



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2024 – 06:41 PM JST

PDB ID : 5H74  
Title : Crystal structure of T2R-TTL-14b complex  
Authors : Wang, Y.; Yu, Y.; Chen, Q.; Yang, J.  
Deposited on : 2016-11-17  
Resolution : 2.60 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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

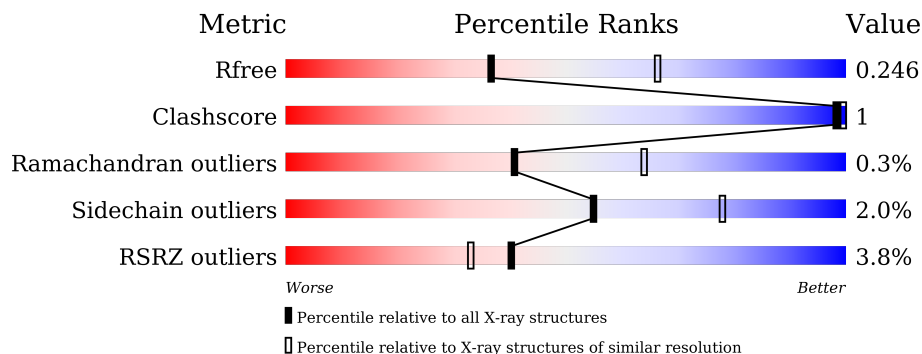
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	 2% 94%
1	C	450	 94%
2	B	445	 94%
2	D	445	 4% 91% 5%
3	E	143	 3% 82% 15%
4	F	384	 12% 84% 13%

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
9	MES	C	504	-	-	-	X

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 17862 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	437	Total	C	N	O	S	0	0	0
			3416	2163	581	650	22			
1	C	440	Total	C	N	O	S	0	0	0
			3437	2175	584	656	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	428	Total	C	N	O	S	0	0	0
			3369	2115	577	650	27			
2	D	424	Total	C	N	O	S	0	0	0
			3333	2093	568	645	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	0	0
			1000	617	181	197	5			

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

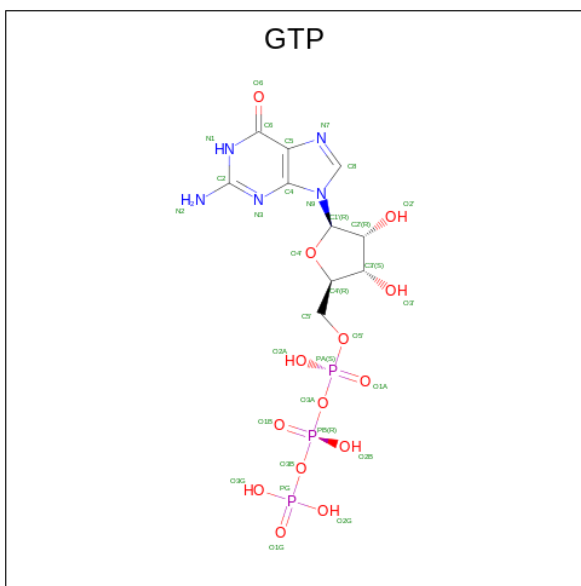
- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	334	Total	C	N	O	S	0	0	0
			2744	1761	470	499	14			

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		
5	D	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
			Total	Mg		
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		

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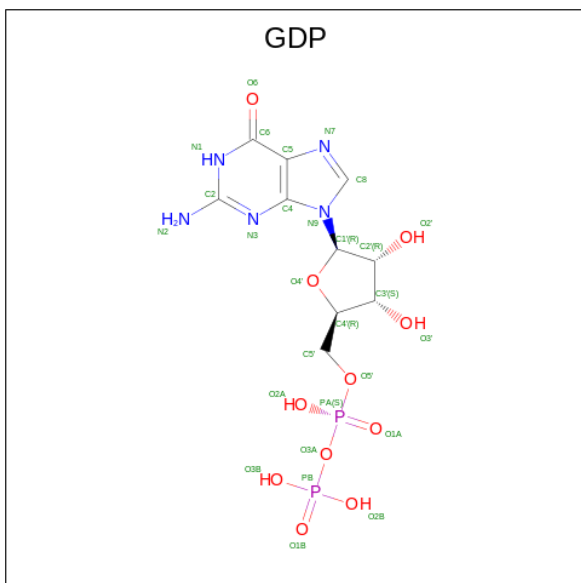
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mg	0	0
			1	1		

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

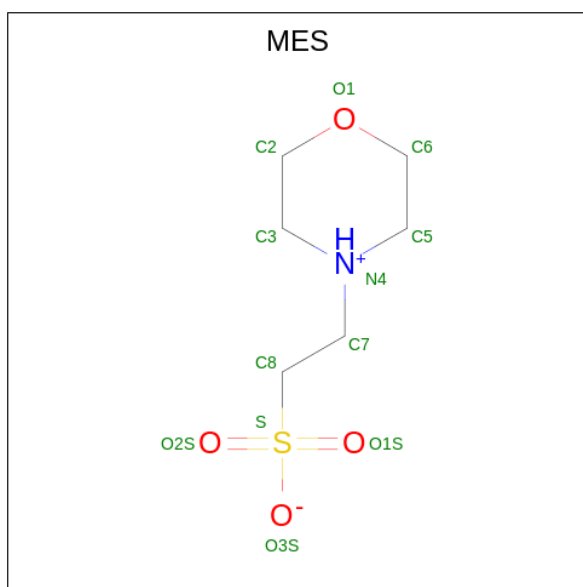
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- 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>).



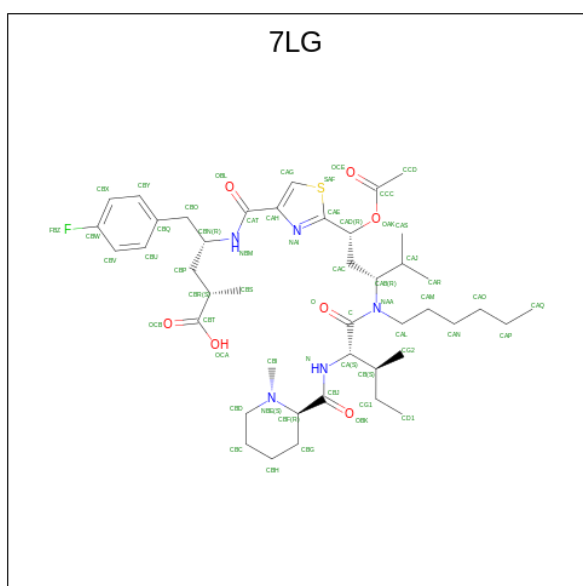
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- 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).



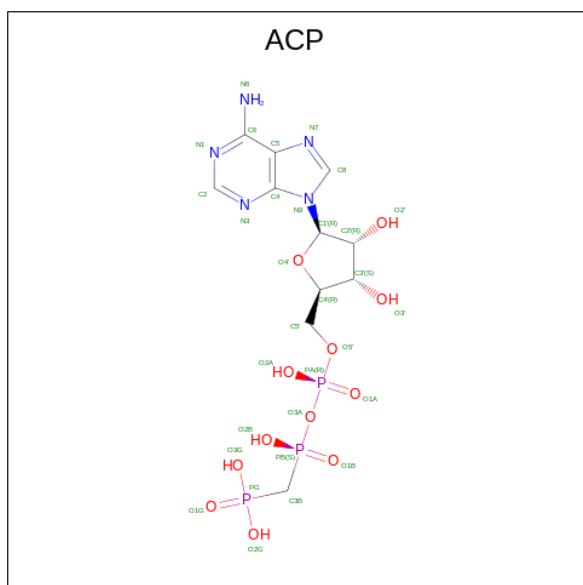
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	S			
9	B	1	Total	12	6	1	4	1	0	0
9	B	1	Total	12	6	1	4	1	0	0
9	C	1	Total	12	6	1	4	1	0	0

- Molecule 10 is (2 {S},4 {R})-4-[[2-[(1 {R},3 {R})-1-acetyloxy-3-[hexyl-[(2 {S},3 {S})-3-methyl-2-[[[(2 {R})-1-methylpiperidin-2-yl]carbonylamino]pentanoyl]amino]-4-methyl-pentyl]-1,3-thiazol-4-yl]carbonylamino]-5-(4-fluorophenyl)-2-methyl-pentanoic acid (three-letter code: 7LG) (formula: C<sub>43</sub>H<sub>66</sub>FN<sub>5</sub>O<sub>7</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	N	O			S
10	B	1	57	43	1	5	7	1	0	0
10	D	1	57	43	1	5	7	1	0	0

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



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

- Molecule 12 is water.

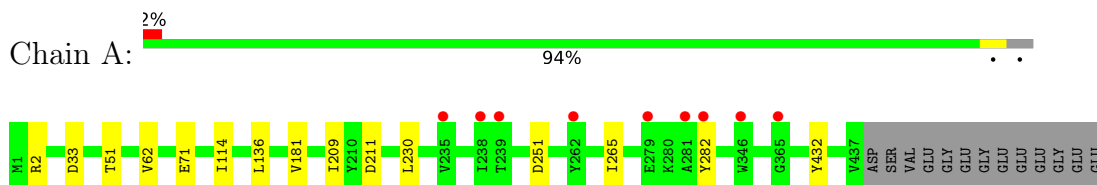
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	64	Total	O	0	0
			64	64		
12	B	67	Total	O	0	0
			67	67		
12	C	87	Total	O	0	0
			87	87		
12	D	12	Total	O	0	0
			12	12		
12	E	6	Total	O	0	0
			6	6		
12	F	16	Total	O	0	0
			16	16		



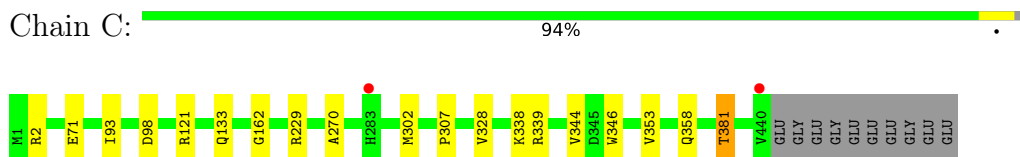
### 3 Residue-property plots [i](#)

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

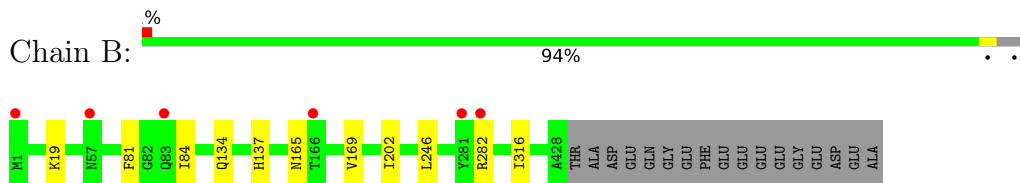
- Molecule 1: Tubulin alpha-1B chain



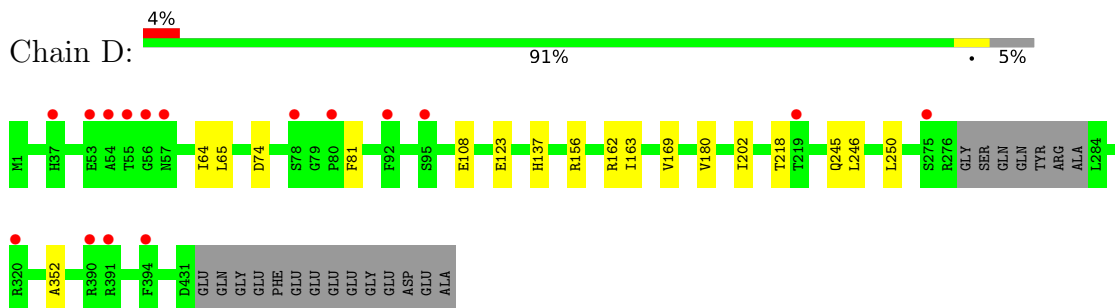
- Molecule 1: Tubulin alpha-1B chain



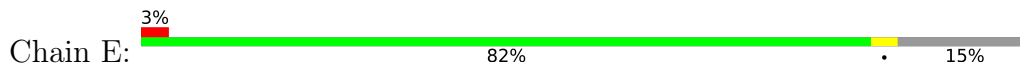
- Molecule 2: Tubulin beta-2B chain

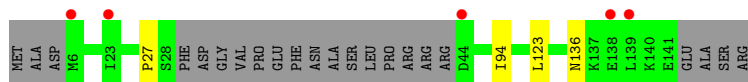


- Molecule 2: Tubulin beta-2B chain

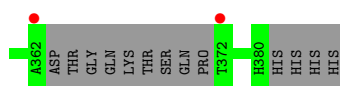
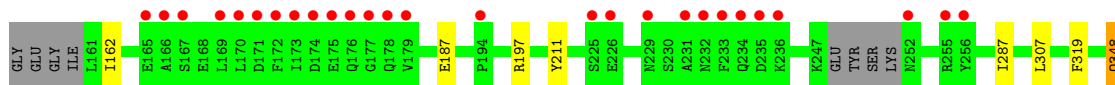
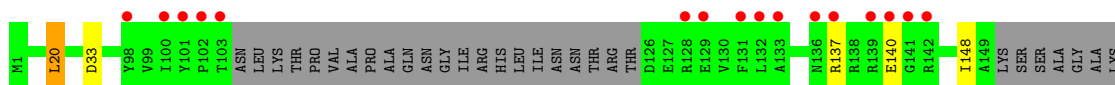
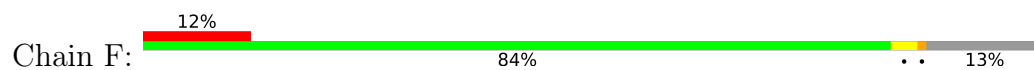


- Molecule 3: Stathmin-4





- Molecule 4: Uncharacterized protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.41Å 154.03Å 185.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 35.46 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.60) 99.8 (35.46-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.38 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.201 , 0.248 0.202 , 0.246	Depositor DCC
$R_{free}$ test set	4591 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.5	Xtrriage
Anisotropy	0.386	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 31.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	17862	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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: 7LG, GTP, GDP, MES, ACP, MG, CA

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	0.40	0/3494	0.61	0/4743
1	C	0.40	0/3515	0.63	0/4772
2	B	0.40	0/3444	0.61	0/4664
2	D	0.40	0/3406	0.60	0/4613
3	E	0.41	0/1008	0.59	0/1337
4	F	0.40	0/2806	0.59	0/3791
All	All	0.40	0/17673	0.61	0/23920

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	3416	0	3331	3	0
1	C	3437	0	3348	8	0
2	B	3369	0	3250	3	0
2	D	3333	0	3214	4	0
3	E	1000	0	1018	1	0
4	F	2744	0	2709	3	0
5	A	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
5	D	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
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
9	B	24	0	26	0	0
9	C	12	0	13	0	0
10	B	57	0	0	0	0
10	D	57	0	0	0	0
11	F	31	0	14	0	0
12	A	64	0	0	0	0
12	B	67	0	0	0	0
12	C	87	0	0	0	0
12	D	12	0	0	0	0
12	E	6	0	0	0	0
12	F	16	0	0	0	0
All	All	17862	0	16971	21	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 1.

The worst 5 of 21 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:265:ILE:HG23	1:A:432:TYR:CE1	2.37	0.59
2:D:246:LEU:HD12	2:D:352:ALA:HB2	1.91	0.52
2:D:64:ILE:HD11	2:D:123:GLU:HG3	1.91	0.51
2:B:134:GLN:HA	2:B:165:ASN:O	2.09	0.51
2:D:163:ILE:HG21	2:D:250:LEU:HB3	1.92	0.51

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	435/450 (97%)	427 (98%)	7 (2%)	1 (0%)	47	71
1	C	438/450 (97%)	425 (97%)	11 (2%)	2 (0%)	29	52
2	B	426/445 (96%)	417 (98%)	9 (2%)	0	100	100
2	D	420/445 (94%)	407 (97%)	12 (3%)	1 (0%)	47	71
3	E	117/143 (82%)	115 (98%)	0	2 (2%)	9	18
4	F	324/384 (84%)	309 (95%)	15 (5%)	0	100	100
All	All	2160/2317 (93%)	2100 (97%)	54 (2%)	6 (0%)	41	64

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	338	LYS
3	E	136	ASN
1	A	282	TYR
1	C	339	ARG
3	E	27	PRO

### 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	368/378 (97%)	360 (98%)	8 (2%)	52	76
1	C	371/378 (98%)	366 (99%)	5 (1%)	69	86
2	B	370/383 (97%)	365 (99%)	5 (1%)	67	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	367/383 (96%)	358 (98%)	9 (2%)	47 73
3	E	109/127 (86%)	108 (99%)	1 (1%)	78 91
4	F	301/342 (88%)	292 (97%)	9 (3%)	41 67
All	All	1886/1991 (95%)	1849 (98%)	37 (2%)	55 78

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	20	LEU
4	F	307	LEU
4	F	33	ASP
4	F	187	GLU
2	B	316	ILE

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	B	245	GLN
2	D	8	GLN
4	F	252	ASN
1	A	406	HIS
1	A	11	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

Of 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 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
8	GDP	B	501	-	24,30,30	0.90	0	30,47,47	1.02	2 (6%)
9	MES	B	503	-	12,12,12	1.96	1 (8%)	14,16,16	6.54	6 (42%)
9	MES	C	504	-	12,12,12	2.18	1 (8%)	14,16,16	1.33	2 (14%)
5	GTP	A	501	6	26,34,34	1.00	2 (7%)	32,54,54	1.11	3 (9%)
10	7LG	B	505	-	57,59,59	1.44	5 (8%)	66,80,80	1.95	9 (13%)
9	MES	B	504	-	12,12,12	2.39	1 (8%)	14,16,16	1.49	1 (7%)
11	ACP	F	401	-	27,33,33	1.79	7 (25%)	32,52,52	1.32	4 (12%)
5	GTP	D	501	6	26,34,34	0.91	0	32,54,54	1.15	4 (12%)
5	GTP	C	501	6	26,34,34	0.87	1 (3%)	32,54,54	1.03	1 (3%)
10	7LG	D	503	-	57,59,59	1.54	6 (10%)	66,80,80	1.51	13 (19%)

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
8	GDP	B	501	-	-	3/12/32/32	0/3/3/3
9	MES	B	503	-	-	1/6/14/14	0/1/1/1
9	MES	C	504	-	-	3/6/14/14	0/1/1/1
5	GTP	A	501	6	-	4/18/38/38	0/3/3/3
10	7LG	B	505	-	-	3/60/79/79	1/3/3/3
9	MES	B	504	-	-	3/6/14/14	0/1/1/1
11	ACP	F	401	-	-	1/15/38/38	0/3/3/3
5	GTP	D	501	6	-	3/18/38/38	0/3/3/3
5	GTP	C	501	6	-	5/18/38/38	0/3/3/3
10	7LG	D	503	-	-	3/60/79/79	1/3/3/3



The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-7.98	1.66	1.77
9	C	504	MES	C8-S	-7.21	1.67	1.77
9	B	503	MES	C8-S	-6.31	1.68	1.77
10	D	503	7LG	CAH-CAT	-6.03	1.36	1.50
10	B	505	7LG	CAH-CAT	-5.85	1.36	1.50

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	503	MES	O2S-S-C8	-14.89	88.98	106.92
9	B	503	MES	O3S-S-O2S	-12.02	81.91	111.27
10	B	505	7LG	CAD-OAK-CCC	11.72	127.58	117.37
9	B	503	MES	O2S-S-O1S	-9.19	82.14	113.95
9	B	503	MES	O1S-S-C8	9.15	117.94	106.92

There are no chirality outliers.

5 of 29 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	PB-O3B-PG-O2G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A

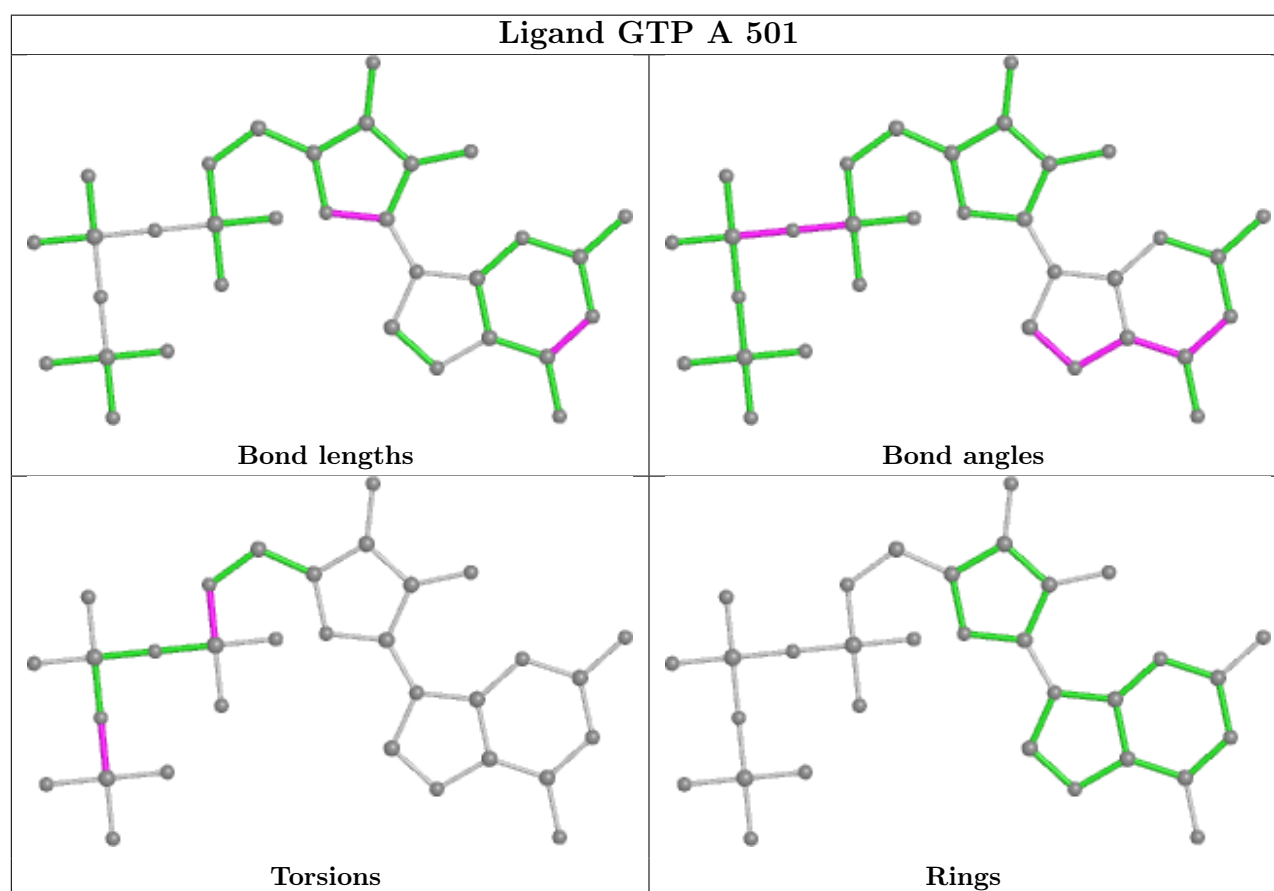
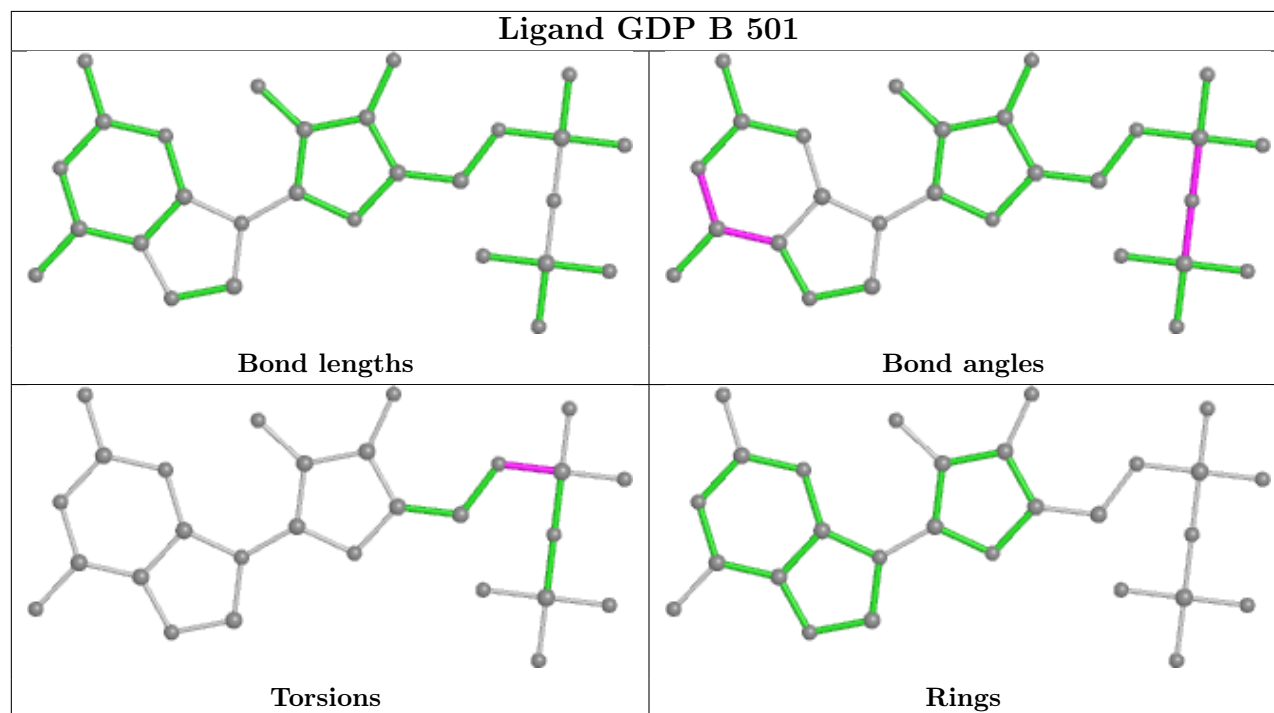
All (2) ring outliers are listed below:

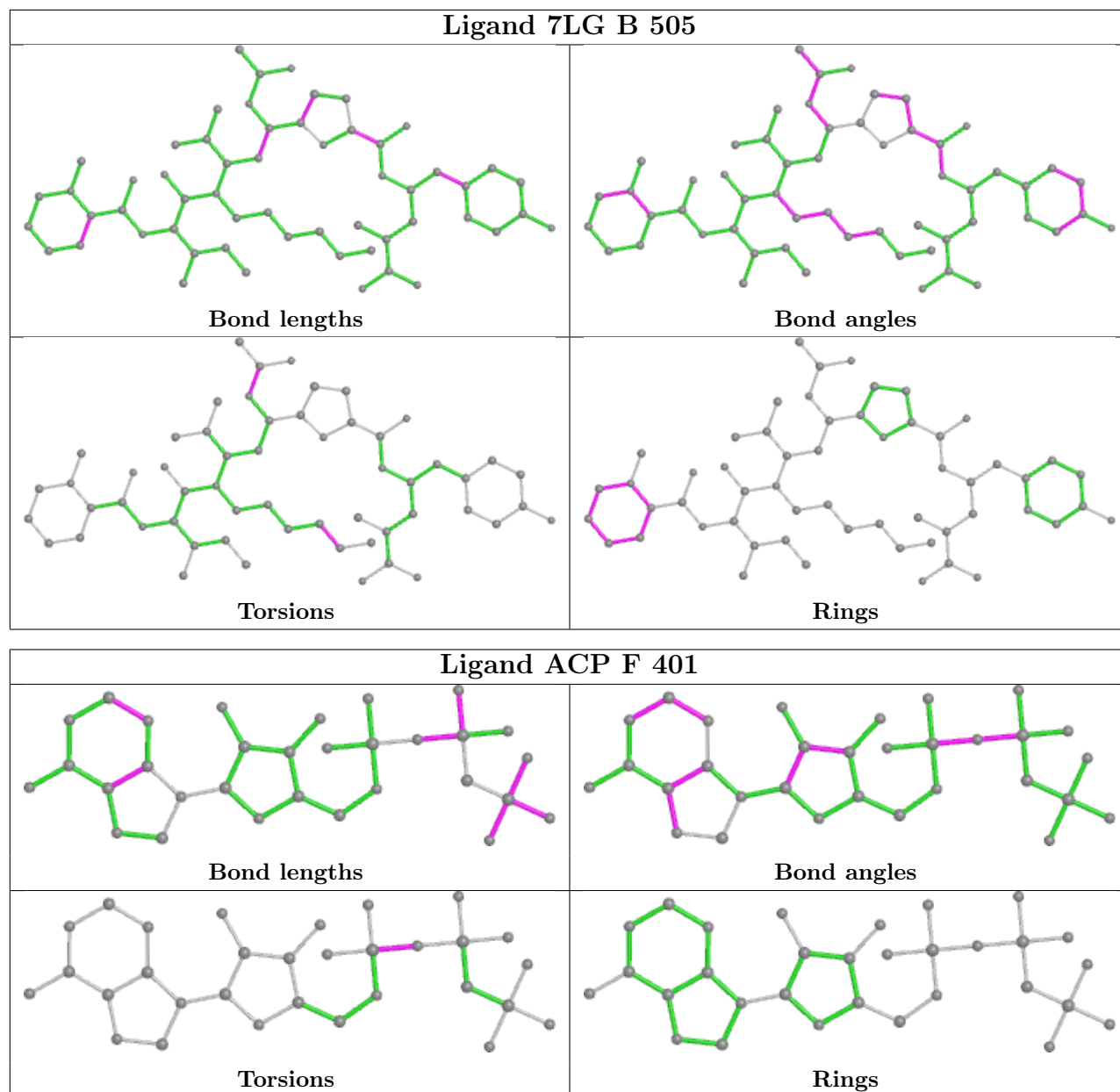
Mol	Chain	Res	Type	Atoms
10	B	505	7LG	CBC-CBD-CBF-CBG-CBH-NBE
10	D	503	7LG	CBC-CBD-CBF-CBG-CBH-NBE

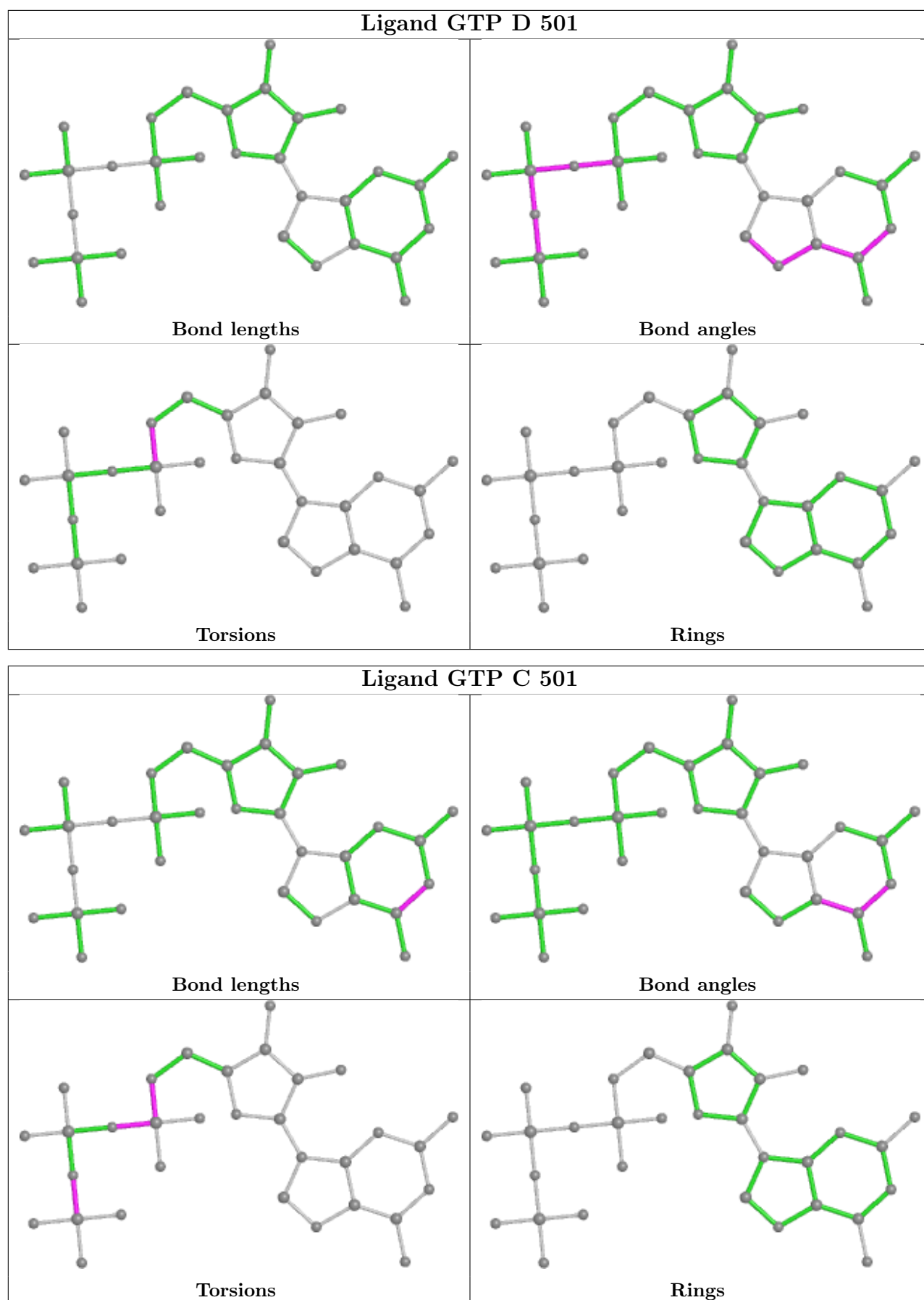
No monomer is involved in short contacts.

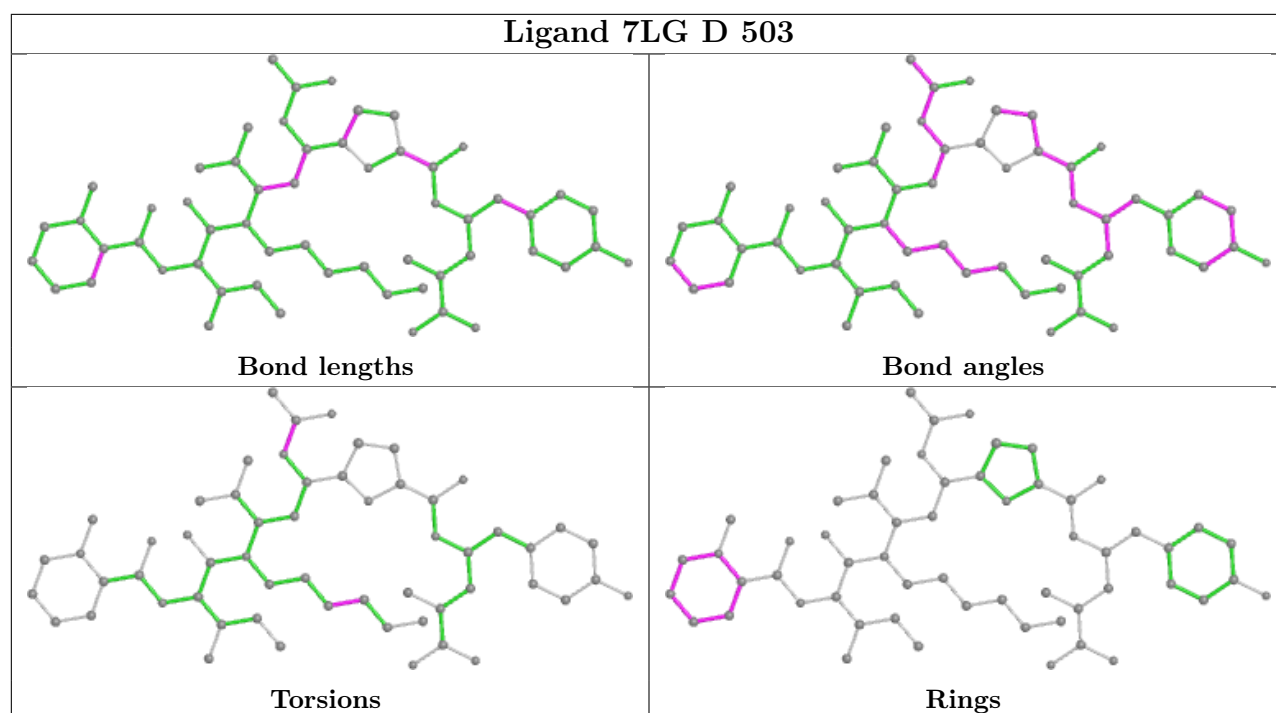
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	437/450 (97%)	-0.17	9 (2%) 63 58	26, 42, 65, 114	0
1	C	440/450 (97%)	-0.42	2 (0%) 91 89	23, 36, 57, 89	0
2	B	428/445 (96%)	-0.29	6 (1%) 75 71	24, 37, 67, 95	0
2	D	424/445 (95%)	0.18	16 (3%) 40 33	33, 56, 86, 112	0
3	E	121/143 (84%)	0.25	5 (4%) 37 30	36, 57, 84, 101	0
4	F	334/384 (86%)	0.40	45 (13%) 3 1	34, 65, 118, 141	0
All	All	2184/2317 (94%)	-0.07	83 (3%) 40 33	23, 46, 87, 141	0

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	372	THR	6.4
4	F	137	ARG	5.8
1	A	282	TYR	5.6
4	F	177	GLY	5.0
4	F	175	GLU	5.0

### 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

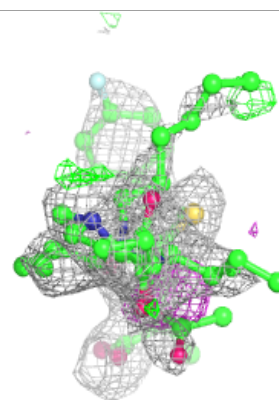
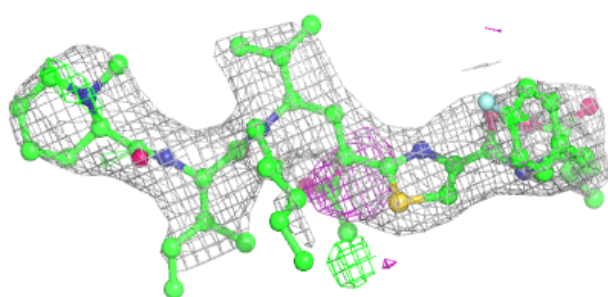
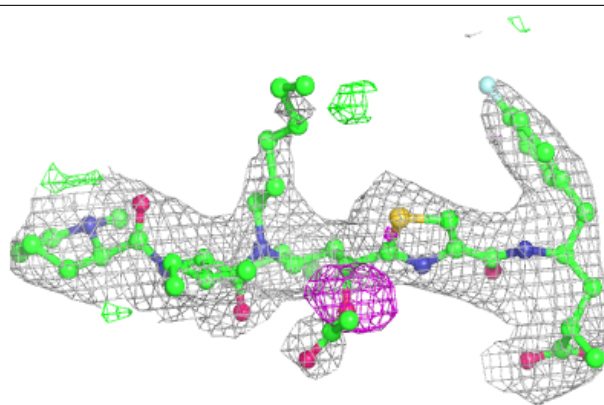
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
9	MES	C	504	12/12	0.70	0.49	104,108,127,129	0
10	7LG	D	503	57/57	0.86	0.38	70,74,87,91	0
6	MG	C	502	1/1	0.87	0.12	36,36,36,36	0
11	ACP	F	401	31/31	0.87	0.17	77,86,112,116	0
6	MG	D	502	1/1	0.88	0.21	71,71,71,71	0
9	MES	B	504	12/12	0.91	0.17	61,65,74,74	0
5	GTP	D	501	32/32	0.92	0.18	44,49,80,86	0
7	CA	C	503	1/1	0.93	0.07	46,46,46,46	0
9	MES	B	503	12/12	0.94	0.17	68,69,70,71	0
10	7LG	B	505	57/57	0.94	0.17	31,36,44,47	0
7	CA	A	503	1/1	0.97	0.06	58,58,58,58	0
6	MG	B	502	1/1	0.97	0.22	38,38,38,38	0
5	GTP	A	501	32/32	0.98	0.12	27,29,32,32	0
8	GDP	B	501	28/28	0.98	0.17	25,28,30,31	0
6	MG	A	502	1/1	0.98	0.06	34,34,34,34	0
5	GTP	C	501	32/32	0.98	0.11	25,26,29,29	0

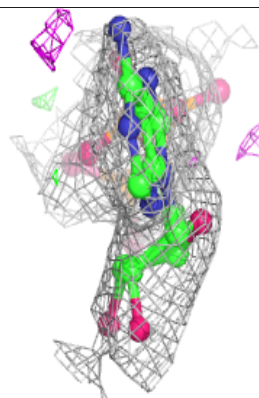
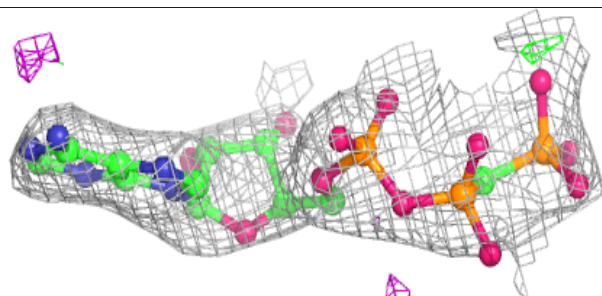
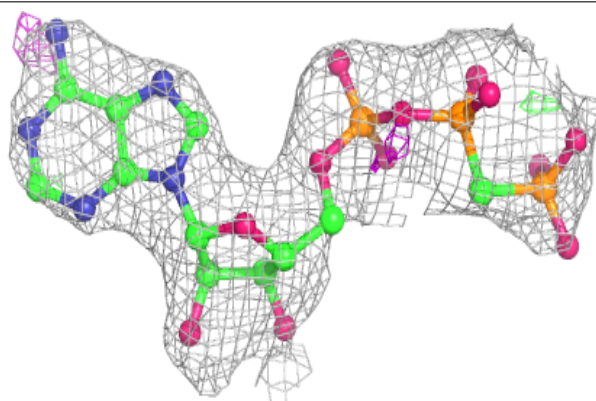
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 7LG 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:**

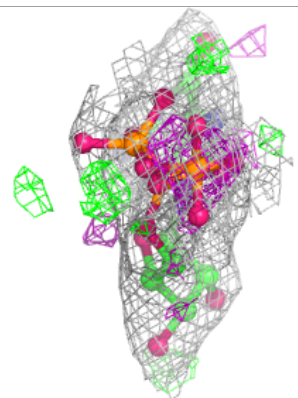
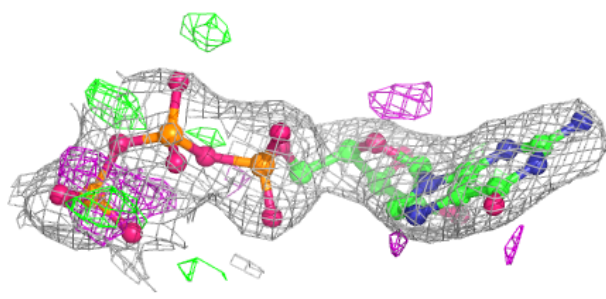
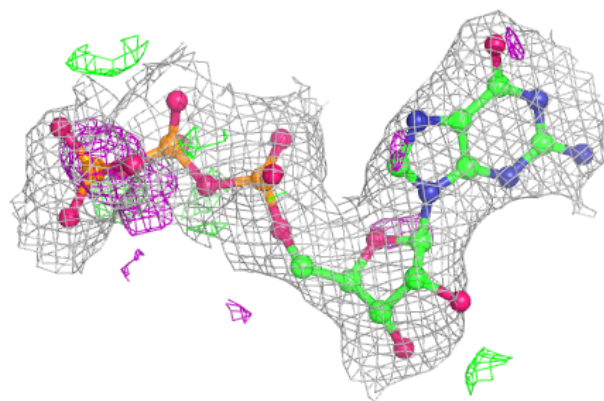
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



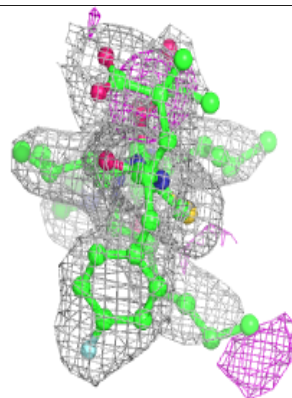
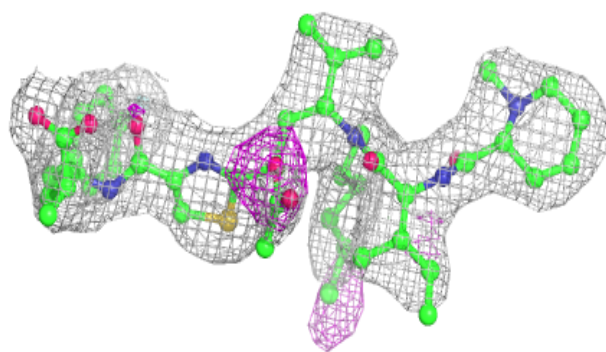
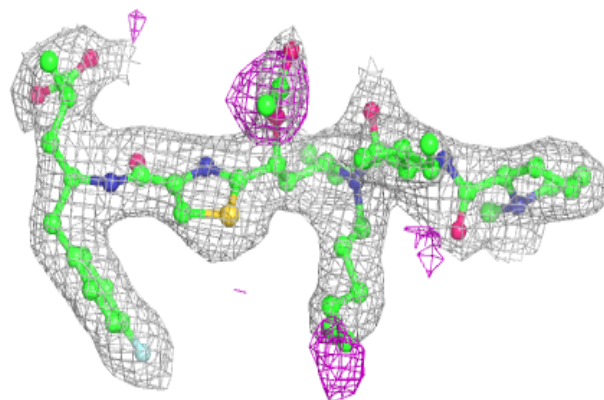


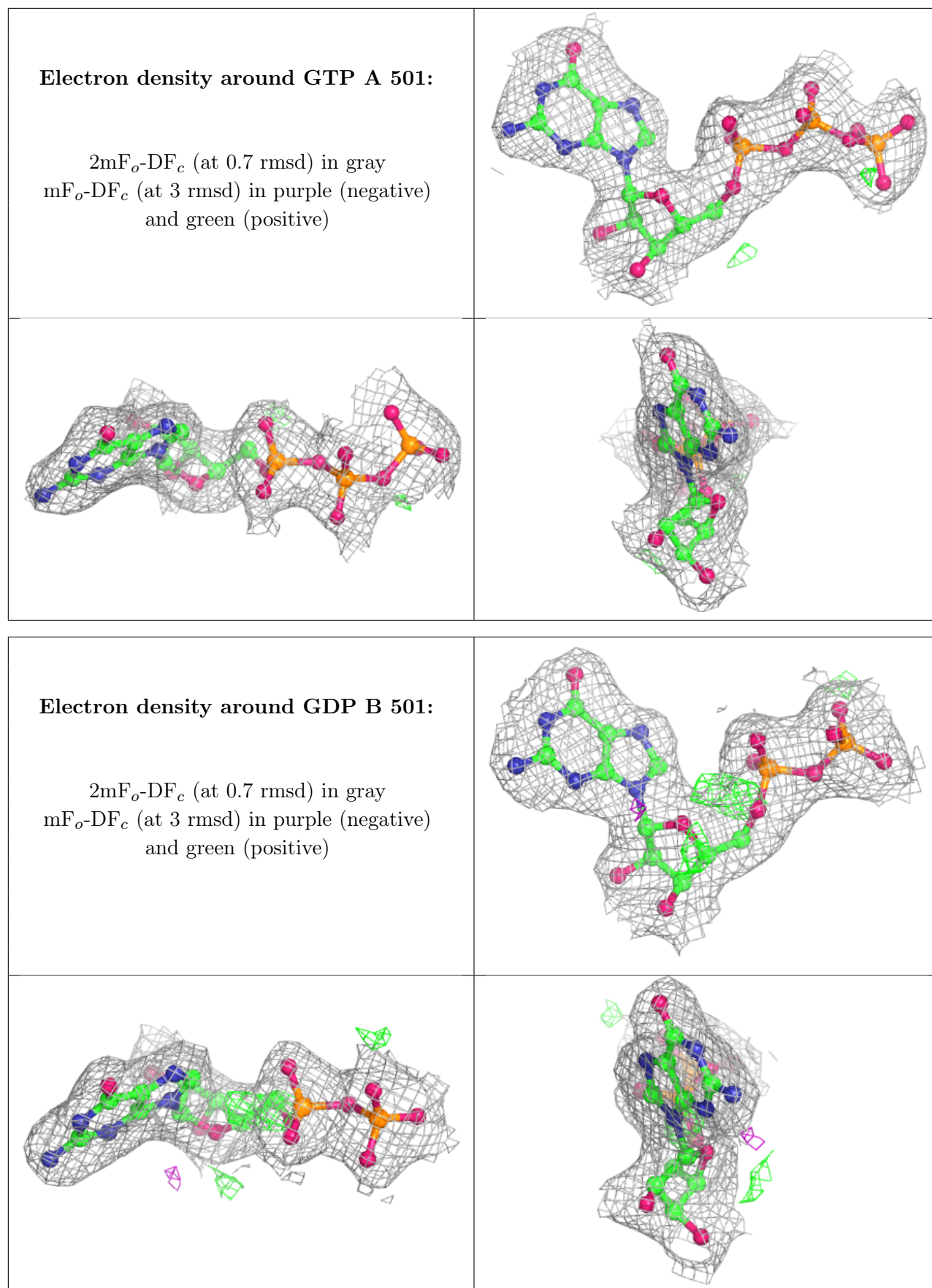
**Electron density around GTP D 501:**

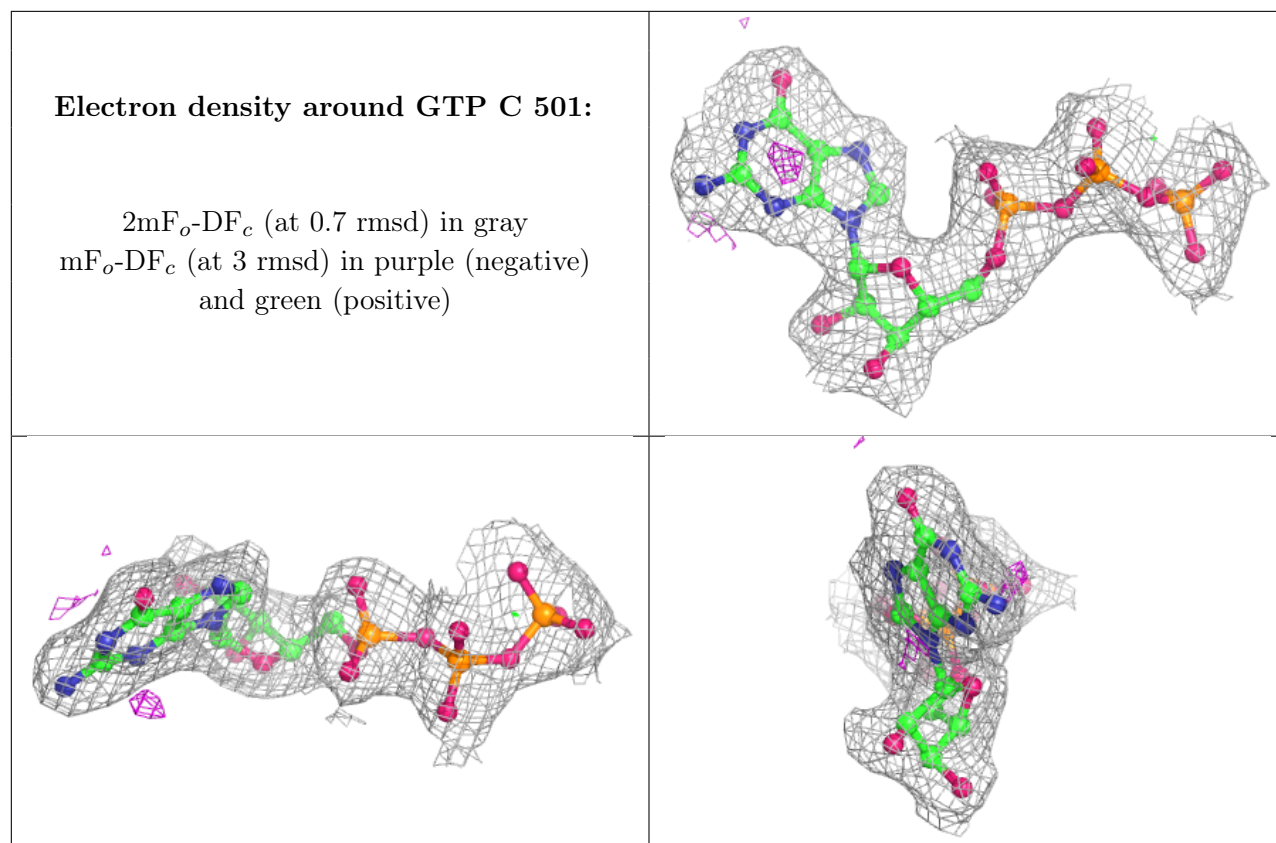
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around 7LG B 505:**

$2mF_o-DF_c$  (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.