06	28,41,47,52	0
7	CA	C	503	1/1	0.99	0.03	51,51,51,51	0
6	MG	B	502	1/1	1.00	0.07	43,43,43,43	0

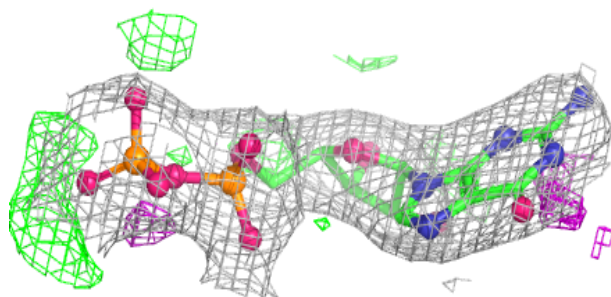
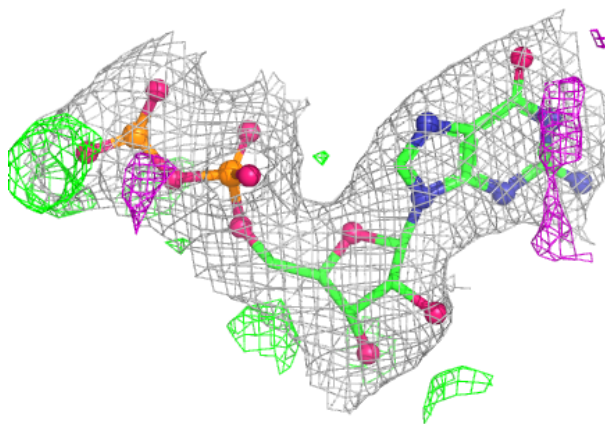
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

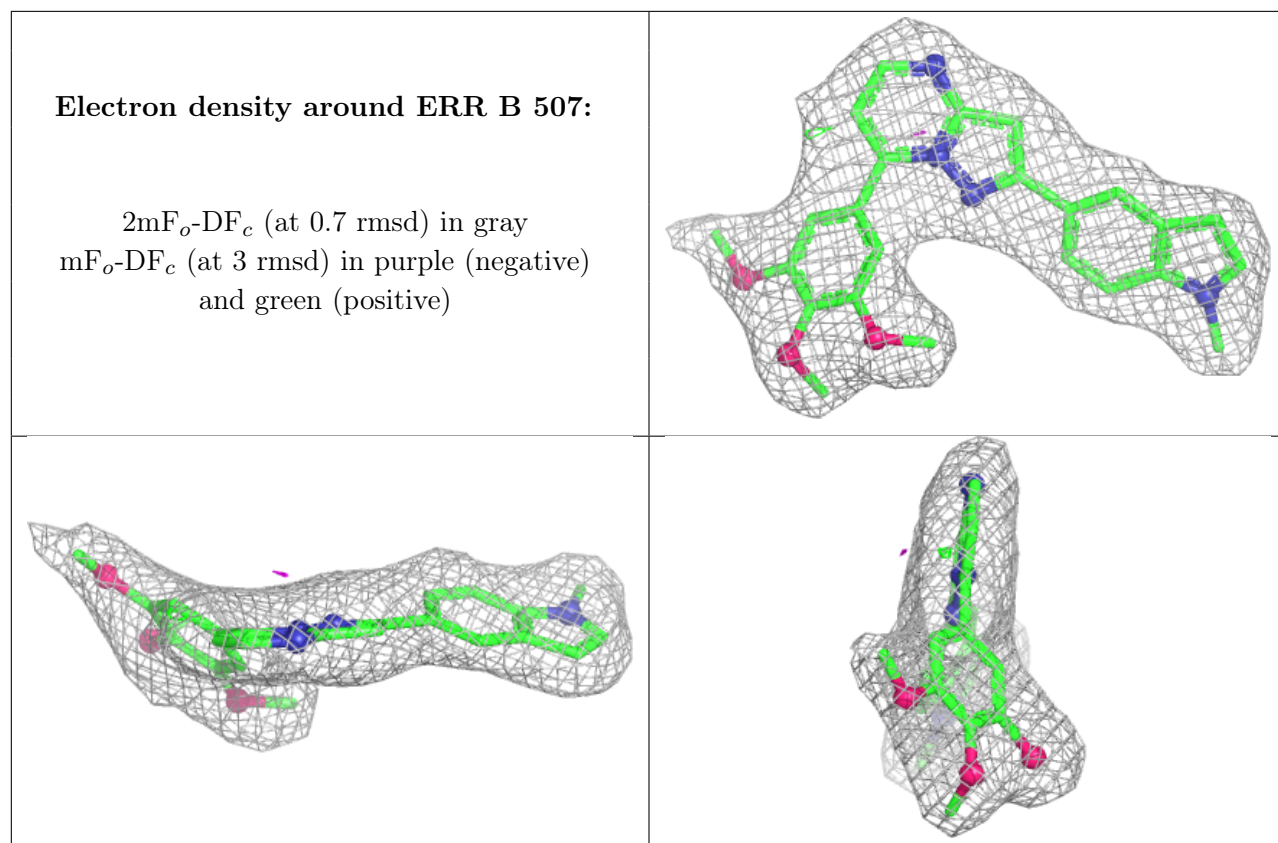
**Electron density around ACP F 402:**

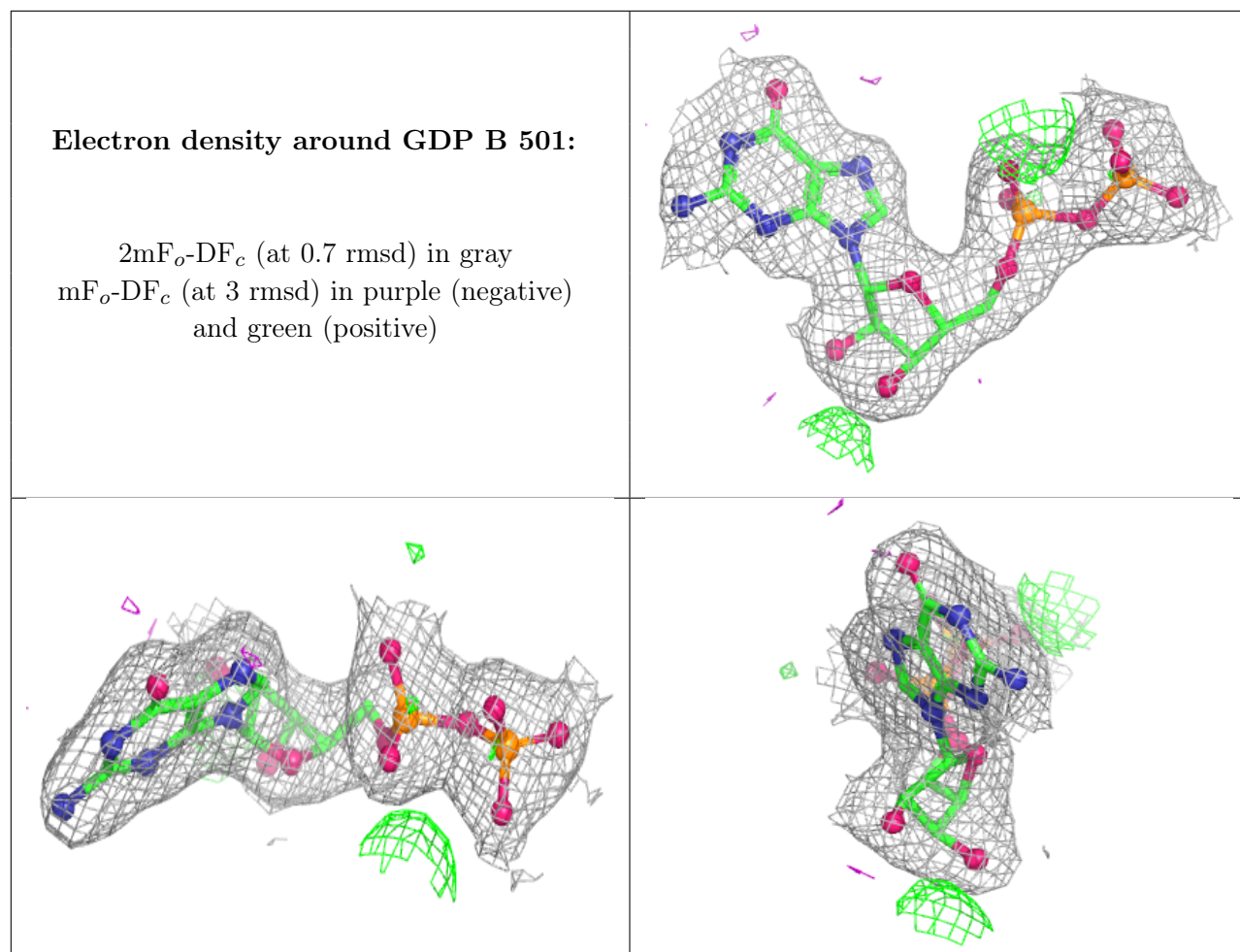
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

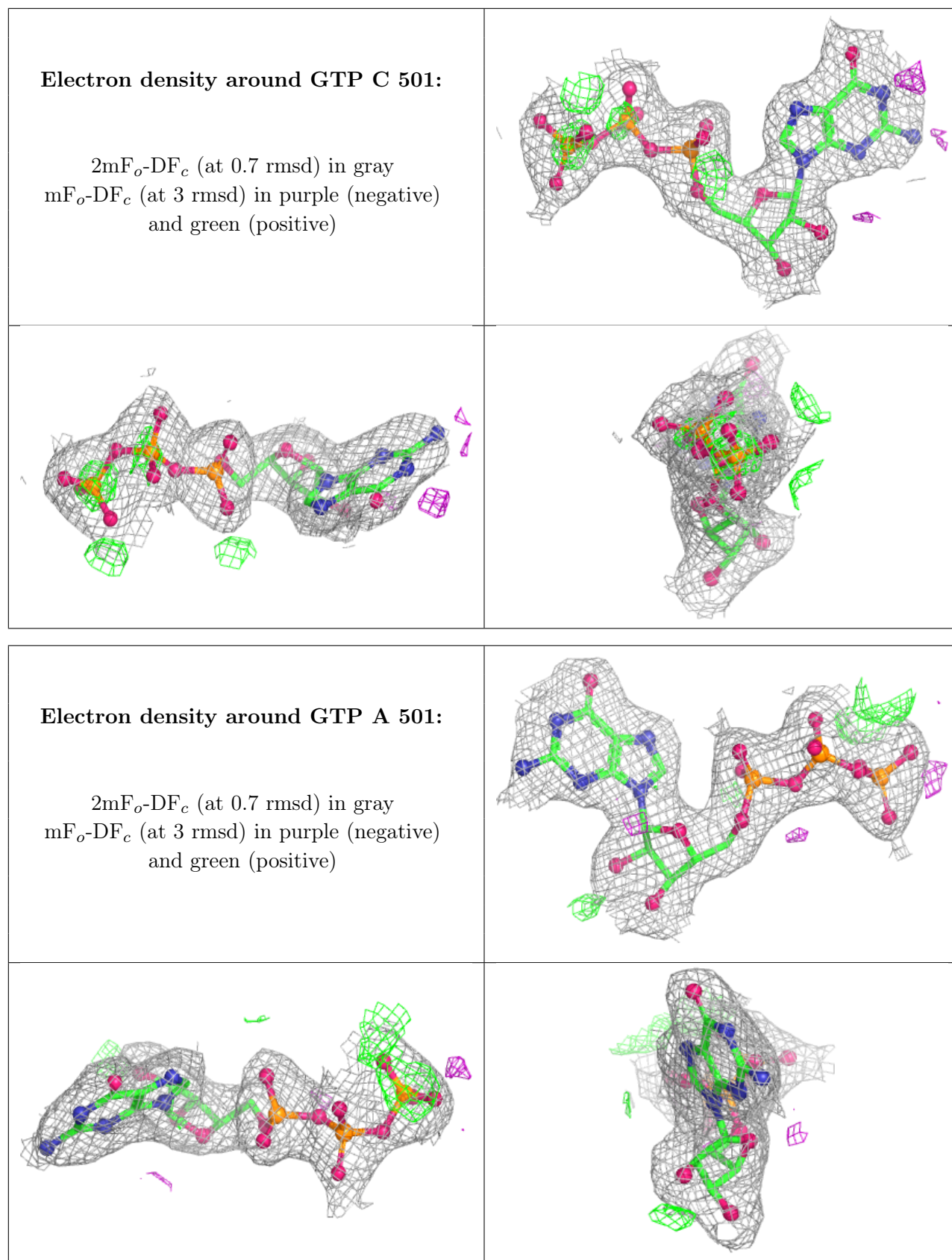
**Electron density around GDP D 600:**

$2mF_o-DF_c$  (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.