



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 20, 2023 – 12:21 pm GMT

PDB ID : 7ZYW
Title : Crystal structure of T2R-TTL-PM534 complex
Authors : Oliva, M.A.; Diaz, J.F.; Cuevas, C.
Deposited on : 2022-05-25
Resolution : 2.45 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

<https://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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

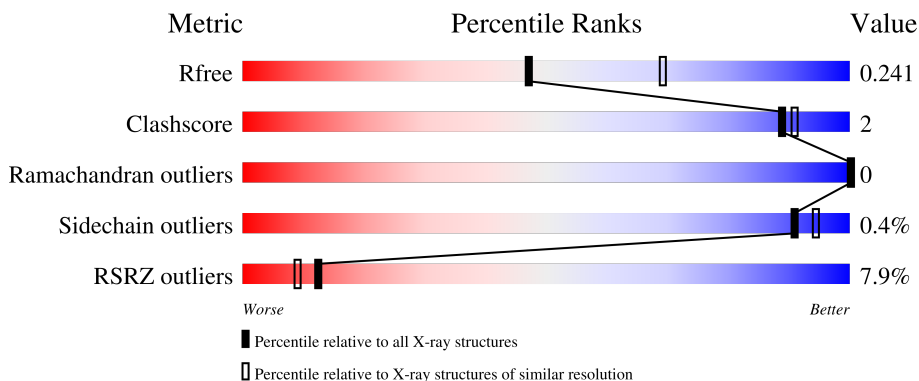
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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.



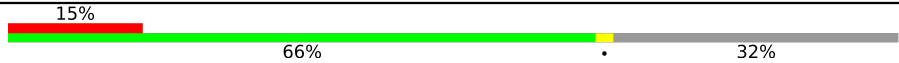
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	451	 4% 89% 7%
1	C	451	 2% 94%
2	B	445	 3% 88% 6% 7%
2	D	445	 11% 87% 7% 7%
3	E	189	 8% 61% 37%

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Mol	Chain	Length	Quality of chain
4	F	384	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a red segment on the left labeled '15%', a green segment in the middle labeled '66%', and a grey segment on the right labeled '32%'. A small yellow dot is located at the end of the green segment.</p>

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 33801 atoms, of which 16646 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	435	Total	C	H	N	O	S	0	15	0
			6896	2206	3426	586	654	24			
1	C	440	Total	C	H	N	O	S	0	18	0
			6955	2224	3438	594	673	26			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	B	416	Total	C	H	N	O	S	0	16	0
			6613	2111	3261	573	642	26			
2	D	414	Total	C	H	N	O	S	0	5	0
			6449	2066	3168	558	631	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
3	E	119	Total	C	H	N	O	S	0	3	0
			2010	614	1014	181	196	5			

- Molecule 4 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
4	F	261	Total	C	H	N	O	S	0	4	0
			4345	1407	2181	367	378	12			

There are 6 discrepancies between the modelled and reference sequences:

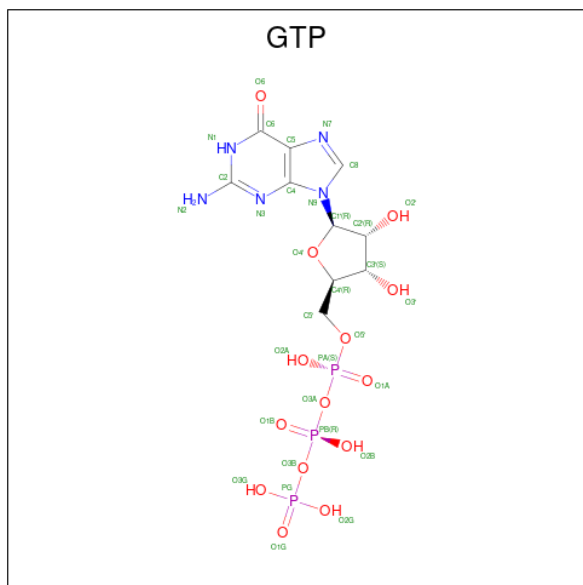
Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43

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Chain	Residue	Modelled	Actual	Comment	Reference
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

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



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

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

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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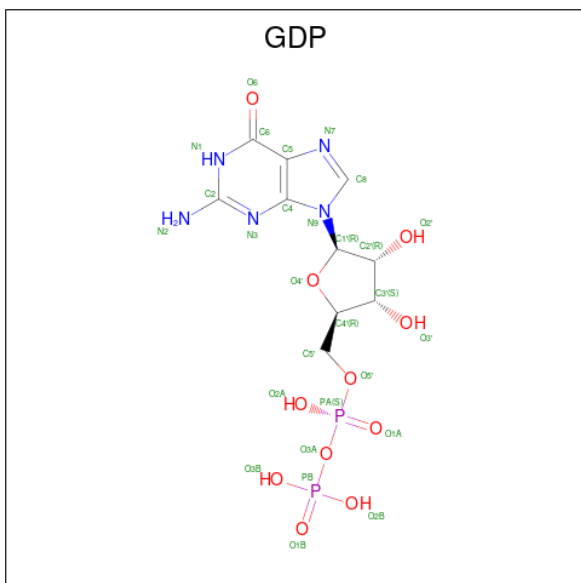
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total Mg 1 1	0	0
8	D	1	Total Mg 1 1	0	0

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 10 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



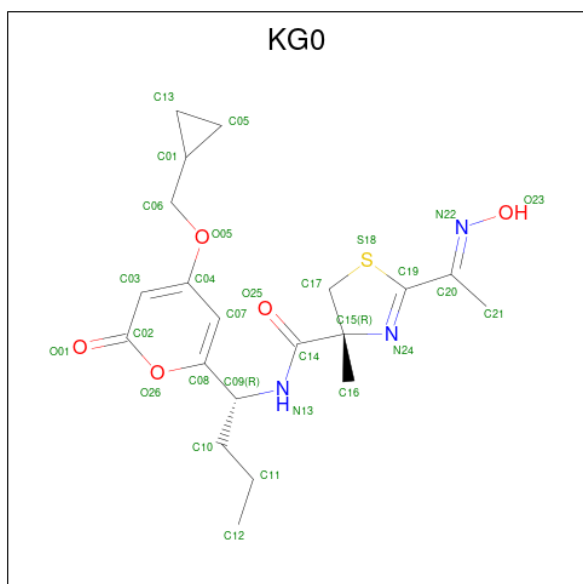
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C H N O P 38 10 10 5 11 2	0	0
10	D	1	Total C H N O P 38 10 10 5 11 2	0	0

- Molecule 11 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 12 is (4R)-N-[(1R)-1-[4-(cyclopropylmethoxy)-6-oxidanylidene-pyran-2-yl]butyl]-4-methyl-2-[(E)-C-methyl-N-oxidanyl-carbonimidoyl]-5H-1,3-thiazole-4-carboxamide (three-letter code: KG0) (formula: C₂₀H₂₇N₃O₅S) (labeled as "Ligand of Interest" by depositor).



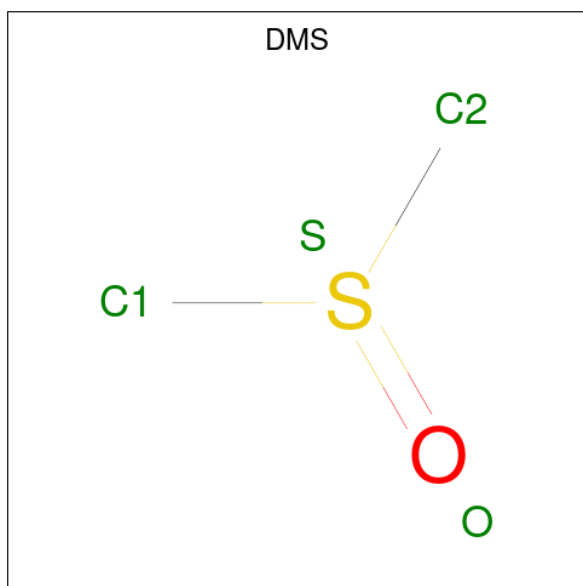
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			S
12	B	1	56	20	27	3	5	1	0	0

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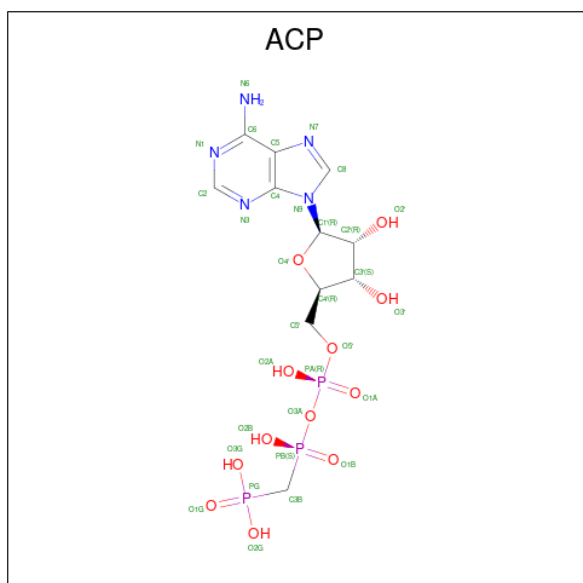
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			S
12	D	1	56	20	27	3	5	1	0	0

- Molecule 13 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	S		
13	C	1	10	2	6	1	1	0	0

- Molecule 14 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



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

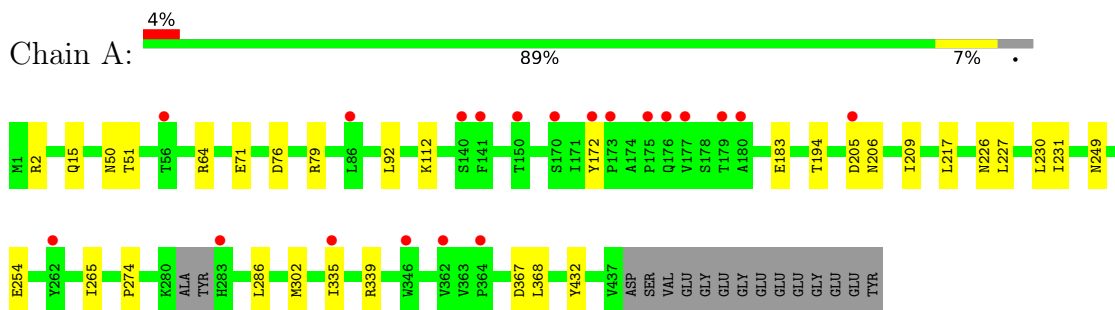
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	17	Total	O	0	0
			17	17		
15	B	27	Total	O	0	0
			27	27		
15	C	64	Total	O	0	0
			64	64		
15	D	6	Total	O	0	0
			6	6		
15	E	1	Total	O	0	0
			1	1		
15	F	3	Total	O	0	0
			3	3		

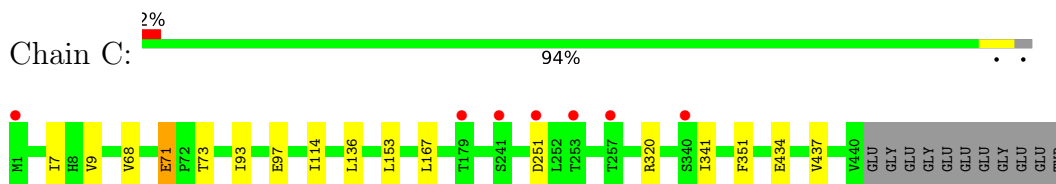
3 Residue-property plots [i](#)

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

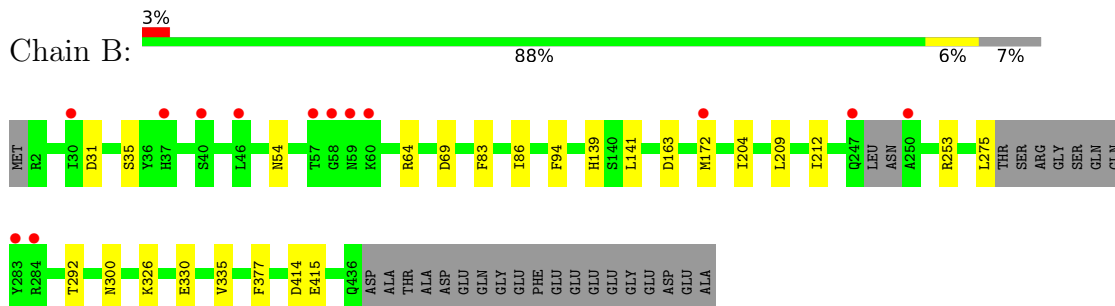
- Molecule 1: Tubulin alpha-1B chain



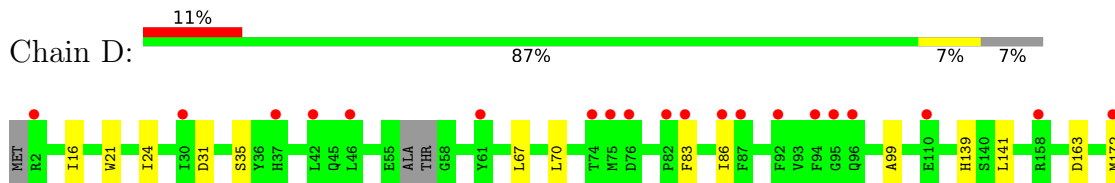
- Molecule 1: Tubulin alpha-1B chain

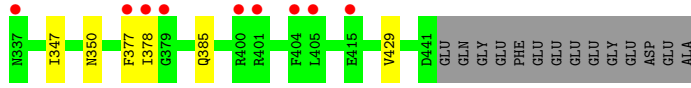
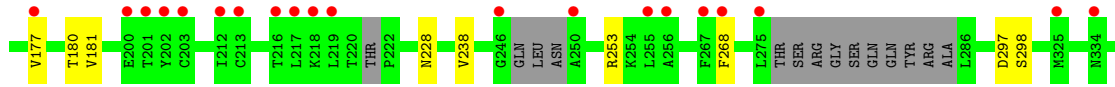


- Molecule 2: Tubulin beta-2B chain

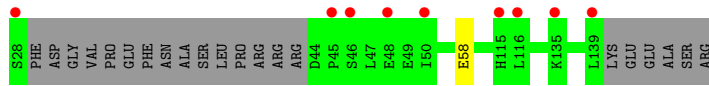
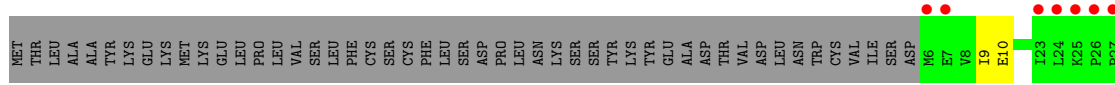


- Molecule 2: Tubulin beta-2B chain

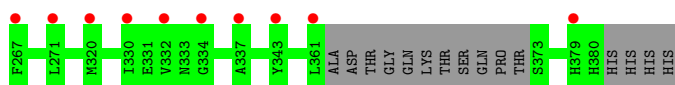
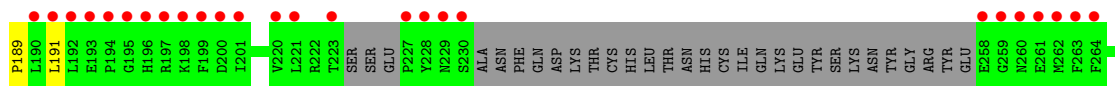
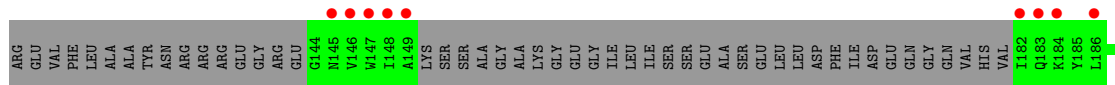
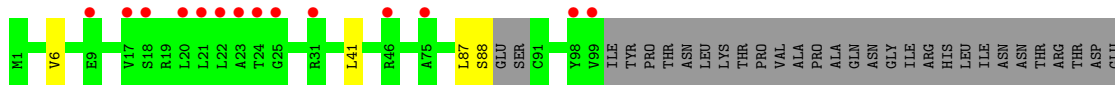




● Molecule 3: Stathmin-4



● Molecule 4: Tubulin beta-2B chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.80Å 158.03Å 181.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.66 – 2.45 49.66 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.66-2.45) 99.5 (49.66-2.45)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.45Å)	Xtrriage
Refinement program	PHENIX 1.19	Depositor
R, R_{free}	0.218 , 0.244 0.216 , 0.241	Depositor DCC
R_{free} test set	5500 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	58.4	Xtrriage
Anisotropy	0.194	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	33801	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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: GOL, MG, KG0, MES, CA, GDP, GTP, ACP, DMS, CL

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	0.25	0/3592	0.47	0/4874
1	C	0.25	0/3650	0.47	0/4959
2	B	0.25	0/3489	0.48	0/4722
2	D	0.24	0/3367	0.46	0/4552
3	E	0.24	0/1016	0.43	0/1348
4	F	0.24	0/2225	0.46	0/3002
All	All	0.25	0/17339	0.47	0/23457

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3470	3426	3409	21	0
1	C	3517	3438	3409	9	0
2	B	3352	3261	3204	12	0
2	D	3281	3168	3150	18	0
3	E	996	1014	1000	2	0
4	F	2164	2181	2175	3	0
5	A	32	10	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	9	12	0	0
6	A	12	16	16	0	0
6	B	12	16	16	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	1	0	0	0	0
10	B	28	10	12	0	0
10	D	28	10	12	0	0
11	B	12	13	13	0	0
12	B	29	27	0	0	0
12	D	29	27	0	0	0
13	C	4	6	6	0	0
14	F	31	14	14	0	0
15	A	17	0	0	0	0
15	B	27	0	0	0	0
15	C	64	0	0	0	0
15	D	6	0	0	0	0
15	E	1	0	0	0	0
15	F	3	0	0	0	0
All	All	17155	16646	16460	63	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 2.

The worst 5 of 63 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:209[B]:ILE:HD13	1:A:231:ILE:HD11	1.75	0.67
2:D:163:ASP:O	2:D:253[B]:ARG:NH2	2.29	0.65
1:A:209[B]:ILE:CD1	1:A:231:ILE:HD11	2.27	0.65
1:C:97:GLU:OE2	2:D:253[A]:ARG:NH1	2.30	0.65
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.80	0.63

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	446/451 (99%)	434 (97%)	12 (3%)	0	100	100
1	C	456/451 (101%)	446 (98%)	10 (2%)	0	100	100
2	B	426/445 (96%)	421 (99%)	5 (1%)	0	100	100
2	D	409/445 (92%)	396 (97%)	13 (3%)	0	100	100
3	E	118/189 (62%)	117 (99%)	1 (1%)	0	100	100
4	F	251/384 (65%)	244 (97%)	7 (3%)	0	100	100
All	All	2106/2365 (89%)	2058 (98%)	48 (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	381/379 (100%)	379 (100%)	2 (0%)	88	93
1	C	389/379 (103%)	387 (100%)	2 (0%)	88	93
2	B	376/383 (98%)	374 (100%)	2 (0%)	88	93
2	D	362/383 (94%)	360 (99%)	2 (1%)	86	91
3	E	110/171 (64%)	110 (100%)	0	100	100
4	F	240/342 (70%)	240 (100%)	0	100	100
All	All	1858/2037 (91%)	1850 (100%)	8 (0%)	91	94

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	377	PHE
2	D	139	HIS
1	C	71	GLU
2	B	377	PHE
1	C	251	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 8 are monoatomic - leaving 13 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	KG0	B	506	-	29,31,31	8.92	14 (48%)	30,44,44	5.33	7 (23%)
6	GOL	A	502	-	5,5,5	0.87	0	5,5,5	1.00	0
12	KG0	D	503	-	29,31,31	8.96	14 (48%)	30,44,44	5.09	6 (20%)
6	GOL	B	503	-	5,5,5	0.86	0	5,5,5	0.99	0
6	GOL	A	503	-	5,5,5	0.89	0	5,5,5	0.97	0
6	GOL	B	504	-	5,5,5	0.95	0	5,5,5	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	GDP	D	501	8	24,30,30	0.96	1 (4%)	30,47,47	1.21	5 (16%)
10	GDP	B	501	8	24,30,30	1.00	1 (4%)	30,47,47	1.07	3 (10%)
13	DMS	C	502	-	3,3,3	0.67	0	3,3,3	0.60	0
14	ACP	F	401	-	27,33,33	0.85	1 (3%)	32,52,52	1.47	2 (6%)
5	GTP	A	501	8	26,34,34	1.13	2 (7%)	32,54,54	1.45	5 (15%)
5	GTP	C	501	8	26,34,34	1.13	2 (7%)	32,54,54	1.39	5 (15%)
11	MES	B	502	-	12,12,12	2.13	1 (8%)	14,16,16	1.59	3 (21%)

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	KG0	B	506	-	-	7/24/41/41	0/3/3/3
6	GOL	A	502	-	-	0/4/4/4	-
12	KG0	D	503	-	-	6/24/41/41	0/3/3/3
6	GOL	B	503	-	-	0/4/4/4	-
6	GOL	A	503	-	-	0/4/4/4	-
6	GOL	B	504	-	-	2/4/4/4	-
10	GDP	D	501	8	-	3/12/32/32	0/3/3/3
10	GDP	B	501	8	-	4/12/32/32	0/3/3/3
14	ACP	F	401	-	-	3/15/38/38	0/3/3/3
5	GTP	A	501	8	-	6/18/38/38	0/3/3/3
5	GTP	C	501	8	-	9/18/38/38	0/3/3/3
11	MES	B	502	-	-	5/6/14/14	0/1/1/1

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	503	KG0	C19-N24	37.41	1.53	1.27
12	B	506	KG0	C19-N24	37.26	1.53	1.27
12	D	503	KG0	C17-S18	-13.70	1.63	1.81
12	D	503	KG0	C19-S18	-13.43	1.58	1.76
12	B	506	KG0	C17-S18	-13.41	1.64	1.81

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	506	KG0	C17-S18-C19	27.06	106.35	89.94
12	D	503	KG0	C17-S18-C19	25.59	105.47	89.94
12	D	503	KG0	S18-C19-N24	-8.81	107.69	118.19
12	B	506	KG0	S18-C19-N24	-8.60	107.94	118.19
14	F	401	ACP	PB-O3A-PA	-6.43	112.16	132.56

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

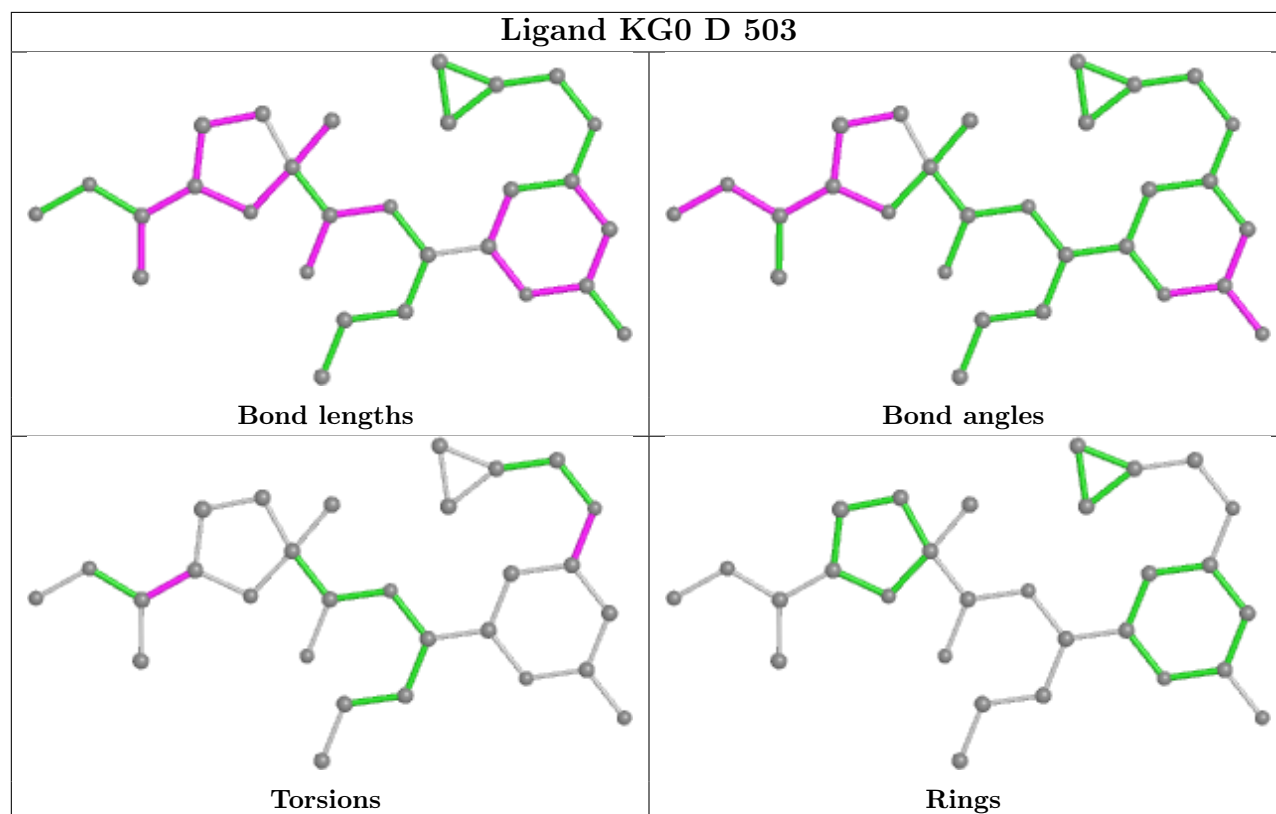
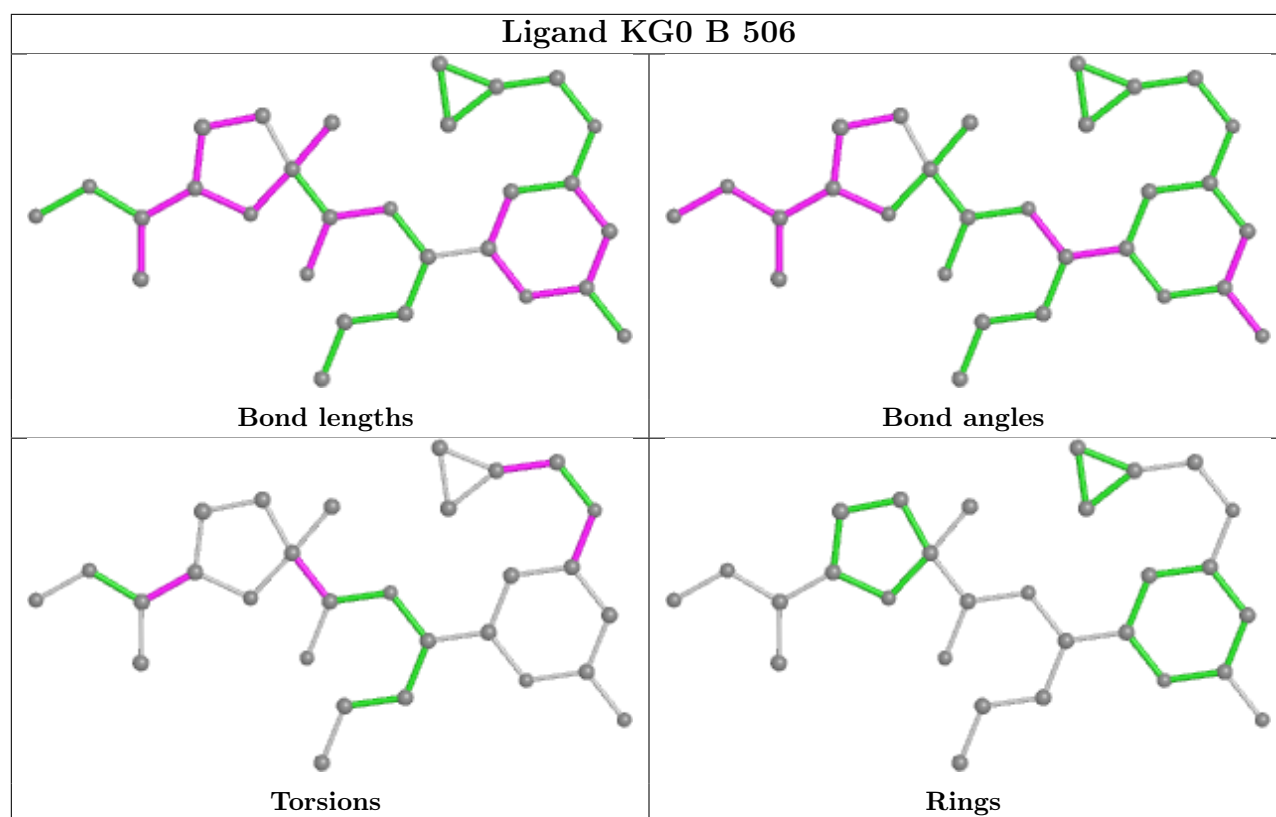
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A

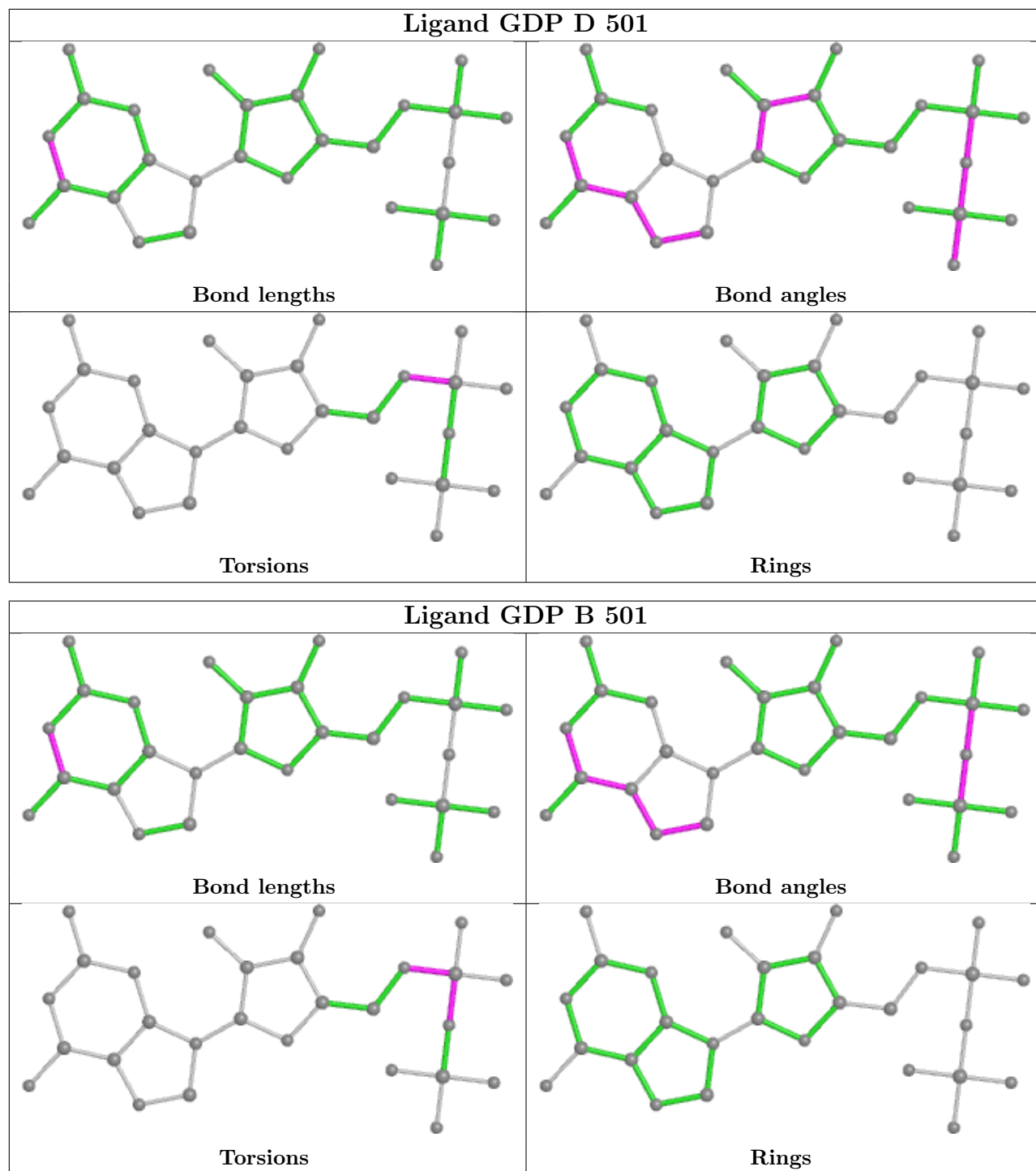
There are no ring outliers.

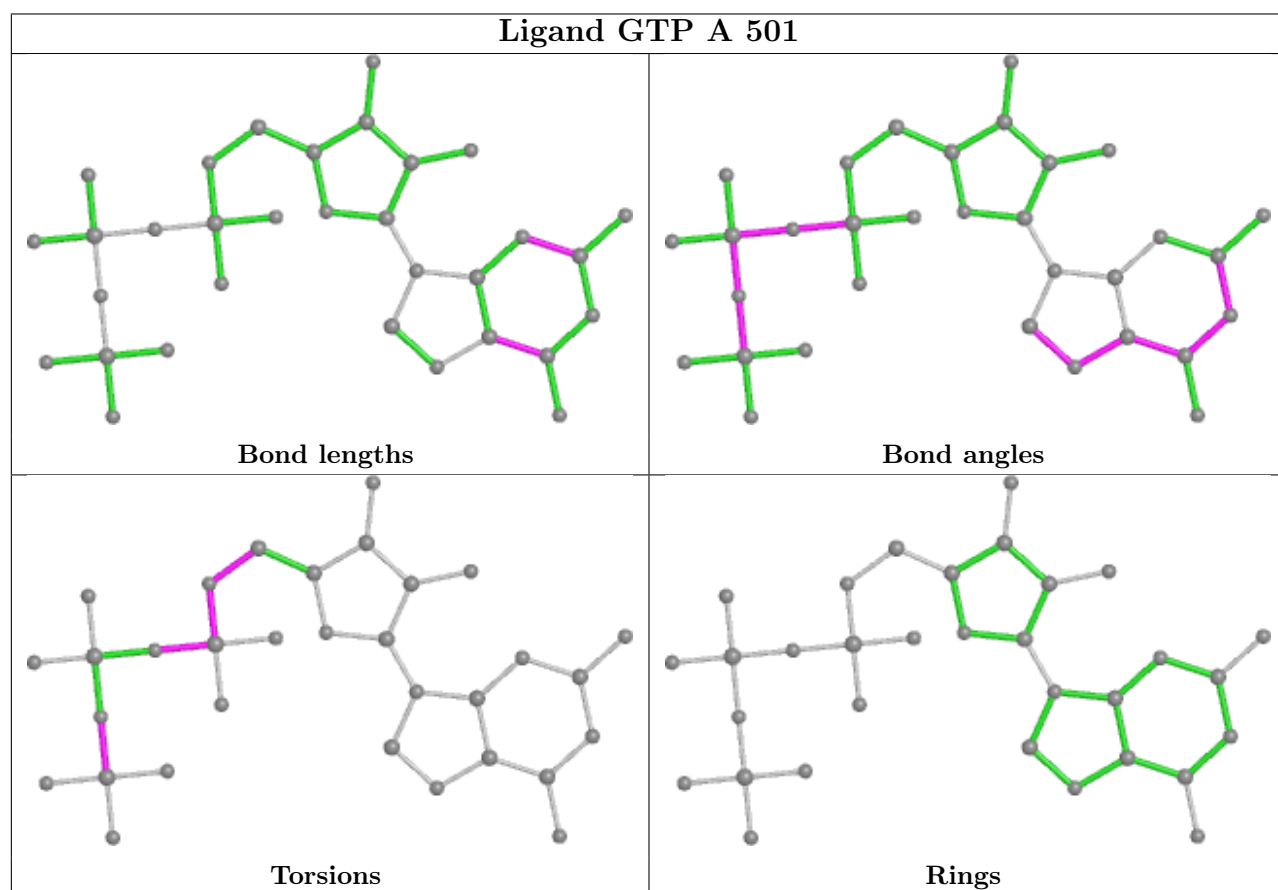
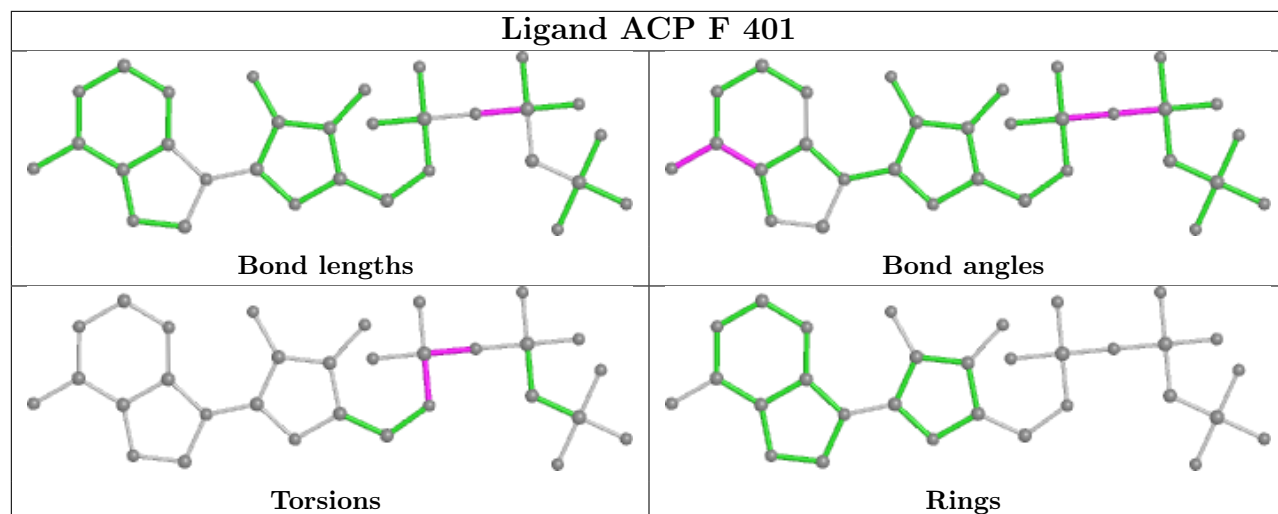
1 monomer is involved in 1 short contact:

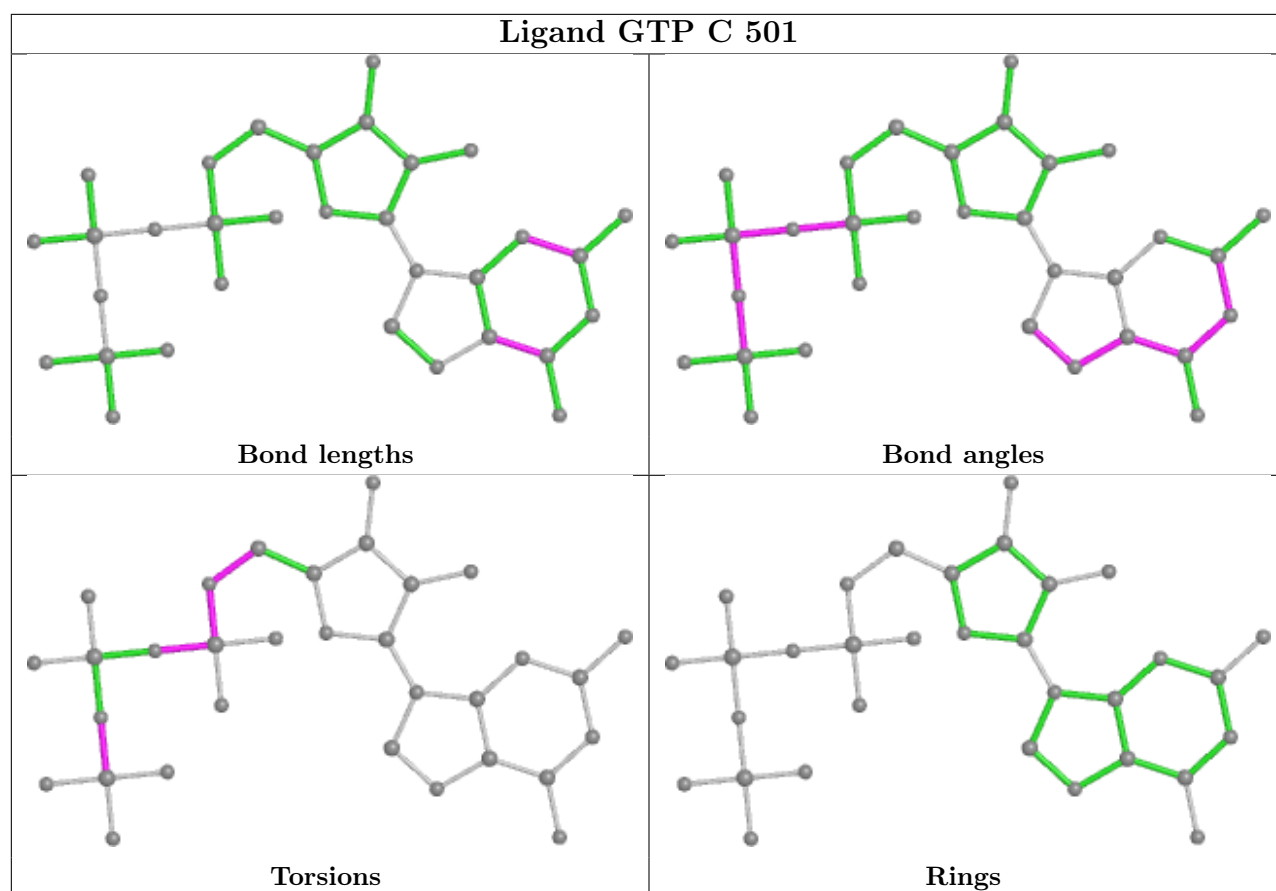
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0

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.









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	435/451 (96%)	0.47	20 (4%) 32 30	47, 72, 108, 131	0
1	C	440/451 (97%)	0.15	7 (1%) 72 69	38, 56, 93, 141	0
2	B	416/445 (93%)	0.34	13 (3%) 49 45	36, 64, 107, 159	0
2	D	414/445 (93%)	0.77	49 (11%) 4 3	50, 92, 132, 180	0
3	E	119/189 (62%)	0.71	16 (13%) 3 2	52, 91, 134, 152	0
4	F	261/384 (67%)	1.01	59 (22%) 0 0	52, 94, 134, 171	0
All	All	2085/2365 (88%)	0.52	164 (7%) 12 9	36, 74, 122, 180	0

The worst 5 of 164 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	59	ASN	8.0
4	F	182	ILE	7.7
4	F	186	LEU	6.9
3	E	27	PRO	6.3
4	F	147	TRP	5.8

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

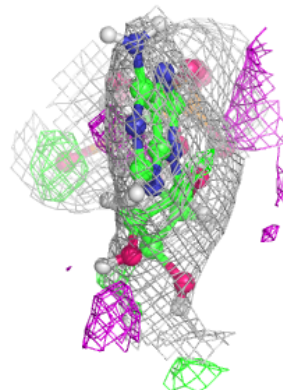
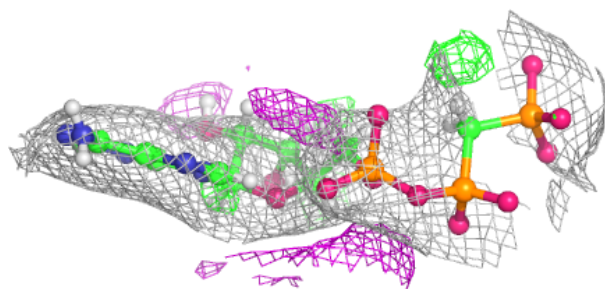
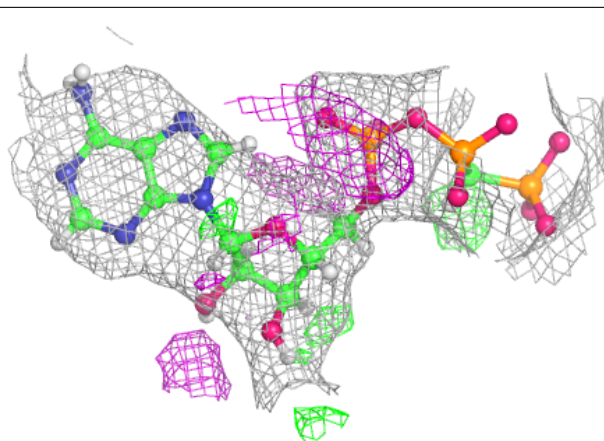
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	CL	A	506	1/1	0.77	0.11	79,79,79,79	0
6	GOL	A	502	6/6	0.79	0.25	66,72,82,82	14
14	ACP	F	401	31/31	0.79	0.21	107,120,143,157	0
6	GOL	B	503	6/6	0.80	0.14	78,87,95,95	0
6	GOL	A	503	6/6	0.82	0.21	80,82,92,92	0
13	DMS	C	502	4/4	0.85	0.19	53,66,83,84	0
6	GOL	B	504	6/6	0.86	0.18	61,70,82,82	0
8	MG	D	502	1/1	0.89	0.04	85,85,85,85	0
7	CA	B	507	1/1	0.91	0.10	84,84,84,84	0
12	KG0	B	506	29/29	0.93	0.24	48,54,63,76	0
10	GDP	D	501	28/28	0.93	0.15	72,78,88,93	0
11	MES	B	502	12/12	0.93	0.13	57,59,71,85	0
12	KG0	D	503	29/29	0.94	0.25	56,63,69,86	0
7	CA	A	504	1/1	0.95	0.04	83,83,83,83	0
8	MG	A	505	1/1	0.96	0.22	50,50,50,50	0
5	GTP	A	501	32/32	0.97	0.27	44,53,57,63	0
10	GDP	B	501	28/28	0.97	0.26	39,47,54,59	0
8	MG	B	505	1/1	0.97	0.26	37,37,37,37	0
7	CA	C	503	1/1	0.97	0.10	70,70,70,70	0
8	MG	C	504	1/1	0.98	0.17	46,46,46,46	0
5	GTP	C	501	32/32	0.98	0.18	41,46,50,56	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.

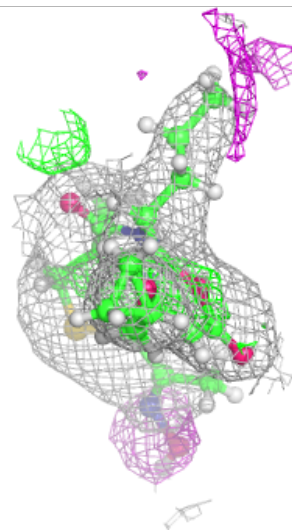
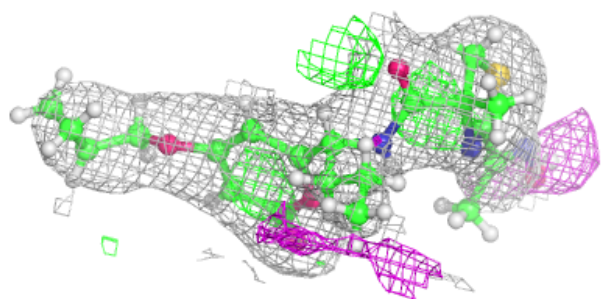
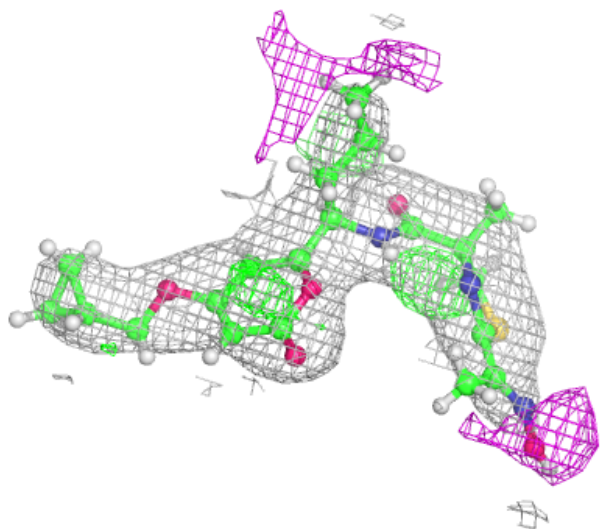
Electron density around ACP F 401:

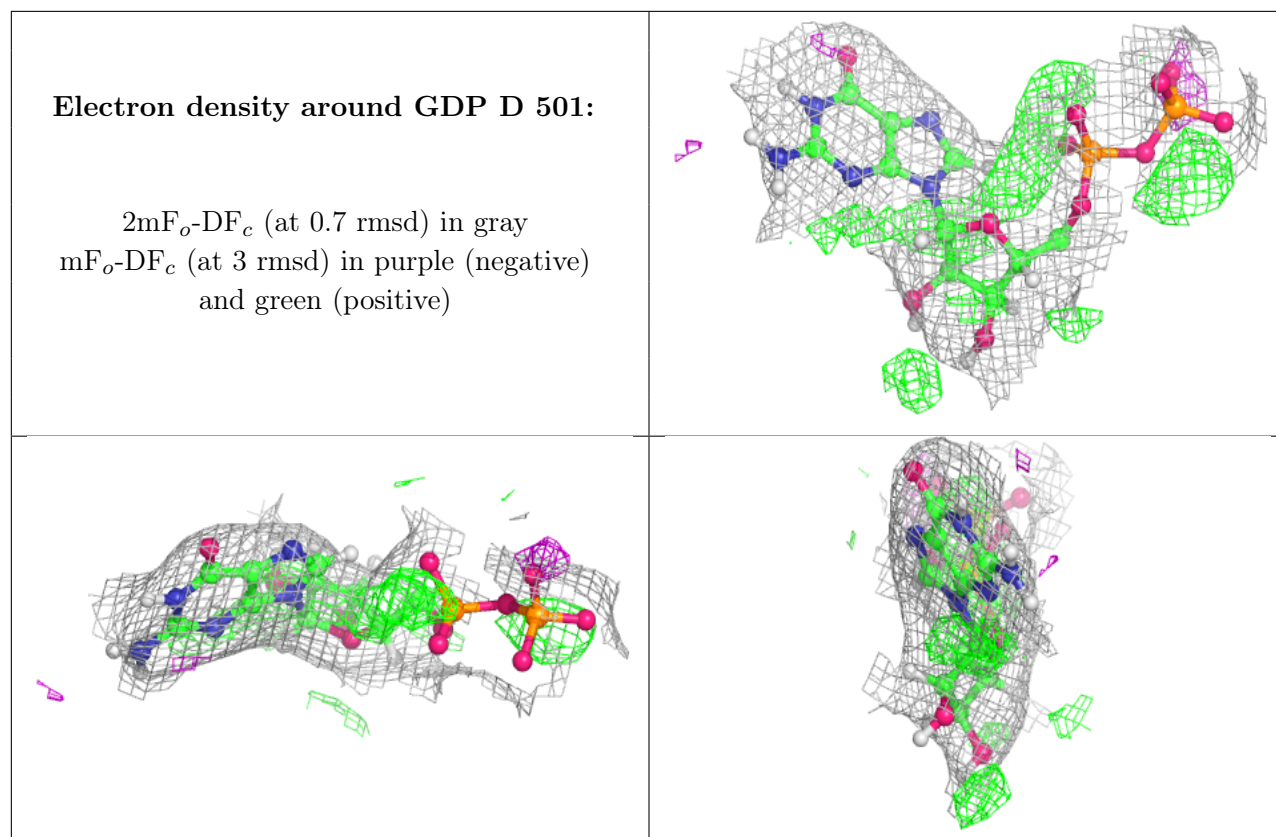
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around KG0 B 506:

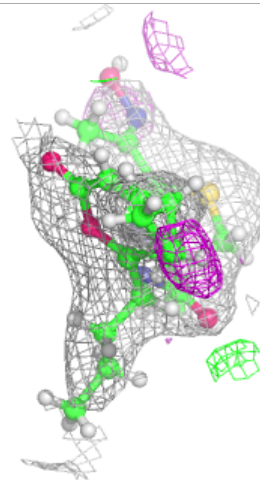
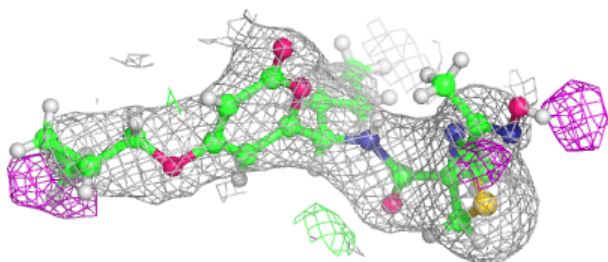
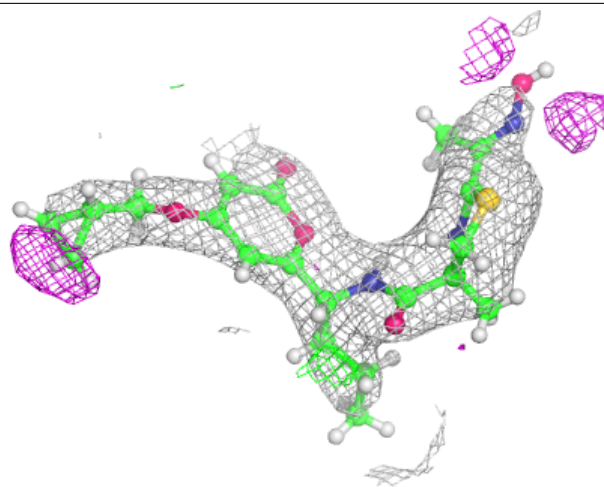
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

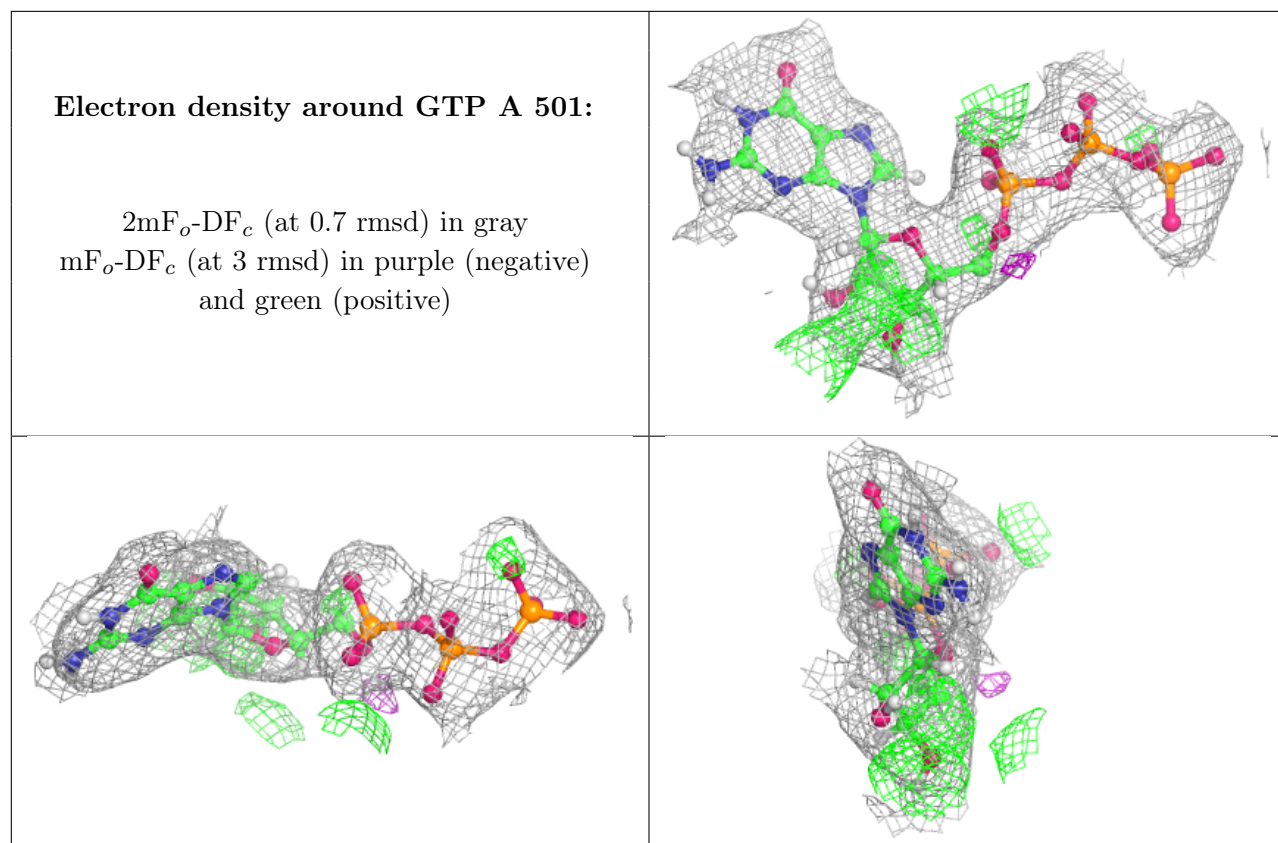




Electron density around KG0 D 503:

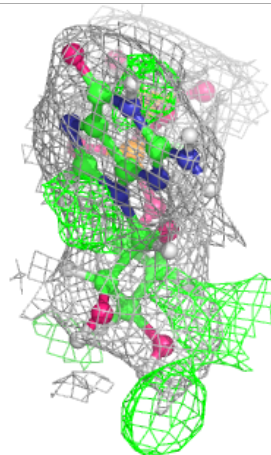
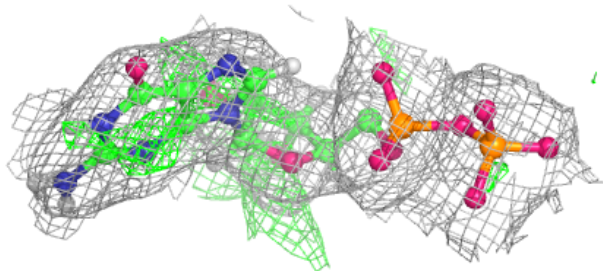
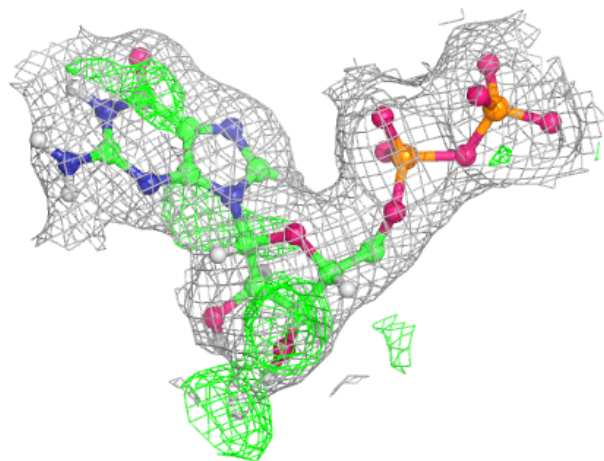
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

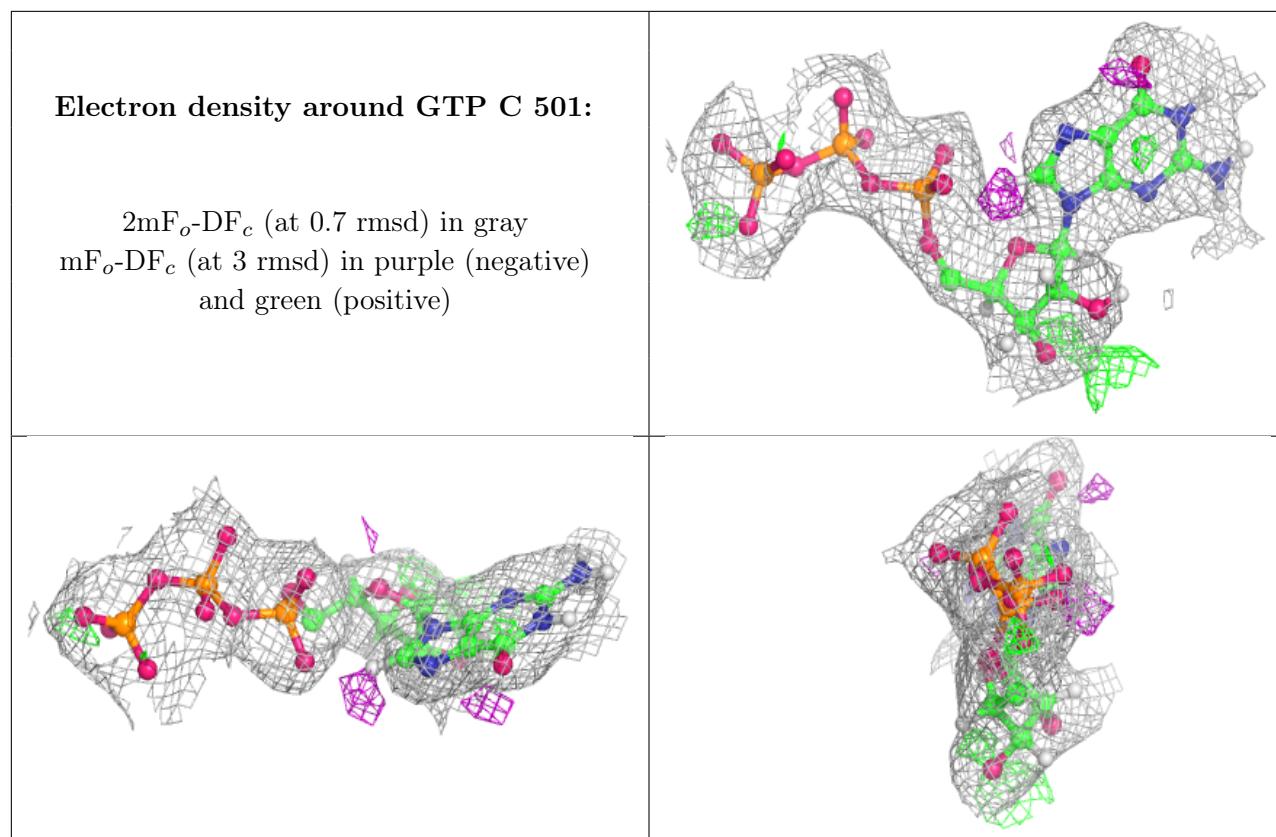




Electron density around GDP B 501:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.