



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 8, 2025 – 02:30 pm BST

PDB ID : 9GNU / pdb_00009gnu
Title : Tubulin in complex with a dioxane analog of zampanolide
Authors : Oliva, M.A.; Diaz, J.F.; Altmann, K.H.
Deposited on : 2024-09-04
Resolution : 2.20 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

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>.

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

MolProbity : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

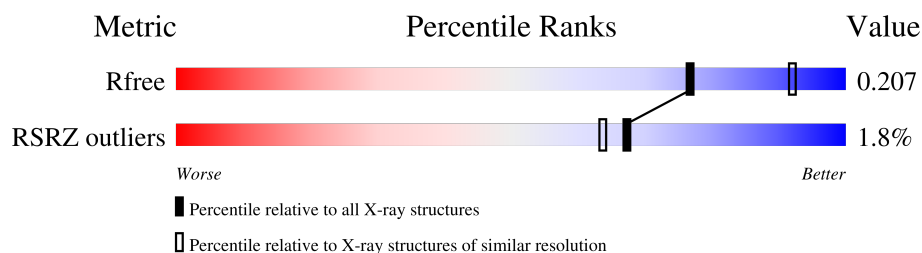
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	164625	5791 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 35660 atoms, of which 17150 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	434	Total	C	H	N	O	S	108	7	0
			6803	2173	3365	583	658	24			
1	C	439	Total	C	H	N	O	S	115	14	0
			6966	2225	3436	600	680	25			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	417	Total	C	H	N	O	S	102	10	0
			6605	2108	3241	572	657	27			
2	D	429	Total	C	H	N	O	S	105	5	0
			6701	2137	3292	583	661	28			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	114	Total	C	H	N	O	S	18	4	0
			1986	604	1008	181	189	4			

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	319	Total	C	H	N	O	S	77	3	0
			5283	1702	2637	449	482	13			

There are 39 discrepancies between the modelled and reference sequences:

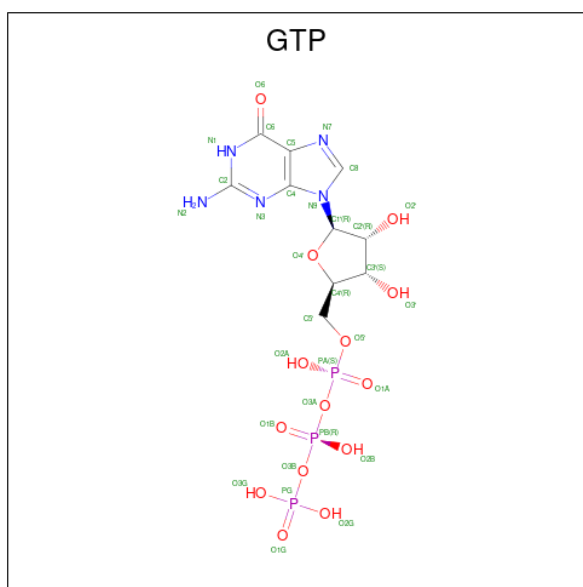
Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	MET	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	PRO	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	LYS	deletion	UNP A0A8V0Z8P0
F	?	-	ASN	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	PHE	deletion	UNP A0A8V0Z8P0
F	379	HIS	-	expression tag	UNP A0A8V0Z8P0
F	380	HIS	-	expression tag	UNP A0A8V0Z8P0
F	381	HIS	-	expression tag	UNP A0A8V0Z8P0
F	382	HIS	-	expression tag	UNP A0A8V0Z8P0
F	383	HIS	-	expression tag	UNP A0A8V0Z8P0
F	384	HIS	-	expression tag	UNP A0A8V0Z8P0

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	A	1	Total 44	C 10	H 12	N 5	O 14	P 3	2	0
5	C	1	Total 44	C 10	H 12	N 5	O 14	P 3	2	0
5	D	1	Total 44	C 10	H 12	N 5	O 14	P 3	2	0

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

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

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

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

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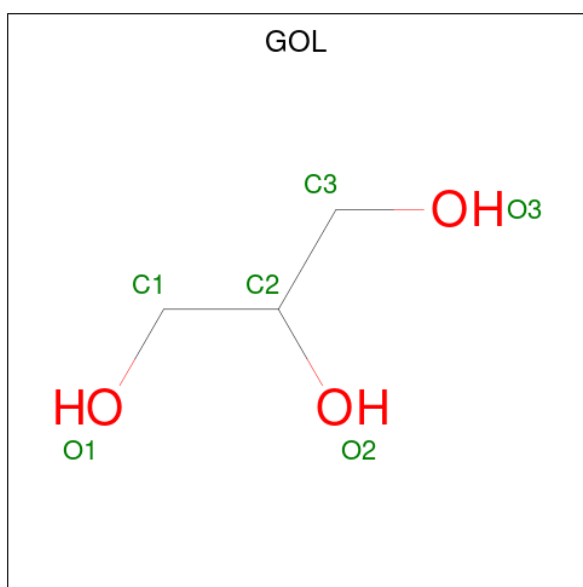
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

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

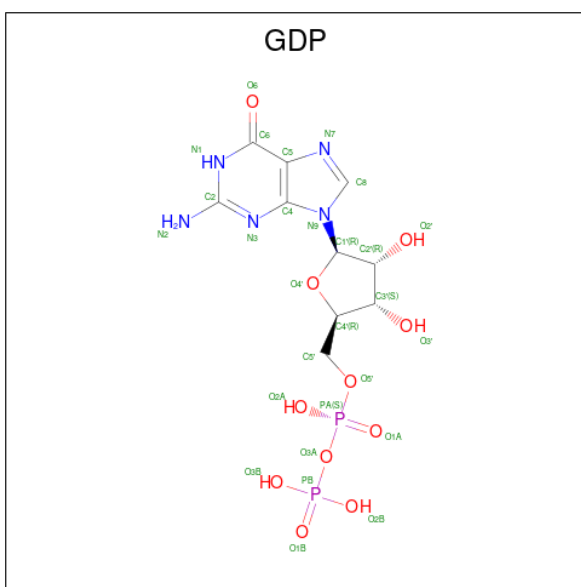
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



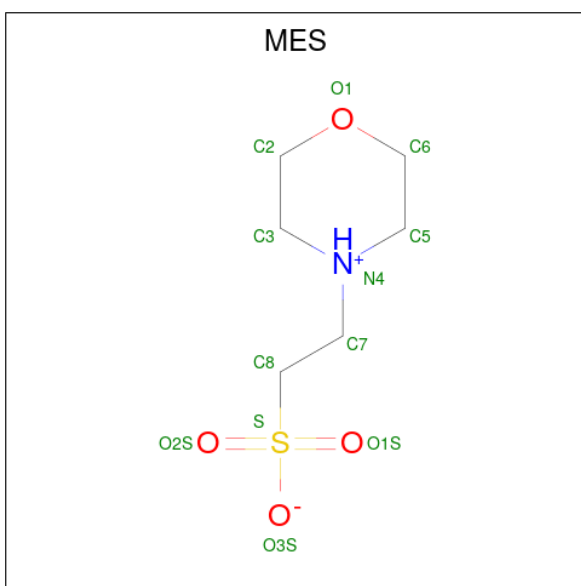
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	H	O	3	0
			14	3	8	3		
9	B	1	Total	C	H	O	3	0
			14	3	8	3		
9	C	1	Total	C	H	O	3	0
			14	3	8	3		

- Molecule 10 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	P	2	0
			40	10	12	5	11	2		

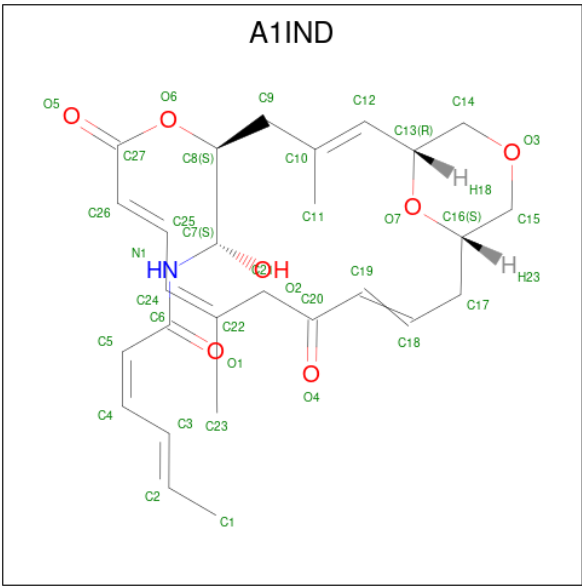
- Molecule 11 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
11	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

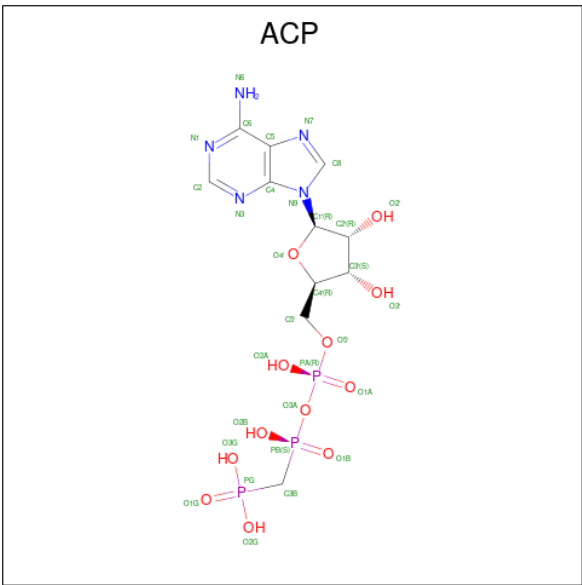
- Molecule 12 is (2Z,4E)-N-((S)-((1R,2E,5S,8E,10Z,14E,17S)-3,11-dimethyl-7,13-dioxo-6,19,21-trioxabicyclo[15.3.1]henicosa-2,8,10,14-tetraen-5-yl)(hydroxy)methyl)hexa-2,4-dienamide

(CCD ID: A1IND) (formula: C₂₇H₃₅NO₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	B	1	Total	C	H	N	O	10	0
			71	27	36	1	7		
12	D	1	Total	C	H	N	O	10	0
			71	27	36	1	7		

- Molecule 13 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
13	F	1	Total	C	H	N	O	P	2	0
			45	11	14	5	12	3		

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	169	Total	O	0	0
			169	169		
14	B	149	Total	O	0	0
			149	149		
14	C	296	Total	O	0	0
			296	296		
14	D	141	Total	O	0	0
			141	141		
14	E	43	Total	O	0	0
			43	43		
14	F	82	Total	O	0	0
			82	82		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.20Å 159.17Å 178.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.14 – 2.20 48.14 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.14-2.20) 99.9 (48.14-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.164 , 0.206 0.165 , 0.207	Depositor DCC
R_{free} test set	7610 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	43.5	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	35660	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 10 are monoatomic - leaving 11 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
12	A1IND	D	503	2	34,36,36	1.74	3 (8%)	34,46,46	2.02	6 (17%)
5	GTP	D	501	6	26,34,34	1.50	6 (23%)	32,54,54	0.96	2 (6%)
5	GTP	C	501	6	26,34,34	1.13	2 (7%)	32,54,54	1.11	2 (6%)
5	GTP	A	501	6	26,34,34	1.31	4 (15%)	32,54,54	1.18	3 (9%)
10	GDP	B	501	6	24,30,30	1.15	1 (4%)	30,47,47	0.73	0
13	ACP	F	401	6	27,33,33	1.06	2 (7%)	32,52,52	1.14	4 (12%)
12	A1IND	B	506	2	34,36,36	1.42	1 (2%)	34,46,46	2.26	8 (23%)
9	GOL	A	506	-	5,5,5	0.47	0	5,5,5	0.91	0
11	MES	B	502	-	12,12,12	0.91	0	14,16,16	1.21	2 (14%)
9	GOL	C	504	-	5,5,5	0.16	0	5,5,5	0.49	0
9	GOL	B	503	-	5,5,5	0.32	0	5,5,5	0.74	0

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
12	A1IND	D	503	2	-	6/41/51/51	0/0/2/2
5	GTP	D	501	6	-	7/18/38/38	0/3/3/3
5	GTP	C	501	6	-	6/18/38/38	0/3/3/3
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
10	GDP	B	501	6	-	4/12/32/32	0/3/3/3
13	ACP	F	401	6	-	4/15/38/38	0/3/3/3
12	A1IND	B	506	2	-	5/41/51/51	0/0/2/2
9	GOL	A	506	-	-	2/4/4/4	-
11	MES	B	502	-	-	2/6/14/14	0/1/1/1
9	GOL	C	504	-	-	2/4/4/4	-
9	GOL	B	503	-	-	0/4/4/4	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	503	A1IND	C19-C18	7.86	1.52	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	506	A1IND	C19-C18	7.53	1.51	1.32
5	D	501	GTP	C5-C6	-4.33	1.38	1.47
10	B	501	GDP	C5-C6	-3.53	1.40	1.47
12	D	503	A1IND	O7-C13	-3.40	1.35	1.44
5	A	501	GTP	C5-C6	-3.02	1.41	1.47
5	C	501	GTP	PG-O2G	-2.98	1.43	1.54
5	A	501	GTP	O4'-C1'	2.94	1.45	1.41
13	F	401	ACP	PG-O1G	2.90	1.56	1.50
5	C	501	GTP	C5-C6	-2.71	1.41	1.47
13	F	401	ACP	PB-O3A	2.56	1.61	1.58
12	D	503	A1IND	C25-C24	-2.40	1.36	1.43
5	D	501	GTP	C8-N7	-2.31	1.31	1.35
5	A	501	GTP	C5-C4	-2.31	1.37	1.43
5	D	501	GTP	PG-O1G	2.23	1.57	1.50
5	D	501	GTP	C5-C4	-2.22	1.37	1.43
5	A	501	GTP	C8-N7	-2.21	1.31	1.35
5	D	501	GTP	PG-O3G	2.08	1.62	1.54
5	D	501	GTP	C6-N1	2.03	1.40	1.37

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	506	A1IND	O1-C6-N1	-9.14	110.28	122.35
12	D	503	A1IND	C17-C18-C19	-6.14	112.28	126.00
12	D	503	A1IND	O7-C16-C15	4.44	113.71	109.68
12	B	506	A1IND	C7-N1-C6	4.11	126.02	121.30
12	D	503	A1IND	O1-C6-N1	-4.11	116.92	122.35
12	D	503	A1IND	O3-C15-C16	-4.10	102.92	111.40
12	B	506	A1IND	C17-C18-C19	-3.56	118.03	126.00
12	B	506	A1IND	O1-C6-C5	3.53	131.09	123.03
12	D	503	A1IND	C7-N1-C6	3.50	125.33	121.30
12	B	506	A1IND	O7-C16-C15	3.44	112.80	109.68
5	C	501	GTP	O2A-PA-O1A	2.87	126.43	112.24
12	D	503	A1IND	O4-C20-C19	2.83	129.94	120.50
13	F	401	ACP	O3G-PG-C3B	2.79	113.16	106.40
11	B	502	MES	O2S-S-C8	-2.78	103.57	106.92
5	D	501	GTP	PB-O3B-PG	-2.72	123.48	132.83
13	F	401	ACP	O1G-PG-C3B	-2.52	105.82	111.24
5	A	501	GTP	O3G-PG-O2G	2.47	117.08	107.64
12	B	506	A1IND	C14-C13-C12	2.47	115.65	111.83
12	B	506	A1IND	C4-C5-C6	2.41	128.63	122.57
13	F	401	ACP	O2G-PG-C3B	-2.31	100.80	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	O2'-C2'-C3'	2.27	119.16	111.82
11	B	502	MES	O1S-S-C8	-2.17	104.30	106.92
5	C	501	GTP	O6-C6-C5	2.17	128.61	124.37
13	F	401	ACP	C5-C6-N6	2.14	123.61	120.35
5	D	501	GTP	PA-O3A-PB	-2.13	125.53	132.83
5	A	501	GTP	O6-C6-C5	2.01	128.30	124.37
12	B	506	A1IND	C5-C6-N1	2.01	118.42	114.56

There are no chirality outliers.

All (44) 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	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	PB-O3B-PG-O2G
5	D	501	GTP	C5'-O5'-PA-O1A
5	D	501	GTP	C5'-O5'-PA-O2A
9	C	504	GOL	C1-C2-C3-O3
10	B	501	GDP	C5'-O5'-PA-O1A
10	B	501	GDP	C5'-O5'-PA-O2A
12	B	506	A1IND	O7-C16-C17-C18
12	B	506	A1IND	O4-C20-C21-C22
12	B	506	A1IND	C17-C18-C19-C20
13	F	401	ACP	C5'-O5'-PA-O1A
13	F	401	ACP	C5'-O5'-PA-O3A
12	B	506	A1IND	C15-C16-C17-C18
12	D	503	A1IND	C15-C16-C17-C18
12	D	503	A1IND	O4-C20-C21-C22
12	D	503	A1IND	O7-C16-C17-C18
11	B	502	MES	C8-C7-N4-C5
9	C	504	GOL	O2-C2-C3-O3
5	A	501	GTP	PB-O3B-PG-O3G
5	D	501	GTP	PB-O3B-PG-O3G
9	A	506	GOL	O1-C1-C2-O2
12	D	503	A1IND	C19-C20-C21-C22
5	C	501	GTP	C4'-C5'-O5'-PA
11	B	502	MES	C8-C7-N4-C3
5	A	501	GTP	PB-O3B-PG-O1G

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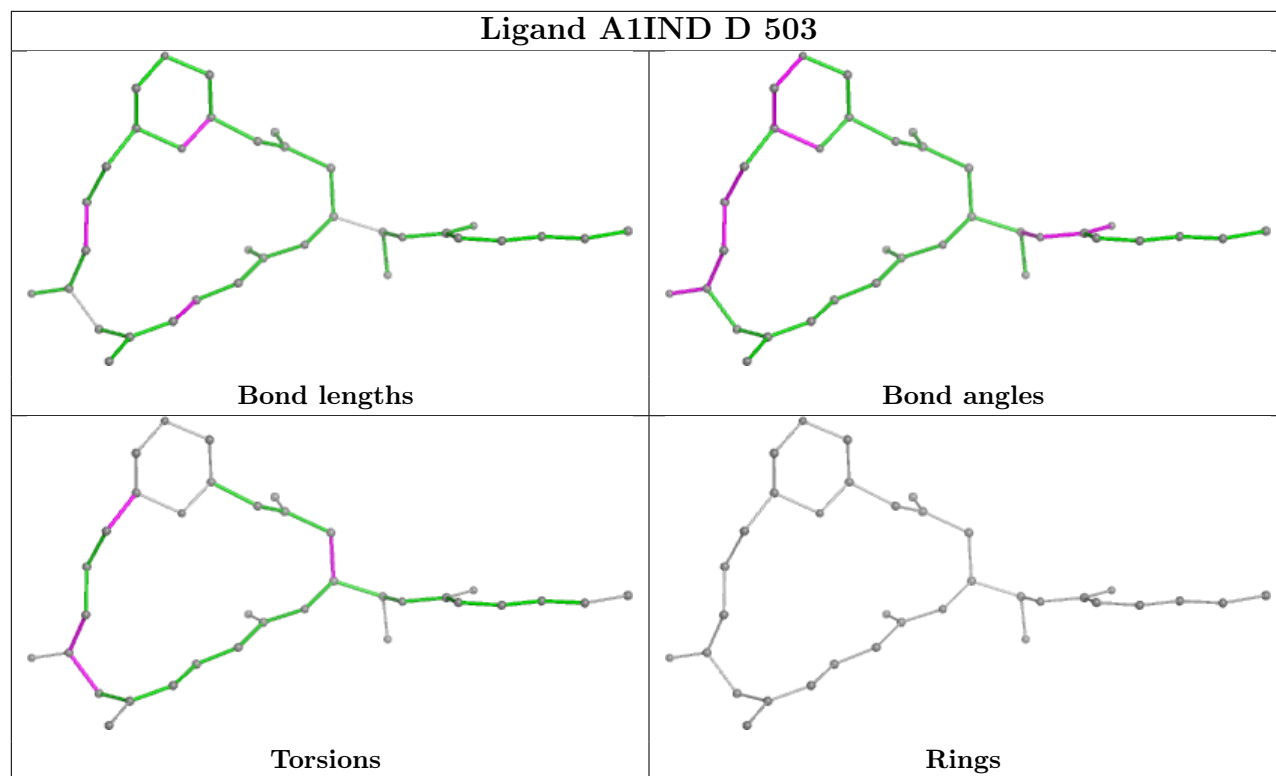
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C4'-C5'-O5'-PA
10	B	501	GDP	C4'-C5'-O5'-PA
12	B	506	A1IND	C7-C8-C9-C10
12	D	503	A1IND	C7-C8-C9-C10
13	F	401	ACP	PB-O3A-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O3A
10	B	501	GDP	C5'-O5'-PA-O3A
5	D	501	GTP	PB-O3A-PA-O1A
9	A	506	GOL	O1-C1-C2-C3
12	D	503	A1IND	C18-C19-C20-C21
13	F	401	ACP	C5'-O5'-PA-O2A
5	D	501	GTP	C4'-C5'-O5'-PA

There are no ring outliers.

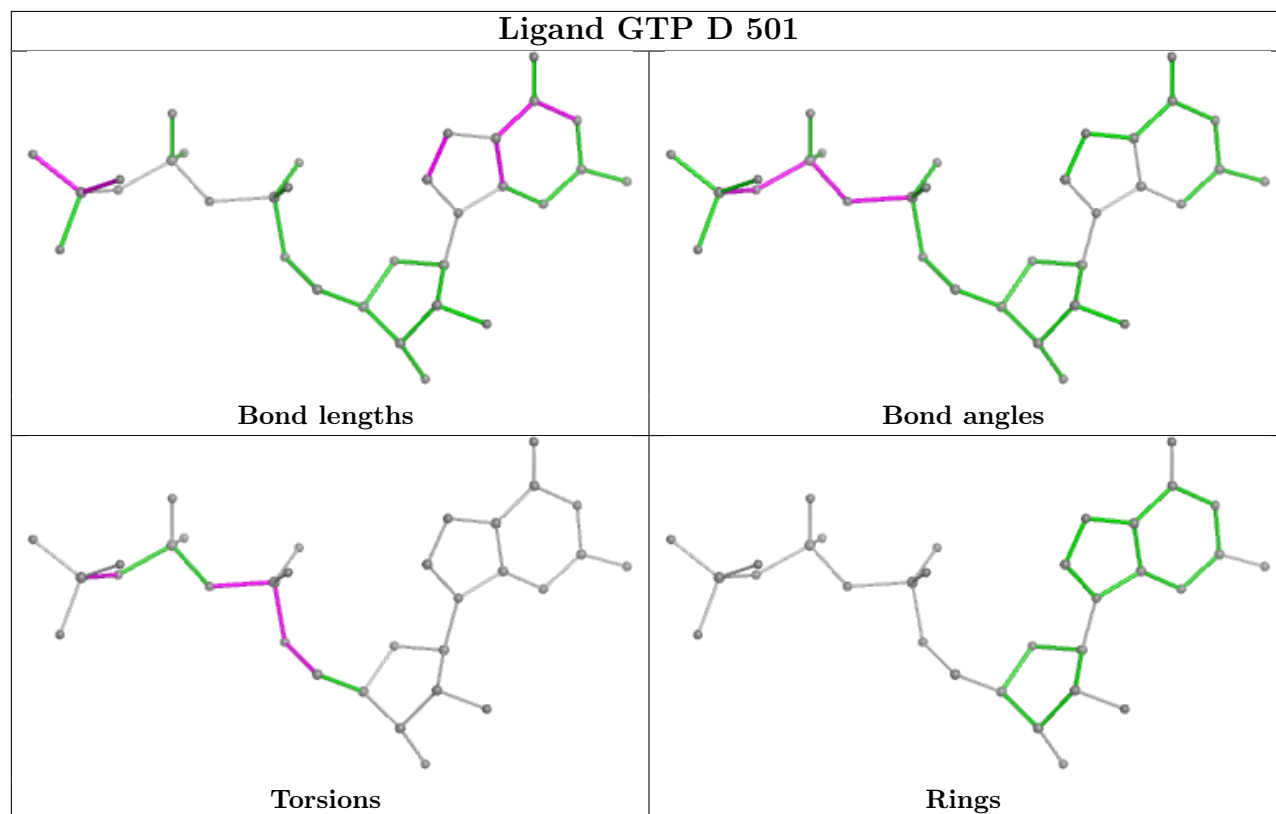
No monomer is involved in short contacts.

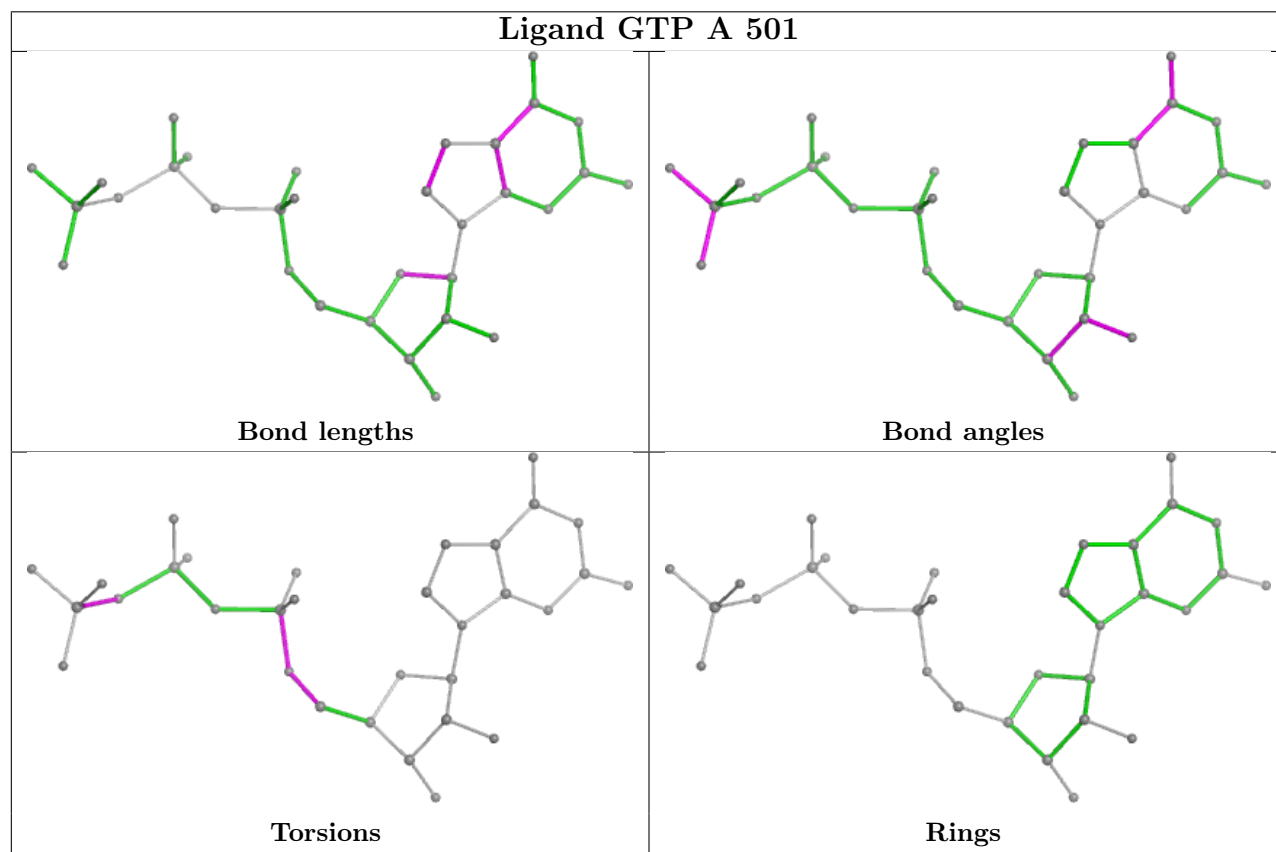
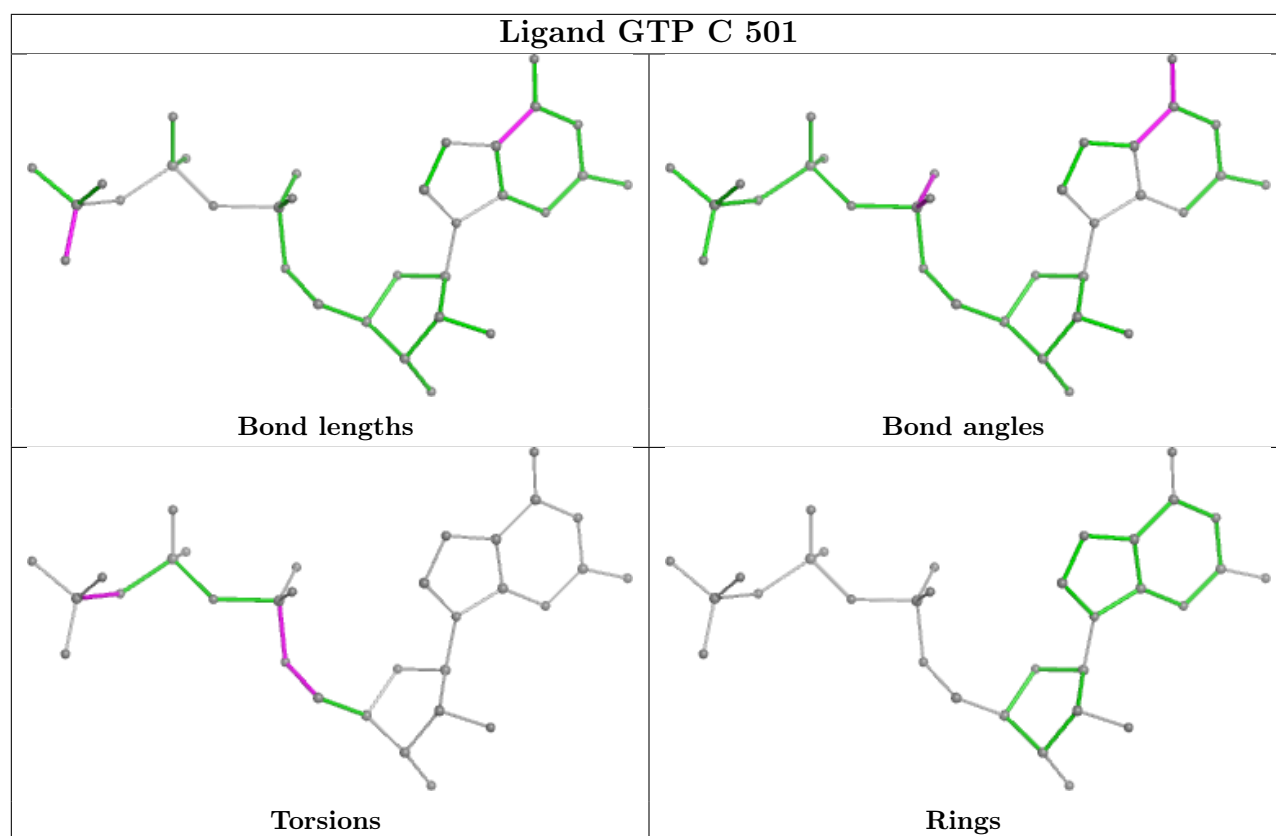
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

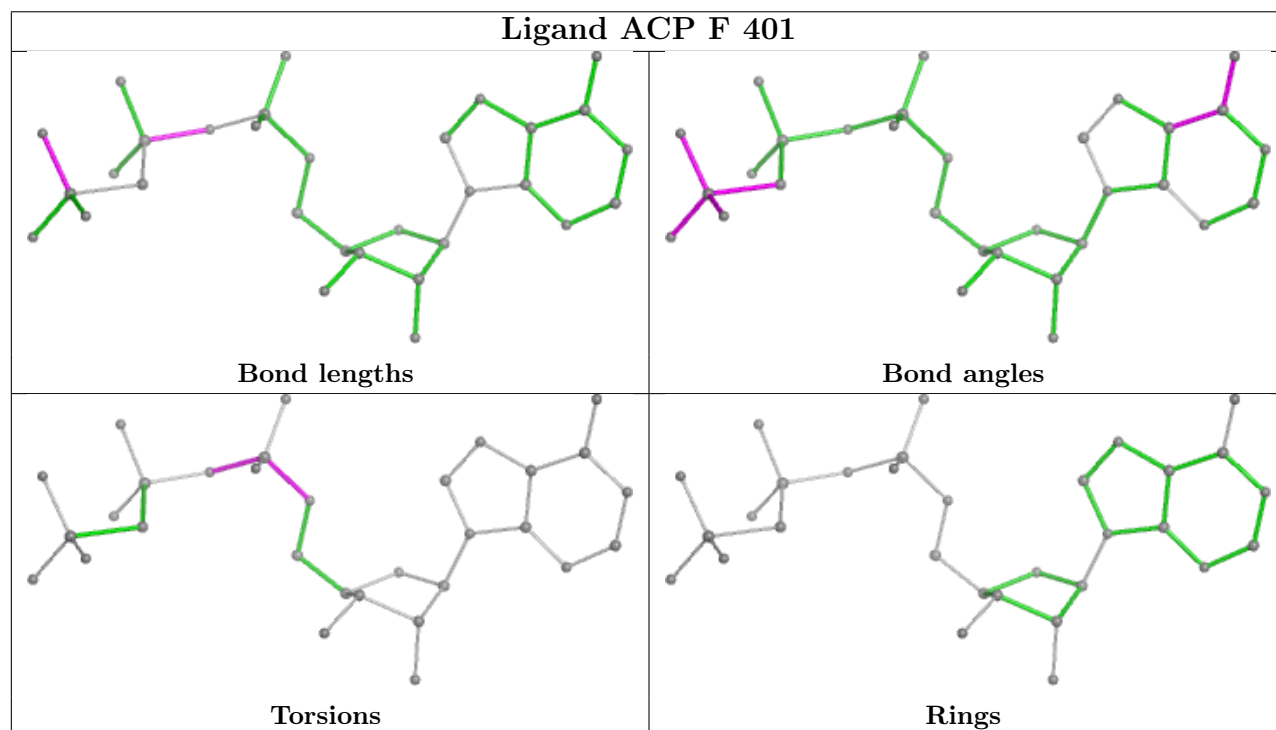
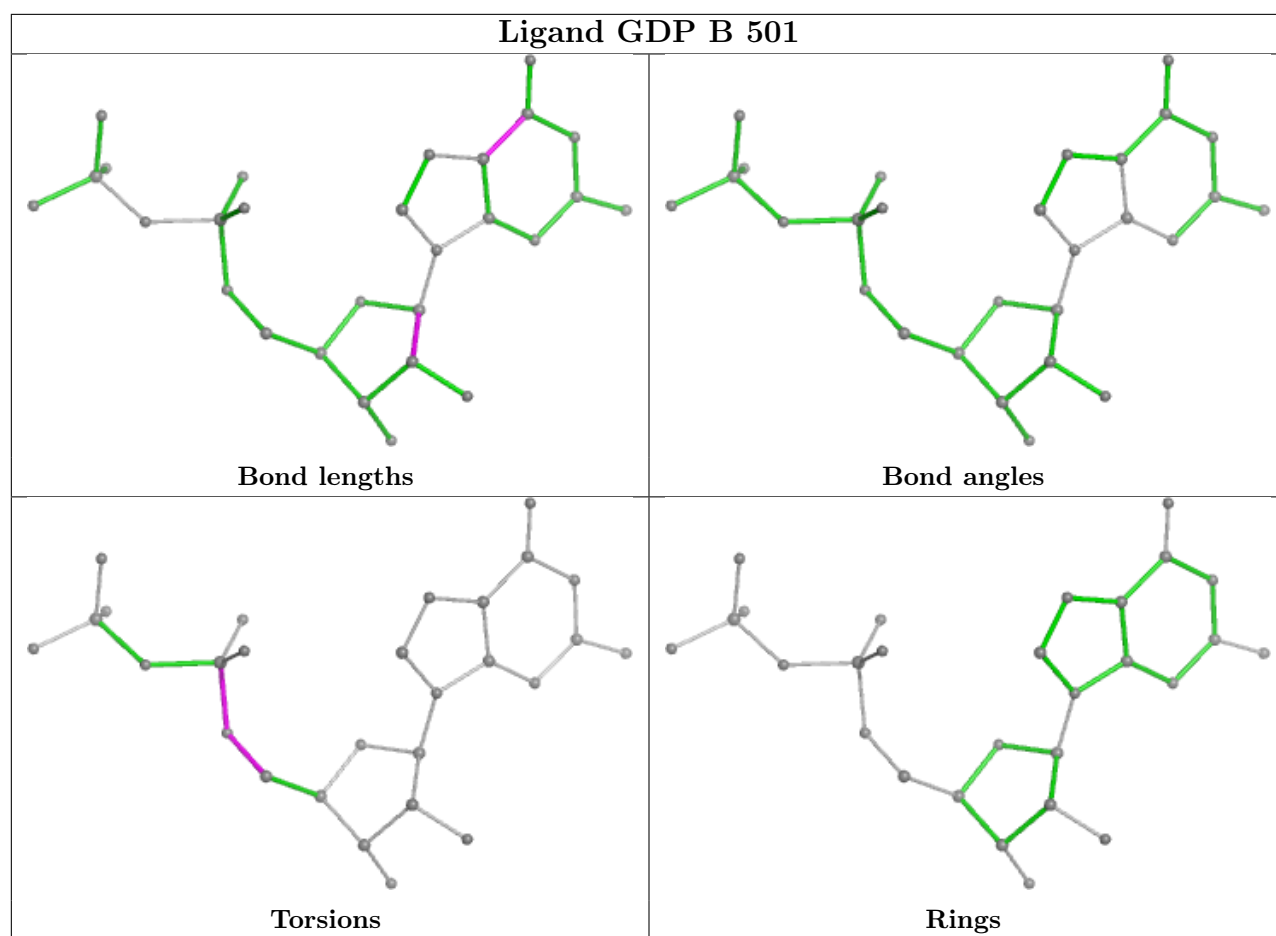
Ligand A1IND D 503

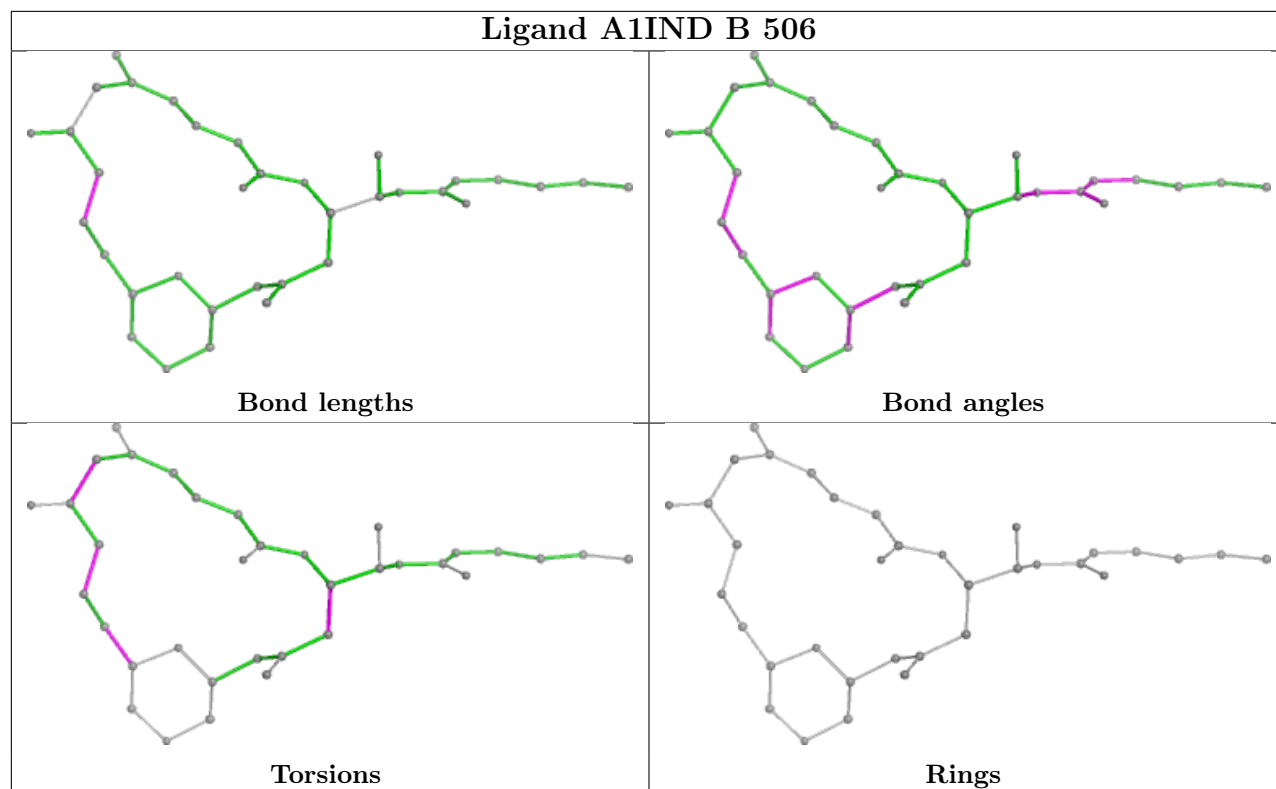


Ligand GTP D 501









4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 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, 95th 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 ²)	Q<0.9
1	A	434/451 (96%)	-0.57	6 (1%)	73 70	19, 47, 78, 108	7 (1%)
1	C	439/451 (97%)	-0.69	8 (1%)	67 64	14, 38, 66, 103	14 (3%)
2	B	417/445 (93%)	-0.43	6 (1%)	73 70	16, 48, 87, 125	12 (2%)
2	D	429/445 (96%)	-0.44	4 (0%)	81 78	18, 50, 84, 112	9 (2%)
3	E	114/189 (60%)	-0.07	3 (2%)	57 54	19, 59, 97, 118	4 (3%)
4	F	319/384 (83%)	-0.30	11 (3%)	48 45	21, 60, 95, 122	3 (0%)
All	All	2152/2365 (90%)	-0.48	38 (1%)	67 64	14, 48, 87, 125	49 (2%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	237	THR	4.7
3	E	27	PRO	4.4
3	E	139	LEU	4.2
1	C	163	LYS	4.1
1	C	340	SER	3.9
1	A	346	TRP	3.8
2	B	438	ALA	3.6
4	F	125	THR	3.6
4	F	152	SER	3.3
1	C	358[A]	GLN	3.2
2	D	82	PRO	3.2
1	C	440	VAL	3.2
4	F	379	HIS	3.1
2	B	325	MET	3.1
4	F	362	ALA	2.9
4	F	373	SER	2.8
1	A	262	TYR	2.8
1	A	438	ASP	2.8
4	F	240	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	196[A]	GLU	2.7
1	C	283	HIS	2.6
4	F	131	PHE	2.6
4	F	179	VAL	2.5
1	A	279	GLU	2.5
2	D	440	ALA	2.5
1	C	245	ASP	2.4
2	B	1	MET	2.4
1	A	437	VAL	2.4
2	D	407	TRP	2.4
2	D	57	THR	2.3
1	A	284	GLU	2.2
2	B	176	LYS	2.2
4	F	230	SER	2.2
1	C	2	ARG	2.1
4	F	136	ASN	2.1
2	B	333	LEU	2.1
2	B	26[A]	ASP	2.0
3	E	115[A]	HIS	2.0

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

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 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, 95th 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 ²)	Q<0.9
6	MG	D	502	1/1	0.78	0.29	74,74,74,74	0
9	GOL	A	506	6/6	0.90	0.14	30,72,78,78	3
6	MG	F	402	1/1	0.91	0.17	59,59,59,59	0
7	CA	B	505	1/1	0.94	0.07	82,82,82,82	0

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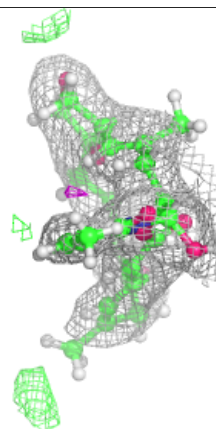
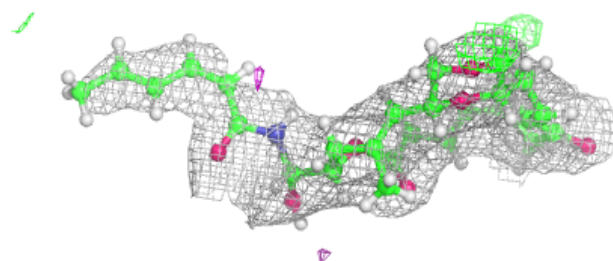
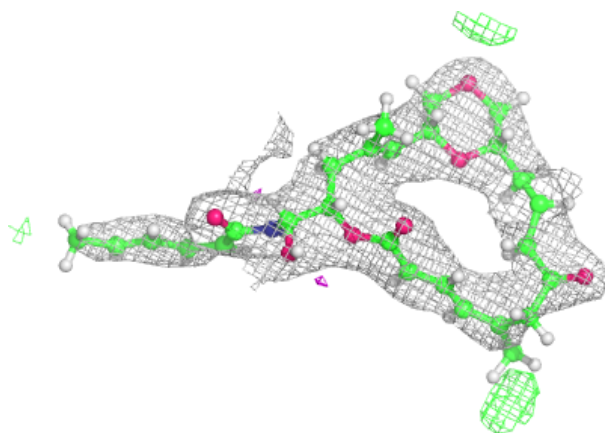
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	GOL	B	503	6/6	0.94	0.12	30,70,74,75	3
9	GOL	C	504	6/6	0.94	0.14	30,75,80,94	3
12	A1IND	B	506	35/35	0.94	0.10	30,63,76,77	10
13	ACP	F	401	31/31	0.95	0.06	30,64,85,99	2
7	CA	A	505	1/1	0.96	0.08	92,92,92,92	0
11	MES	B	502	12/12	0.97	0.07	44,52,59,81	0
5	GTP	D	501	32/32	0.98	0.05	30,48,69,88	2
12	A1IND	D	503	35/35	0.98	0.06	30,47,60,66	10
8	CL	A	504	1/1	0.98	0.06	67,67,67,67	0
10	GDP	B	501	28/28	0.99	0.04	30,35,41,42	2
5	GTP	C	501	32/32	0.99	0.04	26,30,33,35	2
5	GTP	A	501	32/32	0.99	0.03	30,34,38,39	2
6	MG	A	502	1/1	0.99	0.07	36,36,36,36	0
6	MG	C	502	1/1	0.99	0.08	31,31,31,31	0
6	MG	B	504	1/1	1.00	0.06	29,29,29,29	0
7	CA	A	503	1/1	1.00	0.04	60,60,60,60	0
7	CA	C	503	1/1	1.00	0.01	50,50,50,50	0

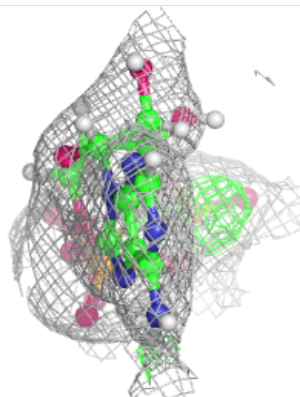
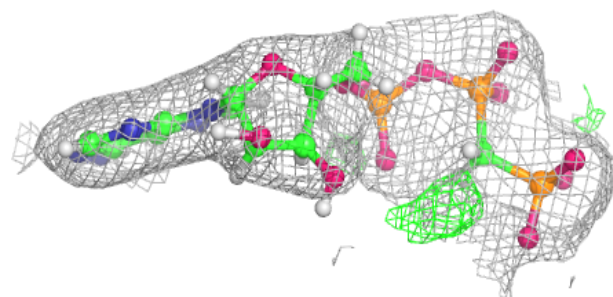
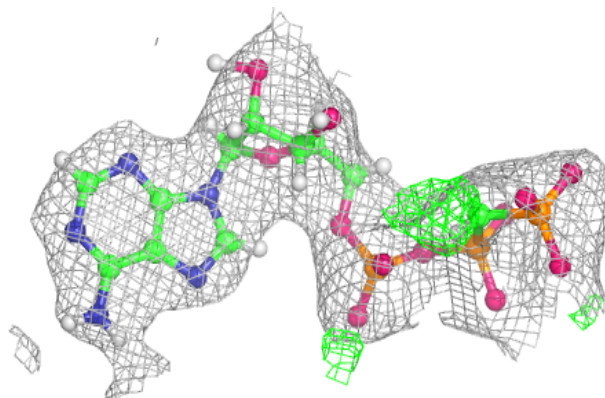
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1IND 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)

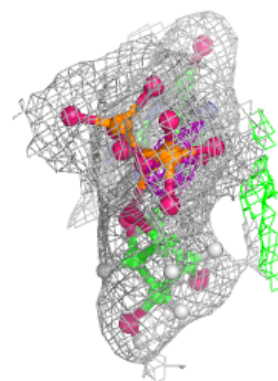
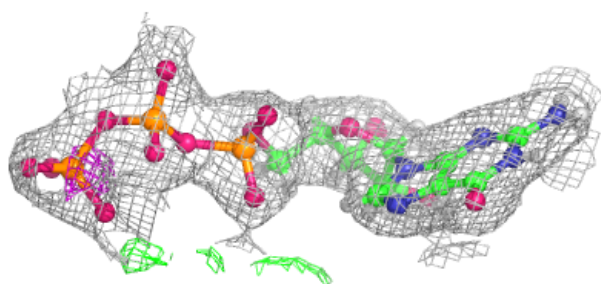
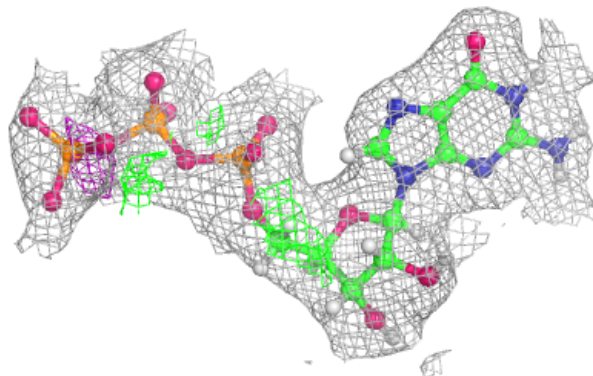
**Electron density around ACP F 401:**

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

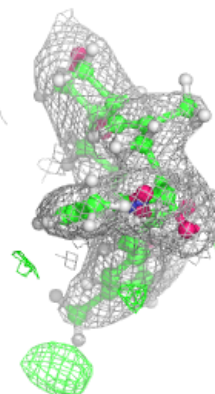
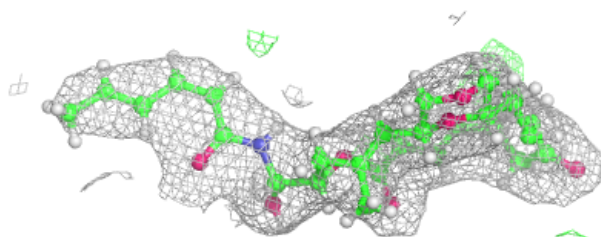
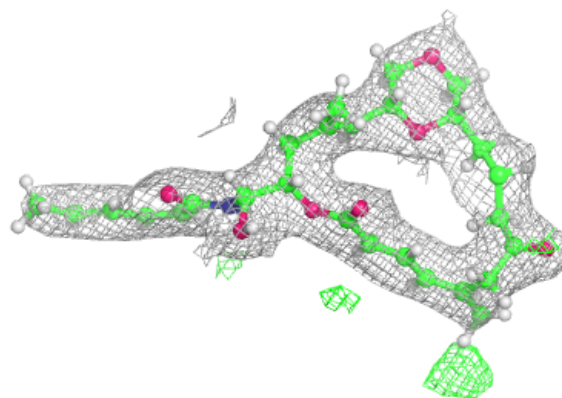


Electron density around GTP D 501:

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

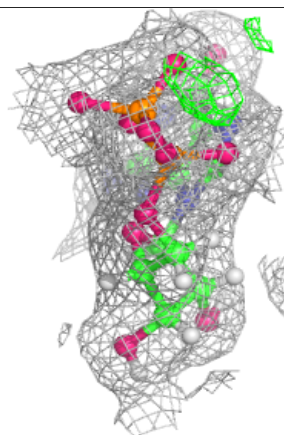
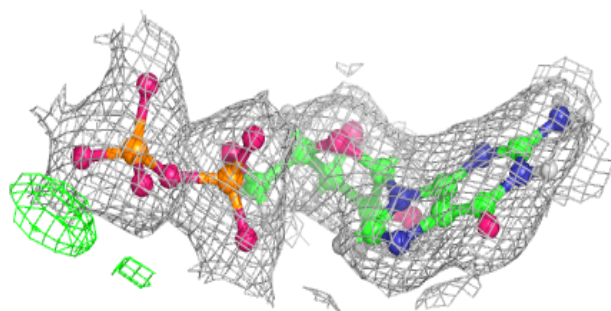
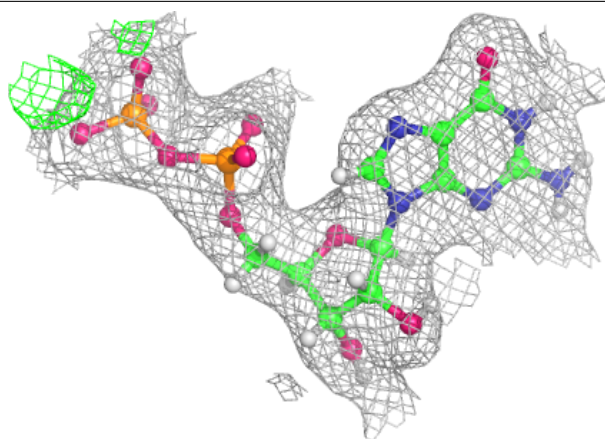
**Electron density around A1IND D 503:**

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



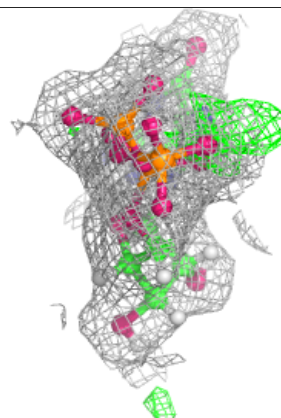
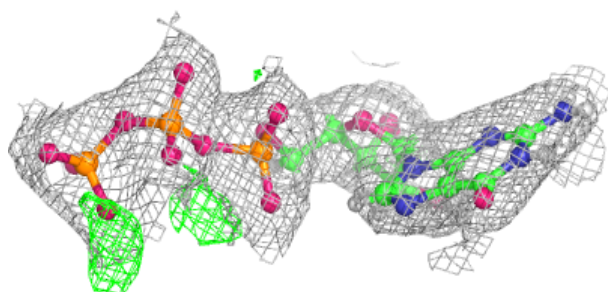
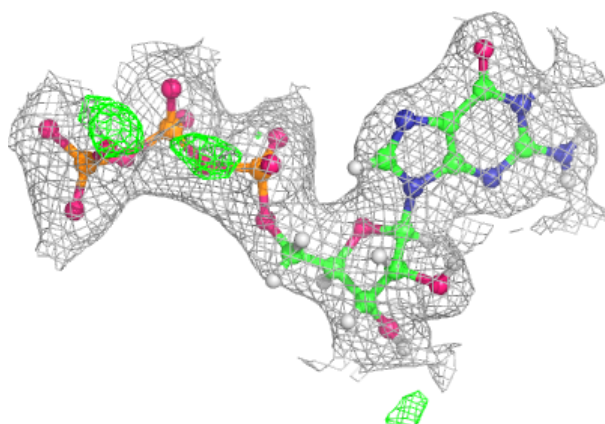
Electron density around GDP B 501:

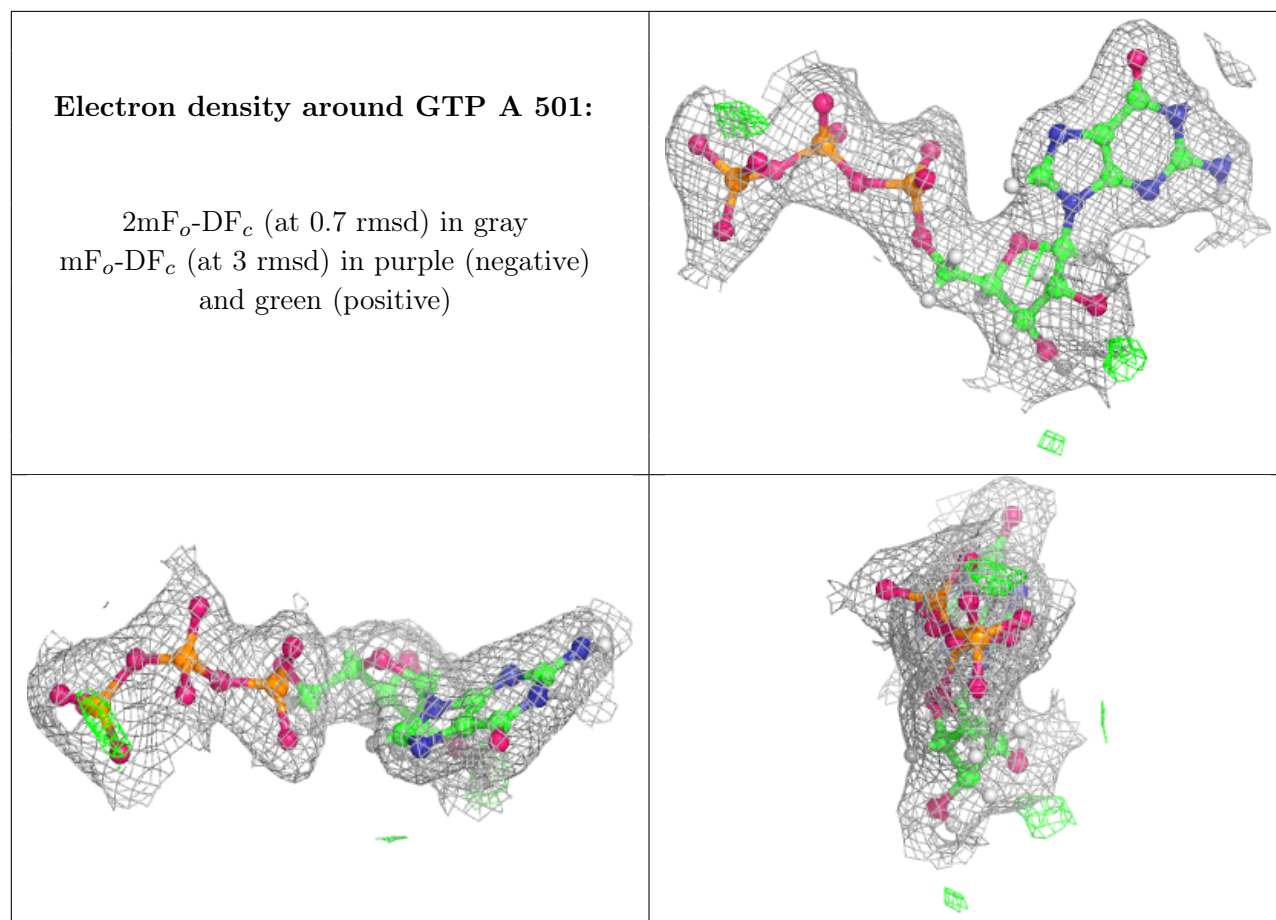
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





5.5 Other polymers ⓘ

There are no such residues in this entry.