wwPDB X-ray Structure Validation Summary Report (i)

Oct 26, 2026 – 06:19 pm GMT

PDB ID	:	30DD / pdb_000030dd
Title	:	T2R-TTL-compound 63 complex
Authors	:	Prota, A.E.; Steinmetz, M.O.; Vishnudas, V.K.
Deposited on	:	2026-04-21
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

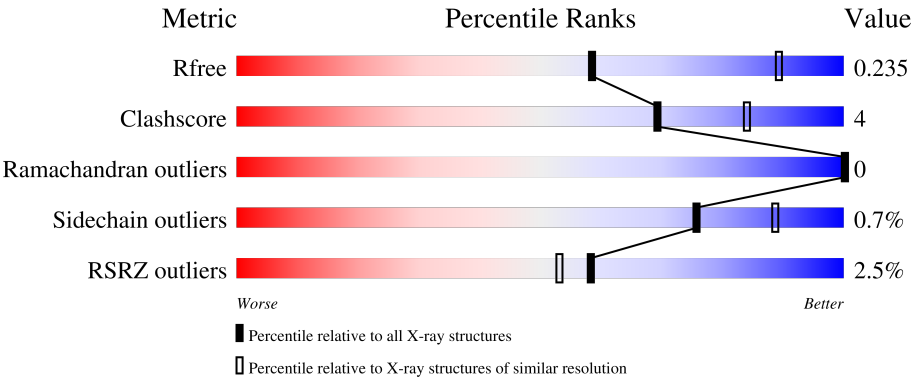
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

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 >=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 <=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	2% 87% 10% ·
1	C	451	% 92% 6% ·
2	B	445	86% 8% 6%
2	D	445	3% 88% 8% ·
3	E	143	5% 81% · 16%

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Mol	Chain	Length	Quality of chain
4	F	384	

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 34479 atoms, of which 16935 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	438	Total	C	H	N	O	S	0	0	0
			6759	2167	3335	582	653	22			
1	C	440	Total	C	H	N	O	S	0	1	0
			6788	2175	3351	584	656	22			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	419	Total	C	H	N	O	S	0	2	0
			6494	2077	3189	564	638	26			
2	D	427	Total	C	H	N	O	S	0	0	0
			6576	2101	3228	571	649	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	120	Total	C	H	N	O	S	0	0	0
			2001	611	1010	180	196	4			

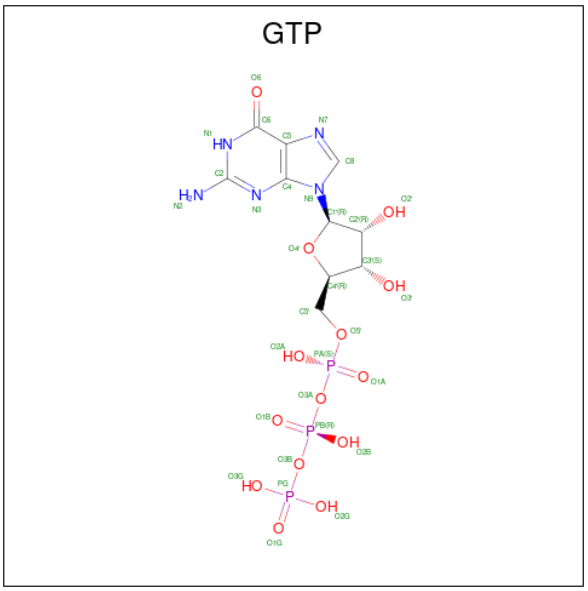
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	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
4	F	338	Total	C	H	N	O	S	0	0	0
			5515	1780	2743	476	502	14			

- 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 H N O P 44 10 12 5 14 3	0	0
5	C	1	Total C H N O P 44 10 12 5 14 3	0	0

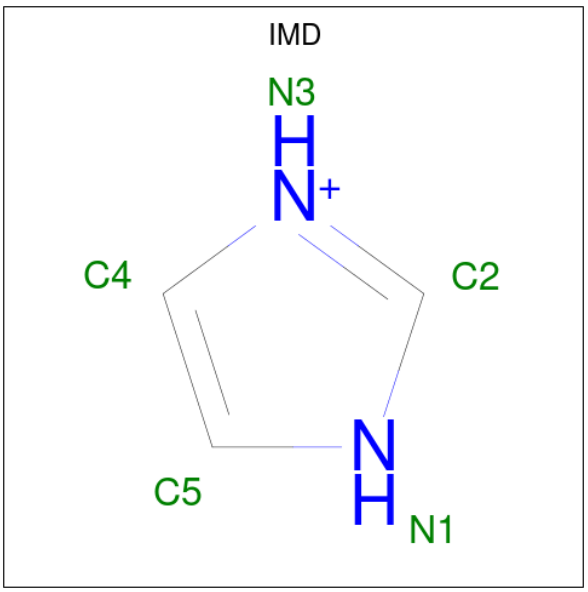
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

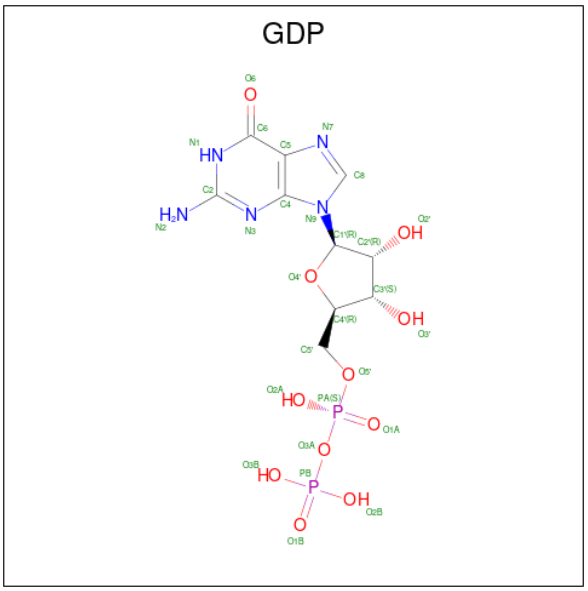
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0

- Molecule 8 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



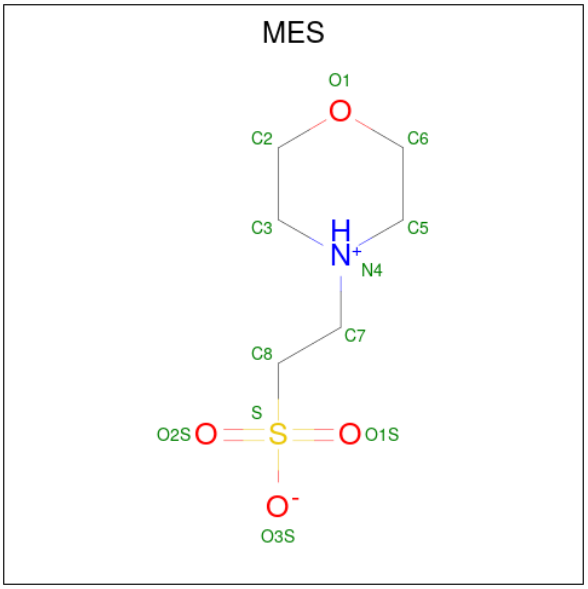
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	N		
8	A	1	10	3	5	2	0	0

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



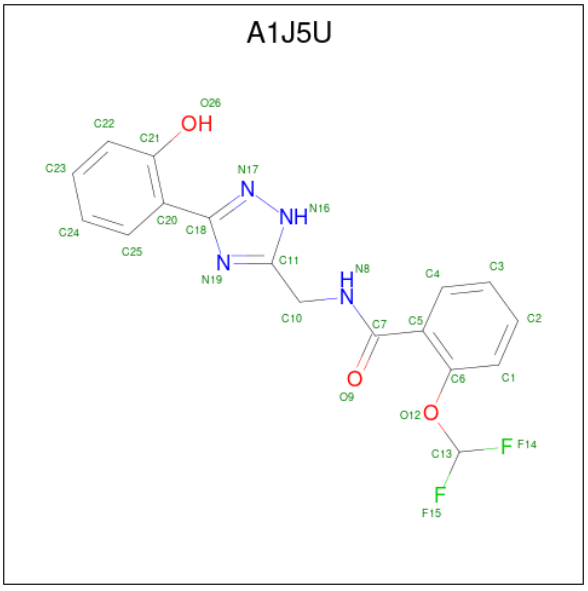
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
9	B	1	40	10	12	5	11	2	0	0
			Total	C	H	N	O	P		
9	D	1	40	10	12	5	11	2	0	0

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



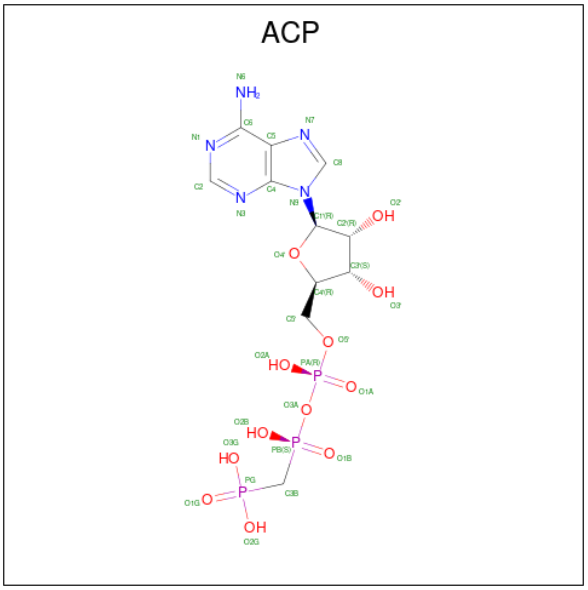
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	S		
10	B	1	25	6	13	1	4	1	0	0

- Molecule 11 is 2-[bis(fluoranyl)methoxy]- {N}-[[3-(2-hydroxyphenyl)-1 {H}-1,2,4-triazol-5 -yl]methyl]benzamide (CCD ID: A1J5U) (formula: $C_{17}H_{14}F_2N_4O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	F	N	O	0	0
			26	17	2	4	3		
11	D	1	Total	C	F	N	O	0	0
			26	17	2	4	3		

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
12	F	1	Total	C	H	N	O	P	0	0
			44	11	13	5	12	3		

- Molecule 13 is water.

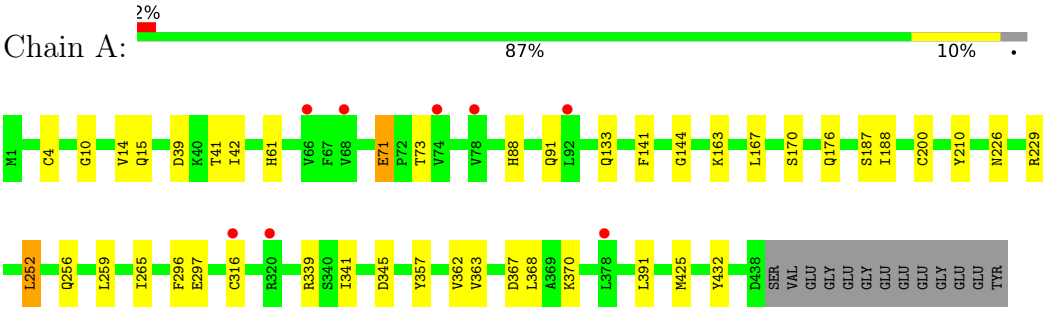
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	6	Total	O	0	0
			6	6		
13	B	18	Total	O	0	0
			18	18		
13	C	14	Total	O	0	0
			14	14		
13	D	2	Total	O	0	0
			2	2		

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.

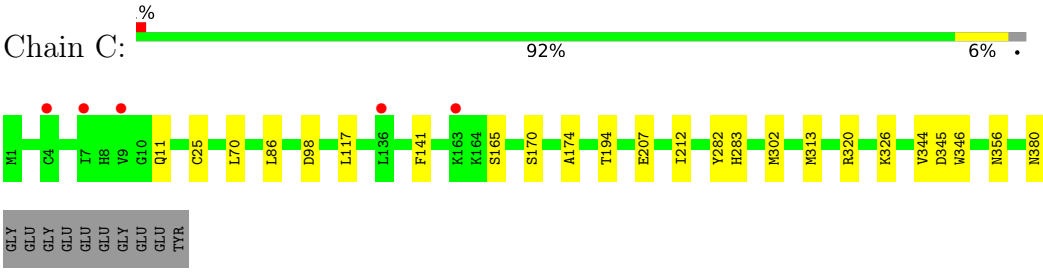
• Molecule 1: Tubulin alpha-1B chain

Chain A:



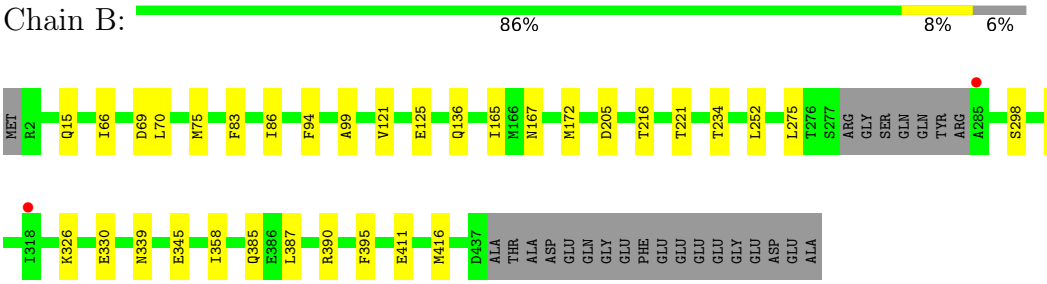
• Molecule 1: Tubulin alpha-1B chain

Chain C:



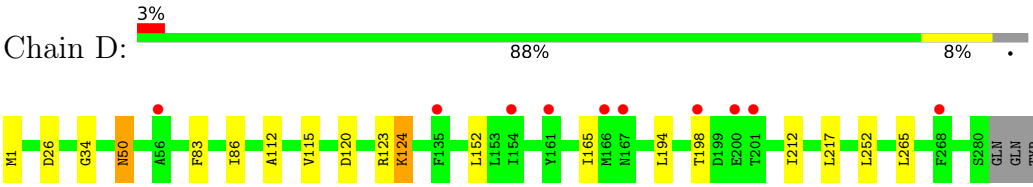
• Molecule 2: Tubulin beta-2B chain

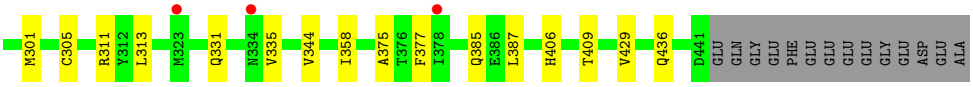
Chain B:



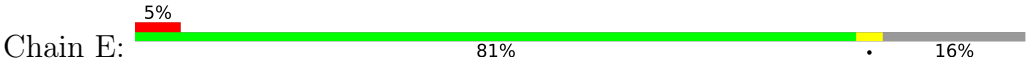
• Molecule 2: Tubulin beta-2B chain

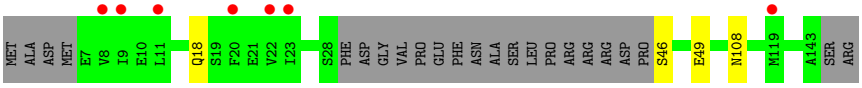
Chain D:



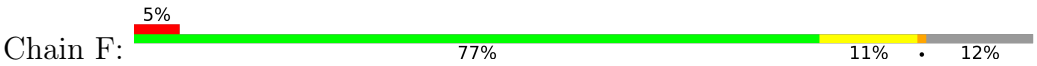


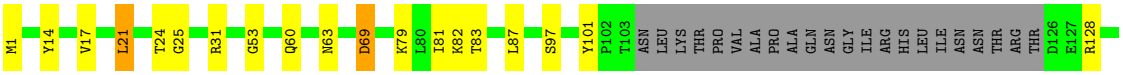
• Molecule 3: Stathmin-4

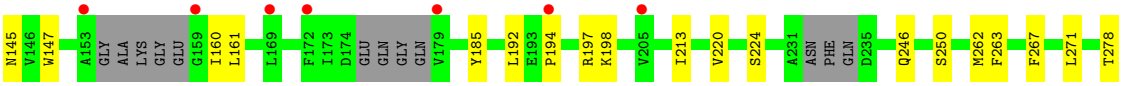


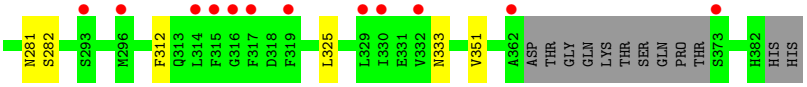


• Molecule 4: Tubulin–tyrosine ligase









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.21Å 156.66Å 182.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.96 – 2.61 49.96 – 2.61	Depositor EDS
% Data completeness (in resolution range)	96.2 (49.96-2.61) 99.3 (49.96-2.61)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 2.61Å)	Xtriage
Refinement program	PHENIX 2.0_5936	Depositor
R, R_{free}	0.193 , 0.229 0.205 , 0.235	Depositor DCC
R_{free} test set	2024 reflections (2.20%)	wwPDB-VP
Wilson B-factor (Å^2)	86.1	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 79.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	34479	wwPDB-VP
Average B, all atoms (Å^2)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ACP, MES, MG, IMD, A1J5U, GTP, CA, GDP

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	0.11	0/3502	0.26	0/4754
1	C	0.15	0/3524	0.28	0/4784
2	B	0.12	0/3387	0.27	0/4586
2	D	0.11	0/3421	0.25	0/4633
3	E	0.10	0/998	0.20	0/1323
4	F	0.10	0/2835	0.25	0/3827
All	All	0.12	0/17667	0.26	0/23907

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

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	3424	3335	3334	34	0
1	C	3437	3351	3342	14	1
2	B	3305	3189	3173	22	1
2	D	3348	3228	3227	25	0
3	E	991	1010	1009	2	0
4	F	2772	2743	2742	26	0
5	A	32	12	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	12	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	1	0	0	0	0
7	C	1	0	0	0	0
8	A	5	5	5	0	0
9	B	28	12	11	1	0
9	D	28	12	11	0	0
10	B	12	13	13	0	0
11	B	26	0	0	0	0
11	D	26	0	0	0	0
12	F	31	13	14	1	0
13	A	6	0	0	0	0
13	B	18	0	0	1	0
13	C	14	0	0	0	0
13	D	2	0	0	0	0
All	All	17544	16935	16905	121	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 4.

The worst 5 of 121 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:14:TYR:HA	4:F:17:VAL:HG12	1.72	0.71
2:B:83:PHE:O	2:B:86:ILE:HG22	1.93	0.68
1:A:4:CYS:SG	1:A:252:LEU:HD21	2.34	0.68
2:D:295:MET:HE2	2:D:375:ALA:HB1	1.77	0.66
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.32	0.63

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:411:GLU:OE1	1:C:282:TYR:OH[4_555]	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	436/451 (97%)	422 (97%)	14 (3%)	0	100	100
1	C	439/451 (97%)	430 (98%)	9 (2%)	0	100	100
2	B	417/445 (94%)	400 (96%)	17 (4%)	0	100	100
2	D	423/445 (95%)	413 (98%)	10 (2%)	0	100	100
3	E	116/143 (81%)	113 (97%)	3 (3%)	0	100	100
4	F	326/384 (85%)	312 (96%)	14 (4%)	0	100	100
All	All	2157/2319 (93%)	2090 (97%)	67 (3%)	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	369/379 (97%)	367 (100%)	2 (0%)	81	91
1	C	372/379 (98%)	369 (99%)	3 (1%)	73	87
2	B	365/383 (95%)	363 (100%)	2 (0%)	81	91
2	D	368/383 (96%)	364 (99%)	4 (1%)	65	83
3	E	107/127 (84%)	106 (99%)	1 (1%)	70	86
4	F	304/342 (89%)	302 (99%)	2 (1%)	76	89
All	All	1885/1993 (95%)	1871 (99%)	14 (1%)	76	89

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	26	ASP
2	D	50	ASN
4	F	69	ASP
3	E	108	ASN
4	F	21	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	35	GLN
1	C	372	GLN
4	F	196	HIS
1	C	285	GLN
2	D	136	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 7 are monoatomic - leaving 9 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	30,34,34	3.74	14 (46%)	46,54,54	1.70	14 (30%)
9	GDP	B	501	6	28,30,30	4.01	15 (53%)	44,47,47	1.67	10 (22%)
11	A1J5U	B	504	-	28,28,28	1.41	3 (10%)	35,38,38	2.28	10 (28%)
5	GTP	A	501	6	30,34,34	3.73	13 (43%)	46,54,54	1.71	14 (30%)
10	MES	B	503	-	12,12,12	1.10	1 (8%)	14,16,16	0.93	1 (7%)
11	A1J5U	D	503	-	28,28,28	1.39	3 (10%)	35,38,38	2.19	10 (28%)
12	ACP	F	401	6	30,33,33	3.41	13 (43%)	45,52,52	2.22	15 (33%)
9	GDP	D	501	-	28,30,30	4.04	15 (53%)	44,47,47	1.75	12 (27%)
8	IMD	A	504	-	5,5,5	0.37	0	5,5,5	0.80	0

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
8	IMD	A	504	-	-	-	0/1/1/1
5	GTP	C	501	6	-	8/22/38/38	0/3/3/3
11	A1J5U	B	504	-	-	0/17/17/17	0/3/3/3
5	GTP	A	501	6	-	6/22/38/38	0/3/3/3
10	MES	B	503	-	-	0/6/14/14	0/1/1/1
11	A1J5U	D	503	-	-	2/17/17/17	0/3/3/3
12	ACP	F	401	6	-	3/19/38/38	0/3/3/3
9	GDP	D	501	-	-	4/16/32/32	0/3/3/3
9	GDP	B	501	6	-	5/16/32/32	0/3/3/3

The worst 5 of 77 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	501	GDP	C3'-C4'	-11.19	1.24	1.53
9	D	501	GDP	C3'-C4'	-11.19	1.24	1.53
5	A	501	GTP	C3'-C4'	-10.72	1.25	1.53
5	C	501	GTP	C3'-C4'	-10.69	1.25	1.53
12	F	401	ACP	C3'-C4'	-9.25	1.29	1.53

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	504	A1J5U	N16-C11-N19	7.76	116.10	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	D	503	A1J5U	N16-C11-N19	7.17	115.63	110.05
11	B	504	A1J5U	C11-N16-N17	-5.57	102.21	110.02
12	F	401	ACP	N3-C2-N1	-5.47	120.05	128.60
11	D	503	A1J5U	C11-N16-N17	-5.41	102.44	110.02

There are no chirality outliers.

5 of 28 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	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O1A

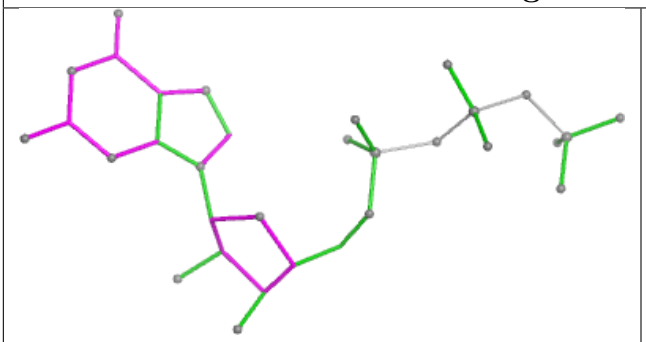
There are no ring outliers.

4 monomers are involved in 5 short contacts:

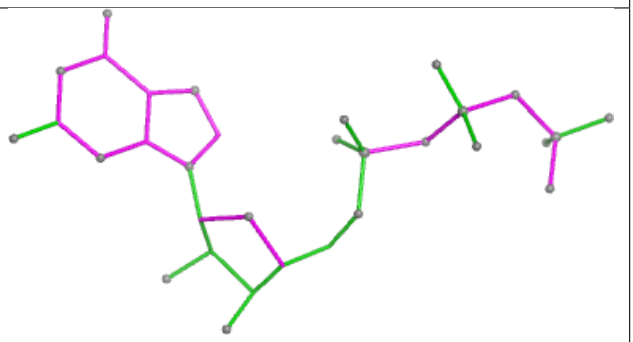
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	501	GTP	1	0
9	B	501	GDP	1	0
5	A	501	GTP	2	0
12	F	401	ACP	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

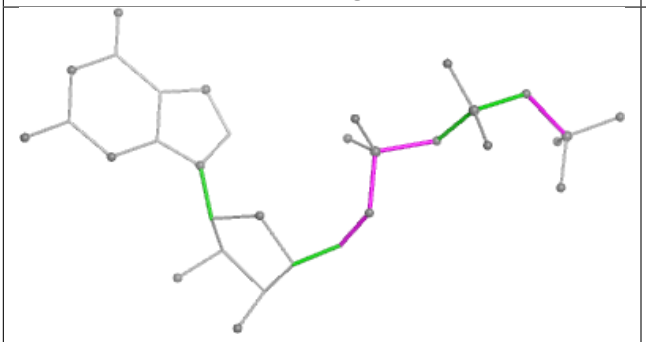
Ligand GTP C 501



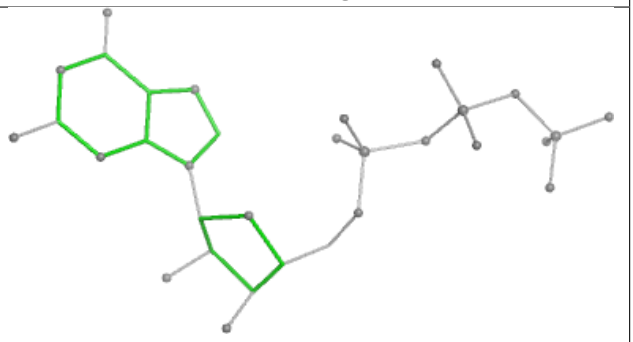
Bond lengths



Bond angles

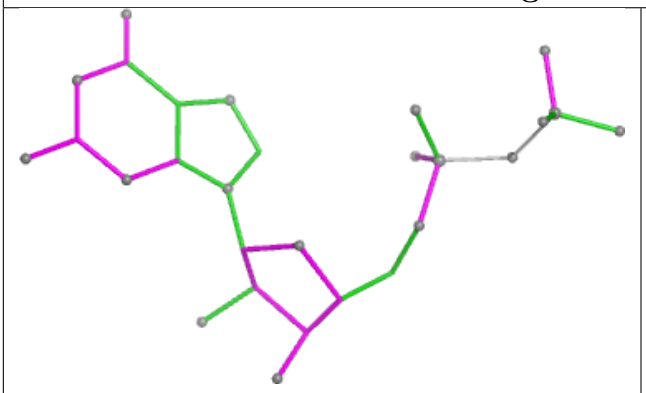


Torsions

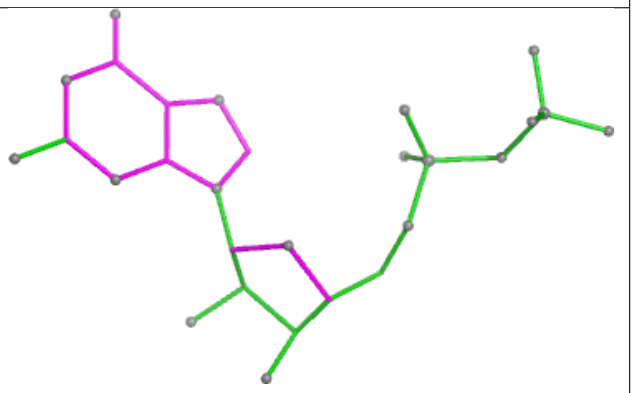


Rings

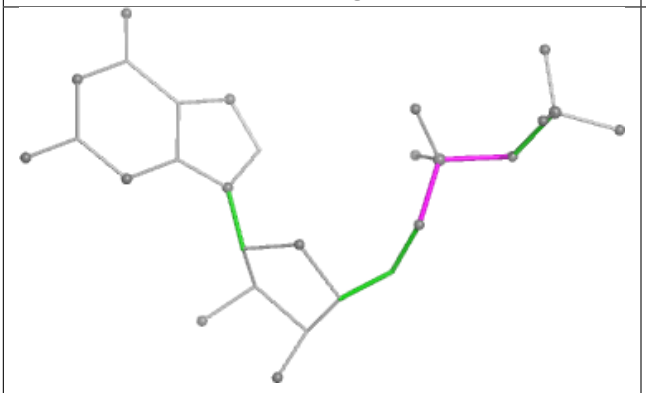
Ligand GDP B 501



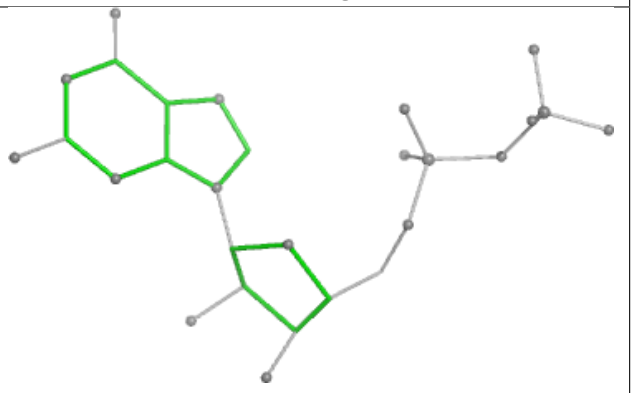
Bond lengths



Bond angles

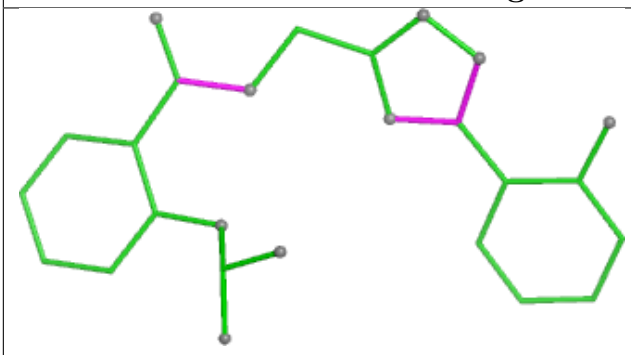


Torsions

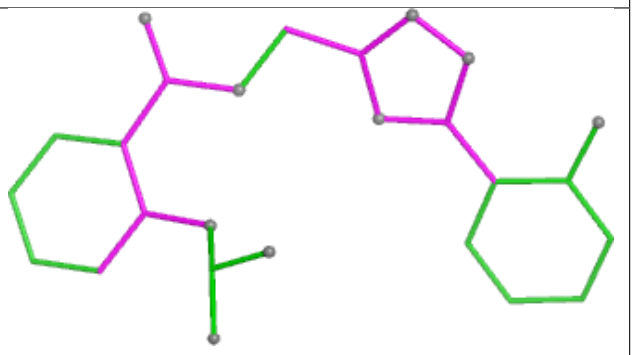


Rings

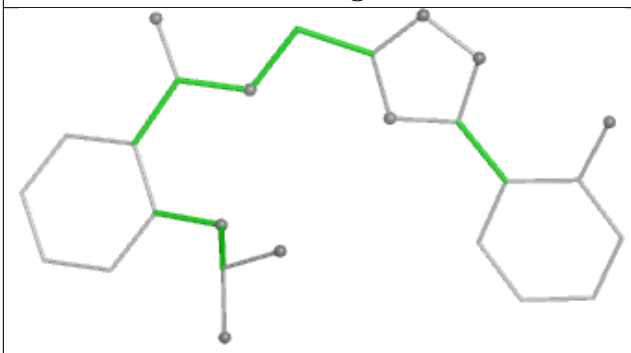
Ligand A1J5U B 504



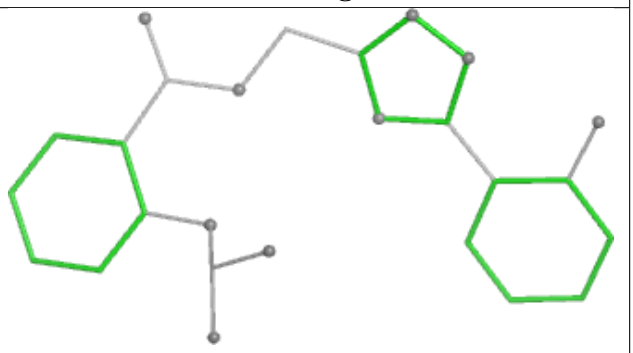
Bond lengths



Bond angles

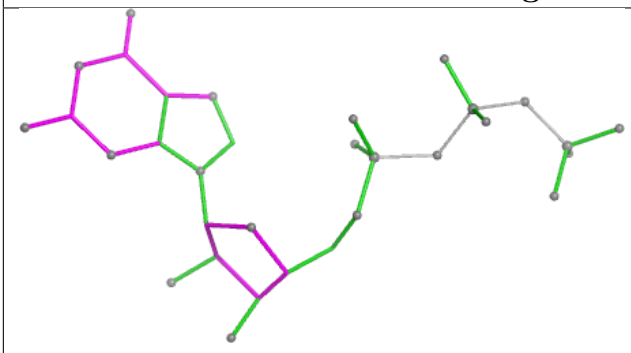


Torsions

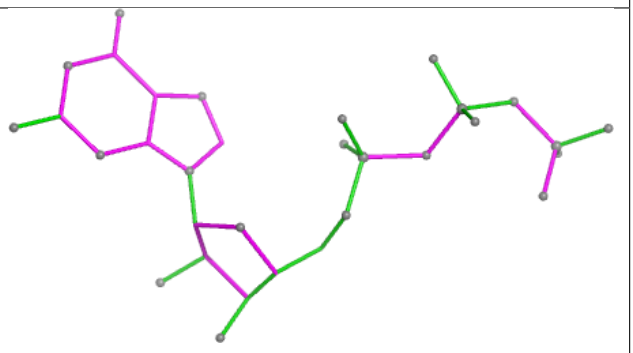


Rings

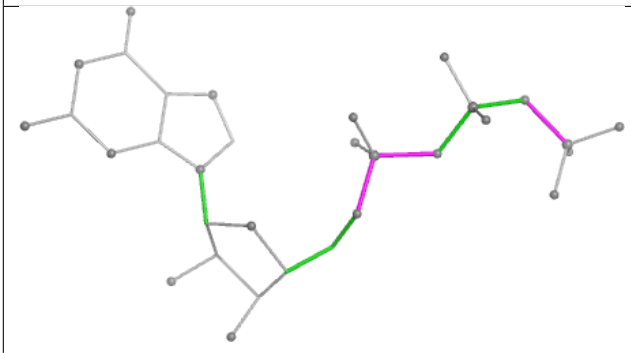
Ligand GTP A 501



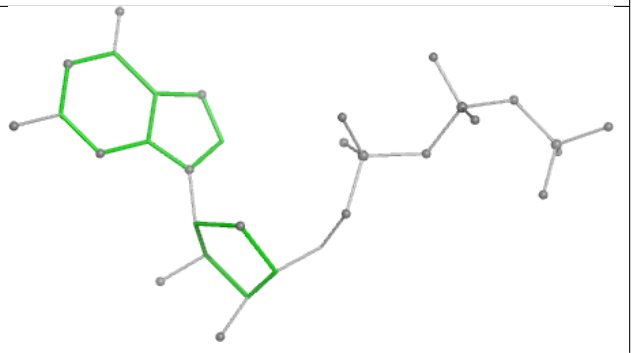
Bond lengths



Bond angles

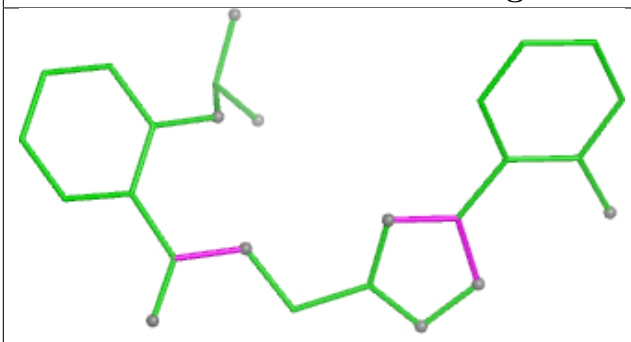


Torsions

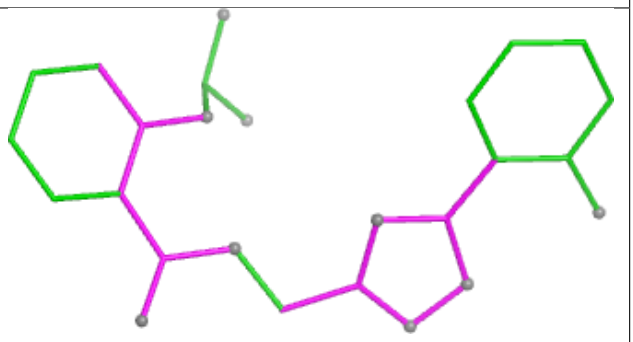


Rings

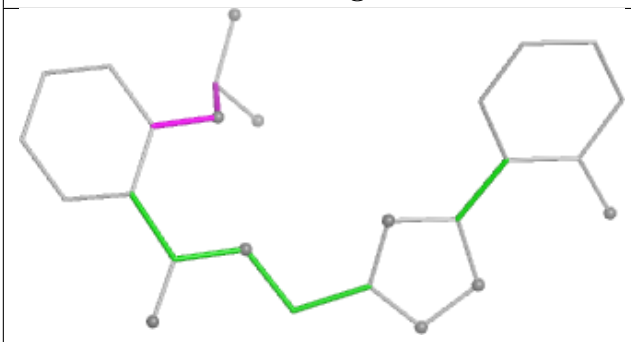
Ligand A1J5U D 503



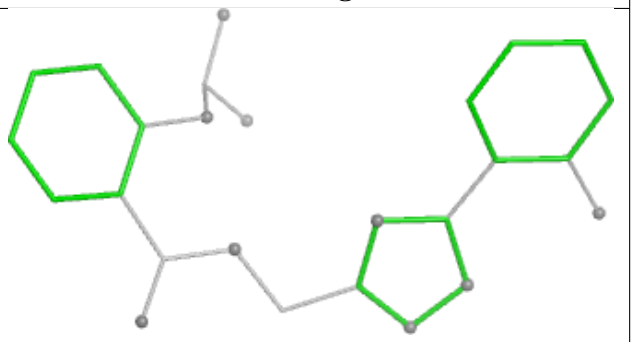
Bond lengths



Bond angles

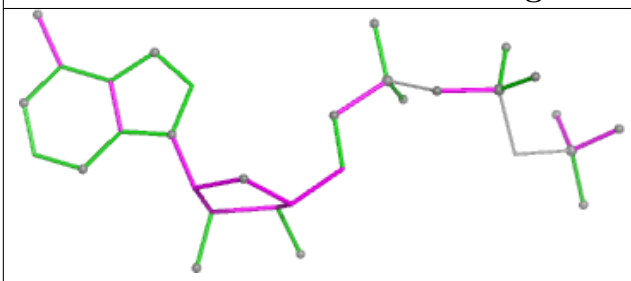


Torsions

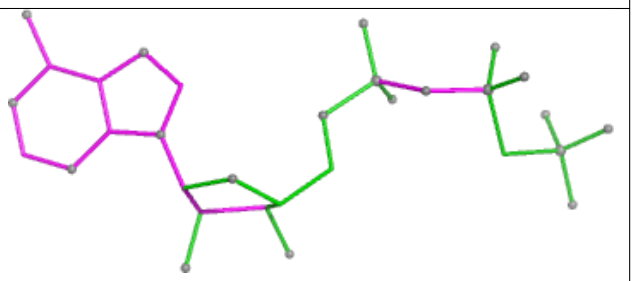


Rings

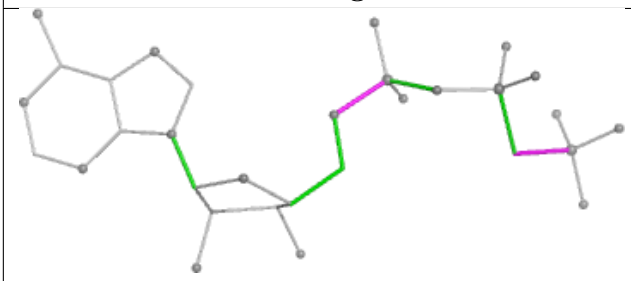
Ligand ACP F 401



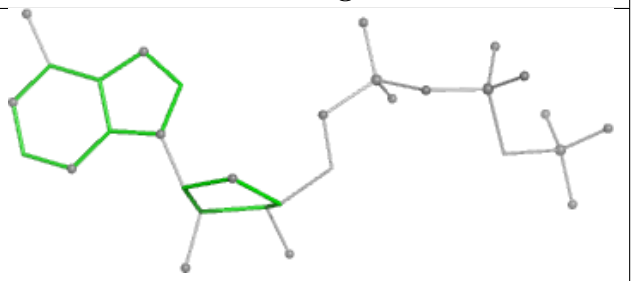
Bond lengths



Bond angles

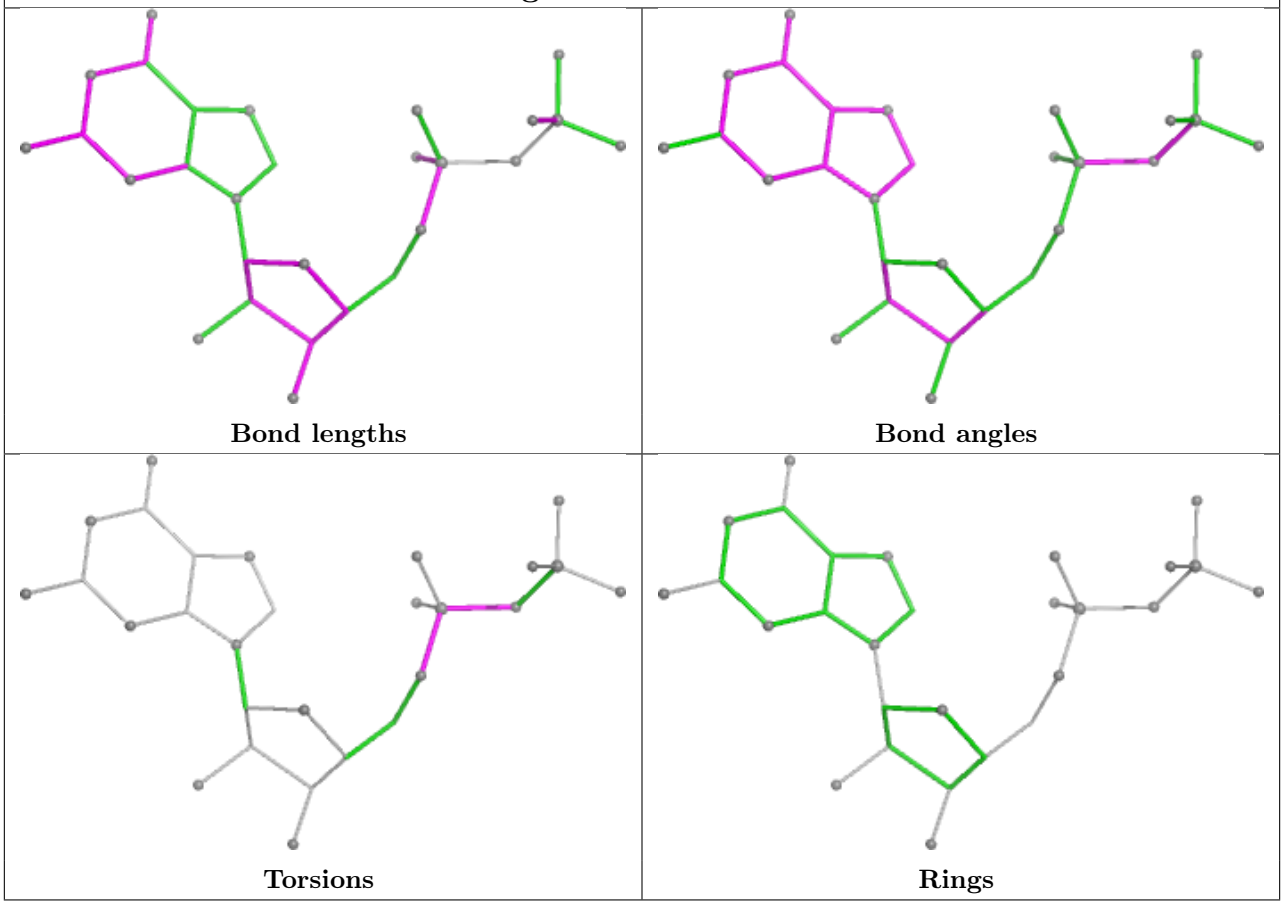


Torsions



Rings

Ligand GDP D 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95^{th} 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	438/451 (97%)	0.11	8 (1%)	67	63	82, 121, 165, 233	0
1	C	440/451 (97%)	-0.15	5 (1%)	78	74	67, 90, 132, 185	0
2	B	419/445 (94%)	-0.19	2 (0%)	87	85	57, 101, 148, 187	1 (0%)
2	D	427/445 (95%)	0.23	14 (3%)	49	44	89, 146, 189, 212	0
3	E	120/143 (83%)	0.25	7 (5%)	29	24	90, 136, 191, 209	0
4	F	338/384 (88%)	0.29	19 (5%)	30	25	103, 162, 222, 238	0
All	All	2182/2319 (94%)	0.06	55 (2%)	58	53	57, 122, 194, 238	1 (0%)

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	11	LEU	5.0
4	F	316	GLY	4.2
4	F	315	PHE	4.2
4	F	362	ALA	4.0
3	E	8	VAL	3.9

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands (i)

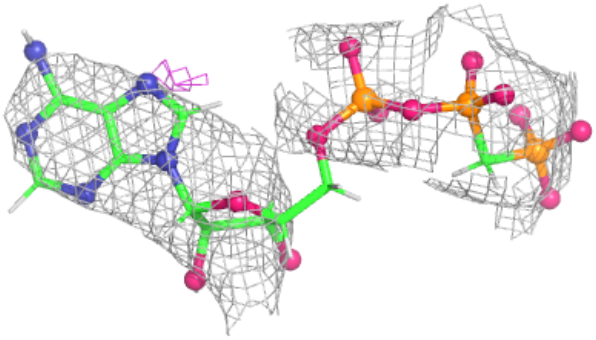
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

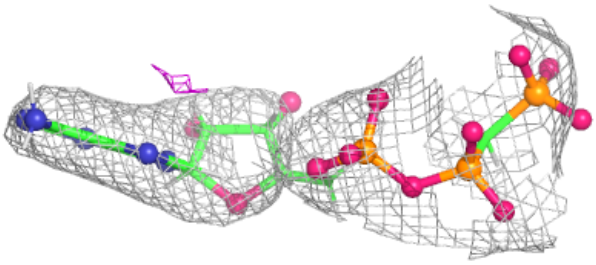
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	D	502	1/1	0.58	0.20	146,146,146,146	0
6	MG	F	402	1/1	0.67	0.09	156,156,156,156	0
8	IMD	A	504	5/5	0.87	0.18	113,129,151,155	0
12	ACP	F	401	31/31	0.88	0.07	136,181,222,229	0
5	GTP	A	501	32/32	0.95	0.08	63,82,107,114	0
9	GDP	B	501	28/28	0.96	0.08	51,76,96,103	0
9	GDP	D	501	28/28	0.96	0.08	114,134,161,166	0
10	MES	B	503	12/12	0.96	0.07	68,93,109,122	0
6	MG	B	502	1/1	0.96	0.10	87,87,87,87	0
7	CA	A	503	1/1	0.97	0.06	142,142,142,142	0
11	A1J5U	B	504	26/26	0.97	0.10	71,84,100,145	0
11	A1J5U	D	503	26/26	0.97	0.11	79,98,119,145	0
5	GTP	C	501	32/32	0.97	0.06	48,76,94,97	0
6	MG	C	502	1/1	0.98	0.06	69,69,69,69	0
7	CA	C	503	1/1	0.99	0.03	112,112,112,112	0
6	MG	A	502	1/1	0.99	0.04	78,78,78,78	0

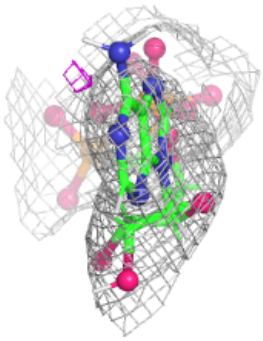
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

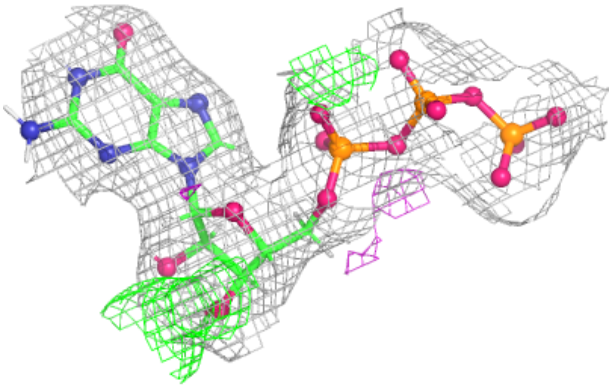


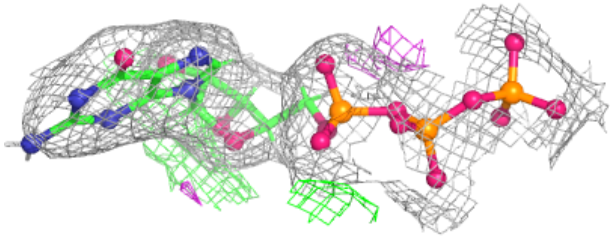


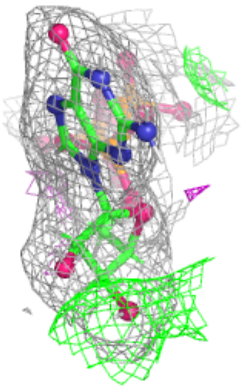


Electron density around GTP A 501:

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

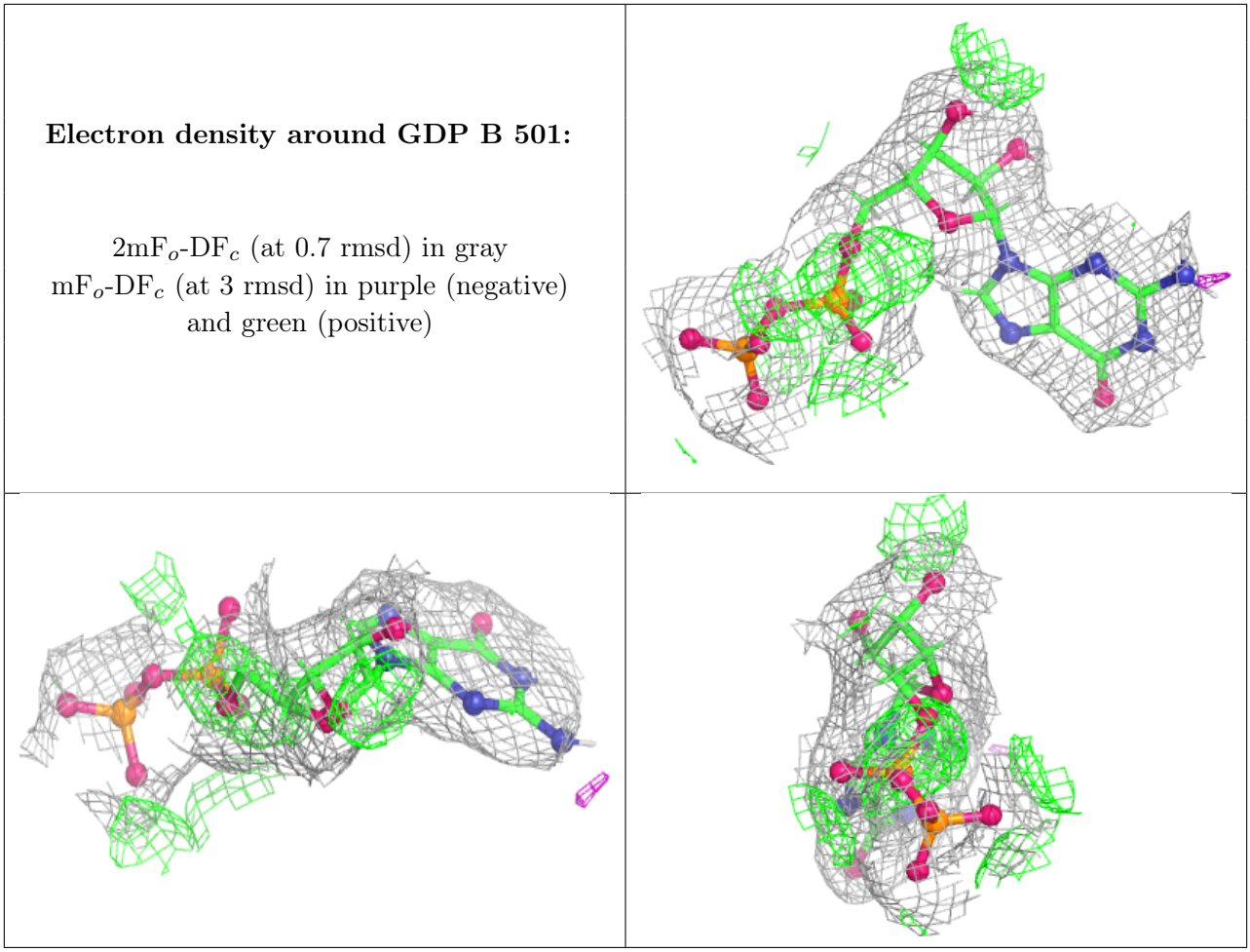






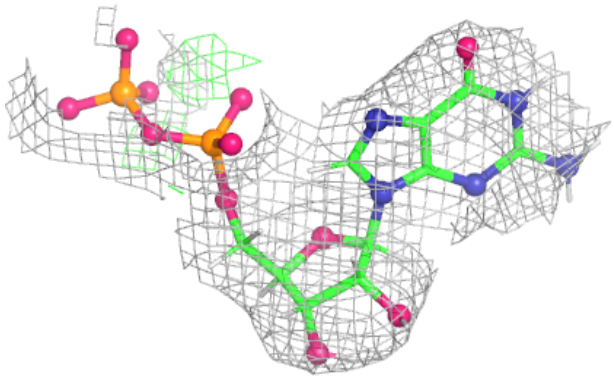
Electron density around GDP B 501:

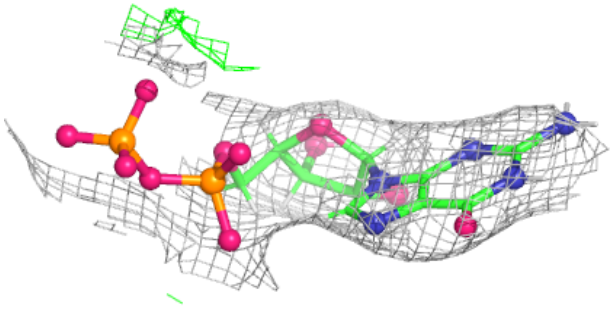
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

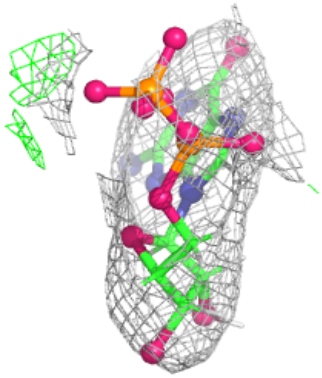


Electron density around GDP D 501:

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

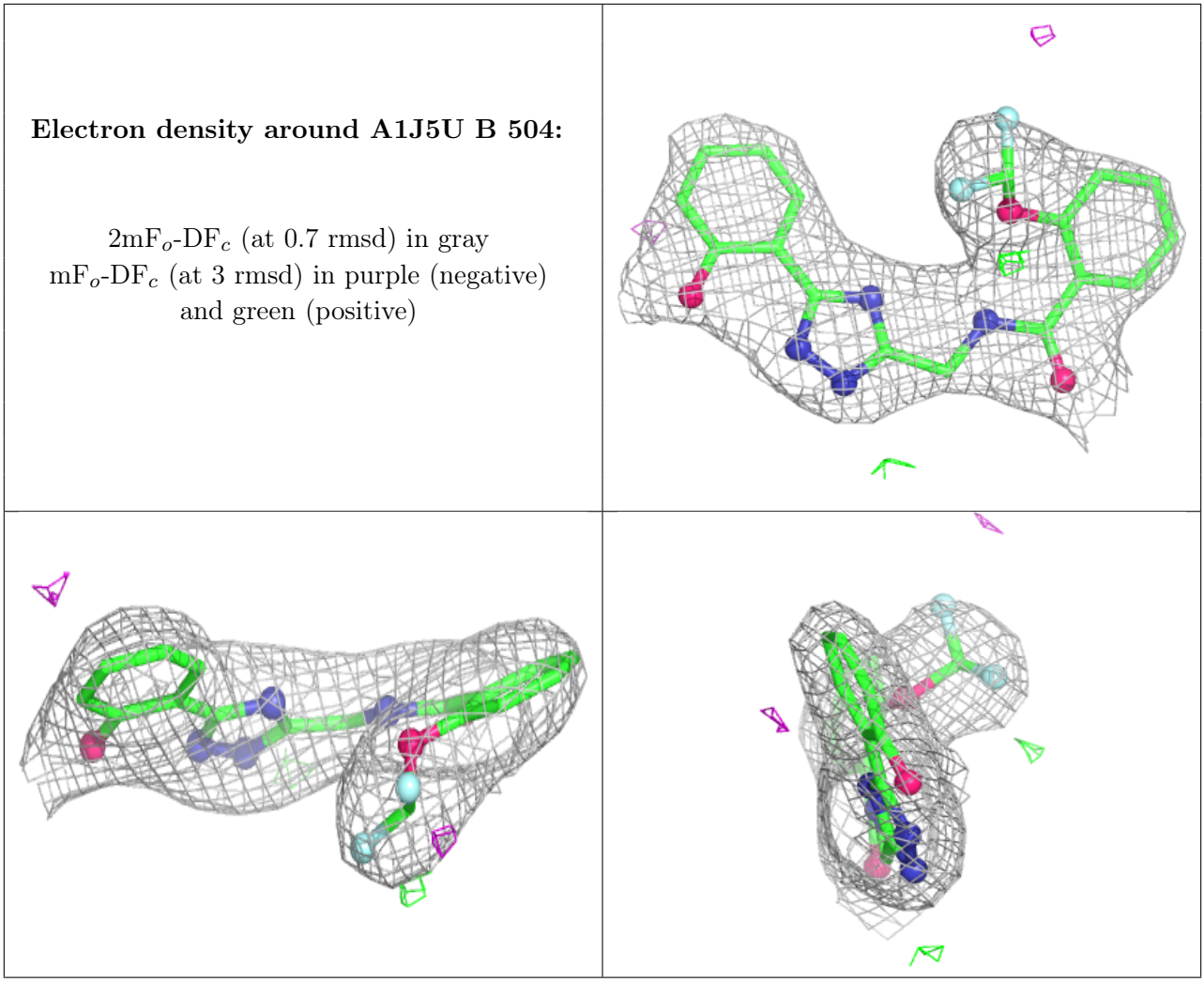






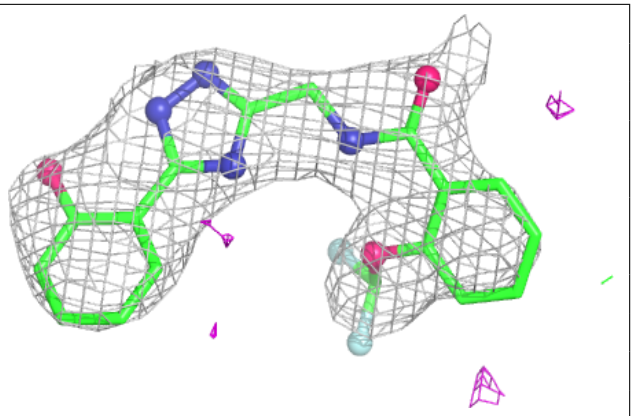
Electron density around A1J5U B 504:

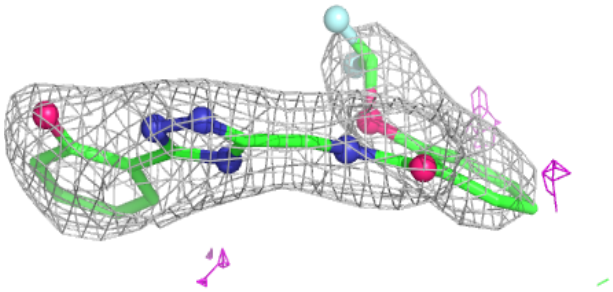
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

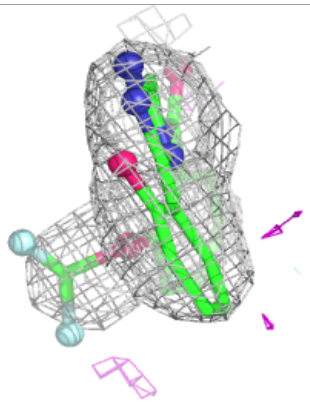


Electron density around A1J5U D 503:

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

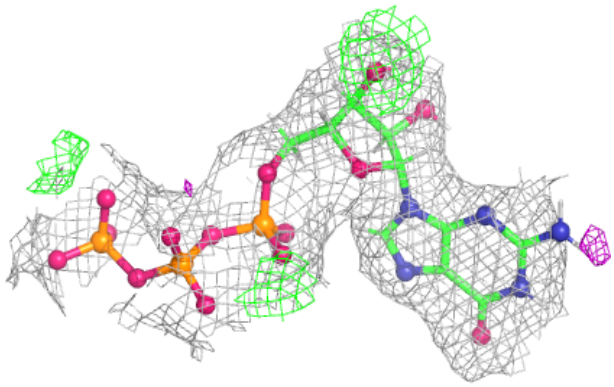


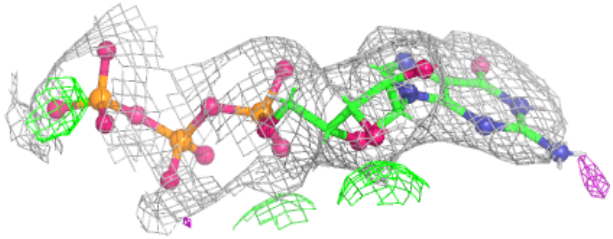


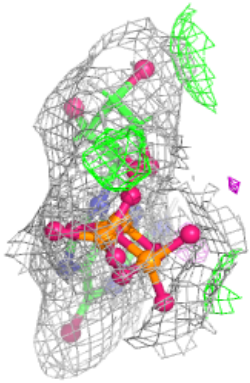


Electron density around GTP C 501:

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







6.5 Other polymers (i)

There are no such residues in this entry.