



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 07:17 am BST

PDB ID : 6FKL
Title : Tubulin-TUB015 complex
Authors : Prota, A.E.; Steinmetz, M.O.; Priego, E.-M.
Deposited on : 2018-01-24
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

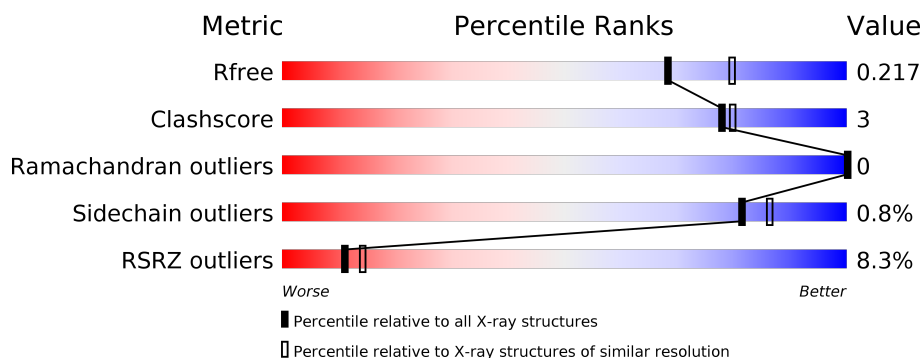
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 on 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	<div> <div>3%</div> <div>89%</div> <div>8%</div> <div>•</div> </div>
1	C	451	<div> <div>%</div> <div>91%</div> <div>6%</div> <div>•</div> </div>
2	B	445	<div> <div>3%</div> <div>87%</div> <div>9%</div> <div>•</div> </div>
2	D	445	<div> <div>8%</div> <div>86%</div> <div>9%</div> <div>5%</div> </div>
3	E	143	<div> <div>9%</div> <div>78%</div> <div>7%</div> <div>15%</div> </div>
4	F	384	<div> <div>26%</div> <div>82%</div> <div>9%</div> <div>9%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	DLK	B	507	X	-	-	-
11	DLK	D	503	X	-	-	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 18310 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	439	Total	C	N	O	S	0	8	0
			3463	2196	583	660	24			
1	C	439	Total	C	N	O	S	0	14	0
			3496	2216	592	666	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	425	Total	C	N	O	S	0	4	0
			3363	2114	573	649	27			
2	D	422	Total	C	N	O	S	0	2	0
			3317	2085	563	643	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	122	Total	C	N	O	S	0	3	0
			1022	632	184	201	5			

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	-	cloning artifact	UNP P63043

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	349	Total	C	N	O	S	0	1	0
			2852	1827	488	523	14			

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 (three-letter code: 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		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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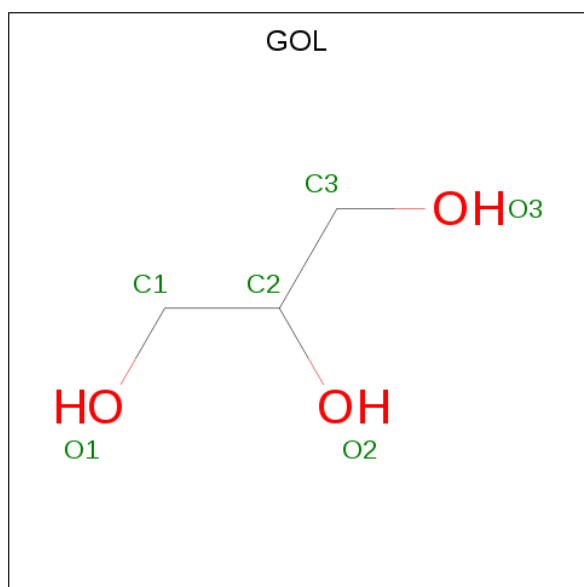
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

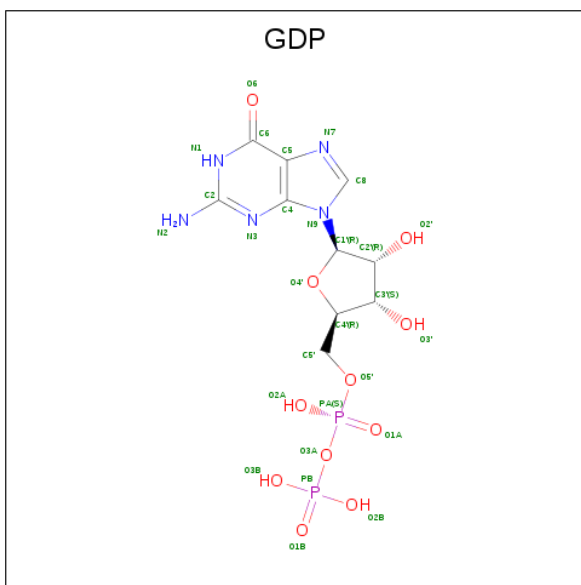
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Ca	0	0
			2	2		
7	A	2	Total	Ca	0	0
			2	2		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



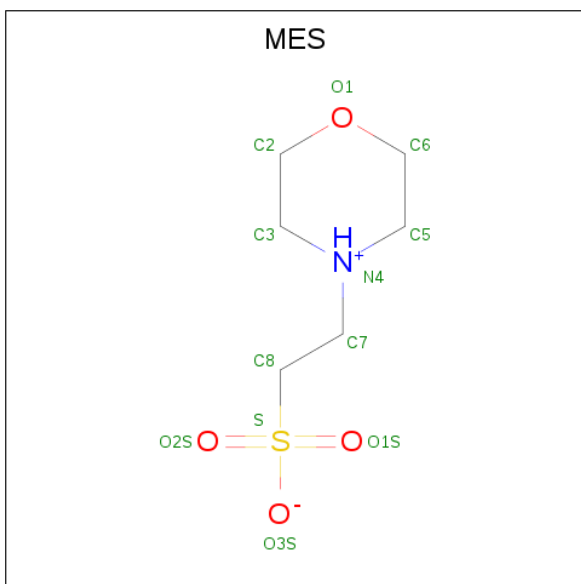
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



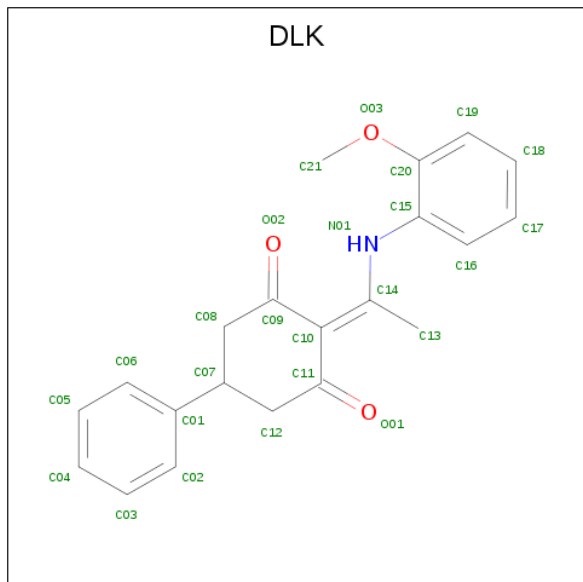
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
9	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $\text{C}_6\text{H}_{13}\text{NO}_4\text{S}$).



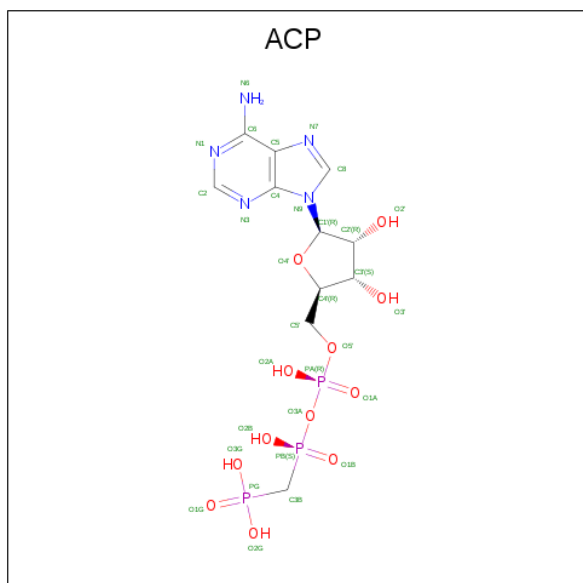
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is 2-{1-[(2-Methoxyphenyl)amino]ethylidene}-5-phenyl-1,3-cyclohexanedione (three-letter code: DLK) (formula: $C_{21}H_{21}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			25	21	1	3		
11	D	1	Total	C	N	O	0	0
			25	21	1	3		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

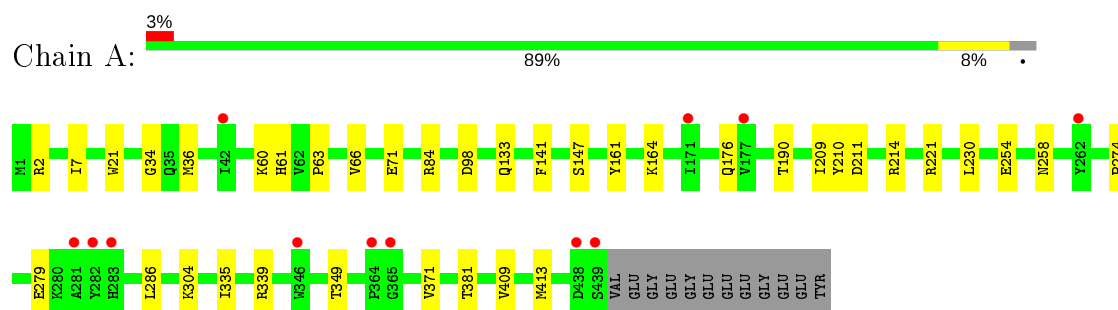
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	125	Total	O	0	0
			125	125		
13	B	120	Total	O	0	0
			120	120		
13	C	212	Total	O	0	0
			212	212		
13	D	53	Total	O	0	0
			53	53		
13	E	20	Total	O	0	0
			20	20		
13	F	32	Total	O	0	0
			32	32		

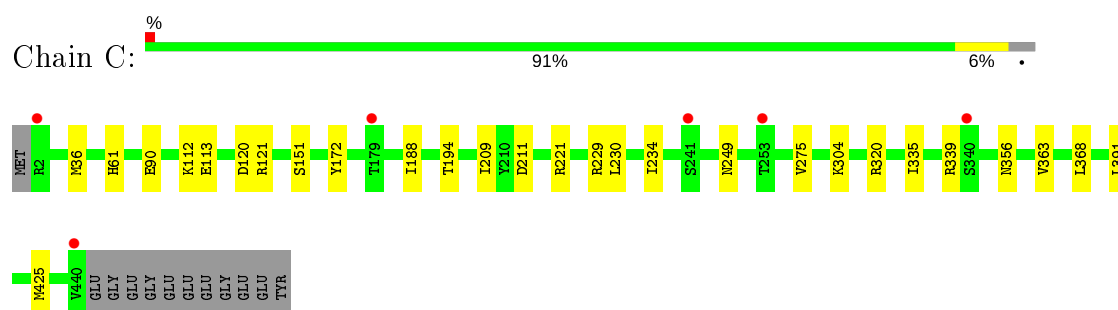
3 Residue-property plots [i](#)

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

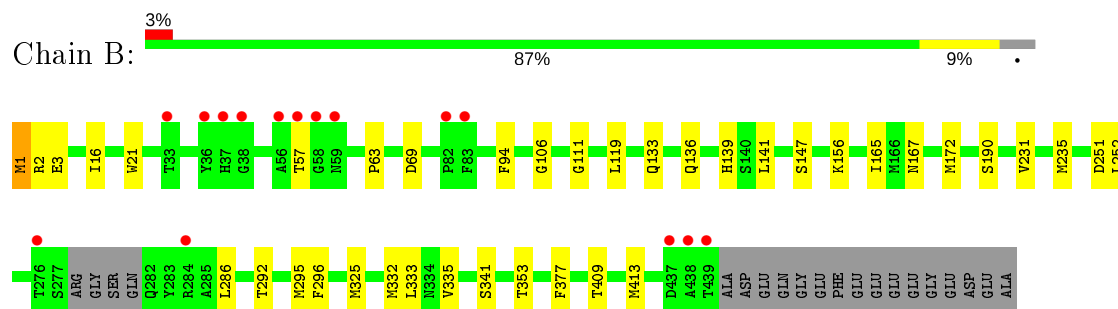
- Molecule 1: Tubulin alpha-1B chain



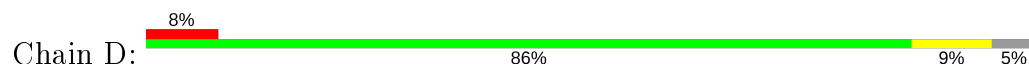
- Molecule 1: Tubulin alpha-1B chain

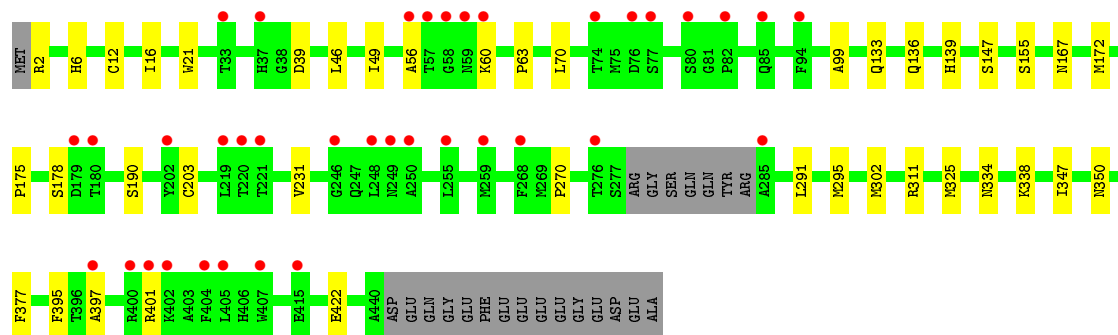


- Molecule 2: Tubulin beta-2B chain

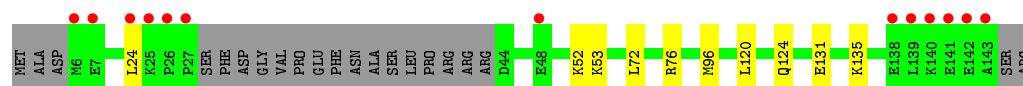
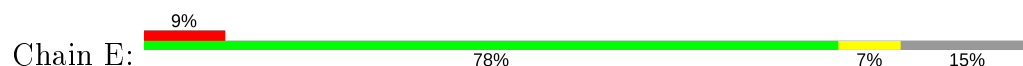


- Molecule 2: Tubulin beta-2B chain

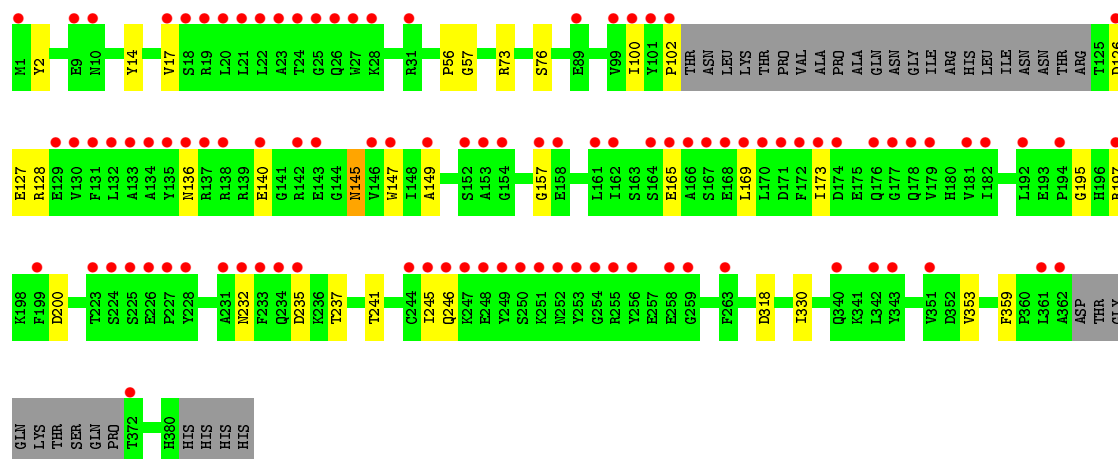
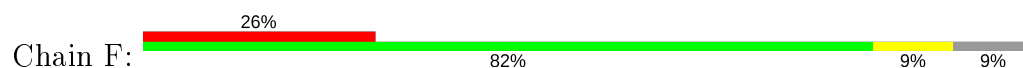




- Molecule 3: Stathmin-4



- Molecule 4: Tubulin tyrosine ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.75Å 157.76Å 179.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.44 – 2.10 49.44 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.44-2.10) 98.4 (49.44-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.10Å)	Xtriage
Refinement program	PHENIX (dev_2863: ???)	Depositor
R, R_{free}	0.178 , 0.217 0.178 , 0.217	Depositor DCC
R_{free} test set	8575 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.1	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	0.96	EDS
Total number of atoms	18310	wwPDB-VP
Average B, all atoms (Å ²)	57.0	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.27	0/3565	0.45	0/4840
1	C	0.29	0/3616	0.46	0/4911
2	B	0.27	0/3449	0.45	0/4670
2	D	0.26	0/3396	0.44	0/4601
3	E	0.25	0/1040	0.37	0/1381
4	F	0.25	0/2920	0.42	0/3944
All	All	0.27	0/17986	0.44	0/24347

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3463	0	3393	20	0
1	C	3496	0	3436	18	0
2	B	3363	0	3255	20	0
2	D	3317	0	3200	23	0
3	E	1022	0	1043	5	0
4	F	2852	0	2821	21	0
5	A	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	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
6	F	1	0	0	0	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0
8	A	6	0	8	0	0
8	B	6	0	8	0	0
9	B	28	0	12	0	0
9	D	28	0	12	1	0
10	B	12	0	12	0	0
11	B	25	0	0	0	0
11	D	25	0	0	0	0
12	F	31	0	14	2	0
13	A	125	0	0	0	0
13	B	120	0	0	0	0
13	C	212	0	0	1	0
13	D	53	0	0	1	0
13	E	20	0	0	0	0
13	F	32	0	0	1	0
All	All	18310	0	17238	101	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 101 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:147[A]:SER:HG	2:D:190:SER:HG	1.39	0.69
1:C:120[B]:ASP:OD2	1:C:121[B]:ARG:NH2	2.24	0.68
2:B:332:MET:HG3	2:B:353:THR:HG21	1.80	0.63
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.80	0.63
1:C:249:ASN:OD1	1:C:356[A]:ASN:ND2	2.29	0.62

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	445/451 (99%)	439 (99%)	6 (1%)	0	100	100
1	C	450/451 (100%)	439 (98%)	11 (2%)	0	100	100
2	B	425/445 (96%)	418 (98%)	7 (2%)	0	100	100
2	D	420/445 (94%)	413 (98%)	7 (2%)	0	100	100
3	E	121/143 (85%)	119 (98%)	2 (2%)	0	100	100
4	F	344/384 (90%)	333 (97%)	11 (3%)	0	100	100
All	All	2205/2319 (95%)	2161 (98%)	44 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	378/379 (100%)	375 (99%)	3 (1%)	81	86
1	C	384/379 (101%)	384 (100%)	0	100	100
2	B	372/383 (97%)	366 (98%)	6 (2%)	62	69
2	D	366/383 (96%)	362 (99%)	4 (1%)	73	79
3	E	112/127 (88%)	111 (99%)	1 (1%)	78	84
4	F	312/342 (91%)	309 (99%)	3 (1%)	76	82
All	All	1924/1993 (96%)	1907 (99%)	17 (1%)	81	84

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	286	LEU
2	B	341	SER
3	E	96	MET
2	B	139	HIS
4	F	145	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	301	GLN
2	D	294	GLN
4	F	145	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 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	$\# Z > 2$
11	DLK	B	507	-	27,27,27	1.60	4 (14%)	37,37,37	1.97	10 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GOL	A	505	-	5,5,5	0.88	0	5,5,5	1.04	0
9	GDP	D	501	6	24,30,30	1.21	2 (8%)	31,47,47	1.91	7 (22%)
9	GDP	B	501	6	24,30,30	1.16	2 (8%)	31,47,47	1.93	7 (22%)
5	GTP	C	501	6	26,34,34	1.00	1 (3%)	33,54,54	1.71	6 (18%)
5	GTP	A	501	6	26,34,34	0.97	1 (3%)	33,54,54	1.71	7 (21%)
10	MES	B	506	-	12,12,12	2.23	1 (8%)	14,16,16	2.11	7 (50%)
12	ACP	F	402	6	27,33,33	1.68	6 (22%)	32,52,52	1.32	4 (12%)
8	GOL	B	505	-	5,5,5	1.04	0	5,5,5	0.87	0
11	DLK	D	503	-	27,27,27	1.66	4 (14%)	37,37,37	2.03	11 (29%)

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
11	DLK	B	507	-	1/1/5/6	4/14/30/30	0/3/3/3
8	GOL	A	505	-	-	4/4/4/4	-
9	GDP	D	501	6	-	5/12/32/32	0/3/3/3
9	GDP	B	501	6	-	5/12/32/32	0/3/3/3
5	GTP	C	501	6	-	9/18/38/38	0/3/3/3
5	GTP	A	501	6	-	7/18/38/38	0/3/3/3
10	MES	B	506	-	-	1/6/14/14	0/1/1/1
12	ACP	F	402	6	-	5/15/38/38	0/3/3/3
8	GOL	B	505	-	-	2/4/4/4	-
11	DLK	D	503	-	1/1/5/6	6/14/30/30	0/3/3/3

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	506	MES	C8-S	-7.43	1.66	1.77
11	D	503	DLK	O02-C09	6.34	1.35	1.23
11	B	507	DLK	O02-C09	6.05	1.35	1.23
9	D	501	GDP	C6-C5	4.25	1.48	1.41
12	F	402	ACP	PB-O1B	4.10	1.61	1.51

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
11	D	503	DLK	C09-C10-C14	7.02	123.72	120.55
11	B	507	DLK	C09-C10-C14	6.41	123.44	120.55
5	C	501	GTP	N3-C2-N1	-5.29	120.17	127.22
5	A	501	GTP	N3-C2-N1	-5.23	120.24	127.22
9	B	501	GDP	C2-N3-C4	4.95	121.02	115.36

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	B	507	DLK	C10
11	D	503	DLK	C10

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	F	402	ACP	PG-C3B-PB-O3A
12	F	402	ACP	C5'-O5'-PA-O1A
12	F	402	ACP	C5'-O5'-PA-O3A
9	D	501	GDP	C5'-O5'-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O2A

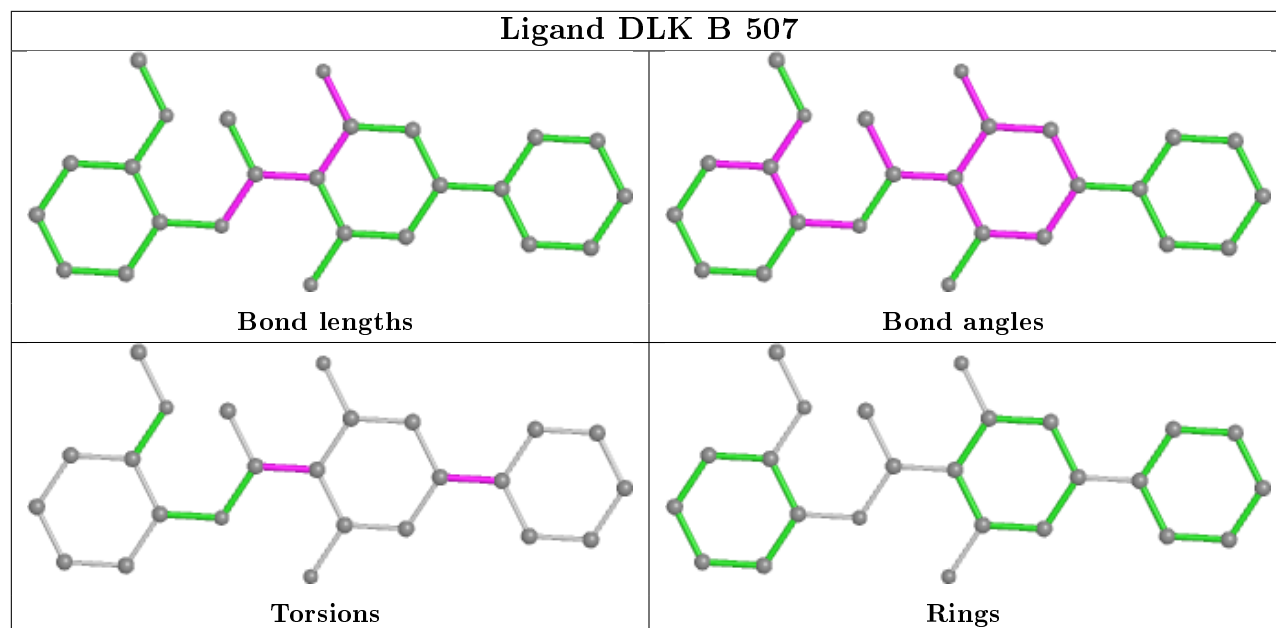
There are no ring outliers.

2 monomers are involved in 3 short contacts:

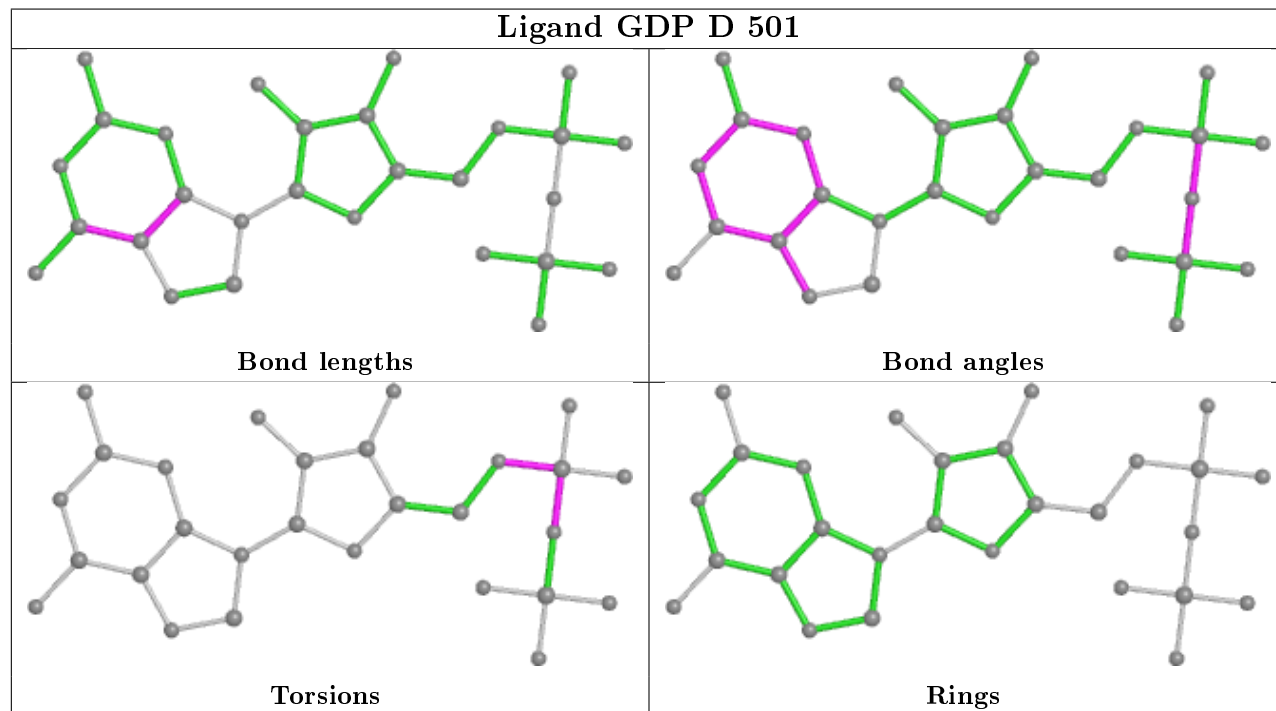
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	501	GDP	1	0
12	F	402	ACP	2	0

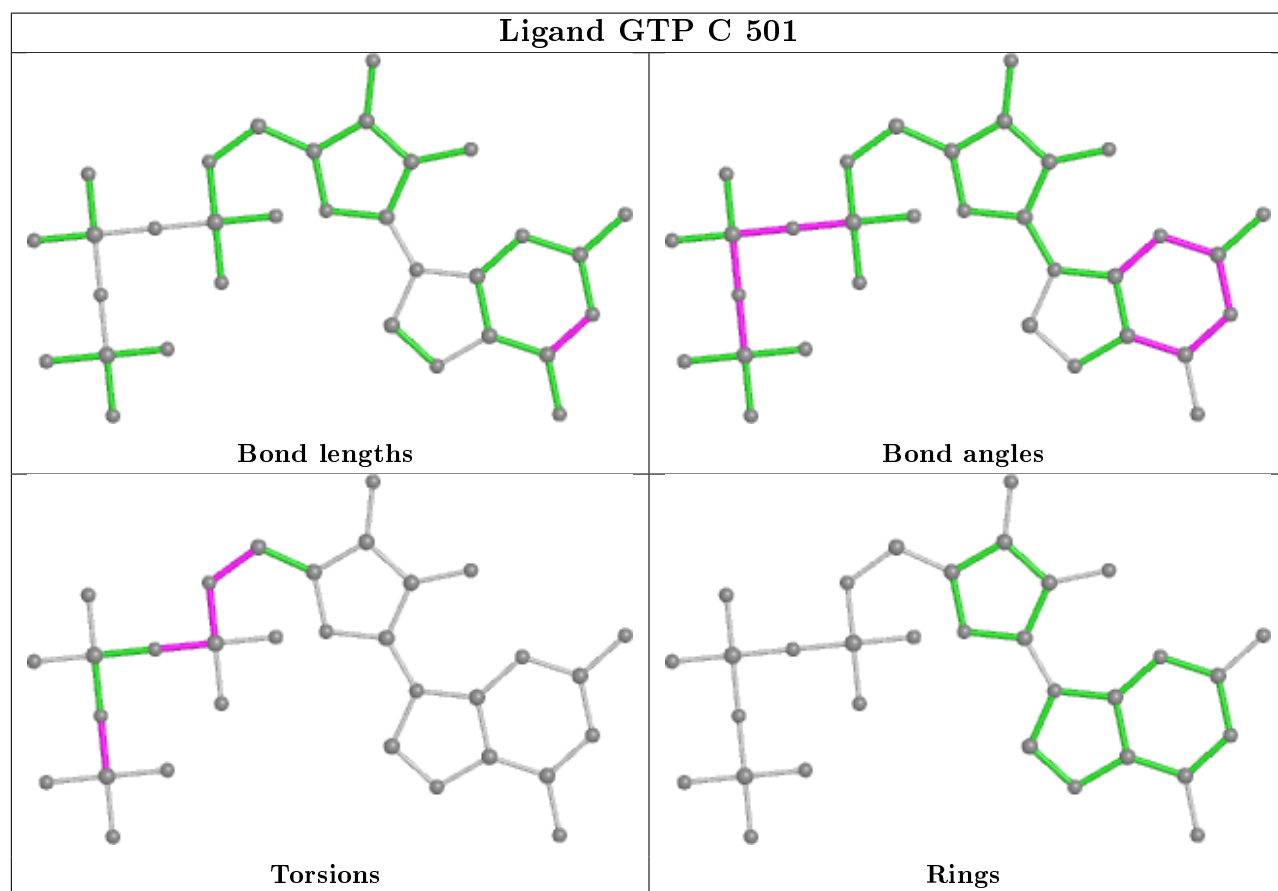
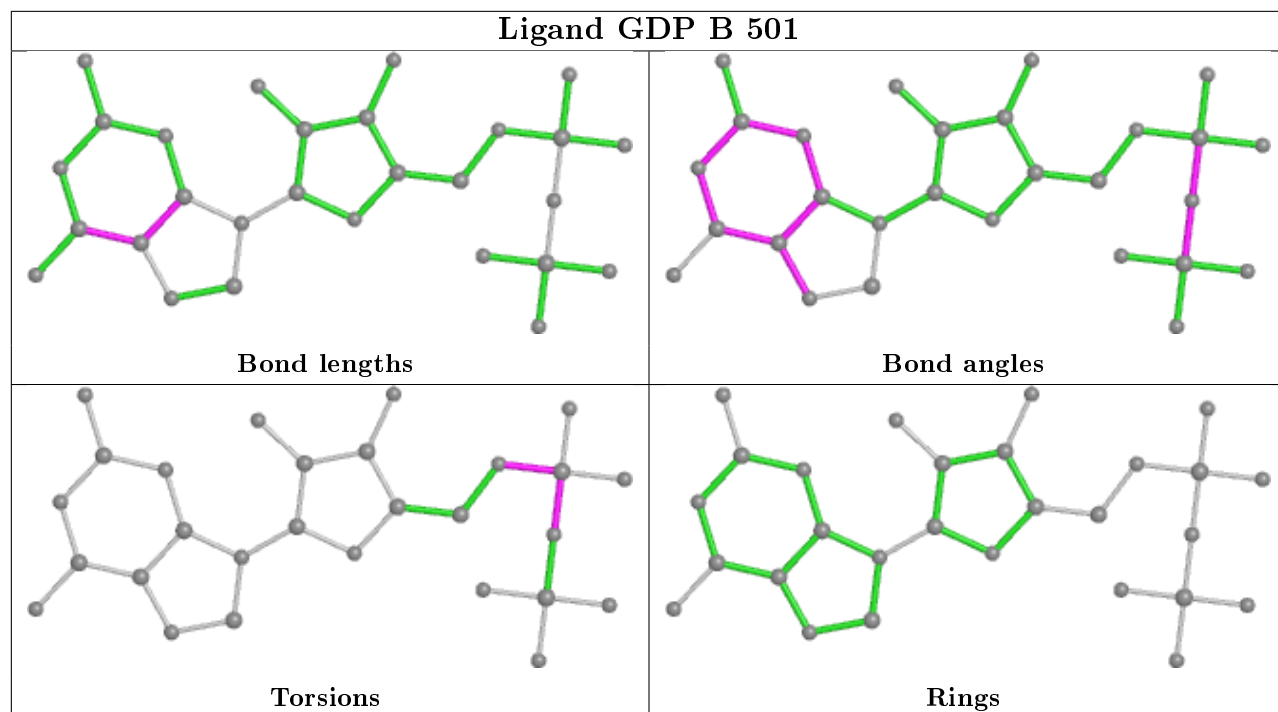
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

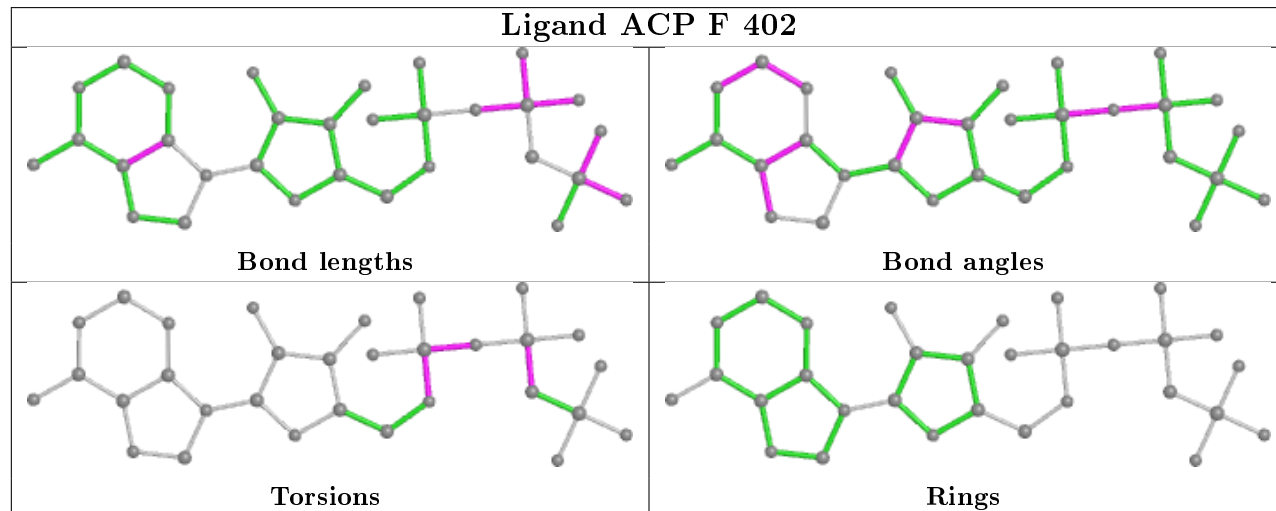
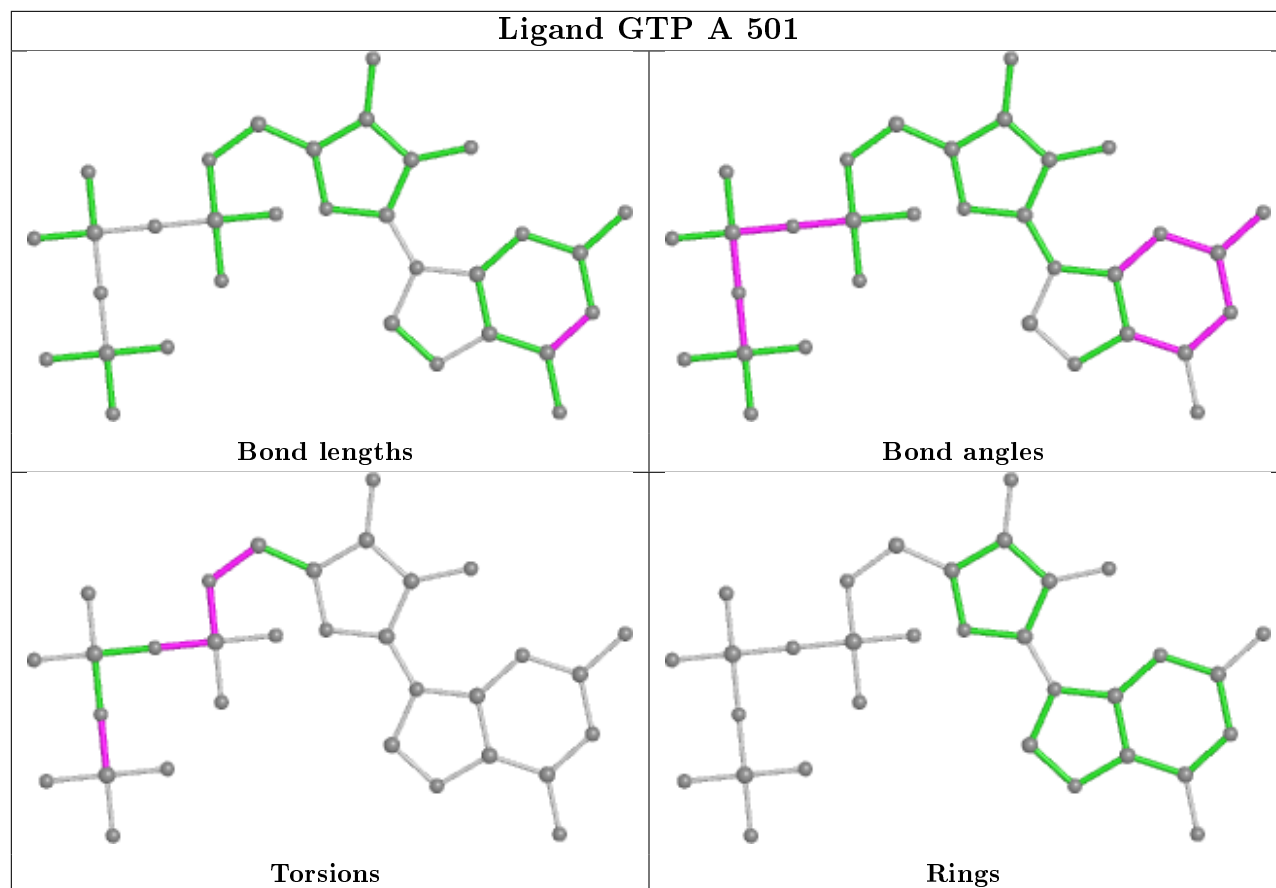
Ligand DLK B 507

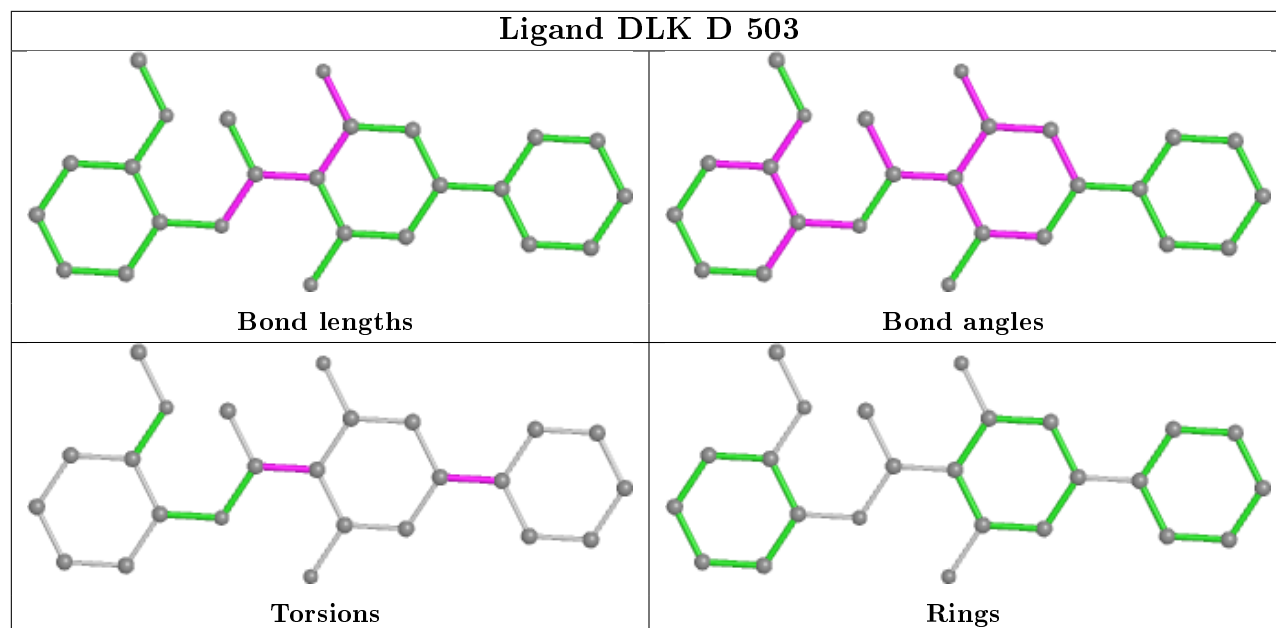


Ligand GDP D 501









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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	439/451 (97%)	0.28	12 (2%) 54 60	32, 49, 81, 138	0
1	C	439/451 (97%)	0.06	6 (1%) 75 78	26, 38, 65, 95	0
2	B	425/445 (95%)	0.26	15 (3%) 44 50	26, 45, 82, 115	0
2	D	422/445 (94%)	0.48	37 (8%) 10 12	34, 58, 89, 143	0
3	E	122/143 (85%)	0.46	13 (10%) 6 7	38, 64, 100, 122	0
4	F	349/384 (90%)	1.25	100 (28%) 0 0	39, 78, 143, 170	0
All	All	2196/2319 (94%)	0.44	183 (8%) 11 14	26, 51, 103, 170	0

The worst 5 of 183 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	173	ILE	9.5
2	D	57	THR	8.6
4	F	130	VAL	7.6
4	F	249	TYR	7.0
4	F	233	PHE	6.8

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

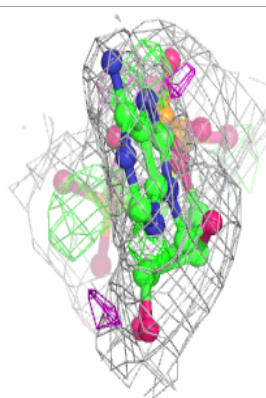
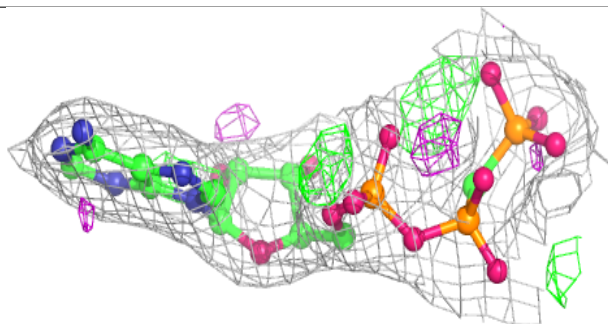
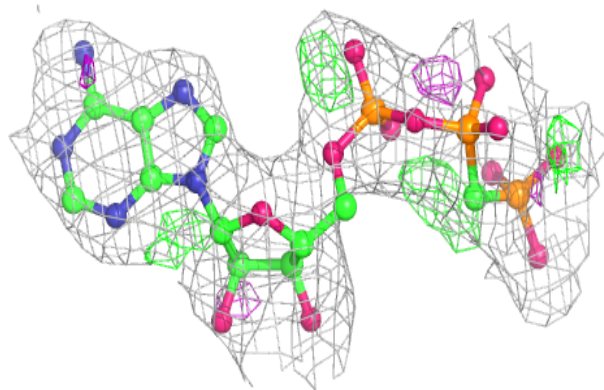
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	GOL	B	505	6/6	0.70	0.29	51,72,73,77	0
12	ACP	F	402	31/31	0.86	0.14	68,78,107,108	0
6	MG	F	401	1/1	0.86	0.06	76,76,76,76	0
11	DLK	D	503	25/25	0.87	0.26	48,69,77,79	0
6	MG	D	502	1/1	0.89	0.09	55,55,55,55	0
7	CA	A	504	1/1	0.91	0.08	101,101,101,101	0
8	GOL	A	505	6/6	0.91	0.19	59,68,72,76	0
7	CA	B	504	1/1	0.93	0.11	122,122,122,122	0
10	MES	B	506	12/12	0.95	0.15	41,51,77,89	0
7	CA	B	503	1/1	0.95	0.09	94,94,94,94	0
7	CA	A	503	1/1	0.97	0.04	63,63,63,63	0
11	DLK	B	507	25/25	0.97	0.14	30,36,43,47	0
9	GDP	D	501	28/28	0.97	0.11	44,51,56,62	0
5	GTP	A	501	32/32	0.98	0.18	24,33,40,42	0
6	MG	A	502	1/1	0.98	0.12	32,32,32,32	0
5	GTP	C	501	32/32	0.99	0.14	21,29,32,38	0
7	CA	C	503	1/1	0.99	0.04	49,49,49,49	0
6	MG	C	502	1/1	0.99	0.14	28,28,28,28	0
9	GDP	B	501	28/28	0.99	0.16	27,31,36,36	0
6	MG	B	502	1/1	1.00	0.21	24,24,24,24	0

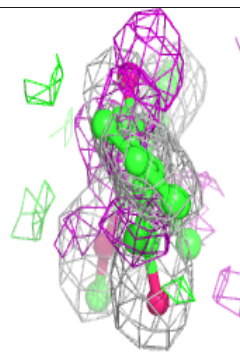
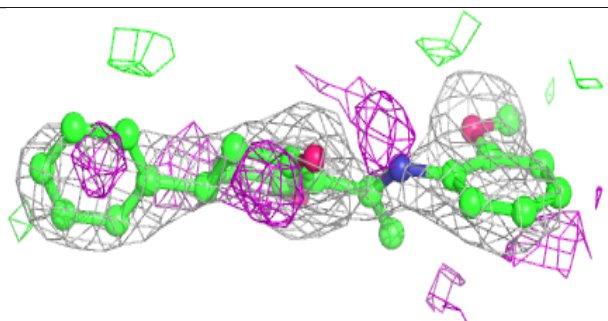
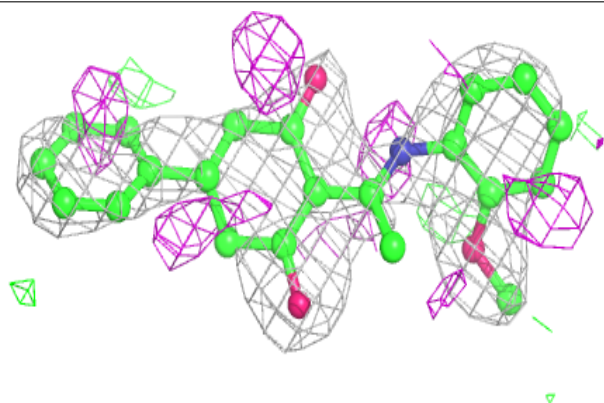
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

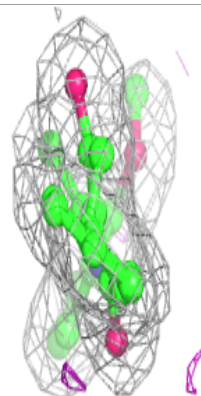
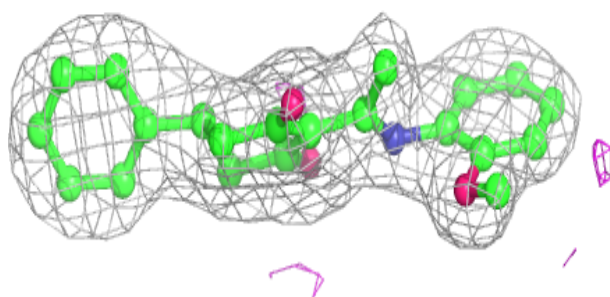
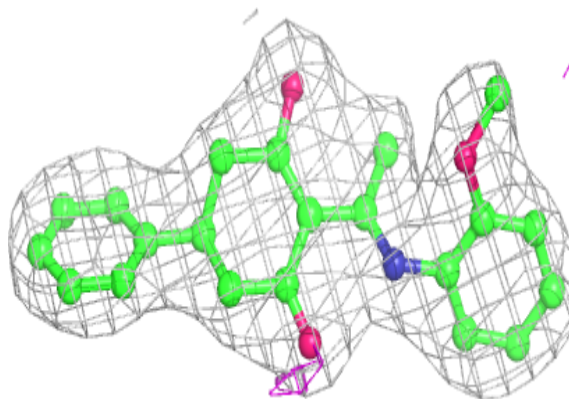
**Electron density around DLK D 503:**

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

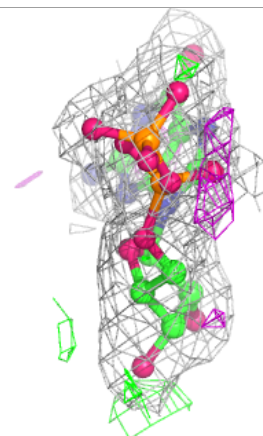
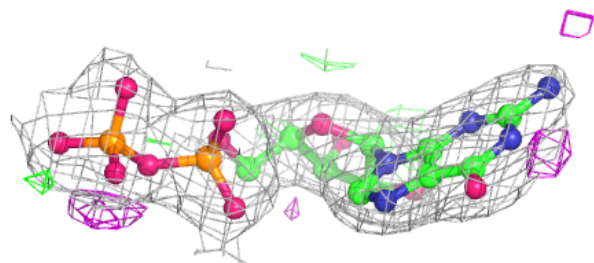
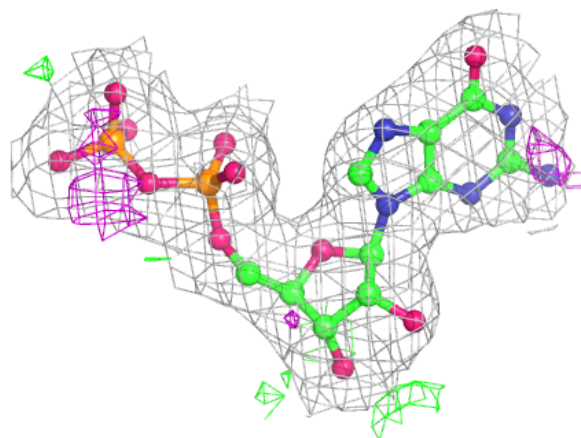


Electron density around DLK B 507:

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

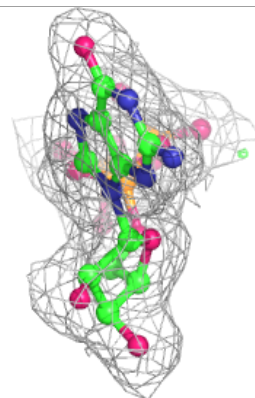
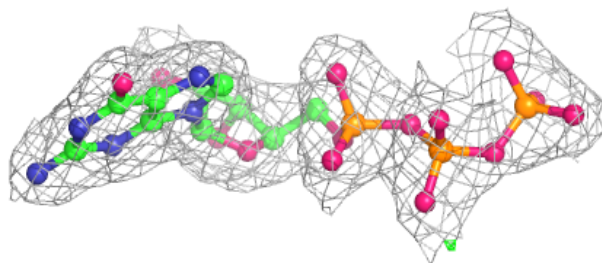
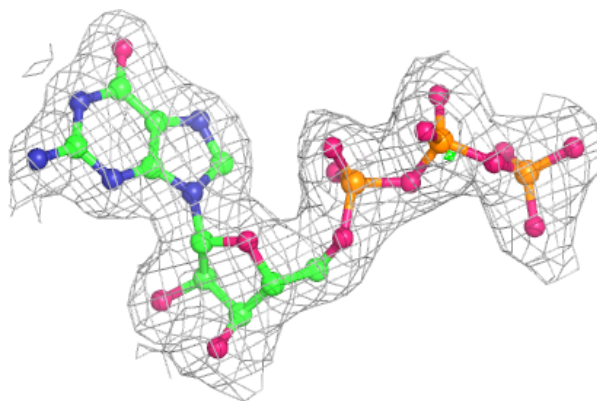
**Electron density around GDP D 501:**

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

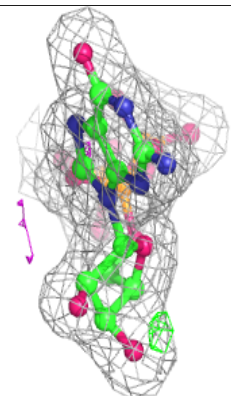
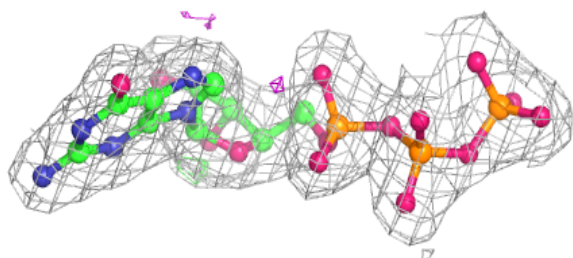
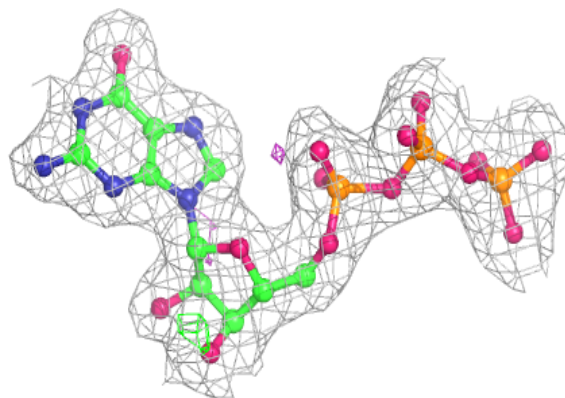


Electron density around GTP A 501:

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

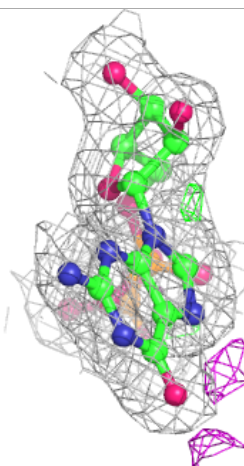
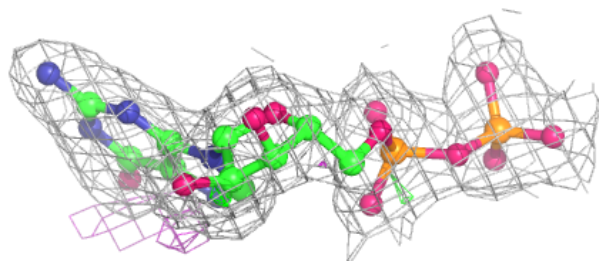
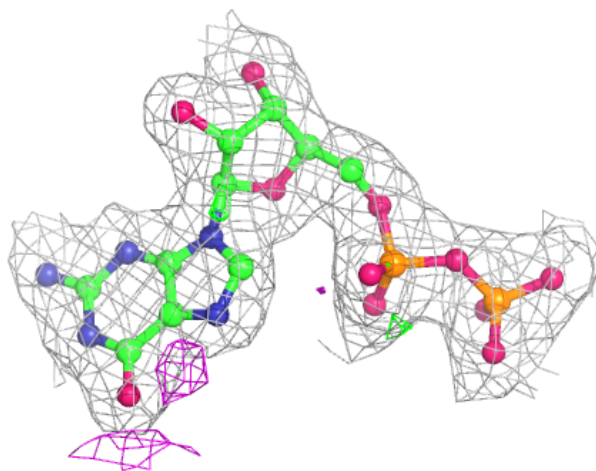
**Electron density around GTP C 501:**

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.