



wwPDB X-ray Structure Validation Summary Report ⓘ

May 18, 2020 – 11:29 am BST

PDB ID : 5NJH
Title : Triazolopyrimidines stabilize microtubules by binding to the vinca inhibitor site of tubulin
Authors : Sharma, A.; Calvo, G.S.; Prota, A.E.; Diaz, J.F.; Steinmetz, M.O.
Deposited on : 2017-03-28
Resolution : 2.39 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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 : 2.11
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) : 2.11

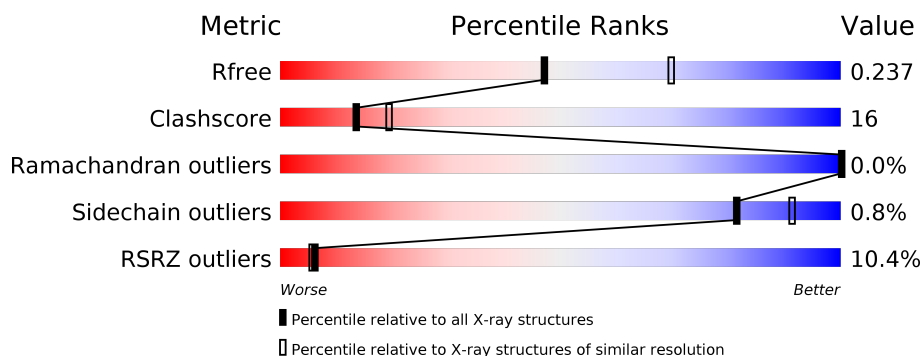
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 ≥ 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>6%</div> <div> <div></div> <div>74%</div> <div>21%</div> <div>..</div> </div> </div>
1	C	450	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>18%</div> <div>.</div> </div> </div>
2	B	445	<div> <div>8%</div> <div> <div></div> <div>71%</div> <div>21%</div> <div>7%</div> </div> </div>
2	D	445	<div> <div>11%</div> <div> <div></div> <div>75%</div> <div>20%</div> <div>5%</div> </div> </div>
3	E	143	<div> <div>10%</div> <div> <div></div> <div>69%</div> <div>15%</div> <div>15%</div> </div> </div>
4	F	384	<div> <div>20%</div> <div> <div></div> <div>64%</div> <div>23%</div> <div>12%</div> </div> </div>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 17810 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
1	A	435	Total	C	N	O	S	0	0	0
			3393	2147	577	647	22			
1	C	439	Total	C	N	O	S	0	11	0
			3480	2207	585	665	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	413	Total	C	N	O	S	3	4	0
			3258	2049	552	631	26			
2	D	424	Total	C	N	O	S	1	5	0
			3350	2107	568	647	28			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	1	0
			1006	621	182	198	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	ILE	conflict	UNP P63043
E	4	ALA	SER	conflict	UNP P63043

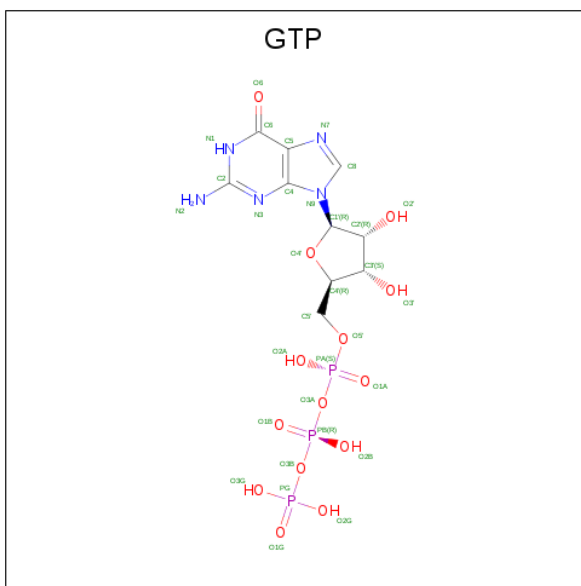
- Molecule 4 is a protein called tubulin tyrosine ligase TTL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	339	Total	C	N	O	S	0	0	0
			2777	1781	475	507	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
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

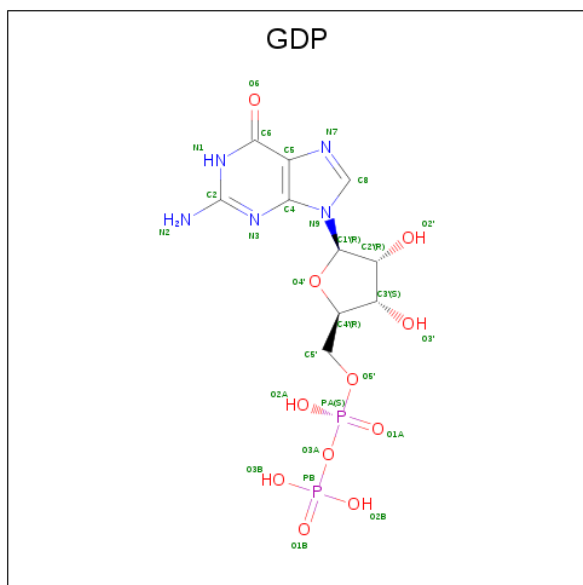
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		
6	A	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		

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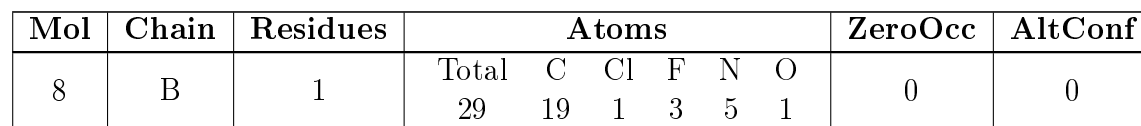
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 8 is 5-chloranyl-7-[(1 {R},5 {S})-3-methoxy-8-azabicyclo[3.2.1]octan-8-yl]-6-[2,4,6-tris(fluoranyl)phenyl]-[1,2,4]triazolo[1,5-a]pyrimidine (three-letter code: 8Z8) (formula: $C_{19}H_{17}ClF_3N_5O$).



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- The chemical structure of ACP (Adenosine Cyclic Phosphate) is shown. It consists of a nucleoside moiety (adenine base and ribose sugar) linked to a cyclic pyrophosphate group. The adenine base is represented by a blue-colored ring system with atoms labeled N1, N3, N7, N9, C2, C4, C6, and C8. The ribose sugar is a five-membered ring with oxygen atoms O4' and O3', and carbon atoms C3', C4', and C5'. The pyrophosphate group is shown as two phosphorus atoms (P1 and P2) bridged by an oxygen atom (O5'). The phosphate groups are further linked to oxygen atoms O1A, O1B, O1C, O2A, O2B, O2C, O3A, O3B, O3C, O4A, O4B, and O4C. The structure is labeled "ACP" at the top.

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

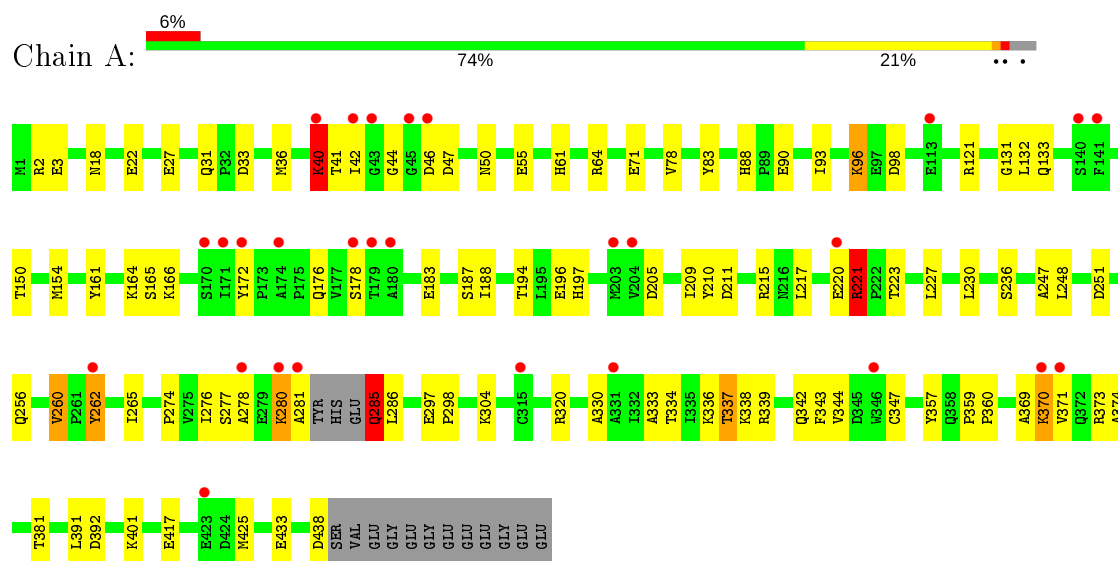
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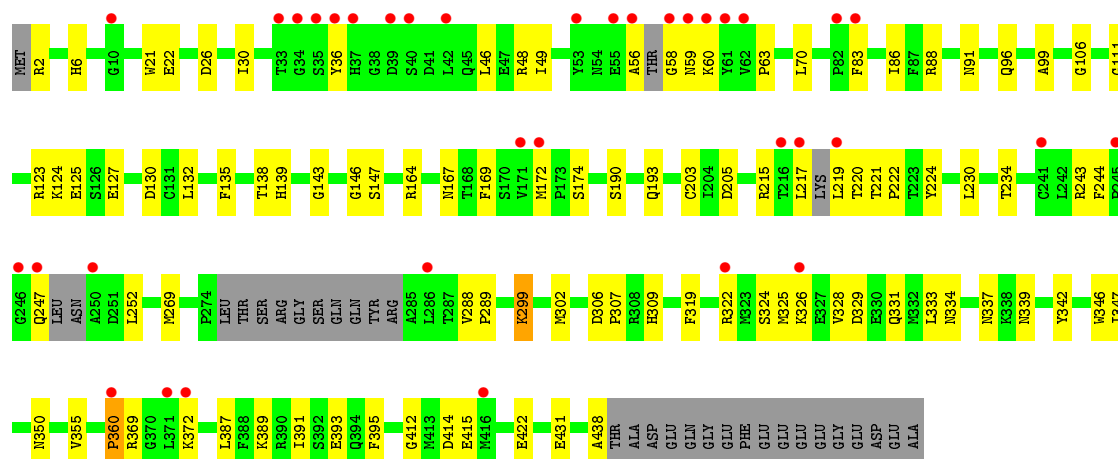
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	79	Total 79	O 79	0	0
10	B	59	Total 59	O 59	0	0
10	C	98	Total 98	O 98	0	0
10	D	62	Total 62	O 62	0	0
10	E	18	Total 18	O 18	0	0
10	F	45	Total 45	O 45	0	0

3 Residue-property plots [i](#)

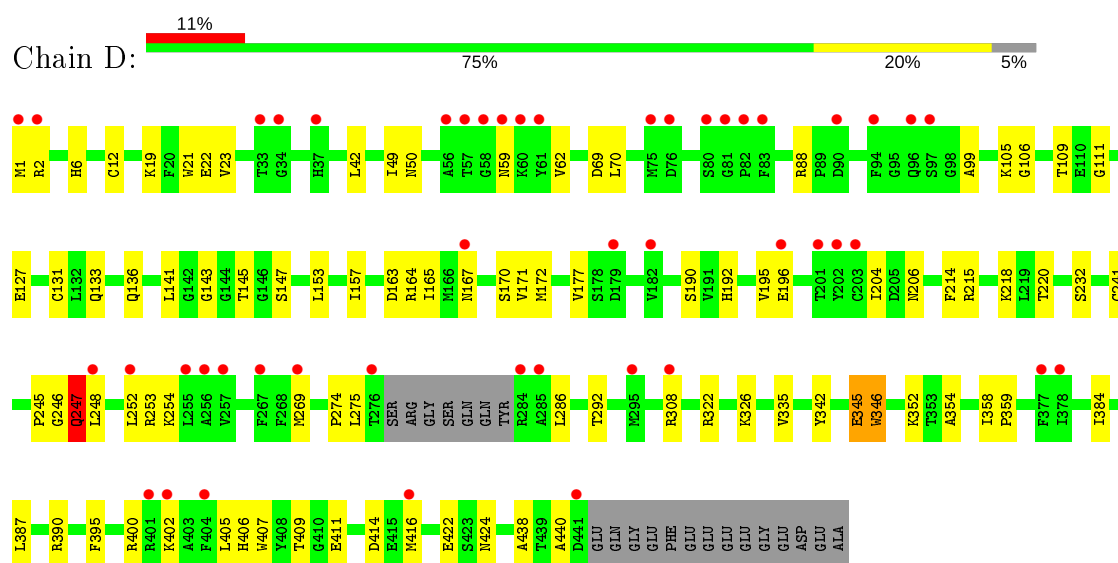
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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

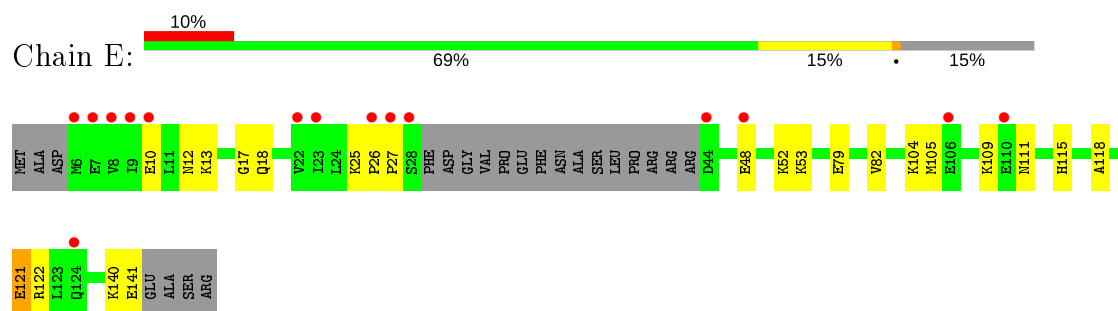




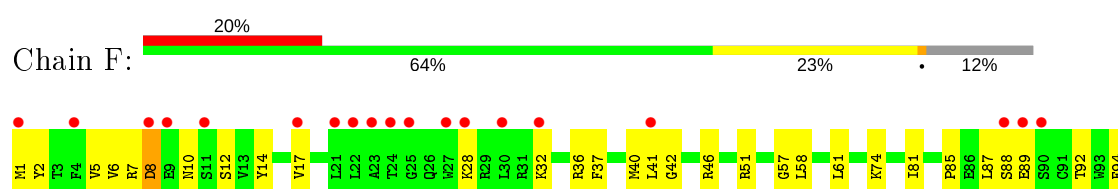
• Molecule 2: Tubulin beta-2B chain

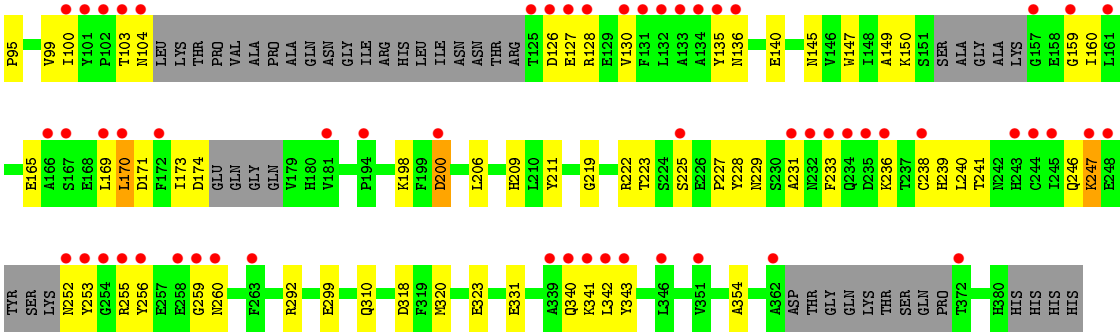


• Molecule 3: Stathmin-4



• Molecule 4: tubulin tyrosine ligase TTL





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.43Å 158.35Å 173.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.09 – 2.39 48.09 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.09-2.39) 99.7 (48.09-2.39)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.39Å)	Xtriage
Refinement program	PHENIX (dev_2420: ???)	Depositor
R, R_{free}	0.217 , 0.237 0.217 , 0.237	Depositor DCC
R_{free} test set	2000 reflections (1.78%)	wwPDB-VP
Wilson B-factor (Å ²)	50.9	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17810	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.63% 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.

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, GTP, MG, ACP, 8Z8

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.45	0/3468	0.66	4/4706 (0.1%)
1	C	0.35	0/3591	0.61	5/4878 (0.1%)
2	B	0.46	1/3340 (0.0%)	0.57	2/4519 (0.0%)
2	D	0.50	2/3438 (0.1%)	0.57	3/4657 (0.1%)
3	E	0.33	0/1017	0.58	1/1349 (0.1%)
4	F	0.28	0/2838	0.56	3/3832 (0.1%)
All	All	0.42	3/17692 (0.0%)	0.60	18/23941 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	C	0	2
2	D	0	3
3	E	0	1
4	F	0	1
All	All	0	13

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	360	PRO	C-N	-20.77	0.86	1.34
2	D	345	GLU	C-N	-17.66	0.93	1.34
2	D	346	TRP	C-N	-17.37	0.94	1.34

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3	GLU	C-N-CA	12.26	152.36	121.70
2	D	346	TRP	O-C-N	-10.51	105.88	122.70
1	A	285	GLN	O-C-N	-7.88	110.10	122.70
1	C	4[A]	CYS	CA-C-O	7.24	135.30	120.10
1	C	4[B]	CYS	CA-C-O	7.24	135.30	120.10

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	196	GLU	Mainchain
1	A	285	GLN	Mainchain
1	A	40	LYS	Mainchain
1	A	46	ASP	Mainchain
1	A	96	LYS	Mainchain

5.2 Too-close contacts ⓘ

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	3393	0	3312	138	0
1	C	3480	0	3409	78	0
2	B	3258	0	3134	128	0
2	D	3350	0	3245	84	0
3	E	1006	0	1026	29	0
4	F	2777	0	2743	136	0
5	A	32	0	12	0	0
5	C	32	0	12	3	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	B	28	0	12	1	0
7	D	28	0	12	1	0
8	B	29	0	0	1	0
9	F	31	0	14	6	0
10	A	79	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	59	0	0	2	0
10	C	98	0	0	10	0
10	D	62	0	0	9	0
10	E	18	0	0	3	0
10	F	45	0	0	8	0
All	All	17810	0	16931	548	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 16.

The worst 5 of 548 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)
4:F:252:ASN:HD22	4:F:255:ARG:NH2	1.09	1.44
2:B:59:ASN:HB2	2:B:60:LYS:NZ	1.36	1.34
4:F:1:MET:HB3	4:F:28:LYS:NZ	1.42	1.33
4:F:252:ASN:ND2	4:F:255:ARG:NH2	1.80	1.29
2:B:59:ASN:CB	2:B:60:LYS:HZ2	1.52	1.22

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	431/450 (96%)	423 (98%)	8 (2%)	0	100	100
1	C	448/450 (100%)	436 (97%)	12 (3%)	0	100	100
2	B	407/445 (92%)	402 (99%)	5 (1%)	0	100	100
2	D	425/445 (96%)	416 (98%)	9 (2%)	0	100	100
3	E	118/143 (82%)	115 (98%)	2 (2%)	1 (1%)	19	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	F	327/384 (85%)	322 (98%)	5 (2%)	0	100	100
All	All	2156/2317 (93%)	2114 (98%)	41 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	27	PRO

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	366/378 (97%)	360 (98%)	6 (2%)	62	79
1	C	381/378 (101%)	379 (100%)	2 (0%)	88	95
2	B	360/383 (94%)	359 (100%)	1 (0%)	92	97
2	D	371/383 (97%)	370 (100%)	1 (0%)	92	97
3	E	110/127 (87%)	110 (100%)	0	100	100
4	F	305/342 (89%)	300 (98%)	5 (2%)	62	79
All	All	1893/1991 (95%)	1878 (99%)	15 (1%)	81	91

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	299	LYS
1	C	2	ARG
4	F	200	ASP
1	A	370	LYS
4	F	145	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	293	ASN
2	D	167	ASN
3	E	115	HIS
1	C	285	GLN
3	E	124	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	$\# Z > 2$
7	GDP	D	501	6	24,30,30	1.20	2 (8%)	31,47,47	1.97	7 (22%)
5	GTP	A	501	6	26,34,34	1.24	3 (11%)	33,54,54	1.83	7 (21%)
7	GDP	B	501	-	24,30,30	1.19	2 (8%)	31,47,47	1.97	8 (25%)
5	GTP	C	501	6	26,34,34	0.99	1 (3%)	33,54,54	1.78	7 (21%)
8	8Z8	B	503	-	27,33,33	3.66	7 (25%)	33,50,50	3.32	15 (45%)
9	ACP	F	402	6	27,33,33	1.27	2 (7%)	32,52,52	1.47	4 (12%)

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
7	GDP	D	501	6	-	5/12/32/32	0/3/3/3
5	GTP	A	501	6	-	3/18/38/38	0/3/3/3
7	GDP	B	501	-	-	7/12/32/32	0/3/3/3
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3
8	8Z8	B	503	-	-	0/6/31/31	0/5/5/5
9	ACP	F	402	6	-	5/15/38/38	0/3/3/3

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	503	8Z8	CAK-NAH	-11.09	1.36	1.47
8	B	503	8Z8	CAU-NAH	-10.98	1.37	1.47
8	B	503	8Z8	CAZ-CAY	-6.28	1.36	1.54
8	B	503	8Z8	OAW-CAI	-6.02	1.29	1.43
7	B	501	GDP	C6-C5	4.24	1.48	1.41

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	503	8Z8	CAQ-CAL-CAM	8.24	122.65	114.56
8	B	503	8Z8	CAF-NAE-CAD	7.04	120.52	116.64
8	B	503	8Z8	CAY-CAK-NAH	-6.52	97.76	102.11
8	B	503	8Z8	CAZ-CAU-NAH	-5.77	98.27	102.11
8	B	503	8Z8	CAA-CAF-NAE	-5.50	119.45	125.91

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

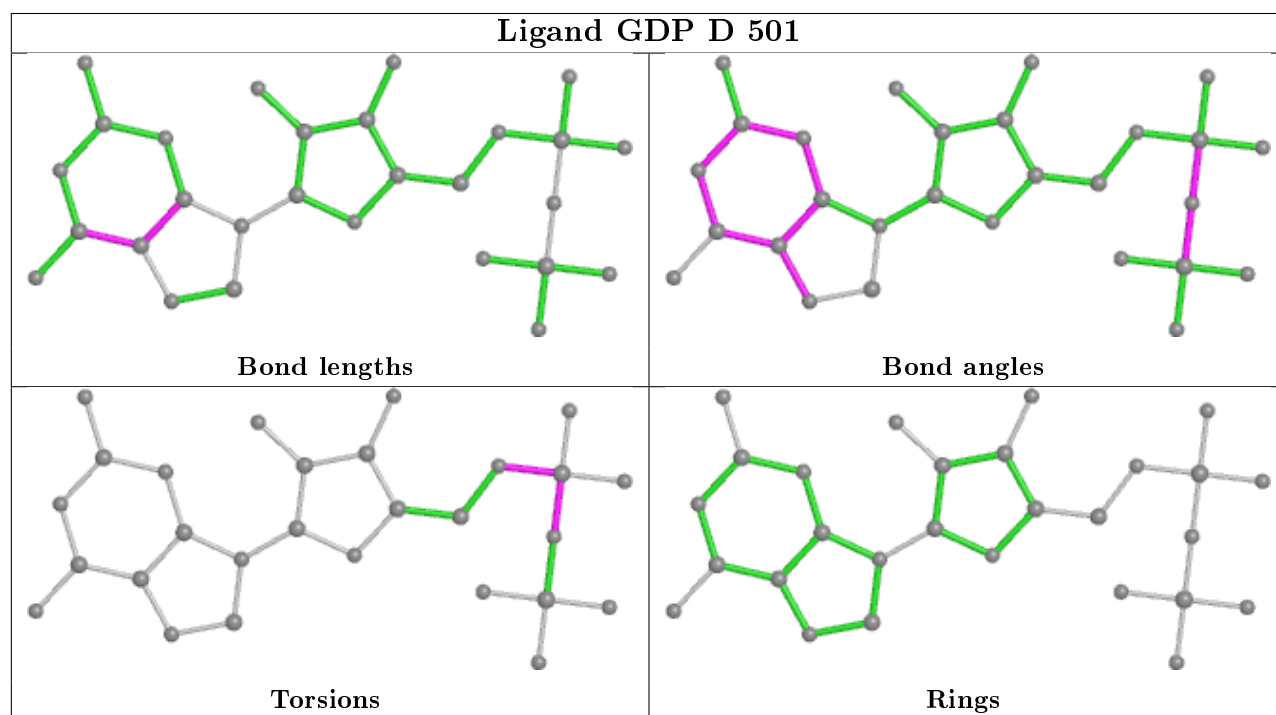
Mol	Chain	Res	Type	Atoms
7	D	501	GDP	C5'-O5'-PA-O1A
7	D	501	GDP	C5'-O5'-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A

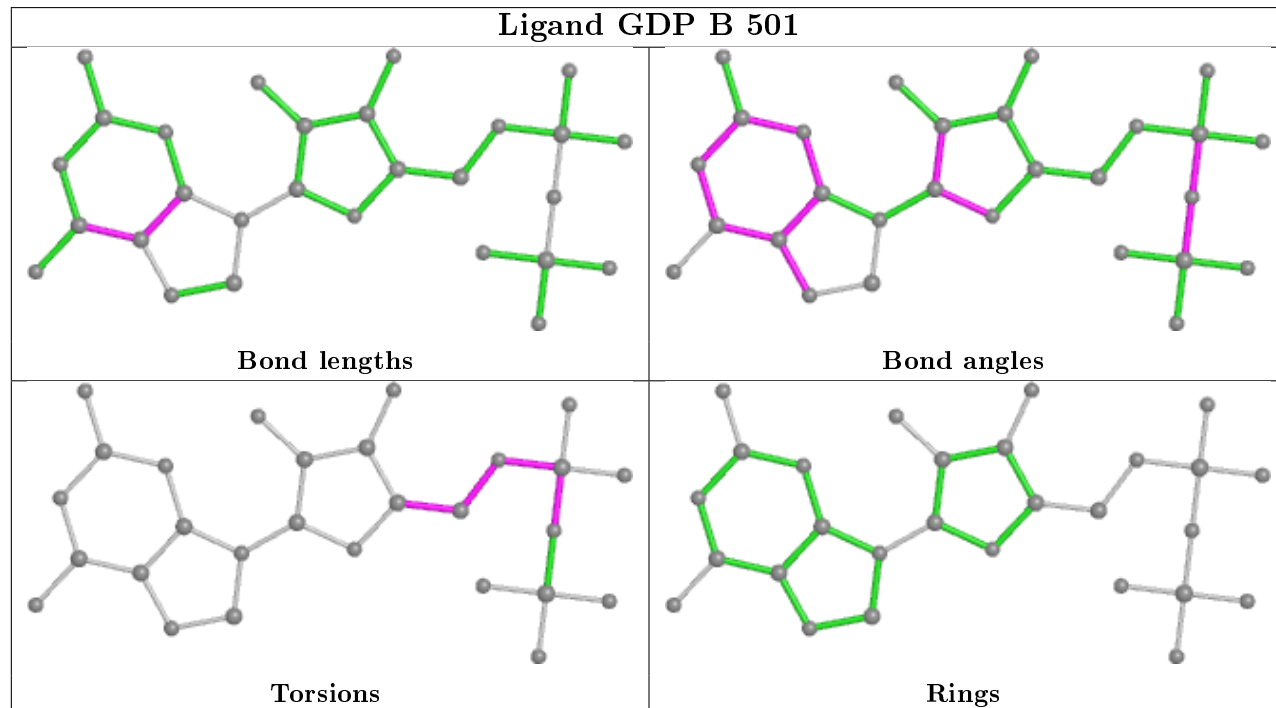
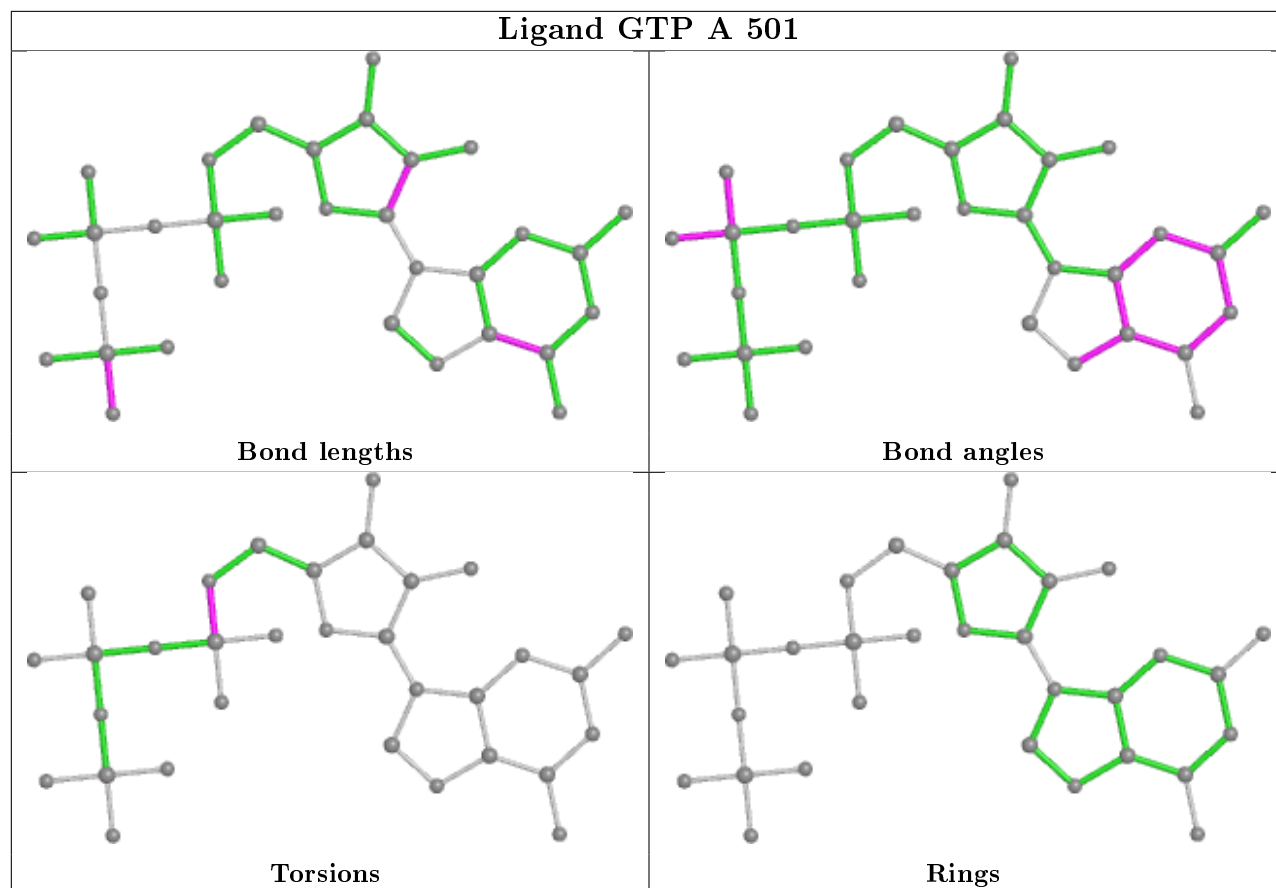
There are no ring outliers.

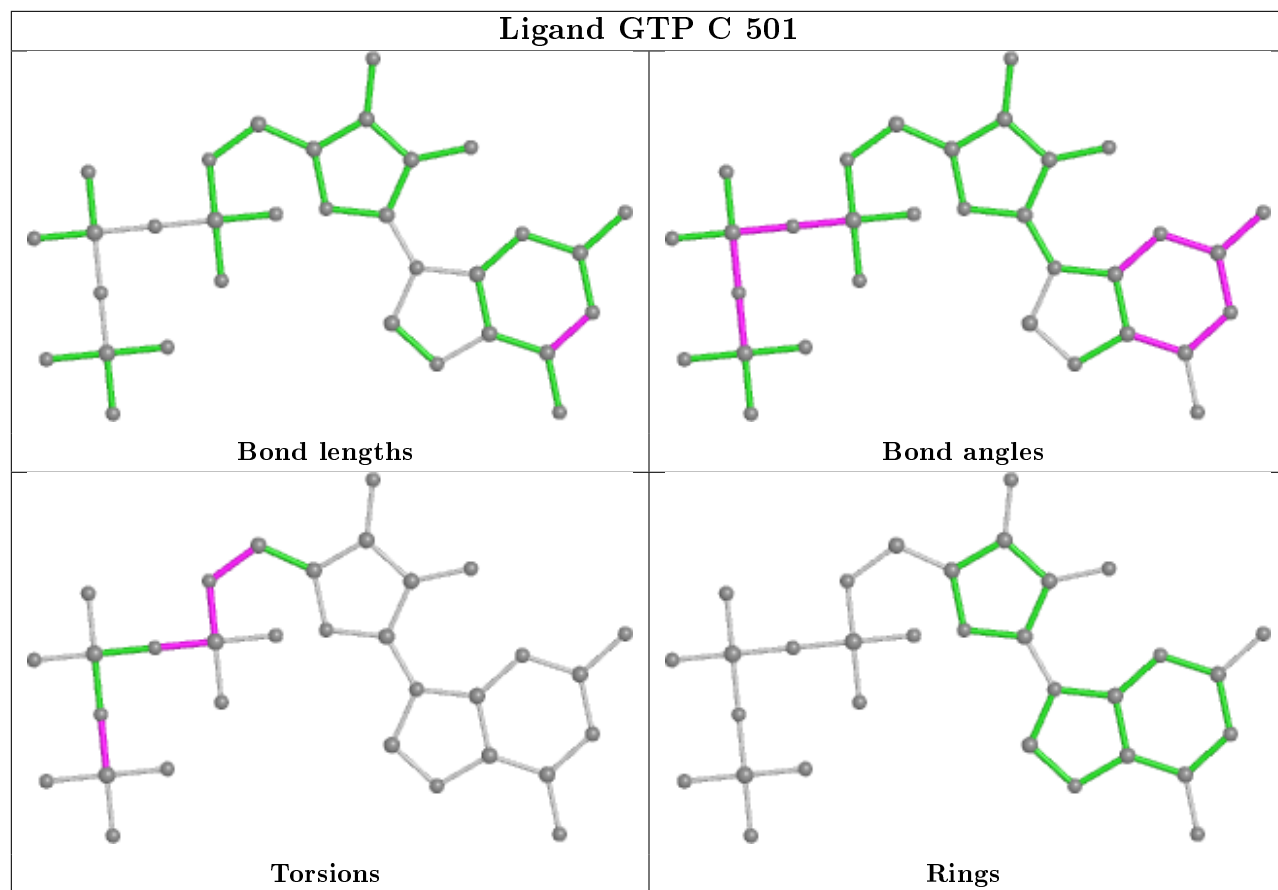
5 monomers are involved in 12 short contacts:

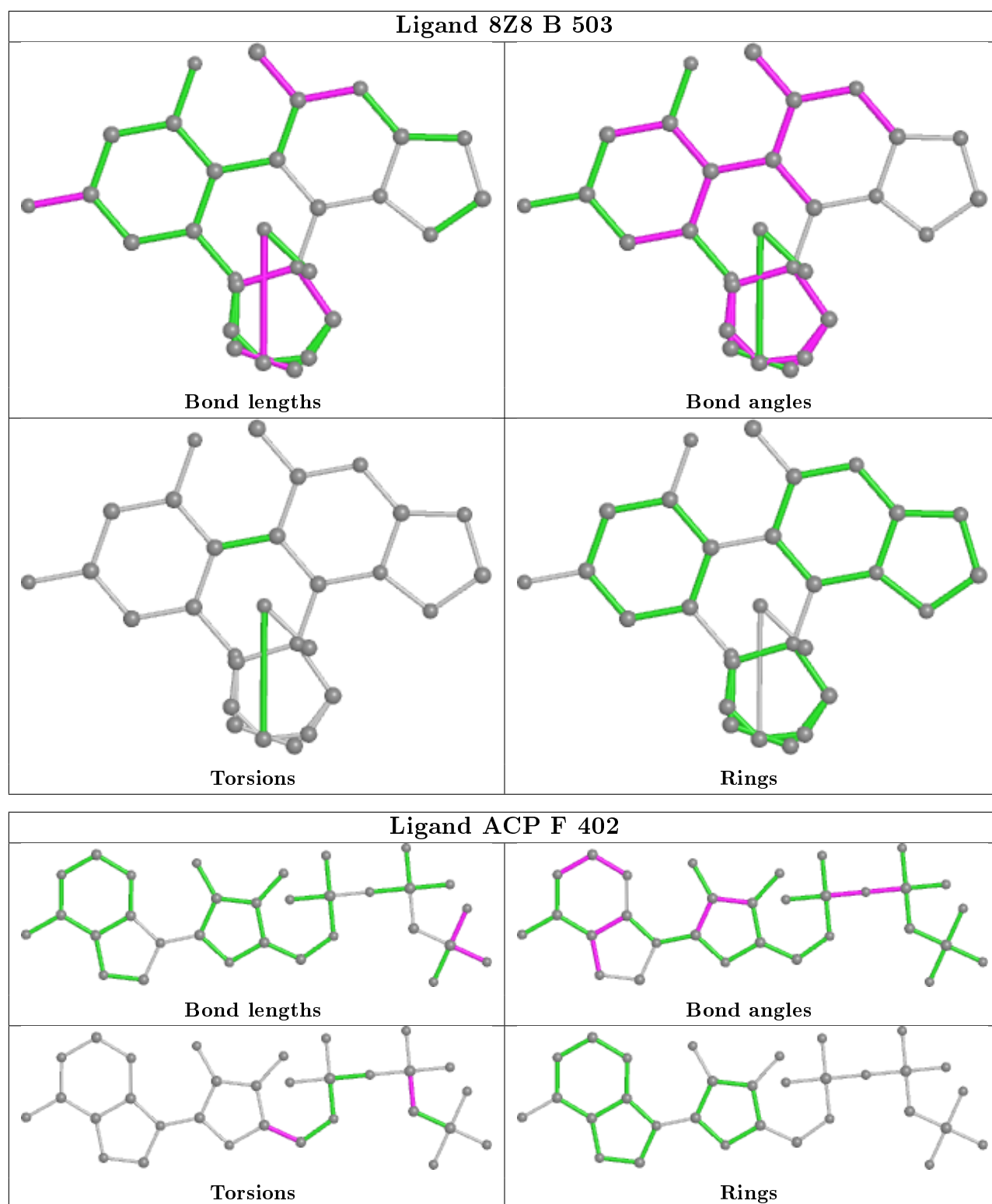
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	501	GDP	1	0
7	B	501	GDP	1	0
5	C	501	GTP	3	0
8	B	503	8Z8	1	0
9	F	402	ACP	6	0

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	2
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	346:TRP	C	347:ILE	N	0.94
1	D	345:GLU	C	346:TRP	N	0.93
1	B	360:PRO	C	369:ARG	N	0.86

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, 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	435/450 (96%)	0.60	28 (6%)	19 18	35, 56, 94, 123	0
1	C	439/450 (97%)	0.44	23 (5%)	27 26	30, 48, 81, 129	0
2	B	413/445 (92%)	0.71	36 (8%)	10 9	32, 54, 97, 146	1 (0%)
2	D	424/445 (95%)	0.73	47 (11%)	5 4	35, 59, 97, 140	3 (0%)
3	E	121/143 (84%)	0.91	15 (12%)	4 3	40, 68, 108, 146	0
4	F	339/384 (88%)	1.06	77 (22%)	0 0	42, 77, 129, 171	0
All	All	2171/2317 (93%)	0.70	226 (10%)	6 6	30, 57, 105, 171	4 (0%)

The worst 5 of 226 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1	MET	7.8
2	D	57	THR	7.1
1	A	262	TYR	6.9
2	B	59	ASN	6.6
3	E	7	GLU	6.6

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

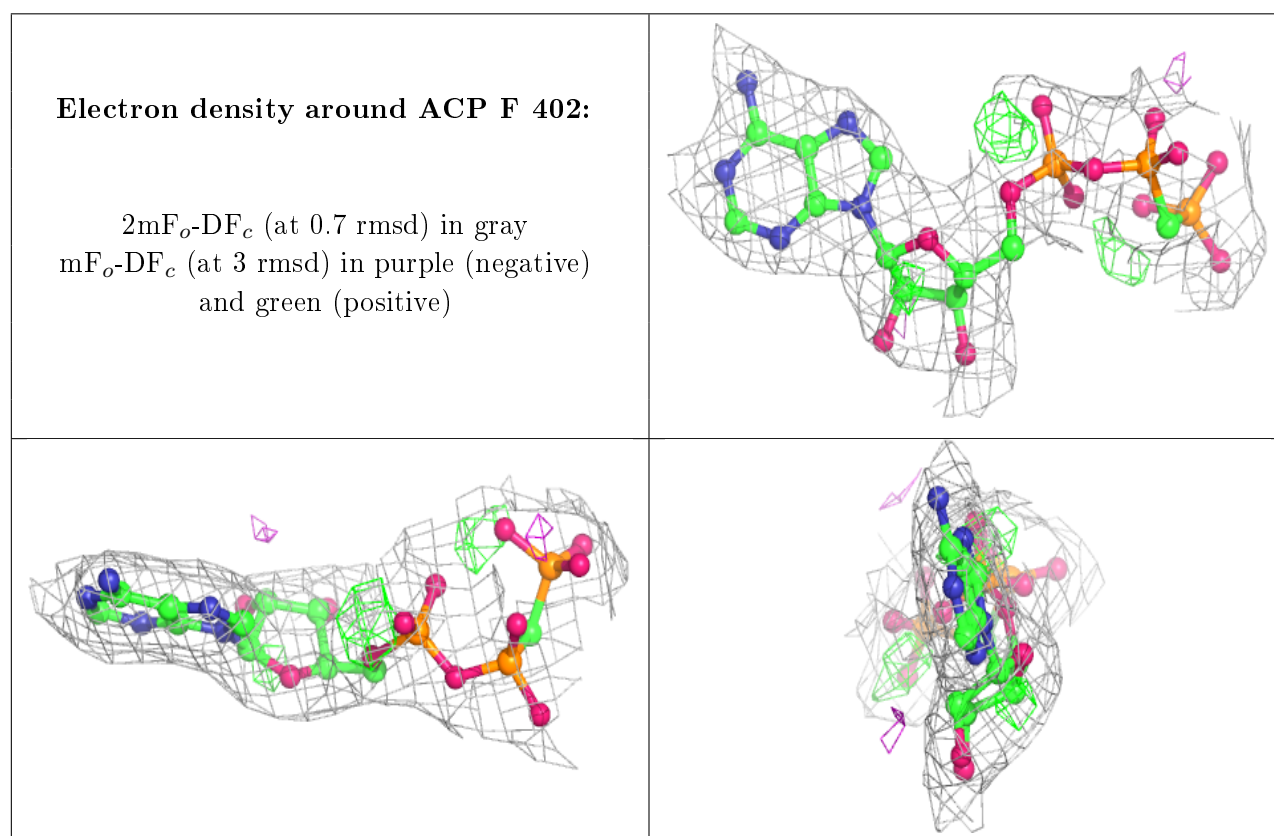
There are no carbohydrates in this entry.

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, 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.

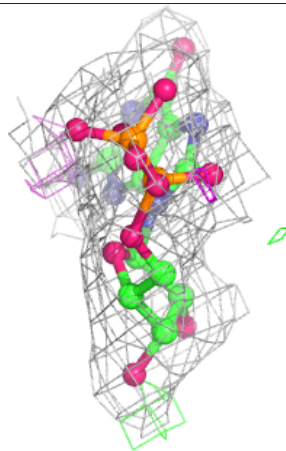
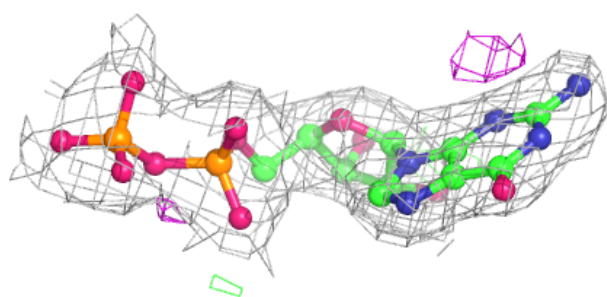
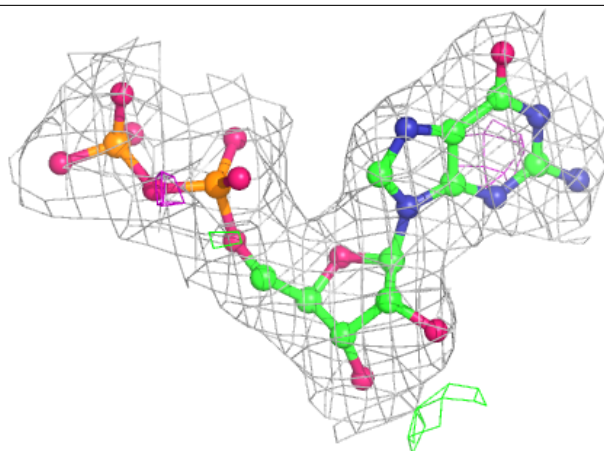
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	F	401	1/1	0.80	0.12	110,110,110,110	0
6	MG	A	502	1/1	0.81	0.12	45,45,45,45	0
9	ACP	F	402	31/31	0.89	0.13	58,86,141,142	0
6	MG	B	502	1/1	0.90	1.03	73,73,73,73	0
6	MG	D	502	1/1	0.91	0.08	54,54,54,54	0
6	MG	C	502	1/1	0.92	0.14	44,44,44,44	0
7	GDP	D	501	28/28	0.96	0.13	49,55,61,63	0
8	8Z8	B	503	29/29	0.96	0.15	45,52,58,62	0
5	GTP	C	501	32/32	0.97	0.16	38,47,61,71	0
7	GDP	B	501	28/28	0.97	0.23	40,57,66,73	0
5	GTP	A	501	32/32	0.98	0.22	36,45,51,55	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.



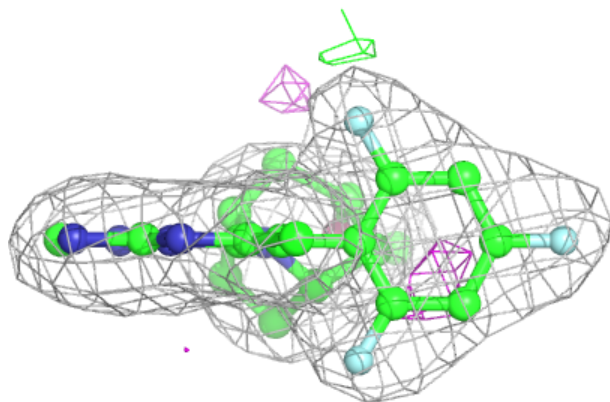
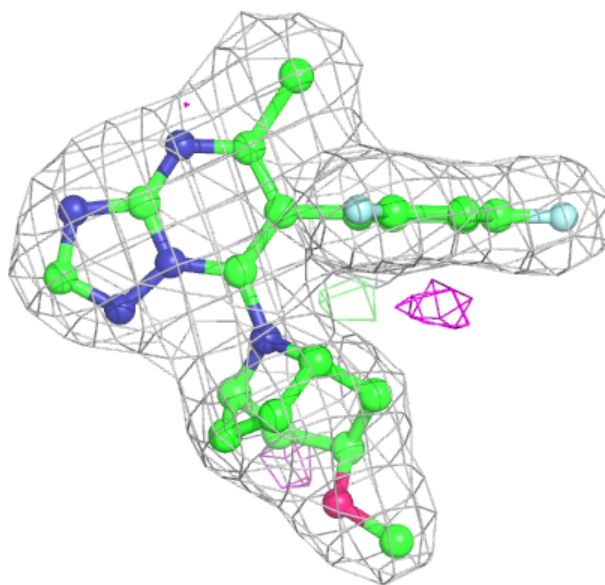
Electron density around GDP D 501:

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



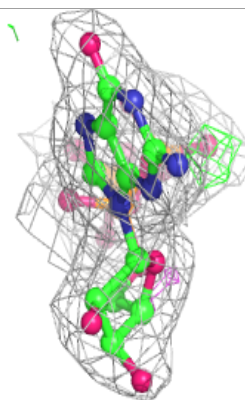
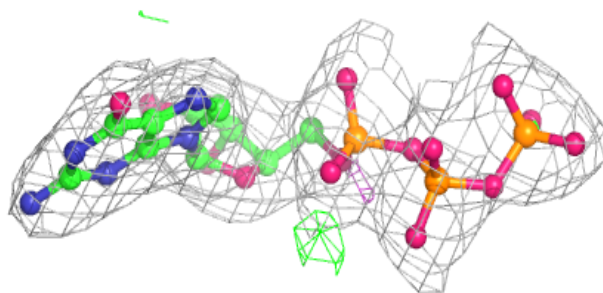
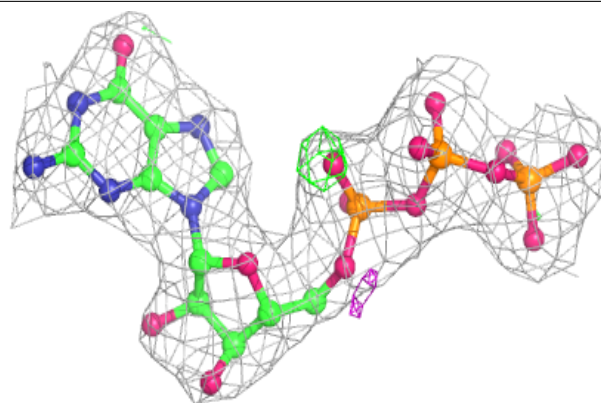
Electron density around 8Z8 B 503:

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

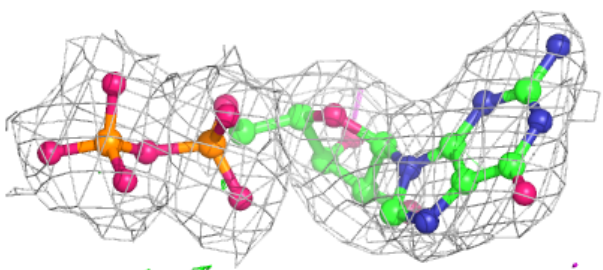
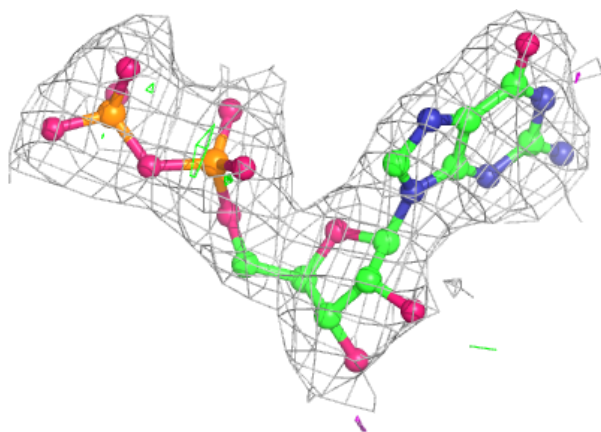


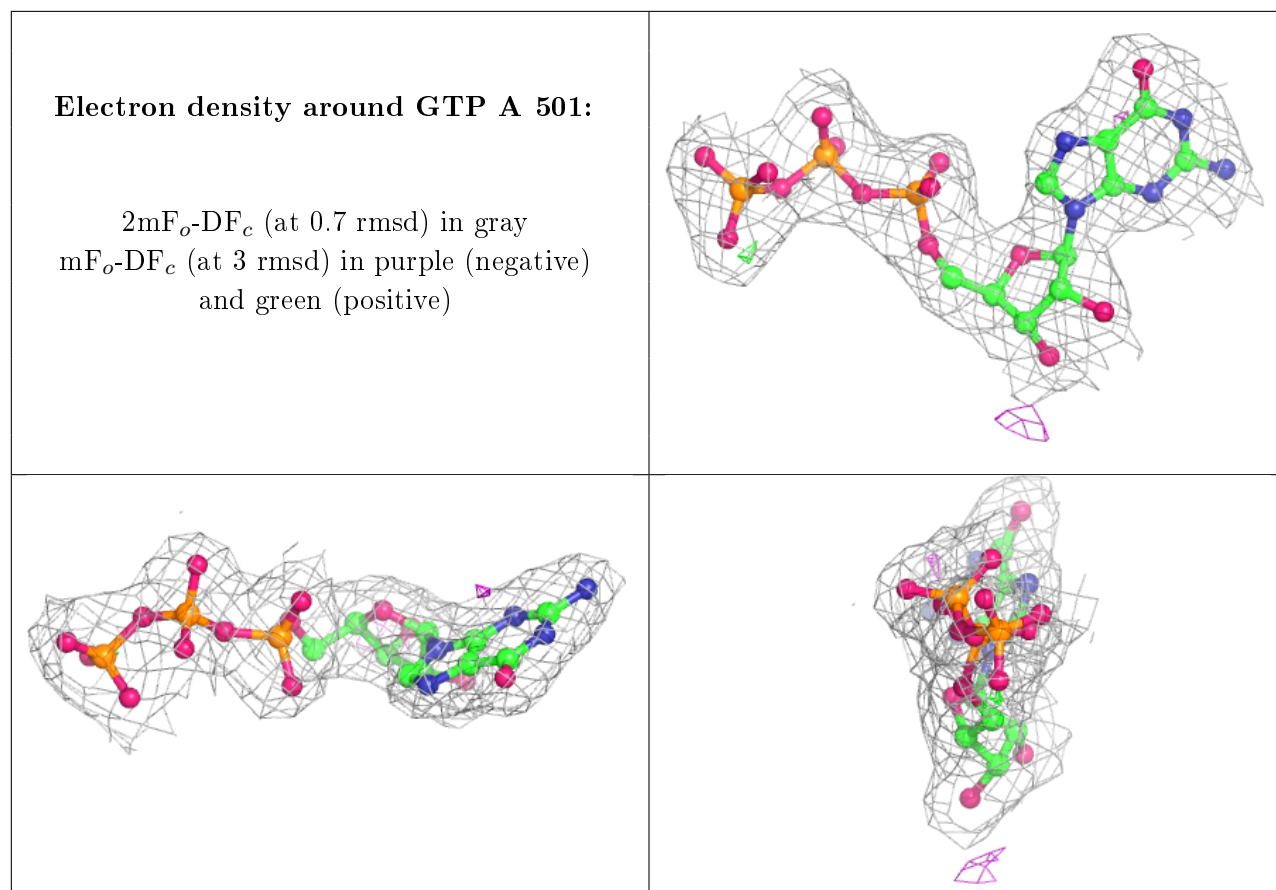
Electron density around GTP C 501:

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

**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)





6.5 Other polymers ⓘ

There are no such residues in this entry.