wwPDB X-ray Structure Validation Summary Report (i)

Mar 3, 2024 – 07:19 PM EST

PDB ID	:	6MZF
Title	:	Structural Basis of Tubulin Recruitment and Assembly by Microtubule Polymerases with Tumor Overexpressed Gene (TOG) Domain Arrays
Authors	:	Nithianantham, S.; Al-Bassam, J.
Deposited on	:	2018-11-05
Resolution	:	4.40 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:

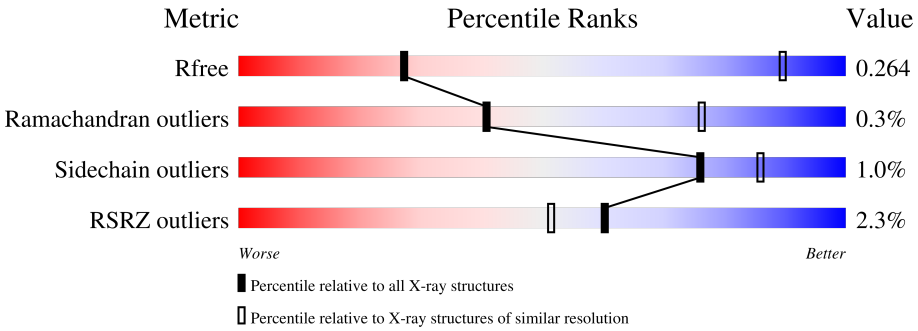
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.40 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	1043 (5.00-3.80)
Ramachandran outliers	138981	1059 (5.00-3.80)
Sidechain outliers	138945	1041 (5.00-3.80)
RSRZ outliers	127900	1095 (5.08-3.70)

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	3% 93% 6%
1	C	451	% 94% 6%
1	H	451	% 93% 6%
1	J	451	3% 94% 6%
1	O	451	6% 93% 6%
1	Q	451	93% 6%

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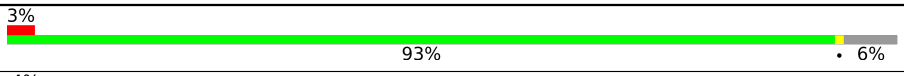
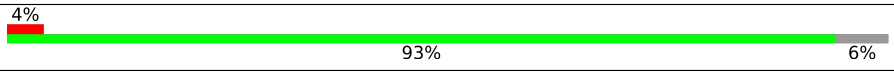
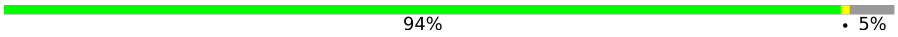
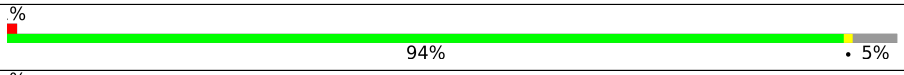
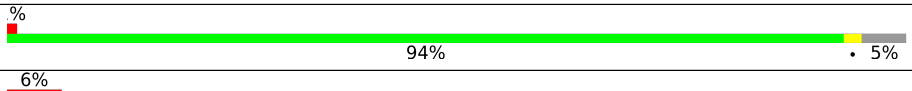
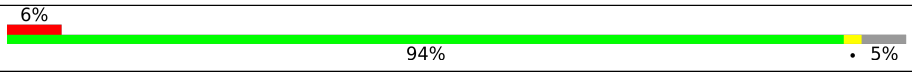
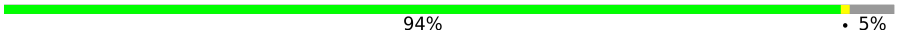
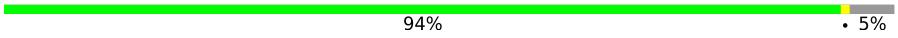
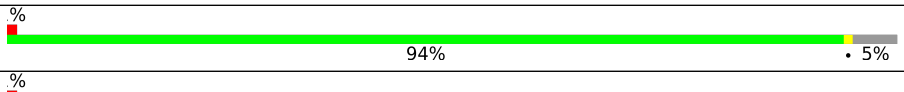
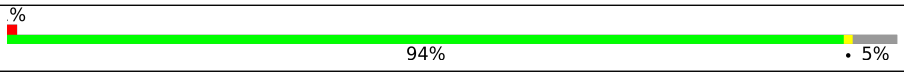
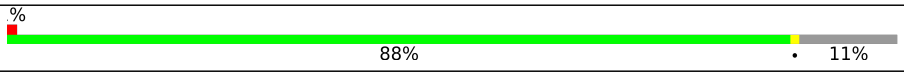
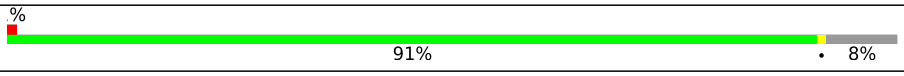
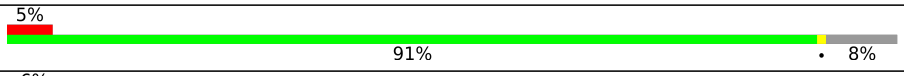
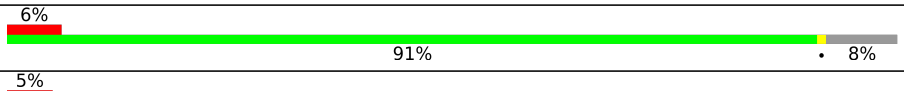
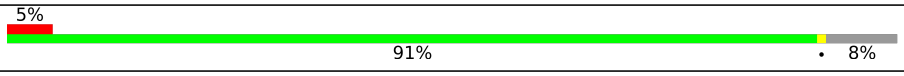
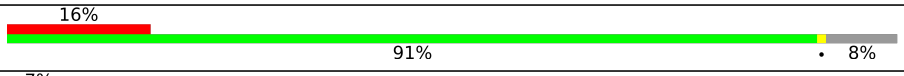
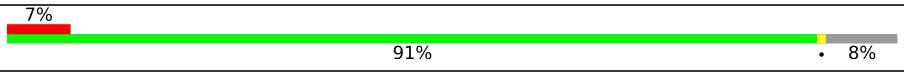
Mol	Chain	Length	Quality of chain
1	V	451	
1	X	451	
2	B	445	
2	D	445	
2	I	445	
2	K	445	
2	P	445	
2	R	445	
2	W	445	
2	Y	445	
3	E	554	
3	L	554	
3	S	554	
3	Z	554	
4	F	169	
4	G	169	
4	M	169	
4	N	169	
4	T	169	
4	U	169	
4	a	169	
4	b	169	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 78030 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-1A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	423	Total	C	N	O	S	0	0	0
			3265	2068	553	623	21			
1	C	423	Total	C	N	O	S	0	0	0
			3265	2068	553	623	21			
1	H	423	Total	C	N	O	S	0	0	0
			3265	2068	553	623	21			
1	J	423	Total	C	N	O	S	0	0	0
			3265	2068	553	623	21			
1	O	423	Total	C	N	O	S	0	0	0
			3265	2068	553	623	21			
1	Q	423	Total	C	N	O	S	0	0	0
			3265	2068	553	623	21			
1	V	423	Total	C	N	O	S	0	0	0
			3265	2068	553	623	21			
1	X	423	Total	C	N	O	S	0	0	0
			3265	2068	553	623	21			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	0	0
			3308	2078	565	639	26			
2	D	424	Total	C	N	O	S	0	0	0
			3308	2078	565	639	26			
2	I	424	Total	C	N	O	S	0	0	0
			3308	2078	565	639	26			
2	K	424	Total	C	N	O	S	0	0	0
			3308	2078	565	639	26			
2	P	424	Total	C	N	O	S	0	0	0
			3308	2078	565	639	26			
2	R	424	Total	C	N	O	S	0	0	0
			3308	2078	565	639	26			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	W	424	Total	C	N	O	S	0	0	0
			3308	2078	565	639	26			
2	Y	424	Total	C	N	O	S	0	0	0
			3308	2078	565	639	26			

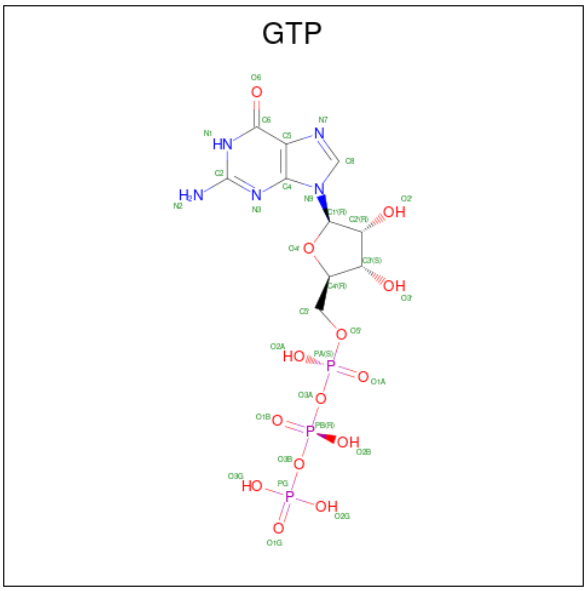
- Molecule 3 is a protein called Protein Stu2p/Alp14p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	491	Total	C	N	O	S	0	0	0
			3949	2525	667	741	16			
3	L	494	Total	C	N	O	S	0	0	0
			3976	2540	672	748	16			
3	S	493	Total	C	N	O	S	0	0	0
			3967	2535	670	746	16			
3	Z	495	Total	C	N	O	S	0	0	0
			3984	2546	673	749	16			

- Molecule 4 is a protein called Designed ankyrin repeat protein (DARPIN) D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	155	Total	C	N	O	S	0	0	0
			1135	713	195	224	3			
4	G	155	Total	C	N	O	S	0	0	0
			1135	713	195	224	3			
4	M	155	Total	C	N	O	S	0	0	0
			1135	713	195	224	3			
4	N	155	Total	C	N	O	S	0	0	0
			1135	713	195	224	3			
4	T	155	Total	C	N	O	S	0	0	0
			1135	713	195	224	3			
4	U	155	Total	C	N	O	S	0	0	0
			1135	713	195	224	3			
4	a	155	Total	C	N	O	S	0	0	0
			1129	707	195	224	3			
4	b	155	Total	C	N	O	S	0	0	0
			1135	713	195	224	3			

- 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		
5	H	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	J	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	O	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	Q	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	V	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	X	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	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		
6	D	1	Total	Mg	0	0
			1	1		

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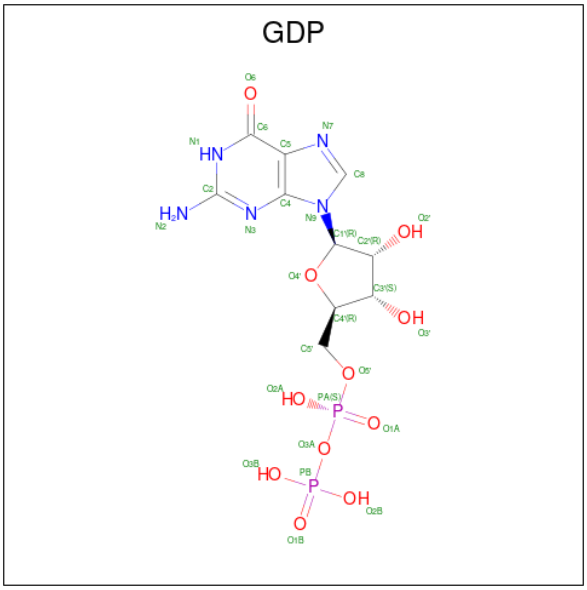
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total Mg 1 1	0	0
6	I	1	Total Mg 1 1	0	0
6	J	1	Total Mg 1 1	0	0
6	K	1	Total Mg 1 1	0	0
6	O	1	Total Mg 1 1	0	0
6	P	1	Total Mg 1 1	0	0
6	Q	1	Total Mg 1 1	0	0
6	R	1	Total Mg 1 1	0	0
6	V	1	Total Mg 1 1	0	0
6	W	1	Total Mg 1 1	0	0
6	X	1	Total Mg 1 1	0	0
6	Y	1	Total Mg 1 1	0	0

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



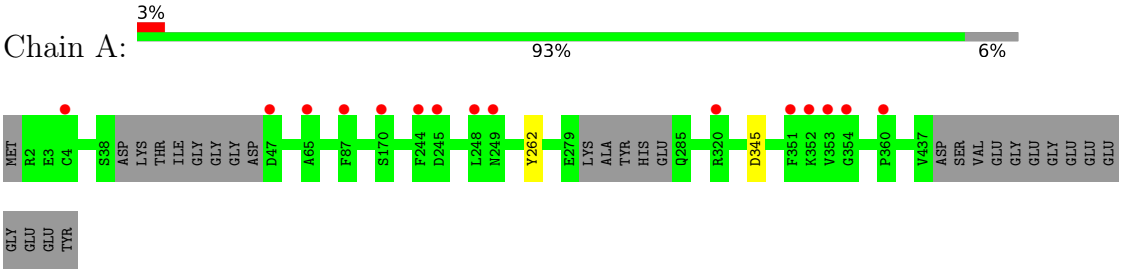
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
7	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
7	I	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
7	K	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
7	P	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
7	R	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
7	W	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
7	Y	1	Total	C	N	O	P	0	0
			28	10	5	11	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.

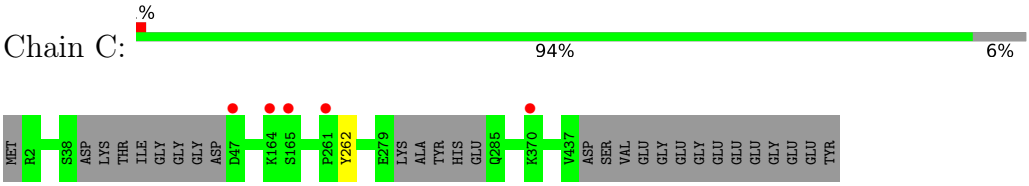
• Molecule 1: Tubulin alpha-1A chain

Chain A:



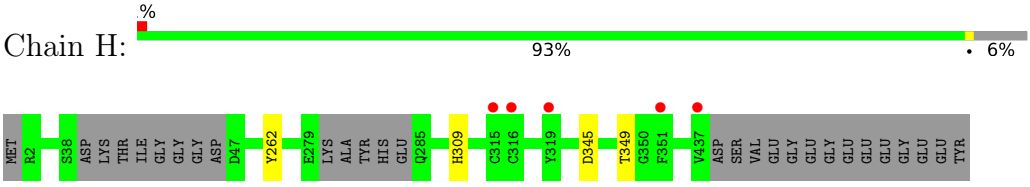
• Molecule 1: Tubulin alpha-1A chain

Chain C:



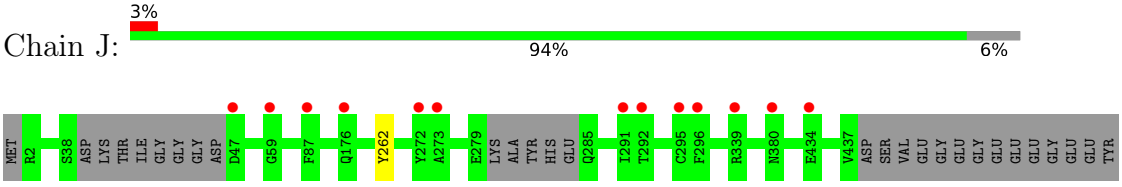
• Molecule 1: Tubulin alpha-1A chain

Chain H:



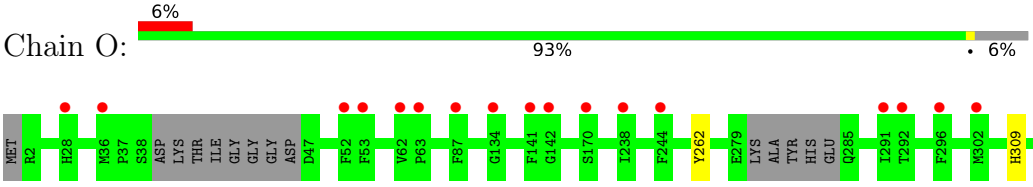
• Molecule 1: Tubulin alpha-1A chain

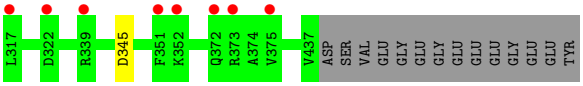
Chain J:



• Molecule 1: Tubulin alpha-1A chain

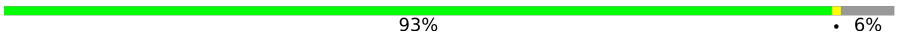
Chain O:

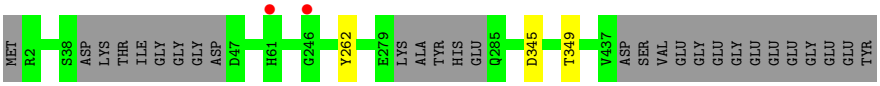




• Molecule 1: Tubulin alpha-1A chain

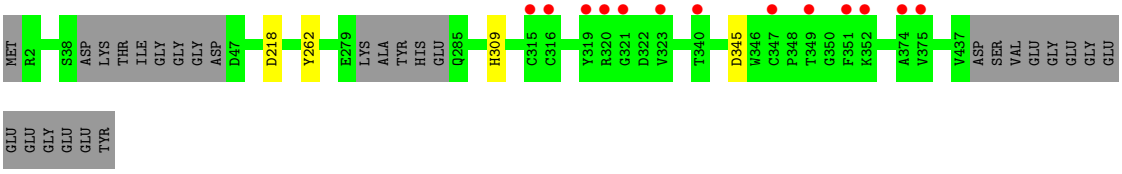
Chain Q:





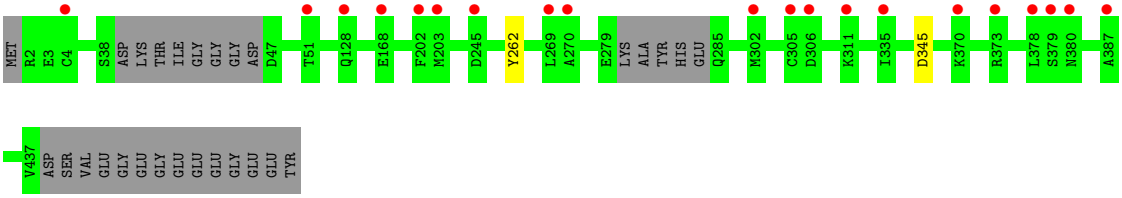
• Molecule 1: Tubulin alpha-1A chain

Chain V:



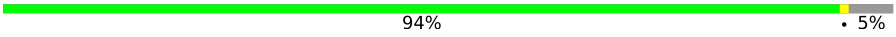
• Molecule 1: Tubulin alpha-1A chain

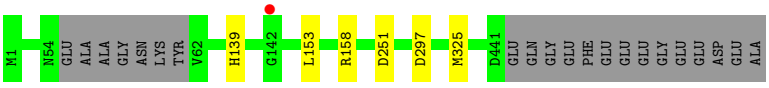
Chain X:



• Molecule 2: Tubulin beta chain

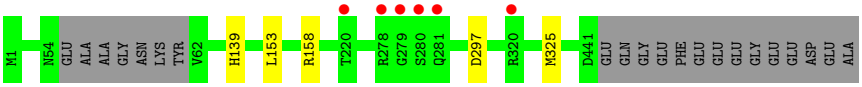
Chain B:





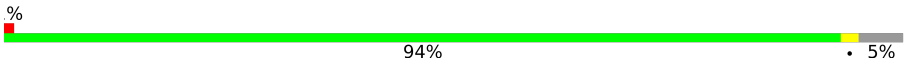
• Molecule 2: Tubulin beta chain

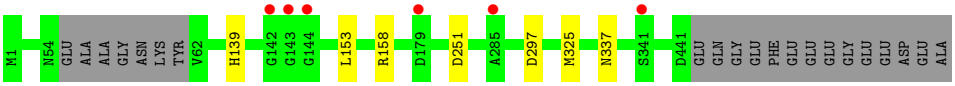
Chain D:



• Molecule 2: Tubulin beta chain

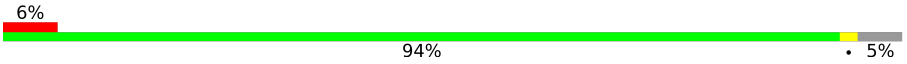
Chain I:

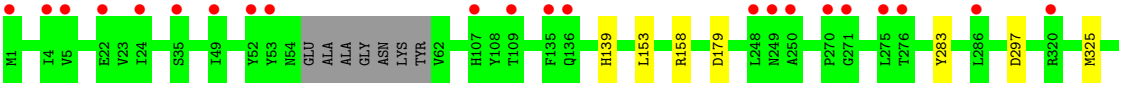


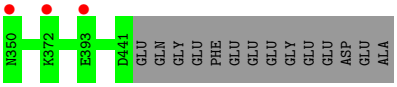


• Molecule 2: Tubulin beta chain

Chain K:

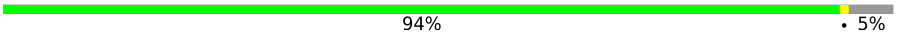






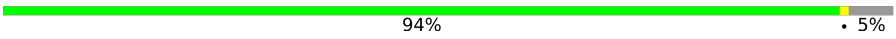
• Molecule 2: Tubulin beta chain

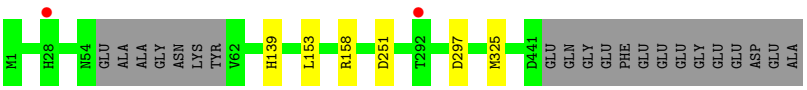
Chain P:



• Molecule 2: Tubulin beta chain

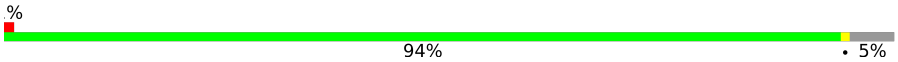
Chain R:

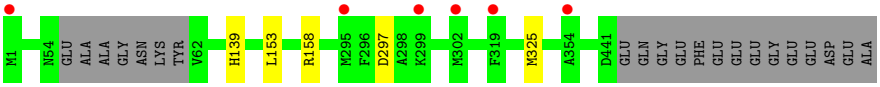




• Molecule 2: Tubulin beta chain

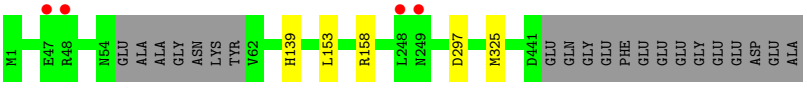
Chain W:





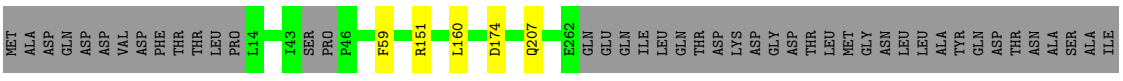
• Molecule 2: Tubulin beta chain

Chain Y:



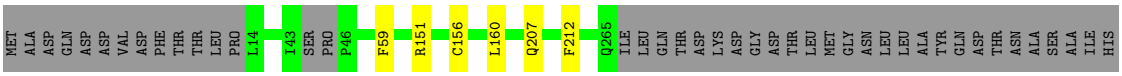
• Molecule 3: Protein Stu2p/Alp14p

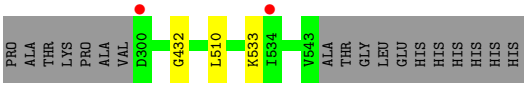
Chain E:



• Molecule 3: Protein Stu2p/Alp14p

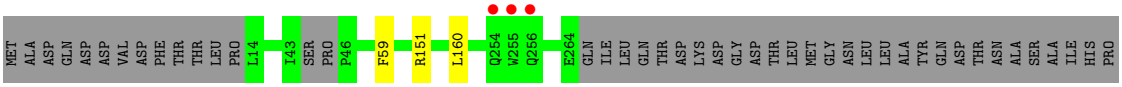
Chain L:





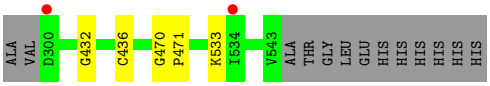
• Molecule 3: Protein Stu2p/Alp14p

Chain S:



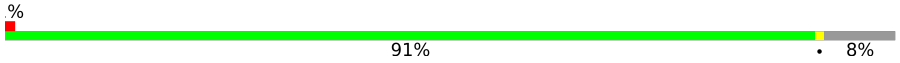
• Molecule 3: Protein Stu2p/Alp14p

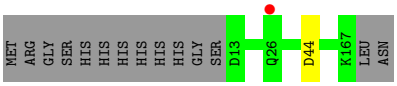
Chain Z:



• Molecule 4: Designed ankyrin repeat protein (DARPIN) D1

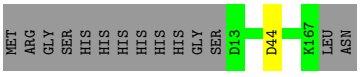
Chain F:





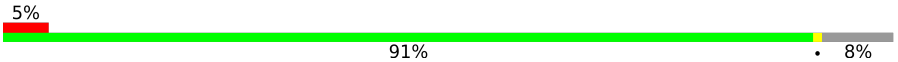
• Molecule 4: Designed ankyrin repeat protein (DARPIN) D1

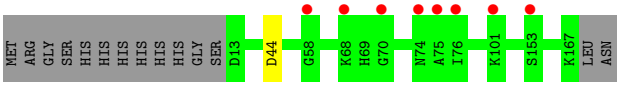
Chain G:



• Molecule 4: Designed ankyrin repeat protein (DARPIN) D1

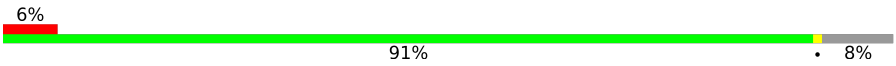
Chain M:

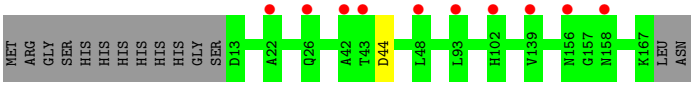




• Molecule 4: Designed ankyrin repeat protein (DARPIN) D1

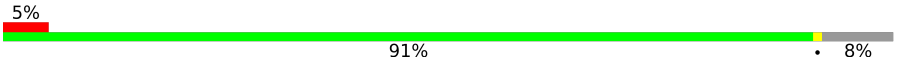
Chain N:

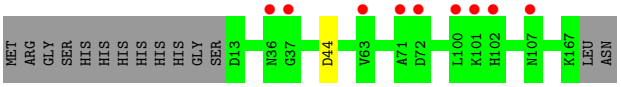




• Molecule 4: Designed ankyrin repeat protein (DARPIN) D1

Chain T:



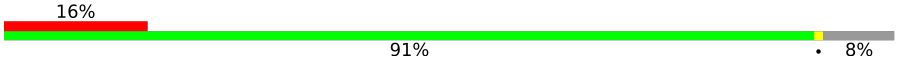


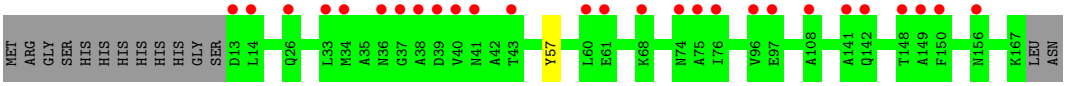
• Molecule 4: Designed ankyrin repeat protein (DARPIN) D1

Chain U:

• Molecule 4: Designed ankyrin repeat protein (DARPIN) D1

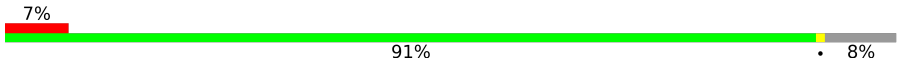
Chain a:

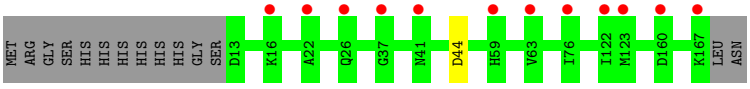




• Molecule 4: Designed ankyrin repeat protein (DARPIN) D1

Chain b:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	218.80Å 107.65Å 282.74Å 90.00° 90.38° 90.00°	Depositor
Resolution (Å)	96.59 – 4.40 96.59 – 4.40	Depositor EDS
% Data completeness (in resolution range)	80.6 (96.59-4.40) 79.4 (96.59-4.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	3.26 (at 4.47Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.225 , 0.252 0.237 , 0.264	Depositor DCC
R_{free} test set	3426 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	82.7	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 59.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.086 for h,-k,-l	Xtriage
Reported twinning fraction	0.120 for h,-k,-l	Depositor
Outliers	1 of 68039 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	78030	wwPDB-VP
Average B, all atoms (Å^2)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GTP, 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	0.24	0/3339	0.40	0/4539
1	C	0.24	0/3339	0.40	0/4539
1	H	0.24	0/3339	0.41	0/4539
1	J	0.24	0/3339	0.40	0/4539
1	O	0.24	0/3339	0.40	0/4539
1	Q	0.24	0/3339	0.40	0/4539
1	V	0.24	0/3339	0.40	0/4539
1	X	0.24	0/3339	0.40	0/4539
2	B	0.25	0/3380	0.42	0/4581
2	D	0.24	0/3380	0.41	0/4581
2	I	0.24	0/3380	0.41	0/4581
2	K	0.24	0/3380	0.41	0/4581
2	P	0.24	0/3380	0.41	0/4581
2	R	0.25	0/3380	0.42	0/4581
2	W	0.24	0/3380	0.41	0/4581
2	Y	0.24	0/3380	0.41	0/4581
3	E	0.25	0/4021	0.44	0/5449
3	L	0.24	0/4048	0.44	0/5485
3	S	0.25	0/4039	0.44	0/5473
3	Z	0.25	0/4056	0.44	0/5496
4	F	0.24	0/1150	0.40	0/1565
4	G	0.23	0/1150	0.40	0/1565
4	M	0.23	0/1150	0.40	0/1565
4	N	0.23	0/1150	0.40	0/1565
4	T	0.23	0/1150	0.40	0/1565
4	U	0.24	0/1150	0.40	0/1565
4	a	0.24	0/1143	0.47	0/1556
4	b	0.24	0/1150	0.40	0/1565
All	All	0.24	0/79109	0.41	0/107374

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)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	417/451 (92%)	390 (94%)	27 (6%)	0	100	100
1	C	417/451 (92%)	389 (93%)	28 (7%)	0	100	100
1	H	417/451 (92%)	389 (93%)	27 (6%)	1 (0%)	47	81
1	J	417/451 (92%)	389 (93%)	28 (7%)	0	100	100
1	O	417/451 (92%)	390 (94%)	27 (6%)	0	100	100
1	Q	417/451 (92%)	388 (93%)	28 (7%)	1 (0%)	47	81
1	V	417/451 (92%)	391 (94%)	26 (6%)	0	100	100
1	X	417/451 (92%)	389 (93%)	28 (7%)	0	100	100
2	B	420/445 (94%)	406 (97%)	13 (3%)	1 (0%)	47	81
2	D	420/445 (94%)	406 (97%)	13 (3%)	1 (0%)	47	81
2	I	420/445 (94%)	406 (97%)	13 (3%)	1 (0%)	47	81
2	K	420/445 (94%)	404 (96%)	14 (3%)	2 (0%)	29	68
2	P	420/445 (94%)	406 (97%)	13 (3%)	1 (0%)	47	81
2	R	420/445 (94%)	406 (97%)	13 (3%)	1 (0%)	47	81
2	W	420/445 (94%)	406 (97%)	13 (3%)	1 (0%)	47	81
2	Y	420/445 (94%)	406 (97%)	13 (3%)	1 (0%)	47	81
3	E	485/554 (88%)	450 (93%)	32 (7%)	3 (1%)	25	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	L	488/554 (88%)	450 (92%)	37 (8%)	1 (0%)	47 81
3	S	487/554 (88%)	452 (93%)	31 (6%)	4 (1%)	19 60
3	Z	489/554 (88%)	451 (92%)	35 (7%)	3 (1%)	25 65
4	F	153/169 (90%)	143 (94%)	9 (6%)	1 (1%)	22 62
4	G	153/169 (90%)	145 (95%)	7 (5%)	1 (1%)	22 62
4	M	153/169 (90%)	144 (94%)	8 (5%)	1 (1%)	22 62
4	N	153/169 (90%)	144 (94%)	8 (5%)	1 (1%)	22 62
4	T	153/169 (90%)	144 (94%)	8 (5%)	1 (1%)	22 62
4	U	153/169 (90%)	145 (95%)	7 (5%)	1 (1%)	22 62
4	a	153/169 (90%)	138 (90%)	15 (10%)	0	100 100
4	b	153/169 (90%)	144 (94%)	8 (5%)	1 (1%)	22 62
All	All	9869/10736 (92%)	9311 (94%)	529 (5%)	29 (0%)	41 76

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Q	349	THR
3	S	433	PHE
4	F	44	ASP
4	G	44	ASP
3	L	432	GLY

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	346/377 (92%)	344 (99%)	2 (1%)	86 92
1	C	346/377 (92%)	345 (100%)	1 (0%)	92 95
1	H	346/377 (92%)	343 (99%)	3 (1%)	78 88
1	J	346/377 (92%)	345 (100%)	1 (0%)	92 95
1	O	346/377 (92%)	343 (99%)	3 (1%)	78 88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	Q	346/377 (92%)	344 (99%)	2 (1%)	86 92
1	V	346/377 (92%)	342 (99%)	4 (1%)	71 84
1	X	346/377 (92%)	344 (99%)	2 (1%)	86 92
2	B	361/381 (95%)	356 (99%)	5 (1%)	67 81
2	D	361/381 (95%)	357 (99%)	4 (1%)	73 85
2	I	361/381 (95%)	355 (98%)	6 (2%)	60 78
2	K	361/381 (95%)	356 (99%)	5 (1%)	67 81
2	P	361/381 (95%)	357 (99%)	4 (1%)	73 85
2	R	361/381 (95%)	356 (99%)	5 (1%)	67 81
2	W	361/381 (95%)	357 (99%)	4 (1%)	73 85
2	Y	361/381 (95%)	357 (99%)	4 (1%)	73 85
3	E	451/504 (90%)	444 (98%)	7 (2%)	62 79
3	L	454/504 (90%)	446 (98%)	8 (2%)	59 77
3	S	453/504 (90%)	449 (99%)	4 (1%)	78 88
3	Z	455/504 (90%)	449 (99%)	6 (1%)	69 82
4	F	116/132 (88%)	116 (100%)	0	100 100
4	G	116/132 (88%)	116 (100%)	0	100 100
4	M	116/132 (88%)	116 (100%)	0	100 100
4	N	116/132 (88%)	116 (100%)	0	100 100
4	T	116/132 (88%)	116 (100%)	0	100 100
4	U	116/132 (88%)	116 (100%)	0	100 100
4	a	115/132 (87%)	114 (99%)	1 (1%)	78 88
4	b	116/132 (88%)	116 (100%)	0	100 100
All	All	8396/9136 (92%)	8315 (99%)	81 (1%)	76 86

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	S	151	ARG
2	Y	153	LEU
3	S	533	LYS
2	W	153	LEU
3	Z	151	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	Y	14	ASN
2	Y	136	GLN
4	a	59	HIS
3	Z	249	GLN
3	E	171	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
7	GDP	P	600	6	24,30,30	0.93	1 (4%)	30,47,47	1.14	3 (10%)
7	GDP	I	600	6	24,30,30	0.93	1 (4%)	30,47,47	1.12	3 (10%)
5	GTP	A	600	6	26,34,34	1.12	2 (7%)	32,54,54	1.57	7 (21%)
5	GTP	C	600	6	26,34,34	1.13	2 (7%)	32,54,54	1.57	7 (21%)
5	GTP	V	600	6	26,34,34	1.13	2 (7%)	32,54,54	1.57	7 (21%)
5	GTP	X	600	6	26,34,34	1.13	2 (7%)	32,54,54	1.58	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	GTP	J	600	6	26,34,34	1.11	2 (7%)	32,54,54	1.58	7 (21%)
7	GDP	Y	600	6	24,30,30	0.95	1 (4%)	30,47,47	1.06	3 (10%)
5	GTP	O	600	6	26,34,34	1.13	2 (7%)	32,54,54	1.60	7 (21%)
7	GDP	R	600	6	24,30,30	0.92	1 (4%)	30,47,47	1.07	3 (10%)
7	GDP	K	600	6	24,30,30	0.96	1 (4%)	30,47,47	1.12	3 (10%)
7	GDP	D	600	6	24,30,30	0.94	1 (4%)	30,47,47	1.07	3 (10%)
7	GDP	W	600	-	24,30,30	0.96	1 (4%)	30,47,47	1.09	3 (10%)
5	GTP	H	600	6	26,34,34	1.11	1 (3%)	32,54,54	1.56	7 (21%)
5	GTP	Q	600	6	26,34,34	1.13	2 (7%)	32,54,54	1.56	7 (21%)
7	GDP	B	600	6	24,30,30	0.93	1 (4%)	30,47,47	1.10	3 (10%)

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
7	GDP	P	600	6	-	3/12/32/32	0/3/3/3
7	GDP	I	600	6	-	4/12/32/32	0/3/3/3
5	GTP	A	600	6	-	2/18/38/38	0/3/3/3
5	GTP	C	600	6	-	2/18/38/38	0/3/3/3
5	GTP	V	600	6	-	2/18/38/38	0/3/3/3
5	GTP	X	600	6	-	3/18/38/38	0/3/3/3
5	GTP	J	600	6	-	3/18/38/38	0/3/3/3
7	GDP	Y	600	6	-	3/12/32/32	0/3/3/3
5	GTP	O	600	6	-	2/18/38/38	0/3/3/3
7	GDP	R	600	6	-	4/12/32/32	0/3/3/3
7	GDP	K	600	6	-	3/12/32/32	0/3/3/3
7	GDP	D	600	6	-	4/12/32/32	0/3/3/3
7	GDP	W	600	-	-	4/12/32/32	0/3/3/3
5	GTP	H	600	6	-	3/18/38/38	0/3/3/3
5	GTP	Q	600	6	-	2/18/38/38	0/3/3/3
7	GDP	B	600	6	-	3/12/32/32	0/3/3/3

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	V	600	GTP	C5-C6	-4.01	1.39	1.47
5	Q	600	GTP	C5-C6	-4.00	1.39	1.47
5	O	600	GTP	C5-C6	-3.99	1.39	1.47
5	C	600	GTP	C5-C6	-3.97	1.39	1.47
5	X	600	GTP	C5-C6	-3.96	1.39	1.47

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	600	GTP	PA-O3A-PB	-4.09	118.78	132.83
5	H	600	GTP	PA-O3A-PB	-4.08	118.84	132.83
5	O	600	GTP	PA-O3A-PB	-4.03	118.99	132.83
5	V	600	GTP	PA-O3A-PB	-3.96	119.25	132.83
5	X	600	GTP	PA-O3A-PB	-3.85	119.62	132.83

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

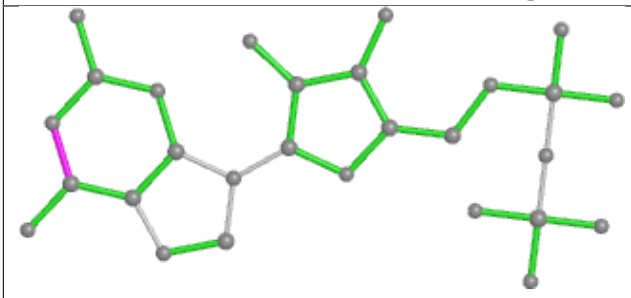
Mol	Chain	Res	Type	Atoms
5	A	600	GTP	PB-O3B-PG-O2G
5	C	600	GTP	PB-O3B-PG-O2G
5	J	600	GTP	PB-O3B-PG-O2G
5	O	600	GTP	PB-O3B-PG-O2G
5	Q	600	GTP	PB-O3B-PG-O2G

There are no ring outliers.

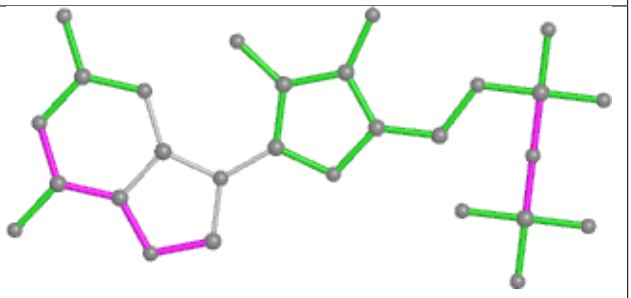
No monomer is involved in short contacts.

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 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.

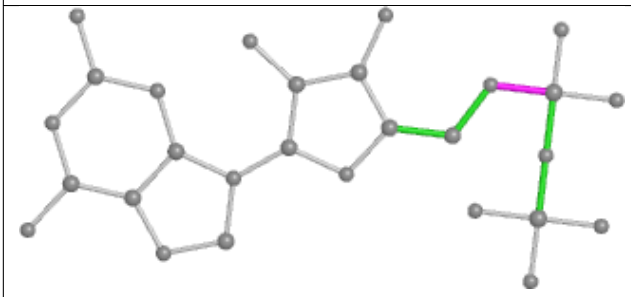
Ligand GDP P 600



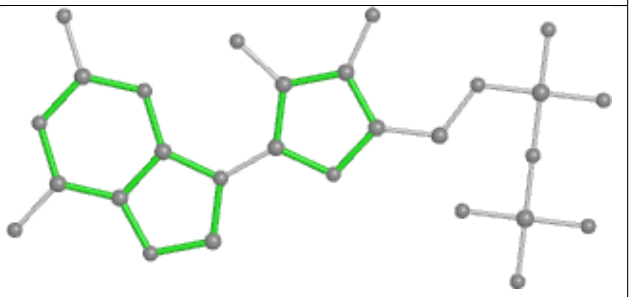
Bond lengths



Bond angles

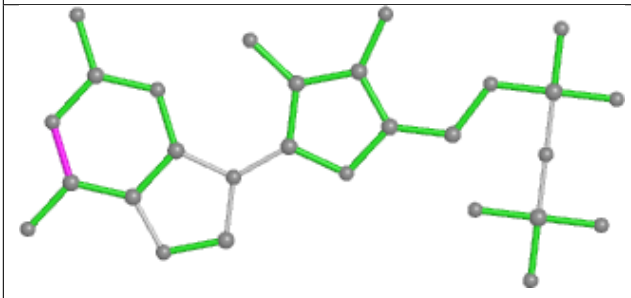


Torsions



Rings

Ligand GDP I 600



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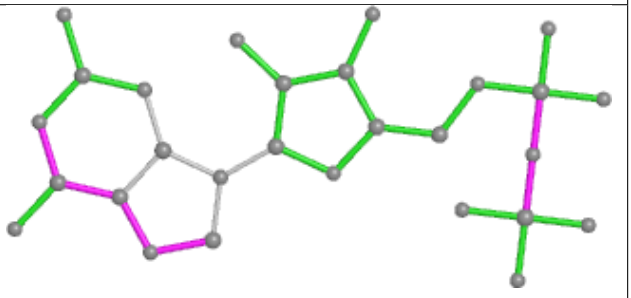

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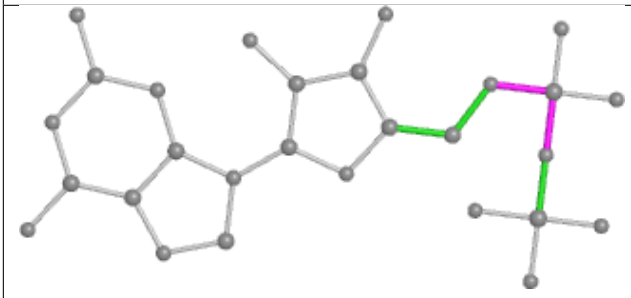

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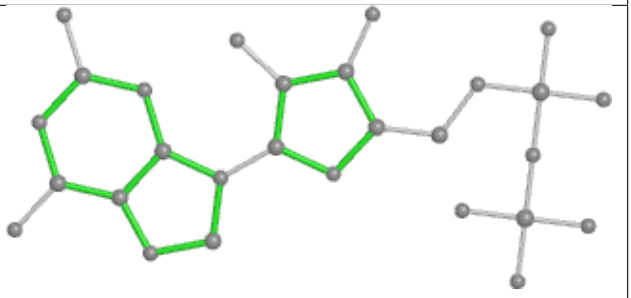

Rings

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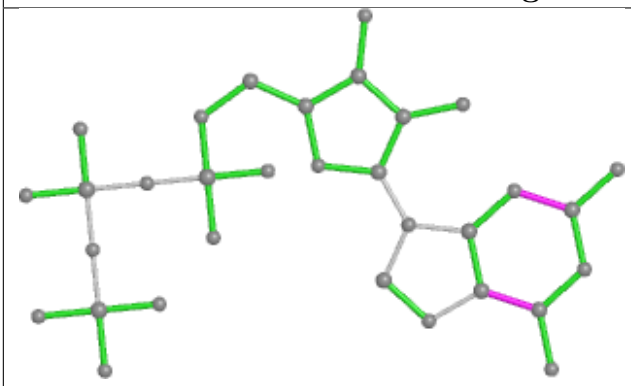

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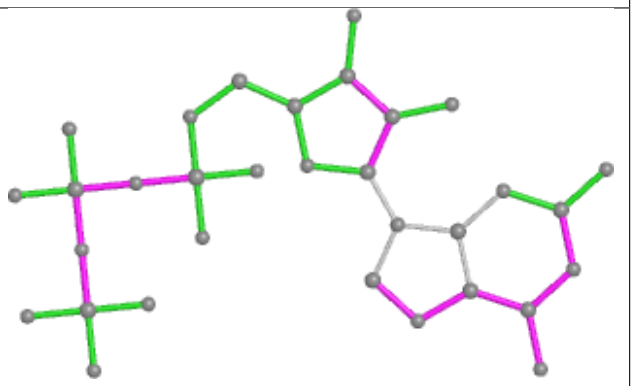
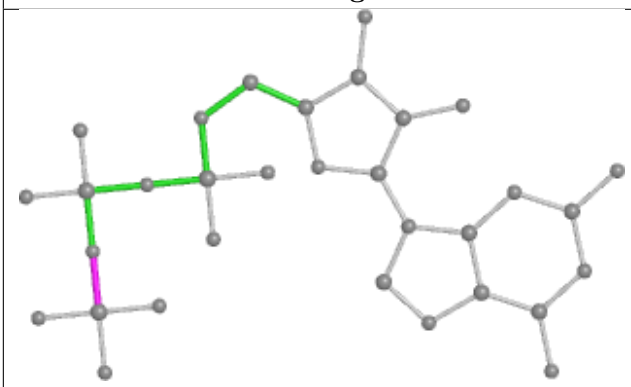


Bond angles



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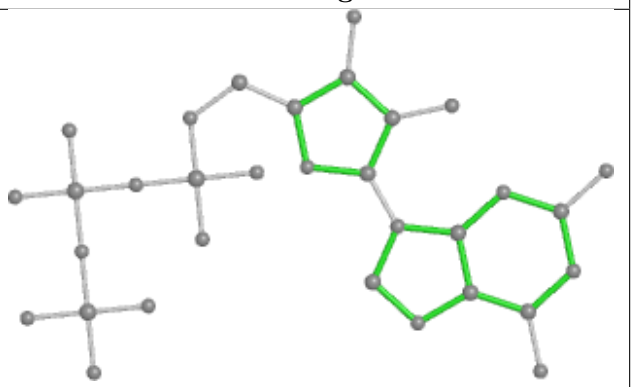
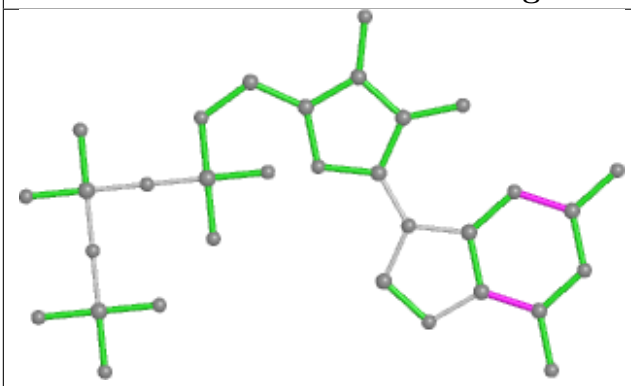
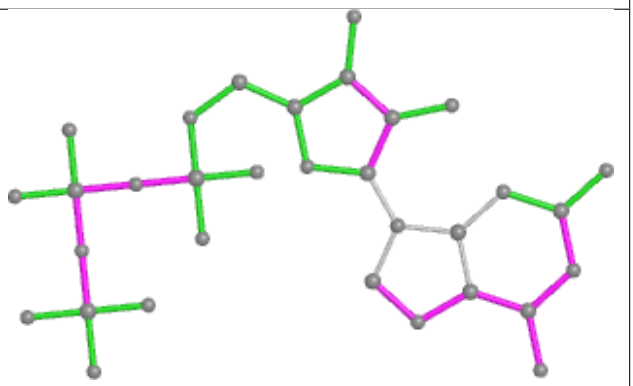


Rings

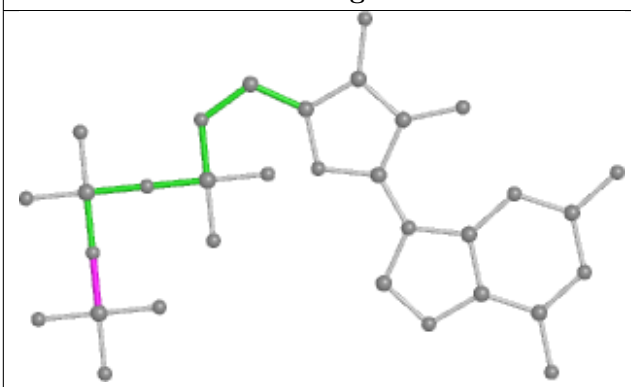
Ligand GTP C 600



Bond lengths



Bond angles



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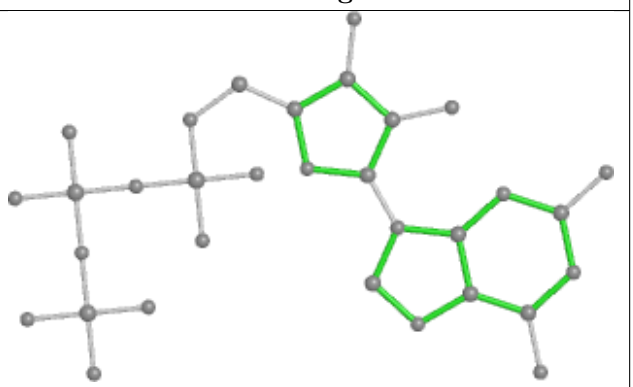

Rings

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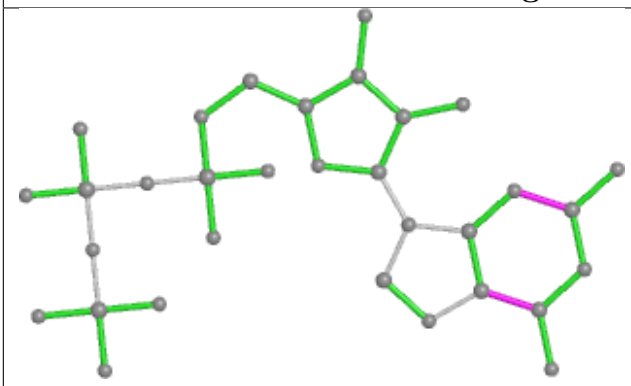

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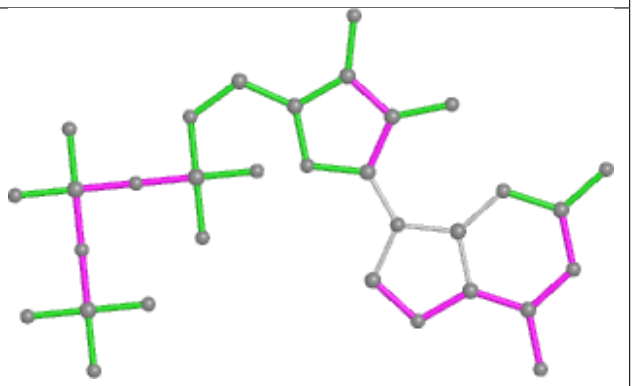

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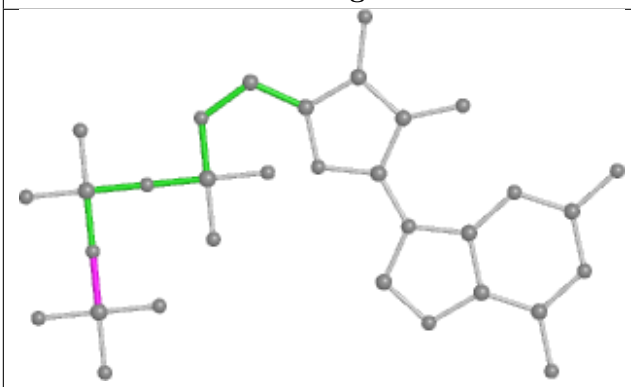

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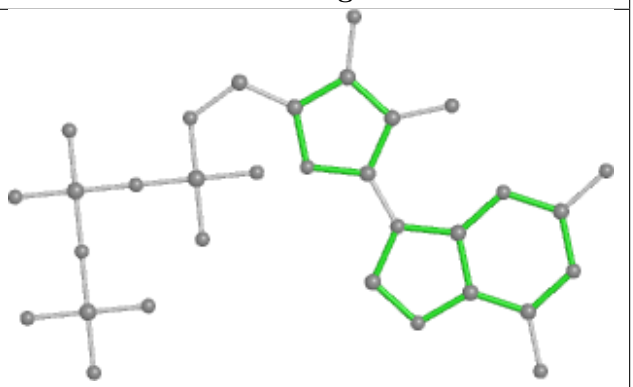

Rings

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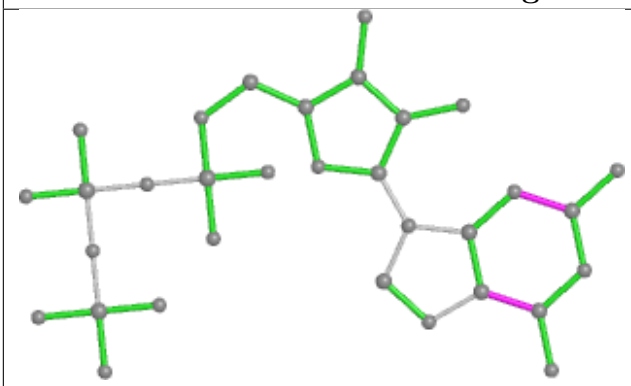

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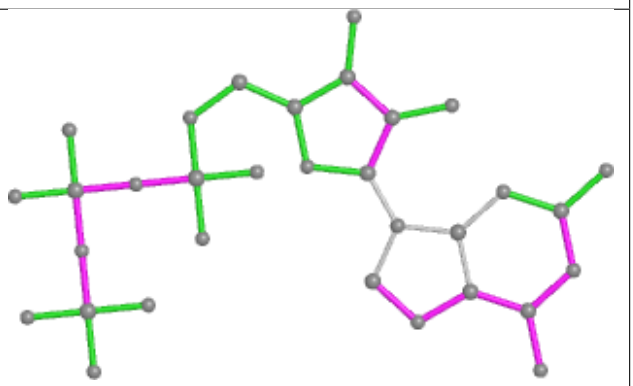
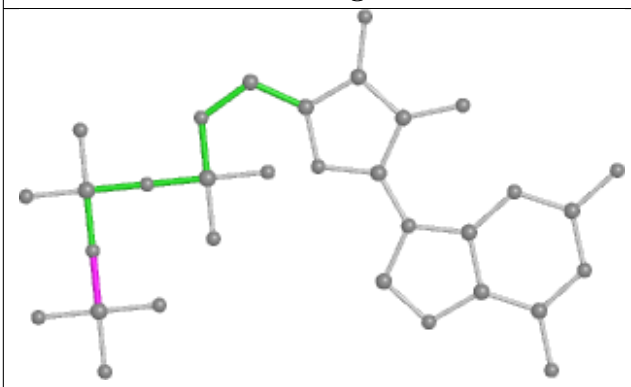


Bond angles



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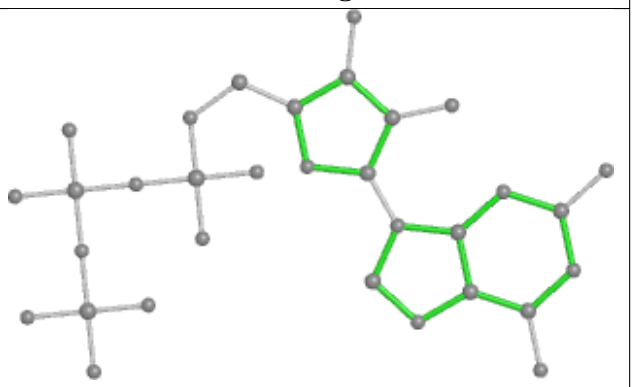

Rings

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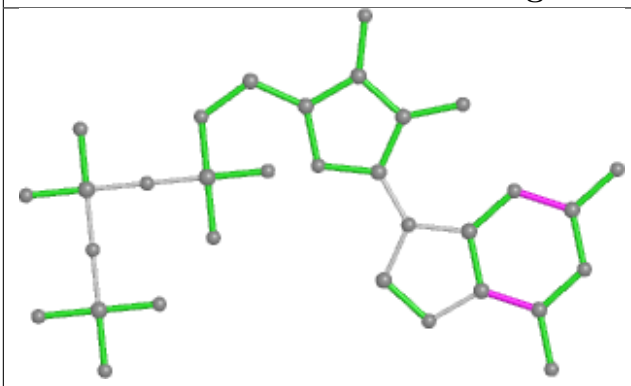

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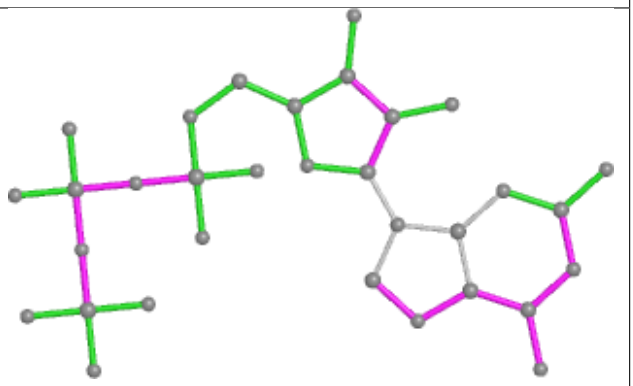
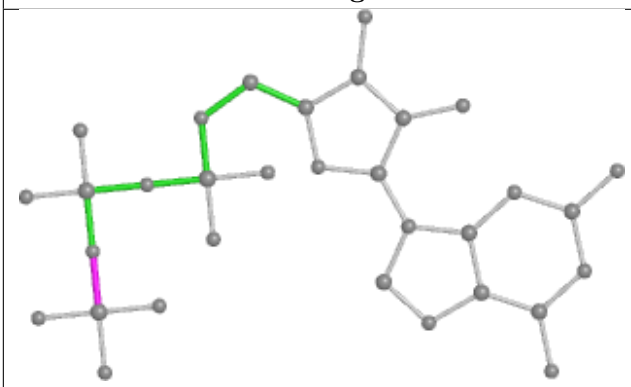


Bond angles



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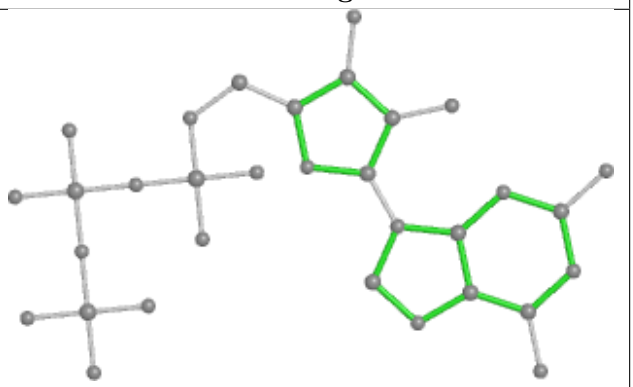
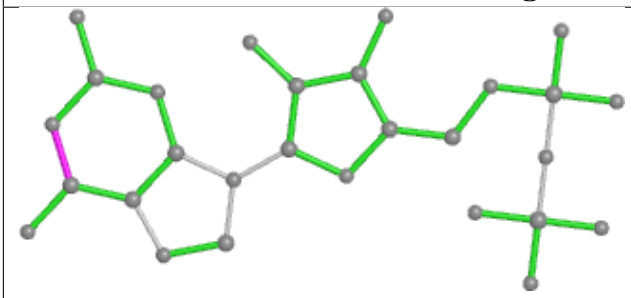
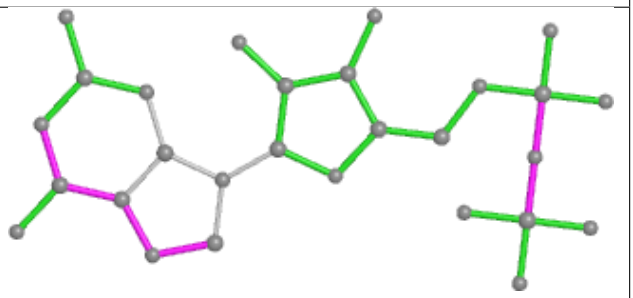


Rings

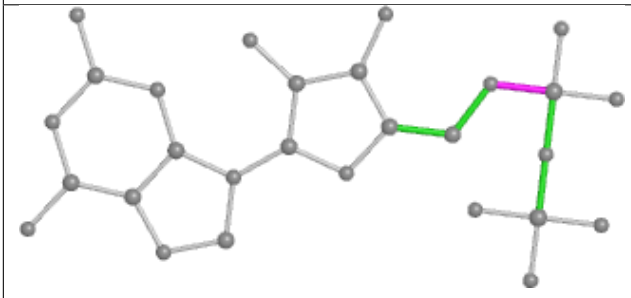
Ligand GDP Y 600



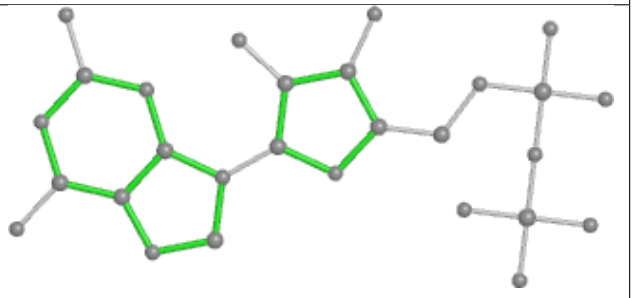
Bond lengths



Bond angles

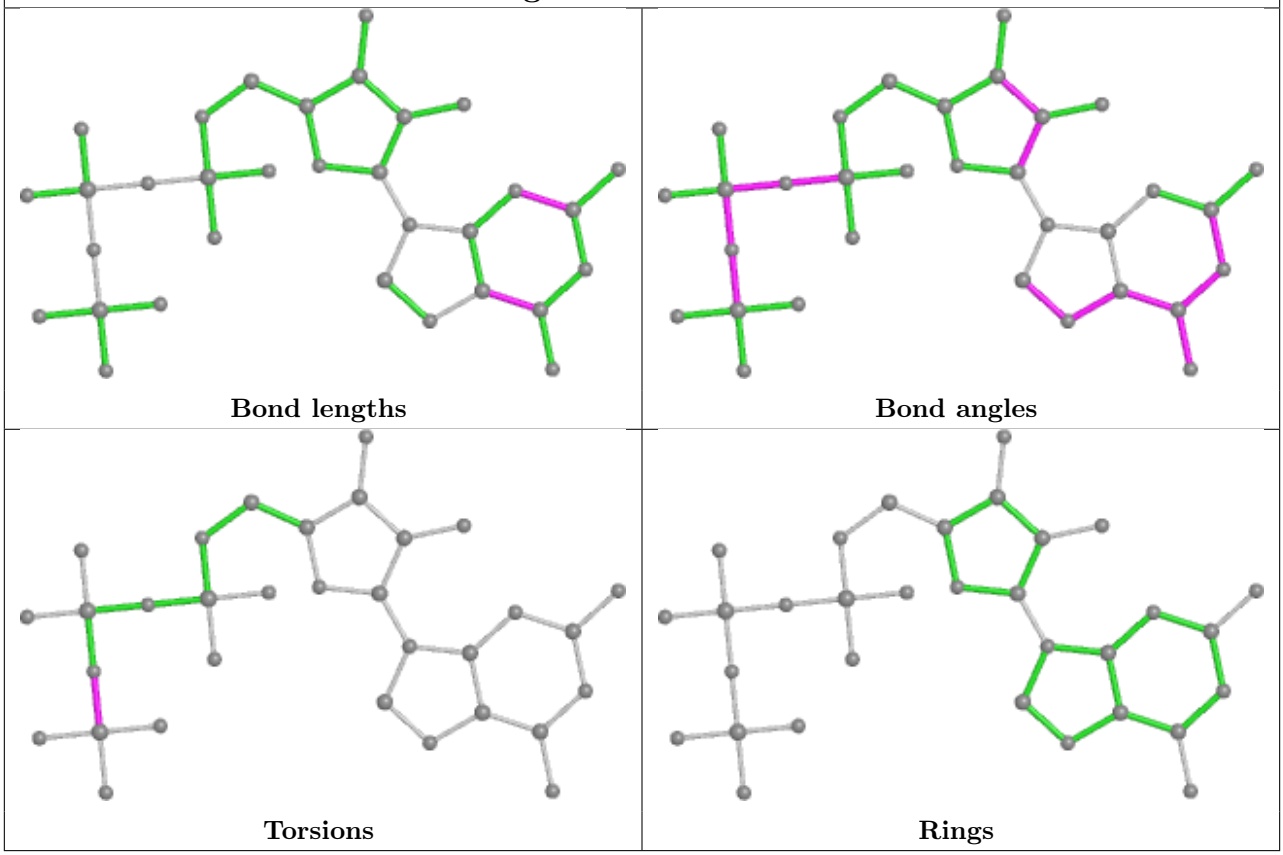


Torsions

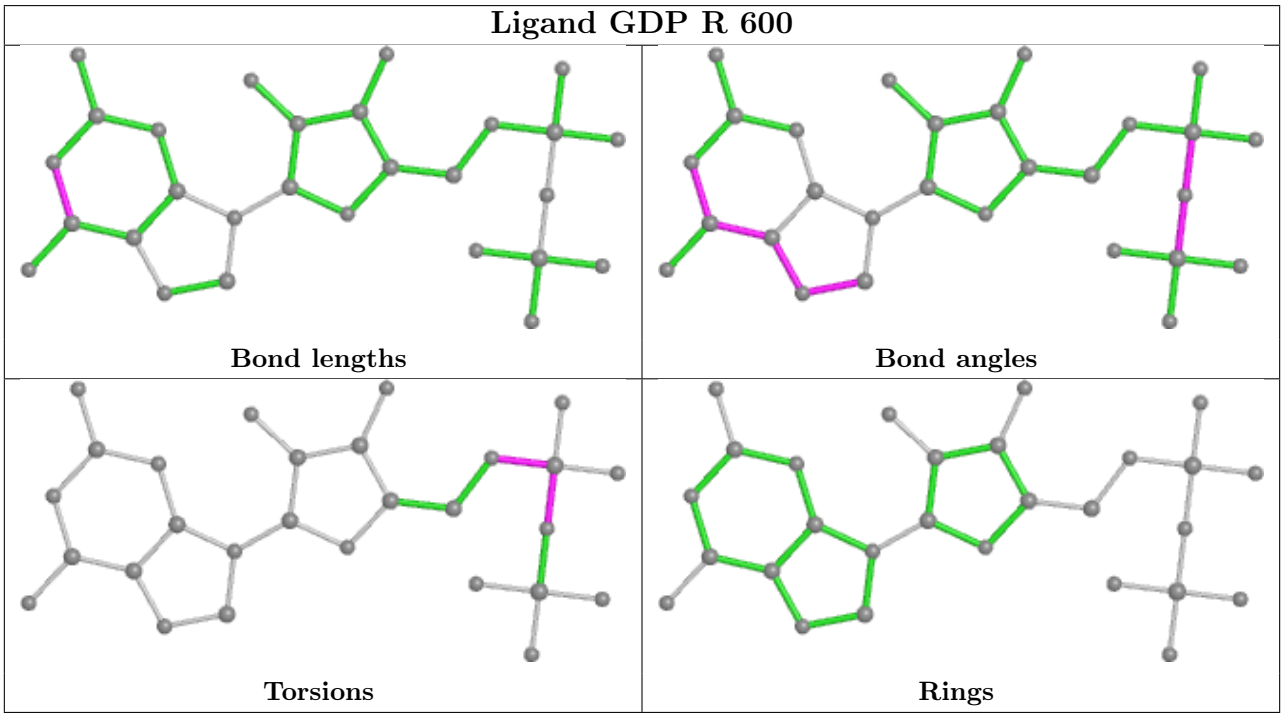


Rings

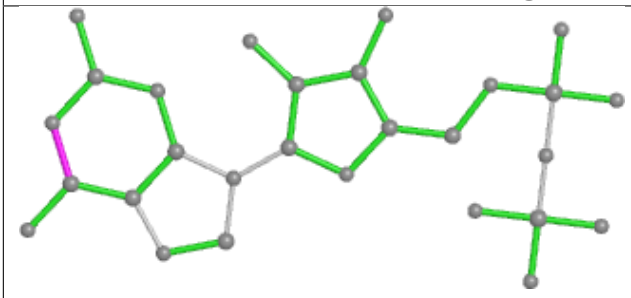
Ligand GTP O 600



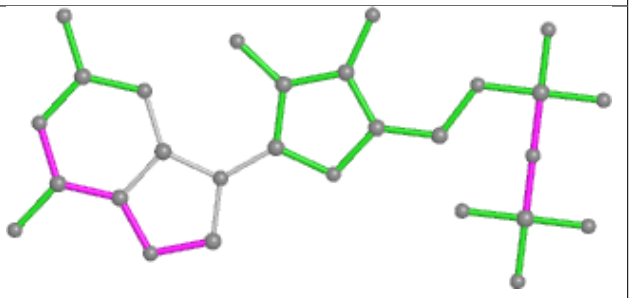
Ligand GDP R 600



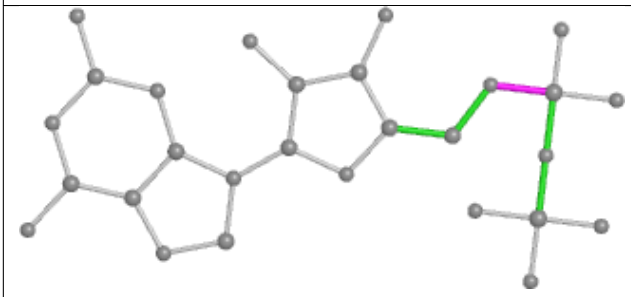
Ligand GDP K 600



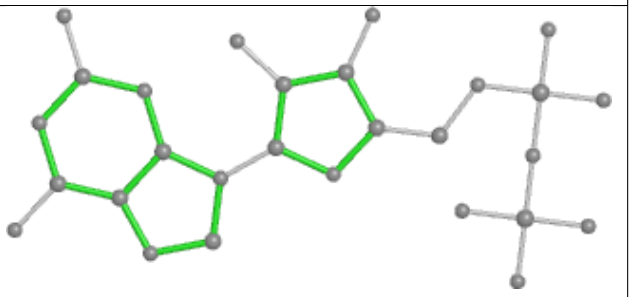
Bond lengths



Bond angles

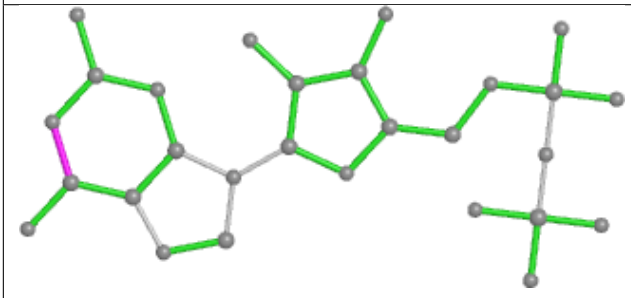


Torsions

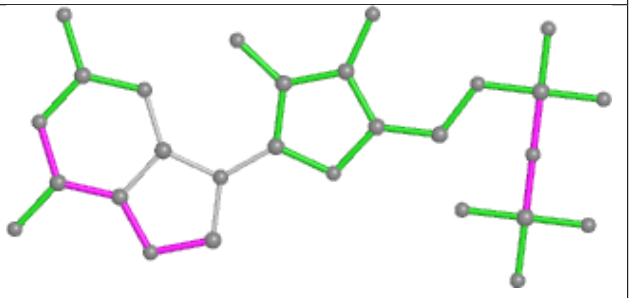


Rings

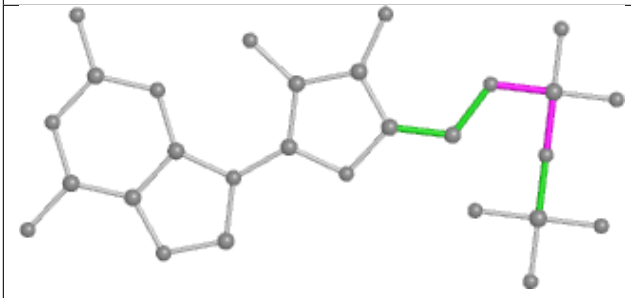
Ligand GDP D 600



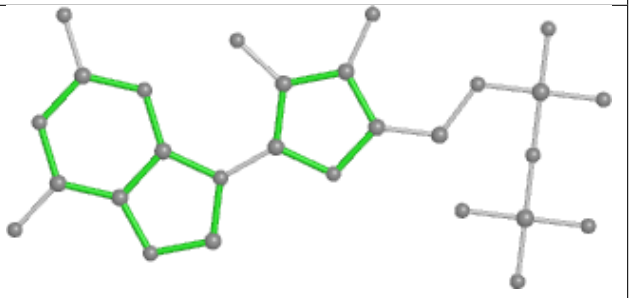
Bond lengths



Bond angles

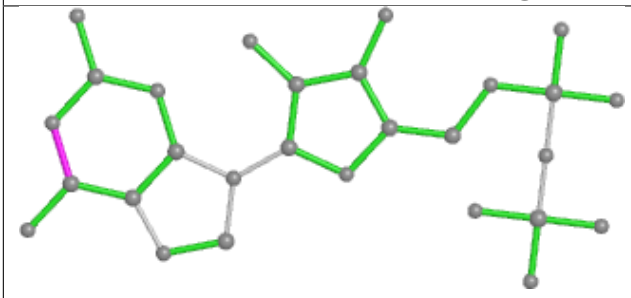


Torsions

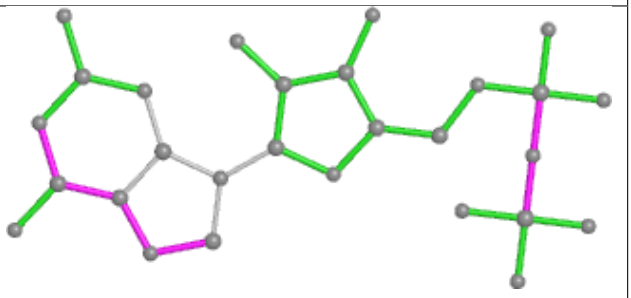


Rings

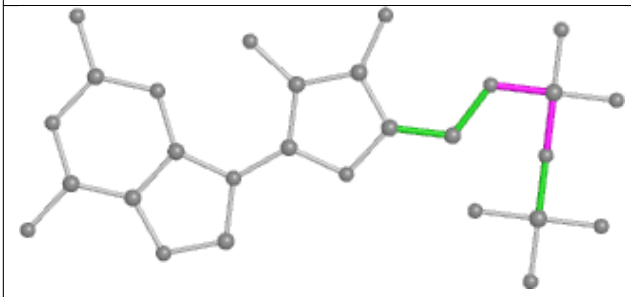
Ligand GDP W 600



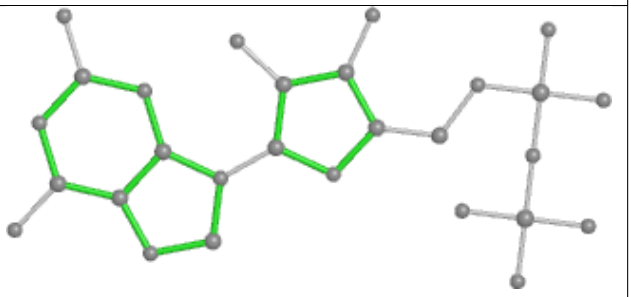
Bond lengths



Bond angles

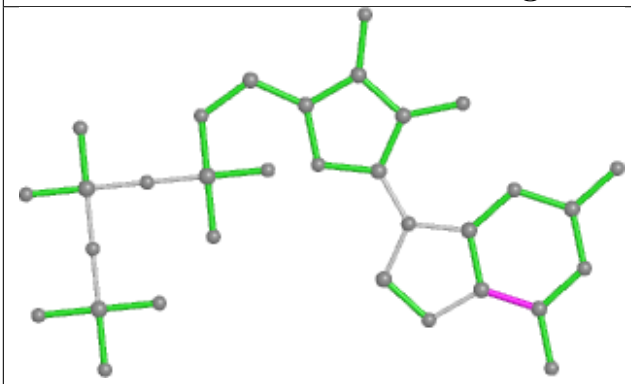


Torsions

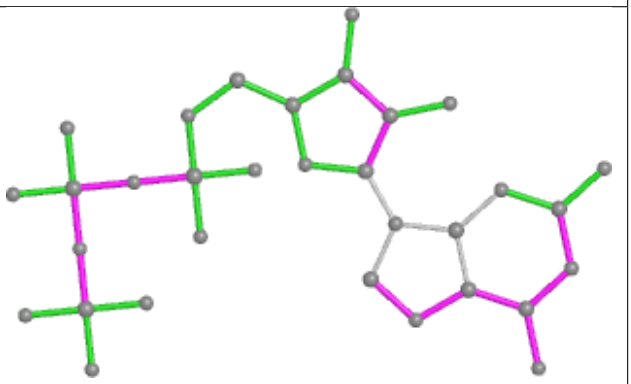


Rings

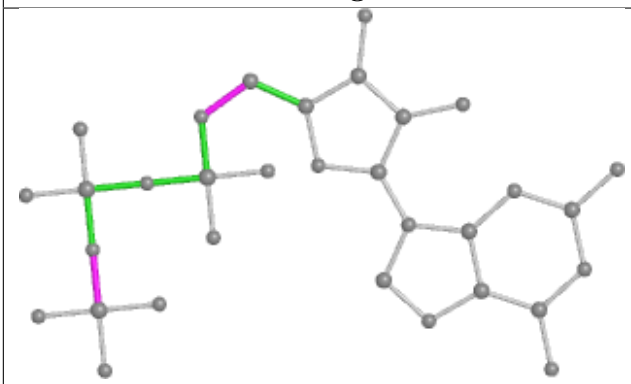
Ligand GTP H 600



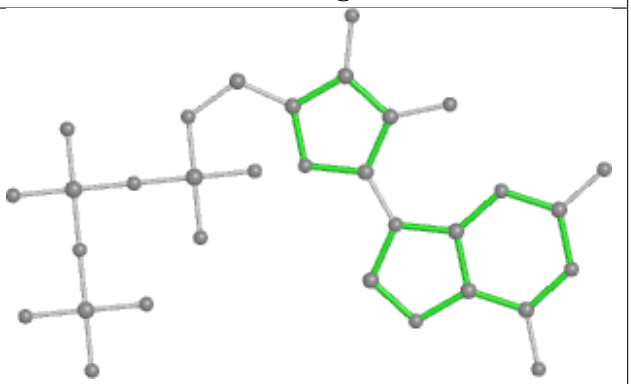
Bond lengths



Bond angles

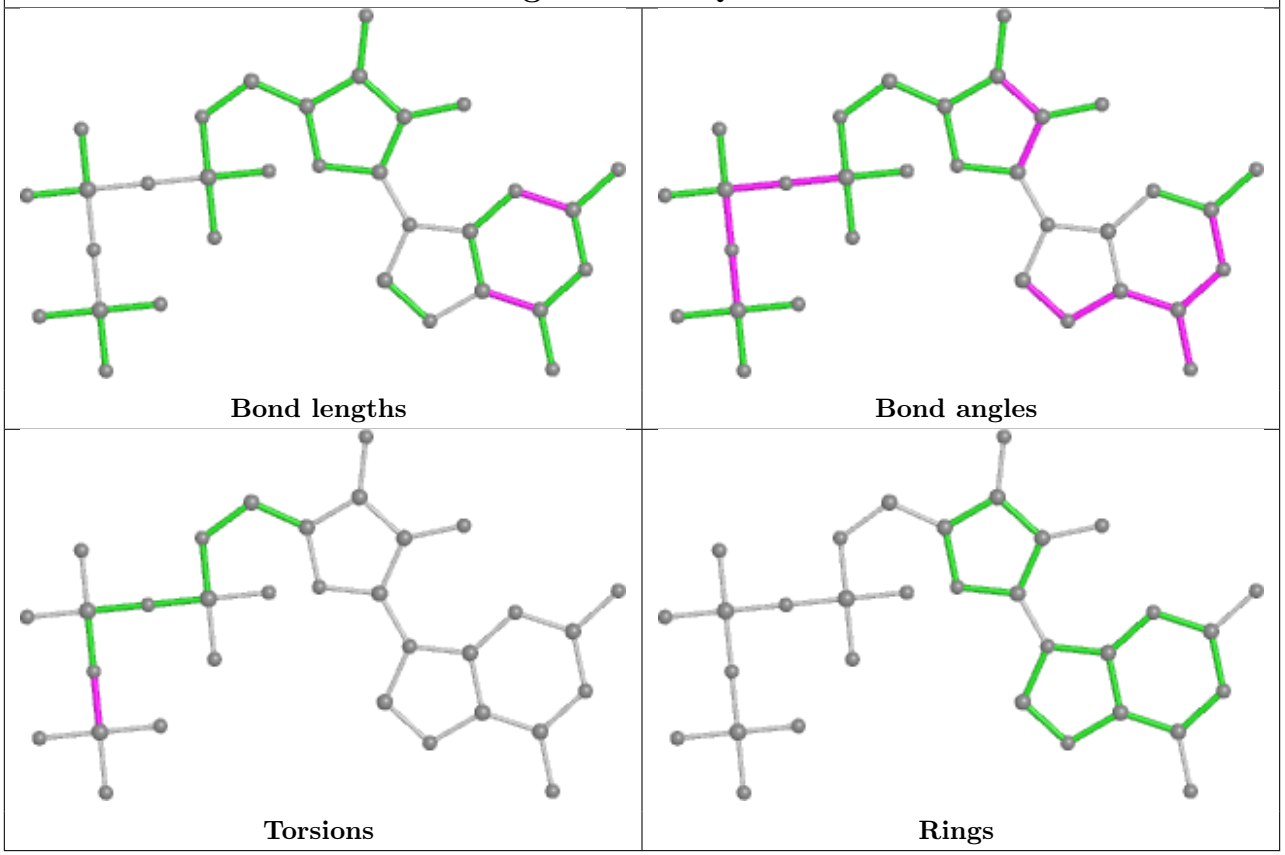


Torsions

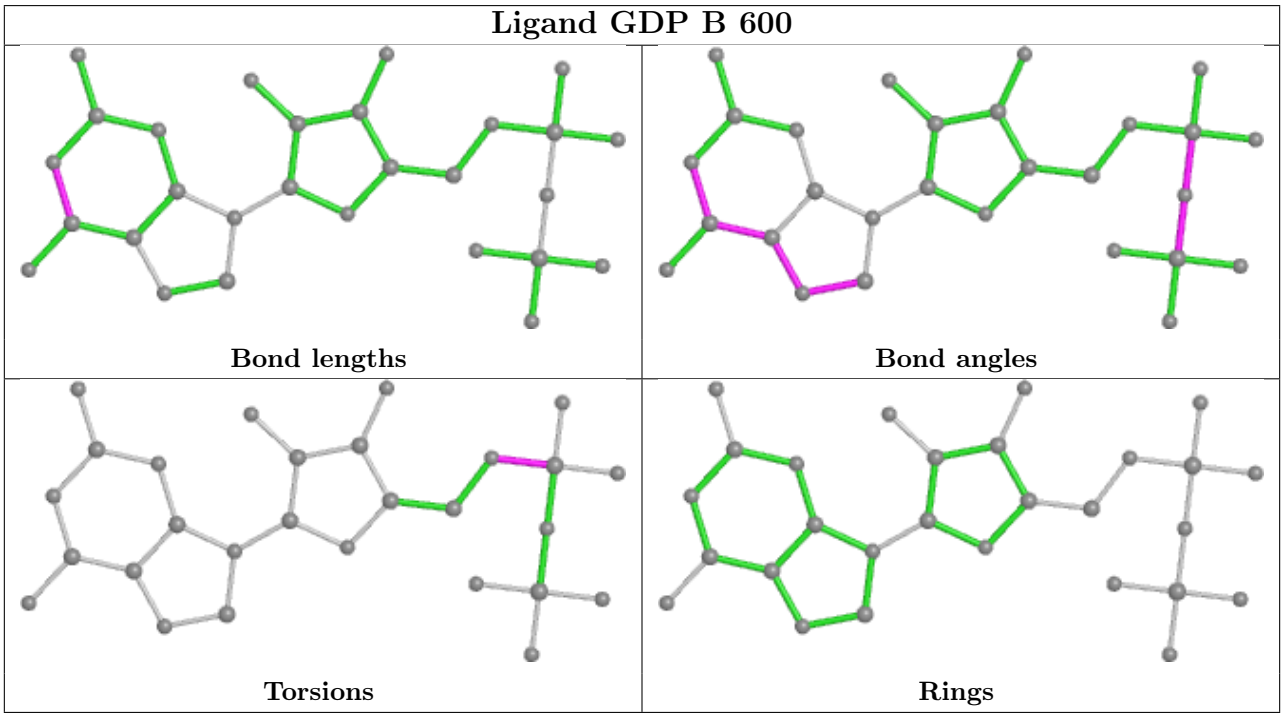


Rings

Ligand GTP Q 600



Ligand GDP B 600



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	423/451 (93%)	0.20	15 (3%) 44 35	49, 113, 165, 235	0
1	C	423/451 (93%)	-0.00	5 (1%) 79 70	54, 97, 139, 163	0
1	H	423/451 (93%)	-0.01	5 (1%) 79 70	39, 97, 143, 207	0
1	J	423/451 (93%)	0.23	13 (3%) 49 39	77, 139, 203, 248	0
1	O	423/451 (93%)	0.42	29 (6%) 16 13	71, 139, 198, 263	0
1	Q	423/451 (93%)	-0.08	2 (0%) 91 85	41, 87, 135, 176	0
1	V	423/451 (93%)	0.10	13 (3%) 49 39	50, 108, 156, 196	0
1	X	423/451 (93%)	0.24	20 (4%) 31 26	62, 124, 183, 294	0
2	B	424/445 (95%)	-0.21	1 (0%) 95 93	32, 58, 92, 130	0
2	D	424/445 (95%)	-0.03	6 (1%) 75 66	43, 82, 130, 182	0
2	I	424/445 (95%)	0.11	6 (1%) 75 66	66, 107, 148, 188	0
2	K	424/445 (95%)	0.28	25 (5%) 22 19	85, 131, 174, 274	0
2	P	424/445 (95%)	-0.14	0 100 100	54, 91, 130, 177	0
2	R	424/445 (95%)	-0.12	2 (0%) 91 85	27, 69, 118, 210	0
2	W	424/445 (95%)	0.15	6 (1%) 75 66	62, 109, 152, 173	0
2	Y	424/445 (95%)	-0.04	4 (0%) 84 77	57, 105, 152, 188	0
3	E	491/554 (88%)	-0.18	0 100 100	45, 81, 123, 158	0
3	L	494/554 (89%)	-0.13	2 (0%) 92 87	63, 93, 133, 187	0
3	S	493/554 (88%)	-0.08	3 (0%) 89 84	40, 92, 139, 165	0
3	Z	495/554 (89%)	-0.15	2 (0%) 92 87	58, 96, 144, 179	0
4	F	155/169 (91%)	-0.17	1 (0%) 89 84	52, 89, 133, 164	0
4	G	155/169 (91%)	-0.28	0 100 100	64, 98, 133, 170	0
4	M	155/169 (91%)	0.41	8 (5%) 27 24	136, 186, 227, 275	0
4	N	155/169 (91%)	0.60	10 (6%) 18 15	150, 222, 280, 383	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
4	T	155/169 (91%)	0.38	9 (5%) 23 19	105, 166, 204, 251	0
4	U	155/169 (91%)	-0.27	0 100 100	44, 78, 111, 127	0
4	a	155/169 (91%)	1.05	27 (17%) 1 2	129, 173, 228, 294	0
4	b	155/169 (91%)	0.65	12 (7%) 13 11	110, 159, 205, 248	0
All	All	9989/10736 (93%)	0.06	226 (2%) 60 51	27, 102, 184, 383	0

The worst 5 of 226 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	a	75	ALA	7.2
4	a	38	ALA	7.0
2	K	1	MET	5.5
4	M	76	ILE	5.4
4	M	75	ALA	5.3

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (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
6	MG	R	601	1/1	0.71	0.35	38,38,38,38	0
6	MG	I	601	1/1	0.77	0.21	70,70,70,70	0
6	MG	K	601	1/1	0.81	0.42	74,74,74,74	0
6	MG	Y	601	1/1	0.83	0.39	69,69,69,69	0
7	GDP	K	600	28/28	0.88	0.24	90,114,123,134	0
6	MG	P	601	1/1	0.91	0.28	48,48,48,48	0
5	GTP	X	600	32/32	0.91	0.23	67,87,98,102	0

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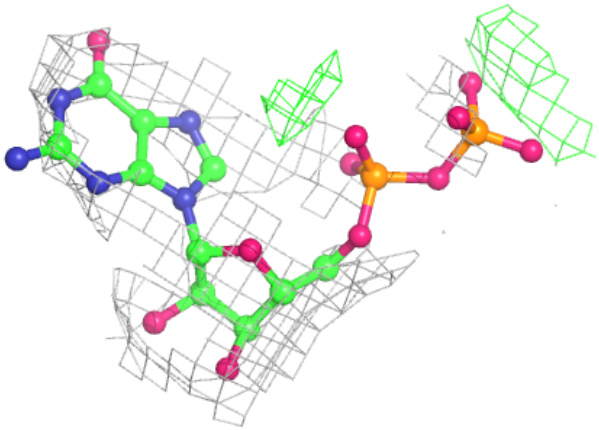
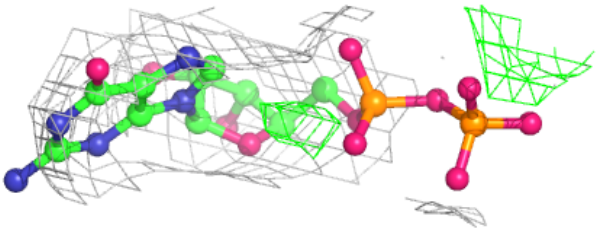
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GTP	J	600	32/32	0.92	0.22	84,109,117,126	0
6	MG	W	601	1/1	0.92	0.22	68,68,68,68	0
6	MG	D	601	1/1	0.94	0.18	25,25,25,25	0
7	GDP	I	600	28/28	0.94	0.27	69,81,89,94	0
5	GTP	C	600	32/32	0.94	0.27	53,75,91,102	0
7	GDP	R	600	28/28	0.94	0.22	41,63,74,74	0
7	GDP	W	600	28/28	0.94	0.27	70,100,108,108	0
7	GDP	Y	600	28/28	0.94	0.20	63,80,101,103	0
5	GTP	O	600	32/32	0.95	0.24	56,95,114,116	0
7	GDP	B	600	28/28	0.95	0.28	36,47,61,87	0
7	GDP	D	600	28/28	0.95	0.23	37,66,79,89	0
5	GTP	A	600	32/32	0.95	0.23	54,79,89,93	0
7	GDP	P	600	28/28	0.96	0.27	55,68,79,84	0
5	GTP	H	600	32/32	0.96	0.25	45,66,81,84	0
5	GTP	Q	600	32/32	0.96	0.20	50,70,82,86	0
5	GTP	V	600	32/32	0.96	0.22	46,70,80,81	0
6	MG	O	601	1/1	0.97	0.24	51,51,51,51	0
6	MG	V	601	1/1	0.97	0.24	36,36,36,36	0
6	MG	B	601	1/1	0.97	0.22	22,22,22,22	0
6	MG	H	601	1/1	0.98	0.23	37,37,37,37	0
6	MG	J	601	1/1	0.98	0.17	54,54,54,54	0
6	MG	X	601	1/1	0.98	0.33	62,62,62,62	0
6	MG	A	601	1/1	0.99	0.23	47,47,47,47	0
6	MG	C	601	1/1	0.99	0.19	46,46,46,46	0
6	MG	Q	601	1/1	1.00	0.27	63,63,63,63	0

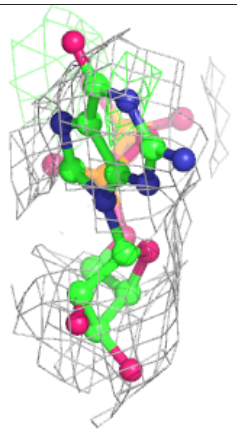
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP K 600:

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

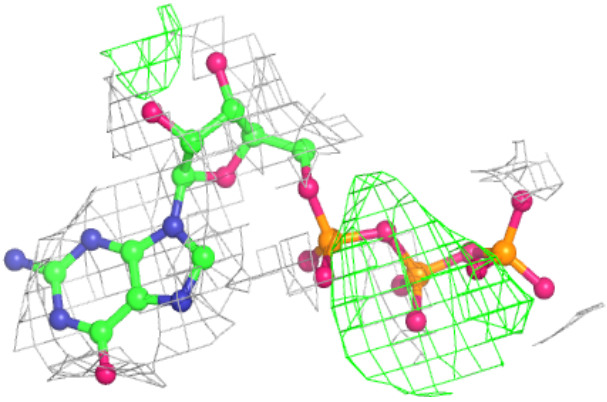


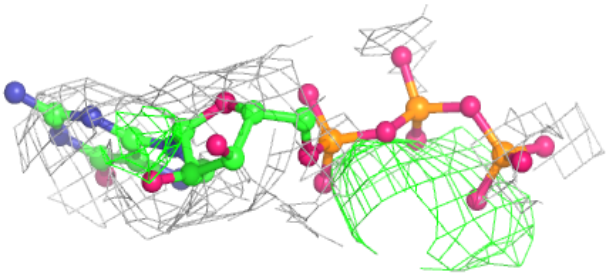


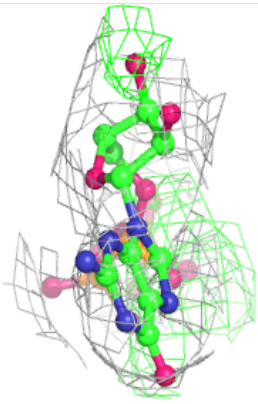


Electron density around GTP X 600:

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

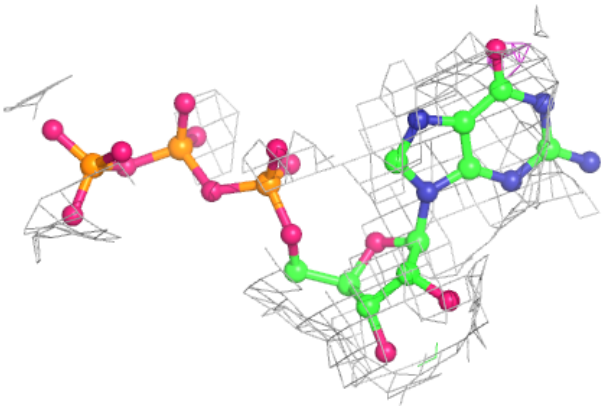


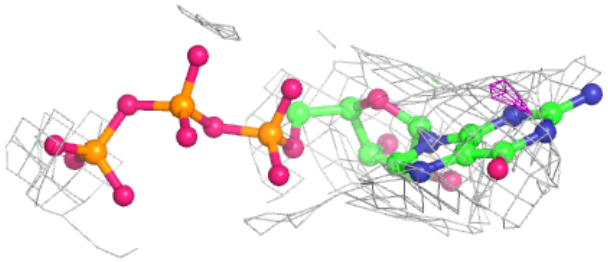


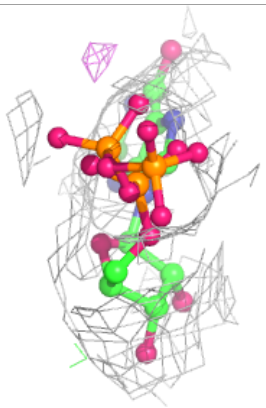


Electron density around GTP J 600:

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

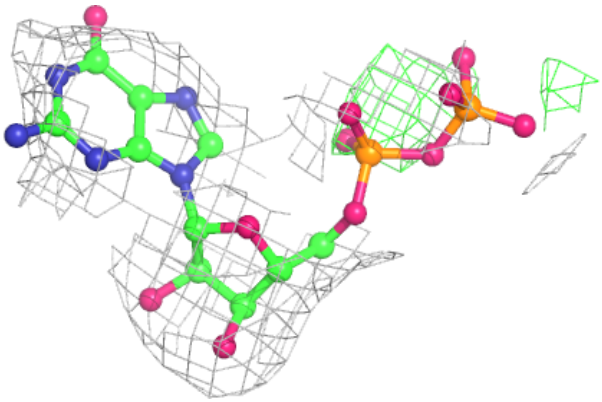


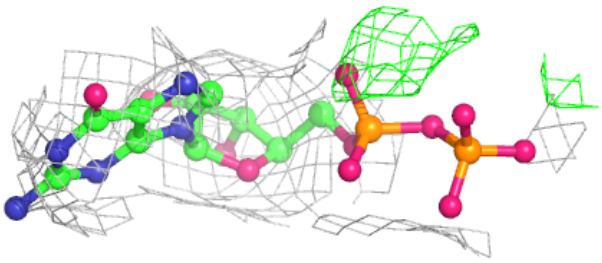


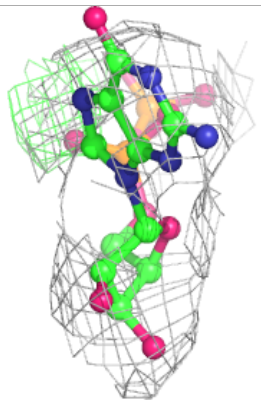


Electron density around GDP I 600:

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

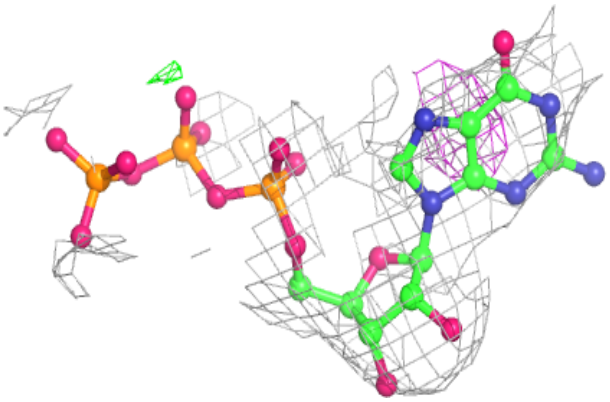


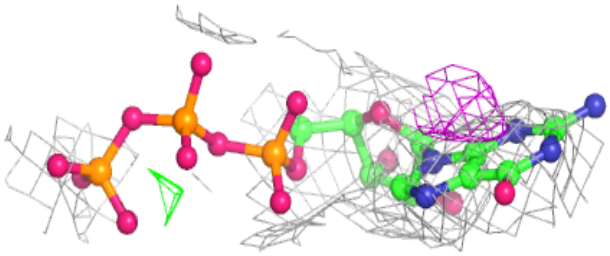


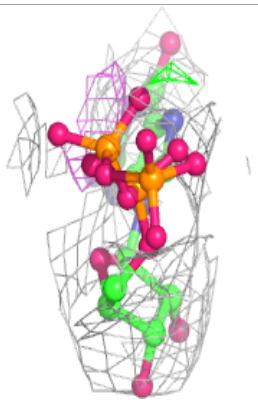


Electron density around GTP C 600:

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

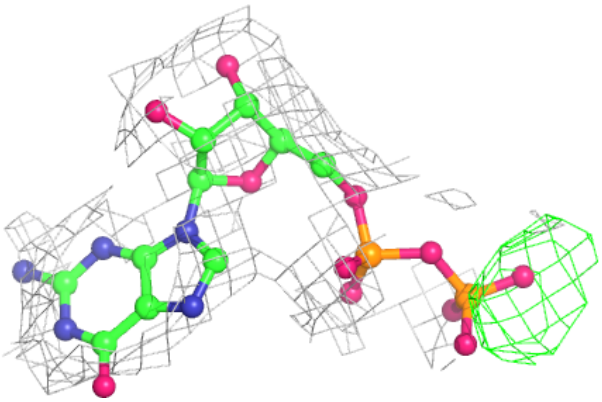


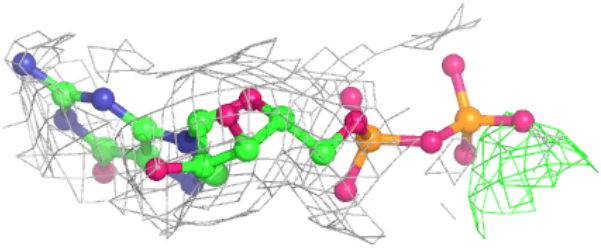


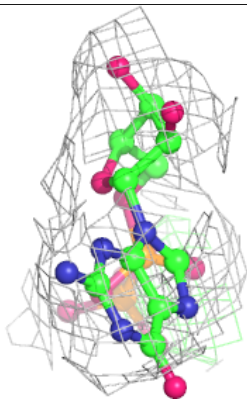


Electron density around GDP R 600:

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

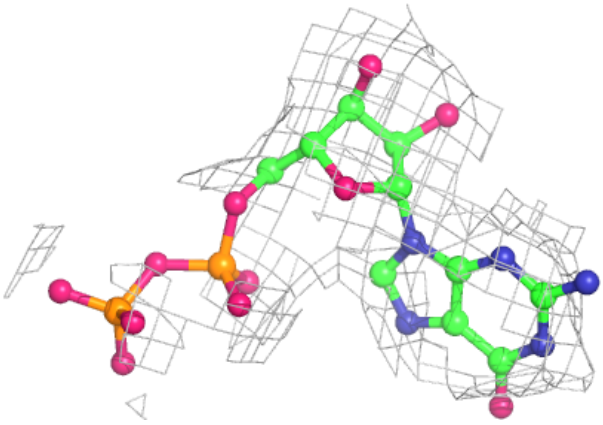


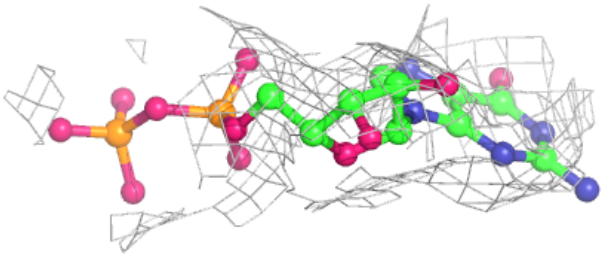


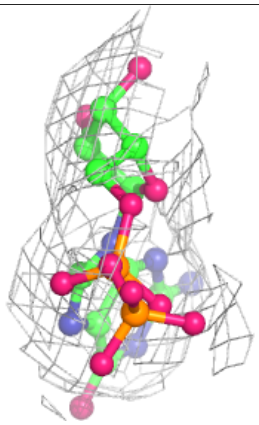


Electron density around GDP W 600:

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

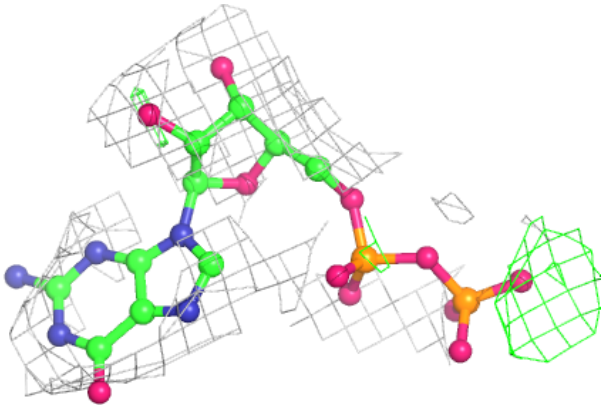


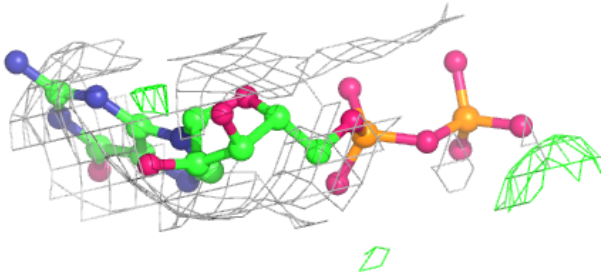


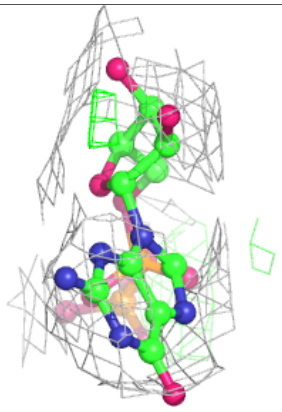


Electron density around GDP Y 600:

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

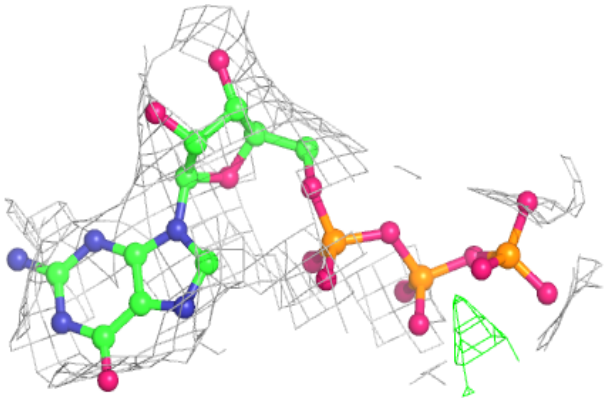


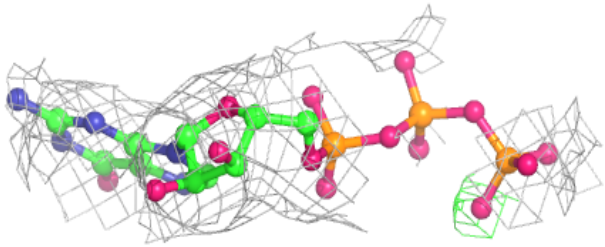


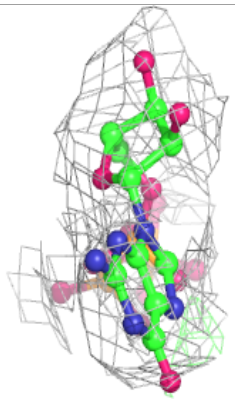


Electron density around GTP O 600:

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

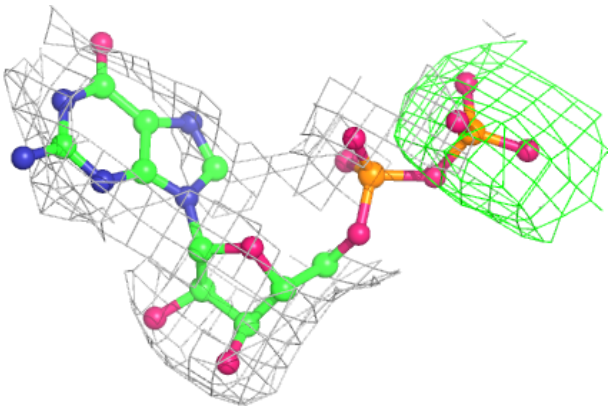


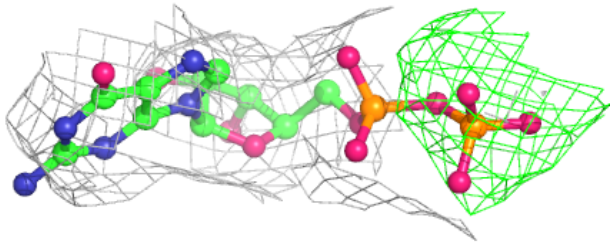


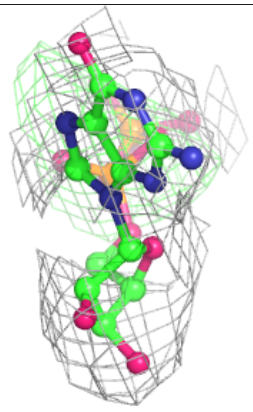


Electron density around GDP B 600:

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

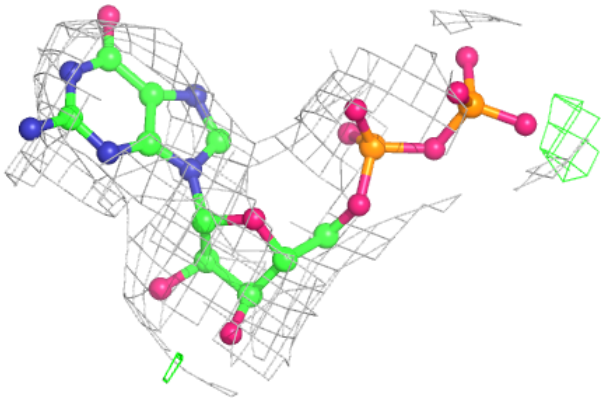


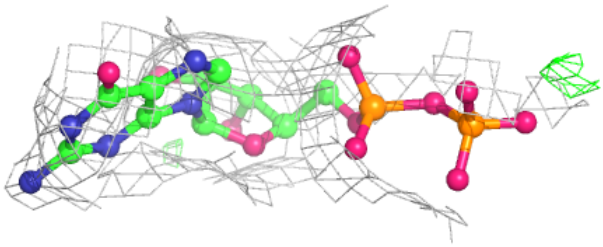


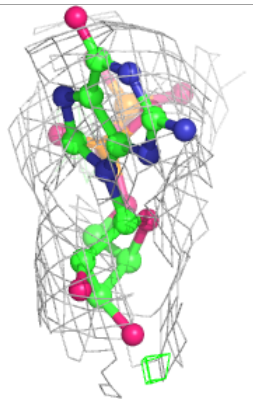


Electron density around GDP D 600:

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

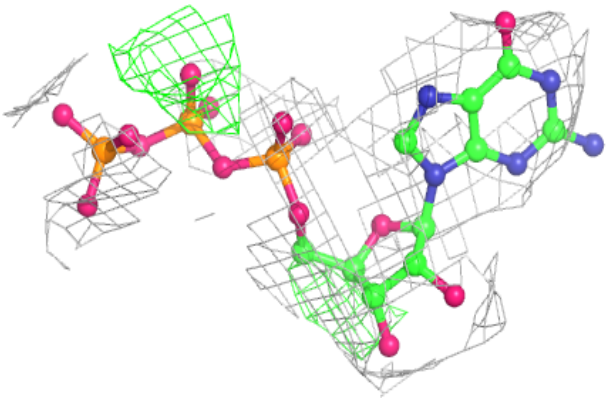


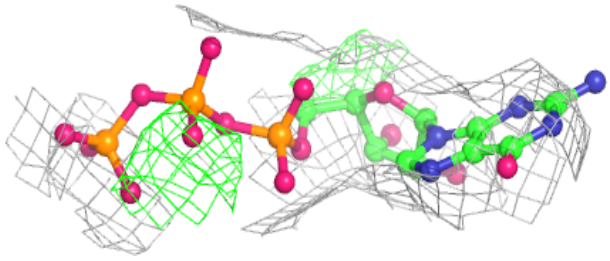


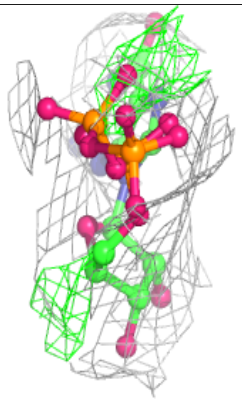


Electron density around GTP A 600:

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

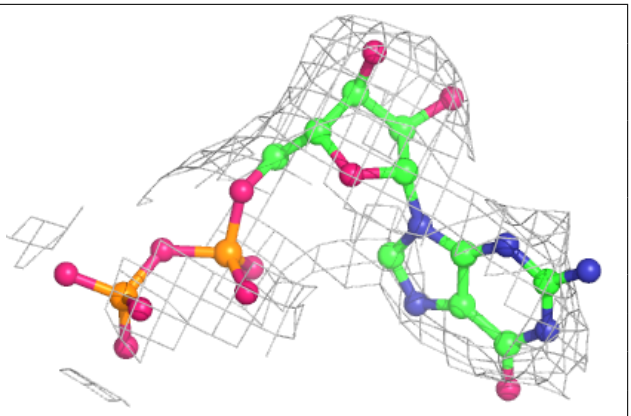


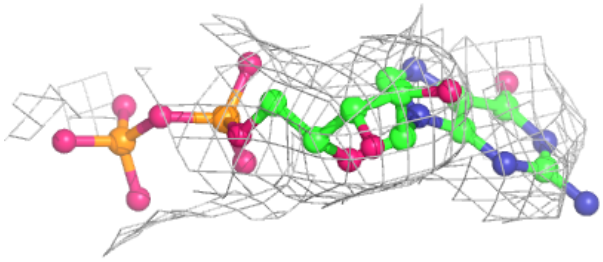


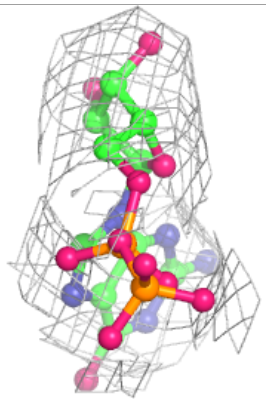


Electron density around GDP P 600:

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

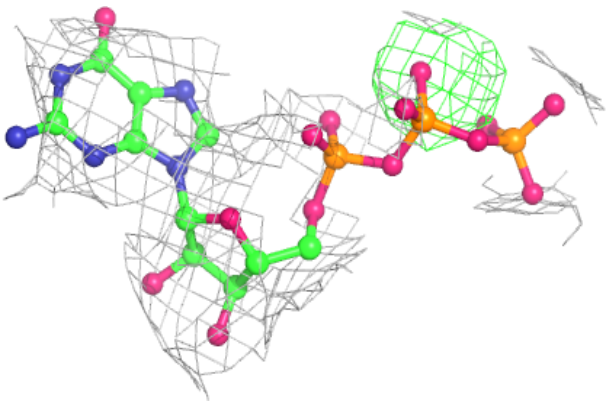


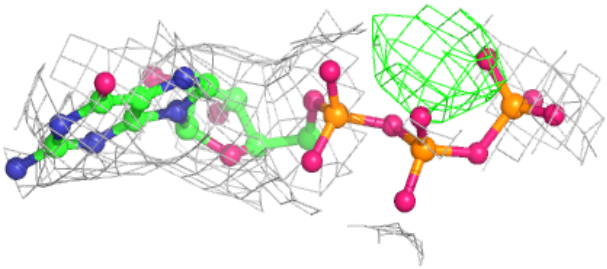


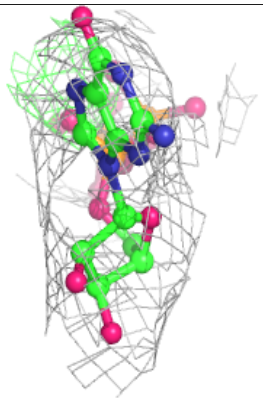


Electron density around GTP H 600:

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

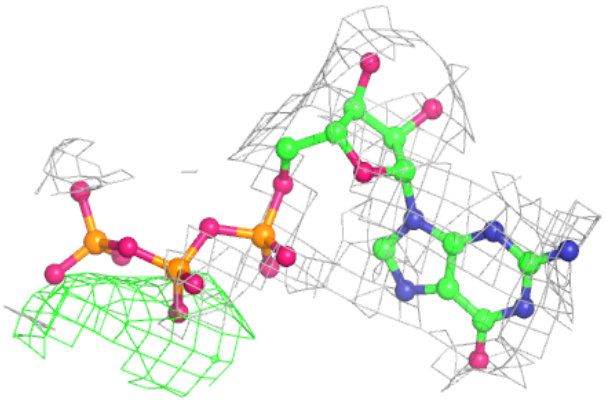


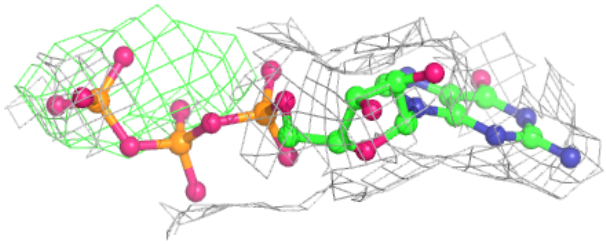


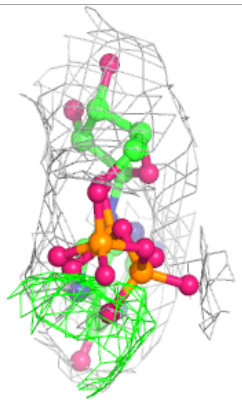


Electron density around GTP Q 600:

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

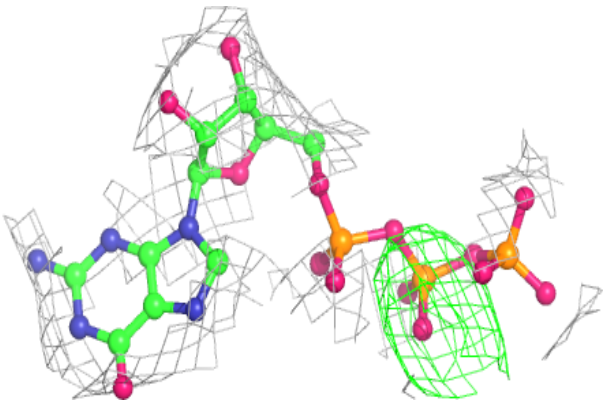


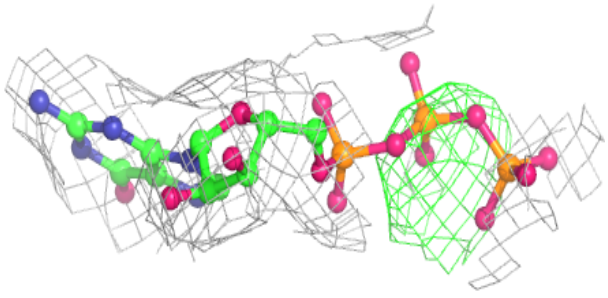


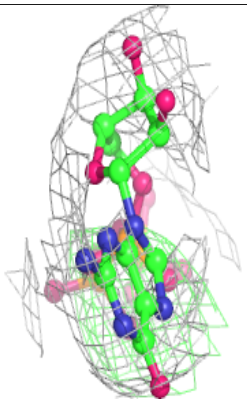


Electron density around GTP V 600:

$2mF_o$-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.