



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 05:30 AM BST

PDB ID : 5YL4  
Title : CRYSTAL STRUCTURE OF T2R-TTL-8WR COMPLEX  
Authors : Fu, Z.Y.; Li, W.B.; Chu, Y.Y.; Hou, Y.W.; Ji, C.P.  
Deposited on : 2017-10-17  
Resolution : 2.64 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

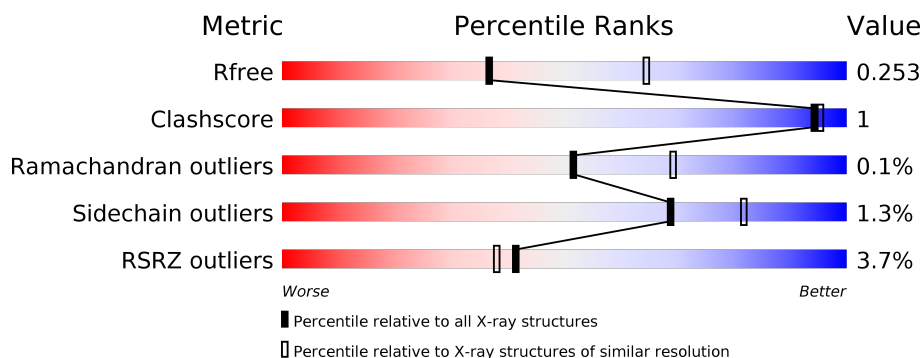
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.64 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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

Mol	Chain	Length	Quality of chain
1	A	450	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 93%; height: 10px; background-color: green;"></div> <div style="width: 5%; height: 10px; background-color: yellow;"></div> <div style="width: 4%; height: 10px; background-color: grey;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>93%</span> <span>5%</span> <span>• •</span> </div> </div>
1	C	450	<div> <div style="width: 93%; height: 10px; background-color: green;"></div> <div style="width: 5%; height: 10px; background-color: yellow;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>93%</span> <span>5%</span> <span>•</span> </div> </div>
2	B	445	<div> <div style="width: 2%; height: 10px; background-color: red;"></div> <div style="width: 91%; height: 10px; background-color: green;"></div> <div style="width: 5%; height: 10px; background-color: yellow;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>91%</span> <span>5%</span> <span>•</span> </div> </div>
2	D	445	<div> <div style="width: 4%; height: 10px; background-color: red;"></div> <div style="width: 91%; height: 10px; background-color: green;"></div> <div style="width: 5%; height: 10px; background-color: yellow;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>4%</span> <span>91%</span> <span>5%</span> <span>•</span> </div> </div>
3	E	143	<div> <div style="width: 3%; height: 10px; background-color: red;"></div> <div style="width: 81%; height: 10px; background-color: green;"></div> <div style="width: 16%; height: 10px; background-color: yellow;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>81%</span> <span>16%</span> <span>•</span> </div> </div>
4	F	384	<div> <div style="width: 12%; height: 10px; background-color: red;"></div> <div style="width: 77%; height: 10px; background-color: green;"></div> <div style="width: 20%; height: 10px; background-color: yellow;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>12%</span> <span>77%</span> <span>20%</span> <span>•</span> </div> </div>

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 17466 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	4	0
			3441	2179	586	652	24			
1	C	440	Total	C	N	O	S	0	9	0
			3482	2200	589	668	25			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	1	0
			3342	2101	570	644	27			
2	D	421	Total	C	N	O	S	0	1	0
			3306	2079	562	638	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	120	Total	C	N	O	S	0	0	0
			994	614	180	195	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	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
4	F	309	Total	C	N	O	S	0	2	0
			2544	1640	437	452	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
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
6	B	1	Total	Mg	0	0
			1	1		
6	A	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		

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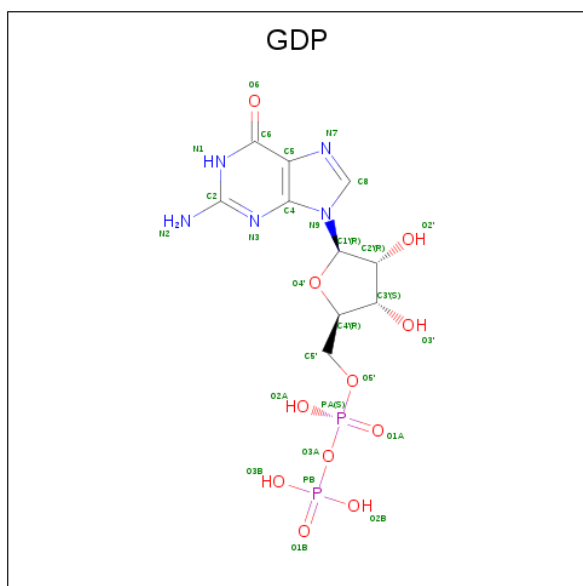
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Mg	0	0
			1	1		

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

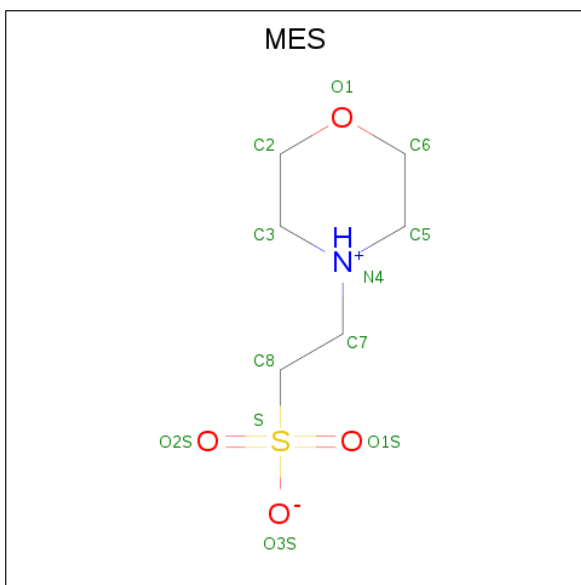
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Ca	0	0
			1	1		
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- 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>).



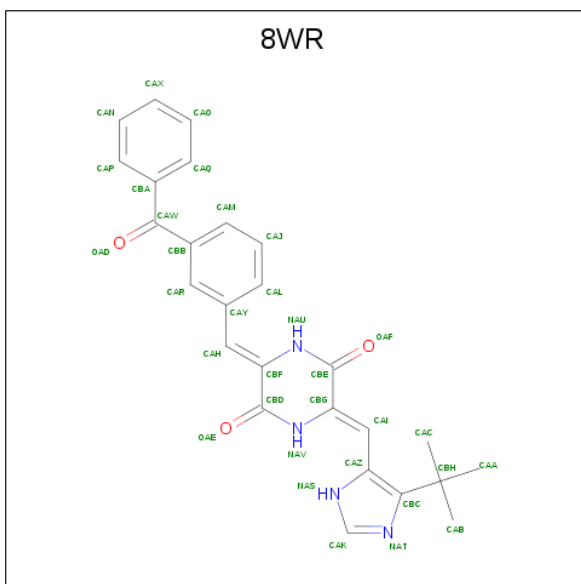
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- 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).



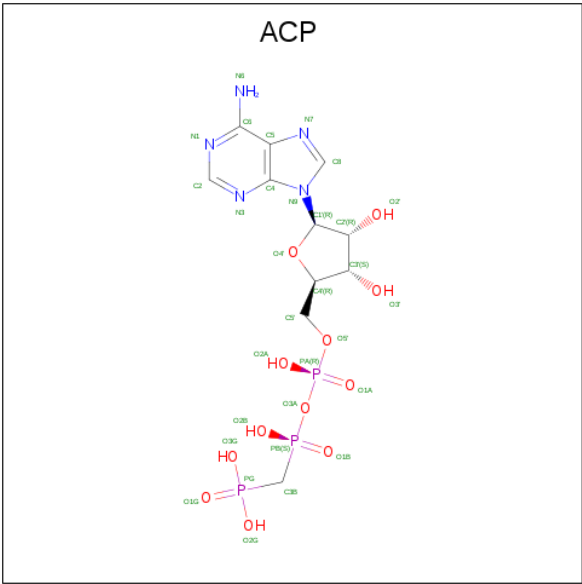
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total 12	C 6	N 1	O 4	S 1	0	0
9	B	1	Total 12	C 6	N 1	O 4	S 1	0	0

- Molecule 10 is (3Z,6Z)-3-[(4-tert-butyl-1H-imidazol-5-yl)methylidene]-6-[[3-(phenylcarbonyl)phenyl]methylidene]piperazine-2,5-dione (three-letter code: 8WR) (formula: C<sub>26</sub>H<sub>24</sub>N<sub>4</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	0	0
			33	26	4	3		

- 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
11	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	26	Total	O	0	0
			26	26		
12	B	43	Total	O	0	0
			43	43		
12	C	62	Total	O	0	0
			62	62		
12	E	3	Total	O	0	0
			3	3		
12	F	4	Total	O	0	0
			4	4		

### 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.

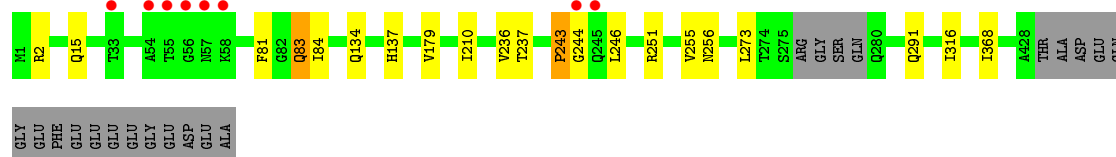
- Molecule 1: Tubulin alpha chain



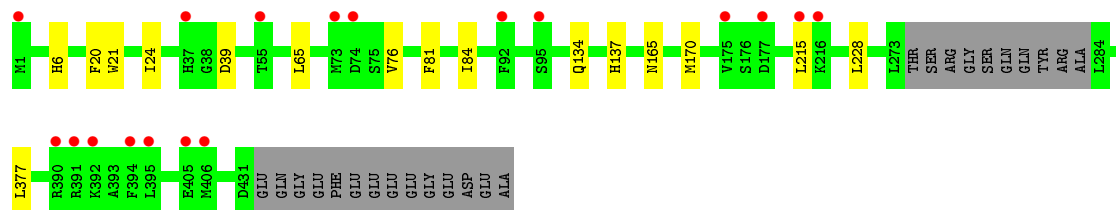
- Molecule 1: Tubulin alpha chain



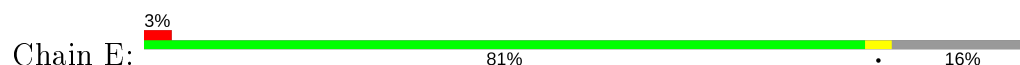
- Molecule 2: Tubulin beta chain



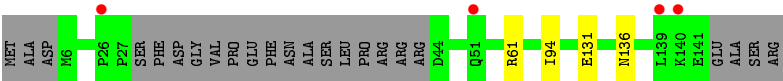
- Molecule 2: Tubulin beta chain



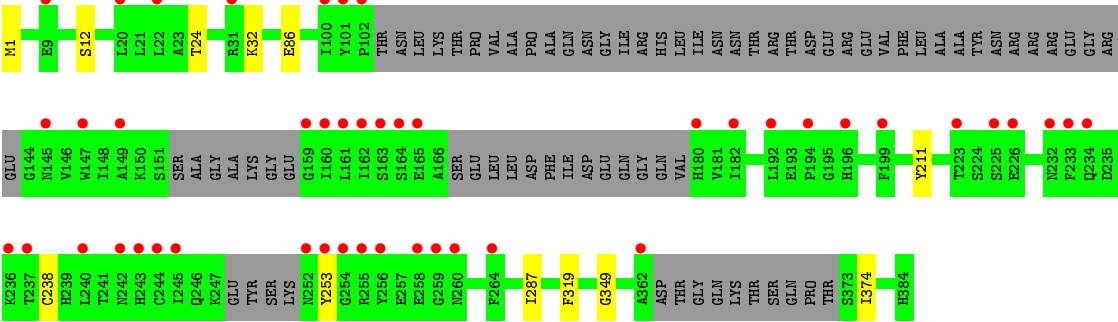
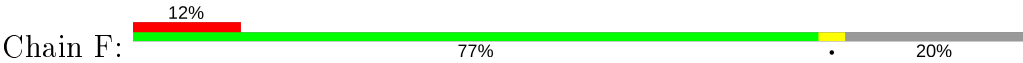
- Molecule 3: Stathmin-4







● 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, $\alpha$ , $\beta$ , $\gamma$	105.46Å 157.73Å 182.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.23 – 2.64 48.23 – 2.64	Depositor EDS
% Data completeness (in resolution range)	97.4 (48.23-2.64) 97.4 (48.23-2.64)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.22 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.218 , 0.256 0.220 , 0.253	Depositor DCC
$R_{free}$ test set	4341 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.3	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 33.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	17466	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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: GDP, MG, CA, 8WR, GTP, ACP, MES

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	0.41	0/3525	0.63	1/4784 (0.0%)
1	C	0.42	0/3572	0.64	0/4850
2	B	0.43	0/3416	0.65	0/4626
2	D	0.41	0/3379	0.58	0/4577
3	E	0.41	0/1002	0.58	0/1329
4	F	0.41	0/2609	0.57	0/3525
All	All	0.41	0/17503	0.62	1/23691 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	402	ARG	NE-CZ-NH1	5.14	122.87	120.30

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	3441	0	3363	14	0
1	C	3482	0	3384	12	0
2	B	3342	0	3216	11	0
2	D	3306	0	3181	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	994	0	1013	2	0
4	F	2544	0	2514	2	0
5	A	32	0	12	0	0
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	B	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
10	B	33	0	0	2	0
11	F	31	0	14	0	0
12	A	26	0	0	0	0
12	B	43	0	0	0	0
12	C	62	0	0	0	0
12	E	3	0	0	0	0
12	F	4	0	0	0	0
All	All	17466	0	16759	44	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.

All (44) 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:229[A]:ARG:HG2	1:A:229[A]:ARG:HH11	1.09	1.17
1:A:229[A]:ARG:HH11	1:A:229[A]:ARG:CG	1.76	0.97
1:A:229[A]:ARG:HG2	1:A:229[A]:ARG:NH1	1.89	0.80
2:B:243:PRO:CB	2:B:244:GLY:HA2	2.19	0.72
1:A:368[B]:LEU:H	1:A:368[B]:LEU:HD12	1.56	0.70
2:B:243:PRO:HB2	2:B:244:GLY:HA2	1.77	0.66
1:A:229[A]:ARG:NH1	1:A:229[A]:ARG:CG	2.47	0.65
1:A:368[B]:LEU:N	1:A:368[B]:LEU:HD12	2.13	0.63
2:B:134:GLN:HB2	10:B:506:8WR:CAQ	2.36	0.56
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.91	0.53
1:A:101:ASN:HD22	2:B:256:ASN:HD21	1.56	0.51
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:170:MET:HG3	2:D:377:LEU:HD11	1.92	0.51
2:B:237:THR:HG22	10:B:506:8WR:CAJ	2.41	0.51
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.92	0.50
1:A:68:VAL:HG11	1:A:149:PHE:CE2	2.48	0.49
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.78	0.48
1:A:265:ILE:HG23	1:A:432:TYR:CE2	2.48	0.48
2:D:134:GLN:HA	2:D:165:ASN:O	2.15	0.47
1:C:178:SER:HB2	1:C:183:GLU:OE2	2.13	0.47
2:D:81:PHE:O	2:D:84:ILE:HG22	2.16	0.46
2:B:236:VAL:HG12	2:B:368:ILE:HD11	1.98	0.46
4:F:349:GLY:HA3	4:F:374:ILE:HD11	1.98	0.46
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.46	0.45
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.56	0.45
2:B:251:ARG:O	2:B:255:VAL:HG23	2.17	0.44
2:B:81:PHE:O	2:B:84:ILE:HG22	2.17	0.44
1:C:271:THR:HG21	1:C:295:CYS:O	2.17	0.44
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.52	0.44
1:C:180:ALA:HB3	1:C:183:GLU:HG3	2.01	0.43
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.54	0.43
1:C:171:ILE:HD12	1:C:171:ILE:N	2.34	0.43
4:F:287:ILE:HG23	4:F:319:PHE:CE2	2.54	0.43
2:B:210:ILE:HG23	2:B:273:LEU:HD13	2.00	0.42
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.55	0.42
2:B:83:GLN:HA	2:B:83:GLN:HE21	1.85	0.42
1:A:275:VAL:HG13	1:A:368[A]:LEU:HD21	2.02	0.41
2:D:65:LEU:CD2	2:D:76:VAL:HG11	2.50	0.41
2:D:215:LEU:HD11	2:D:228:LEU:HD21	2.02	0.41
1:A:411:GLU:O	3:E:61:ARG:NH1	2.54	0.41
1:A:236:SER:OG	1:A:320:ARG:NH1	2.54	0.41
1:C:209:ILE:HG22	1:C:227:LEU:HD22	2.02	0.41
1:C:230:LEU:O	1:C:234:ILE:HD12	2.20	0.41
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.40	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	439/450 (98%)	430 (98%)	9 (2%)	0	100	100
1	C	446/450 (99%)	435 (98%)	11 (2%)	0	100	100
2	B	421/445 (95%)	408 (97%)	12 (3%)	1 (0%)	47	64
2	D	417/445 (94%)	401 (96%)	15 (4%)	1 (0%)	47	64
3	E	116/143 (81%)	114 (98%)	2 (2%)	0	100	100
4	F	299/384 (78%)	289 (97%)	9 (3%)	1 (0%)	41	56
All	All	2138/2317 (92%)	2077 (97%)	58 (3%)	3 (0%)	51	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	243	PRO
2	D	39	ASP
4	F	253	TYR

### 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	372/378 (98%)	366 (98%)	6 (2%)	62	78
1	C	379/378 (100%)	377 (100%)	2 (0%)	88	94
2	B	366/383 (96%)	359 (98%)	7 (2%)	57	74
2	D	362/383 (94%)	361 (100%)	1 (0%)	92	96
3	E	108/127 (85%)	106 (98%)	2 (2%)	57	74
4	F	280/342 (82%)	273 (98%)	7 (2%)	47	66
All	All	1867/1991 (94%)	1842 (99%)	25 (1%)	69	82

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	229[A]	ARG
1	A	229[B]	ARG
1	A	237	SER
1	A	320	ARG
1	A	326	LYS
2	B	2	ARG
2	B	15	GLN
2	B	83	GLN
2	B	137	HIS
2	B	246	LEU
2	B	291	GLN
2	B	316	ILE
1	C	245	ASP
1	C	342	GLN
2	D	137	HIS
3	E	131	GLU
3	E	136	ASN
4	F	1	MET
4	F	12	SER
4	F	24	THR
4	F	32	LYS
4	F	86	GLU
4	F	211	TYR
4	F	238	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
2	B	83	GLN
2	B	292	GLN
1	C	249	ASN
2	D	165	ASN
3	E	136	ASN
4	F	252	ASN

### 5.3.3 RNA ⓘ

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 15 ligands modelled in this entry, 7 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$
9	MES	B	505	-	12,12,12	1.98	1 (8%)	14,16,16	6.48	8 (57%)
5	GTP	A	501	6	26,34,34	1.24	2 (7%)	33,54,54	1.93	9 (27%)
5	GTP	C	501	6	26,34,34	1.13	2 (7%)	33,54,54	1.83	8 (24%)
8	GDP	B	501	6	24,30,30	1.19	3 (12%)	31,47,47	1.96	6 (19%)
9	MES	B	503	-	12,12,12	2.01	1 (8%)	14,16,16	6.96	9 (64%)
5	GTP	D	501	6	26,34,34	1.21	2 (7%)	33,54,54	1.90	8 (24%)
10	8WR	B	506	-	28,36,36	1.41	4 (14%)	33,52,52	1.20	4 (12%)
11	ACP	F	401	-	27,33,33	1.50	6 (22%)	32,52,52	1.31	3 (9%)

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
9	MES	B	505	-	-	2/6/14/14	0/1/1/1
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
5	GTP	C	501	6	-	8/18/38/38	0/3/3/3
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MES	B	503	-	-	3/6/14/14	0/1/1/1
5	GTP	D	501	6	-	6/18/38/38	0/3/3/3
10	8WR	B	506	-	-	3/18/22/22	0/4/4/4
11	ACP	F	401	-	-	5/15/38/38	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	505	MES	C8-S	-6.32	1.68	1.77
9	B	503	MES	C8-S	-6.27	1.68	1.77
5	A	501	GTP	C6-C5	4.38	1.48	1.41
5	D	501	GTP	C6-C5	4.17	1.48	1.41
5	C	501	GTP	C6-C5	3.78	1.47	1.41
10	B	506	8WR	CBG-NAV	3.72	1.41	1.35
11	F	401	ACP	PB-O3A	3.61	1.62	1.58
10	B	506	8WR	CBF-NAU	3.54	1.41	1.35
10	B	506	8WR	CBE-NAU	3.39	1.38	1.33
8	B	501	GDP	C6-C5	3.36	1.47	1.41
11	F	401	ACP	PG-O2G	2.92	1.61	1.54
11	F	401	ACP	PG-O3G	2.88	1.61	1.54
5	D	501	GTP	C5-C4	2.71	1.48	1.40
11	F	401	ACP	C5-C4	2.65	1.48	1.40
5	A	501	GTP	C5-C4	2.57	1.47	1.40
5	C	501	GTP	C5-C4	2.53	1.47	1.40
10	B	506	8WR	CBD-NAV	2.38	1.37	1.33
8	B	501	GDP	C5-C4	2.34	1.47	1.40
8	B	501	GDP	C2'-C1'	-2.30	1.50	1.53
11	F	401	ACP	PB-O2B	2.20	1.61	1.56
11	F	401	ACP	C2-N3	2.12	1.35	1.32

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	503	MES	O3S-S-C8	-13.42	84.07	105.77
9	B	505	MES	O3S-S-O1S	-12.34	81.12	111.27
9	B	503	MES	O3S-S-O2S	-11.67	82.77	111.27
9	B	503	MES	O2S-S-C8	11.44	120.69	106.92
9	B	505	MES	O3S-S-O2S	-11.02	84.34	111.27
9	B	503	MES	O3S-S-O1S	-10.59	85.39	111.27
9	B	505	MES	O2S-S-C8	10.17	119.16	106.92
9	B	505	MES	O3S-S-C8	-9.64	90.17	105.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	505	MES	O1S-S-C8	9.46	118.31	106.92
9	B	503	MES	O1S-S-C8	8.66	117.34	106.92
8	B	501	GDP	C6-N1-C2	4.95	123.79	115.93
9	B	503	MES	C2-C3-N4	4.78	117.36	110.10
5	C	501	GTP	C5-C6-N1	-4.62	117.11	123.43
5	C	501	GTP	C6-N1-C2	4.45	123.00	115.93
5	A	501	GTP	C6-C5-C4	-4.40	116.60	120.80
8	B	501	GDP	C5-C6-N1	-4.35	117.48	123.43
5	A	501	GTP	C6-N1-C2	4.35	122.84	115.93
5	D	501	GTP	C2-N3-C4	4.34	120.32	115.36
5	D	501	GTP	C6-N1-C2	4.34	122.83	115.93
8	B	501	GDP	C2-N3-C4	4.32	120.30	115.36
5	A	501	GTP	C2-N3-C4	4.30	120.27	115.36
8	B	501	GDP	C6-C5-C4	-4.23	116.76	120.80
5	A	501	GTP	C5-C6-N1	-4.23	117.65	123.43
5	C	501	GTP	C6-C5-C4	-4.15	116.84	120.80
5	D	501	GTP	C5-C6-N1	-4.12	117.80	123.43
5	D	501	GTP	C6-C5-C4	-3.95	117.03	120.80
8	B	501	GDP	N3-C2-N1	-3.91	122.00	127.22
11	F	401	ACP	N3-C2-N1	-3.62	123.03	128.68
5	C	501	GTP	C2-N3-C4	3.59	119.46	115.36
10	B	506	8WR	CBD-NAV-CBG	3.47	124.11	116.41
5	D	501	GTP	N3-C2-N1	-3.36	122.75	127.22
5	A	501	GTP	N3-C2-N1	-3.29	122.83	127.22
10	B	506	8WR	CBE-NAU-CBF	3.25	123.61	116.41
5	C	501	GTP	N3-C2-N1	-3.14	123.03	127.22
9	B	505	MES	C6-C5-N4	2.99	114.64	110.10
5	A	501	GTP	C4-C5-N7	-2.92	106.36	109.40
11	F	401	ACP	C4-C5-N7	-2.84	106.44	109.40
11	F	401	ACP	C3'-C2'-C1'	2.75	105.12	100.98
5	D	501	GTP	PA-O3A-PB	-2.73	123.46	132.83
9	B	503	MES	O1-C6-C5	-2.70	105.86	111.80
10	B	506	8WR	CBF-CAH-CAY	-2.62	126.62	130.01
9	B	503	MES	C5-N4-C3	2.48	114.42	108.83
5	C	501	GTP	PA-O3A-PB	-2.47	124.33	132.83
5	A	501	GTP	O3G-PG-O2G	2.44	116.95	107.64
5	D	501	GTP	C4-C5-N7	-2.42	106.88	109.40
5	A	501	GTP	PA-O3A-PB	-2.30	124.92	132.83
8	B	501	GDP	C4-C5-N7	-2.26	107.04	109.40
9	B	505	MES	C5-N4-C3	2.18	113.73	108.83
5	A	501	GTP	C1'-N9-C4	-2.16	122.84	126.64
9	B	505	MES	C7-N4-C5	-2.16	105.70	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	501	GTP	PB-O3B-PG	-2.13	125.53	132.83
5	C	501	GTP	C4-C5-N7	-2.11	107.20	109.40
10	B	506	8WR	CBB-CAW-CBA	2.11	123.75	120.28
5	C	501	GTP	PB-O3B-PG	-2.10	125.63	132.83
9	B	503	MES	C6-C5-N4	2.03	113.18	110.10

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
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
8	B	501	GDP	C5'-O5'-PA-O2A
9	B	503	MES	N4-C7-C8-S
9	B	503	MES	C7-C8-S-O2S
5	D	501	GTP	C5'-O5'-PA-O1A
10	B	506	8WR	CBG-CAI-CAZ-NAS
11	F	401	ACP	PB-C3B-PG-O1G
11	F	401	ACP	PB-C3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O1G
5	D	501	GTP	C5'-O5'-PA-O2A
9	B	505	MES	C7-C8-S-O1S
9	B	505	MES	C7-C8-S-O2S
9	B	503	MES	C7-C8-S-O1S
11	F	401	ACP	PB-C3B-PG-O2G
11	F	401	ACP	O4'-C4'-C5'-O5'
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	C4'-C5'-O5'-PA
5	D	501	GTP	C4'-C5'-O5'-PA
11	F	401	ACP	C3'-C4'-C5'-O5'
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3A-PA-O2A

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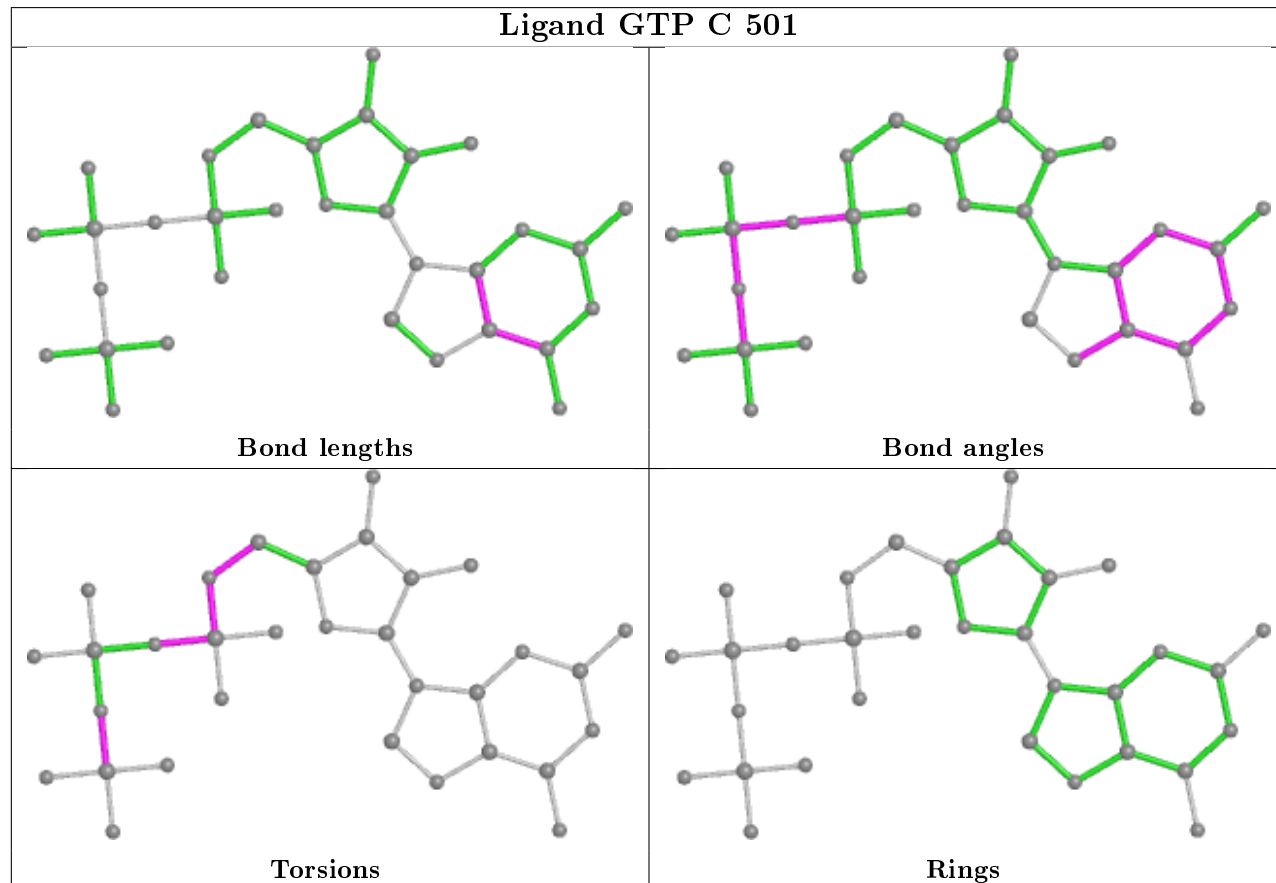
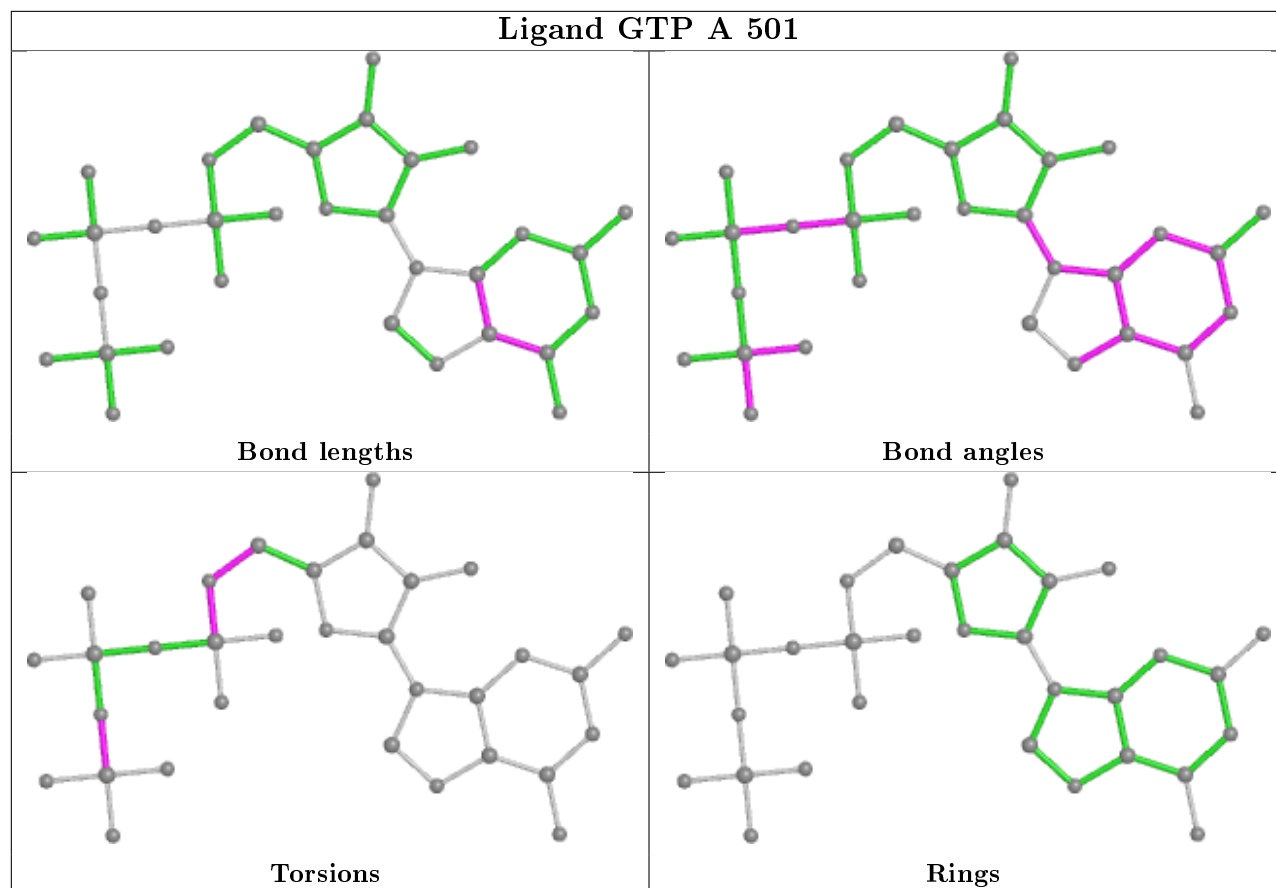
Mol	Chain	Res	Type	Atoms
5	D	501	GTP	PB-O3A-PA-O1A
5	D	501	GTP	PB-O3A-PA-O2A
10	B	506	8WR	CBF-CAH-CAY-CAL
10	B	506	8WR	CBF-CAH-CAY-CAR

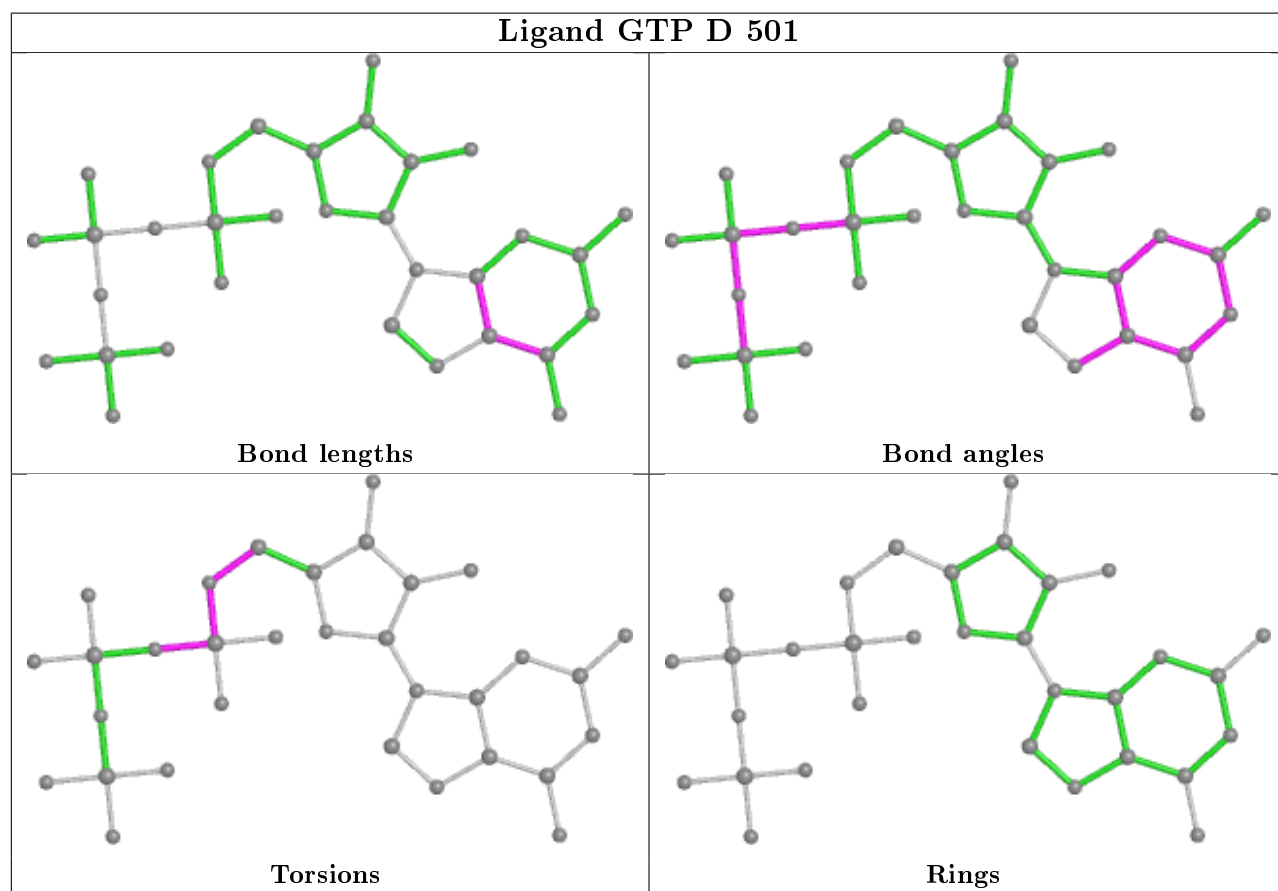
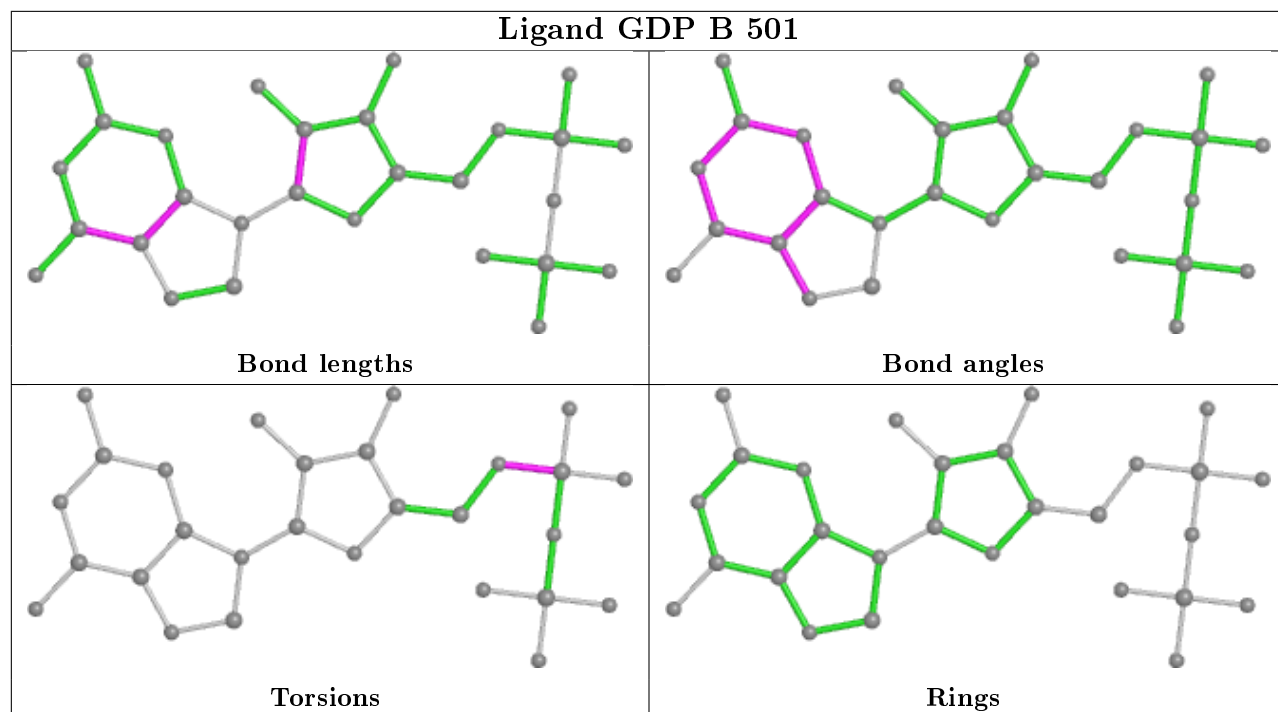
There are no ring outliers.

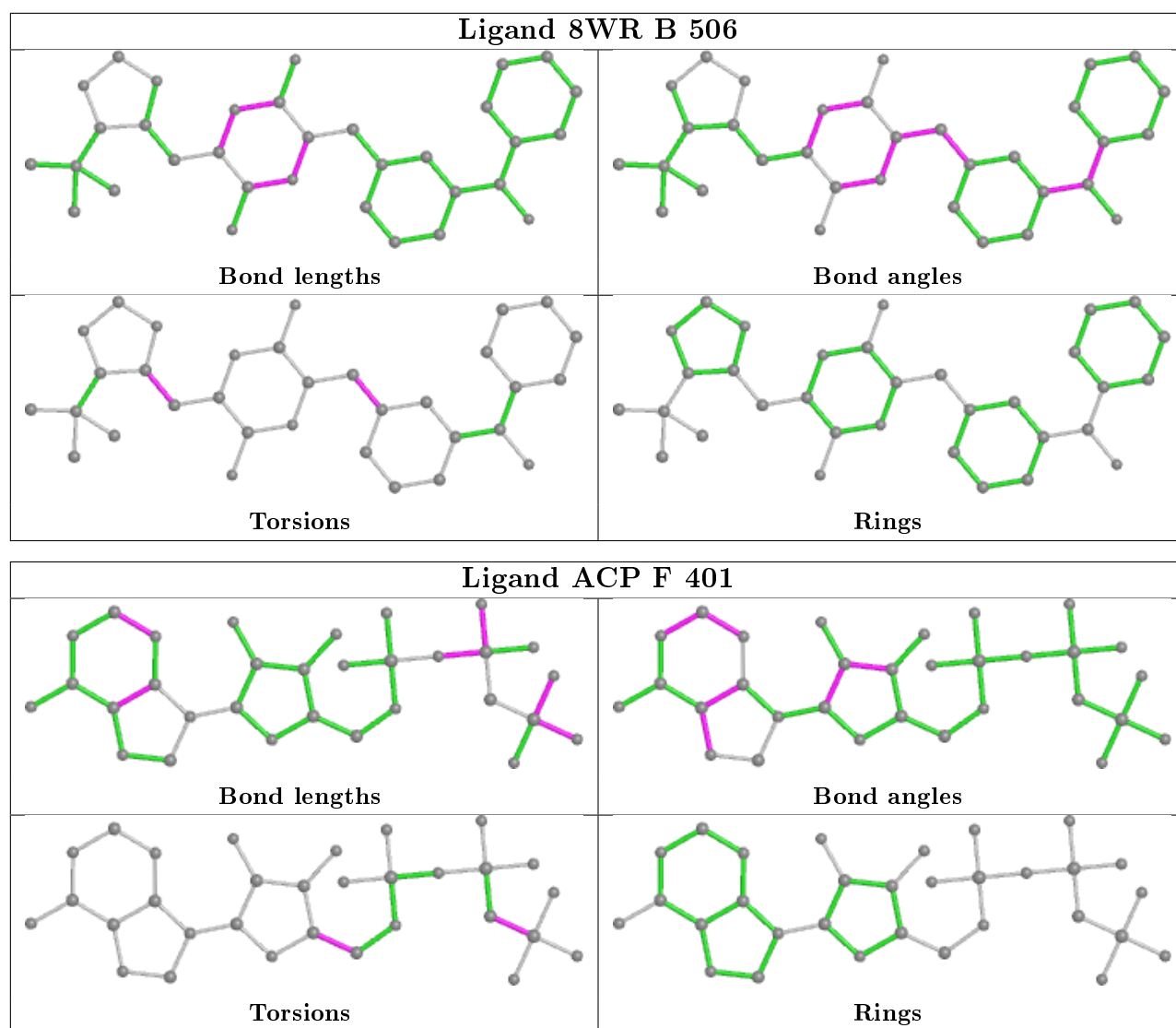
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	506	8WR	2	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	437/450 (97%)	-0.11	3 (0%)	87 86	20, 39, 66, 83	0
1	C	440/450 (97%)	-0.39	1 (0%)	95 96	14, 30, 52, 73	1 (0%)
2	B	424/445 (95%)	-0.13	8 (1%)	66 64	18, 38, 71, 97	1 (0%)
2	D	421/445 (94%)	0.27	18 (4%)	35 31	29, 57, 94, 128	4 (0%)
3	E	120/143 (83%)	0.29	4 (3%)	46 43	30, 57, 89, 102	0
4	F	309/384 (80%)	0.66	46 (14%)	2 1	30, 63, 112, 125	0
All	All	2151/2317 (92%)	0.04	80 (3%)	41 38	14, 45, 87, 128	6 (0%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	244	CYS	6.0
4	F	182	ILE	5.1
4	F	253	TYR	4.9
4	F	362	ALA	4.9
4	F	102	PRO	4.7
4	F	245	ILE	4.5
4	F	163	SER	4.5
4	F	161	LEU	4.2
2	B	57	ASN	4.1
4	F	233	PHE	4.1
4	F	234	GLN	4.0
4	F	225	SER	3.9
4	F	149	ALA	3.9
2	D	55	THR	3.8
2	B	55	THR	3.7
4	F	232	ASN	3.6
4	F	194	PRO	3.6
4	F	256	TYR	3.6
4	F	259	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	391	ARG	3.5
2	D	395	LEU	3.5
2	D	390	ARG	3.4
4	F	240	LEU	3.4
2	D	73	MET	3.3
2	D	394	PHE	3.3
2	B	56	GLY	3.3
4	F	165	GLU	3.2
2	D	177	ASP	3.2
4	F	20	LEU	3.2
4	F	101	TYR	3.2
2	D	215	LEU	3.1
4	F	199	PHE	3.1
2	D	37	HIS	3.0
2	D	1	MET	3.0
2	B	245	GLN	2.9
4	F	236	LYS	2.9
2	D	74	ASP	2.9
4	F	100	ILE	2.8
2	B	54	ALA	2.8
2	B	244	GLY	2.7
4	F	260	ASN	2.7
4	F	254	GLY	2.6
4	F	180	HIS	2.6
2	D	92	PHE	2.6
1	A	41	THR	2.6
4	F	9	GLU	2.6
1	A	57	GLY	2.6
2	B	58	LYS	2.5
1	C	340	SER	2.4
4	F	223	THR	2.4
2	B	33	THR	2.4
4	F	192	LEU	2.4
4	F	22	LEU	2.4
4	F	255	ARG	2.4
4	F	237	THR	2.3
4	F	252	ASN	2.3
2	D	405	GLU	2.3
4	F	242	ASN	2.3
4	F	162	ILE	2.3
3	E	26	PRO	2.3
4	F	159	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
4	F	258	GLU	2.2
4	F	164	SER	2.2
4	F	147	TRP	2.2
1	A	42	ILE	2.2
2	D	175	VAL	2.2
3	E	139	LEU	2.1
2	D	392	LYS	2.1
3	E	140	LYS	2.1
4	F	160	ILE	2.1
2	D	95	SER	2.1
4	F	31	ARG	2.1
3	E	51	GLN	2.1
2	D	216	LYS	2.0
2	D	406	MET	2.0
4	F	243	HIS	2.0
4	F	226	GLU	2.0
4	F	145	ASN	2.0
4	F	264	PHE	2.0
4	F	196	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 monosaccharides 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.

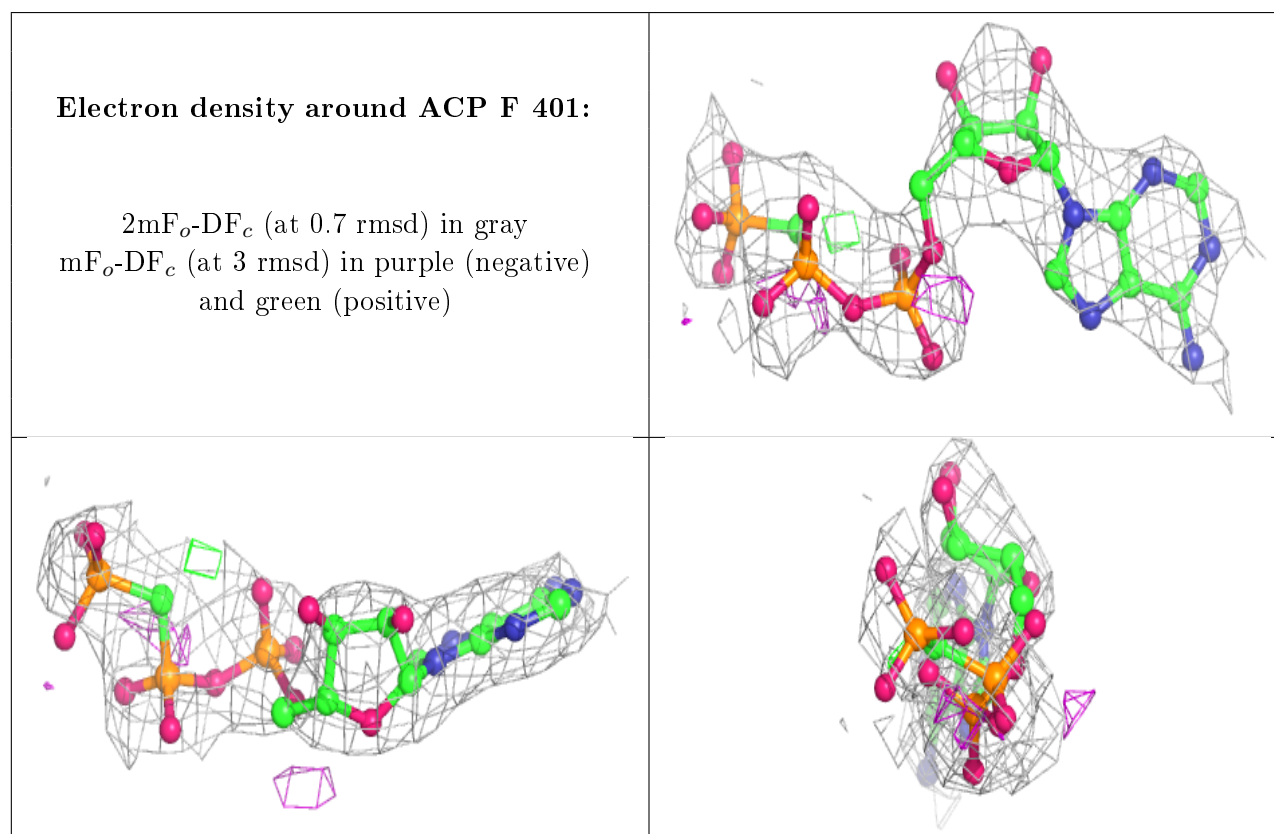
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
11	ACP	F	401	31/31	0.86	0.31	85,92,130,134	0
10	8WR	B	506	33/33	0.89	0.24	35,37,38,39	0
7	CA	A	503	1/1	0.92	0.07	63,63,63,63	0
9	MES	B	503	12/12	0.92	0.20	64,69,75,79	0

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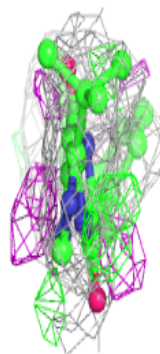
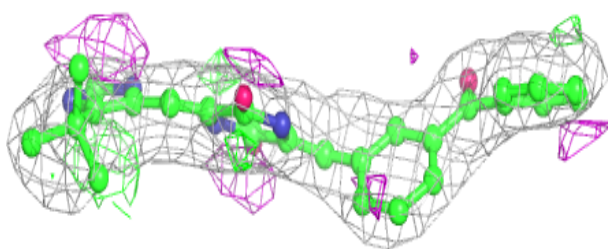
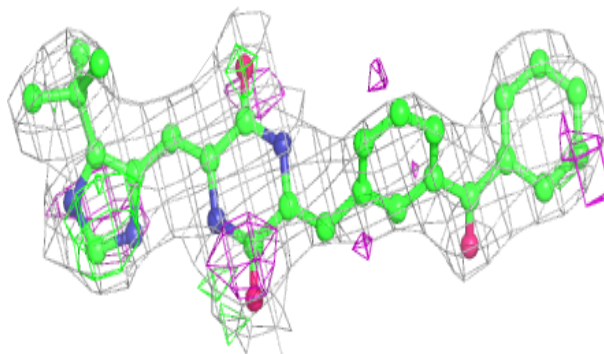
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	MES	B	505	12/12	0.93	0.25	78,81,92,93	0
7	CA	B	504	1/1	0.93	0.07	76,76,76,76	0
7	CA	C	503	1/1	0.94	0.10	49,49,49,49	0
6	MG	D	502	1/1	0.94	0.06	50,50,50,50	0
5	GTP	D	501	32/32	0.95	0.13	39,44,57,65	0
6	MG	B	502	1/1	0.97	0.16	29,29,29,29	0
8	GDP	B	501	28/28	0.98	0.16	19,20,21,23	0
6	MG	A	502	1/1	0.98	0.13	20,20,20,20	0
5	GTP	C	501	32/32	0.99	0.12	19,20,21,21	0
5	GTP	A	501	32/32	0.99	0.16	20,23,24,24	0
6	MG	C	502	1/1	0.99	0.13	20,20,20,20	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.

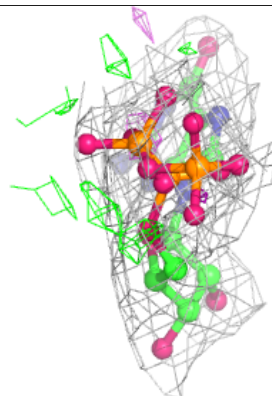
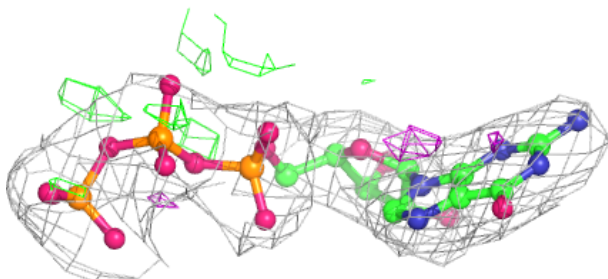
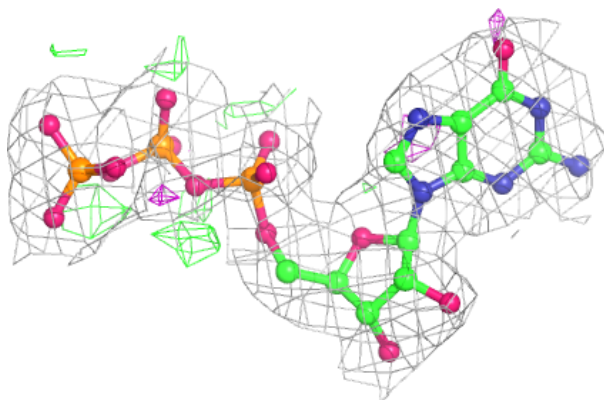


**Electron density around 8WR B 506:**

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

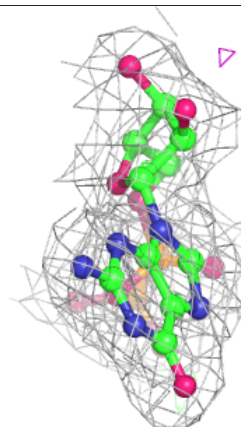
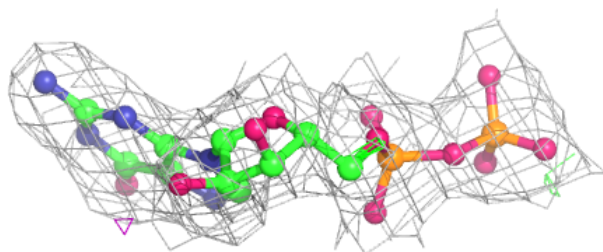
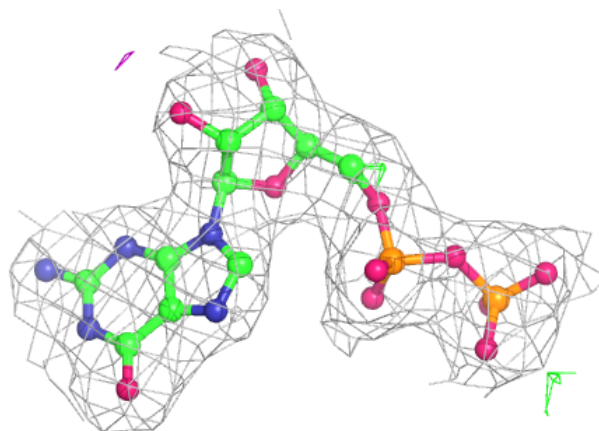
**Electron density around GTP D 501:**

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

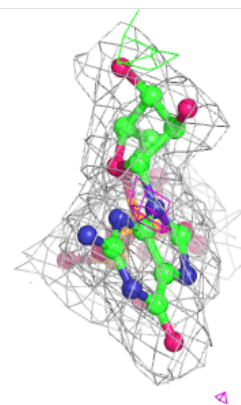
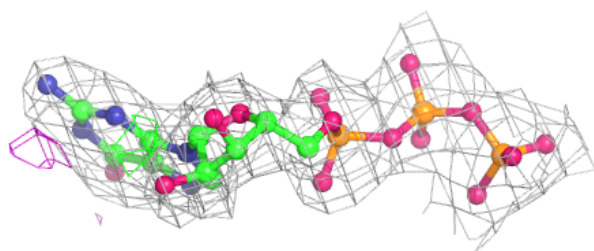
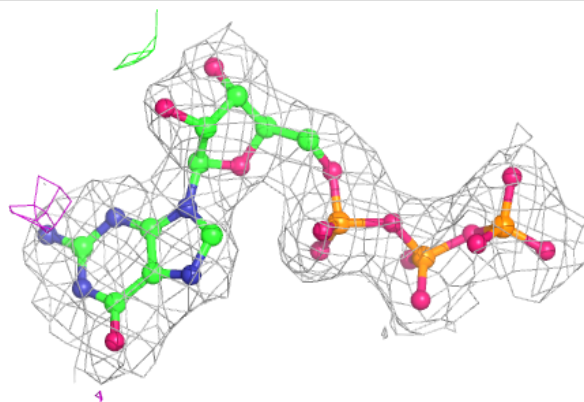


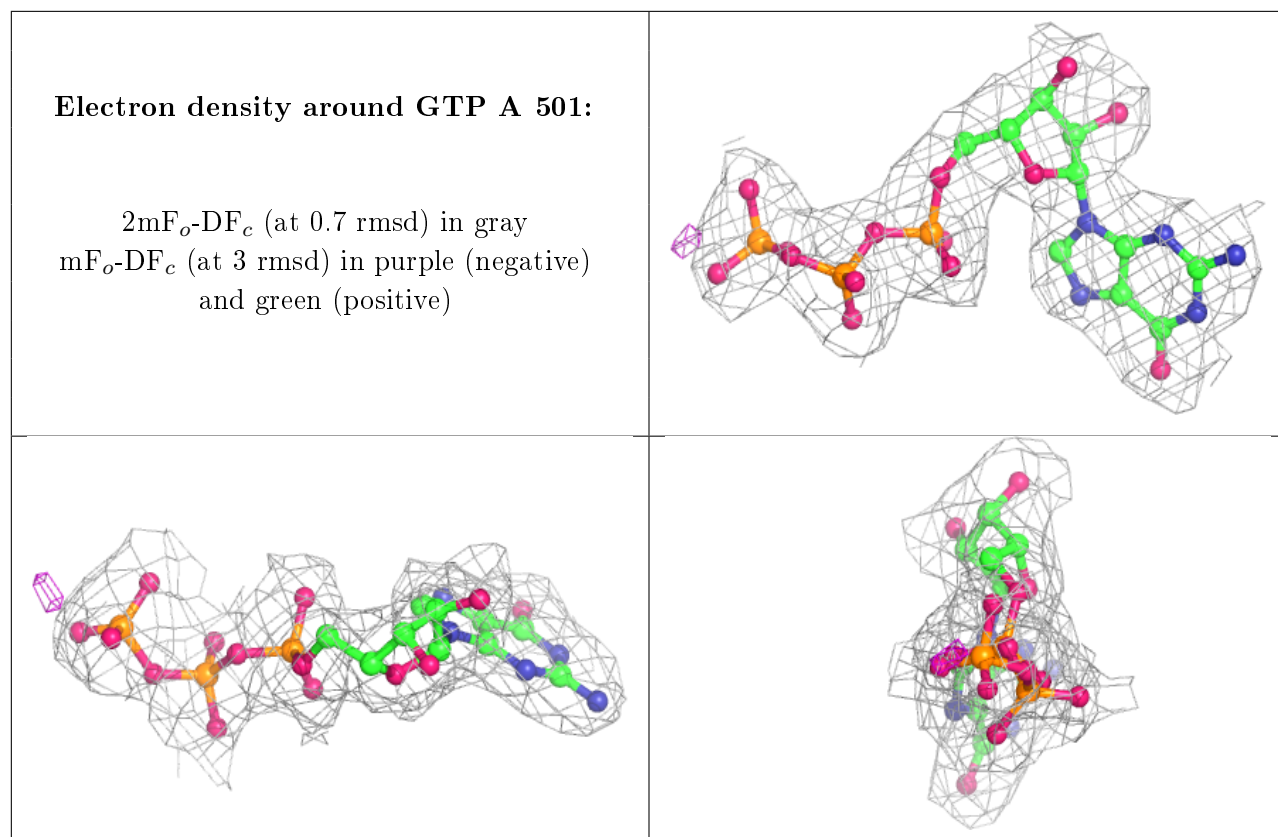
**Electron density around GDP B 501:**

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

**Electron density around GTP C 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.