Full wwPDB X-ray Structure Validation Report ⓘ

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

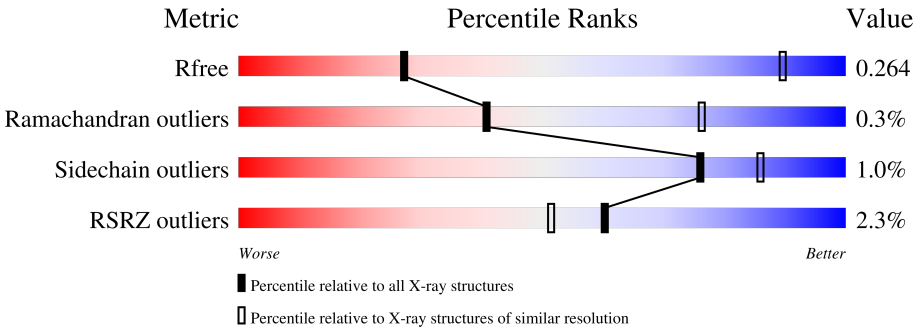
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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	3% 93% 6%
1	X	451	4% 93% 6%
2	B	445	94% 5%
2	D	445	% 94% 5%
2	I	445	% 94% 5%
2	K	445	6% 94% 5%
2	P	445	94% 5%
2	R	445	94% 5%
2	W	445	% 94% 5%
2	Y	445	% 94% 5%
3	E	554	87% 11%
3	L	554	88% 11%
3	S	554	% 88% 11%
3	Z	554	88% 11%
4	F	169	% 91% 8%
4	G	169	91% 8%
4	M	169	5% 91% 8%
4	N	169	6% 91% 8%
4	T	169	5% 91% 8%
4	U	169	91% 8%
4	a	169	16% 91% 8%
4	b	169	7% 91% 8%

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			

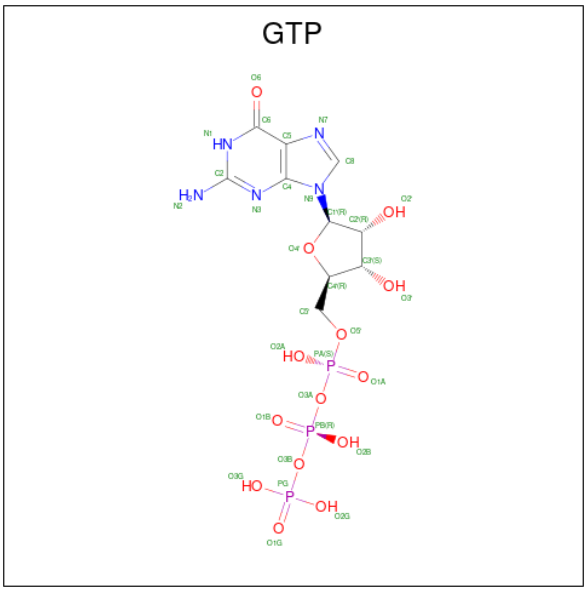
- Molecule 3 is a protein called Protein Stu2p/Alp14p.

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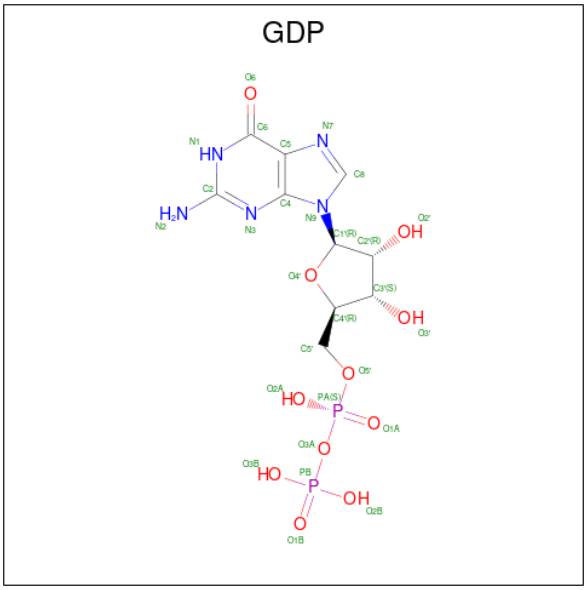
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total Mg 1 1	0	0
6	I	1	Total Mg 1 1	0	0
6	J	1	Total Mg 1 1	0	0
6	K	1	Total Mg 1 1	0	0
6	O	1	Total Mg 1 1	0	0
6	P	1	Total Mg 1 1	0	0
6	Q	1	Total Mg 1 1	0	0
6	R	1	Total Mg 1 1	0	0
6	V	1	Total Mg 1 1	0	0
6	W	1	Total Mg 1 1	0	0
6	X	1	Total Mg 1 1	0	0
6	Y	1	Total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

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



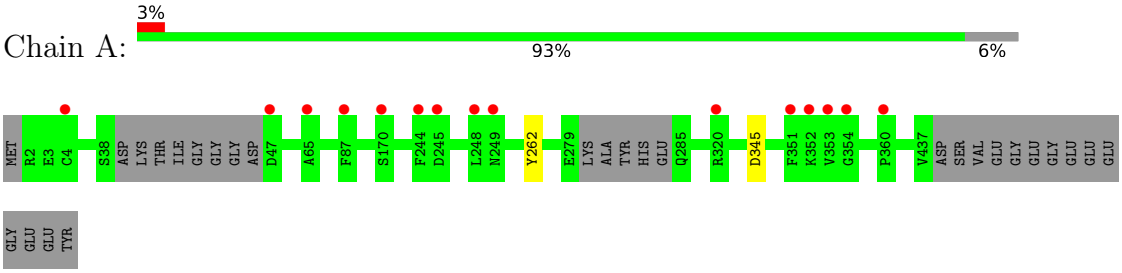
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
7	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
7	I	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
7	K	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
7	P	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
7	R	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
7	W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

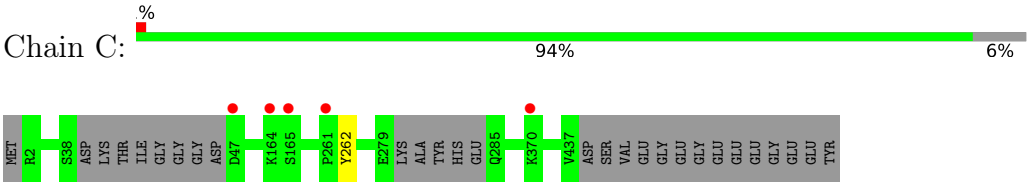
• Molecule 1: Tubulin alpha-1A chain

Chain A:



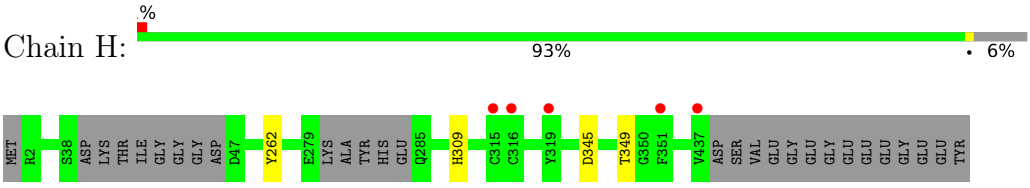
• Molecule 1: Tubulin alpha-1A chain

Chain C:



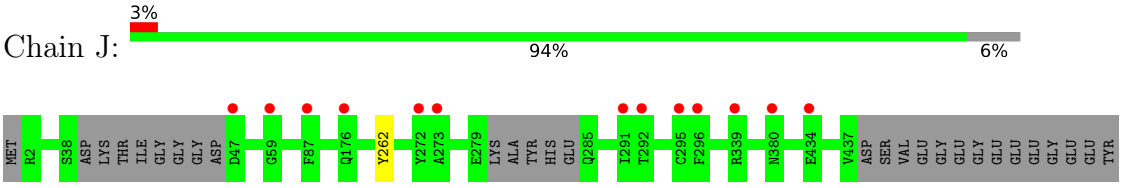
• Molecule 1: Tubulin alpha-1A chain

Chain H:



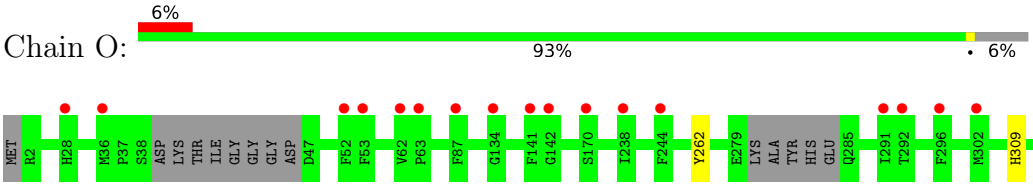
• Molecule 1: Tubulin alpha-1A chain

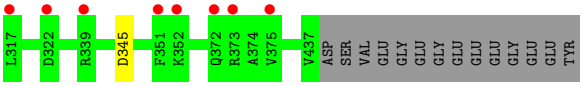
Chain J:



• Molecule 1: Tubulin alpha-1A chain

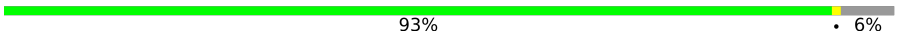
Chain O:

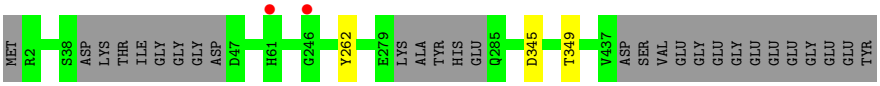




• Molecule 1: Tubulin alpha-1A chain

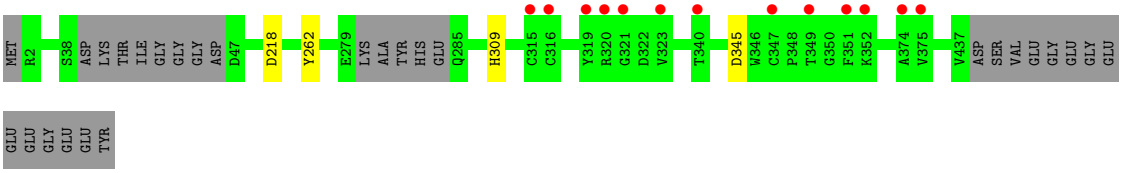
Chain Q:





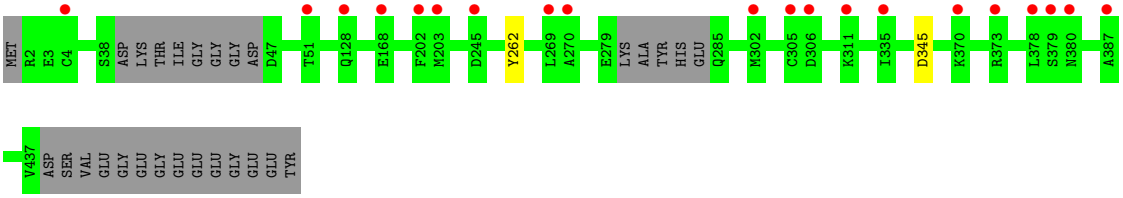
• Molecule 1: Tubulin alpha-1A chain

Chain V:



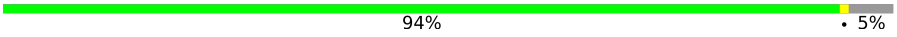
• Molecule 1: Tubulin alpha-1A chain

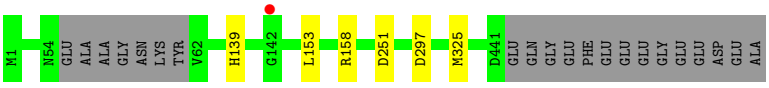
Chain X:



• Molecule 2: Tubulin beta chain

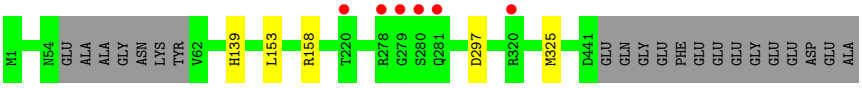
Chain B:





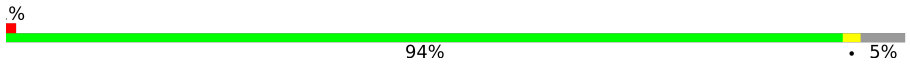
• Molecule 2: Tubulin beta chain

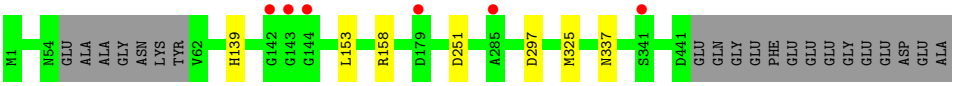
Chain D:



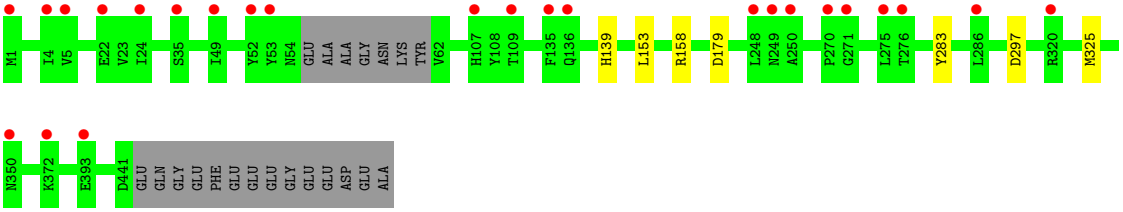
• Molecule 2: Tubulin beta chain

Chain I:





• Molecule 2: Tubulin beta chain



• Molecule 2: Tubulin beta chain

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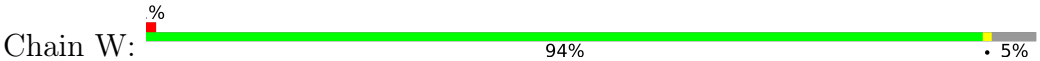
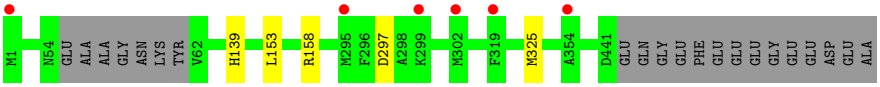
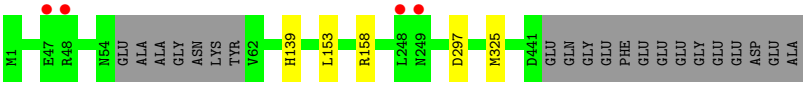
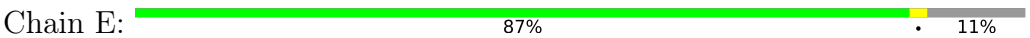


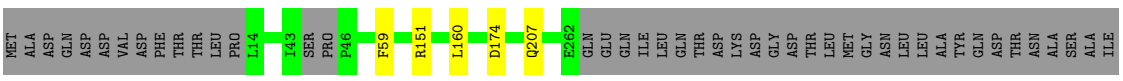


• Molecule 2: Tubulin beta chain



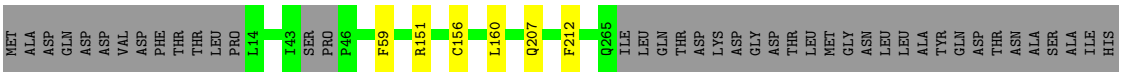
• Molecule 3: Protein Stu2p/Alp14p

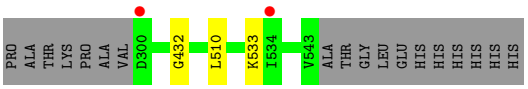




• Molecule 3: Protein Stu2p/Alp14p

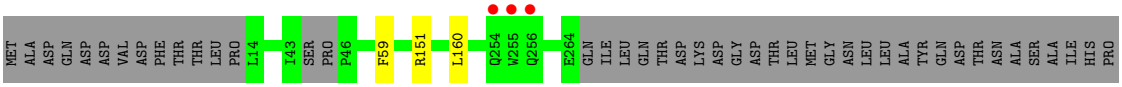
Chain L:





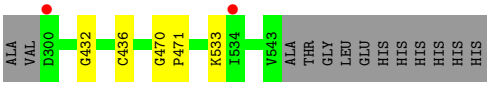
• Molecule 3: Protein Stu2p/Alp14p

Chain S:



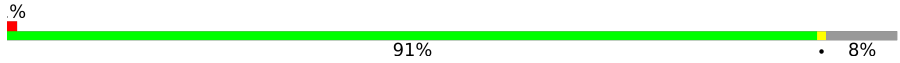
• Molecule 3: Protein Stu2p/Alp14p

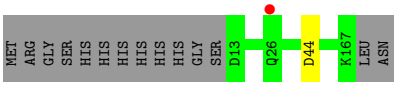
Chain Z:



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

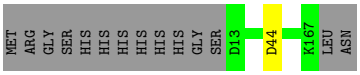
Chain F:





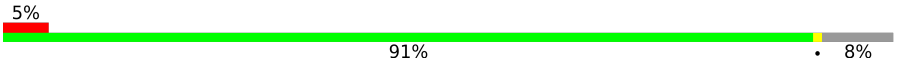
• Molecule 4: Designed ankyrin repeat protein (DARPIN) D1

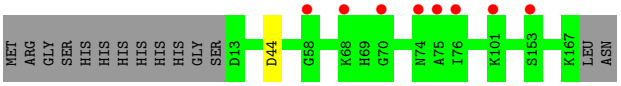
Chain G:



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

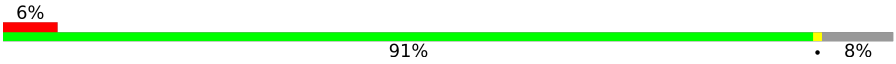
Chain M:

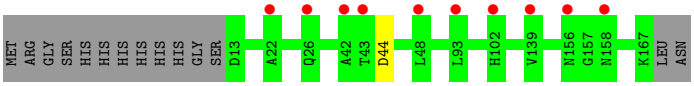




• Molecule 4: Designed ankyrin repeat protein (DARPIN) D1

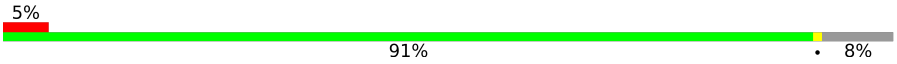
Chain N:

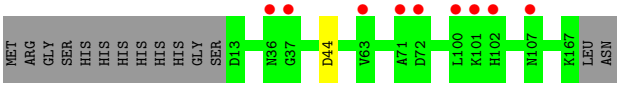




• Molecule 4: Designed ankyrin repeat protein (DARPIN) D1

Chain T:



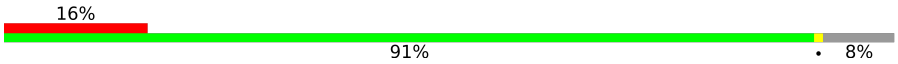


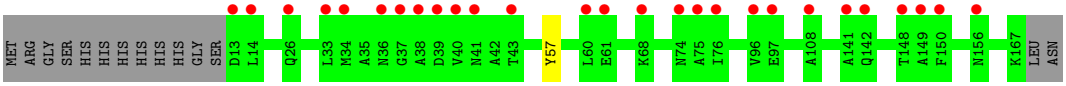
• Molecule 4: Designed ankyrin repeat protein (DARPIN) D1

Chain U:

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

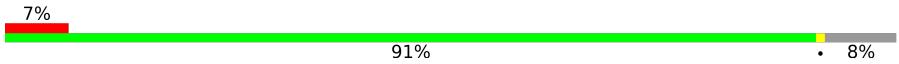
Chain a:

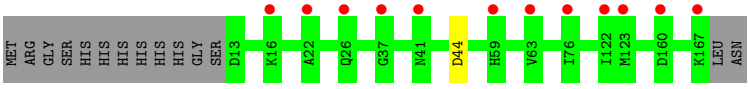




• Molecule 4: Designed ankyrin repeat protein (DARPIN) D1

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

5.1 Standard geometry

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

All (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
4	M	44	ASP
4	N	44	ASP
3	S	432	GLY
4	T	44	ASP
4	U	44	ASP
3	Z	432	GLY
4	b	44	ASP
3	E	174	ASP
3	E	471	PRO
1	H	349	THR
3	S	472	LEU
2	B	297	ASP
2	D	297	ASP
2	I	297	ASP
2	K	283	TYR
2	K	297	ASP
2	P	297	ASP

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Mol	Chain	Res	Type
2	R	297	ASP
2	W	297	ASP
2	Y	297	ASP
3	E	480	LEU
3	S	467	LYS
3	Z	471	PRO
3	Z	470	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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	262	TYR
1	A	345	ASP
2	B	139	HIS
2	B	153	LEU
2	B	158	ARG
2	B	251	ASP
2	B	325	MET
1	C	262	TYR
2	D	139	HIS
2	D	153	LEU
2	D	158	ARG
2	D	325	MET
3	E	59	PHE
3	E	151	ARG
3	E	160	LEU
3	E	207	GLN
3	E	431	CYS
3	E	510	LEU
3	E	533	LYS
1	H	262	TYR
1	H	309	HIS
1	H	345	ASP
2	I	139	HIS

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Mol	Chain	Res	Type
2	I	153	LEU
2	I	158	ARG
2	I	251	ASP
2	I	325	MET
2	I	337	ASN
1	J	262	TYR
2	K	139	HIS
2	K	153	LEU
2	K	158	ARG
2	K	179	ASP
2	K	325	MET
3	L	59	PHE
3	L	151	ARG
3	L	156	CYS
3	L	160	LEU
3	L	207	GLN
3	L	212	PHE
3	L	510	LEU
3	L	533	LYS
1	O	262	TYR
1	O	309	HIS
1	O	345	ASP
2	P	139	HIS
2	P	153	LEU
2	P	158	ARG
2	P	325	MET
1	Q	262	TYR
1	Q	345	ASP
2	R	139	HIS
2	R	153	LEU
2	R	158	ARG
2	R	251	ASP
2	R	325	MET
3	S	59	PHE
3	S	151	ARG
3	S	160	LEU
3	S	533	LYS
1	V	218	ASP
1	V	262	TYR
1	V	309	HIS
1	V	345	ASP
2	W	139	HIS

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Mol	Chain	Res	Type
2	W	153	LEU
2	W	158	ARG
2	W	325	MET
1	X	262	TYR
1	X	345	ASP
2	Y	139	HIS
2	Y	153	LEU
2	Y	158	ARG
2	Y	325	MET
3	Z	59	PHE
3	Z	151	ARG
3	Z	156	CYS
3	Z	160	LEU
3	Z	436	CYS
3	Z	533	LYS
4	a	57	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	300	ASN
3	E	171	ASN
2	Y	14	ASN
2	Y	136	GLN
3	Z	249	GLN
4	a	59	HIS

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%)
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (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
5	A	600	GTP	C5-C6	-3.96	1.39	1.47
5	H	600	GTP	C5-C6	-3.94	1.39	1.47
5	J	600	GTP	C5-C6	-3.91	1.39	1.47
7	K	600	GDP	C6-N1	-2.35	1.34	1.37
7	W	600	GDP	C6-N1	-2.34	1.34	1.37
7	I	600	GDP	C6-N1	-2.34	1.34	1.37
7	D	600	GDP	C6-N1	-2.32	1.34	1.37
7	Y	600	GDP	C6-N1	-2.28	1.34	1.37
7	B	600	GDP	C6-N1	-2.23	1.34	1.37
7	P	600	GDP	C6-N1	-2.21	1.34	1.37
7	R	600	GDP	C6-N1	-2.21	1.34	1.37
5	C	600	GTP	C2-N3	2.20	1.38	1.33
5	V	600	GTP	C2-N3	2.19	1.38	1.33
5	Q	600	GTP	C2-N3	2.18	1.38	1.33
5	J	600	GTP	C2-N3	2.18	1.38	1.33
5	X	600	GTP	C2-N3	2.15	1.38	1.33
5	A	600	GTP	C2-N3	2.11	1.38	1.33
5	O	600	GTP	C2-N3	2.08	1.38	1.33

All (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
5	C	600	GTP	PA-O3A-PB	-3.68	120.20	132.83
5	A	600	GTP	PA-O3A-PB	-3.65	120.30	132.83
5	Q	600	GTP	PA-O3A-PB	-3.48	120.89	132.83
5	Q	600	GTP	PB-O3B-PG	-3.41	121.12	132.83
5	X	600	GTP	PB-O3B-PG	-3.37	121.26	132.83
5	J	600	GTP	PB-O3B-PG	-3.27	121.59	132.83
5	C	600	GTP	PB-O3B-PG	-3.26	121.64	132.83
5	O	600	GTP	PB-O3B-PG	-3.18	121.90	132.83
5	H	600	GTP	PB-O3B-PG	-3.18	121.93	132.83
5	V	600	GTP	C5-C6-N1	3.17	119.56	113.95
5	V	600	GTP	PB-O3B-PG	-3.15	122.00	132.83
5	A	600	GTP	PB-O3B-PG	-3.15	122.02	132.83
5	A	600	GTP	C5-C6-N1	3.13	119.48	113.95
5	C	600	GTP	C5-C6-N1	3.13	119.48	113.95
7	I	600	GDP	PA-O3A-PB	-3.09	122.23	132.83
5	Q	600	GTP	C5-C6-N1	3.07	119.37	113.95
5	O	600	GTP	C5-C6-N1	3.06	119.36	113.95
5	J	600	GTP	C5-C6-N1	3.06	119.36	113.95
5	X	600	GTP	C5-C6-N1	3.03	119.31	113.95
5	O	600	GTP	C8-N7-C5	2.99	108.68	102.99
5	J	600	GTP	C8-N7-C5	2.98	108.67	102.99
7	K	600	GDP	PA-O3A-PB	-2.98	122.61	132.83
5	X	600	GTP	C8-N7-C5	2.97	108.65	102.99
5	A	600	GTP	C8-N7-C5	2.97	108.65	102.99
5	H	600	GTP	C5-C6-N1	2.96	119.17	113.95
5	H	600	GTP	C8-N7-C5	2.94	108.59	102.99
5	C	600	GTP	C8-N7-C5	2.94	108.59	102.99
7	W	600	GDP	PA-O3A-PB	-2.92	122.79	132.83
5	O	600	GTP	C2-N1-C6	-2.92	119.73	125.10
5	A	600	GTP	C2-N1-C6	-2.91	119.73	125.10
5	V	600	GTP	C8-N7-C5	2.90	108.52	102.99
5	X	600	GTP	C2-N1-C6	-2.89	119.78	125.10
5	Q	600	GTP	C8-N7-C5	2.89	108.49	102.99
7	P	600	GDP	PA-O3A-PB	-2.83	123.12	132.83
5	J	600	GTP	C2-N1-C6	-2.79	119.97	125.10
7	B	600	GDP	PA-O3A-PB	-2.78	123.30	132.83
5	V	600	GTP	C2-N1-C6	-2.75	120.04	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	600	GTP	C2-N1-C6	-2.71	120.11	125.10
5	Q	600	GTP	C2-N1-C6	-2.70	120.12	125.10
5	H	600	GTP	C2-N1-C6	-2.70	120.13	125.10
7	R	600	GDP	PA-O3A-PB	-2.58	123.97	132.83
7	D	600	GDP	PA-O3A-PB	-2.55	124.07	132.83
5	J	600	GTP	C3'-C2'-C1'	2.53	104.79	100.98
7	Y	600	GDP	PA-O3A-PB	-2.51	124.21	132.83
5	X	600	GTP	C3'-C2'-C1'	2.45	104.67	100.98
5	C	600	GTP	C3'-C2'-C1'	2.38	104.56	100.98
5	O	600	GTP	C3'-C2'-C1'	2.36	104.53	100.98
5	H	600	GTP	C3'-C2'-C1'	2.34	104.50	100.98
7	Y	600	GDP	C8-N7-C5	2.32	107.42	102.99
7	P	600	GDP	C8-N7-C5	2.30	107.37	102.99
7	K	600	GDP	C5-C6-N1	2.29	118.00	113.95
5	C	600	GTP	O6-C6-C5	-2.29	119.90	124.37
7	W	600	GDP	C8-N7-C5	2.28	107.34	102.99
5	A	600	GTP	C3'-C2'-C1'	2.28	104.41	100.98
7	R	600	GDP	C8-N7-C5	2.27	107.32	102.99
7	I	600	GDP	C8-N7-C5	2.27	107.31	102.99
7	D	600	GDP	C5-C6-N1	2.27	117.95	113.95
5	Q	600	GTP	C3'-C2'-C1'	2.26	104.38	100.98
5	V	600	GTP	O6-C6-C5	-2.25	119.98	124.37
5	O	600	GTP	O6-C6-C5	-2.25	119.99	124.37
7	B	600	GDP	C8-N7-C5	2.23	107.24	102.99
7	D	600	GDP	C8-N7-C5	2.23	107.24	102.99
5	V	600	GTP	C3'-C2'-C1'	2.23	104.34	100.98
7	K	600	GDP	C8-N7-C5	2.23	107.24	102.99
5	Q	600	GTP	O6-C6-C5	-2.22	120.03	124.37
7	B	600	GDP	C5-C6-N1	2.22	117.87	113.95
7	I	600	GDP	C5-C6-N1	2.19	117.82	113.95
7	R	600	GDP	C5-C6-N1	2.18	117.81	113.95
5	A	600	GTP	O6-C6-C5	-2.17	120.14	124.37
5	X	600	GTP	O6-C6-C5	-2.13	120.21	124.37
7	Y	600	GDP	C5-C6-N1	2.13	117.71	113.95
7	P	600	GDP	C5-C6-N1	2.12	117.70	113.95
7	W	600	GDP	C5-C6-N1	2.12	117.69	113.95
5	J	600	GTP	O6-C6-C5	-2.09	120.30	124.37
5	H	600	GTP	O6-C6-C5	-2.04	120.40	124.37

There are no chirality outliers.

All (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
5	X	600	GTP	PB-O3B-PG-O2G
7	B	600	GDP	C5'-O5'-PA-O1A
7	B	600	GDP	C5'-O5'-PA-O2A
7	D	600	GDP	C5'-O5'-PA-O1A
7	D	600	GDP	C5'-O5'-PA-O2A
7	I	600	GDP	C5'-O5'-PA-O1A
7	I	600	GDP	C5'-O5'-PA-O2A
7	K	600	GDP	C5'-O5'-PA-O1A
7	K	600	GDP	C5'-O5'-PA-O2A
7	P	600	GDP	C5'-O5'-PA-O1A
7	P	600	GDP	C5'-O5'-PA-O2A
7	R	600	GDP	C5'-O5'-PA-O1A
7	R	600	GDP	C5'-O5'-PA-O2A
7	W	600	GDP	C5'-O5'-PA-O1A
7	W	600	GDP	C5'-O5'-PA-O2A
7	Y	600	GDP	C5'-O5'-PA-O1A
7	Y	600	GDP	C5'-O5'-PA-O2A
5	J	600	GTP	PB-O3B-PG-O1G
7	D	600	GDP	PB-O3A-PA-O2A
7	R	600	GDP	PB-O3A-PA-O2A
7	W	600	GDP	PB-O3A-PA-O2A
5	A	600	GTP	PB-O3B-PG-O1G
5	C	600	GTP	PB-O3B-PG-O1G
5	O	600	GTP	PB-O3B-PG-O1G
5	Q	600	GTP	PB-O3B-PG-O1G
5	X	600	GTP	PB-O3B-PG-O1G
5	H	600	GTP	PB-O3B-PG-O2G
5	J	600	GTP	PB-O3B-PG-O3G
5	V	600	GTP	PB-O3B-PG-O2G
5	X	600	GTP	PB-O3B-PG-O3G
7	B	600	GDP	C5'-O5'-PA-O3A
7	D	600	GDP	C5'-O5'-PA-O3A
7	I	600	GDP	C5'-O5'-PA-O3A
7	K	600	GDP	C5'-O5'-PA-O3A
7	P	600	GDP	C5'-O5'-PA-O3A
7	R	600	GDP	C5'-O5'-PA-O3A
7	W	600	GDP	C5'-O5'-PA-O3A
7	Y	600	GDP	C5'-O5'-PA-O3A

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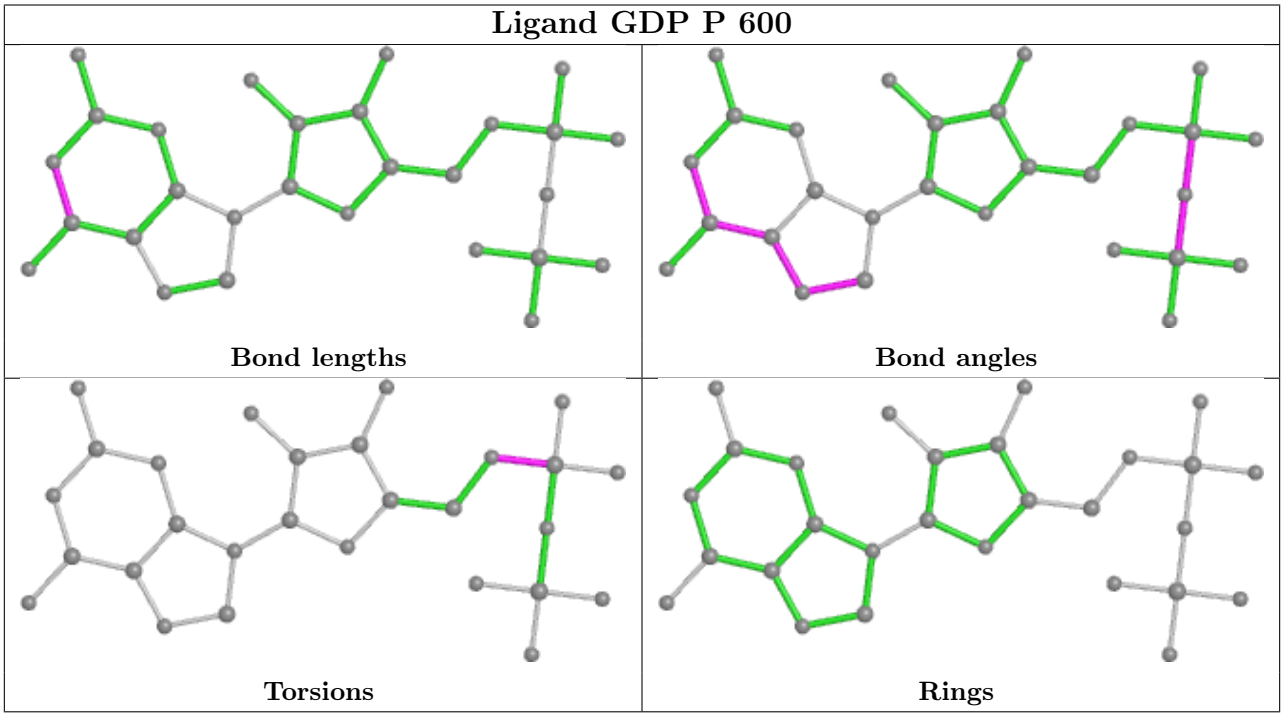
Mol	Chain	Res	Type	Atoms
7	I	600	GDP	PB-O3A-PA-O2A
5	H	600	GTP	PB-O3B-PG-O1G
5	V	600	GTP	PB-O3B-PG-O1G
5	H	600	GTP	C4'-C5'-O5'-PA

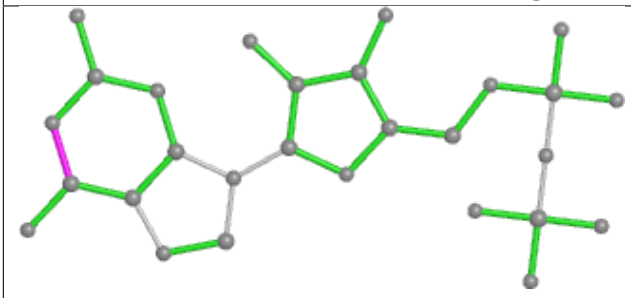
There are no ring outliers.

No monomer is involved in short contacts.

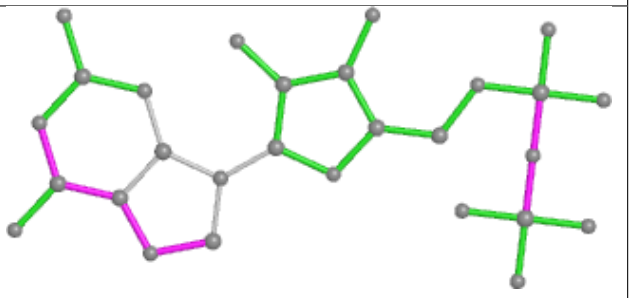
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



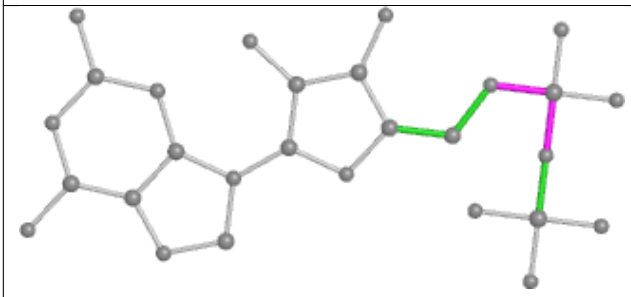
Ligand GDP I 600



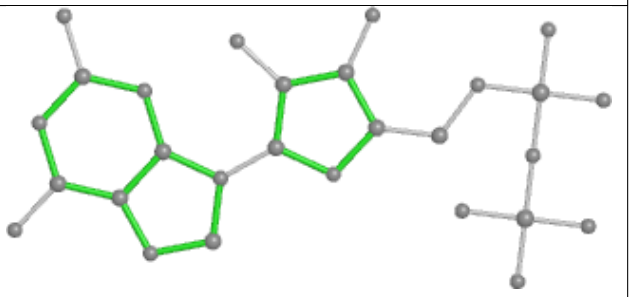
Bond lengths



Bond angles

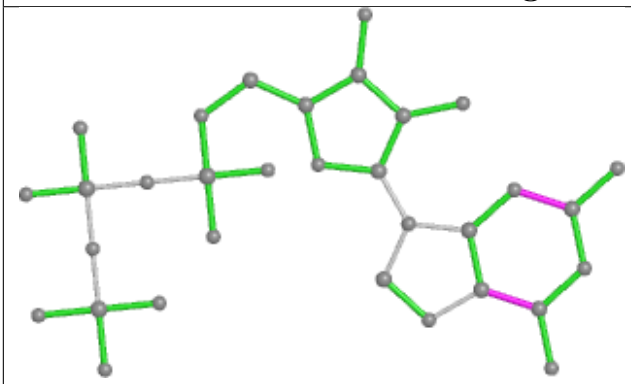


Torsions

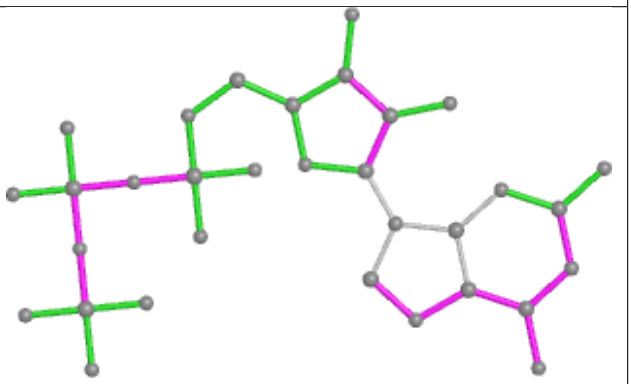


Rings

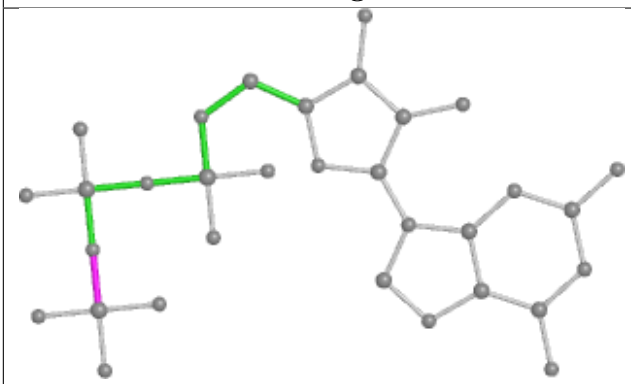
Ligand GTP A 600



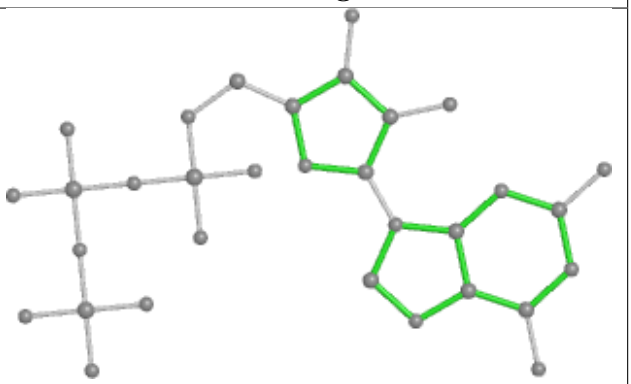
Bond lengths



Bond angles

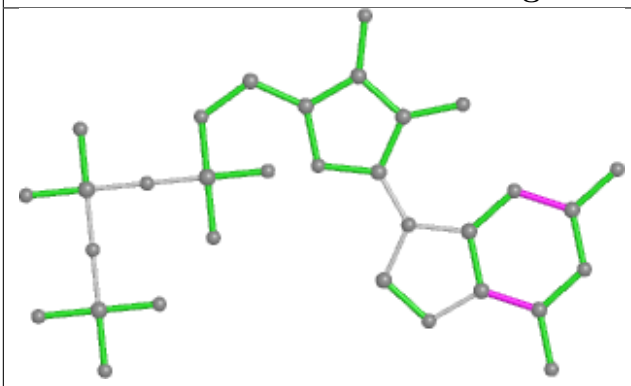


Torsions

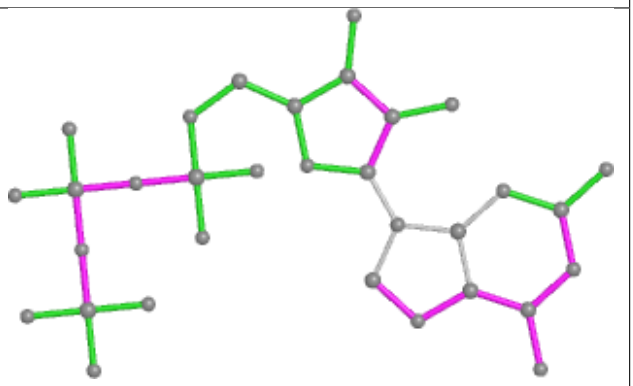


Rings

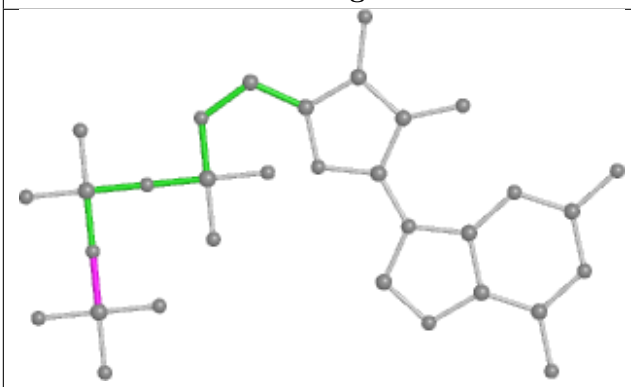
Ligand GTP C 600



Bond lengths



Bond angles



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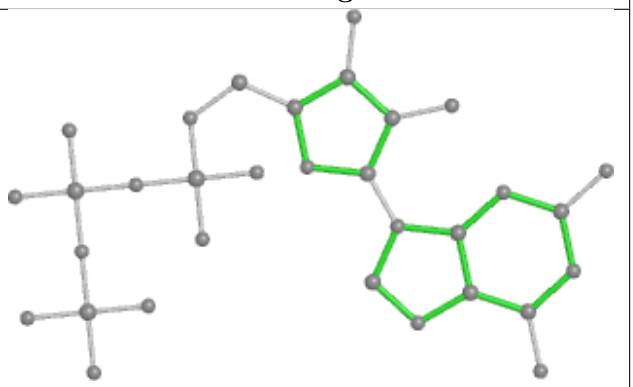
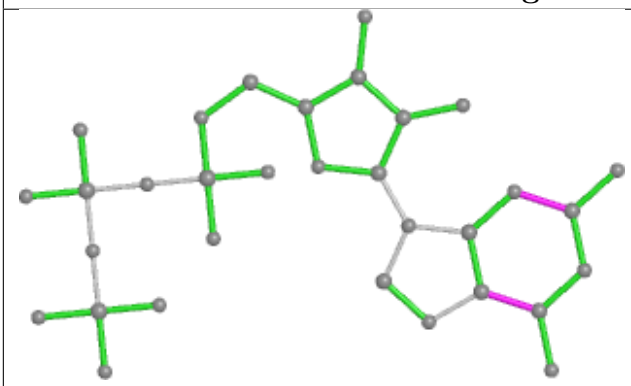
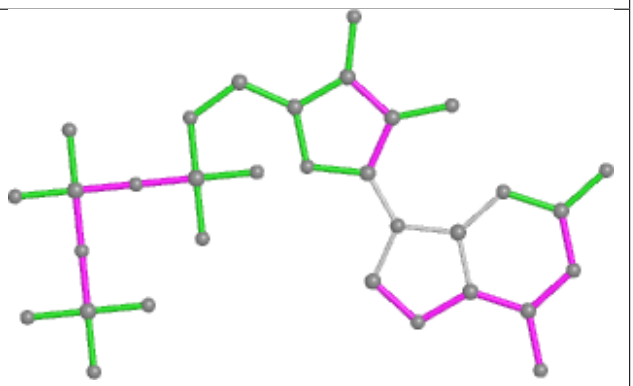


Rings

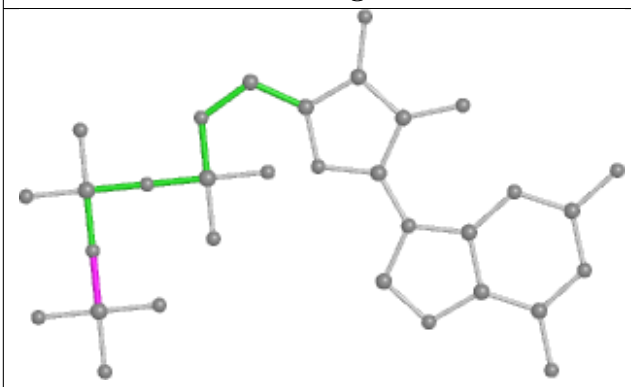
Ligand GTP V 600



Bond lengths



Bond angles



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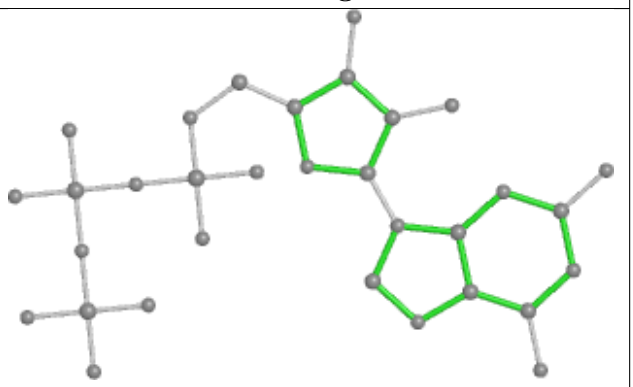
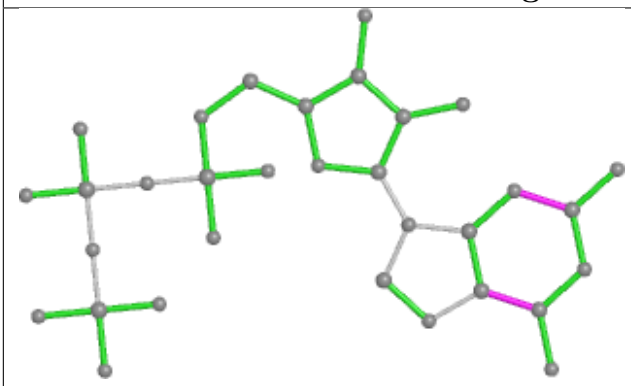
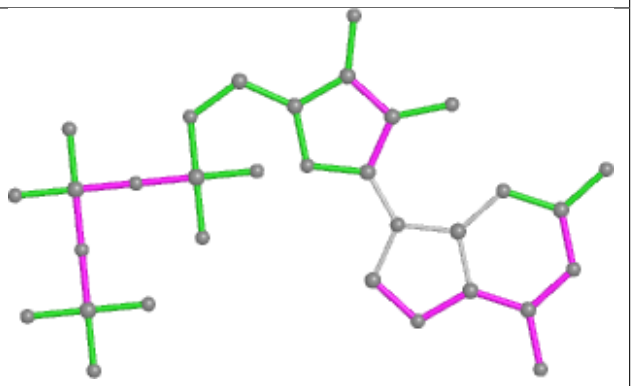


Rings

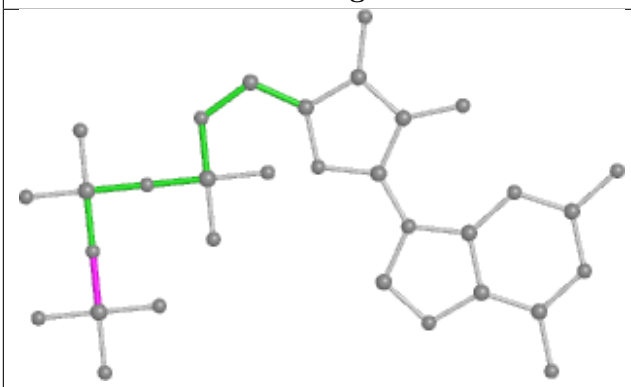
Ligand GTP X 600



Bond lengths



Bond angles



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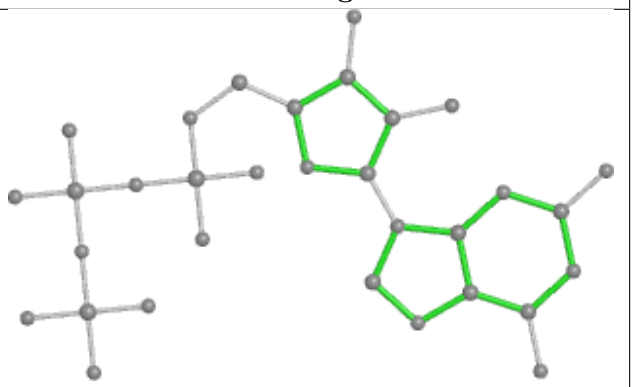
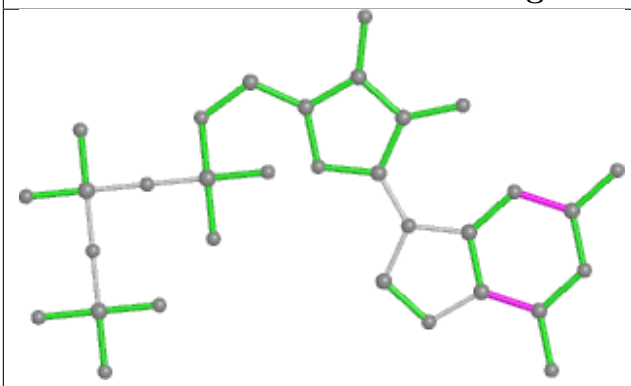
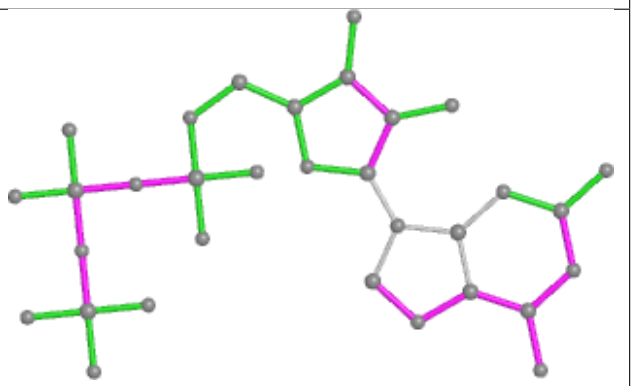


Rings

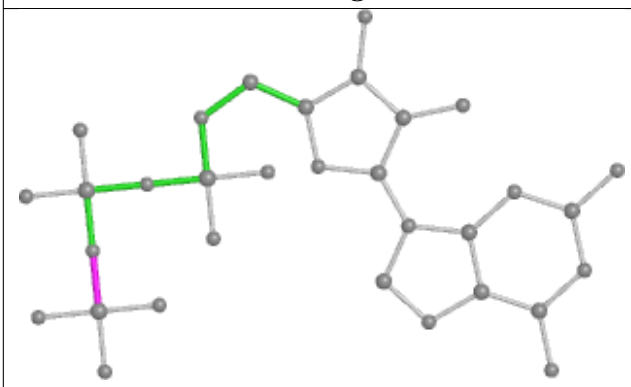
Ligand GTP J 600



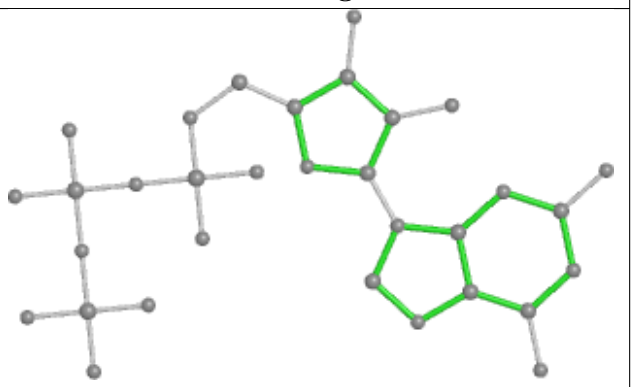
Bond lengths



Bond angles

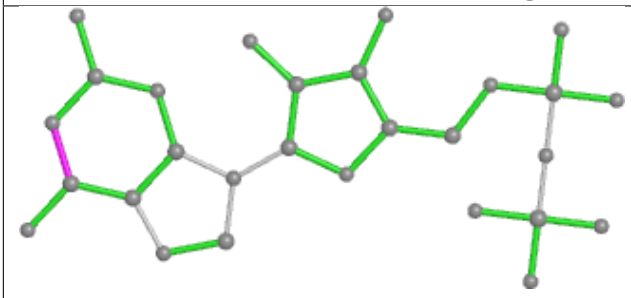


Torsions

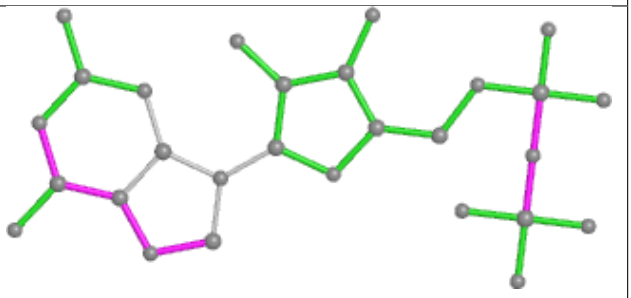


Rings

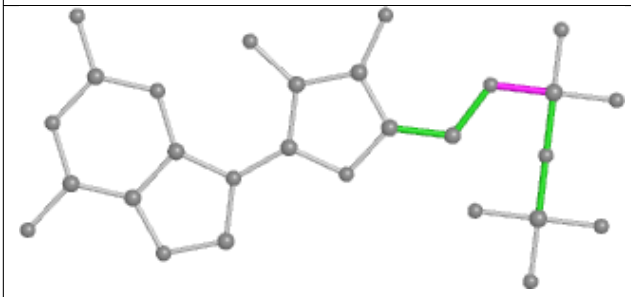
Ligand GDP Y 600



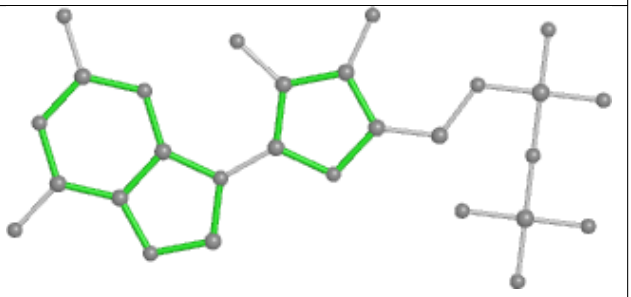
Bond lengths



Bond angles

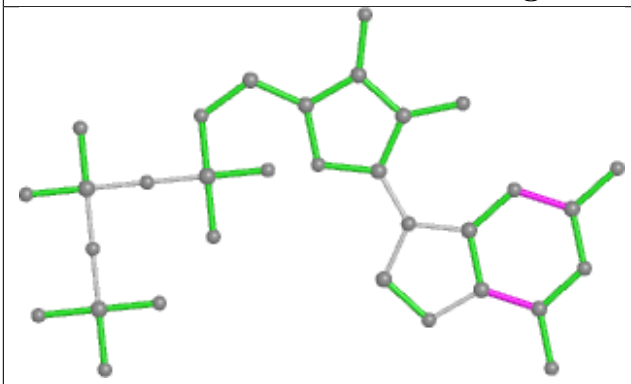


Torsions

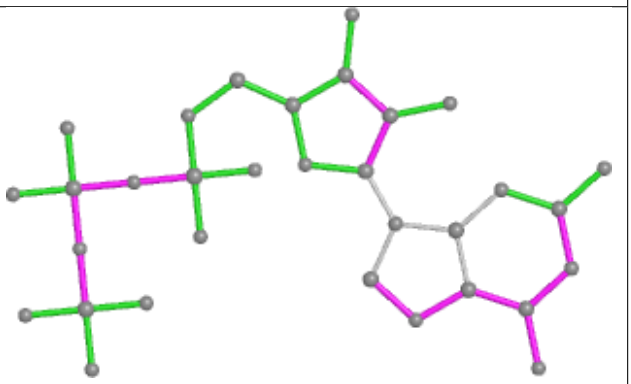


Rings

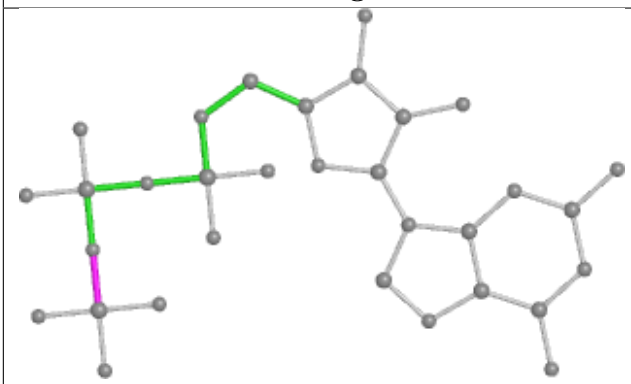
Ligand GTP O 600



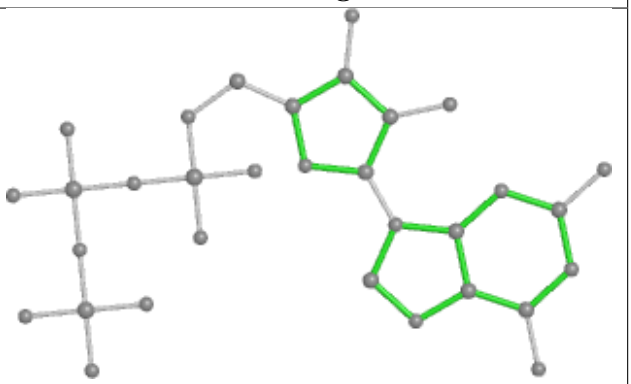
Bond lengths



Bond angles

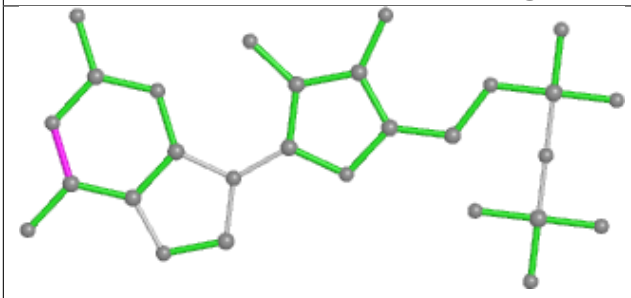


Torsions

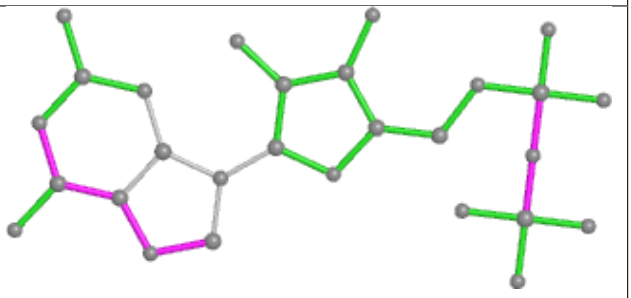


Rings

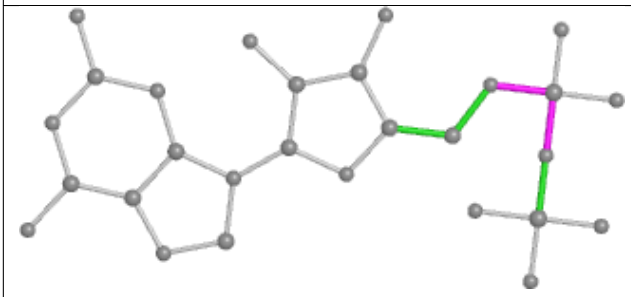
Ligand GDP R 600



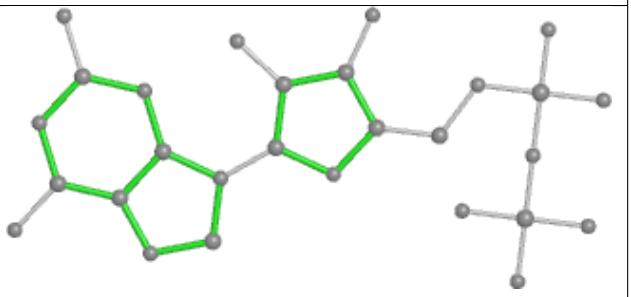
Bond lengths



Bond angles

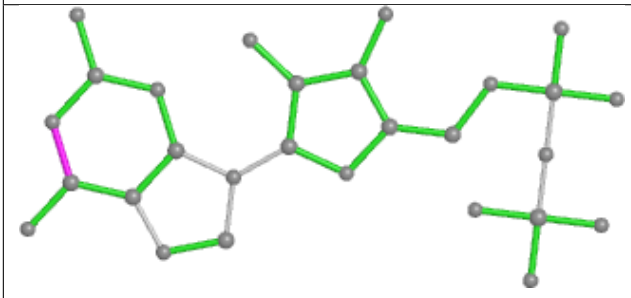


Torsions

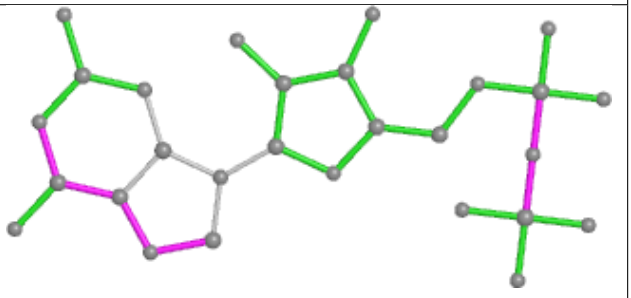


Rings

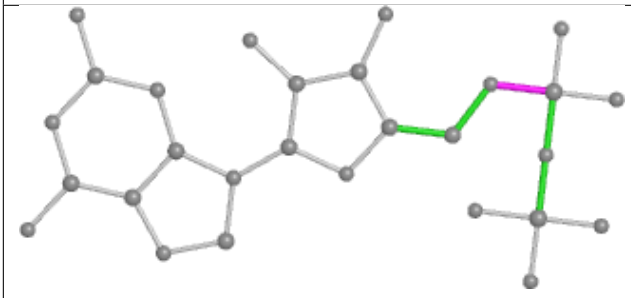
Ligand GDP K 600



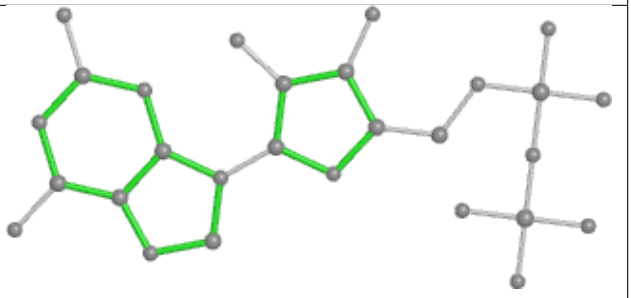
Bond lengths



Bond angles

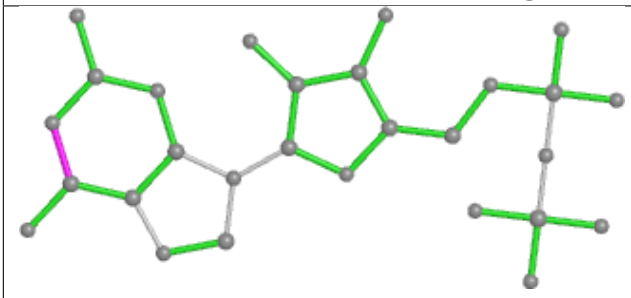


Torsions

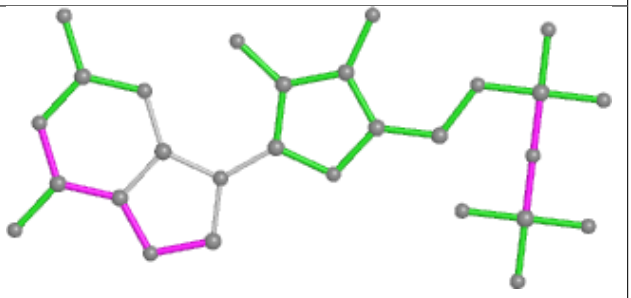


Rings

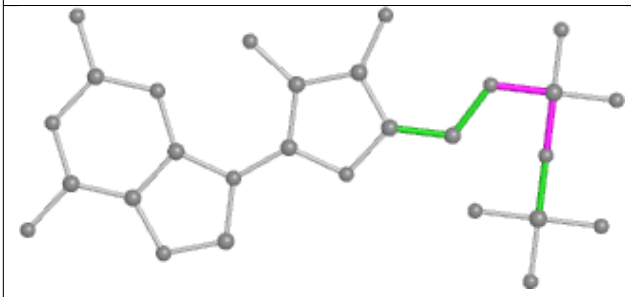
Ligand GDP D 600



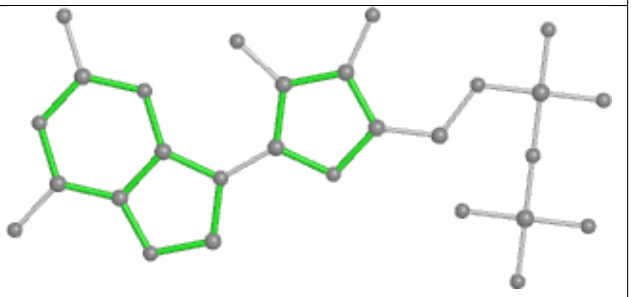
Bond lengths



Bond angles

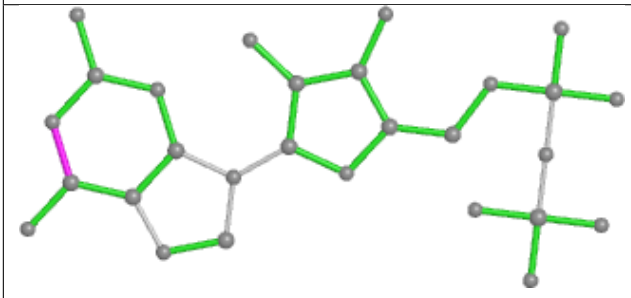


Torsions

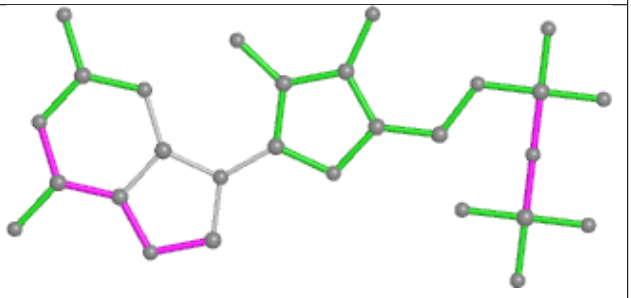


Rings

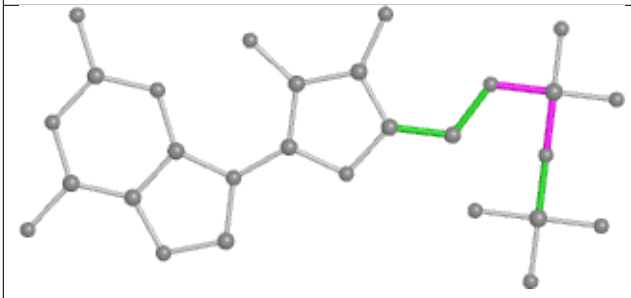
Ligand GDP W 600



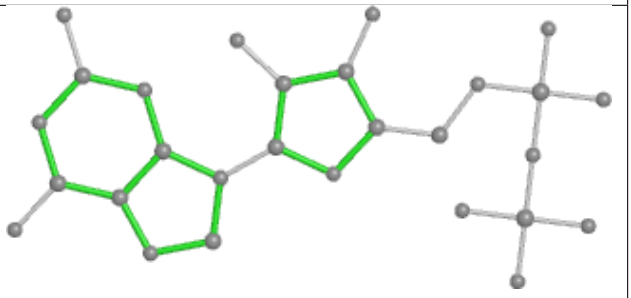
Bond lengths



Bond angles

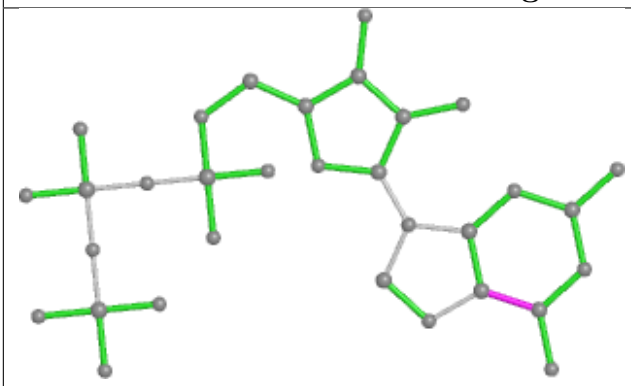


Torsions

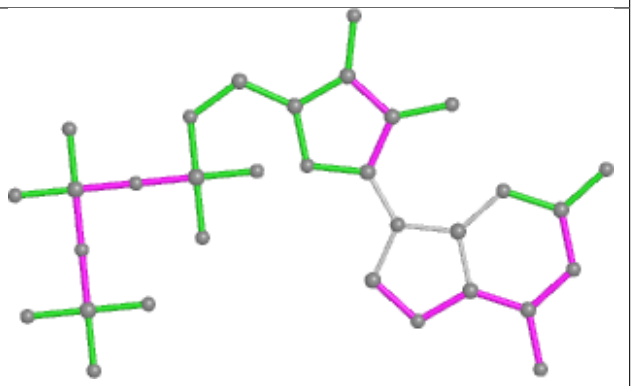


Rings

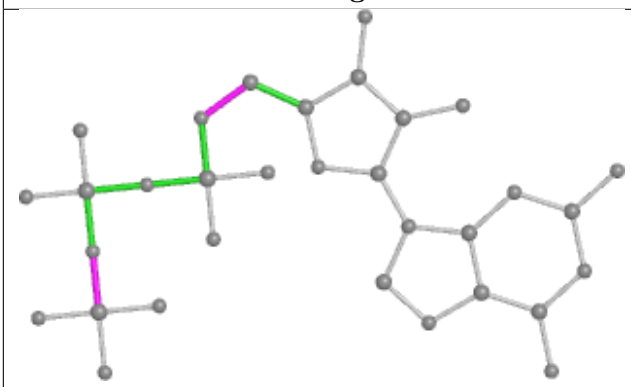
Ligand GTP H 600



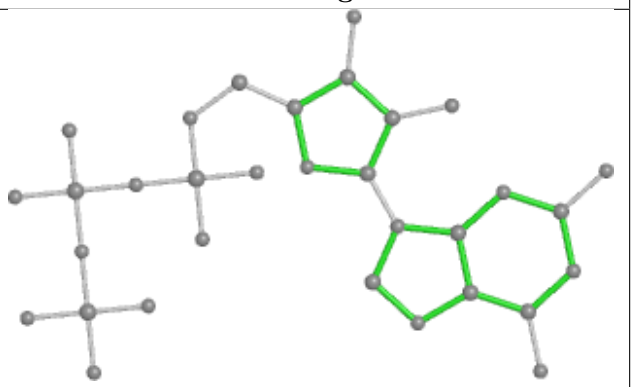
Bond lengths



Bond angles

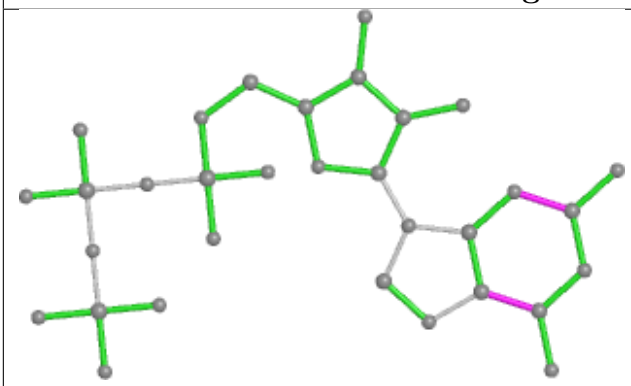


Torsions

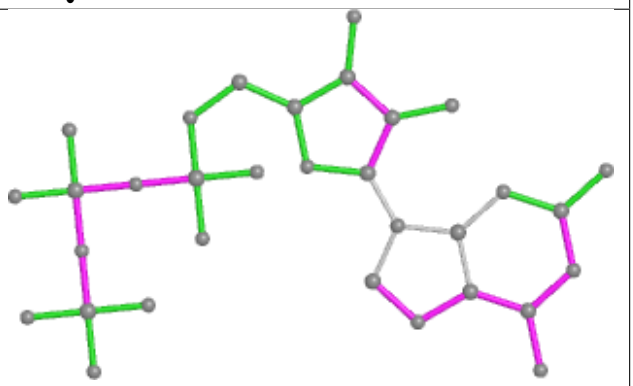


Rings

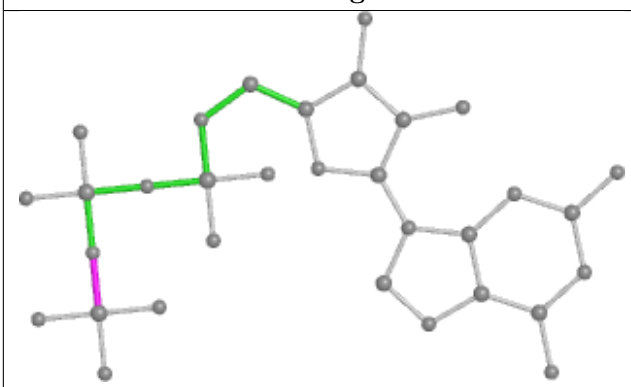
Ligand GTP Q 600



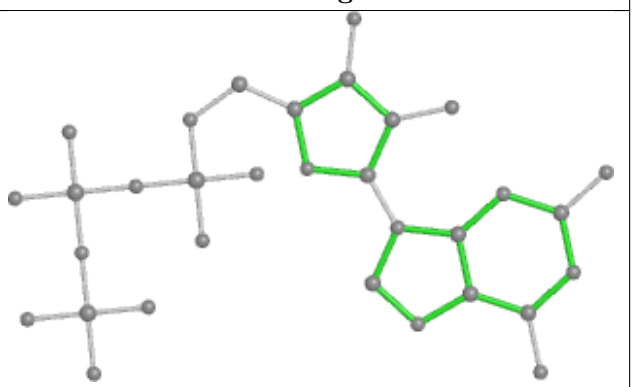
Bond lengths



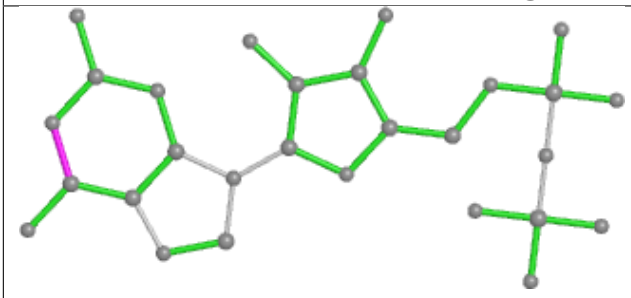
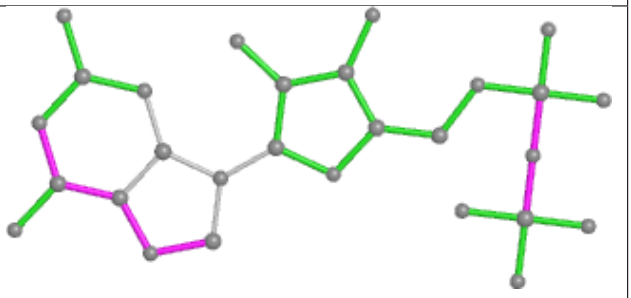
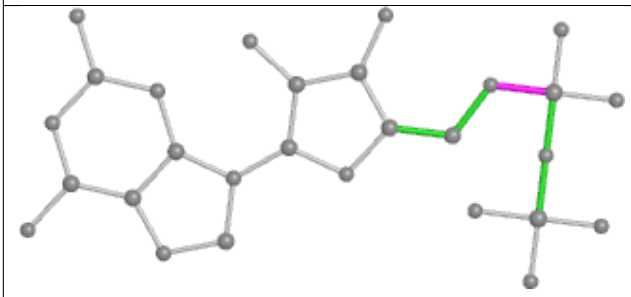
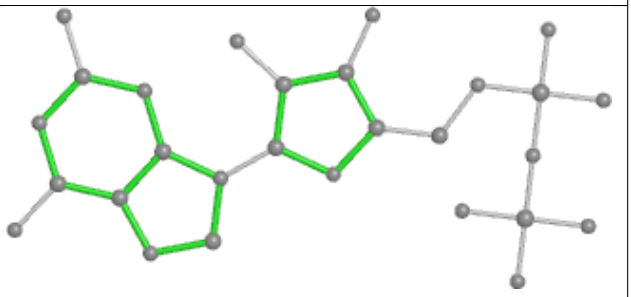
Bond angles



Torsions



Rings

Ligand GDP B 600	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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

All (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
2	I	179	ASP	5.2
1	X	379	SER	5.2
1	X	4	CYS	4.9
2	K	249	ASN	4.7
4	a	37	GLY	4.6
4	a	41	ASN	4.2
1	O	296	PHE	4.2
2	K	49	ILE	4.2
2	D	280	SER	4.0
2	D	279	GLY	4.0
4	a	142	GLN	3.9
1	O	302	MET	3.9
1	A	249	ASN	3.9
1	A	245	ASP	3.8
4	a	34	MET	3.8
4	N	26	GLN	3.7
1	J	296	PHE	3.7
4	N	102	HIS	3.6
1	O	52	PHE	3.6
1	J	295	CYS	3.6
4	a	43	THR	3.6
1	X	168	GLU	3.5
1	J	292	THR	3.5
1	V	315	CYS	3.5
1	O	292	THR	3.5
1	X	380	ASN	3.5
3	L	300	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
2	K	53	TYR	3.4
1	O	315	CYS	3.4
1	J	380	ASN	3.4
4	b	59	HIS	3.3
1	V	319	TYR	3.3
2	K	4	ILE	3.3
1	O	351	PHE	3.3
2	W	319	PHE	3.2
1	X	305	CYS	3.2
2	I	142	GLY	3.2
1	O	134	GLY	3.2
2	K	250	ALA	3.2
1	A	4	CYS	3.2
4	T	101	LYS	3.2
4	a	96	VAL	3.1
4	a	36	ASN	3.1
1	O	28	HIS	3.1
4	N	139	VAL	3.0
2	K	52	TYR	3.0
4	b	41	ASN	3.0
4	M	68	LYS	3.0
1	V	321	GLY	3.0
4	a	148	THR	3.0
1	V	323	VAL	3.0
4	N	93	LEU	3.0
1	H	351	PHE	3.0
4	T	63	VAL	3.0
1	O	373	ARG	3.0
1	J	273	ALA	3.0
2	D	281	GLN	2.9
1	V	374	ALA	2.9
4	M	74	ASN	2.9
4	a	74	ASN	2.9
1	V	351	PHE	2.9
4	a	40	VAL	2.9
1	V	352	LYS	2.9
1	O	62	VAL	2.9
1	H	315	CYS	2.9
4	b	160	ASP	2.9
2	W	1	MET	2.8
1	O	372	GLN	2.8
3	S	255	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
4	b	76	ILE	2.8
1	A	65	ALA	2.8
4	a	141	ALA	2.8
1	X	269	LEU	2.8
2	I	144	GLY	2.8
4	T	102	HIS	2.8
1	O	53	PHE	2.8
4	a	39	ASP	2.8
4	a	61	GLU	2.8
4	b	26	GLN	2.8
4	b	167	LYS	2.8
4	a	108	ALA	2.8
1	V	375	VAL	2.8
4	b	63	VAL	2.7
4	N	43	THR	2.7
1	O	63	PRO	2.7
2	Y	48	ARG	2.7
4	T	37	GLY	2.7
1	C	47	ASP	2.7
3	Z	534	ILE	2.7
1	X	335	ILE	2.7
1	J	87	PHE	2.7
4	N	22	ALA	2.7
2	K	109	THR	2.7
1	O	170	SER	2.7
4	N	156	ASN	2.7
2	Y	249	ASN	2.7
4	a	76	ILE	2.7
1	A	170	SER	2.6
4	a	60	LEU	2.6
4	M	58	GLY	2.6
1	O	352	LYS	2.6
4	b	123	MET	2.6
4	M	101	LYS	2.6
1	O	316	CYS	2.6
1	X	311	LYS	2.6
4	a	149	ALA	2.6
4	N	158	ASN	2.6
1	Q	246	GLY	2.6
1	J	291	ILE	2.5
1	A	248	LEU	2.5
1	H	319	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	O	313	MET	2.5
3	L	534	ILE	2.5
4	a	13	ASP	2.5
1	X	245	ASP	2.5
4	a	68	LYS	2.5
4	a	150	PHE	2.5
1	X	203	MET	2.5
1	A	47	ASP	2.5
1	O	317	LEU	2.5
1	O	291	ILE	2.5
4	T	71	ALA	2.5
2	K	286	LEU	2.4
1	A	244	PHE	2.4
1	O	322	ASP	2.4
2	K	372	LYS	2.4
4	a	33	LEU	2.4
2	R	28	HIS	2.4
1	J	434	GLU	2.4
1	V	320	ARG	2.4
1	H	437	VAL	2.4
4	b	37	GLY	2.4
1	A	351	PHE	2.3
4	a	14	LEU	2.3
1	X	270	ALA	2.3
2	K	320	ARG	2.3
1	A	360	PRO	2.3
1	V	349	THR	2.3
3	Z	300	ASP	2.3
2	K	271	GLY	2.3
1	Q	61	HIS	2.3
1	X	51	THR	2.3
1	O	142	GLY	2.3
4	M	70	GLY	2.3
2	R	292	THR	2.3
2	K	275	LEU	2.3
1	C	370	LYS	2.3
2	W	299	LYS	2.3
4	M	153	SER	2.3
4	N	48	LEU	2.3
1	X	306	ASP	2.3
1	O	141	PHE	2.3
1	X	302	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	O	244	PHE	2.3
1	V	316	CYS	2.3
1	X	378	LEU	2.2
4	a	26	GLN	2.2
1	J	47	ASP	2.2
1	X	373	ARG	2.2
1	V	347	CYS	2.2
2	B	142	GLY	2.2
4	N	42	ALA	2.2
1	O	238	ILE	2.2
1	X	128	GLN	2.2
2	D	220	THR	2.2
1	J	59	GLY	2.2
1	X	387	ALA	2.2
4	T	36	ASN	2.2
2	I	285	ALA	2.2
3	S	254	GLN	2.2
2	I	341	SER	2.2
1	O	339	ARG	2.2
4	b	16	LYS	2.2
1	C	165	SER	2.2
1	O	87	PHE	2.2
3	S	256	GLN	2.2
4	a	156	ASN	2.2
2	K	393	GLU	2.2
1	V	340	THR	2.2
4	a	97	GLU	2.2
2	K	35	SER	2.2
1	C	164	LYS	2.2
1	O	36	MET	2.2
2	K	5	VAL	2.2
2	K	136	GLN	2.2
4	F	26	GLN	2.2
2	I	143	GLY	2.2
1	J	176	GLN	2.1
1	H	316	CYS	2.1
2	D	278	ARG	2.1
2	W	302	MET	2.1
1	A	352	LYS	2.1
1	X	370	LYS	2.1
2	K	22	GLU	2.1
2	K	248	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	339	ARG	2.1
4	T	107	ASN	2.1
1	X	202	PHE	2.1
4	b	22	ALA	2.1
2	D	320	ARG	2.1
2	W	295	MET	2.1
2	K	135	PHE	2.1
2	K	107	HIS	2.1
4	b	122	ILE	2.1
1	A	354	GLY	2.1
2	K	270	PRO	2.0
2	K	276	THR	2.0
1	J	272	TYR	2.0
1	O	314	ALA	2.0
2	K	24	ILE	2.0
4	T	72	ASP	2.0
1	A	87	PHE	2.0
2	K	350	ASN	2.0
2	Y	47	GLU	2.0
4	T	100	LEU	2.0
1	O	375	VAL	2.0
1	C	261	PRO	2.0
1	A	320	ARG	2.0
2	W	354	ALA	2.0
2	Y	248	LEU	2.0
1	A	353	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

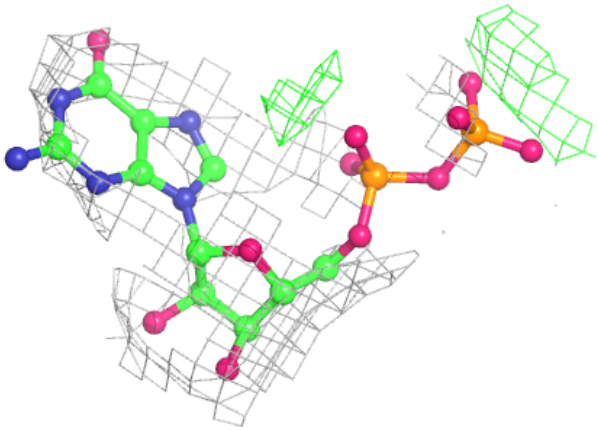
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

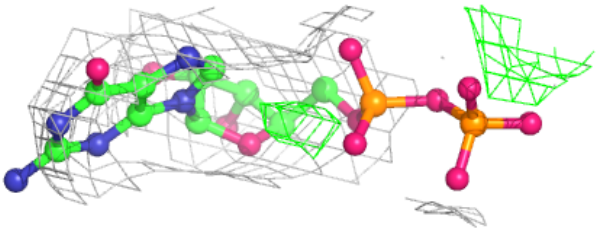
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	R	601	1/1	0.71	0.35	38,38,38,38	0
6	MG	I	601	1/1	0.77	0.21	70,70,70,70	0
6	MG	K	601	1/1	0.81	0.42	74,74,74,74	0
6	MG	Y	601	1/1	0.83	0.39	69,69,69,69	0
7	GDP	K	600	28/28	0.88	0.24	90,114,123,134	0
6	MG	P	601	1/1	0.91	0.28	48,48,48,48	0
5	GTP	X	600	32/32	0.91	0.23	67,87,98,102	0
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

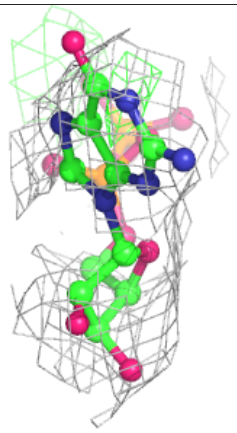
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

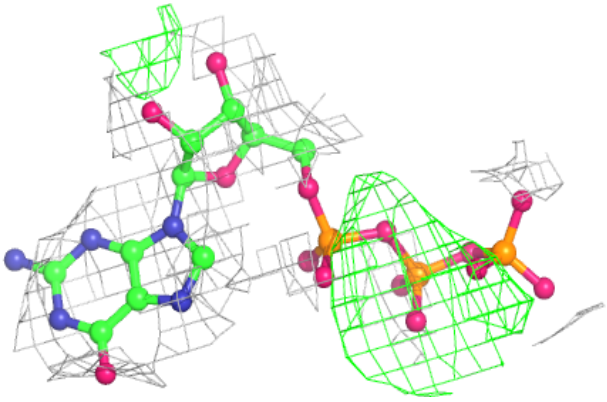


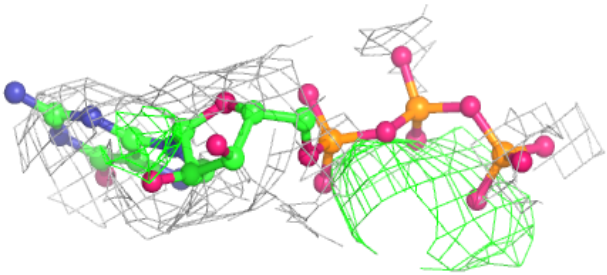


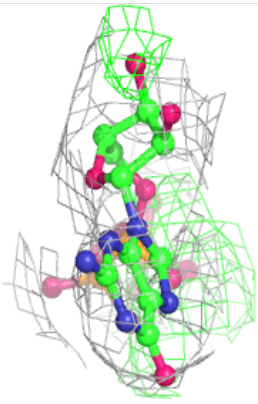


Electron density around GTP X 600:

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

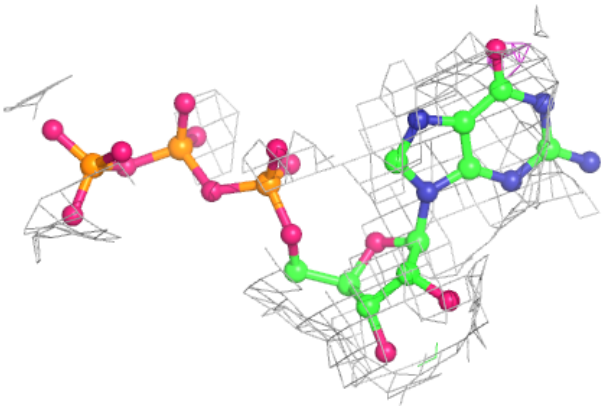


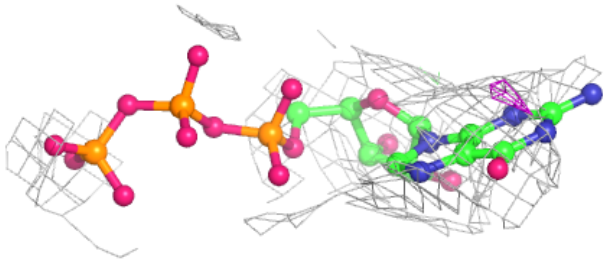


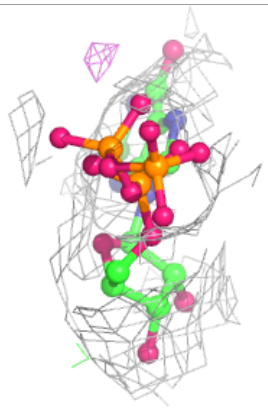


Electron density around GTP J 600:

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

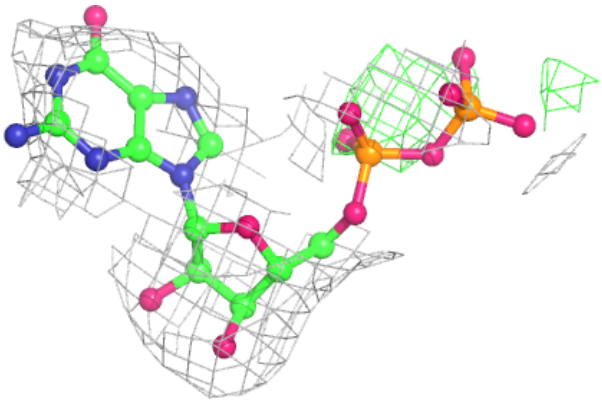


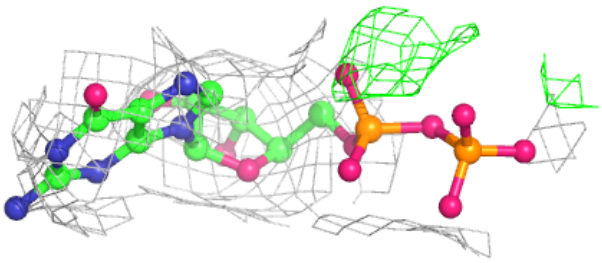


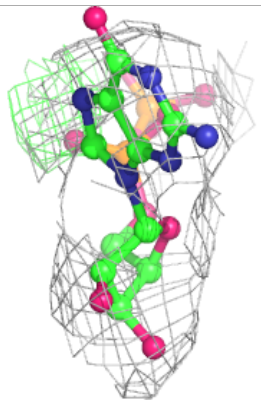


Electron density around GDP I 600:

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

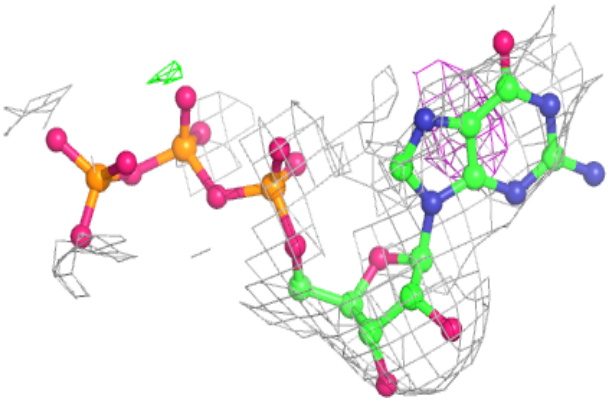


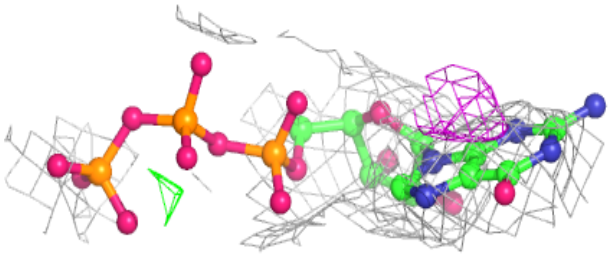


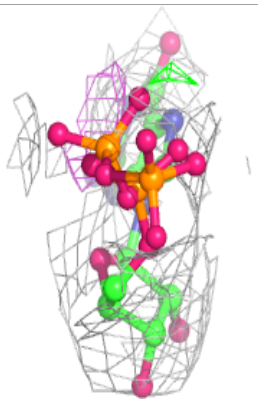


Electron density around GTP C 600:

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

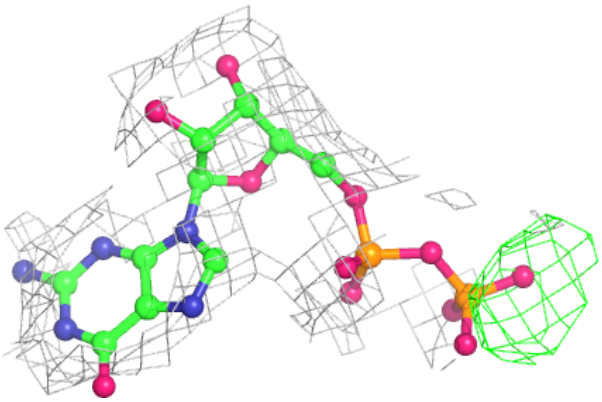


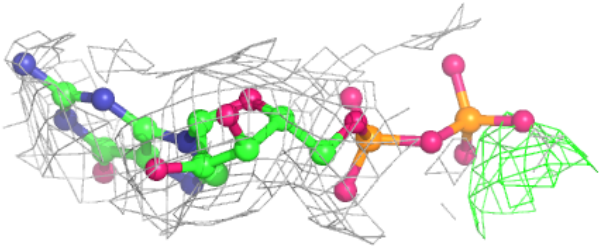


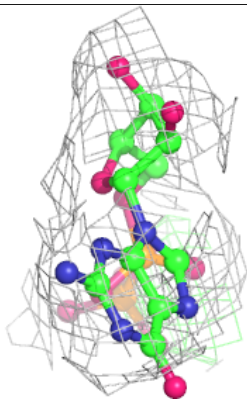


Electron density around GDP R 600:

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

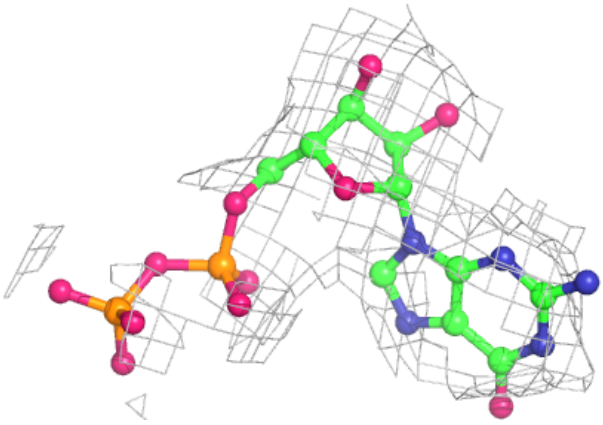


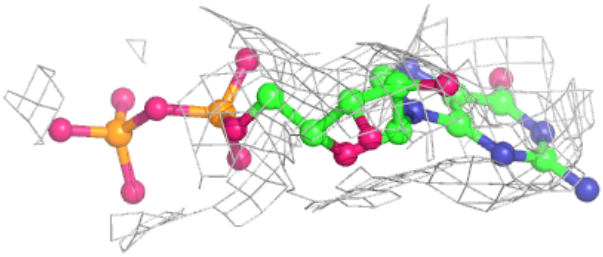


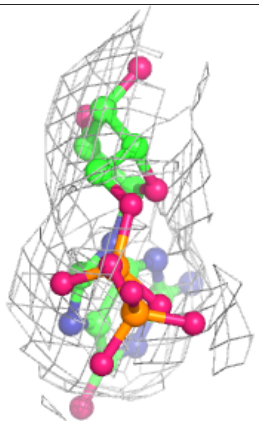


Electron density around GDP W 600:

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

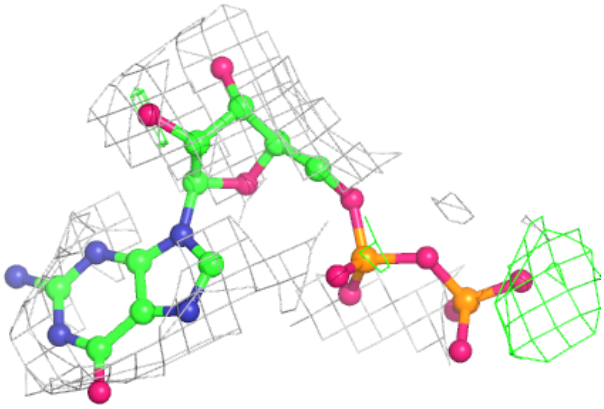


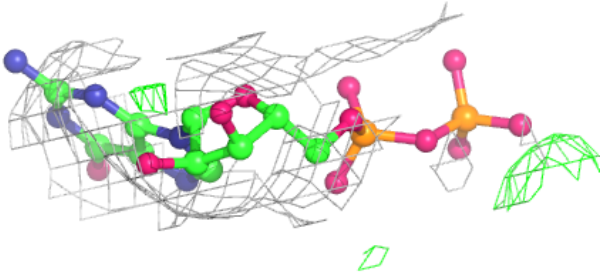


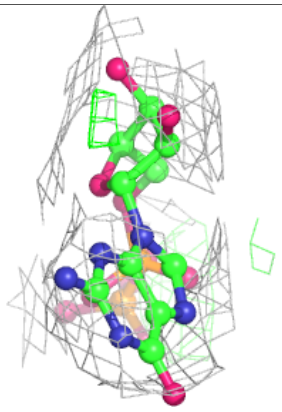


Electron density around GDP Y 600:

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

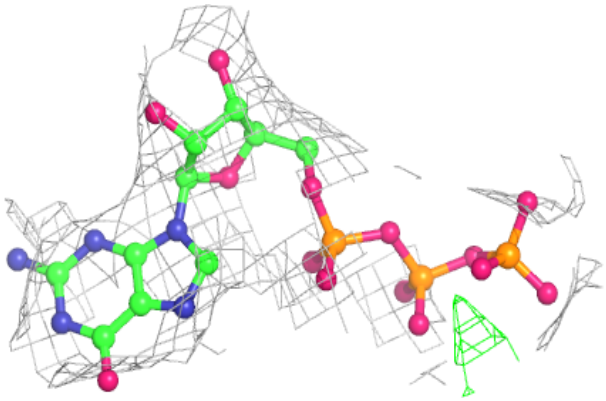


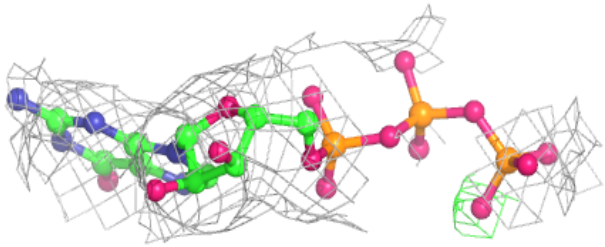


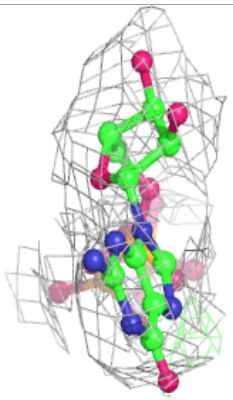


Electron density around GTP O 600:

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

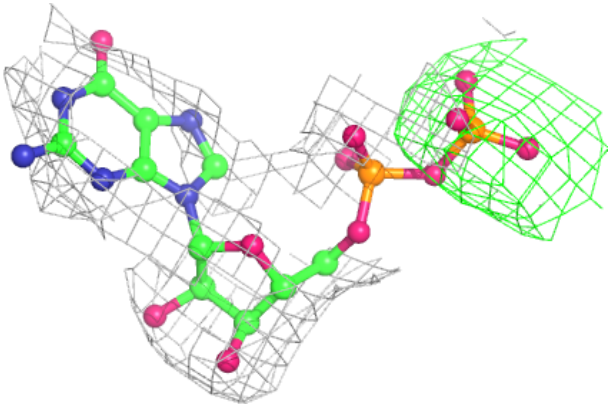


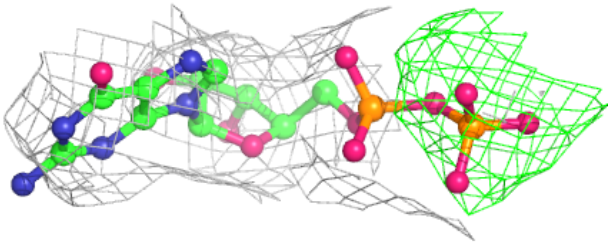


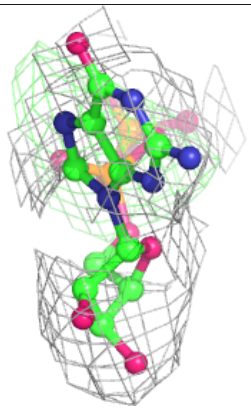


Electron density around GDP B 600:

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

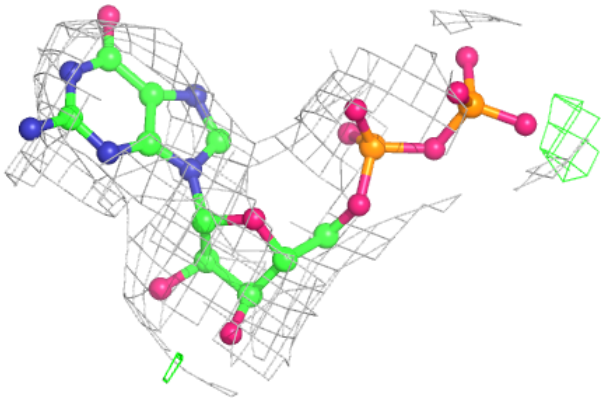


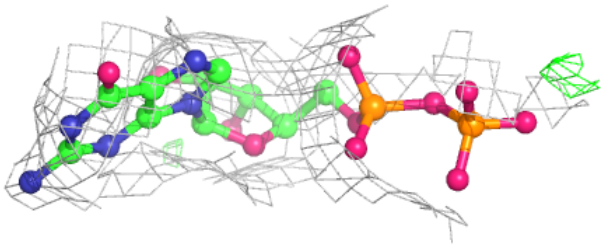


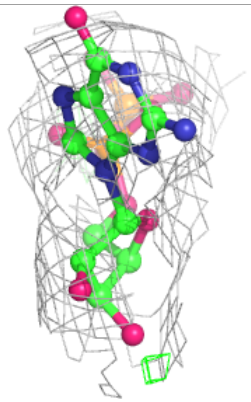


Electron density around GDP D 600:

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

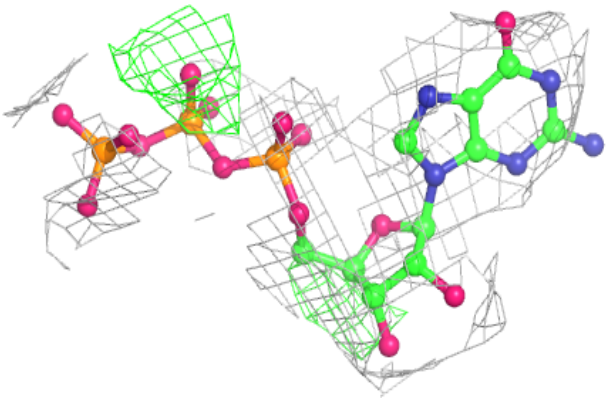


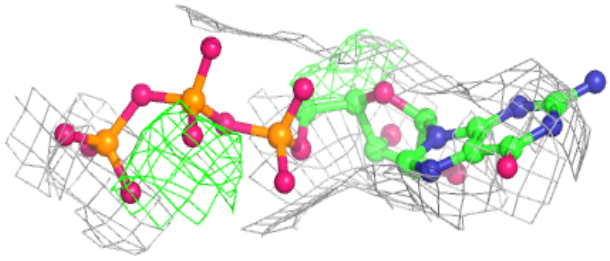


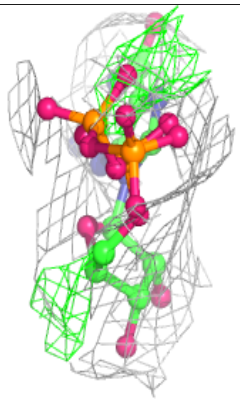


Electron density around GTP A 600:

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

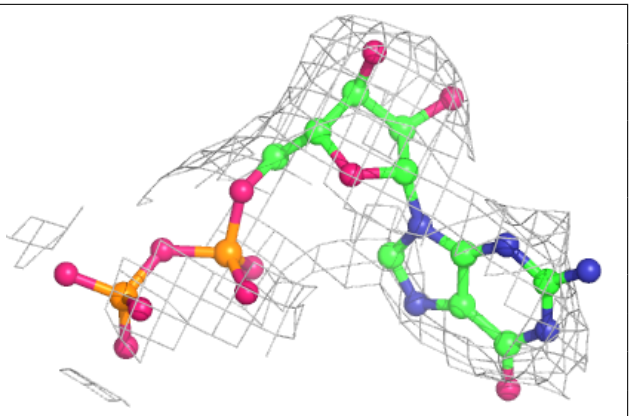


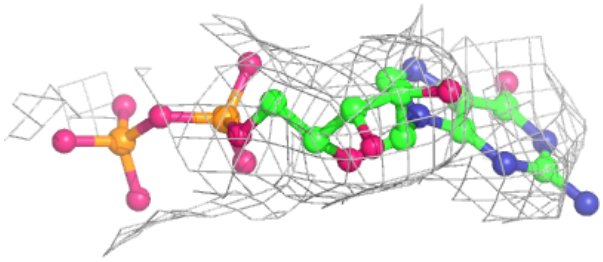


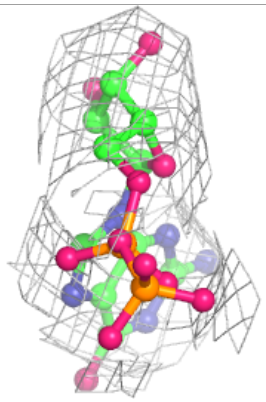


Electron density around GDP P 600:

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

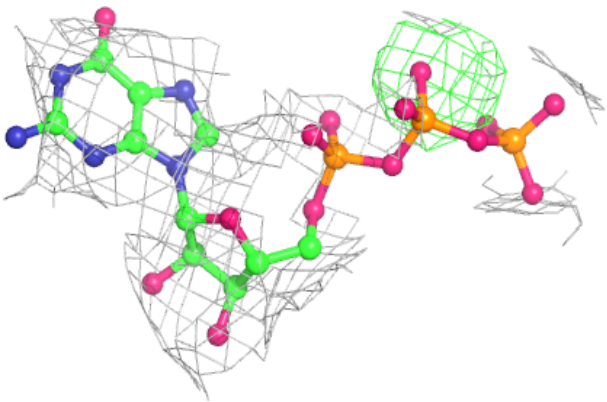


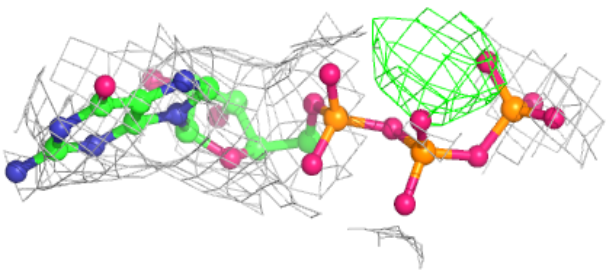


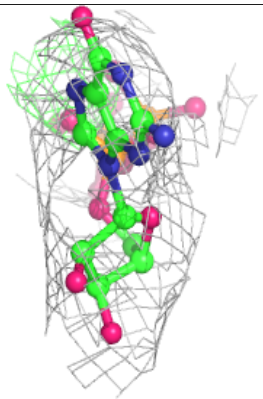


Electron density around GTP H 600:

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

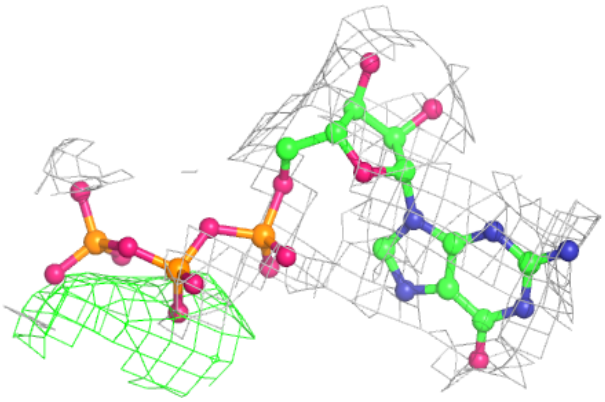


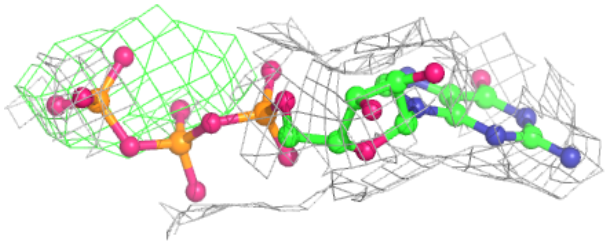


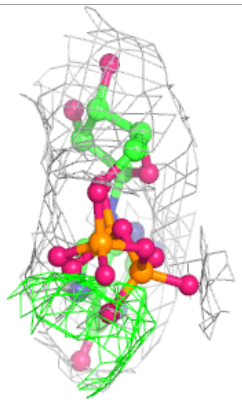


Electron density around GTP Q 600:

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

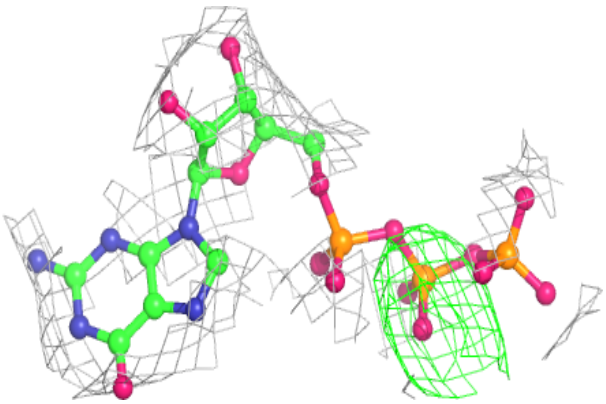


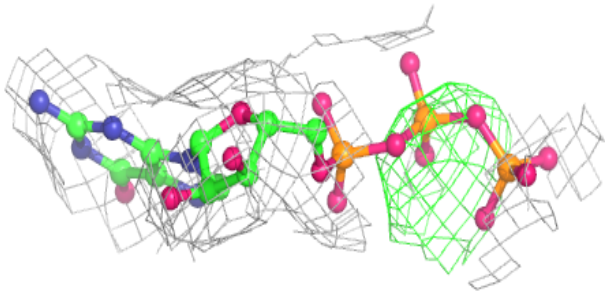


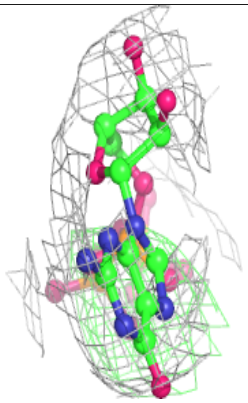


Electron density around GTP V 600:

$2mF_o$-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.