



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2022 – 10:18 AM EST

PDB ID : 5SBD  
Title : Tubulin-maytansinoid-5b-complex  
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Deposited on : 2021-07-20  
Resolution : 2.25 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 : 2.27  
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) : 2.27

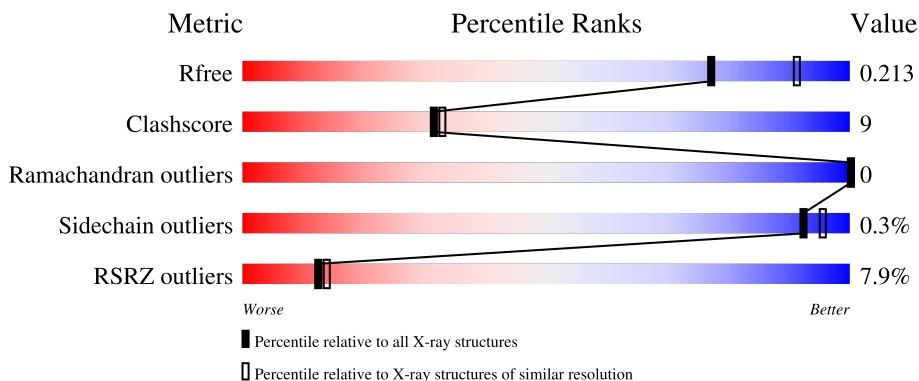
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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.



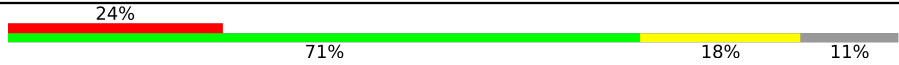
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	 4% 79% 18%
1	C	451	 79% 18%
2	B	445	 5% 71% 24% 5%
2	D	445	 7% 76% 20%
3	E	143	 7% 73% 11% 15%

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Mol	Chain	Length	Quality of chain										
4	F	384	 <p>A horizontal bar chart showing the quality distribution of chain F. The bar is divided into four segments: a red segment (24%), a green segment (71%), a yellow segment (18%), and a grey segment (11%). The percentages are labeled above or below the corresponding segments.</p> <table border="1"><thead><tr><th>Quality Category</th><th>Percentage</th></tr></thead><tbody><tr><td>Red</td><td>24%</td></tr><tr><td>Green</td><td>71%</td></tr><tr><td>Yellow</td><td>18%</td></tr><tr><td>Grey</td><td>11%</td></tr></tbody></table>	Quality Category	Percentage	Red	24%	Green	71%	Yellow	18%	Grey	11%
Quality Category	Percentage												
Red	24%												
Green	71%												
Yellow	18%												
Grey	11%												

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 18541 atoms, of which 13 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	437	Total	C	N	O	S	0	3	0
			3434	2172	584	654	24			
1	C	440	Total	C	N	O	S	0	5	0
			3467	2194	589	661	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	423	Total	C	N	O	S	0	1	0
			3345	2102	572	644	27			
2	D	426	Total	C	N	O	S	0	0	0
			3343	2098	570	648	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	121	Total	C	N	O	S	0	1	0
			1008	622	182	198	6			

There are 2 discrepancies between the modelled and reference sequences:

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

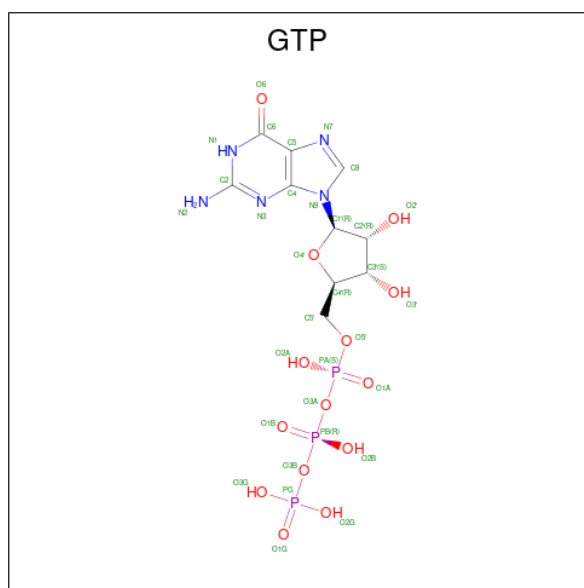
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	341	Total	C	N	O	S	0	3	0
			2815	1806	481	513	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 (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



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 (three-letter code: MG) (formula: Mg).

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

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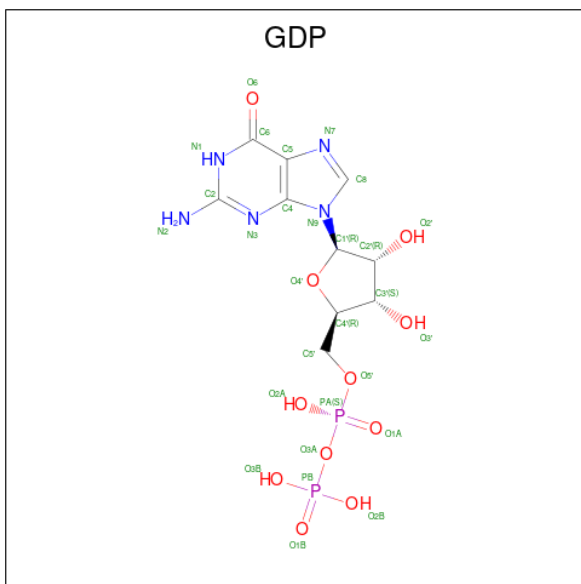
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

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

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



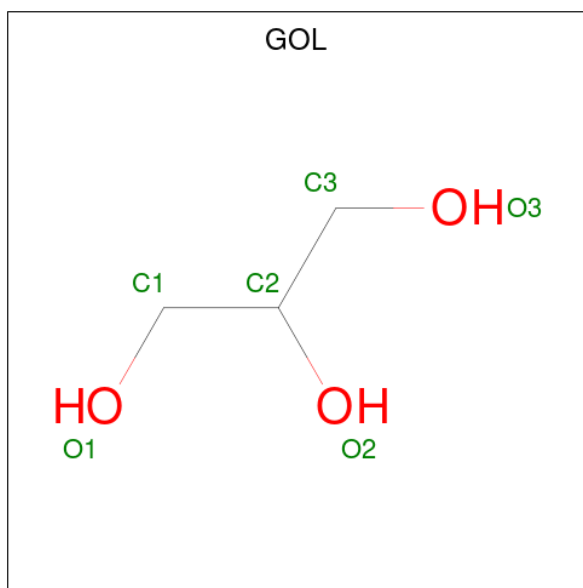
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
8	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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



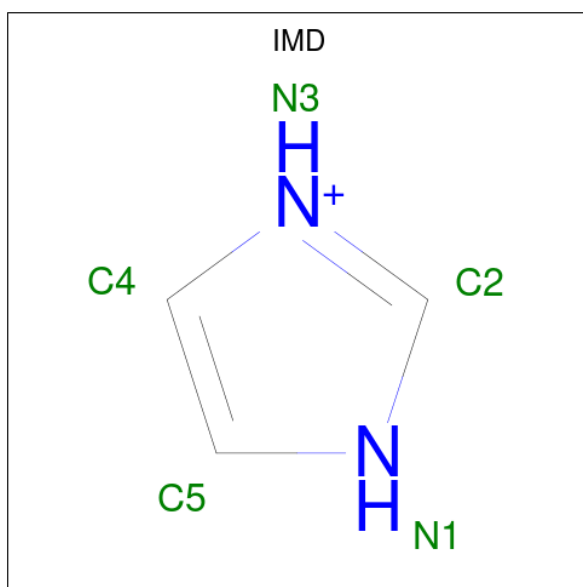
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
9	B	1	12	6	1	4	1	0	0

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



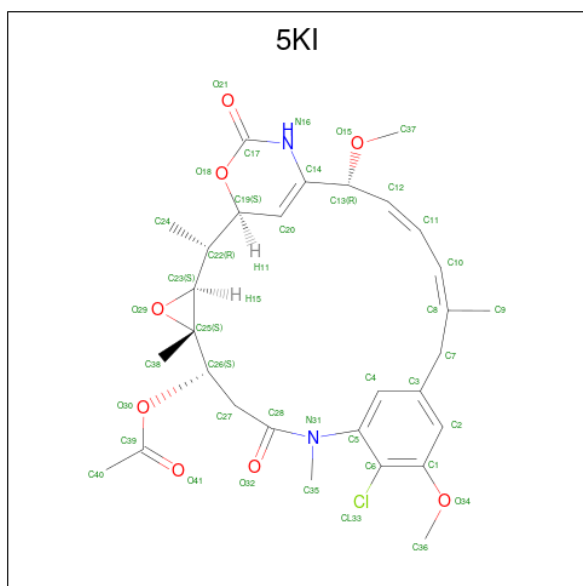
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
10	B	1	14	3	8	3	0	0

- Molecule 11 is IMIDAZOLE (three-letter code: IMD) (formula: C<sub>3</sub>H<sub>5</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	N		
11	C	1	10	3	5	2	0	0

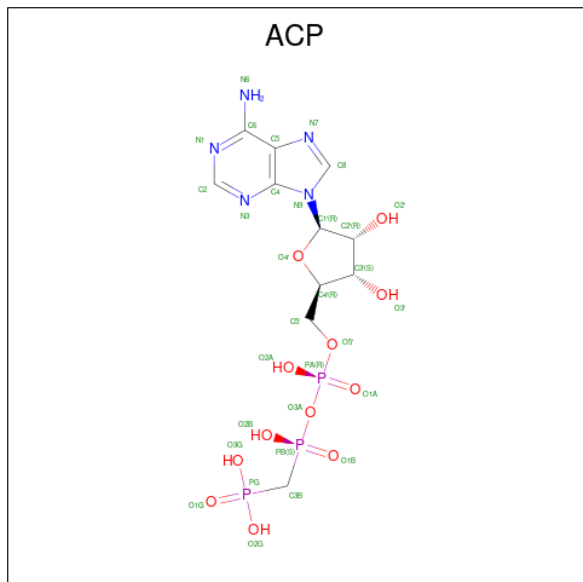
- Molecule 12 is (1S,2R,3S,5S,6S,16E,18E,20R)-11-chloro-12,20-dimethoxy-2,5,9,16-tetramethyl-8,23-dioxo-4,24-dioxa-9,22-diazatetracyclo[19.3.1.1 10,14 .0 3,5 ]hexacosa-10(26),11,13,16,18,21(25)-hexaen-6-yl acetate (three-letter code: 5KI) (formula: C<sub>30</sub>H<sub>37</sub>ClN<sub>2</sub>O<sub>8</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
12	D	1	41	30	1	2	8	0	0



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



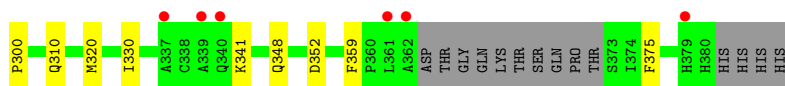
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
13	F	1	31	11	5	12	3	0	0

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	158	Total	O	0	0
			158	158		
14	B	196	Total	O	0	0
			196	196		
14	C	310	Total	O	0	0
			310	310		
14	D	127	Total	O	0	0
			127	127		
14	E	39	Total	O	0	0
			39	39		
14	F	62	Total	O	0	0
			62	62		







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.08Å 158.60Å 180.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.58 – 2.25 49.58 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.58-2.25) 99.6 (49.58-2.25)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 2.25Å)	Xtrriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, $R_{free}$	0.179 , 0.214 0.177 , 0.213	Depositor DCC
$R_{free}$ test set	7151 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.6	Xtrriage
Anisotropy	0.208	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 42.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18541	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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, GTP, GDP, MES, CA, ACP, IMD, GOL, 5KI

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.24	0/3512	0.46	0/4767
1	C	0.24	0/3555	0.46	0/4828
2	B	0.24	0/3419	0.47	0/4629
2	D	0.24	0/3416	0.46	0/4626
3	E	0.23	0/1016	0.41	0/1347
4	F	0.24	0/2878	0.45	0/3886
All	All	0.24	0/17796	0.46	0/24083

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3434	0	3343	63	0
1	C	3467	0	3377	56	0
2	B	3345	0	3227	75	0
2	D	3343	0	3222	63	0
3	E	1008	0	1026	15	0
4	F	2815	0	2781	47	0
5	A	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	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	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	2	0
9	B	12	0	12	1	0
10	B	6	8	8	1	0
11	C	5	5	5	0	0
12	D	41	0	0	1	0
13	F	31	0	14	0	0
14	A	158	0	0	5	0
14	B	196	0	0	12	0
14	C	310	0	0	5	0
14	D	127	0	0	7	1
14	E	39	0	0	1	0
14	F	62	0	0	4	1
All	All	18528	13	17063	311	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 311 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:335:ILE:HG23	1:A:339:ARG:HG3	1.61	0.83
1:A:71:GLU:OE2	1:A:73:THR:OG1	1.95	0.82
3:E:6:MET:HG3	3:E:24:LEU:HD23	1.63	0.80
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.66	0.77
4:F:102:PRO:HB3	4:F:173:ILE:HG22	1.72	0.72

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:D:606:HOH:O	14:F:555:HOH:O[3_545]	2.17	0.03

### 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	438/451 (97%)	431 (98%)	7 (2%)	0	100	100
1	C	443/451 (98%)	432 (98%)	11 (2%)	0	100	100
2	B	420/445 (94%)	416 (99%)	4 (1%)	0	100	100
2	D	422/445 (95%)	414 (98%)	8 (2%)	0	100	100
3	E	118/143 (82%)	118 (100%)	0	0	100	100
4	F	334/384 (87%)	327 (98%)	7 (2%)	0	100	100
All	All	2175/2319 (94%)	2138 (98%)	37 (2%)	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	371/379 (98%)	370 (100%)	1 (0%)	92	95
1	C	376/379 (99%)	374 (100%)	2 (0%)	88	92
2	B	368/383 (96%)	367 (100%)	1 (0%)	92	95
2	D	368/383 (96%)	367 (100%)	1 (0%)	92	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	110/127 (87%)	110 (100%)	0	100	100
4	F	308/342 (90%)	308 (100%)	0	100	100
All	All	1901/1993 (95%)	1896 (100%)	5 (0%)	92	95

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

Mol	Chain	Res	Type
1	A	71	GLU
2	B	139	HIS
1	C	71	GLU
1	C	284	GLU
2	D	139	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	167	ASN
2	D	294	GLN
4	F	348	GLN
1	C	285	GLN
1	A	301	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 9 are monoatomic - leaving 9 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
13	ACP	F	401	6	27,33,33	1.99	7 (25%)	32,52,52	1.27	4 (12%)
10	GOL	B	505	-	5,5,5	0.79	0	5,5,5	0.82	0
11	IMD	C	504	-	3,5,5	0.40	0	4,5,5	0.59	0
12	5KI	D	503	-	43,44,44	1.36	5 (11%)	46,65,65	1.85	11 (23%)
8	GDP	D	501	6	24,30,30	1.19	2 (8%)	31,47,47	1.94	7 (22%)
9	MES	B	504	-	12,12,12	2.24	1 (8%)	14,16,16	1.99	4 (28%)
8	GDP	B	501	6	24,30,30	1.17	2 (8%)	31,47,47	1.90	7 (22%)
5	GTP	C	501	6	26,34,34	0.95	1 (3%)	33,54,54	1.71	6 (18%)
5	GTP	A	501	6	26,34,34	0.97	1 (3%)	33,54,54	1.76	7 (21%)

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
13	ACP	F	401	6	-	6/15/38/38	0/3/3/3
10	GOL	B	505	-	-	2/4/4/4	-
11	IMD	C	504	-	-	-	0/1/1/1
12	5KI	D	503	-	-	12/44/68/68	0/2/4/4
8	GDP	D	501	6	-	3/12/32/32	0/3/3/3
9	MES	B	504	-	-	5/6/14/14	0/1/1/1
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3
5	GTP	C	501	6	-	8/18/38/38	0/3/3/3
5	GTP	A	501	6	-	9/18/38/38	0/3/3/3

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-7.48	1.66	1.77
13	F	401	ACP	PG-O1G	5.44	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	501	GDP	C5-C6	4.22	1.48	1.41
8	B	501	GDP	C5-C6	4.15	1.48	1.41
13	F	401	ACP	PB-O1B	4.12	1.61	1.51

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	503	5KI	C25-O29-C23	6.06	64.43	60.79
5	A	501	GTP	N3-C2-N1	-5.33	120.11	127.22
5	C	501	GTP	N3-C2-N1	-5.23	120.25	127.22
12	D	503	5KI	C6-C5-N31	5.16	126.00	120.71
8	D	501	GDP	C2-N3-C4	4.86	120.91	115.36

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

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

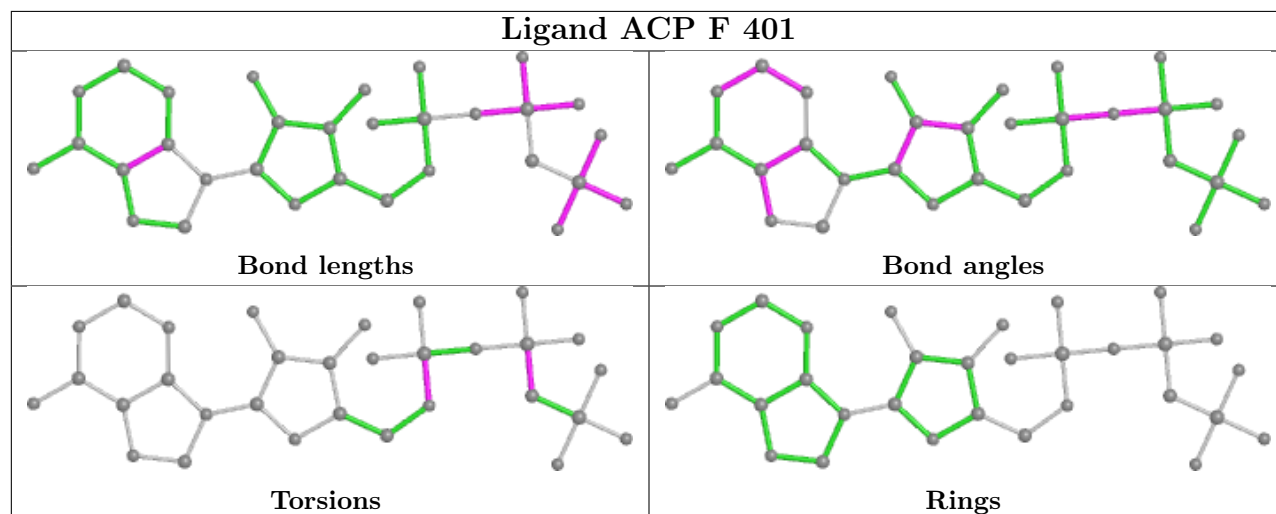
There are no ring outliers.

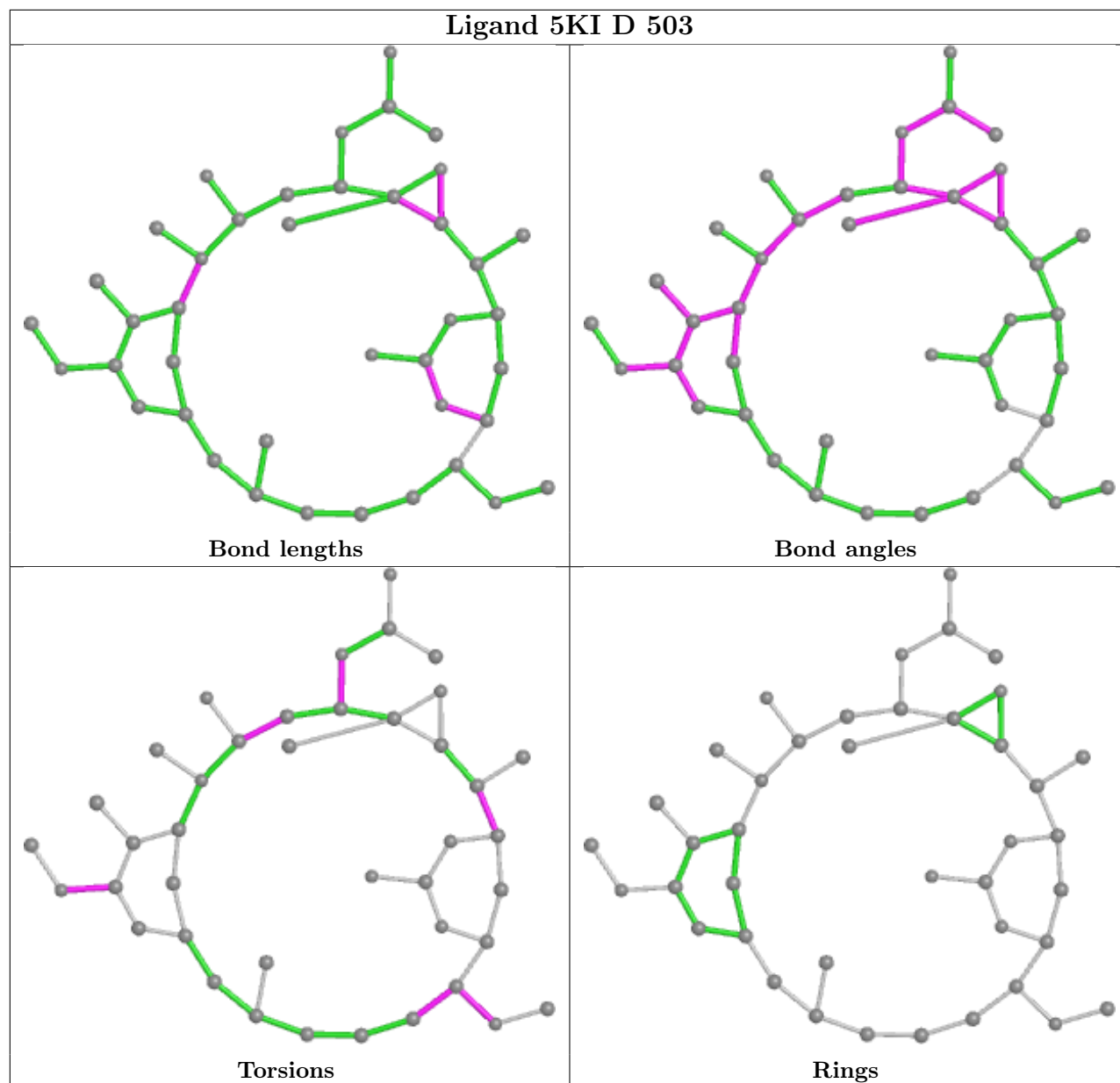
5 monomers are involved in 6 short contacts:

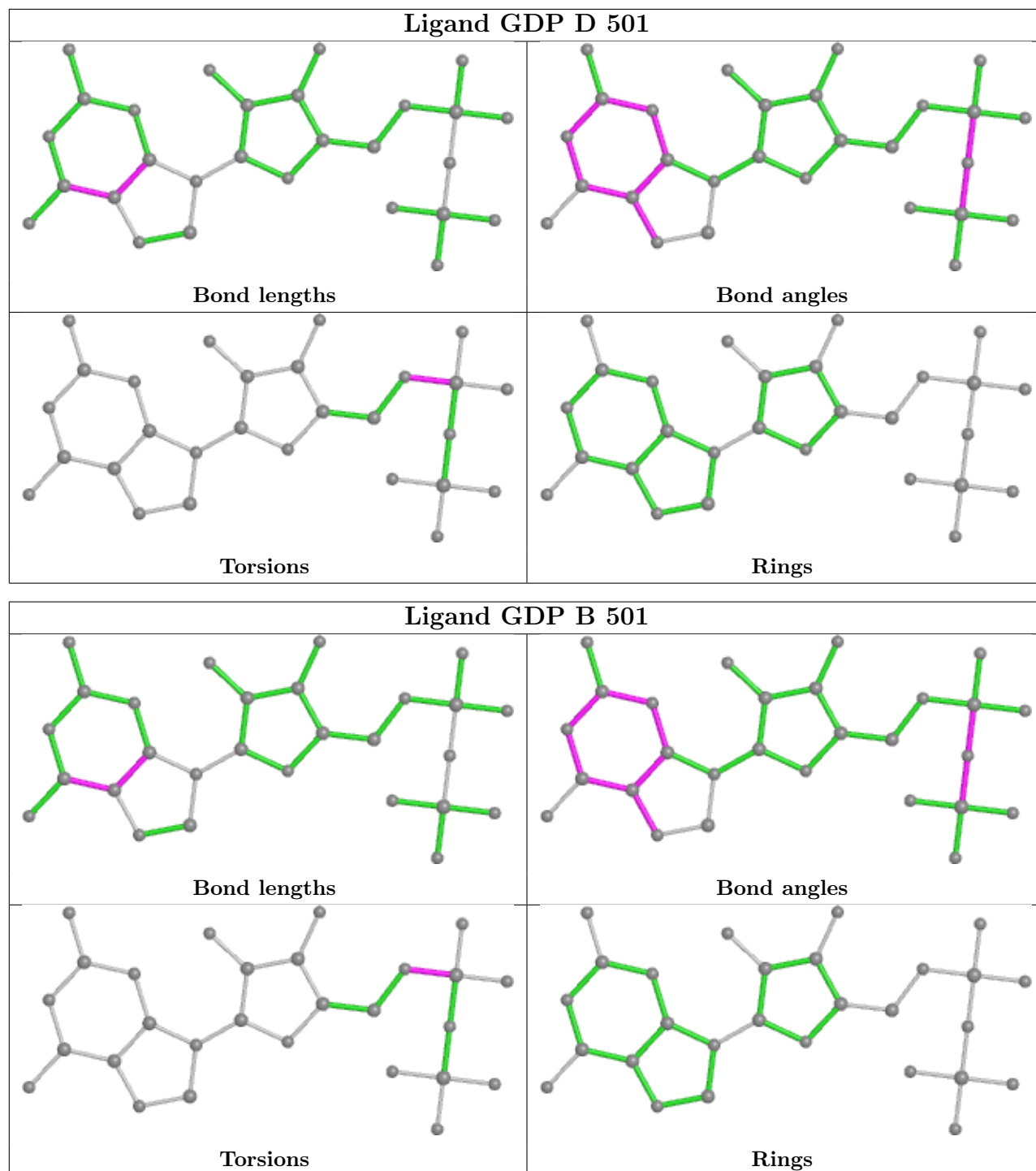
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	505	GOL	1	0
12	D	503	5KI	1	0
8	D	501	GDP	2	0
9	B	504	MES	1	0
5	A	501	GTP	1	0

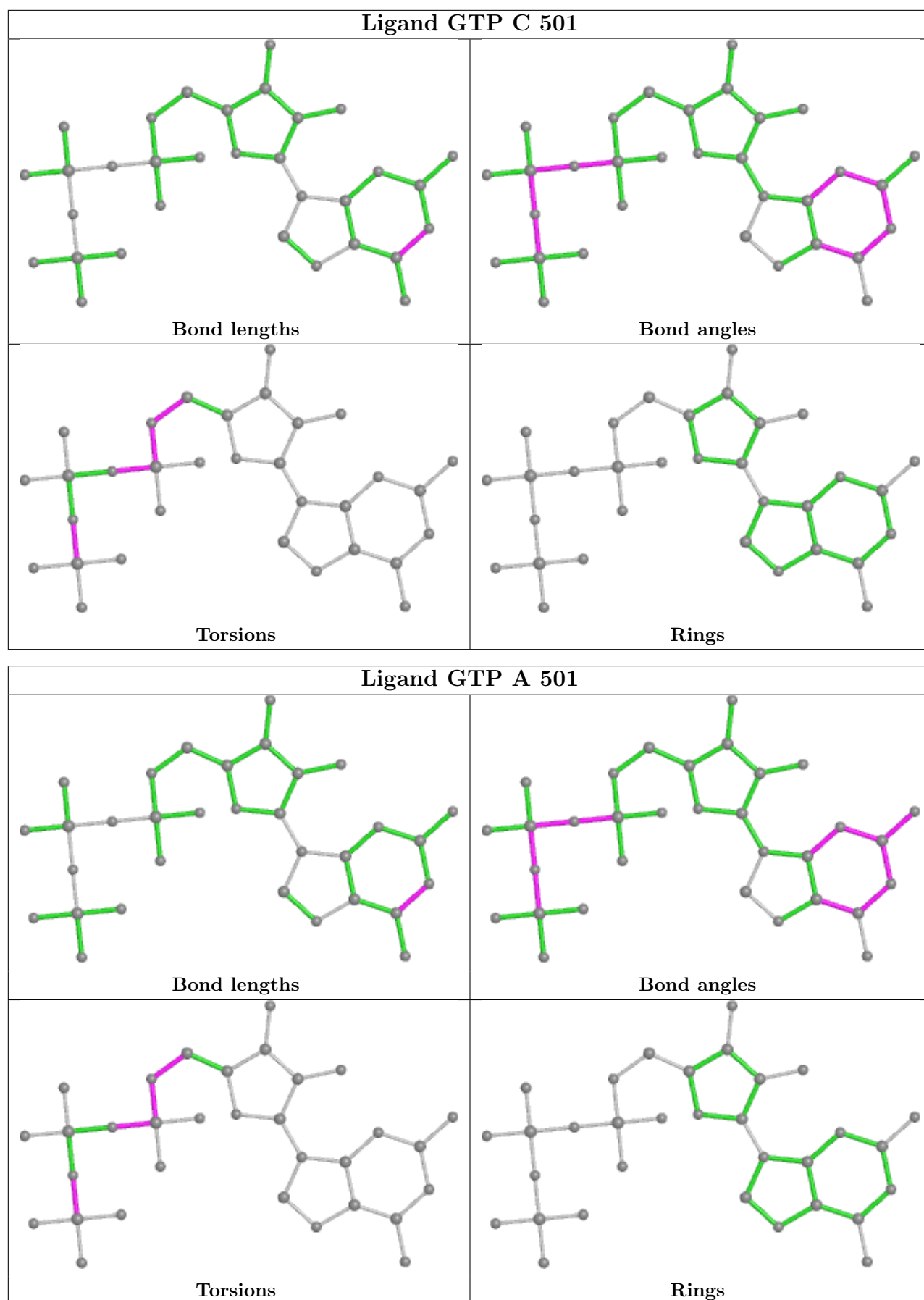
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 [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	437/451 (96%)	0.20	18 (4%) 37 40	32, 50, 79, 120	0
1	C	440/451 (97%)	-0.14	1 (0%) 95 96	27, 39, 63, 105	0
2	B	423/445 (95%)	0.16	23 (5%) 25 28	29, 48, 80, 114	0
2	D	426/445 (95%)	0.34	29 (6%) 17 18	32, 57, 88, 114	0
3	E	121/143 (84%)	0.39	10 (8%) 11 12	43, 63, 92, 105	0
4	F	341/384 (88%)	1.23	92 (26%) 0 0	44, 71, 125, 152	0
All	All	2188/2319 (94%)	0.32	173 (7%) 12 14	27, 52, 96, 152	0

The worst 5 of 173 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	251	LYS	8.1
4	F	250	SER	8.0
4	F	249	TYR	7.1
4	F	173	ILE	7.0
4	F	170	LEU	7.0

### 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 monosaccharides in this entry.

## 6.4 Ligands

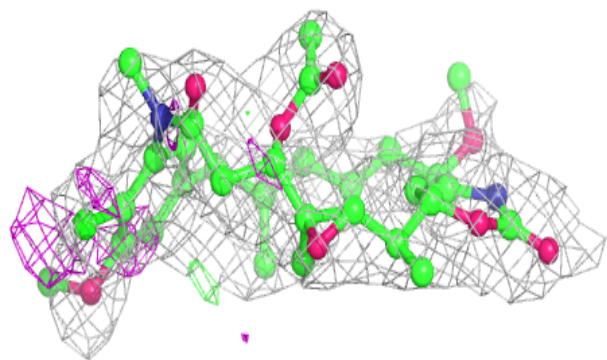
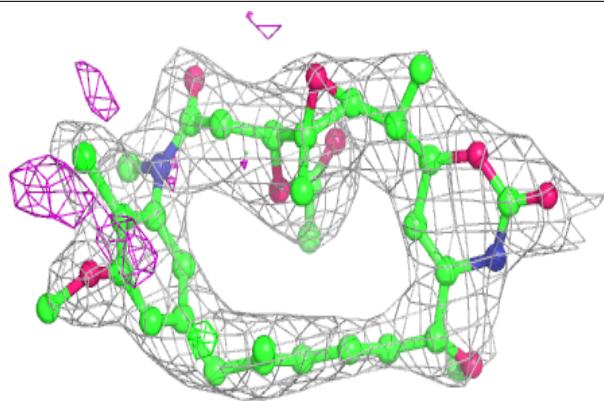
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
10	GOL	B	505	6/6	0.69	0.21	67,82,90,99	0
7	CA	B	503	1/1	0.80	0.24	95,95,95,95	0
12	5KI	D	503	41/41	0.85	0.28	55,72,83,89	0
11	IMD	C	504	5/5	0.88	0.14	54,64,76,80	0
7	CA	E	201	1/1	0.90	0.04	92,92,92,92	0
6	MG	D	502	1/1	0.92	0.15	65,65,65,65	0
13	ACP	F	401	31/31	0.92	0.17	64,82,96,106	0
6	MG	F	402	1/1	0.94	0.04	74,74,74,74	0
7	CA	A	503	1/1	0.95	0.06	60,60,60,60	0
8	GDP	D	501	28/28	0.96	0.12	46,54,64,79	0
7	CA	C	503	1/1	0.97	0.05	49,49,49,49	0
9	MES	B	504	12/12	0.97	0.12	40,51,60,70	0
5	GTP	A	501	32/32	0.97	0.21	22,34,42,45	0
5	GTP	C	501	32/32	0.98	0.15	26,31,37,39	0
6	MG	A	502	1/1	0.98	0.18	34,34,34,34	0
8	GDP	B	501	28/28	0.98	0.20	27,34,44,50	0
6	MG	C	502	1/1	0.99	0.14	29,29,29,29	0
6	MG	B	502	1/1	0.99	0.21	26,26,26,26	0

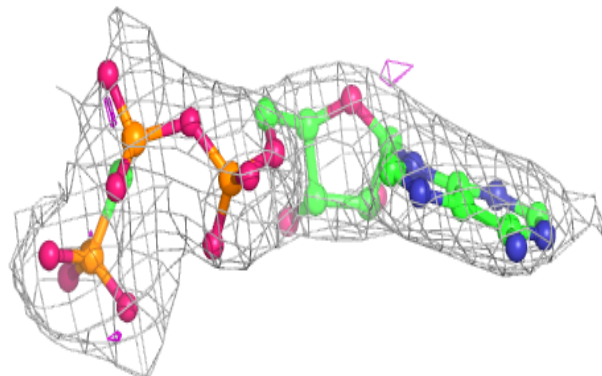
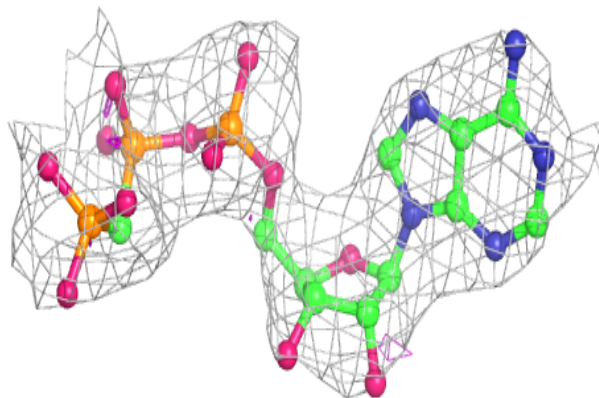
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 5KI 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)

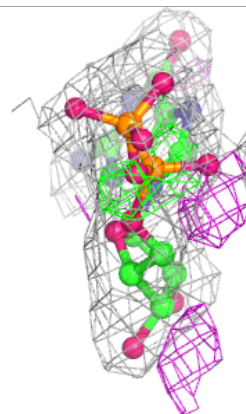
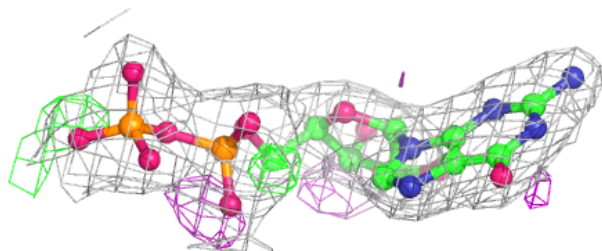
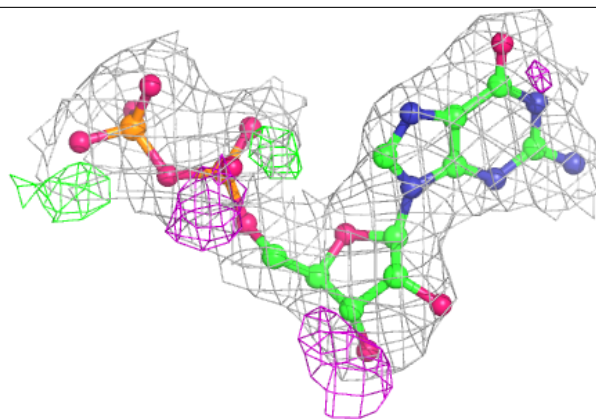
**Electron density around ACP F 401:**

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

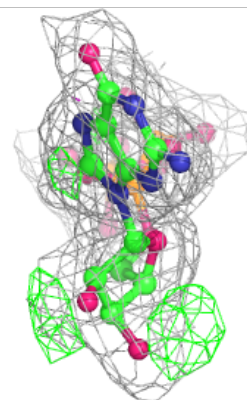
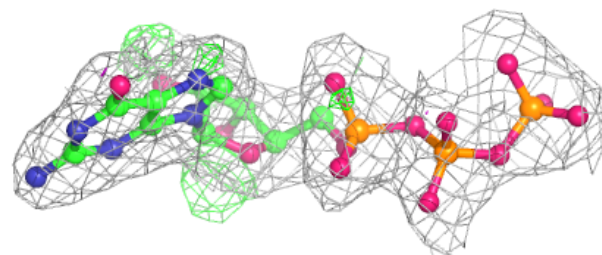
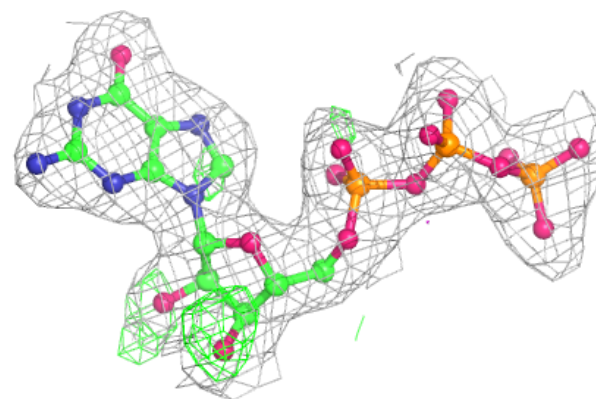


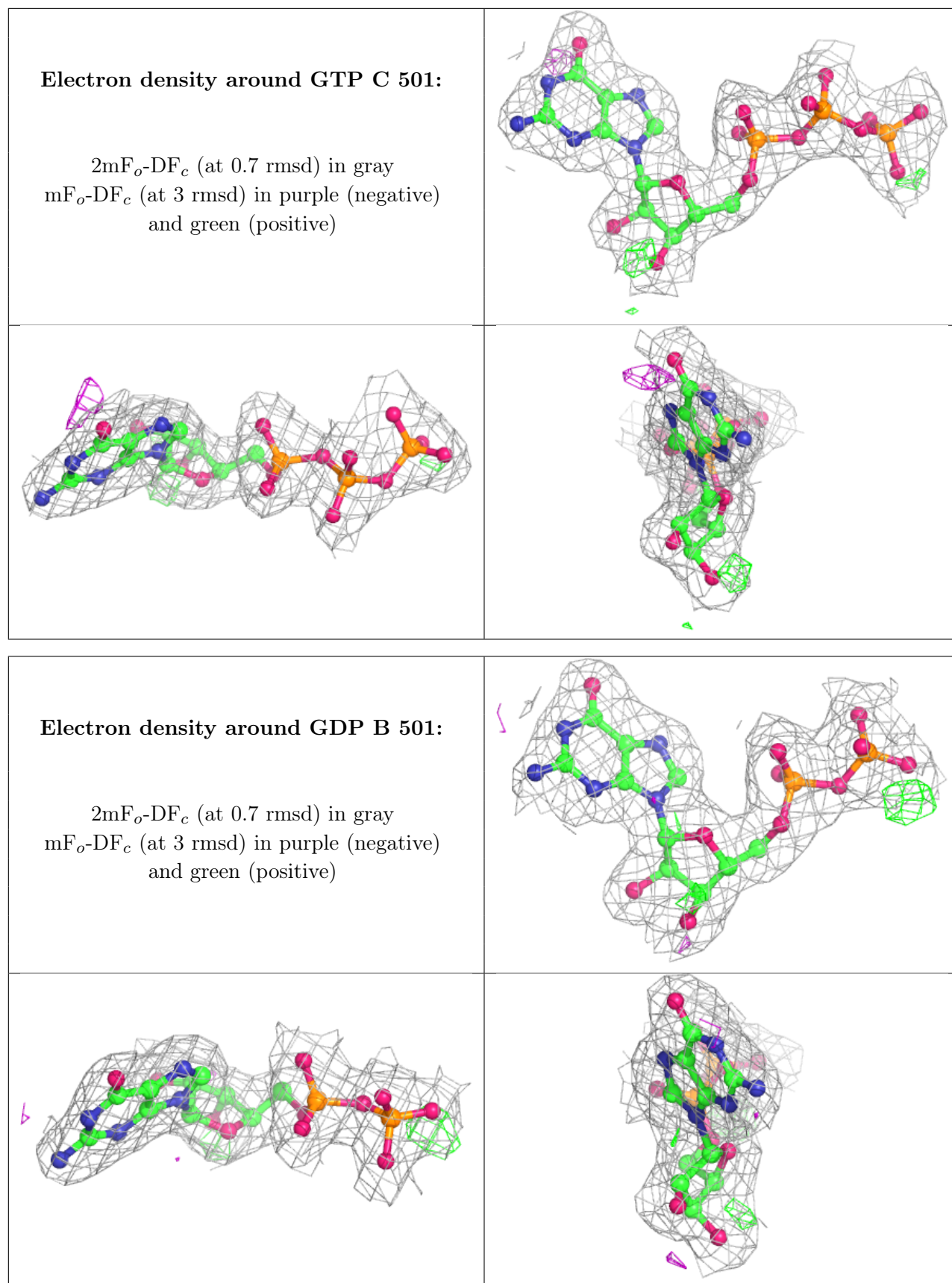
**Electron density around GDP D 501:**

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

**Electron density around 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.