



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 12:22 PM UTC

PDB ID : 7CLD / pdb\_00007cld  
Title : Crystal structure of T2R-TTL-Cevipabulin complex  
Authors : Chen, L.J.; Chen, Q.; Yu, Y.; Yang, J.H.  
Deposited on : 2020-07-20  
Resolution : 2.61 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](mailto:validation@mail.wwpdb.org)

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<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>.

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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)  
Xtrriage (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

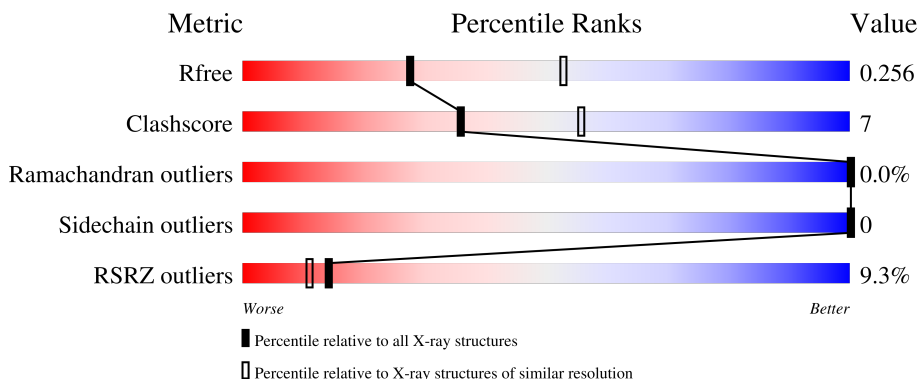
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	450	 5% 84% 14%
1	C	450	 2% 86% 12%
2	B	445	 5% 78% 16% 6%
2	D	445	 12% 78% 18%
3	E	143	 19% 70% 15% 1%

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Mol	Chain	Length	Quality of chain
4	F	384	 <p>A horizontal bar chart showing the quality distribution of chain F. The bar is divided into four segments: 18% red, 69% green, 22% yellow, and 9% grey. The percentages are labeled above or below the corresponding segments.</p>

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 35069 atoms, of which 17070 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	438	6802	2182	3351	588	657	24	0	4	0
1	C	440	6827	2196	3361	587	660	23	0	7	0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	B	418	6491	2077	3184	566	636	28	0	3	0
2	D	426	6563	2100	3217	570	649	27	0	1	0

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
3	E	123	2053	629	1031	185	203	5	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
4	F	351	5696	1838	2824	491	528	15	0	1	0

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 (CCD ID: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



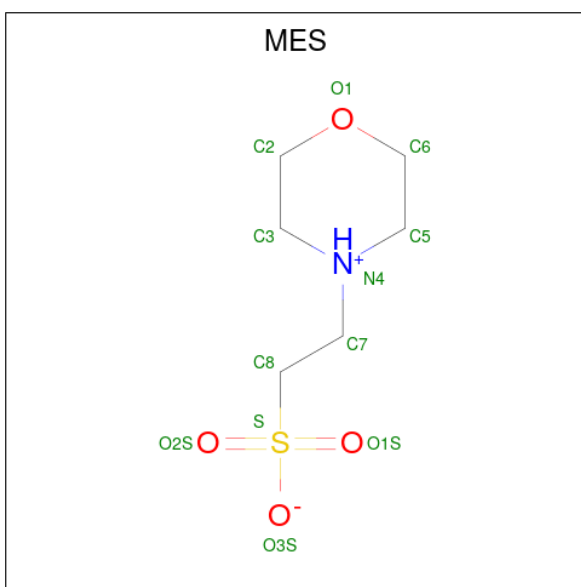
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
5	A	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		
5	C	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		
5	D	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		

- 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		

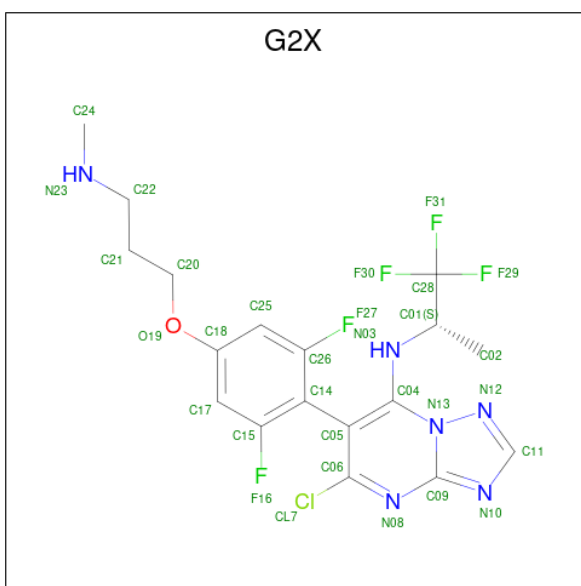
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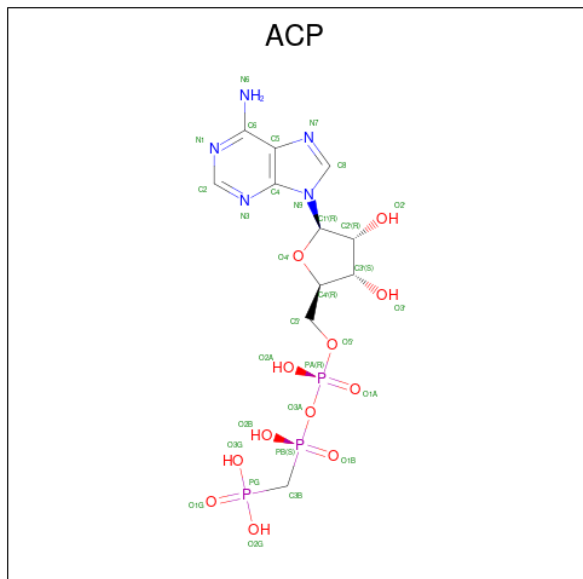
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			S
9	B	1	24	6	12	1	4	1	0	0

- Molecule 10 is 6-[2,6-bis(fluoranyl)-4-[3-(methylamino)propoxy]phenyl]-5-chloranyl-N-[(2S)-1,1,1-tris(fluoranyl)propan-2-yl]-[1,2,4]triazolo[1,5-a]pyrimidin-7-amine (CCD ID: G2X) (formula:  $C_{18}H_{18}ClF_5N_6O$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	
			Total	C	Cl	F	H	N			O
10	B	1	49	18	1	5	18	6	1	0	0
10	C	1	49	18	1	5	18	6	1	0	0

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula:  $C_{11}H_{18}N_5O_{12}P_3$ ).



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

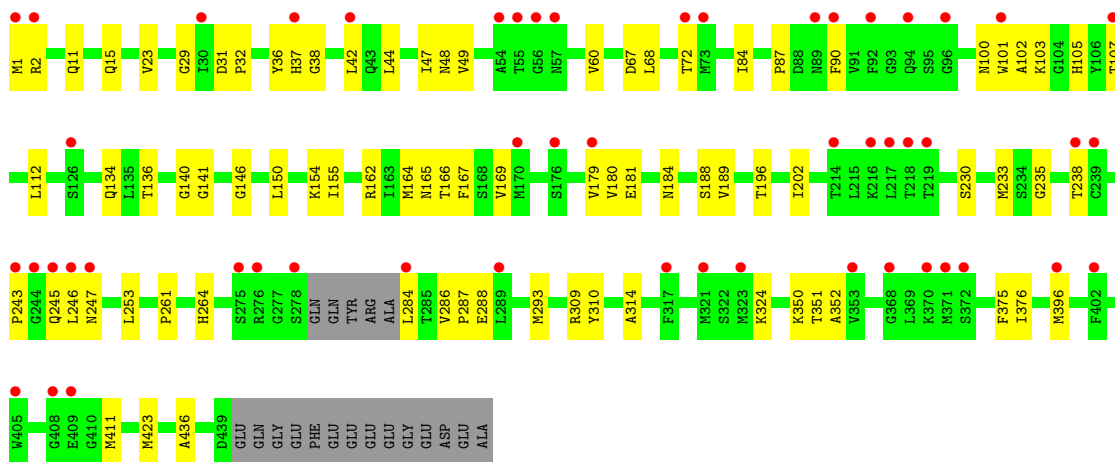
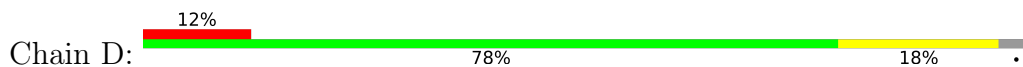
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	72	Total	O	0	0
			72	72		
12	B	53	Total	O	0	0
			53	53		
12	C	104	Total	O	0	0
			104	104		
12	D	32	Total	O	0	0
			32	32		
12	E	13	Total	O	0	0
			13	13		
12	F	20	Total	O	0	0
			20	20		

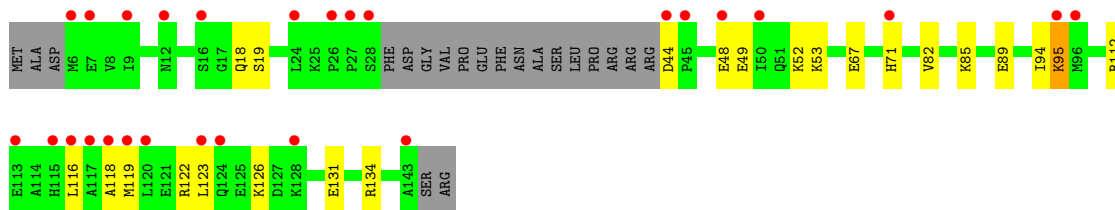




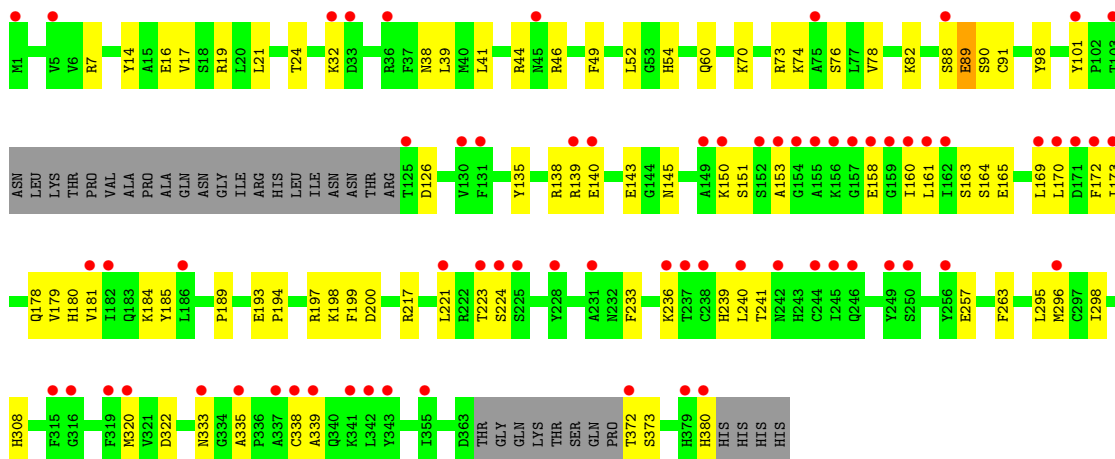
- Molecule 2: Tubulin beta chain



- Molecule 3: Stathmin-4



- Molecule 4: Tubulin tyrosine ligase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.42Å 160.78Å 174.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.03 – 2.61 50.03 – 2.61	Depositor EDS
% Data completeness (in resolution range)	93.4 (50.03-2.61) 93.4 (50.03-2.61)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.64 (at 2.61Å)	Xtrriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, $R_{free}$	0.207 , 0.258 0.207 , 0.256	Depositor DCC
$R_{free}$ test set	1761 reflections (1.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.1	Xtrriage
Anisotropy	0.052	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 46.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	35069	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.17% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MES, ACP, GTP, GDP, MG, CA, G2X

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	0/3532	0.39	0/4794
1	C	0.45	2/3568 (0.1%)	0.51	2/4846 (0.0%)
2	B	0.27	0/3386	0.42	0/4584
2	D	0.25	0/3422	0.38	0/4634
3	E	0.53	2/1030 (0.2%)	0.53	3/1367 (0.2%)
4	F	0.23	0/2937	0.42	0/3967
All	All	0.32	4/17875 (0.0%)	0.44	5/24192 (0.0%)

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	C	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	372	GLN	CD-NE2	-16.83	0.97	1.33
3	E	95	LYS	CG-CD	-9.91	1.22	1.52
3	E	95	LYS	CE-NZ	-8.04	1.25	1.49
1	C	372	GLN	CD-OE1	-6.10	1.11	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	372	GLN	CB-CG-CD	-15.35	86.50	112.60
3	E	95	LYS	CD-CE-NZ	-9.18	82.52	111.90
1	C	372	GLN	N-CA-CB	-7.67	98.82	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	95	LYS	CB-CG-CD	-6.56	96.21	111.30
3	E	95	LYS	CG-CD-CE	6.33	125.85	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	372	GLN	Sidechain

## 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	3451	3351	3362	47	0
1	C	3466	3361	3376	39	0
2	B	3307	3184	3193	45	1
2	D	3346	3217	3227	52	0
3	E	1022	1031	1034	19	1
4	F	2872	2824	2835	66	0
5	A	32	10	12	0	0
5	C	32	10	12	1	0
5	D	32	10	12	1	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	A	2	0	0	0	0
7	B	2	0	0	0	0
7	C	2	0	0	0	0
7	D	1	0	0	0	0
8	B	28	10	12	1	0
9	B	12	12	12	0	0
10	B	31	18	0	0	0
10	C	31	18	0	1	0
11	F	31	14	14	2	0
12	A	72	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	B	53	0	0	2	0
12	C	104	0	0	5	0
12	D	32	0	0	6	0
12	E	13	0	0	2	0
12	F	20	0	0	0	0
All	All	17999	17070	17101	254	1

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 7.

The worst 5 of 254 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:79:ARG:NH1	12:A:601:HOH:O	2.03	0.89
3:E:95:LYS:HD3	3:E:95:LYS:N	1.91	0.86
4:F:296[B]:MET:SD	4:F:380:HIS:ND1	2.51	0.83
4:F:140:GLU:O	4:F:140:GLU:OE1	2.04	0.76
2:B:285:THR:N	2:B:288:GLU:OE1	2.19	0.75

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:ARG:HH21	3:E:131:GLU:OE1[4_455]	1.46	0.14

## 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	440/450 (98%)	431 (98%)	9 (2%)	0	<a href="#">100</a> <a href="#">100</a>
1	C	445/450 (99%)	432 (97%)	13 (3%)	0	<a href="#">100</a> <a href="#">100</a>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	417/445 (94%)	404 (97%)	13 (3%)	0	100	100
2	D	423/445 (95%)	408 (96%)	15 (4%)	0	100	100
3	E	120/143 (84%)	116 (97%)	4 (3%)	0	100	100
4	F	346/384 (90%)	337 (97%)	8 (2%)	1 (0%)	36	56
All	All	2191/2317 (95%)	2128 (97%)	62 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	89	GLU

### 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	373/378 (99%)	373 (100%)	0	100	100
1	C	378/378 (100%)	378 (100%)	0	100	100
2	B	364/383 (95%)	364 (100%)	0	100	100
2	D	369/383 (96%)	369 (100%)	0	100	100
3	E	111/127 (87%)	111 (100%)	0	100	100
4	F	314/342 (92%)	314 (100%)	0	100	100
All	All	1909/1991 (96%)	1909 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	372	GLN
2	D	99	ASN
4	F	252	ASN
2	D	37	HIS

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Mol	Chain	Res	Type
2	D	165	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 12 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GTP	C	501	6	33,34,34	1.03	3 (9%)	50,54,54	1.44	9 (18%)
5	GTP	A	501	6	33,34,34	0.92	2 (6%)	50,54,54	1.54	9 (18%)
5	GTP	D	503	6	33,34,34	1.04	3 (9%)	50,54,54	1.70	11 (22%)
10	G2X	B	506	-	30,33,33	2.32	11 (36%)	37,48,48	1.98	10 (27%)
8	GDP	B	501	-	29,30,30	1.20	3 (10%)	45,47,47	1.81	10 (22%)
10	G2X	C	504	-	30,33,33	2.45	14 (46%)	37,48,48	1.91	11 (29%)
9	MES	B	503	-	12,12,12	2.16	1 (8%)	15,16,16	1.64	3 (20%)
11	ACP	F	402	6	31,33,33	2.46	10 (32%)	47,52,52	2.48	15 (31%)

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
5	GTP	C	501	6	-	7/22/38/38	0/3/3/3
5	GTP	A	501	6	-	6/22/38/38	0/3/3/3
5	GTP	D	503	6	-	5/22/38/38	0/3/3/3
10	G2X	B	506	-	-	3/20/20/20	0/3/3/3
8	GDP	B	501	-	-	3/16/32/32	0/3/3/3
10	G2X	C	504	-	-	1/20/20/20	0/3/3/3
9	MES	B	503	-	-	0/6/14/14	0/1/1/1
11	ACP	F	402	6	-	1/19/38/38	0/3/3/3

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	503	MES	C8-S	-7.17	1.67	1.77
11	F	402	ACP	PB-O3A	5.46	1.64	1.58
10	C	504	G2X	C09-N10	5.38	1.41	1.33
11	F	402	ACP	PA-O3A	5.26	1.65	1.59
10	B	506	G2X	C09-N10	4.49	1.39	1.33

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	402	ACP	C4-N9-C8	8.77	114.95	105.74
10	C	504	G2X	C11-N12-N13	6.46	106.12	100.86
10	B	506	G2X	C11-N12-N13	6.34	106.03	100.86
8	B	501	GDP	C5-C4-N3	-5.66	119.39	128.39
11	F	402	ACP	N3-C4-N9	5.44	136.42	127.17

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

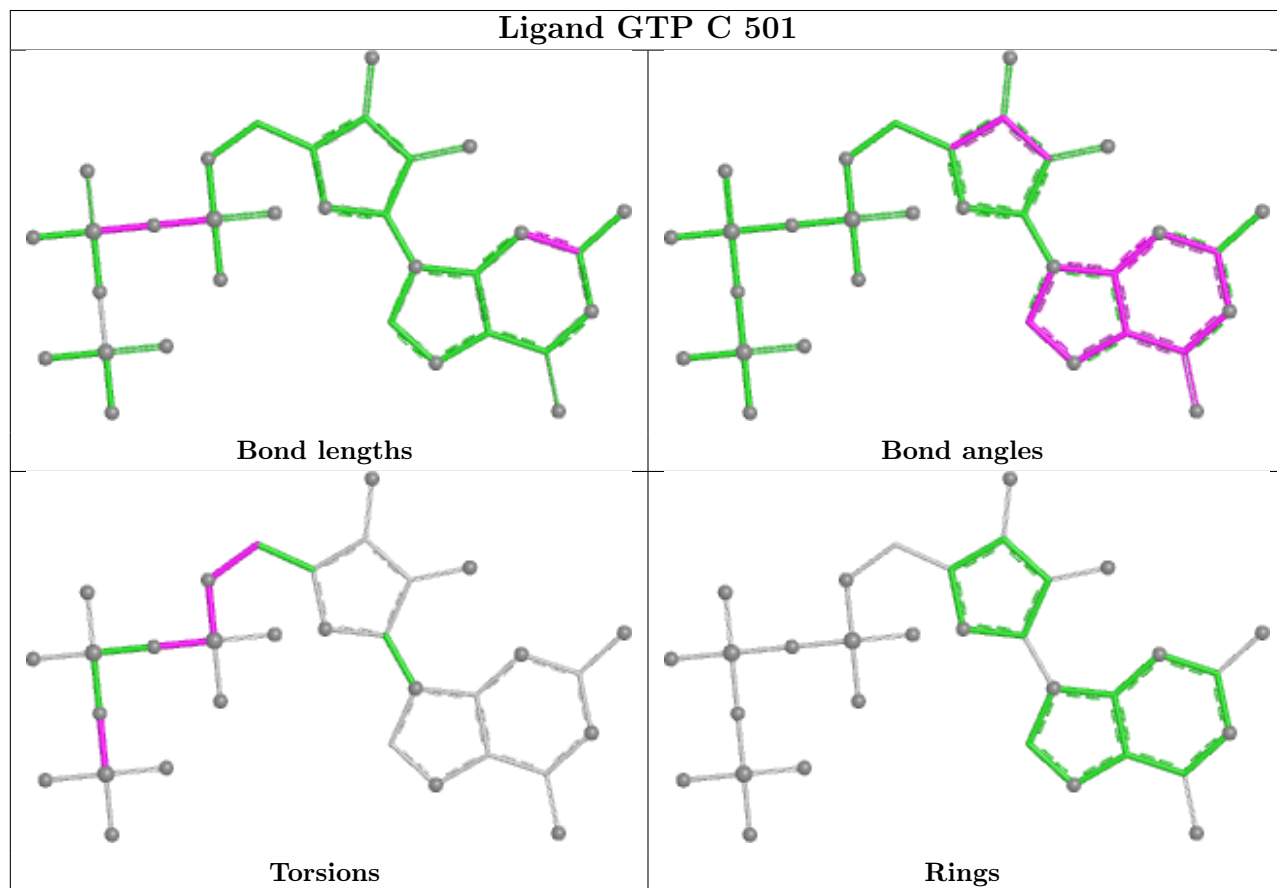
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O3A

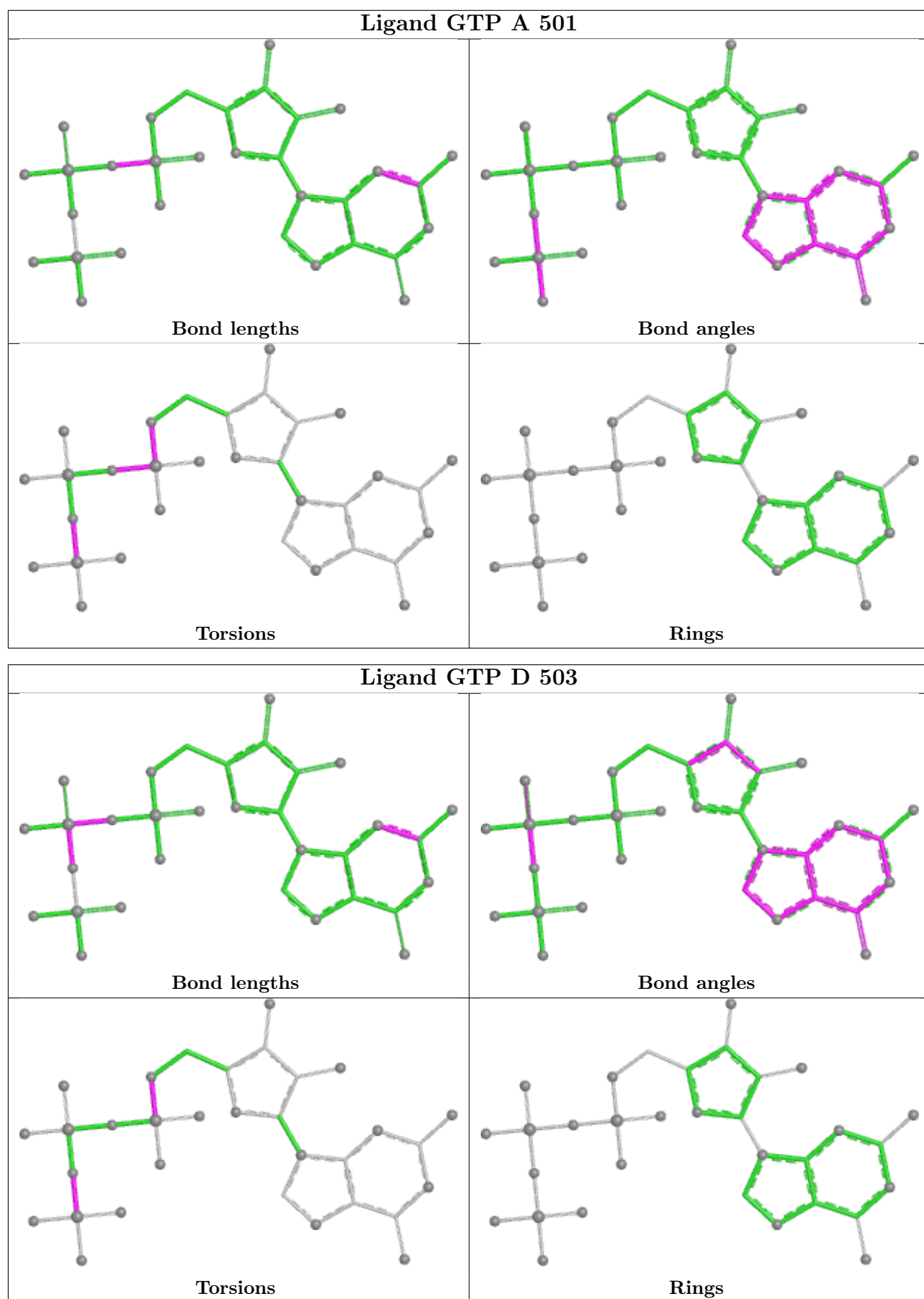
There are no ring outliers.

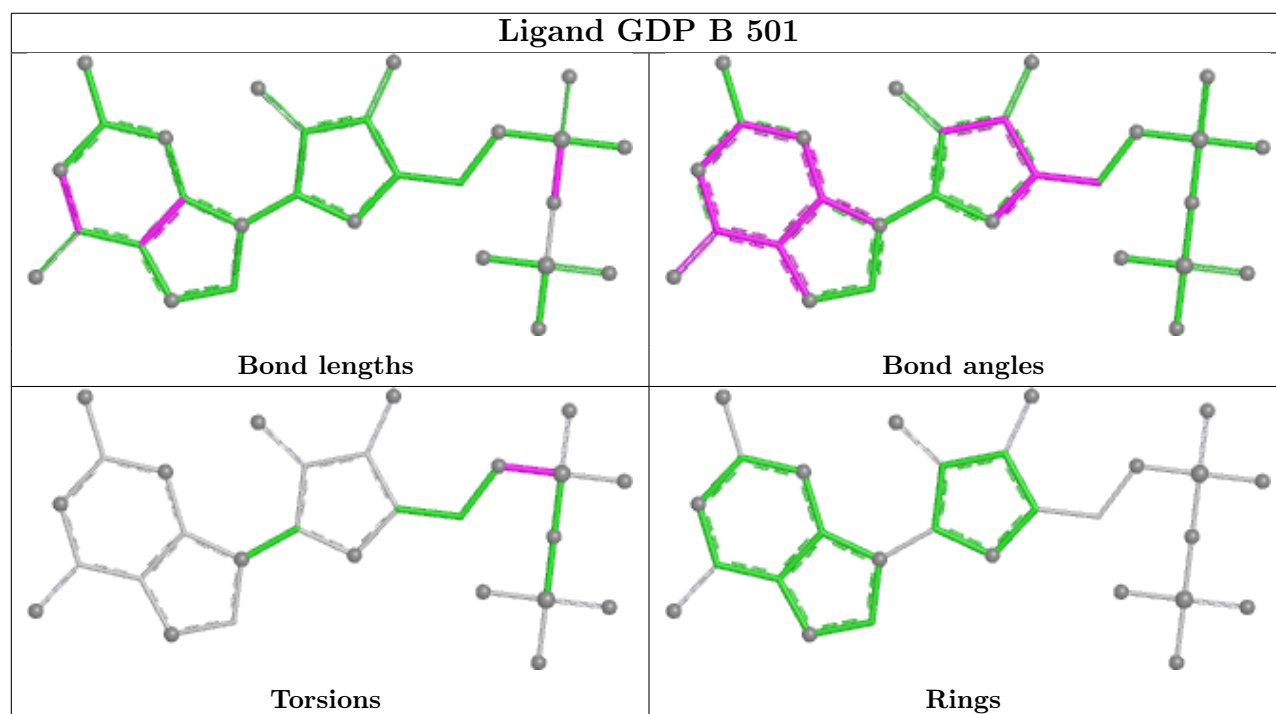
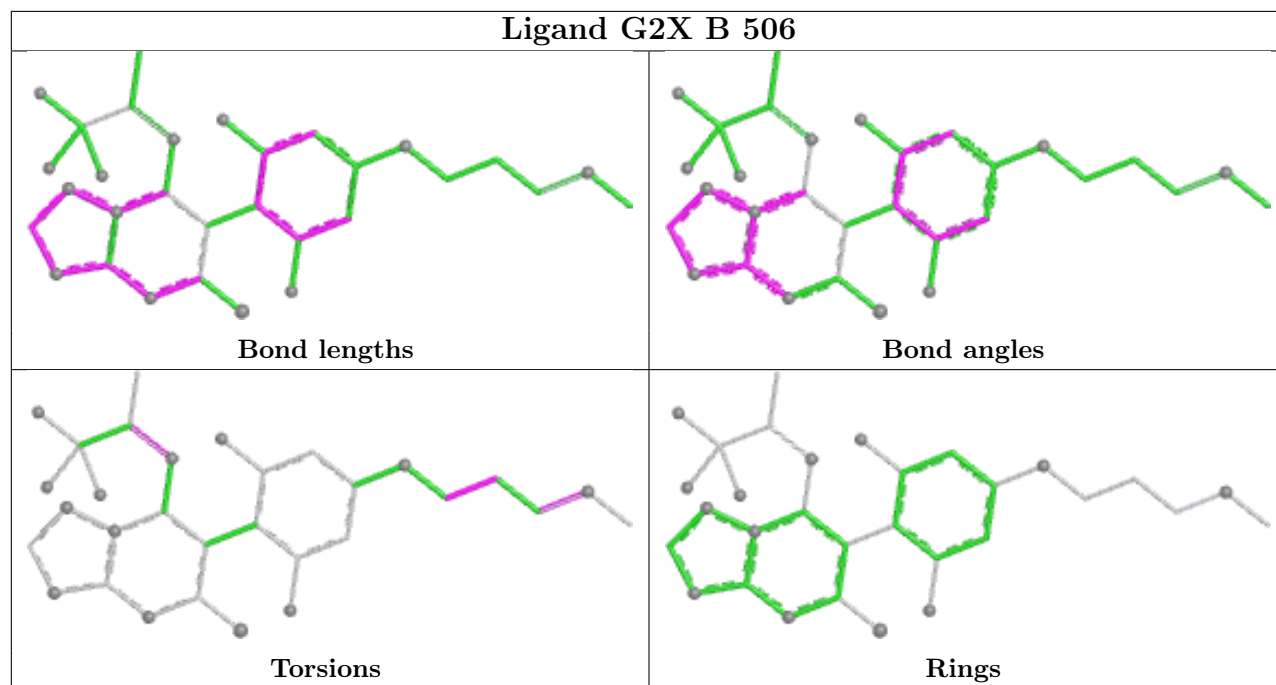
5 monomers are involved in 6 short contacts:

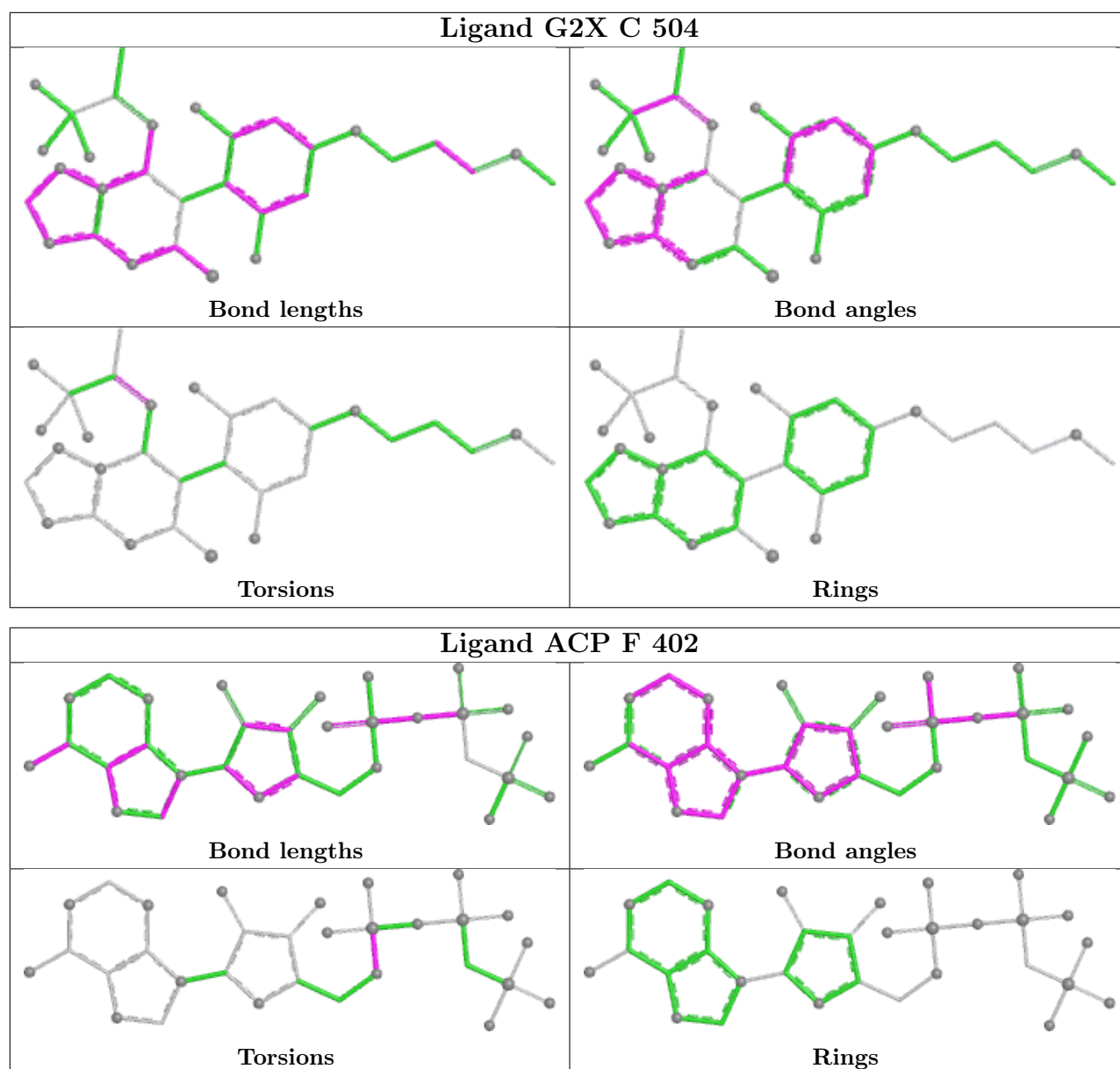
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	501	GTP	1	0
5	D	503	GTP	1	0
8	B	501	GDP	1	0
10	C	504	G2X	1	0
11	F	402	ACP	2	0

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	438/450 (97%)	0.33	23 (5%) 32 27	15, 46, 85, 137	4 (0%)
1	C	440/450 (97%)	-0.21	9 (2%) 65 60	8, 29, 60, 95	6 (1%)
2	B	418/445 (93%)	0.25	23 (5%) 30 25	9, 41, 84, 121	3 (0%)
2	D	426/445 (95%)	0.81	52 (12%) 8 6	17, 57, 98, 136	1 (0%)
3	E	123/143 (86%)	0.99	27 (21%) 2 2	19, 61, 104, 113	1 (0%)
4	F	351/384 (91%)	1.27	70 (19%) 3 2	23, 76, 126, 141	1 (0%)
All	All	2196/2317 (94%)	0.49	204 (9%) 14 11	8, 48, 103, 141	16 (0%)

The worst 5 of 204 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	245	ILE	7.6
1	C	1	MET	6.2
2	D	239	CYS	6.0
2	D	368	GLY	6.0
4	F	103	THR	5.6

### 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

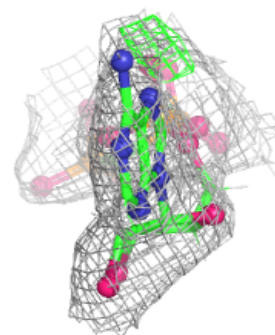
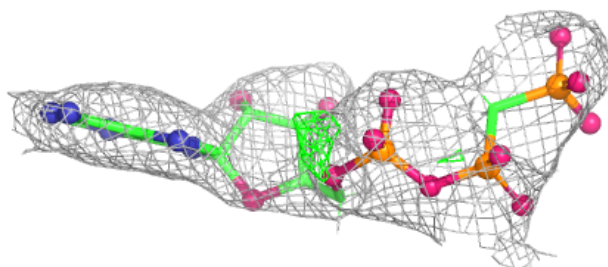
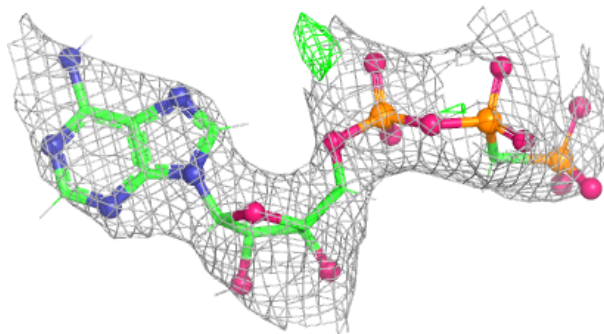
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	MG	D	501	1/1	0.59	0.34	59,59,59,59	0
6	MG	F	401	1/1	0.67	0.22	89,89,89,89	0
7	CA	B	504	1/1	0.79	0.29	119,119,119,119	0
11	ACP	F	402	31/31	0.88	0.16	69,89,110,122	0
6	MG	B	502	1/1	0.89	0.27	44,44,44,44	0
7	CA	B	505	1/1	0.89	0.11	72,72,72,72	0
7	CA	C	503	1/1	0.89	0.16	98,98,98,98	0
7	CA	A	504	1/1	0.89	0.23	98,98,98,98	0
5	GTP	D	503	32/32	0.91	0.12	38,48,61,69	0
10	G2X	B	506	31/31	0.92	0.11	24,37,57,58	0
10	G2X	C	504	31/31	0.93	0.10	18,32,59,62	0
7	CA	D	502	1/1	0.93	0.16	78,78,78,78	0
9	MES	B	503	12/12	0.95	0.09	36,43,51,54	0
5	GTP	C	501	32/32	0.96	0.08	15,27,49,59	0
7	CA	A	503	1/1	0.97	0.05	75,75,75,75	0
8	GDP	B	501	28/28	0.97	0.07	15,28,51,64	0
5	GTP	A	501	32/32	0.98	0.06	10,28,40,49	0
6	MG	A	502	1/1	0.99	0.05	23,23,23,23	0
7	CA	C	505	1/1	0.99	0.03	30,30,30,30	0
6	MG	C	502	1/1	1.00	0.02	19,19,19,19	0

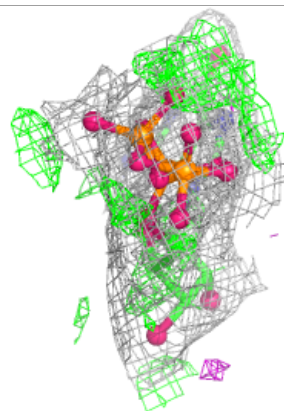
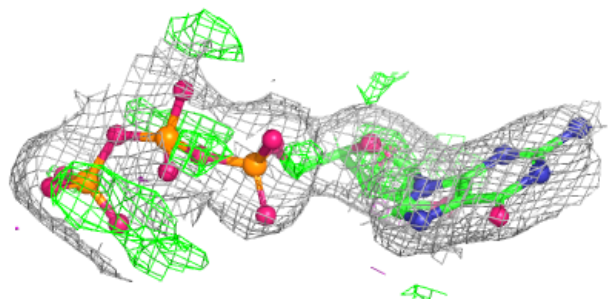
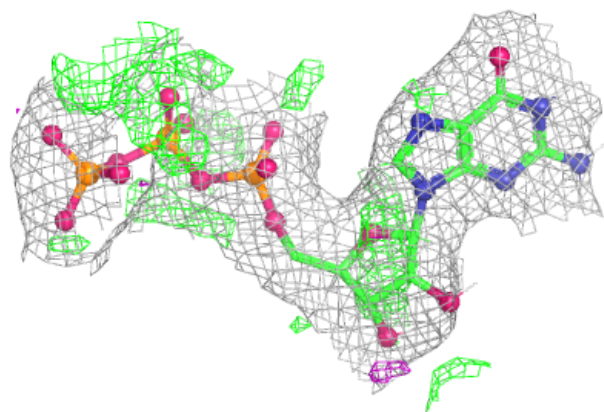
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ACP F 402:**

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

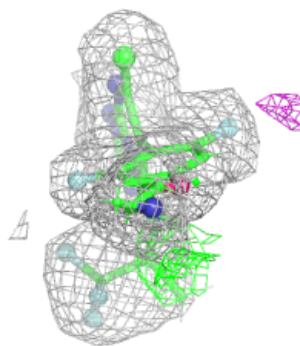
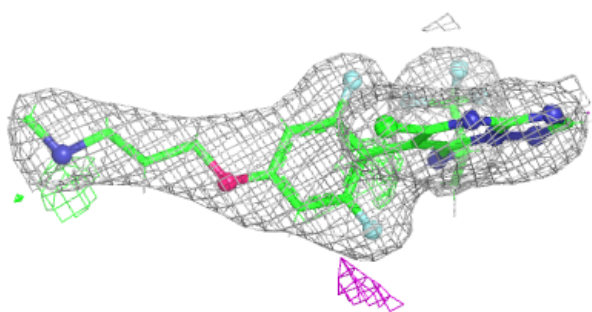
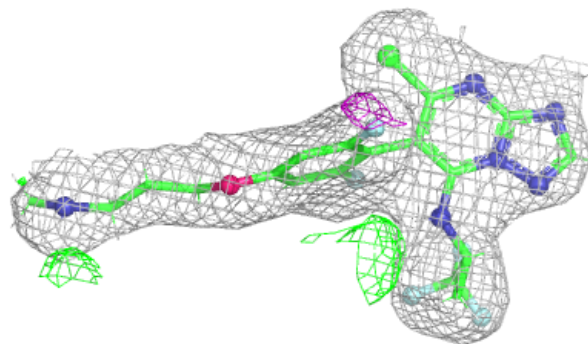
**Electron density around GTP D 503:**

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

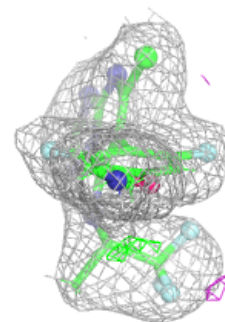
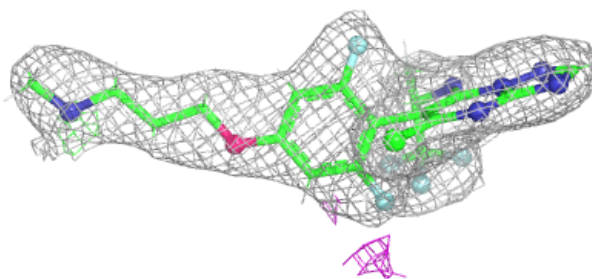
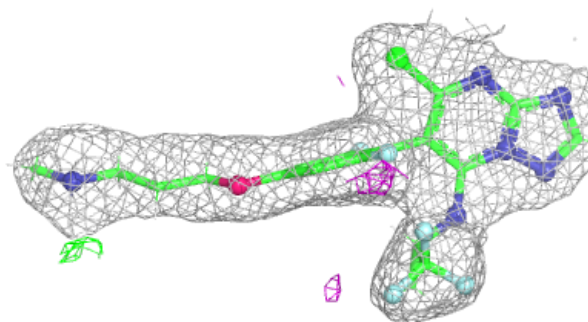


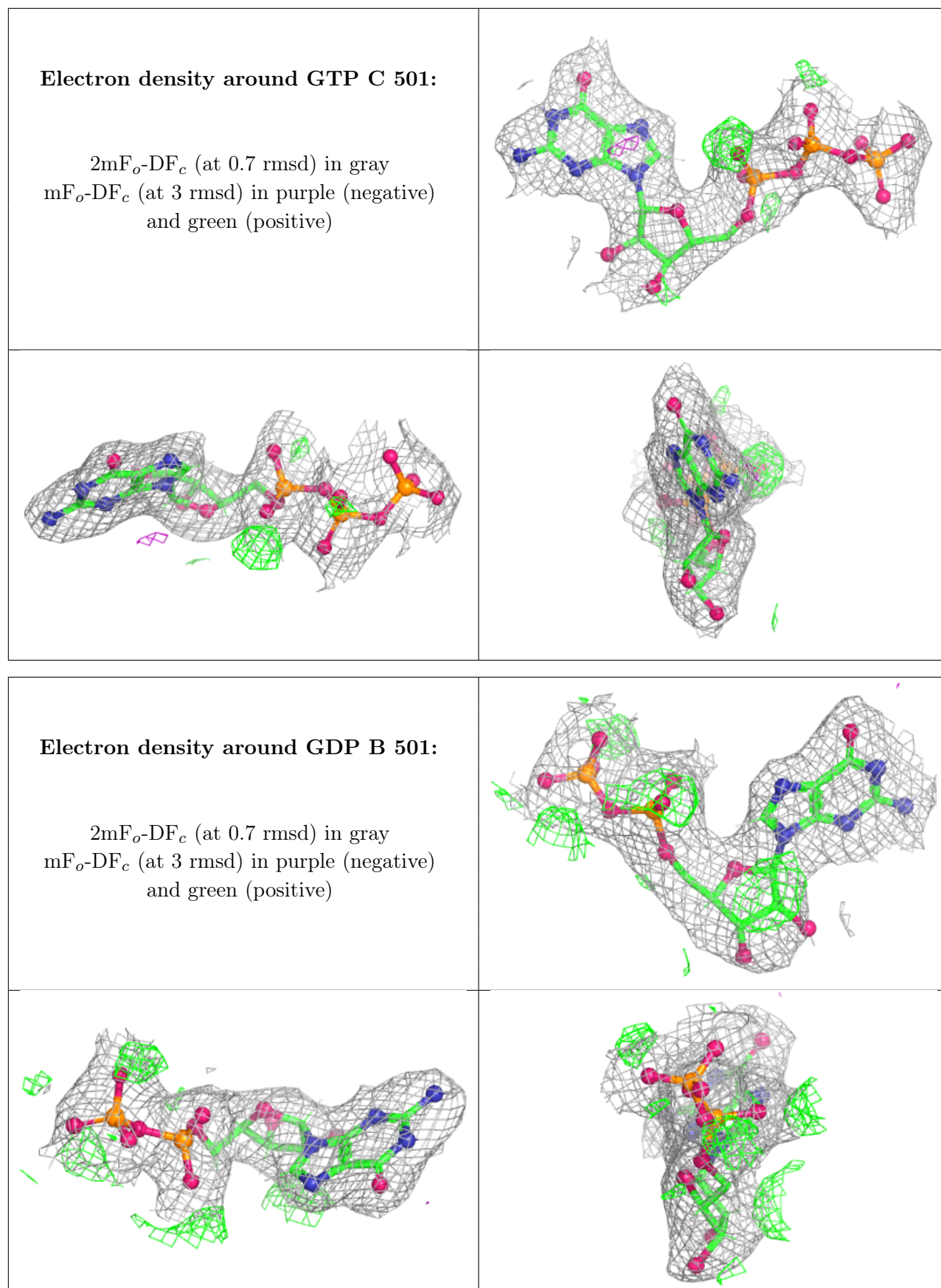
**Electron density around G2X B 506:**

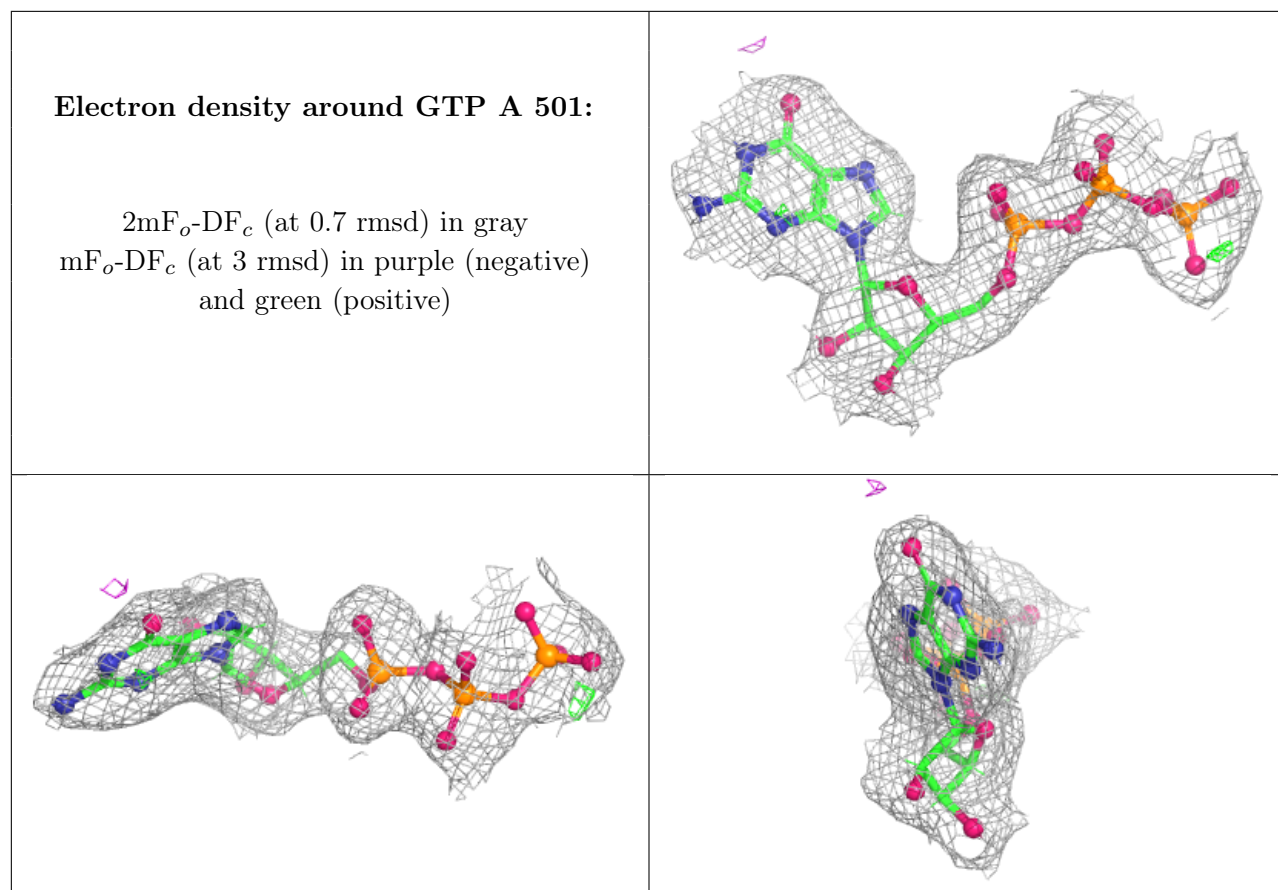
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around G2X C 504:**

$2mF_o-DF_c$  (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.