



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 04:50 PM UTC

PDB ID : 7PJE / pdb_00007pje
Title : Inhibiting parasite proliferation using a rationally designed anti-tubulin agent
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Deposited on : 2021-08-24
Resolution : 1.75 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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

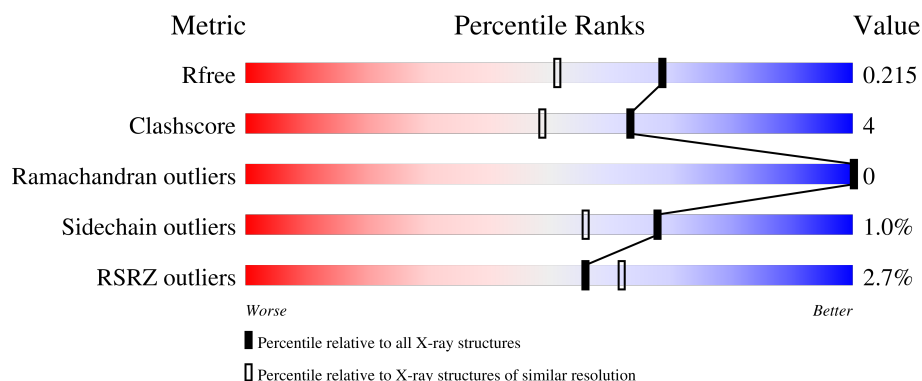
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	449	% 86% 7% 6%
1	C	449	4% 85% 9% 6%
2	B	443	2% 89% 6% .
2	D	443	4% 84% 11% .
3	E	155	% 74% 6% 19%

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Mol	Chain	Length	Quality of chain
3	F	155	% 77% 5% 19%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 31317 atoms, of which 14958 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	422	Total	C	H	N	O	S	0	9	0
			6574	2096	3265	561	628	24			
1	C	424	Total	C	H	N	O	S	0	2	0
			6551	2089	3250	561	629	22			

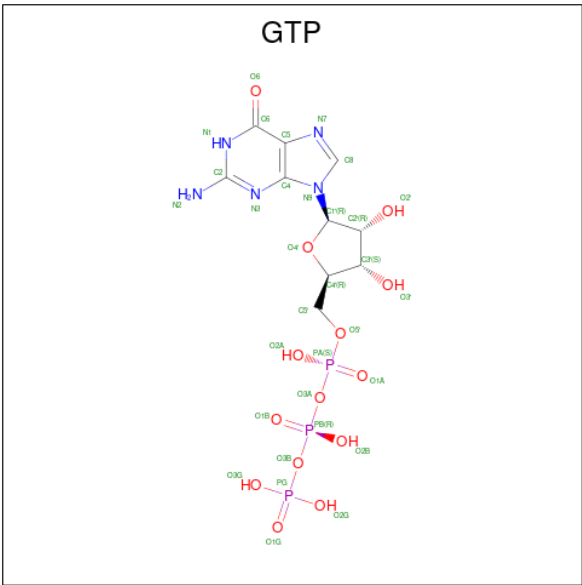
- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	425	Total	C	H	N	O	S	0	11	0
			6673	2124	3295	582	643	29			
2	D	424	Total	C	H	N	O	S	0	4	0
			6553	2091	3227	570	637	28			

- Molecule 3 is a protein called Darpin D1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	F	126	Total	C	H	N	O	S	0	0	0
			1867	588	937	161	178	3			
3	E	125	Total	C	H	N	O	S	0	2	0
			1877	589	946	162	177	3			

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	P	0	0
			41	10	9	5	14	3		
4	B	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		
4	C	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		
4	D	1	Total	C	H	N	O	P	0	0
			41	10	9	5	14	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	241	Total	O	0	0
			241	241		
6	B	280	Total	O	0	0
			280	280		

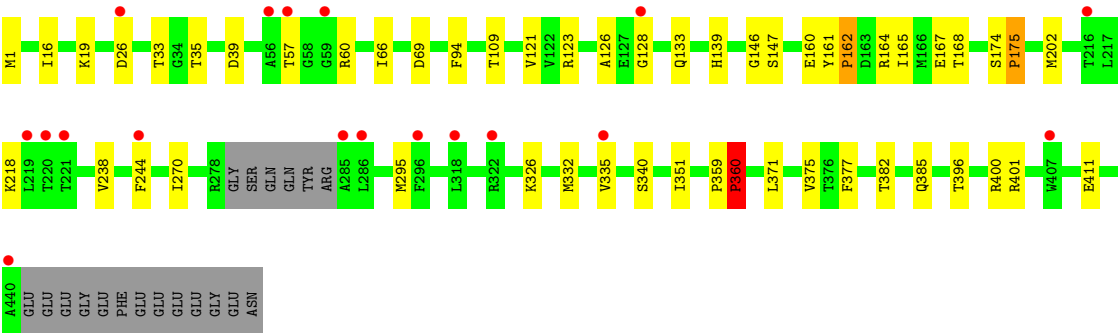
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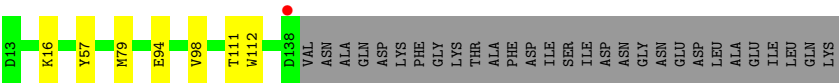
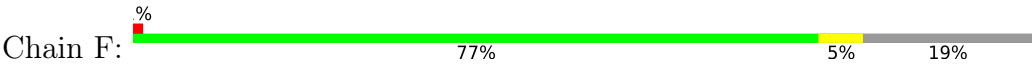
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	67	Total 67	O 67	0	0
6	C	228	Total 228	O 228	0	0
6	D	160	Total 160	O 160	0	0
6	E	77	Total 77	O 77	0	0

- Molecule 1: Tubulin alpha chain

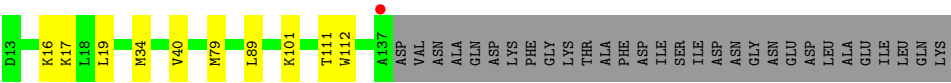
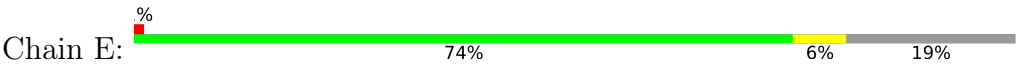




● Molecule 3: Darpin D1



● Molecule 3: Darpin D1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.13Å 183.92Å 118.32Å 90.00° 92.44° 90.00°	Depositor
Resolution (Å)	46.83 – 1.75 46.83 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.4 (46.83-1.75) 98.4 (46.83-1.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.181 , 0.213 0.183 , 0.215	Depositor DCC
R_{free} test set	10973 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.630	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.064 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	31317	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: GTP, MG

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	0.79	8/3429 (0.2%)	0.94	9/4642 (0.2%)
1	C	0.67	3/3380 (0.1%)	0.84	8/4577 (0.2%)
2	B	0.86	11/3495 (0.3%)	1.03	18/4728 (0.4%)
2	D	0.87	11/3417 (0.3%)	1.09	20/4625 (0.4%)
3	E	0.55	0/953	0.66	0/1298
3	F	0.46	0/944	0.66	1/1286 (0.1%)
All	All	0.77	33/15618 (0.2%)	0.95	56/21156 (0.3%)

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
2	D	0	1

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	348	PRO	N-CA	17.04	1.69	1.47
2	D	162	PRO	N-CA	16.46	1.68	1.47
1	C	175	PRO	N-CA	16.43	1.69	1.47
2	D	175	PRO	N-CA	16.40	1.69	1.47
2	B	222	PRO	N-CA	16.35	1.68	1.47

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	174	SER	CA-C-N	14.27	135.59	119.32
1	C	174	SER	C-N-CA	14.27	135.59	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	174	SER	CA-C-N	14.06	135.78	119.47
2	D	174	SER	C-N-CA	14.06	135.78	119.47
1	A	174	SER	CA-C-N	13.86	135.54	119.47

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	360	PRO	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	3309	3265	3215	21	0
1	C	3301	3250	3234	31	0
2	B	3378	3295	3248	24	0
2	D	3326	3227	3200	35	0
3	E	931	946	940	9	0
3	F	930	937	940	3	0
4	A	32	9	12	0	0
4	B	32	10	12	1	0
4	C	32	10	12	0	0
4	D	32	9	12	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	241	0	0	1	0
6	B	280	0	0	5	0
6	C	228	0	0	3	0
6	D	160	0	0	2	0
6	E	77	0	0	1	0
6	F	67	0	0	0	0
All	All	16359	14958	14825	120	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 4.

The worst 5 of 120 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)
2:B:348:PRO:CA	2:B:348:PRO:N	1.69	1.46
1:C:175:PRO:CA	1:C:175:PRO:N	1.69	1.43
2:B:222:PRO:CA	2:B:222:PRO:N	1.68	1.41
1:A:175:PRO:N	1:A:175:PRO:CA	1.68	1.38
2:D:175:PRO:N	2:D:175:PRO:CA	1.69	1.32

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	425/449 (95%)	413 (97%)	12 (3%)	0	100	100
1	C	420/449 (94%)	406 (97%)	14 (3%)	0	100	100
2	B	432/443 (98%)	424 (98%)	8 (2%)	0	100	100
2	D	424/443 (96%)	415 (98%)	9 (2%)	0	100	100
3	E	125/155 (81%)	125 (100%)	0	0	100	100
3	F	124/155 (80%)	124 (100%)	0	0	100	100
All	All	1950/2094 (93%)	1907 (98%)	43 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	366/376 (97%)	364 (100%)	2 (0%)	81	75
1	C	361/376 (96%)	359 (99%)	2 (1%)	78	71
2	B	372/376 (99%)	368 (99%)	4 (1%)	65	52
2	D	363/376 (96%)	357 (98%)	6 (2%)	53	36
3	E	97/120 (81%)	96 (99%)	1 (1%)	68	56
3	F	96/120 (80%)	95 (99%)	1 (1%)	68	56
All	All	1655/1744 (95%)	1639 (99%)	16 (1%)	68	56

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	340	SER
2	D	335	VAL
1	C	339	ARG
2	D	167	GLU
1	C	175	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	433	GLN
2	D	385	GLN
1	C	85	GLN
2	D	136	GLN
1	C	15	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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$
4	GTP	C	502	5	33,34,34	0.95	1 (3%)	50,54,54	1.66	10 (20%)
4	GTP	A	501	5	33,34,34	1.00	2 (6%)	50,54,54	1.57	12 (24%)
4	GTP	D	501	-	33,34,34	1.19	3 (9%)	50,54,54	1.55	10 (20%)
4	GTP	B	501	5	33,34,34	0.99	2 (6%)	50,54,54	1.61	9 (18%)

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
4	GTP	C	502	5	-	7/22/38/38	0/3/3/3
4	GTP	A	501	5	-	6/22/38/38	0/3/3/3
4	GTP	D	501	-	-	5/22/38/38	0/3/3/3
4	GTP	B	501	5	-	6/22/38/38	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	501	GTP	PB-O3A	4.43	1.64	1.59
4	A	501	GTP	PB-O3B	2.61	1.62	1.59
4	A	501	GTP	PB-O3A	2.61	1.62	1.59
4	D	501	GTP	PA-O3A	2.33	1.62	1.59
4	C	502	GTP	PG-O2G	-2.31	1.46	1.54

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	GTP	O2B-PB-O3B	5.48	122.10	107.27
4	D	501	GTP	C5-C4-N3	-4.62	121.04	128.39
4	C	502	GTP	O2B-PB-O3B	4.29	118.86	107.27
4	A	501	GTP	C2-N3-C4	4.28	119.67	112.30
4	C	502	GTP	C2-N3-C4	4.23	119.59	112.30

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	GTP	PB-O3B-PG-O2G
4	A	501	GTP	C5'-O5'-PA-O3A
4	A	501	GTP	C5'-O5'-PA-O1A
4	A	501	GTP	C5'-O5'-PA-O2A
4	B	501	GTP	PB-O3B-PG-O3G

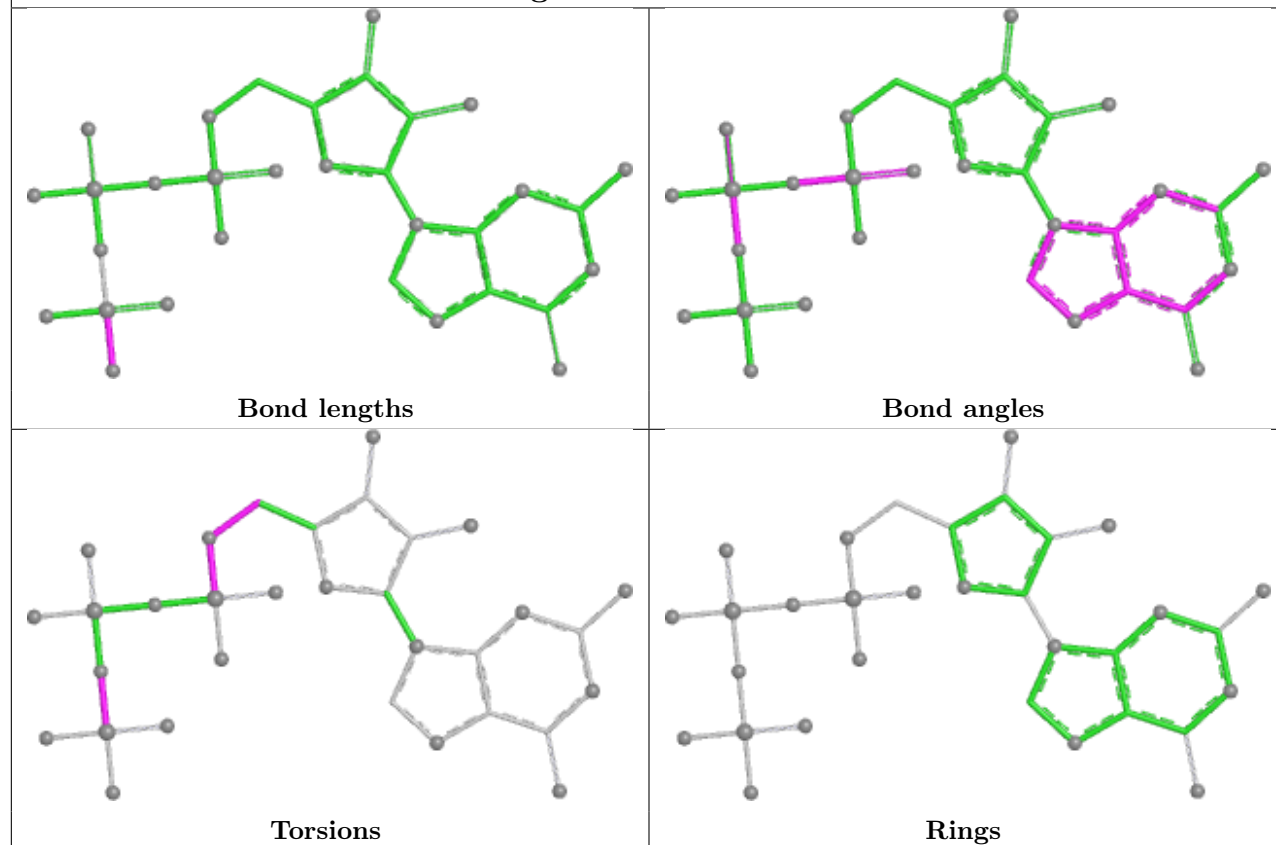
There are no ring outliers.

1 monomer is involved in 1 short contact:

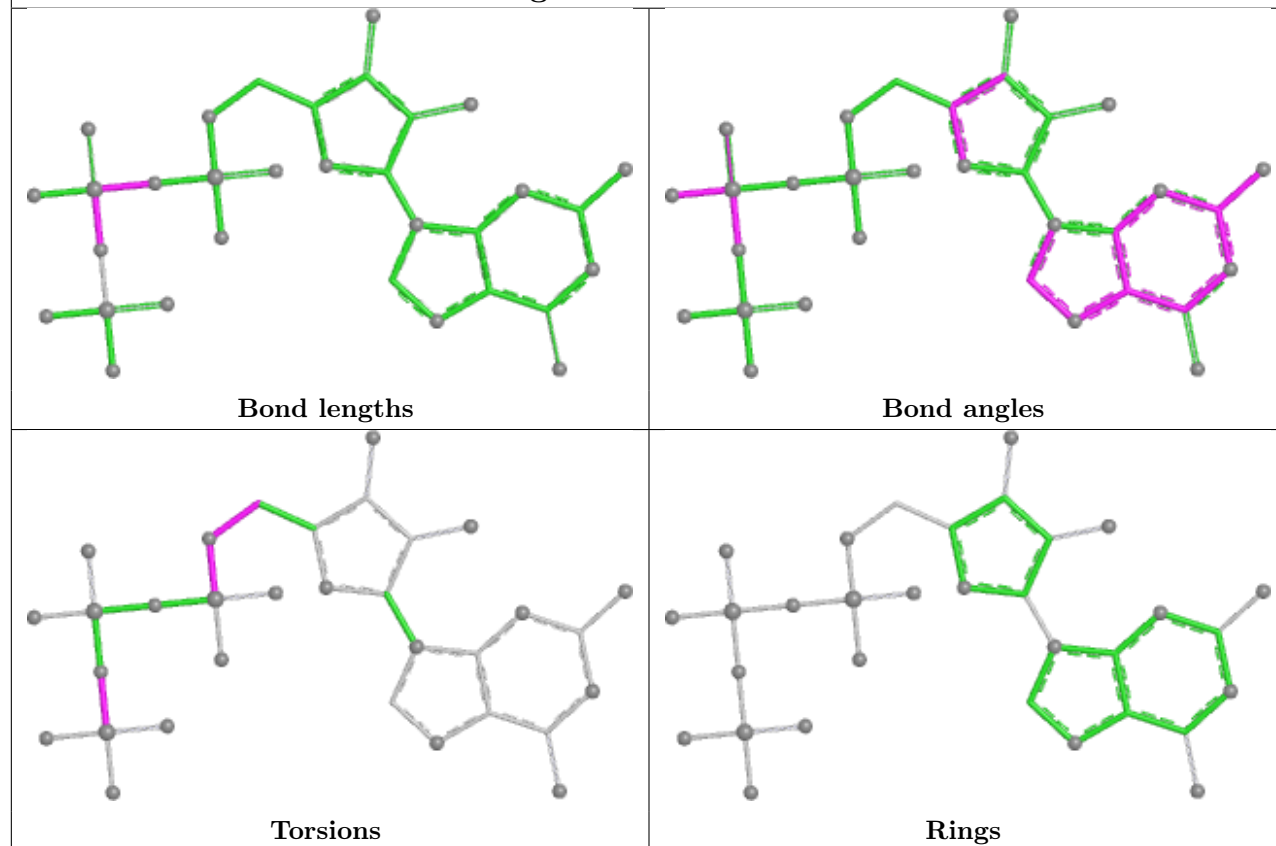
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	GTP	1	0

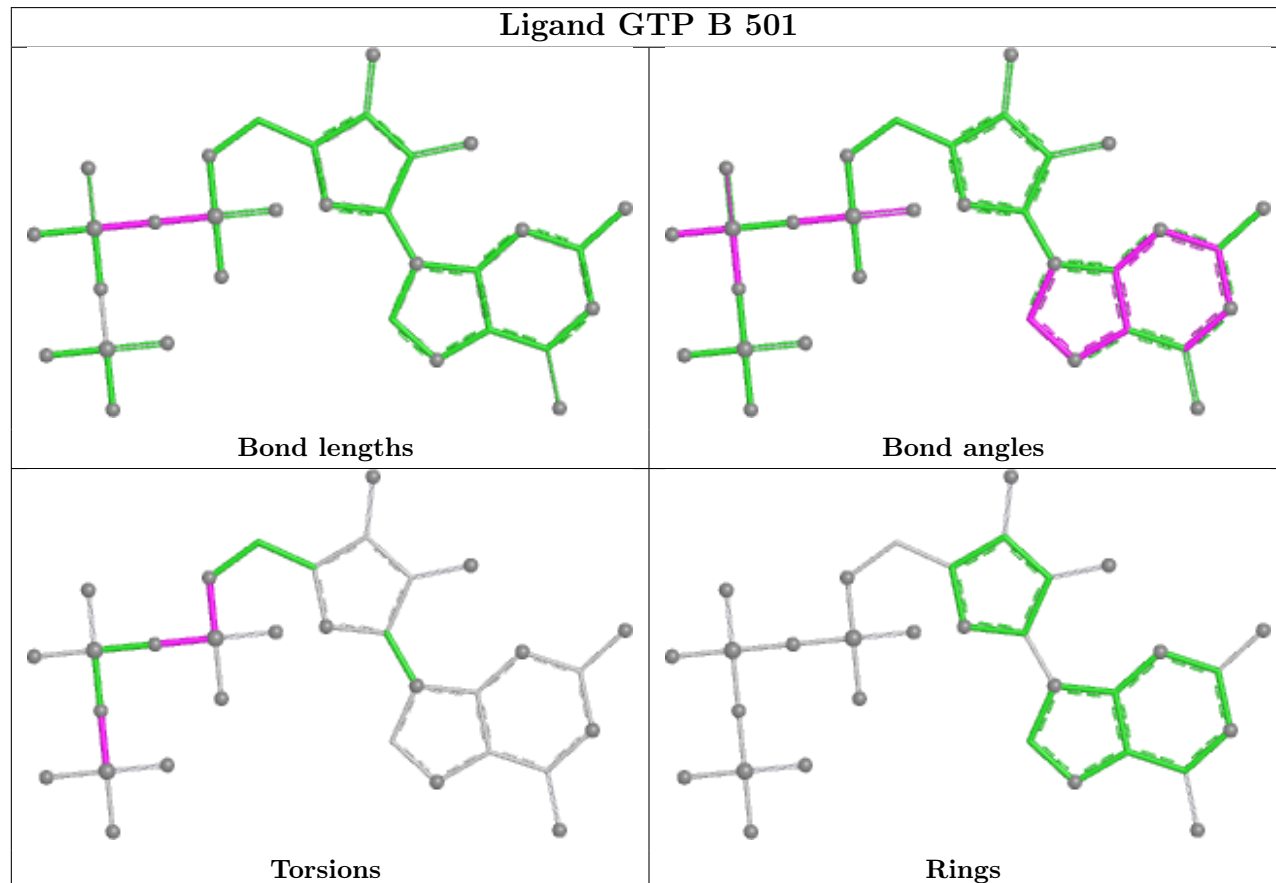
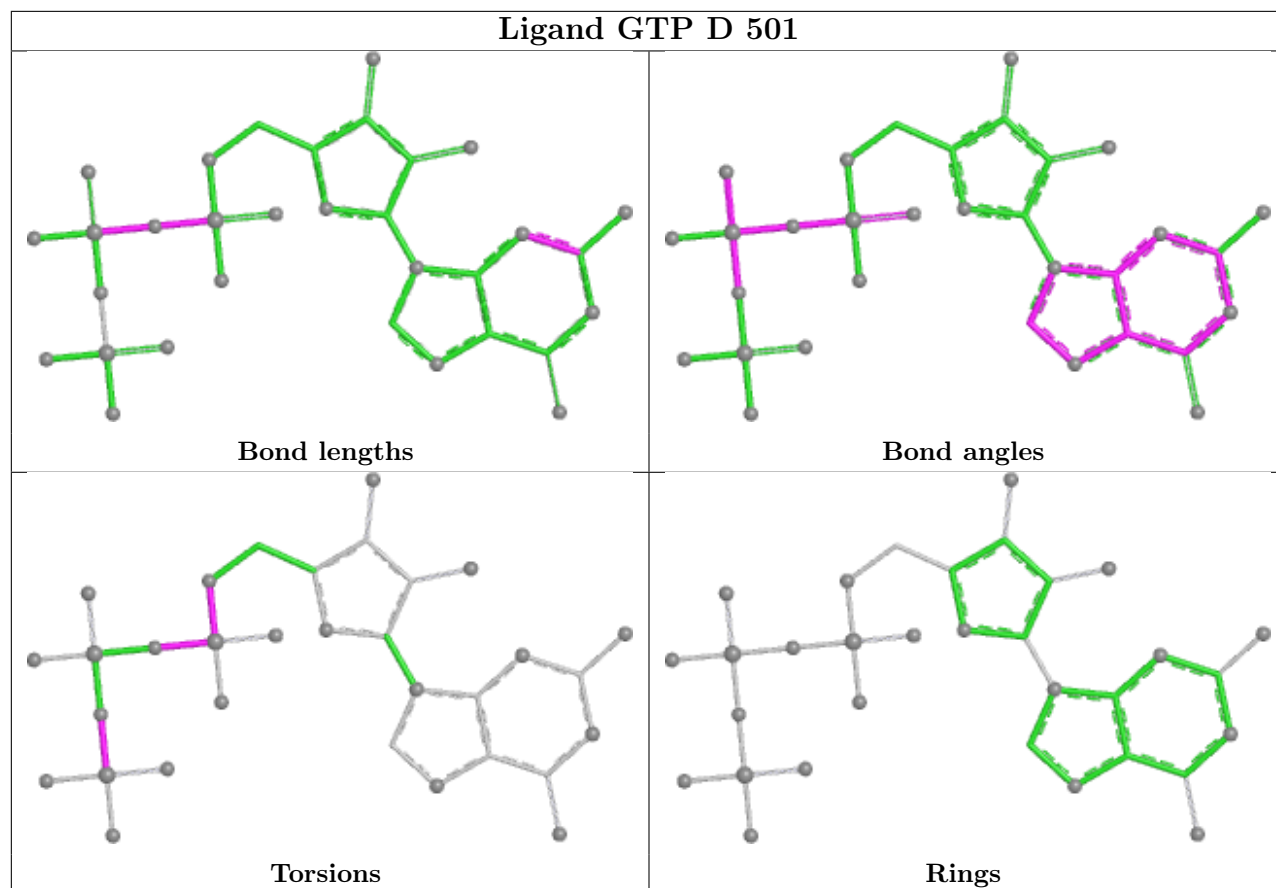
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GTP C 502



Ligand GTP A 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	422/449 (93%)	0.11	6 (1%) 73 80	17, 46, 76, 109	4 (0%)
1	C	424/449 (94%)	0.23	16 (3%) 44 50	19, 46, 82, 138	1 (0%)
2	B	425/443 (95%)	-0.01	10 (2%) 59 66	20, 39, 66, 88	7 (1%)
2	D	424/443 (95%)	0.33	18 (4%) 40 46	25, 51, 85, 129	1 (0%)
3	E	125/155 (80%)	0.05	1 (0%) 82 86	33, 48, 69, 93	1 (0%)
3	F	126/155 (81%)	-0.04	1 (0%) 82 86	34, 45, 69, 83	0
All	All	1946/2094 (92%)	0.15	52 (2%) 56 62	17, 46, 78, 138	14 (0%)

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	296	PHE	4.7
3	E	137	ALA	4.1
1	A	436	GLY	4.1
1	C	37	PRO	4.0
1	C	280	LYS	3.9

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](#)

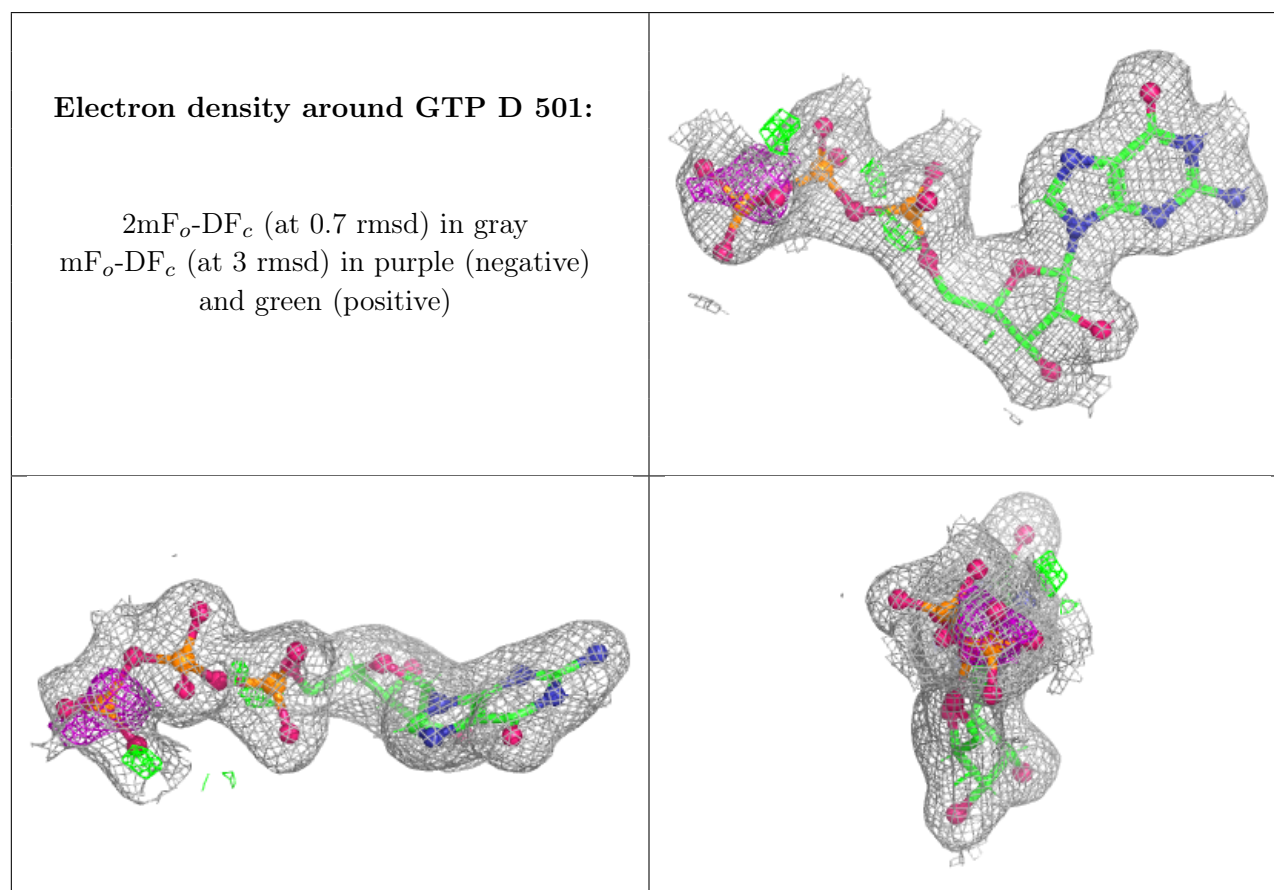
There are no oligosaccharides in this entry.

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, 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.

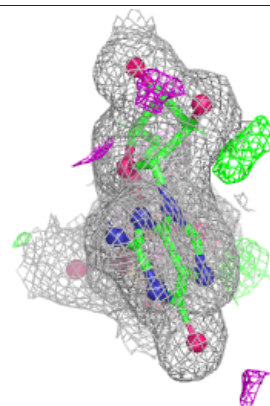
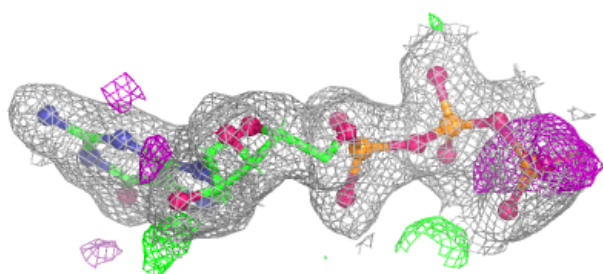
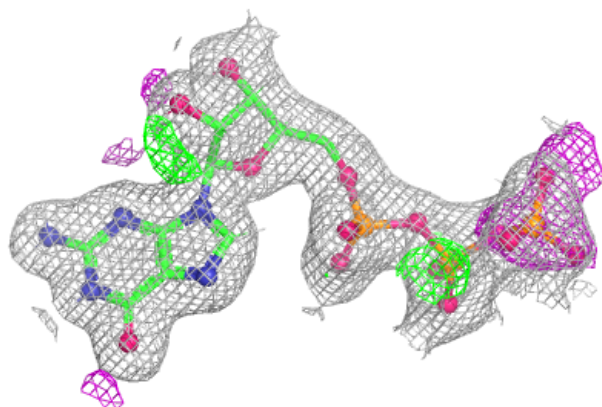
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	B	502	1/1	0.80	0.12	45,45,45,45	0
4	GTP	D	501	32/32	0.96	0.08	31,39,66,77	0
4	GTP	B	501	32/32	0.97	0.06	26,31,38,49	0
5	MG	A	502	1/1	0.98	0.04	31,31,31,31	0
4	GTP	C	502	32/32	0.98	0.05	29,33,40,45	0
5	MG	C	501	1/1	0.98	0.07	37,37,37,37	0
4	GTP	A	501	32/32	0.99	0.04	26,30,35,38	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.

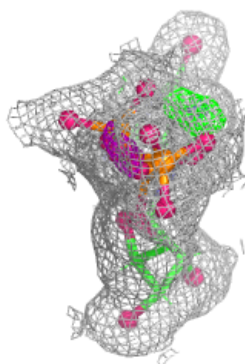
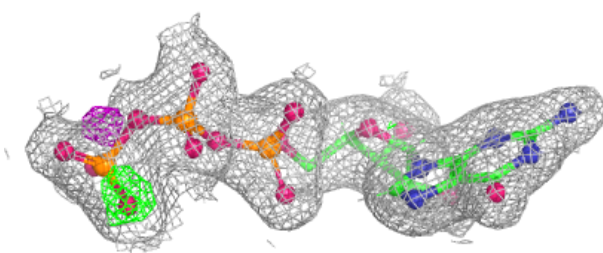
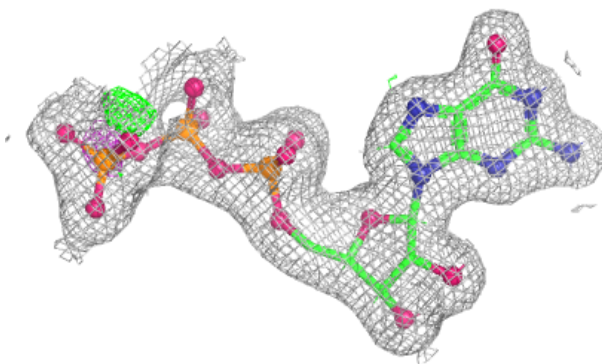


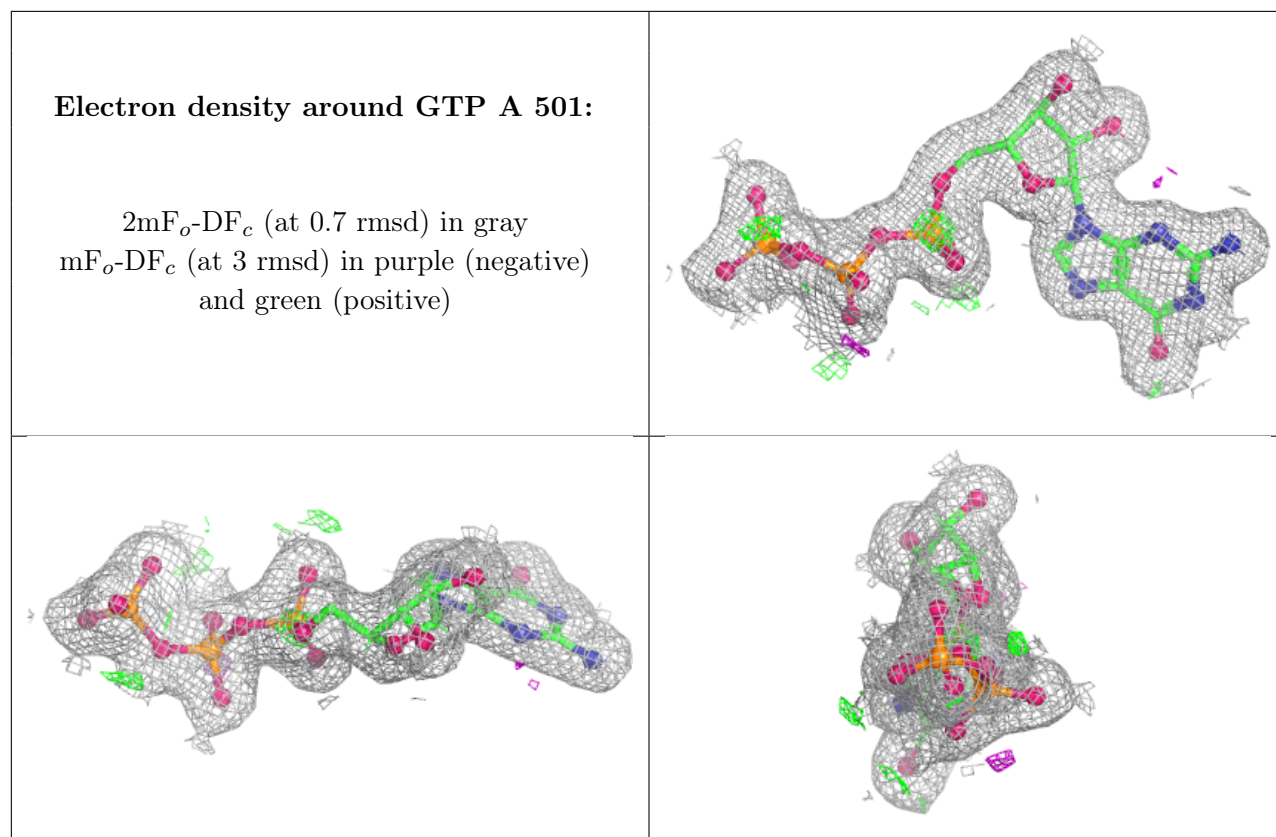
Electron density around GTP B 501:

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

**Electron density around GTP C 502:**

$2mF_o-DF_c$ (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.