



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:49 AM UTC

PDB ID : 5JQG / pdb_00005jqg
Title : An apo tubulin-RB-TTL complex structure used for side-by-side comparison
Authors : Wang, Y.X.; Naismith, J.H.; Zhu, X.
Deposited on : 2016-05-04
Resolution : 2.24 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	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

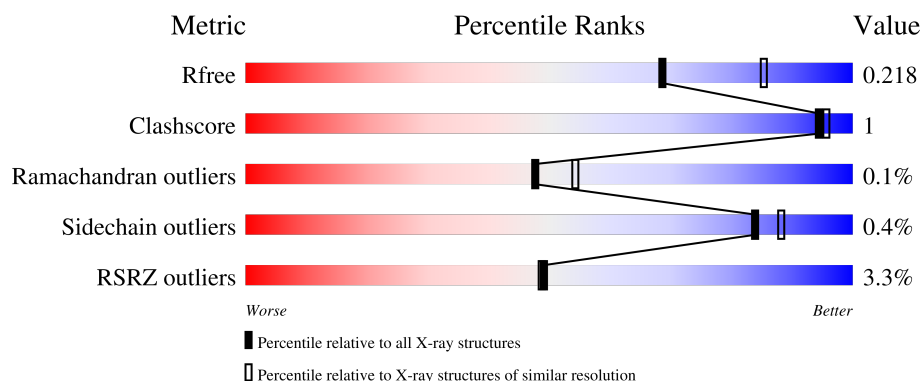
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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	
1	C	451	
2	B	445	
2	D	445	
3	E	143	

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Mol	Chain	Length	Quality of chain
4	F	384	6% 75% 6% 20%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17646 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	437	Total	C	N	O	S	0	3	0
			3430	2173	582	651	24			
1	C	440	Total	C	N	O	S	0	9	0
			3482	2200	589	668	25			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	4	0
			3353	2107	575	646	25			
2	D	420	Total	C	N	O	S	0	1	0
			3296	2073	561	637	25			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	120	Total	C	N	O	S	0	3	0
			1012	627	182	197	6			

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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	309	Total	C	N	O	S	0	3	0
			2553	1645	438	455	15			

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
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		
5	D	1	Total	C	N	O	P	0	0
			32	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
6	D	1	Total	Mg	0	0
			1	1		

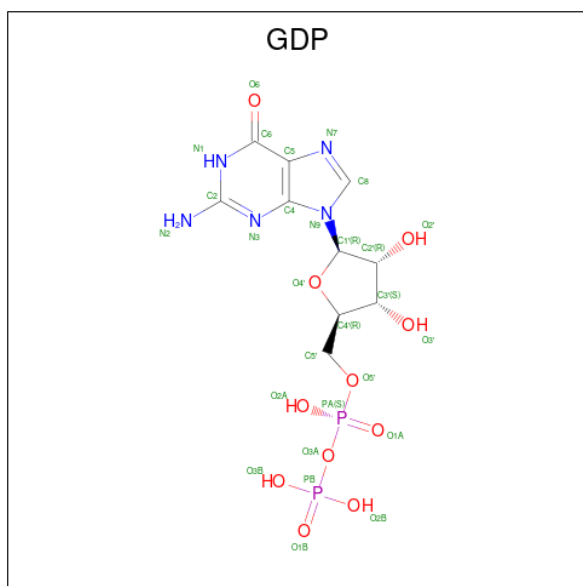
- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	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 CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

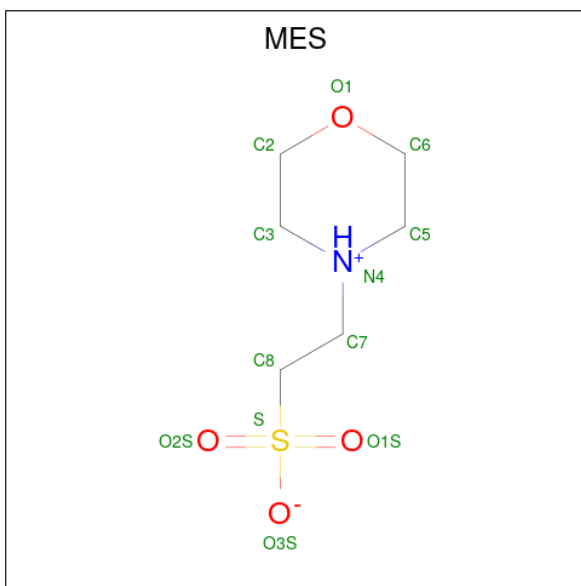
- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

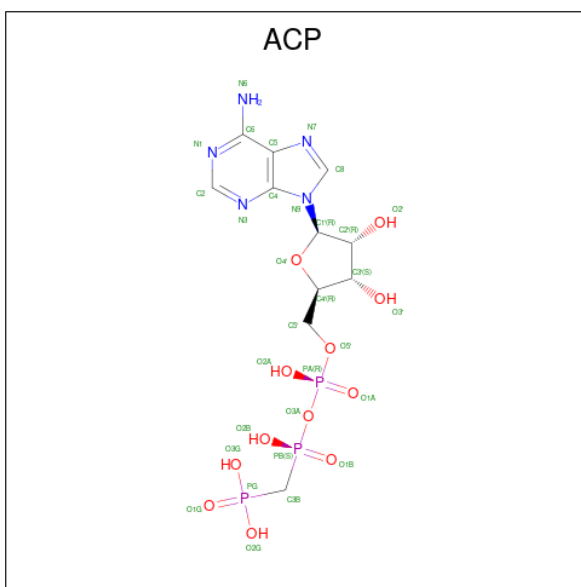
- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES)

(formula: $C_6H_{13}NO_4S$).



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

- 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
11	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

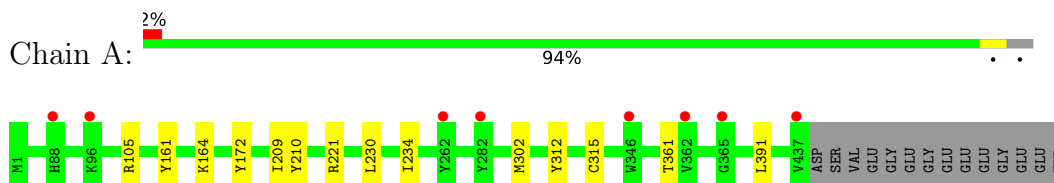
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	78	Total	O	0	0
			78	78		
12	B	62	Total	O	0	0
			62	62		
12	C	131	Total	O	0	0
			131	131		
12	D	35	Total	O	0	0
			35	35		
12	E	6	Total	O	0	0
			6	6		
12	F	21	Total	O	0	0
			21	21		

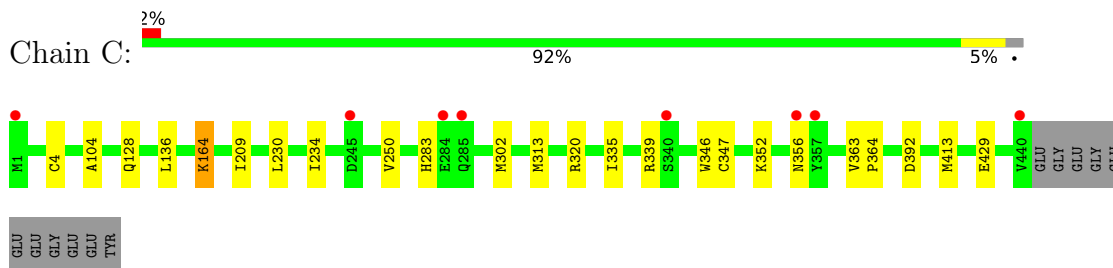
3 Residue-property plots [i](#)

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.

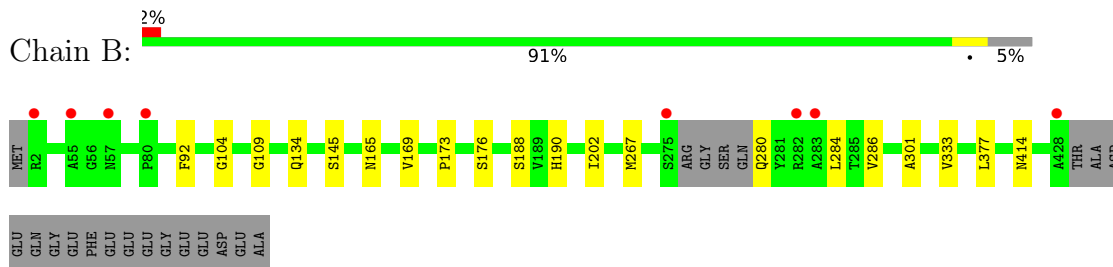
- Molecule 1: Tubulin alpha-1B chain



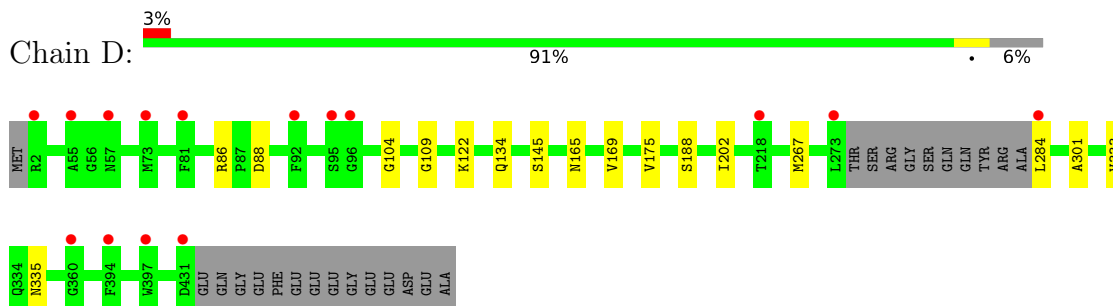
- Molecule 1: Tubulin alpha-1B chain



- Molecule 2: Tubulin beta chain

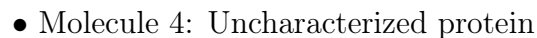


- Molecule 2: Tubulin beta chain



- Molecule 3: Stathmin-4

Chain E:



Chain F:

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.05Å 158.12Å 180.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.22 – 2.24 35.22 – 2.24	Depositor EDS
% Data completeness (in resolution range)	99.9 (35.22-2.24) 99.9 (35.22-2.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.181 , 0.212 0.190 , 0.218	Depositor DCC
R_{free} test set	7246 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.8	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	17646	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 2.43% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MES, ACP, GTP, GDP, CA, MG, 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	1.00	2/3514 (0.1%)	1.01	1/4770 (0.0%)
1	C	1.08	0/3572	1.03	2/4850 (0.0%)
2	B	1.03	2/3433 (0.1%)	0.98	1/4651 (0.0%)
2	D	0.95	0/3369	0.98	2/4566 (0.0%)
3	E	1.02	0/1026	1.12	1/1361 (0.1%)
4	F	0.93	2/2618 (0.1%)	0.94	2/3537 (0.1%)
All	All	1.01	6/17532 (0.0%)	1.00	9/23735 (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
4	F	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	254	GLY	C-O	6.66	1.33	1.24
1	A	105	ARG	C-O	-5.57	1.17	1.24
1	A	105	ARG	CA-C	5.49	1.59	1.52
2	B	92	PHE	C-O	-5.35	1.17	1.23
2	B	286	VAL	CA-CB	5.25	1.57	1.54
4	F	254	GLY	CA-C	5.18	1.58	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	175	VAL	CB-CA-C	6.20	117.25	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	333	VAL	N-CA-CB	6.18	118.94	110.54
4	F	59	VAL	N-CA-C	-5.92	101.08	108.89
1	A	361	THR	N-CA-C	-5.85	101.01	110.32
1	C	335	ILE	N-CA-C	5.53	116.26	110.62
2	B	333	VAL	N-CA-CB	5.47	117.98	110.54
3	E	76	ARG	N-CA-CB	5.26	117.85	110.12
1	C	339	ARG	N-CA-C	5.07	117.86	109.85
4	F	340	GLN	O-C-N	5.04	128.29	122.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	F	165	GLU	Peptide

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	3430	0	3350	7	0
1	C	3482	0	3384	12	0
2	B	3353	0	3233	8	0
2	D	3296	0	3173	8	1
3	E	1012	0	1038	2	0
4	F	2553	0	2519	7	1
5	A	32	0	12	0	0
5	C	32	0	12	0	0
5	D	32	0	12	0	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
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
9	B	28	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	24	0	26	0	0
11	F	31	0	14	0	0
12	A	78	0	0	0	0
12	B	62	0	0	0	0
12	C	131	0	0	1	0
12	D	35	0	0	0	0
12	E	6	0	0	0	0
12	F	21	0	0	0	0
All	All	17646	0	16785	44	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 1.

All (44) 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:C:234:ILE:HD13	1:C:302:MET:SD	2.24	0.77
1:C:128:GLN:OE1	12:C:601:HOH:O	2.05	0.75
1:A:234:ILE:HD13	1:A:302:MET:SD	2.29	0.73
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.32	0.70
1:A:209:ILE:HD11	1:A:302:MET:SD	2.35	0.67
1:C:209:ILE:HD11	1:C:302:MET:SD	2.36	0.66
1:C:346:TRP:CZ3	1:C:347[A]:CYS:SG	2.89	0.65
1:C:313:MET:O	1:C:347[B]:CYS:SG	2.59	0.61
2:B:190:HIS:CE1	2:B:414[B]:ASN:OD1	2.56	0.58
1:C:104:ALA:HB2	1:C:413:MET:SD	2.43	0.58
2:B:173:PRO:HA	2:B:176:SER:HB2	1.93	0.51
2:D:145[A]:SER:HG	2:D:188:SER:HG	1.57	0.51
2:B:145:SER:HG	2:B:188:SER:HG	1.59	0.50
2:D:104:GLY:O	2:D:109:GLY:HA3	2.13	0.49
2:B:267:MET:HG3	2:B:301:ALA:HB3	1.94	0.48
2:D:86:ARG:NH1	2:D:122:LYS:HE2	2.28	0.48
2:D:267:MET:HG3	2:D:301:ALA:HB3	1.95	0.47
1:C:250:VAL:HG11	1:C:352:LYS:HE3	1.95	0.47
2:D:86:ARG:NH1	2:D:88:ASP:HB2	2.29	0.47
2:B:104:GLY:O	2:B:109:GLY:HA3	2.16	0.46
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.98	0.45
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.52	0.45
4:F:292:ARG:NH1	4:F:296[B]:MET:SD	2.90	0.45
1:A:312:TYR:CD2	1:A:315[B]:CYS:SG	3.10	0.45
2:B:134:GLN:HA	2:B:165:ASN:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:162:ILE:HD11	4:F:240:LEU:HD11	2.00	0.44
2:D:134:GLN:HA	2:D:165:ASN:O	2.17	0.44
4:F:349:GLY:HA3	4:F:374:ILE:HD11	2.00	0.43
1:A:161:TYR:HB3	1:A:164:LYS:HG2	1.99	0.43
1:C:320:ARG:HA	1:C:356:ASN:O	2.19	0.42
1:C:392:ASP:OD2	1:C:429:GLU:OE2	2.36	0.42
4:F:255:ARG:HD3	4:F:256:TYR:CZ	2.55	0.42
1:A:209:ILE:HG23	1:A:230:LEU:HD23	2.01	0.42
1:A:210:TYR:OH	1:A:221:ARG:HD3	2.20	0.42
4:F:21:LEU:O	4:F:24:THR:HB	2.20	0.42
3:E:6:MET:HE2	3:E:24:LEU:HD22	2.01	0.42
4:F:70:LYS:O	4:F:76:SER:HB3	2.20	0.42
2:B:169:VAL:HA	2:B:202:ILE:O	2.21	0.41
3:E:135:LYS:O	3:E:136:ASN:C	2.63	0.41
2:B:377:LEU:HD23	2:B:377:LEU:C	2.46	0.41
4:F:200:ASP:OD2	4:F:241:THR:OG1	2.27	0.40
1:C:363:VAL:HG12	1:C:364:PRO:O	2.22	0.40
2:D:122:LYS:HB3	2:D:122:LYS:HE3	1.95	0.40
2:D:169:VAL:HA	2:D:202:ILE:O	2.21	0.40

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:D:335:ASN:OD1	4:F:384:HIS:NE2[3_545]	2.13	0.07

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	438/451 (97%)	429 (98%)	9 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	446/451 (99%)	437 (98%)	7 (2%)	2 (0%)	30	30
2	B	423/445 (95%)	416 (98%)	7 (2%)	0	100	100
2	D	416/445 (94%)	411 (99%)	5 (1%)	0	100	100
3	E	119/143 (83%)	117 (98%)	2 (2%)	0	100	100
4	F	300/384 (78%)	290 (97%)	10 (3%)	0	100	100
All	All	2142/2319 (92%)	2100 (98%)	40 (2%)	2 (0%)	48	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	164	LYS
1	C	283	HIS

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	371/379 (98%)	371 (100%)	0	100	100
1	C	379/379 (100%)	378 (100%)	1 (0%)	86	90
2	B	368/381 (97%)	366 (100%)	2 (0%)	81	86
2	D	361/381 (95%)	360 (100%)	1 (0%)	86	90
3	E	111/127 (87%)	110 (99%)	1 (1%)	70	78
4	F	281/342 (82%)	278 (99%)	3 (1%)	65	74
All	All	1871/1989 (94%)	1863 (100%)	8 (0%)	84	88

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	280	GLN
2	B	284	LEU
1	C	164	LYS
2	D	284	LEU

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Mol	Chain	Res	Type
3	E	77	GLU
4	F	12	SER
4	F	32	LYS
4	F	86	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	85	GLN
1	A	309	HIS
1	A	393	HIS
2	B	8	GLN
2	B	14	ASN
2	B	57	ASN
2	B	94	GLN
2	B	134	GLN
2	B	329	GLN
2	B	347	ASN
2	B	426	GLN
1	C	31	GLN
1	C	393	HIS
2	D	8	GLN
2	D	14	ASN
2	D	134	GLN
2	D	195	ASN
2	D	396	HIS
3	E	84	GLN
4	F	229	ASN
4	F	243	HIS

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 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 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	D	501	6	33,34,34	1.20	5 (15%)	50,54,54	1.62	7 (14%)
10	MES	B	505	-	12,12,12	2.27	1 (8%)	15,16,16	1.04	1 (6%)
5	GTP	A	501	6	33,34,34	1.39	6 (18%)	50,54,54	1.61	8 (16%)
10	MES	B	504	-	12,12,12	2.03	1 (8%)	15,16,16	1.36	2 (13%)
9	GDP	B	501	6	29,30,30	1.21	3 (10%)	45,47,47	1.76	10 (22%)
11	ACP	F	401	-	31,33,33	1.94	11 (35%)	47,52,52	1.73	9 (19%)
5	GTP	C	501	6	33,34,34	1.15	3 (9%)	50,54,54	1.56	8 (16%)

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	D	501	6	-	6/22/38/38	0/3/3/3
10	MES	B	505	-	-	0/6/14/14	0/1/1/1
5	GTP	A	501	6	-	4/22/38/38	0/3/3/3
10	MES	B	504	-	-	3/6/14/14	0/1/1/1
9	GDP	B	501	6	-	4/16/32/32	0/3/3/3
11	ACP	F	401	-	-	3/19/38/38	0/3/3/3
5	GTP	C	501	6	-	6/22/38/38	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	505	MES	C8-S	-7.47	1.67	1.77
10	B	504	MES	C8-S	-6.66	1.68	1.77
11	F	401	ACP	C5-C4	4.81	1.47	1.39
11	F	401	ACP	PB-O1B	4.58	1.62	1.51
5	A	501	GTP	PB-O3B	3.83	1.63	1.59
11	F	401	ACP	PB-O2B	-3.25	1.48	1.56
11	F	401	ACP	PG-O2G	3.09	1.61	1.55
5	D	501	GTP	C5-C4	2.95	1.46	1.38
9	B	501	GDP	C5-C4	2.92	1.46	1.38
5	D	501	GTP	PB-O3B	2.83	1.62	1.59
5	A	501	GTP	C5-C4	2.80	1.46	1.38
5	A	501	GTP	PA-O3A	2.79	1.62	1.59
11	F	401	ACP	C5-N7	-2.72	1.34	1.39
11	F	401	ACP	PG-O3G	2.68	1.61	1.55
5	A	501	GTP	C4-N9	-2.67	1.31	1.38
9	B	501	GDP	PA-O3A	2.66	1.62	1.59
5	C	501	GTP	PA-O3A	2.54	1.62	1.59
5	C	501	GTP	C6-N1	-2.54	1.34	1.38
11	F	401	ACP	C5-C6	2.53	1.48	1.41
11	F	401	ACP	PA-O3A	2.49	1.62	1.59
11	F	401	ACP	C4-N9	-2.37	1.32	1.37
5	C	501	GTP	C5-C4	2.37	1.45	1.38
5	A	501	GTP	C6-N1	-2.35	1.34	1.38
11	F	401	ACP	PB-O3A	2.32	1.61	1.58
5	D	501	GTP	PA-O3A	2.19	1.61	1.59
9	B	501	GDP	C4-N9	-2.11	1.32	1.38
11	F	401	ACP	C8-N7	2.10	1.35	1.31
5	D	501	GTP	C4-N9	-2.05	1.32	1.38
5	D	501	GTP	C5-N7	-2.04	1.35	1.39
5	A	501	GTP	C5-N7	-2.01	1.35	1.39

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	C5-C4-N3	-5.27	119.47	126.72
5	D	501	GTP	C5-C4-N3	-5.02	120.39	128.39
5	D	501	GTP	C2-N3-C4	4.81	120.58	112.30
5	A	501	GTP	C5-C4-N3	-4.63	121.02	128.39
11	F	401	ACP	N3-C4-N9	4.52	134.86	127.17
9	B	501	GDP	C2-N3-C4	4.45	119.97	112.30
5	C	501	GTP	C5-C4-N3	-4.44	121.32	128.39
9	B	501	GDP	C5-C4-N3	-4.43	121.34	128.39
5	C	501	GTP	N9-C4-N3	4.15	134.26	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	C2-N3-C4	3.99	119.17	112.30
5	A	501	GTP	C2-N3-C4	3.96	119.12	112.30
5	A	501	GTP	N9-C4-N3	3.95	133.85	125.95
9	B	501	GDP	C6-C5-N7	3.88	137.35	130.29
9	B	501	GDP	N9-C4-N3	3.79	133.54	125.95
5	D	501	GTP	C6-C5-N7	3.72	137.05	130.29
11	F	401	ACP	N3-C2-N1	-3.71	122.96	128.58
11	F	401	ACP	C2-N3-C4	3.56	120.53	111.83
5	D	501	GTP	N9-C4-N3	3.56	133.07	125.95
5	A	501	GTP	C6-C5-N7	3.15	136.02	130.29
11	F	401	ACP	C4-N9-C8	3.13	109.03	105.74
5	C	501	GTP	C6-C5-N7	3.02	135.78	130.29
11	F	401	ACP	C4-C5-N7	-3.00	107.15	110.58
9	B	501	GDP	O2A-PA-O1A	2.96	126.23	112.44
5	A	501	GTP	O3G-PG-O1G	2.86	121.98	110.83
9	B	501	GDP	O4'-C1'-N9	-2.68	102.29	108.36
9	B	501	GDP	O6-C6-C5	-2.65	119.54	126.53
5	D	501	GTP	O6-C6-C5	-2.63	119.58	126.53
9	B	501	GDP	C6-C5-C4	-2.62	114.89	118.83
5	A	501	GTP	O6-C6-C5	-2.55	119.81	126.53
5	C	501	GTP	O3A-PA-O1A	-2.52	103.12	110.70
5	C	501	GTP	C8-N9-C4	2.50	110.71	106.03
10	B	505	MES	O3S-S-C8	2.44	110.78	106.00
11	F	401	ACP	C5-N7-C8	2.38	107.19	103.45
10	B	504	MES	C5-N4-C3	2.37	113.94	108.84
5	D	501	GTP	C4-C5-N7	-2.31	107.01	110.67
10	B	504	MES	O2S-S-C8	2.30	110.20	106.73
5	A	501	GTP	C8-N9-C4	2.27	110.28	106.03
9	B	501	GDP	C8-N9-C4	2.20	110.15	106.03
5	C	501	GTP	O3G-PG-O1G	2.14	119.19	110.83
9	B	501	GDP	C5-C6-N1	2.14	118.71	113.25
5	A	501	GTP	O3G-PG-O3B	-2.13	97.50	104.64
5	D	501	GTP	C5-C6-N1	2.11	118.63	113.25
11	F	401	ACP	N9-C8-N7	-2.11	110.95	113.94
5	C	501	GTP	O6-C6-C5	-2.11	120.97	126.53
11	F	401	ACP	C2-N1-C6	2.10	122.18	118.73

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A

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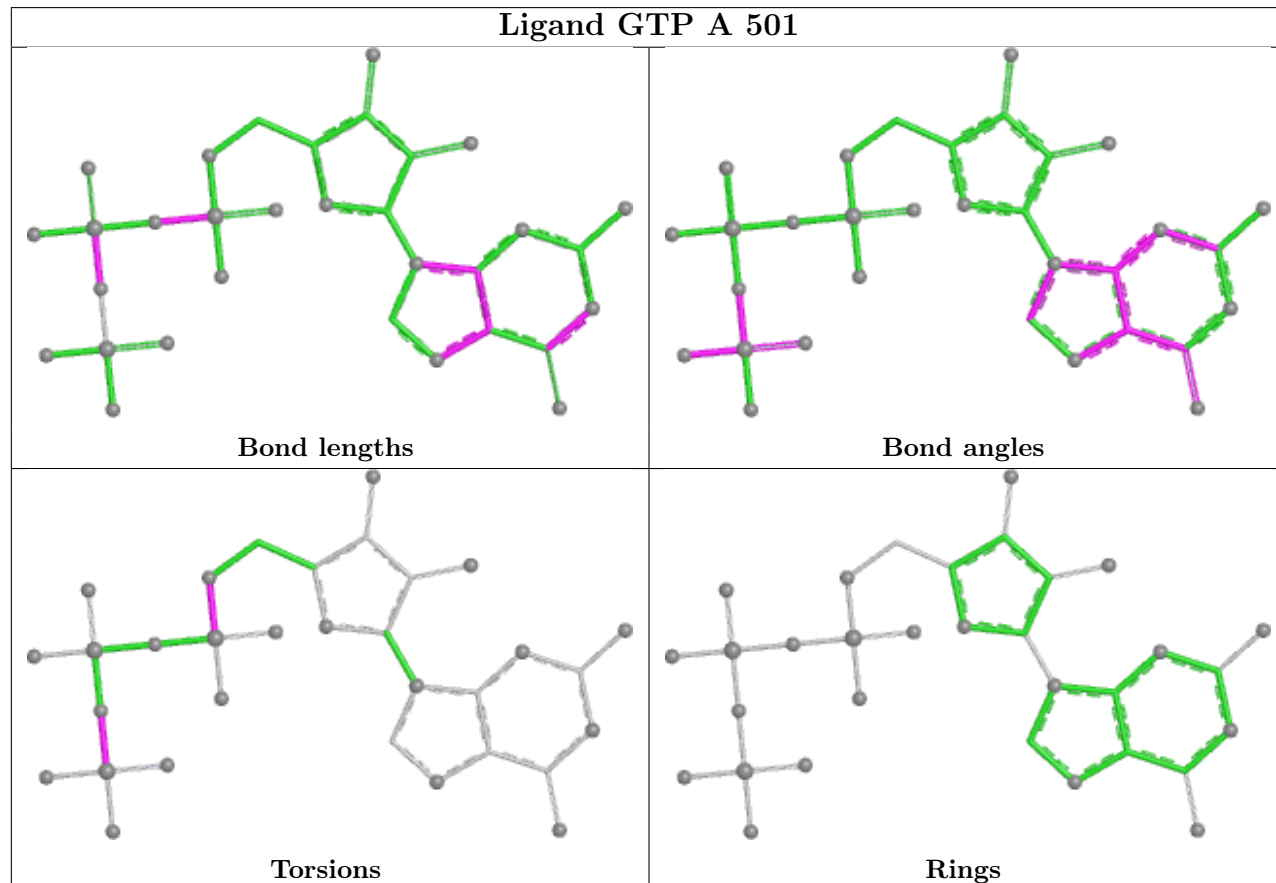
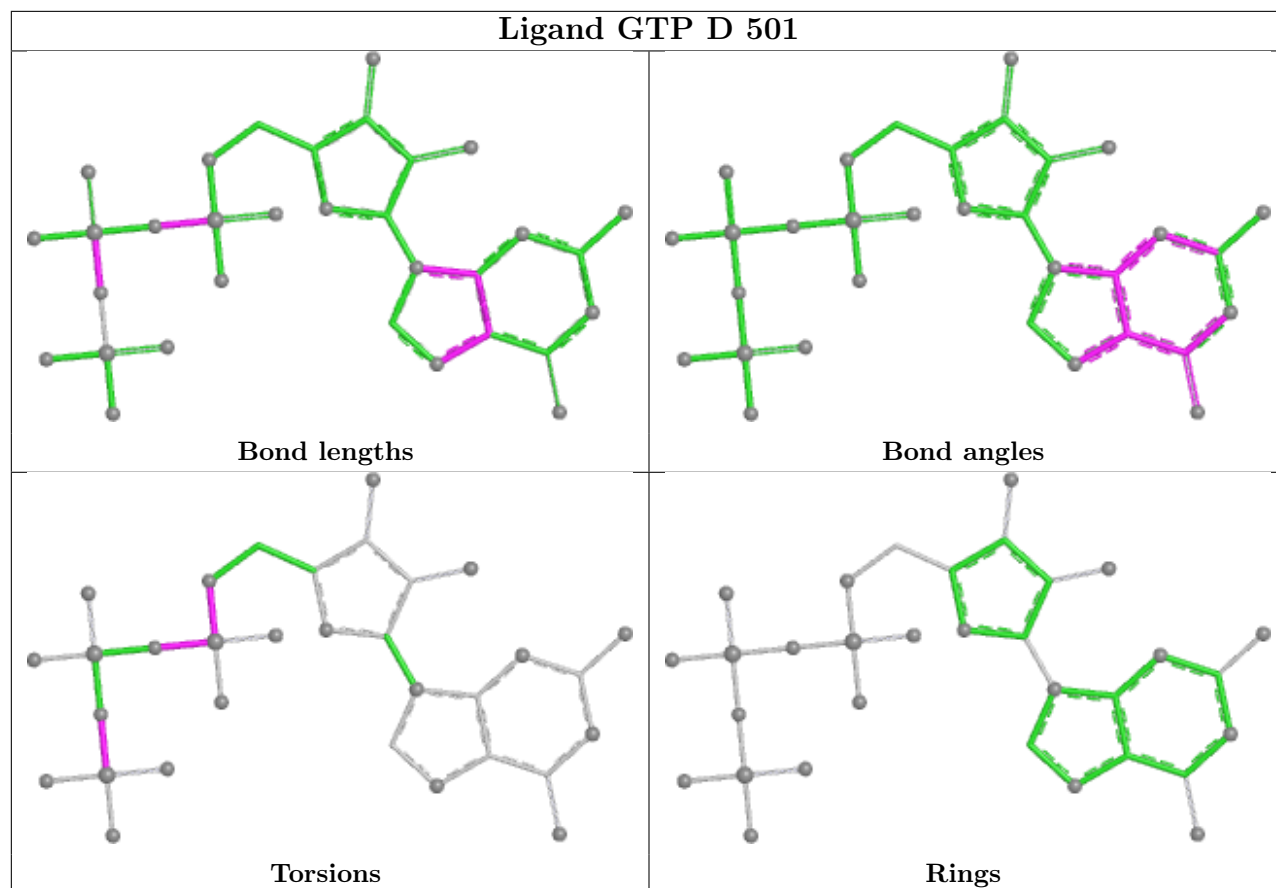
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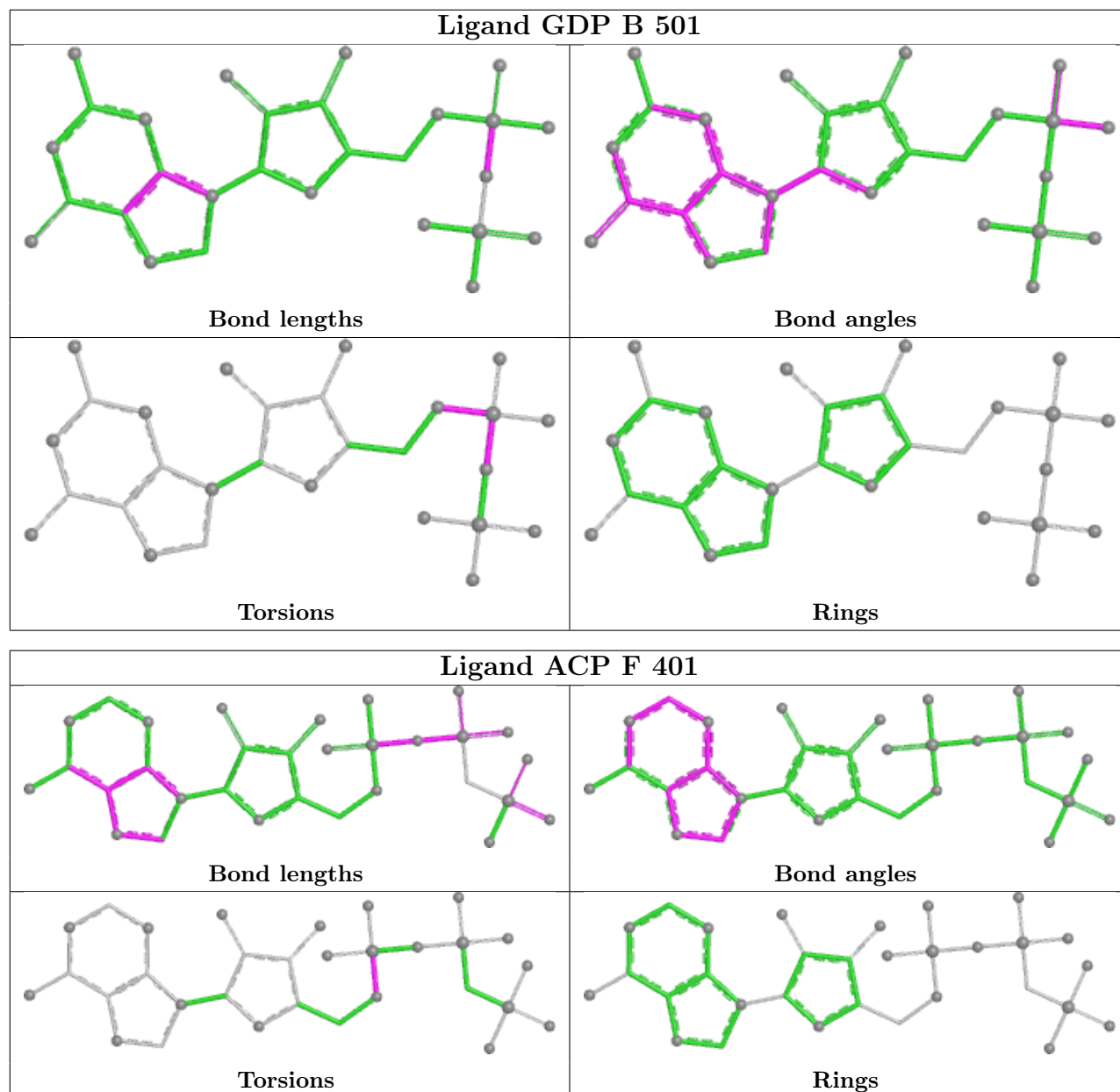
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	PB-O3B-PG-O3G
5	D	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O1A
5	D	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
10	B	504	MES	C7-C8-S-O1S
10	B	504	MES	C7-C8-S-O2S
11	F	401	ACP	C5'-O5'-PA-O1A
10	B	504	MES	C7-C8-S-O3S
5	A	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O2A
11	F	401	ACP	C5'-O5'-PA-O2A
11	F	401	ACP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3A-PA-O1A
5	D	501	GTP	PB-O3A-PA-O1A
5	D	501	GTP	PB-O3A-PA-O2A
9	B	501	GDP	PB-O3A-PA-O1A

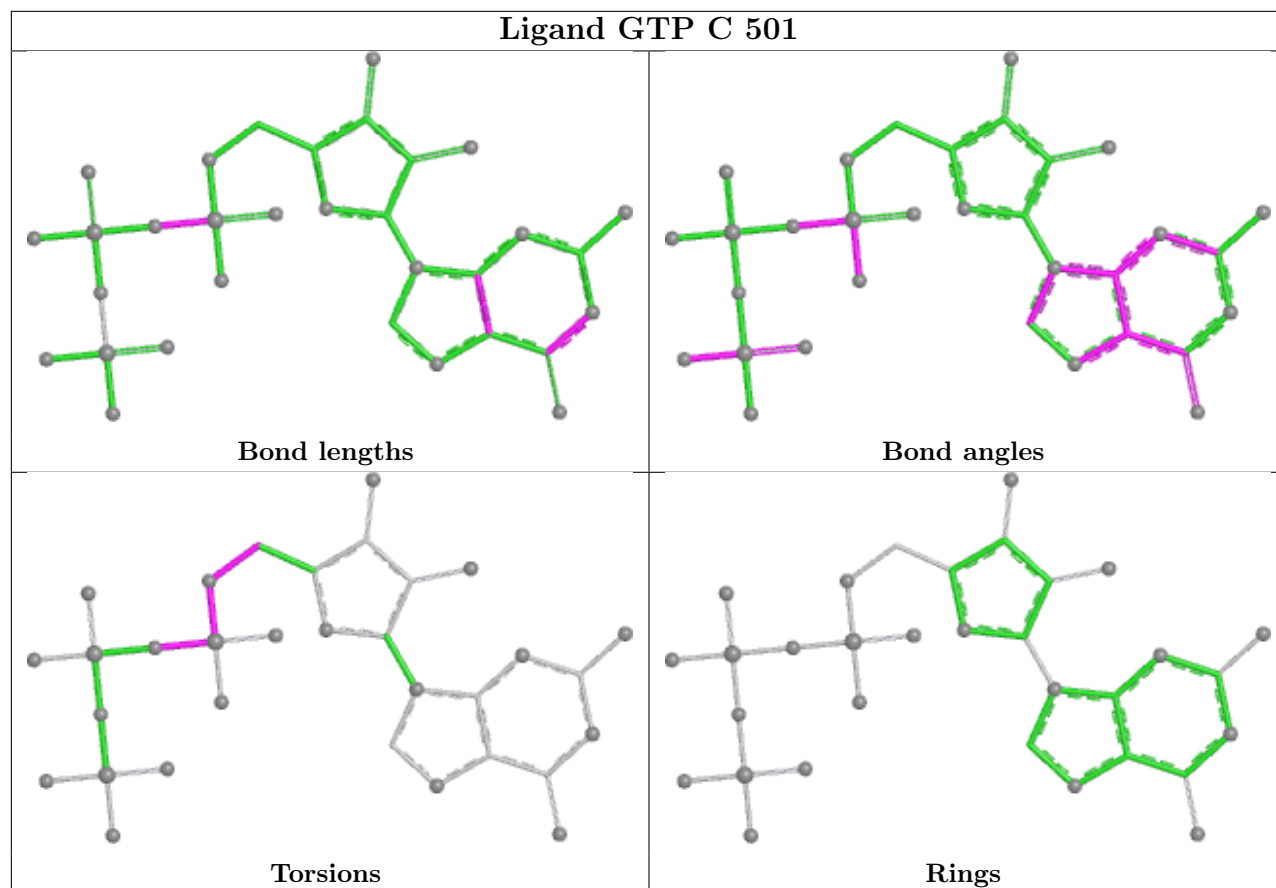
There are no ring outliers.

No monomer is involved in short contacts.

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







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 ⓘ

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	437/451 (96%)	-0.13	8 (1%) 67 69	24, 43, 71, 92	3 (0%)
1	C	440/451 (97%)	-0.31	8 (1%) 67 69	15, 34, 59, 90	9 (2%)
2	B	423/445 (95%)	-0.05	8 (1%) 66 68	19, 42, 72, 97	5 (1%)
2	D	420/445 (94%)	0.19	15 (3%) 46 46	30, 53, 86, 111	4 (0%)
3	E	120/143 (83%)	0.46	8 (6%) 24 22	26, 56, 91, 105	3 (2%)
4	F	309/384 (80%)	0.41	24 (7%) 19 17	19, 59, 96, 123	3 (0%)
All	All	2149/2319 (92%)	0.02	71 (3%) 49 49	15, 46, 82, 123	27 (1%)

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	166	ALA	6.2
4	F	102	PRO	5.7
4	F	247	LYS	5.4
4	F	159	GLY	4.9
4	F	182	ILE	4.3
1	A	262	TYR	4.2
2	D	96	GLY	4.1
1	C	1	MET	4.1
2	B	283	ALA	3.9
4	F	161	LEU	3.7
1	C	440	VAL	3.7
3	E	12[A]	ASN	3.7
4	F	383	HIS	3.6
2	D	394	PHE	3.6
4	F	252	ASN	3.5
4	F	382	HIS	3.4
2	B	282	ARG	3.3
1	A	437	VAL	3.3
3	E	139	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
4	F	144	GLY	3.2
4	F	245	ILE	3.2
2	D	95	SER	3.1
4	F	381	HIS	3.1
3	E	6	MET	3.1
4	F	237	THR	3.1
2	D	73	MET	3.0
2	B	428	ALA	3.0
2	D	431	ASP	2.9
1	A	346	TRP	2.9
1	A	282	TYR	2.9
1	C	357	TYR	2.8
4	F	362	ALA	2.8
2	D	284	LEU	2.7
4	F	384	HIS	2.7
4	F	233	PHE	2.7
1	A	88	HIS	2.7
2	B	55	ALA	2.7
2	D	218	THR	2.7
3	E	27	PRO	2.7
2	D	55	ALA	2.6
1	C	340	SER	2.5
4	F	100	ILE	2.5
2	D	397	TRP	2.5
2	D	92	PHE	2.4
4	F	234	GLN	2.4
2	B	275	SER	2.4
4	F	31	ARG	2.4
2	D	57	ASN	2.3
1	A	365	GLY	2.3
2	D	360	GLY	2.3
4	F	373	SER	2.3
4	F	99	VAL	2.3
1	C	356	ASN	2.3
4	F	101	TYR	2.3
1	C	285	GLN	2.3
1	C	245	ASP	2.2
3	E	140	LYS	2.2
2	D	2	ARG	2.2
4	F	243	HIS	2.2
1	A	362	VAL	2.2
2	B	80	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
3	E	45	PRO	2.2
1	A	96	LYS	2.2
4	F	236	LYS	2.1
3	E	7	GLU	2.1
2	D	273	LEU	2.1
3	E	90	ASN	2.1
2	D	81	PHE	2.1
1	C	284	GLU	2.0
2	B	57	ASN	2.0
2	B	2	ARG	2.0

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(Å ²)	Q<0.9
7	CA	B	503	1/1	0.80	0.16	81,81,81,81	0
8	CL	A	504	1/1	0.85	0.14	69,69,69,69	0
6	MG	D	502	1/1	0.88	0.08	54,54,54,54	0
10	MES	B	505	12/12	0.90	0.13	58,66,93,94	0
11	ACP	F	401	31/31	0.90	0.10	55,65,84,94	0
10	MES	B	504	12/12	0.94	0.11	38,46,54,58	0
7	CA	A	503	1/1	0.96	0.07	50,50,50,50	0
5	GTP	D	501	32/32	0.96	0.07	37,46,58,60	0
6	MG	B	502	1/1	0.97	0.04	29,29,29,29	0
6	MG	A	502	1/1	0.98	0.03	32,32,32,32	0
5	GTP	C	501	32/32	0.99	0.04	22,26,30,31	0
9	GDP	B	501	28/28	0.99	0.04	25,29,34,38	0
5	GTP	A	501	32/32	0.99	0.04	25,30,33,33	0

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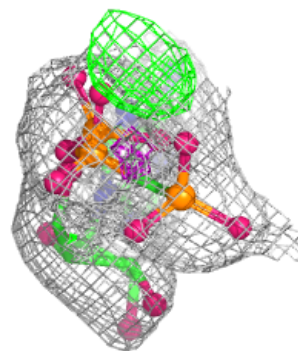
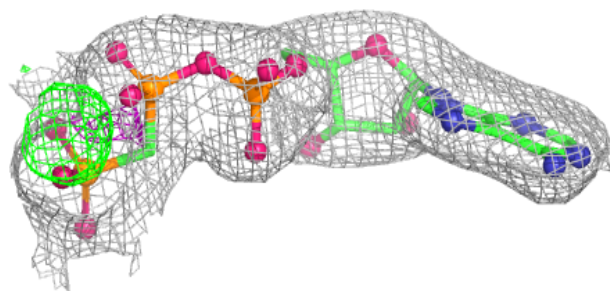
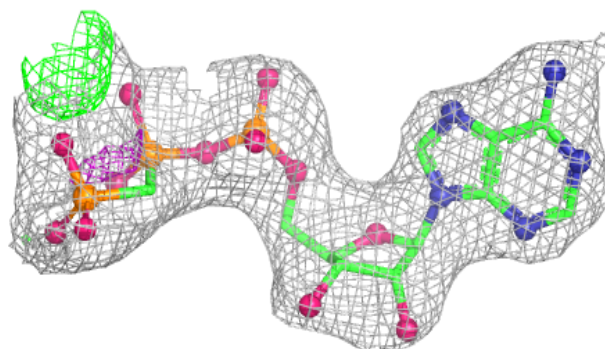
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	C	502	1/1	0.99	0.02	28,28,28,28	0
7	CA	C	503	1/1	0.99	0.08	39,39,39,39	0

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.

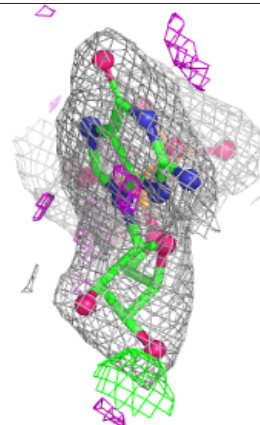
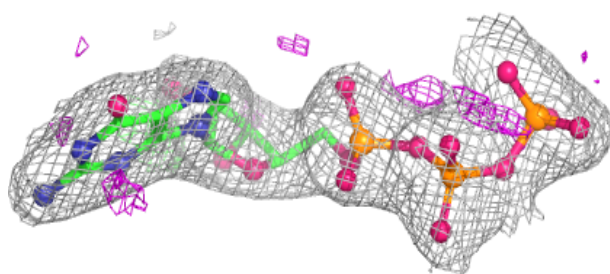
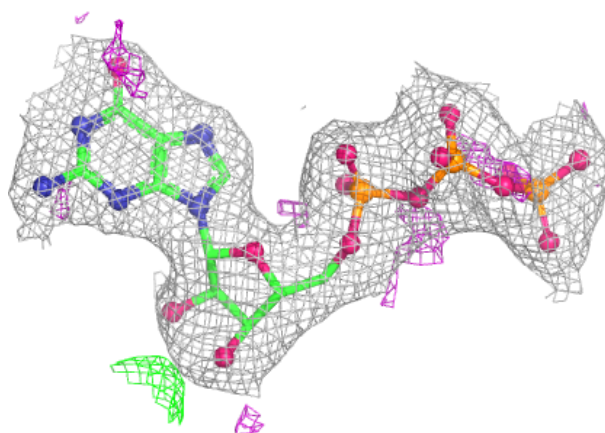
Electron density around ACP F 401:

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

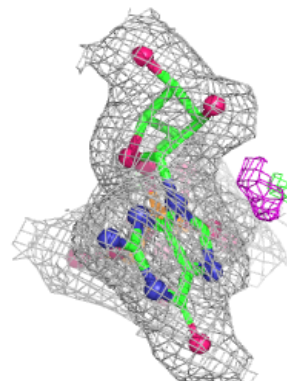
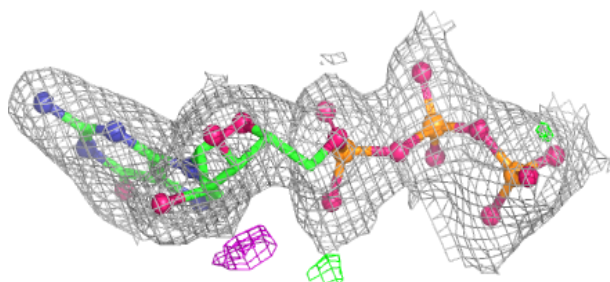
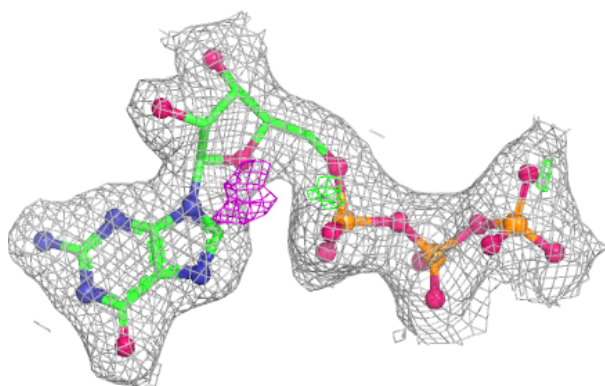


Electron density around GTP D 501:

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

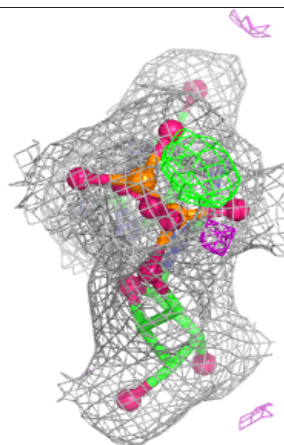
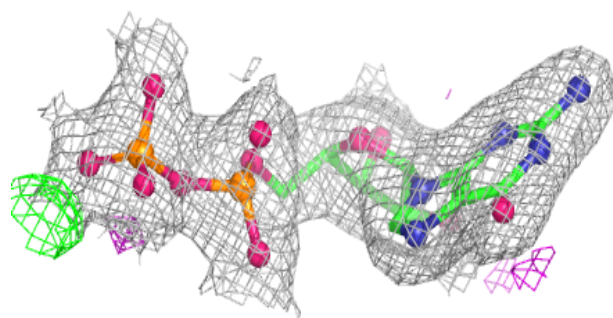
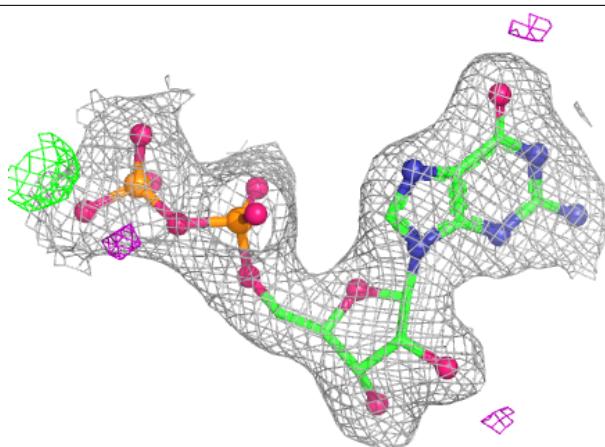
**Electron density around GTP C 501:**

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



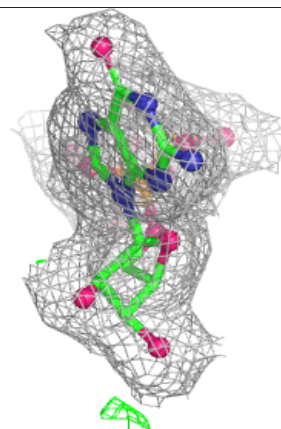
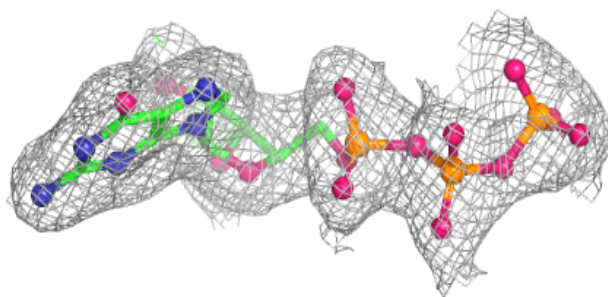
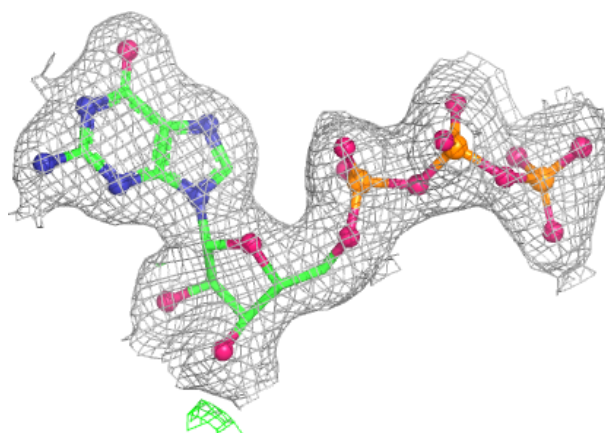
Electron density around GDP B 501:

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



Electron density around GTP A 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.