Full wwPDB X-ray Structure Validation Report (i)

Mar 3, 2024 – 08:30 PM EST

PDB ID	:	6MZE
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	:	3.60 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 (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:

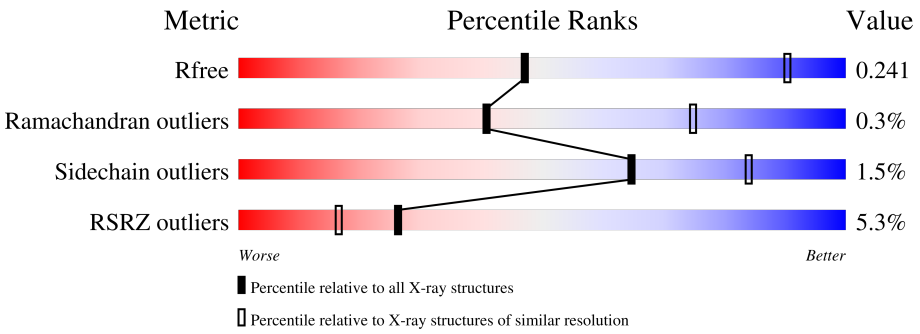
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.60 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	1257 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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	2% 93% • 6%
1	H	451	% 92% • 6%
1	J	451	8% 93% • 6%
1	O	451	12% 93% • 6%
1	Q	451	93% • 6%

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Mol	Chain	Length	Quality of chain
1	V	451	4% 93% 6%
1	X	451	9% 93% 6%
2	B	445	94% 5%
2	D	445	2% 93% 5%
2	I	445	2% 93% 5%
2	K	445	6% 94% 5%
2	P	445	93% 5%
2	R	445	% 94% 5%
2	W	445	% 94% 5%
2	Y	445	3% 94% 5%
3	E	536	% 89% 8%
3	L	536	2% 89% 8%
3	S	536	3% 88% 9%
3	Z	536	2% 89% 8%
4	F	169	3% 92% 8%
4	G	169	4% 92% 8%
4	M	169	29% 92% 8%
4	N	169	31% 92% 8%
4	T	169	29% 92% 8%
4	U	169	92% 8%
4	a	169	32% 91% 8%
4	b	169	12% 92% 8%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	MG	B	601	-	-	-	X
6	MG	R	601	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 77878 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
			Total	C	N	O	S			
1	A	423	3265	2068	553	623	21	0	0	0
1	C	423	3265	2068	553	623	21	0	0	0
1	H	423	3265	2068	553	623	21	0	0	0
1	J	423	3265	2068	553	623	21	0	0	0
1	O	423	3265	2068	553	623	21	0	0	0
1	Q	423	3265	2068	553	623	21	0	0	0
1	V	423	3265	2068	553	623	21	0	0	0
1	X	423	3265	2068	553	623	21	0	0	0

- Molecule 2 is a protein called Tubulin beta chain.

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

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

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

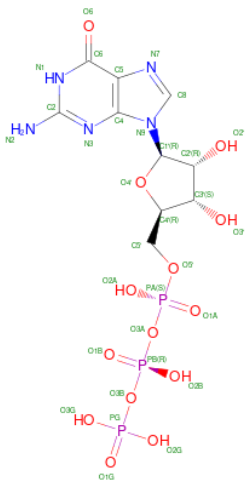
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	492	3936	2521	665	734	16	0	0	0
3	L	491	3924	2514	661	733	16	0	0	0
3	S	490	3922	2513	662	731	16	0	0	0
3	Z	492	3936	2521	665	734	16	0	0	0

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

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

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

GTP



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	32	10	5	14	3	0	0
5	C	1	32	10	5	14	3	0	0
5	H	1	32	10	5	14	3	0	0
5	J	1	32	10	5	14	3	0	0
5	O	1	32	10	5	14	3	0	0
5	Q	1	32	10	5	14	3	0	0
5	V	1	32	10	5	14	3	0	0
5	X	1	32	10	5	14	3	0	0

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

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

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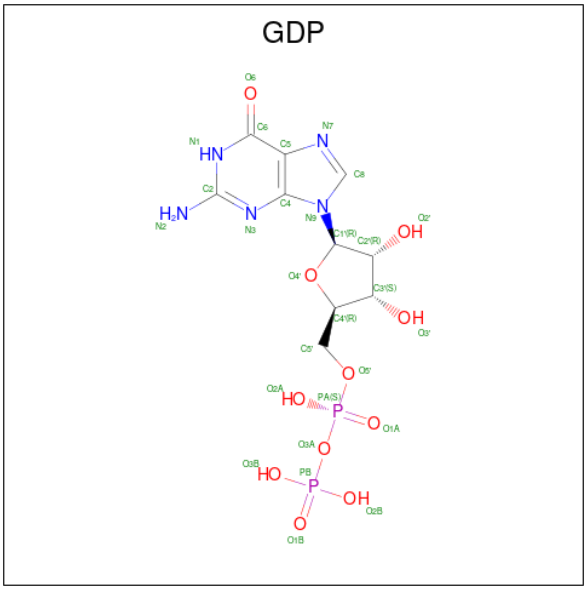
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total Mg 1 1	0	0
6	I	1	Total Mg 1 1	0	0
6	J	1	Total Mg 1 1	0	0
6	K	1	Total Mg 1 1	0	0
6	O	1	Total Mg 1 1	0	0
6	P	1	Total Mg 1 1	0	0
6	Q	1	Total Mg 1 1	0	0
6	R	1	Total Mg 1 1	0	0
6	V	1	Total Mg 1 1	0	0
6	W	1	Total Mg 1 1	0	0
6	X	1	Total Mg 1 1	0	0
6	Y	1	Total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

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



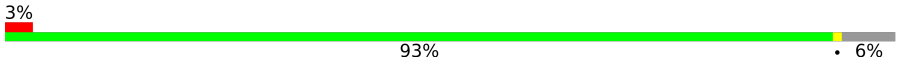
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
7	B	1	28	10	5	11	2	0	0
7	D	1	28	10	5	11	2	0	0
7	I	1	28	10	5	11	2	0	0
7	K	1	28	10	5	11	2	0	0
7	P	1	28	10	5	11	2	0	0
7	R	1	28	10	5	11	2	0	0
7	W	1	28	10	5	11	2	0	0
7	Y	1	28	10	5	11	2	0	0

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.

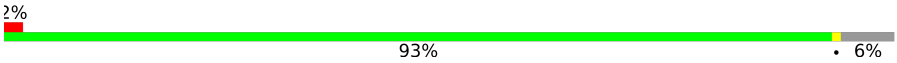
• Molecule 1: Tubulin alpha-1A chain

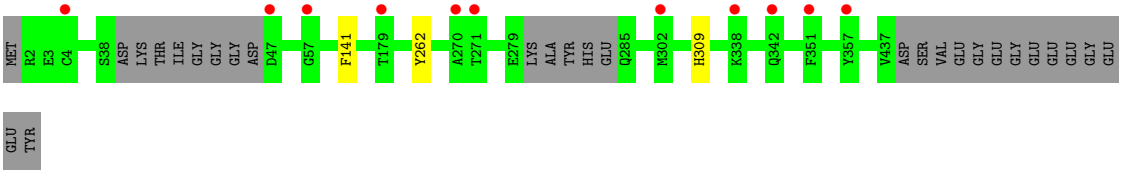
Chain A:



• Molecule 1: Tubulin alpha-1A chain

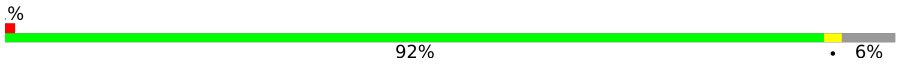
Chain C:

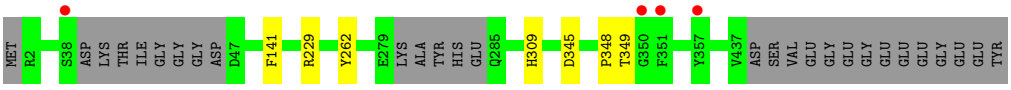




• Molecule 1: Tubulin alpha-1A chain

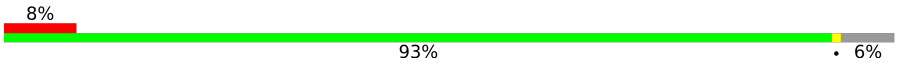
Chain H:

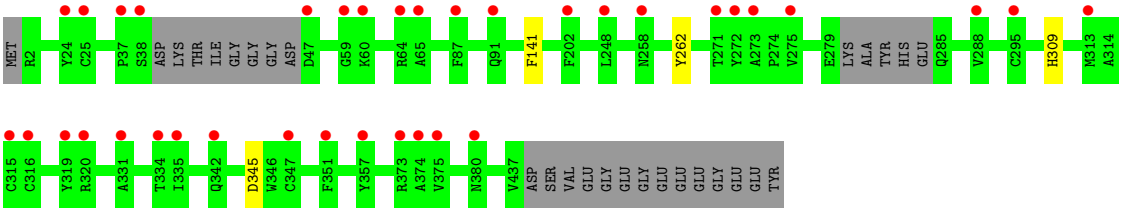




• Molecule 1: Tubulin alpha-1A chain

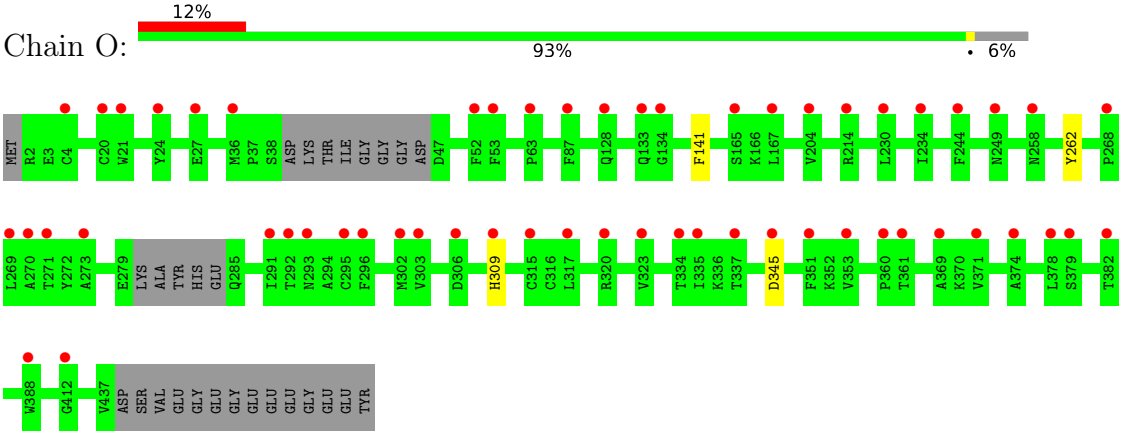
Chain J:





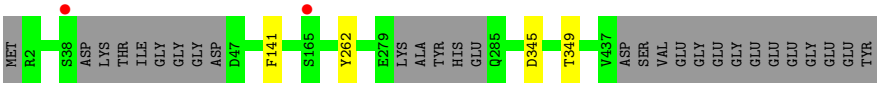
• Molecule 1: Tubulin alpha-1A chain

Chain O:



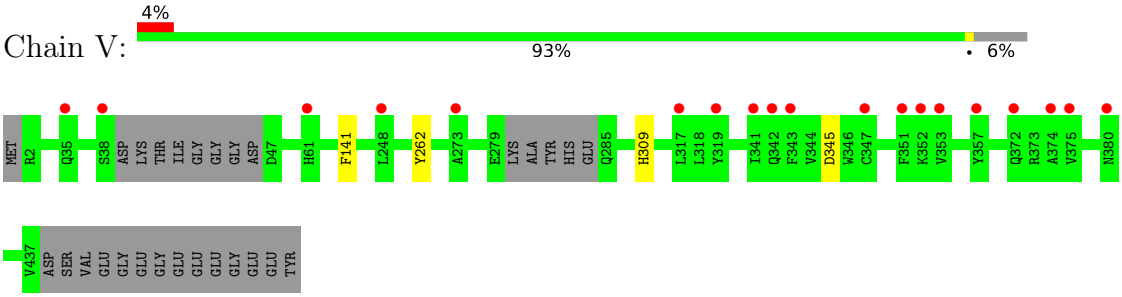
• Molecule 1: Tubulin alpha-1A chain

Chain Q:



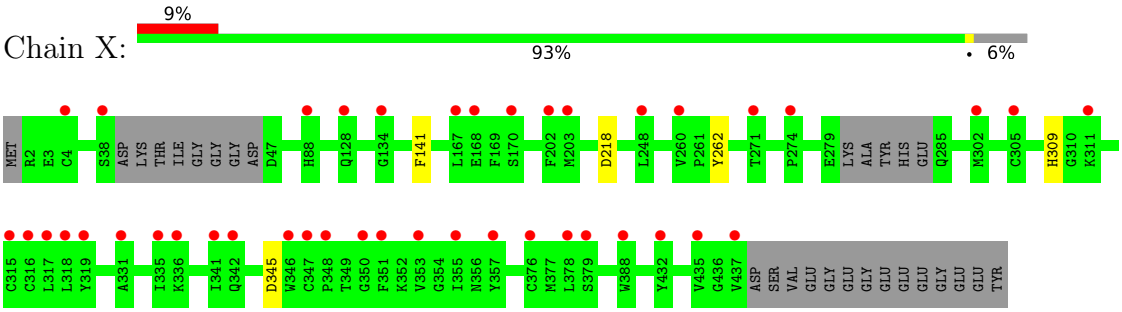
• Molecule 1: Tubulin alpha-1A chain

Chain V:



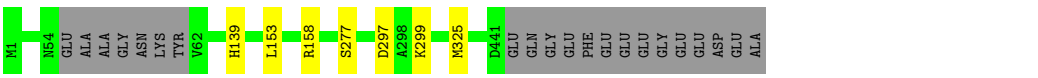
• Molecule 1: Tubulin alpha-1A chain

Chain X:



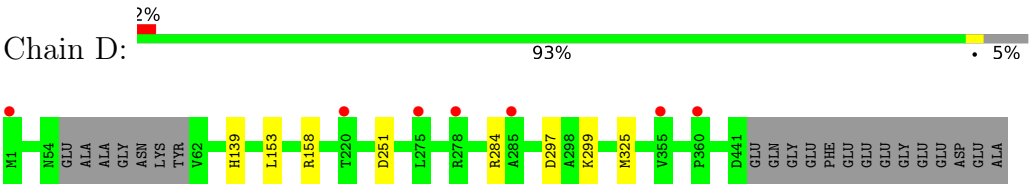
• Molecule 2: Tubulin beta chain

Chain B:



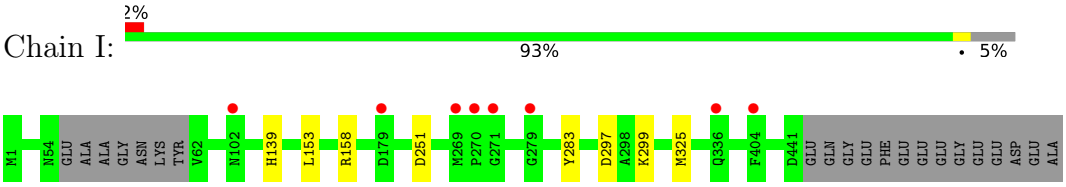
• Molecule 2: Tubulin beta chain

Chain D:



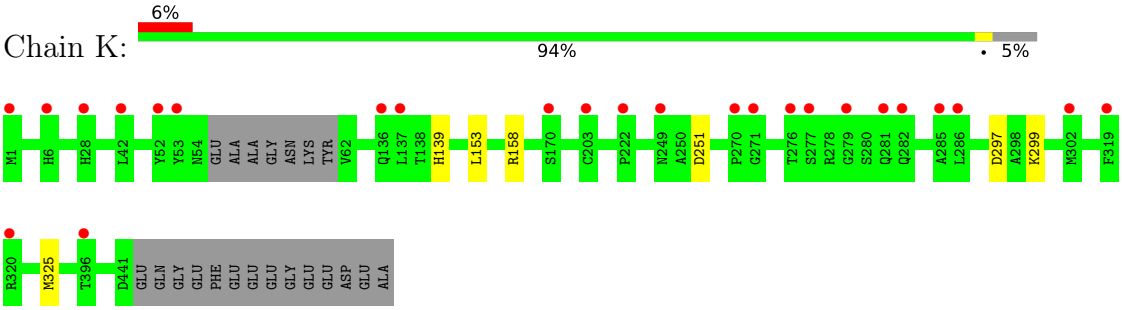
• Molecule 2: Tubulin beta chain

Chain I:



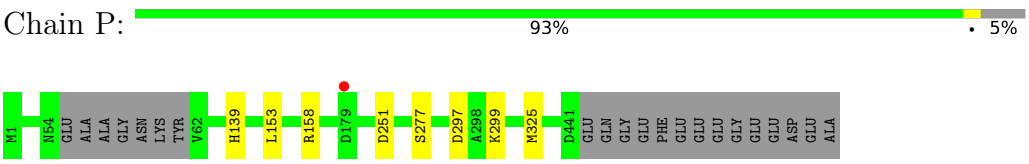
• Molecule 2: Tubulin beta chain

Chain K:



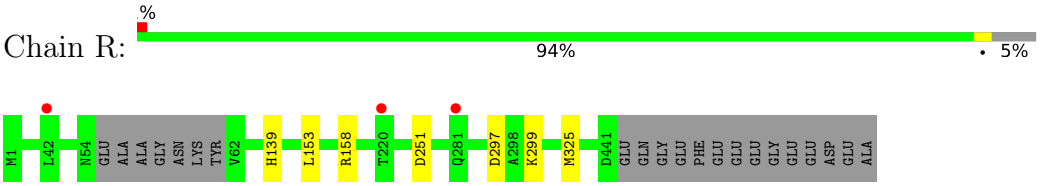
• Molecule 2: Tubulin beta chain

Chain P:



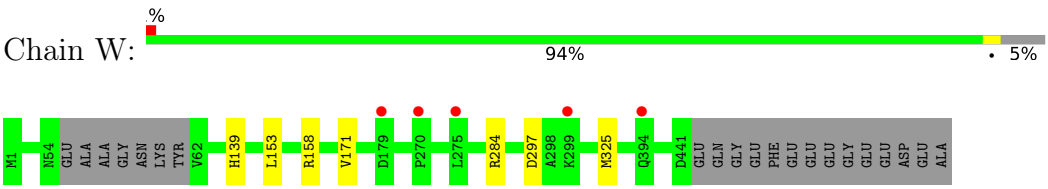
• Molecule 2: Tubulin beta chain

Chain R:



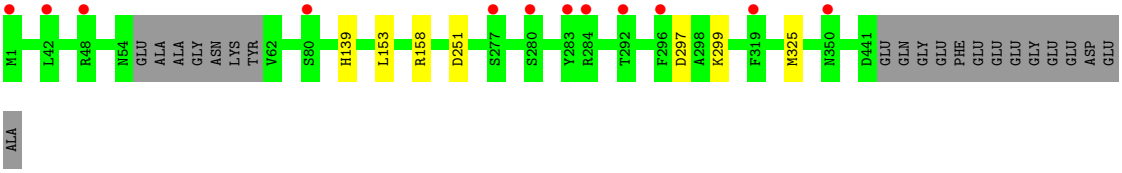
• Molecule 2: Tubulin beta chain

Chain W:



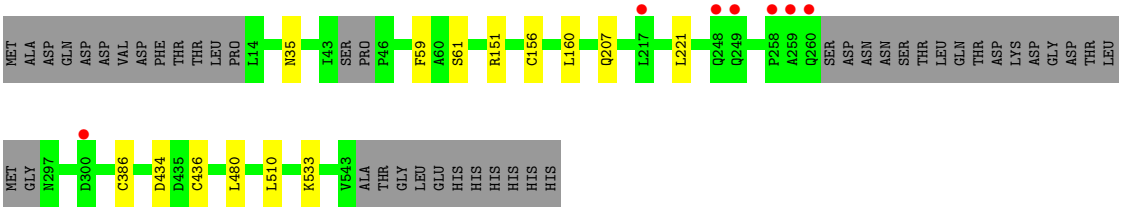
• Molecule 2: Tubulin beta chain

Chain Y:



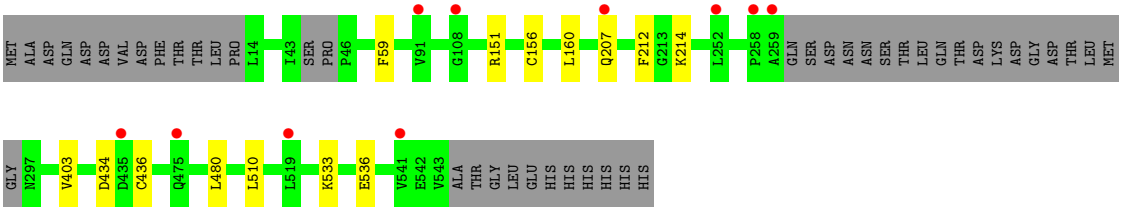
- Molecule 3: Protein Stu2p/Alp14p

Chain E:



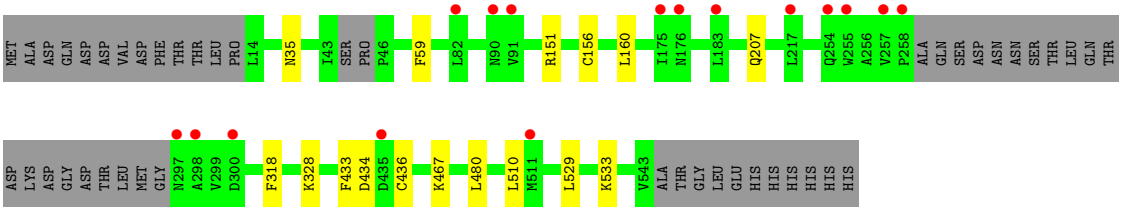
- Molecule 3: Protein Stu2p/Alp14p

Chain L:



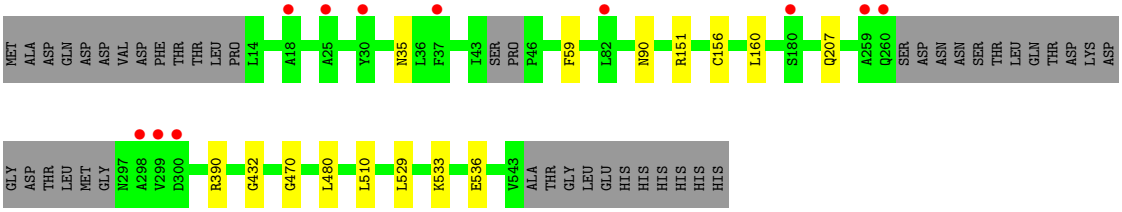
- Molecule 3: Protein Stu2p/Alp14p

Chain S:



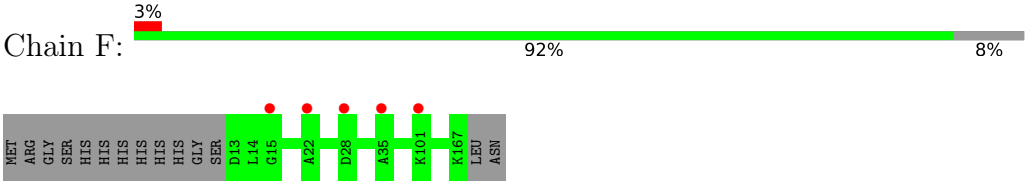
- Molecule 3: Protein Stu2p/Alp14p

Chain Z:



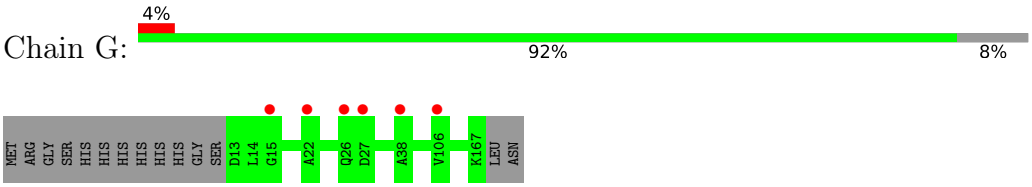
• Molecule 4: Designed ankyrin repeat protein (DARPIN) D1

Chain F:



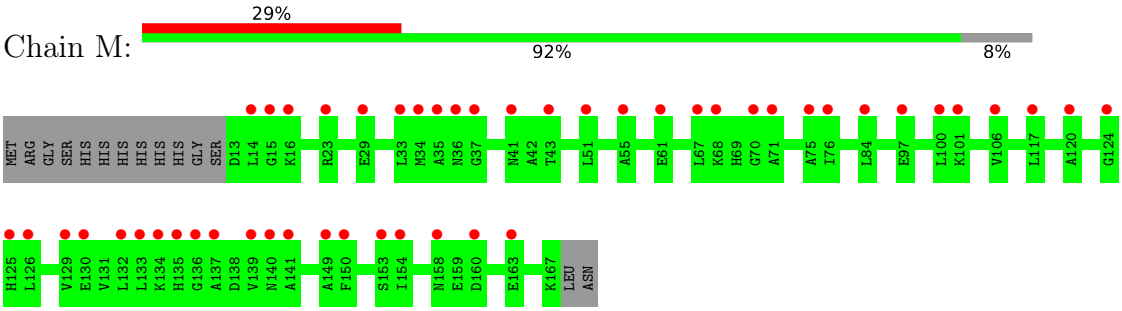
• Molecule 4: Designed ankyrin repeat protein (DARPIN) D1

Chain G:



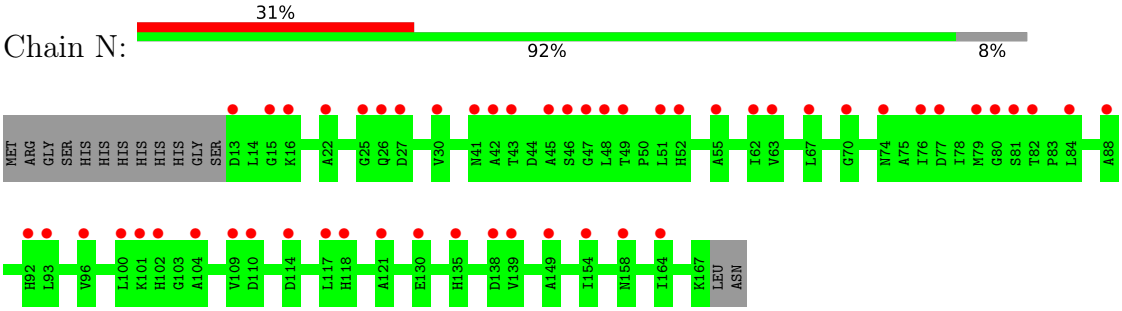
• Molecule 4: Designed ankyrin repeat protein (DARPIN) D1

Chain M:



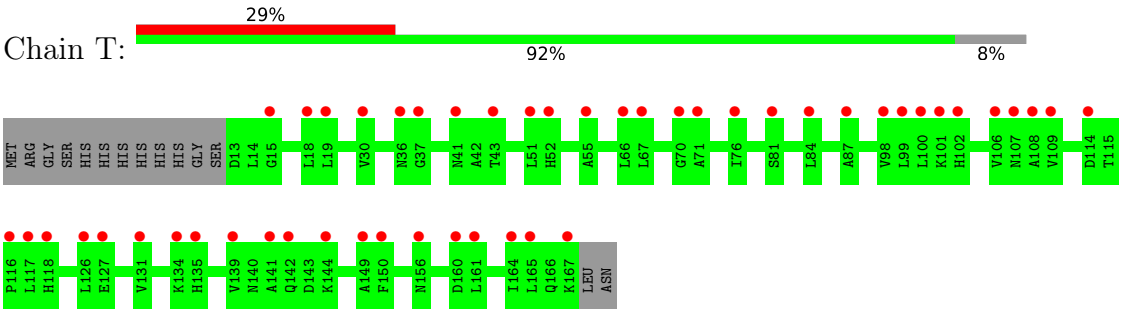
• Molecule 4: Designed ankyrin repeat protein (DARPIN) D1

Chain N:



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

Chain T:

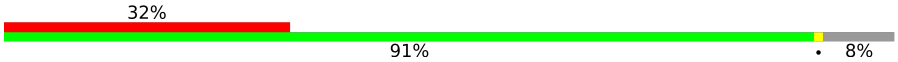


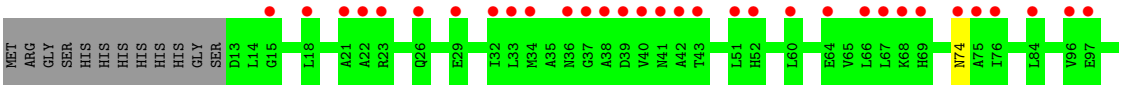
• Molecule 4: Designed ankyrin repeat protein (DARPIN) D1

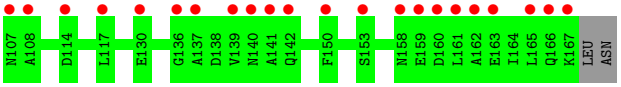
Chain U:

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

Chain a:

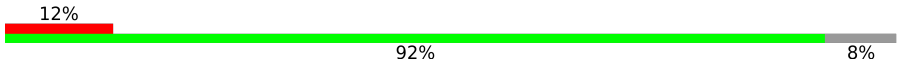


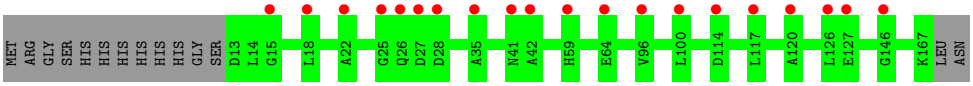




• Molecule 4: Designed ankyrin repeat protein (DARPIN) D1

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	218.48Å 106.15Å 282.23Å 90.00° 90.39° 90.00°	Depositor
Resolution (Å)	59.45 – 3.60 59.45 – 3.58	Depositor EDS
% Data completeness (in resolution range)	79.4 (59.45-3.60) 79.4 (59.45-3.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	2.96 (at 3.57Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.202 , 0.245 0.199 , 0.241	Depositor DCC
R_{free} test set	5975 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	81.4	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 92.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.004 for h,-k,-l	Xtriage
Reported twinning fraction	0.010 for h,-k,-l	Depositor
Outliers	1 of 121943 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	77878	wwPDB-VP
Average B, all atoms (Å^2)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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	0.41	0/4539
1	C	0.24	0/3339	0.41	0/4539
1	H	0.26	0/3339	0.42	0/4539
1	J	0.24	0/3339	0.41	0/4539
1	O	0.24	0/3339	0.41	0/4539
1	Q	0.24	0/3339	0.41	0/4539
1	V	0.24	0/3339	0.41	0/4539
1	X	0.24	0/3339	0.41	0/4539
2	B	0.26	0/3380	0.43	0/4581
2	D	0.25	0/3380	0.43	0/4581
2	I	0.25	0/3380	0.43	0/4581
2	K	0.25	0/3380	0.43	0/4581
2	P	0.25	0/3380	0.43	0/4581
2	R	0.25	0/3380	0.43	0/4581
2	W	0.26	0/3380	0.44	0/4581
2	Y	0.25	0/3380	0.42	0/4581
3	E	0.28	0/4009	0.50	0/5438
3	L	0.27	0/3997	0.50	0/5423
3	S	0.27	0/3995	0.49	0/5419
3	Z	0.28	0/4009	0.48	0/5438
4	F	0.24	0/1150	0.41	0/1565
4	G	0.24	0/1150	0.41	0/1565
4	M	0.24	0/1150	0.41	0/1565
4	N	0.25	0/1150	0.43	0/1565
4	T	0.23	0/1150	0.41	0/1565
4	U	0.24	0/1150	0.41	0/1565
4	a	0.26	0/1150	0.51	0/1565
4	b	0.24	0/1150	0.41	0/1565
All	All	0.25	0/78962	0.44	0/107198

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%)	389 (93%)	28 (7%)	0	100	100
1	C	417/451 (92%)	389 (93%)	28 (7%)	0	100	100
1	H	417/451 (92%)	387 (93%)	28 (7%)	2 (0%)	29	68
1	J	417/451 (92%)	389 (93%)	28 (7%)	0	100	100
1	O	417/451 (92%)	387 (93%)	30 (7%)	0	100	100
1	Q	417/451 (92%)	388 (93%)	28 (7%)	1 (0%)	47	79
1	V	417/451 (92%)	389 (93%)	28 (7%)	0	100	100
1	X	417/451 (92%)	389 (93%)	28 (7%)	0	100	100
2	B	420/445 (94%)	403 (96%)	16 (4%)	1 (0%)	47	79
2	D	420/445 (94%)	403 (96%)	15 (4%)	2 (0%)	29	68
2	I	420/445 (94%)	402 (96%)	16 (4%)	2 (0%)	29	68
2	K	420/445 (94%)	403 (96%)	16 (4%)	1 (0%)	47	79
2	P	420/445 (94%)	403 (96%)	16 (4%)	1 (0%)	47	79
2	R	420/445 (94%)	404 (96%)	15 (4%)	1 (0%)	47	79
2	W	420/445 (94%)	402 (96%)	16 (4%)	2 (0%)	29	68
2	Y	420/445 (94%)	404 (96%)	15 (4%)	1 (0%)	47	79
3	E	486/536 (91%)	448 (92%)	36 (7%)	2 (0%)	34	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L	485/536 (90%)	448 (92%)	35 (7%)	2 (0%)	34	71
3	S	484/536 (90%)	449 (93%)	30 (6%)	5 (1%)	15	55
3	Z	486/536 (91%)	453 (93%)	29 (6%)	4 (1%)	19	59
4	F	153/169 (90%)	145 (95%)	8 (5%)	0	100	100
4	G	153/169 (90%)	145 (95%)	8 (5%)	0	100	100
4	M	153/169 (90%)	145 (95%)	8 (5%)	0	100	100
4	N	153/169 (90%)	145 (95%)	8 (5%)	0	100	100
4	T	153/169 (90%)	145 (95%)	8 (5%)	0	100	100
4	U	153/169 (90%)	145 (95%)	8 (5%)	0	100	100
4	a	153/169 (90%)	140 (92%)	12 (8%)	1 (1%)	22	61
4	b	153/169 (90%)	145 (95%)	8 (5%)	0	100	100
All	All	9861/10664 (92%)	9284 (94%)	549 (6%)	28 (0%)	41	75

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	349	THR
2	I	283	TYR
2	W	284	ARG
2	D	284	ARG
3	S	467	LYS
3	Z	432	GLY
2	K	297	ASP
1	Q	349	THR
2	R	297	ASP
3	Z	90	ASN
2	B	297	ASP
2	D	297	ASP
2	I	297	ASP
2	P	297	ASP
3	S	318	PHE
3	S	433	PHE
2	W	297	ASP
2	Y	297	ASP
4	a	74	ASN
3	E	434	ASP
3	E	480	LEU
3	L	480	LEU

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Mol	Chain	Res	Type
3	S	434	ASP
3	S	480	LEU
3	Z	470	GLY
3	Z	480	LEU
3	L	434	ASP
1	H	348	PRO

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%)	342 (99%)	4 (1%)	71	87
1	C	346/377 (92%)	343 (99%)	3 (1%)	78	90
1	H	346/377 (92%)	341 (99%)	5 (1%)	67	85
1	J	346/377 (92%)	342 (99%)	4 (1%)	71	87
1	O	346/377 (92%)	342 (99%)	4 (1%)	71	87
1	Q	346/377 (92%)	343 (99%)	3 (1%)	78	90
1	V	346/377 (92%)	342 (99%)	4 (1%)	71	87
1	X	346/377 (92%)	341 (99%)	5 (1%)	67	85
2	B	361/381 (95%)	355 (98%)	6 (2%)	60	82
2	D	361/381 (95%)	355 (98%)	6 (2%)	60	82
2	I	361/381 (95%)	355 (98%)	6 (2%)	60	82
2	K	361/381 (95%)	355 (98%)	6 (2%)	60	82
2	P	361/381 (95%)	354 (98%)	7 (2%)	57	80
2	R	361/381 (95%)	355 (98%)	6 (2%)	60	82
2	W	361/381 (95%)	356 (99%)	5 (1%)	67	85
2	Y	361/381 (95%)	355 (98%)	6 (2%)	60	82
3	E	448/488 (92%)	436 (97%)	12 (3%)	44	73
3	L	447/488 (92%)	435 (97%)	12 (3%)	44	73
3	S	447/488 (92%)	436 (98%)	11 (2%)	47	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Z	448/488 (92%)	437 (98%)	11 (2%)	47	75
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	116/132 (88%)	116 (100%)	0	100	100
4	b	116/132 (88%)	116 (100%)	0	100	100
All	All	8374/9072 (92%)	8248 (98%)	126 (2%)	65	84

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	PHE
1	A	262	TYR
1	A	309	HIS
1	A	345	ASP
2	B	139	HIS
2	B	153	LEU
2	B	158	ARG
2	B	277	SER
2	B	299	LYS
2	B	325	MET
1	C	141	PHE
1	C	262	TYR
1	C	309	HIS
2	D	139	HIS
2	D	153	LEU
2	D	158	ARG
2	D	251	ASP
2	D	299	LYS
2	D	325	MET
3	E	35	ASN
3	E	59	PHE
3	E	61	SER
3	E	151	ARG
3	E	156	CYS
3	E	160	LEU

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Mol	Chain	Res	Type
3	E	207	GLN
3	E	221	LEU
3	E	386	CYS
3	E	436	CYS
3	E	510	LEU
3	E	533	LYS
1	H	141	PHE
1	H	229	ARG
1	H	262	TYR
1	H	309	HIS
1	H	345	ASP
2	I	139	HIS
2	I	153	LEU
2	I	158	ARG
2	I	251	ASP
2	I	299	LYS
2	I	325	MET
1	J	141	PHE
1	J	262	TYR
1	J	309	HIS
1	J	345	ASP
2	K	139	HIS
2	K	153	LEU
2	K	158	ARG
2	K	251	ASP
2	K	299	LYS
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	214	LYS
3	L	403	VAL
3	L	436	CYS
3	L	510	LEU
3	L	533	LYS
3	L	536	GLU
1	O	141	PHE
1	O	262	TYR
1	O	309	HIS

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Mol	Chain	Res	Type
1	O	345	ASP
2	P	139	HIS
2	P	153	LEU
2	P	158	ARG
2	P	251	ASP
2	P	277	SER
2	P	299	LYS
2	P	325	MET
1	Q	141	PHE
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	299	LYS
2	R	325	MET
3	S	35	ASN
3	S	59	PHE
3	S	151	ARG
3	S	156	CYS
3	S	160	LEU
3	S	207	GLN
3	S	328	LYS
3	S	436	CYS
3	S	510	LEU
3	S	529	LEU
3	S	533	LYS
1	V	141	PHE
1	V	262	TYR
1	V	309	HIS
1	V	345	ASP
2	W	139	HIS
2	W	153	LEU
2	W	158	ARG
2	W	171	VAL
2	W	325	MET
1	X	141	PHE
1	X	218	ASP
1	X	262	TYR
1	X	309	HIS
1	X	345	ASP

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Mol	Chain	Res	Type
2	Y	139	HIS
2	Y	153	LEU
2	Y	158	ARG
2	Y	251	ASP
2	Y	299	LYS
2	Y	325	MET
3	Z	35	ASN
3	Z	59	PHE
3	Z	151	ARG
3	Z	156	CYS
3	Z	160	LEU
3	Z	207	GLN
3	Z	390	ARG
3	Z	510	LEU
3	Z	529	LEU
3	Z	533	LYS
3	Z	536	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	E	90	ASN
1	O	216	ASN
3	S	90	ASN
3	Z	249	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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	B	600	6	24,30,30	0.93	1 (4%)	30,47,47	1.11	3 (10%)
5	GTP	J	600	6	26,34,34	1.12	2 (7%)	32,54,54	1.58	7 (21%)
5	GTP	X	600	6	26,34,34	1.13	2 (7%)	32,54,54	1.57	7 (21%)
5	GTP	O	600	6	26,34,34	1.12	2 (7%)	32,54,54	1.58	7 (21%)
5	GTP	C	600	6	26,34,34	1.12	2 (7%)	32,54,54	1.59	7 (21%)
5	GTP	A	600	6	26,34,34	1.13	2 (7%)	32,54,54	1.60	7 (21%)
7	GDP	K	600	6	24,30,30	0.94	1 (4%)	30,47,47	1.09	3 (10%)
7	GDP	D	600	6	24,30,30	0.93	1 (4%)	30,47,47	1.08	3 (10%)
5	GTP	H	600	6	26,34,34	1.18	2 (7%)	32,54,54	2.08	7 (21%)
7	GDP	W	600	6	24,30,30	0.92	1 (4%)	30,47,47	1.08	3 (10%)
5	GTP	V	600	6	26,34,34	1.12	2 (7%)	32,54,54	1.57	7 (21%)
7	GDP	Y	600	6	24,30,30	0.95	1 (4%)	30,47,47	1.08	3 (10%)
7	GDP	R	600	6	24,30,30	0.93	1 (4%)	30,47,47	1.13	3 (10%)
5	GTP	Q	600	6	26,34,34	1.13	2 (7%)	32,54,54	1.60	7 (21%)
7	GDP	I	600	6	24,30,30	0.93	1 (4%)	30,47,47	1.10	3 (10%)
7	GDP	P	600	6	24,30,30	0.92	1 (4%)	30,47,47	1.12	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	B	600	6	-	3/12/32/32	0/3/3/3
5	GTP	J	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	O	600	6	-	3/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	C	600	6	-	2/18/38/38	0/3/3/3
5	GTP	A	600	6	-	2/18/38/38	0/3/3/3
7	GDP	K	600	6	-	3/12/32/32	0/3/3/3
7	GDP	D	600	6	-	3/12/32/32	0/3/3/3
5	GTP	H	600	6	-	2/18/38/38	0/3/3/3
7	GDP	W	600	6	-	4/12/32/32	0/3/3/3
5	GTP	V	600	6	-	1/18/38/38	0/3/3/3
7	GDP	Y	600	6	-	3/12/32/32	0/3/3/3
7	GDP	R	600	6	-	3/12/32/32	0/3/3/3
5	GTP	Q	600	6	-	2/18/38/38	0/3/3/3
7	GDP	I	600	6	-	4/12/32/32	0/3/3/3
7	GDP	P	600	6	-	3/12/32/32	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	600	GTP	C5-C6	-4.03	1.39	1.47
5	X	600	GTP	C5-C6	-3.99	1.39	1.47
5	V	600	GTP	C5-C6	-3.97	1.39	1.47
5	Q	600	GTP	C5-C6	-3.95	1.39	1.47
5	O	600	GTP	C5-C6	-3.95	1.39	1.47
5	J	600	GTP	C5-C6	-3.92	1.39	1.47
5	C	600	GTP	C5-C6	-3.91	1.39	1.47
5	H	600	GTP	C5-C6	-3.69	1.39	1.47
5	H	600	GTP	C2-N3	2.65	1.39	1.33
7	Y	600	GDP	C6-N1	-2.29	1.34	1.37
7	B	600	GDP	C6-N1	-2.25	1.34	1.37
7	D	600	GDP	C6-N1	-2.22	1.34	1.37
7	R	600	GDP	C6-N1	-2.22	1.34	1.37
7	W	600	GDP	C6-N1	-2.21	1.34	1.37
7	K	600	GDP	C6-N1	-2.18	1.34	1.37
7	P	600	GDP	C6-N1	-2.18	1.34	1.37
5	X	600	GTP	C2-N3	2.15	1.38	1.33
5	C	600	GTP	C2-N3	2.15	1.38	1.33
5	V	600	GTP	C2-N3	2.14	1.38	1.33
5	Q	600	GTP	C2-N3	2.14	1.38	1.33
5	J	600	GTP	C2-N3	2.13	1.38	1.33
7	I	600	GDP	C6-N1	-2.11	1.34	1.37
5	A	600	GTP	C2-N3	2.10	1.38	1.33
5	O	600	GTP	C2-N3	2.07	1.38	1.33

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	600	GTP	C2-N1-C6	-5.76	114.49	125.10
5	H	600	GTP	C5-C6-N1	4.75	122.34	113.95
5	H	600	GTP	PA-O3A-PB	-4.16	118.57	132.83
5	H	600	GTP	O6-C6-C5	-4.03	116.49	124.37
5	V	600	GTP	PA-O3A-PB	-3.79	119.82	132.83
5	C	600	GTP	PA-O3A-PB	-3.78	119.84	132.83
5	X	600	GTP	PA-O3A-PB	-3.78	119.86	132.83
5	O	600	GTP	PA-O3A-PB	-3.78	119.87	132.83
5	A	600	GTP	PA-O3A-PB	-3.76	119.92	132.83
5	Q	600	GTP	PA-O3A-PB	-3.75	119.95	132.83
5	J	600	GTP	PA-O3A-PB	-3.74	120.00	132.83
5	H	600	GTP	PB-O3B-PG	-3.36	121.31	132.83
5	J	600	GTP	PB-O3B-PG	-3.33	121.41	132.83
5	O	600	GTP	PB-O3B-PG	-3.32	121.43	132.83
5	A	600	GTP	PB-O3B-PG	-3.31	121.46	132.83
5	V	600	GTP	PB-O3B-PG	-3.30	121.51	132.83
5	Q	600	GTP	C5-C6-N1	3.29	119.77	113.95
5	V	600	GTP	C5-C6-N1	3.29	119.76	113.95
5	H	600	GTP	C3'-C2'-C1'	3.28	105.92	100.98
5	Q	600	GTP	PB-O3B-PG	-3.28	121.58	132.83
5	A	600	GTP	C5-C6-N1	3.28	119.74	113.95
5	X	600	GTP	PB-O3B-PG	-3.27	121.59	132.83
5	O	600	GTP	C5-C6-N1	3.25	119.69	113.95
5	C	600	GTP	C5-C6-N1	3.22	119.63	113.95
5	C	600	GTP	PB-O3B-PG	-3.21	121.80	132.83
5	J	600	GTP	C5-C6-N1	3.20	119.61	113.95
5	X	600	GTP	C5-C6-N1	3.19	119.59	113.95
5	C	600	GTP	C8-N7-C5	2.88	108.47	102.99
5	O	600	GTP	C2-N1-C6	-2.87	119.82	125.10
5	J	600	GTP	C8-N7-C5	2.86	108.45	102.99
5	V	600	GTP	C8-N7-C5	2.86	108.43	102.99
5	X	600	GTP	C8-N7-C5	2.85	108.42	102.99
5	O	600	GTP	C8-N7-C5	2.85	108.42	102.99
5	Q	600	GTP	C8-N7-C5	2.85	108.41	102.99
7	W	600	GDP	PA-O3A-PB	-2.85	123.06	132.83
5	A	600	GTP	C8-N7-C5	2.84	108.41	102.99
7	R	600	GDP	PA-O3A-PB	-2.84	123.07	132.83
7	I	600	GDP	PA-O3A-PB	-2.84	123.08	132.83
5	A	600	GTP	C2-N1-C6	-2.84	119.87	125.10
7	K	600	GDP	PA-O3A-PB	-2.82	123.14	132.83
7	D	600	GDP	PA-O3A-PB	-2.80	123.22	132.83
7	P	600	GDP	PA-O3A-PB	-2.80	123.22	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	600	GDP	PA-O3A-PB	-2.78	123.28	132.83
5	J	600	GTP	C2-N1-C6	-2.76	120.01	125.10
7	Y	600	GDP	PA-O3A-PB	-2.75	123.40	132.83
5	V	600	GTP	C2-N1-C6	-2.75	120.04	125.10
5	Q	600	GTP	C2-N1-C6	-2.72	120.08	125.10
5	X	600	GTP	C2-N1-C6	-2.72	120.08	125.10
5	C	600	GTP	C2-N1-C6	-2.67	120.17	125.10
5	H	600	GTP	C8-N7-C5	2.63	108.00	102.99
7	I	600	GDP	C5-C6-N1	2.53	118.42	113.95
7	Y	600	GDP	C5-C6-N1	2.51	118.39	113.95
7	R	600	GDP	C5-C6-N1	2.50	118.36	113.95
7	P	600	GDP	C5-C6-N1	2.48	118.33	113.95
7	K	600	GDP	C5-C6-N1	2.47	118.31	113.95
7	W	600	GDP	C5-C6-N1	2.42	118.22	113.95
7	B	600	GDP	C5-C6-N1	2.40	118.19	113.95
7	D	600	GDP	C5-C6-N1	2.37	118.13	113.95
5	A	600	GTP	O6-C6-C5	-2.30	119.87	124.37
7	R	600	GDP	C8-N7-C5	2.30	107.37	102.99
7	P	600	GDP	C8-N7-C5	2.30	107.37	102.99
5	C	600	GTP	C3'-C2'-C1'	2.28	104.41	100.98
7	Y	600	GDP	C8-N7-C5	2.28	107.33	102.99
7	K	600	GDP	C8-N7-C5	2.27	107.31	102.99
5	X	600	GTP	O6-C6-C5	-2.27	119.95	124.37
5	X	600	GTP	C3'-C2'-C1'	2.25	104.37	100.98
7	I	600	GDP	C8-N7-C5	2.25	107.27	102.99
5	Q	600	GTP	O6-C6-C5	-2.24	119.99	124.37
7	D	600	GDP	C8-N7-C5	2.24	107.26	102.99
7	W	600	GDP	C8-N7-C5	2.24	107.26	102.99
7	B	600	GDP	C8-N7-C5	2.24	107.26	102.99
5	O	600	GTP	O6-C6-C5	-2.23	120.02	124.37
5	V	600	GTP	C3'-C2'-C1'	2.22	104.32	100.98
5	V	600	GTP	O6-C6-C5	-2.21	120.05	124.37
5	A	600	GTP	C3'-C2'-C1'	2.20	104.29	100.98
5	J	600	GTP	O6-C6-C5	-2.20	120.08	124.37
5	O	600	GTP	C3'-C2'-C1'	2.18	104.26	100.98
5	J	600	GTP	C3'-C2'-C1'	2.18	104.25	100.98
5	Q	600	GTP	C3'-C2'-C1'	2.17	104.24	100.98
5	C	600	GTP	O6-C6-C5	-2.15	120.17	124.37

There are no chirality outliers.

All (43) torsion outliers are listed below:

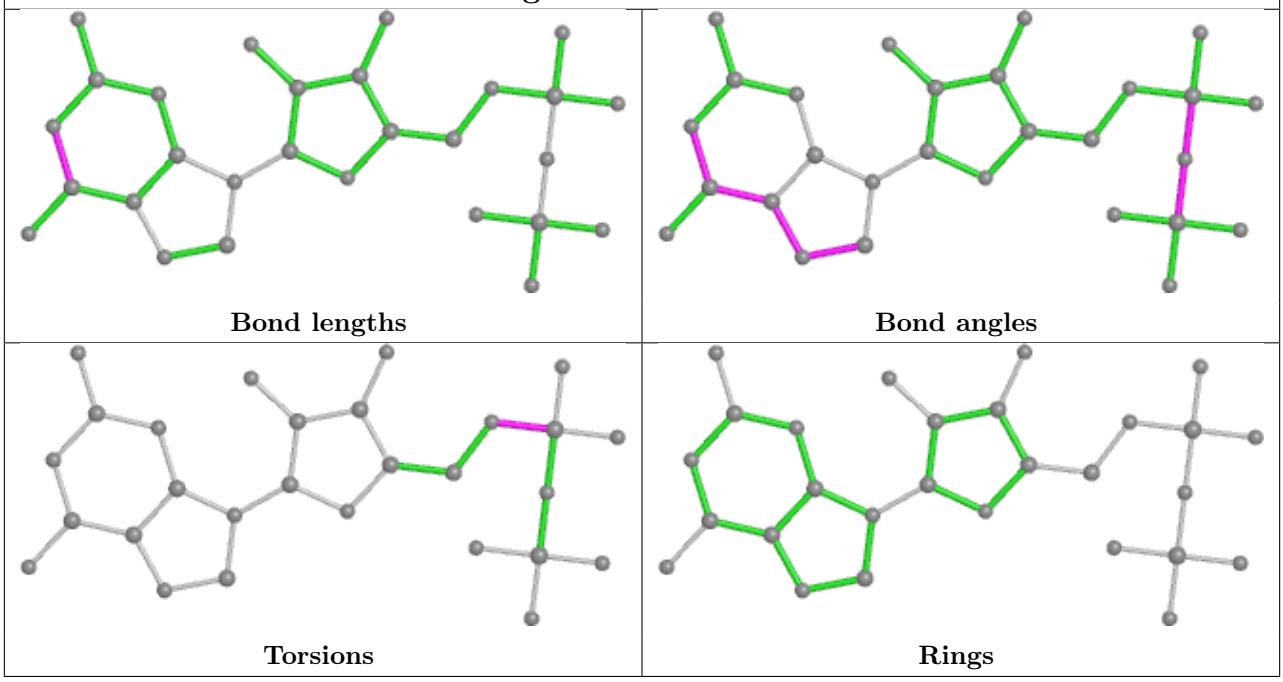
Mol	Chain	Res	Type	Atoms
5	A	600	GTP	PB-O3B-PG-O2G
5	C	600	GTP	PB-O3B-PG-O2G
5	J	600	GTP	PB-O3B-PG-O2G
5	O	600	GTP	PB-O3B-PG-O2G
5	Q	600	GTP	PB-O3B-PG-O2G
5	X	600	GTP	PB-O3B-PG-O2G
7	B	600	GDP	C5'-O5'-PA-O1A
7	B	600	GDP	C5'-O5'-PA-O2A
7	D	600	GDP	C5'-O5'-PA-O1A
7	D	600	GDP	C5'-O5'-PA-O2A
7	I	600	GDP	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	X	600	GTP	PB-O3B-PG-O1G
5	A	600	GTP	PB-O3B-PG-O1G
5	C	600	GTP	PB-O3B-PG-O1G
5	J	600	GTP	PB-O3B-PG-O1G
5	Q	600	GTP	PB-O3B-PG-O1G
5	H	600	GTP	PB-O3B-PG-O2G
5	O	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
7	I	600	GDP	PB-O3A-PA-O1A
7	W	600	GDP	PB-O3A-PA-O1A
5	H	600	GTP	PB-O3B-PG-O1G
5	O	600	GTP	PB-O3B-PG-O1G

There are no ring outliers.

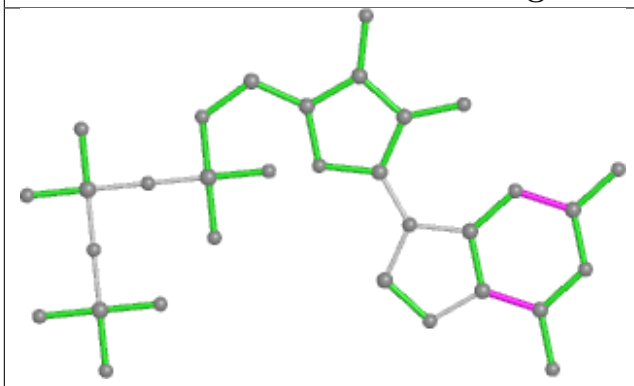
No monomer is involved in short contacts.

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.

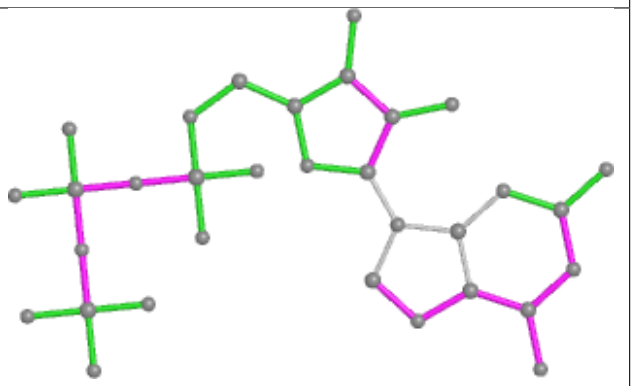
Ligand GDP B 600



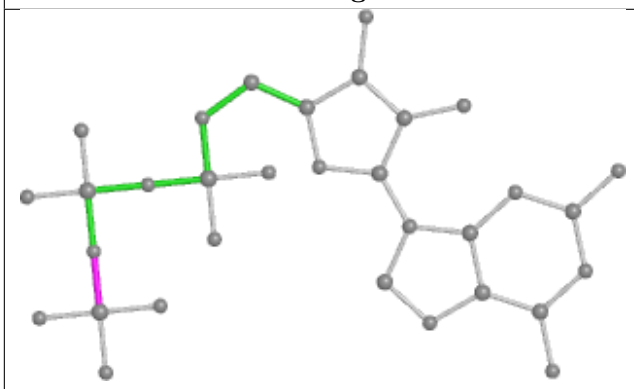
Ligand GTP J 600



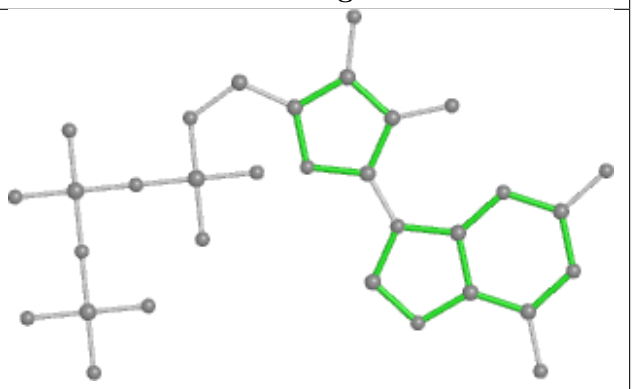
Bond lengths



Bond angles

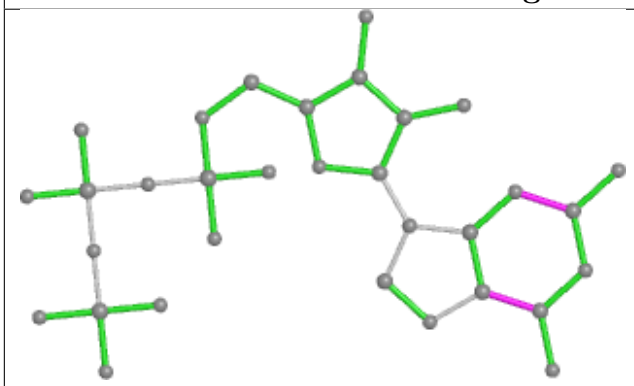


Torsions



Rings

Ligand GTP X 600



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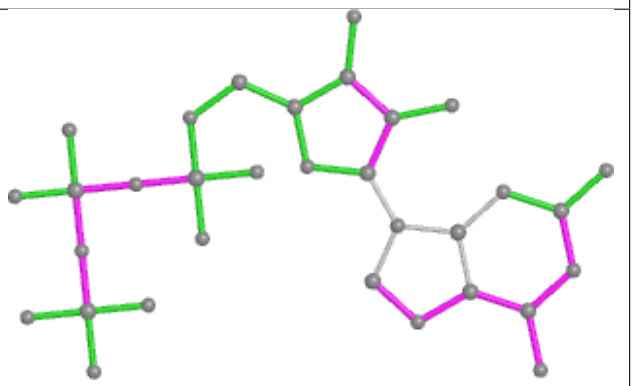

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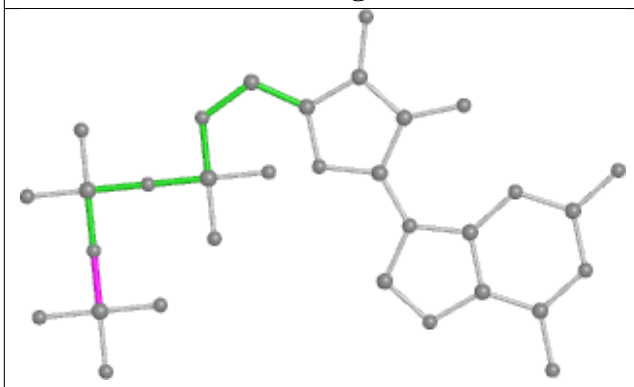

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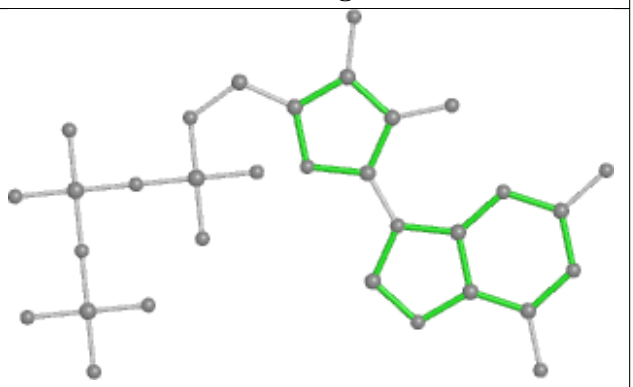
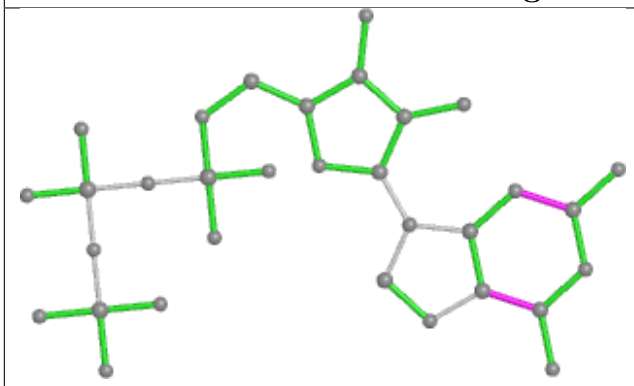
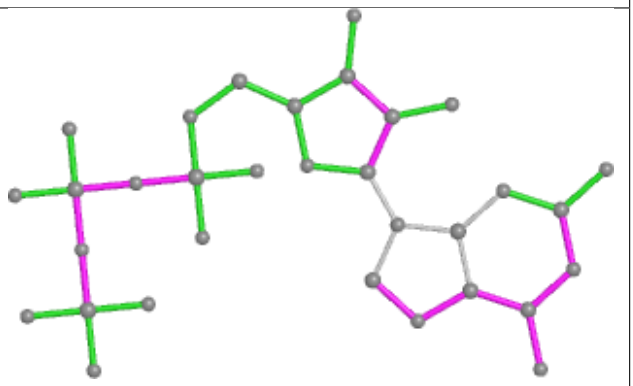


Rings

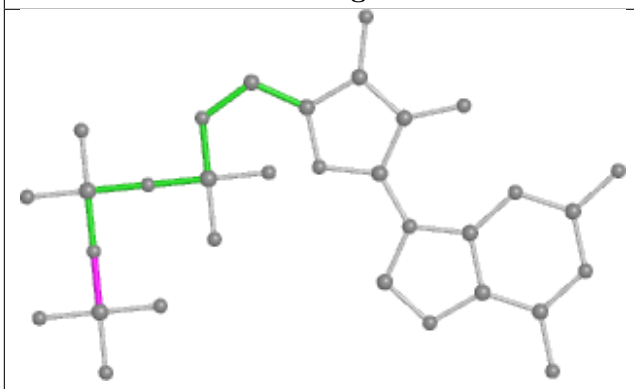
Ligand GTP O 600



Bond lengths



Bond angles



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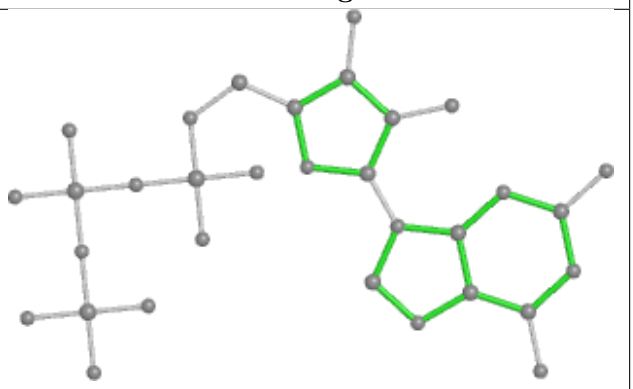

Rings

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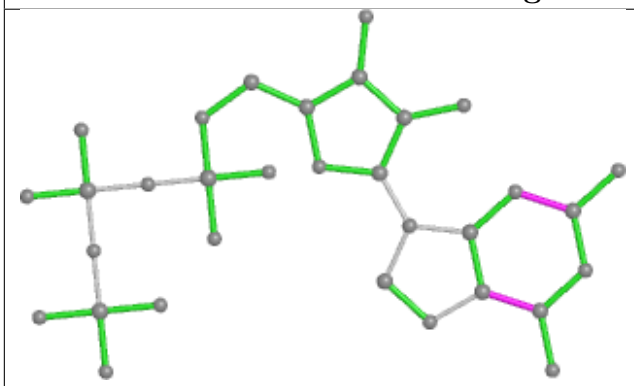

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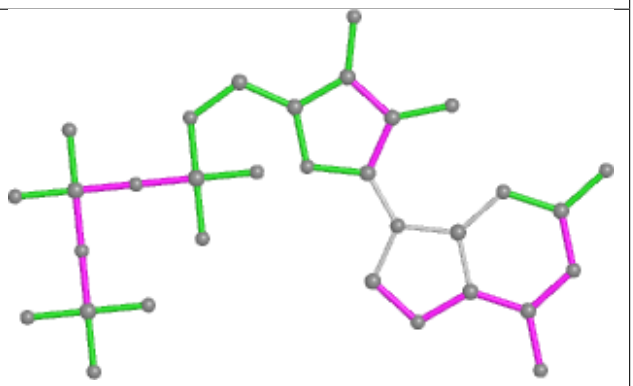
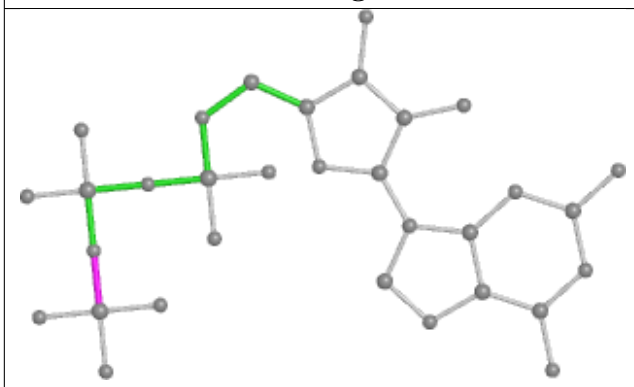


Bond angles



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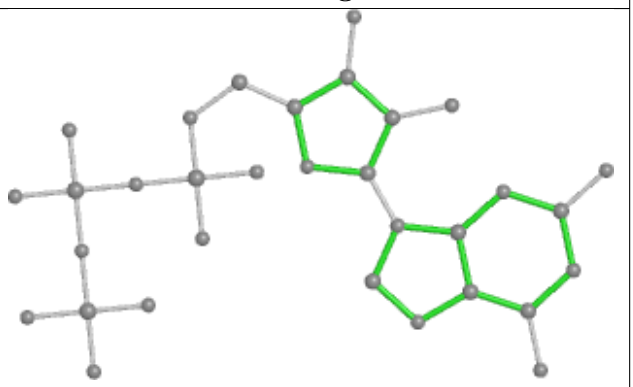
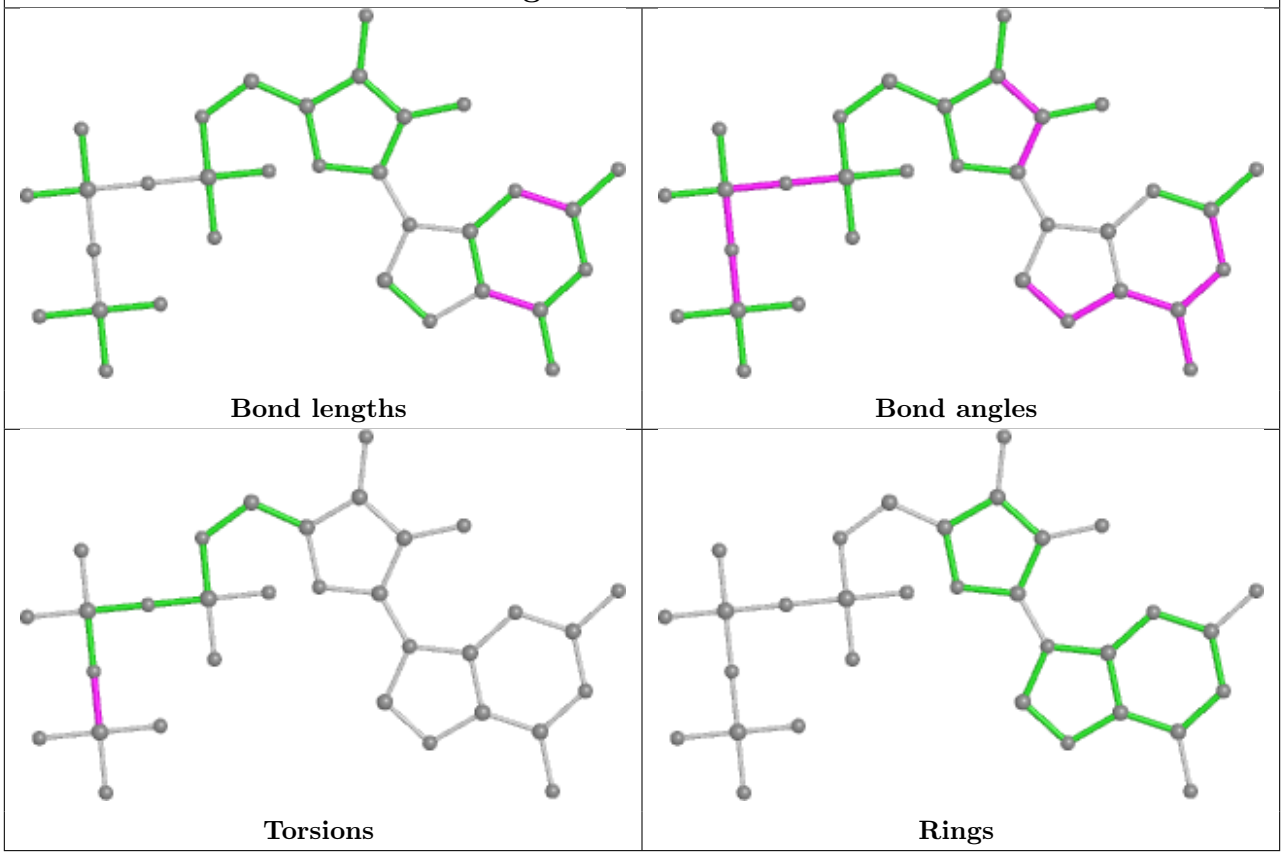


Rings

Ligand GTP A 600



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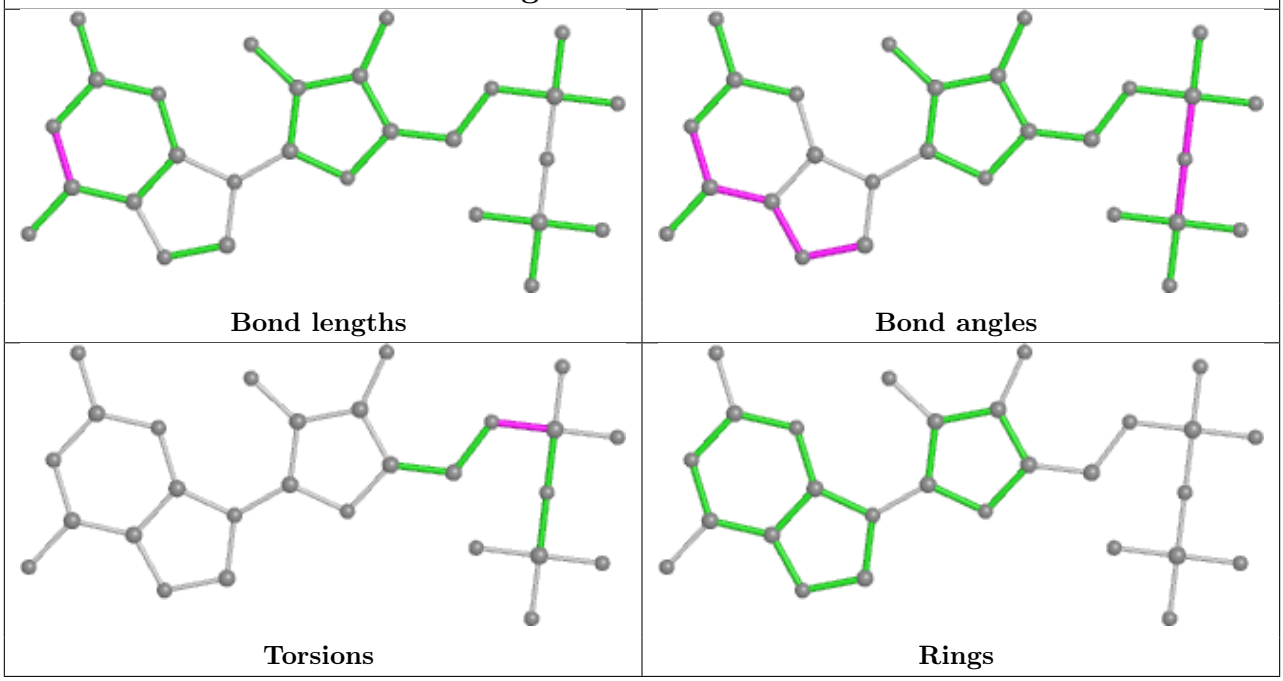

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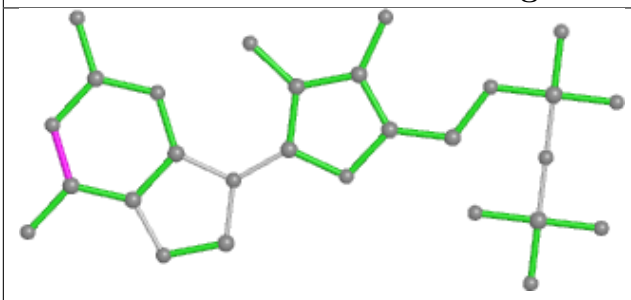
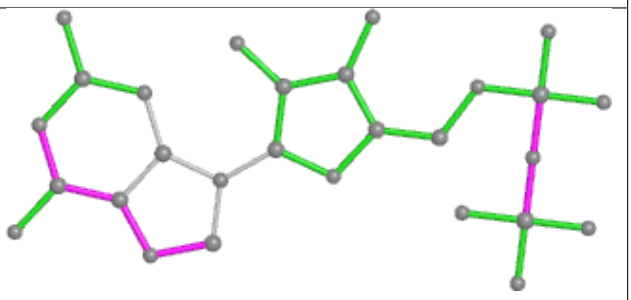
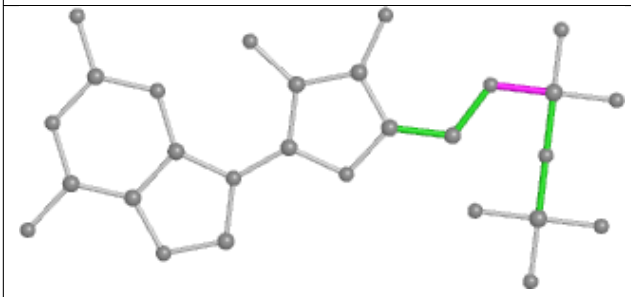


Bond lengths



Bond angles



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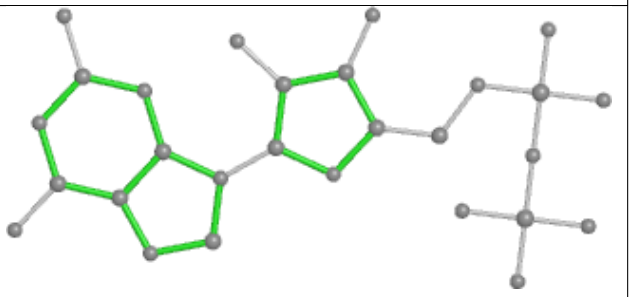

Rings

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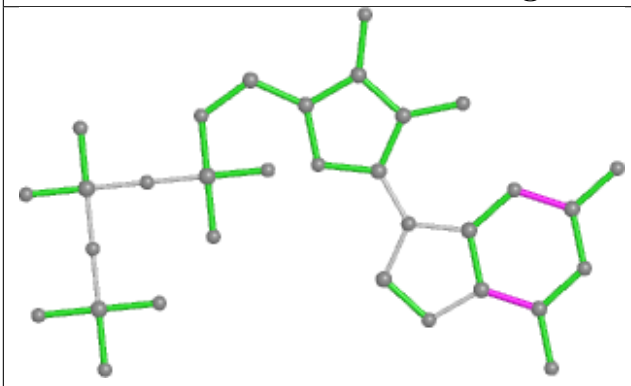
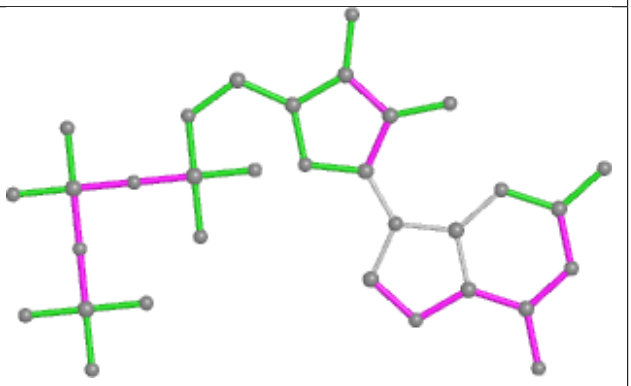
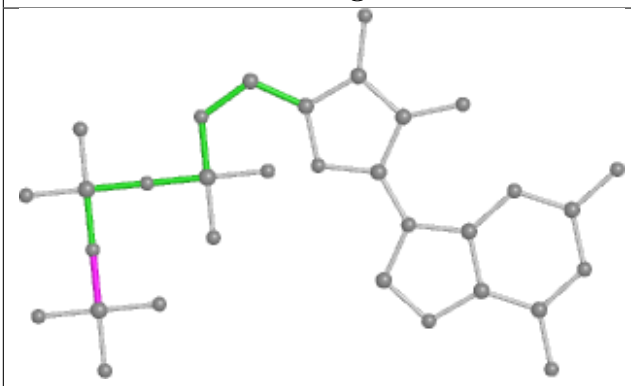


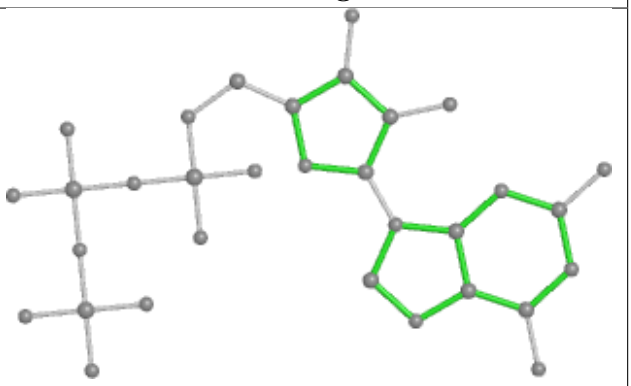
Bond lengths



Bond angles

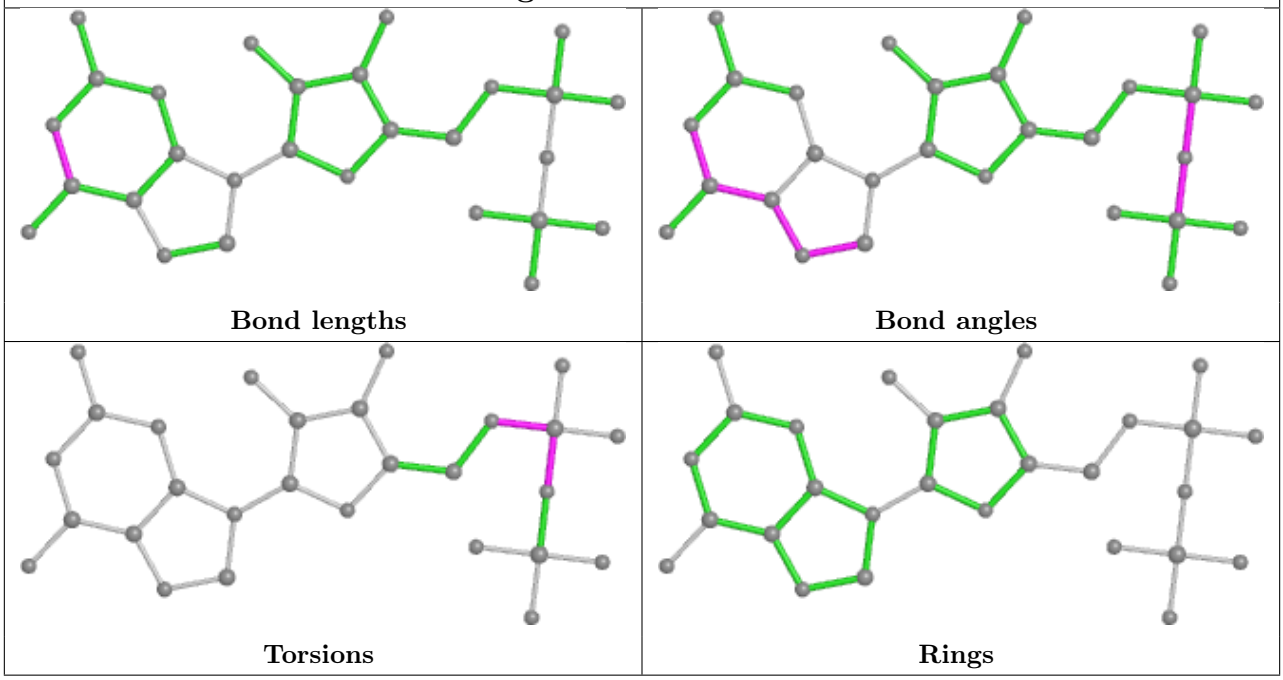


Torsions

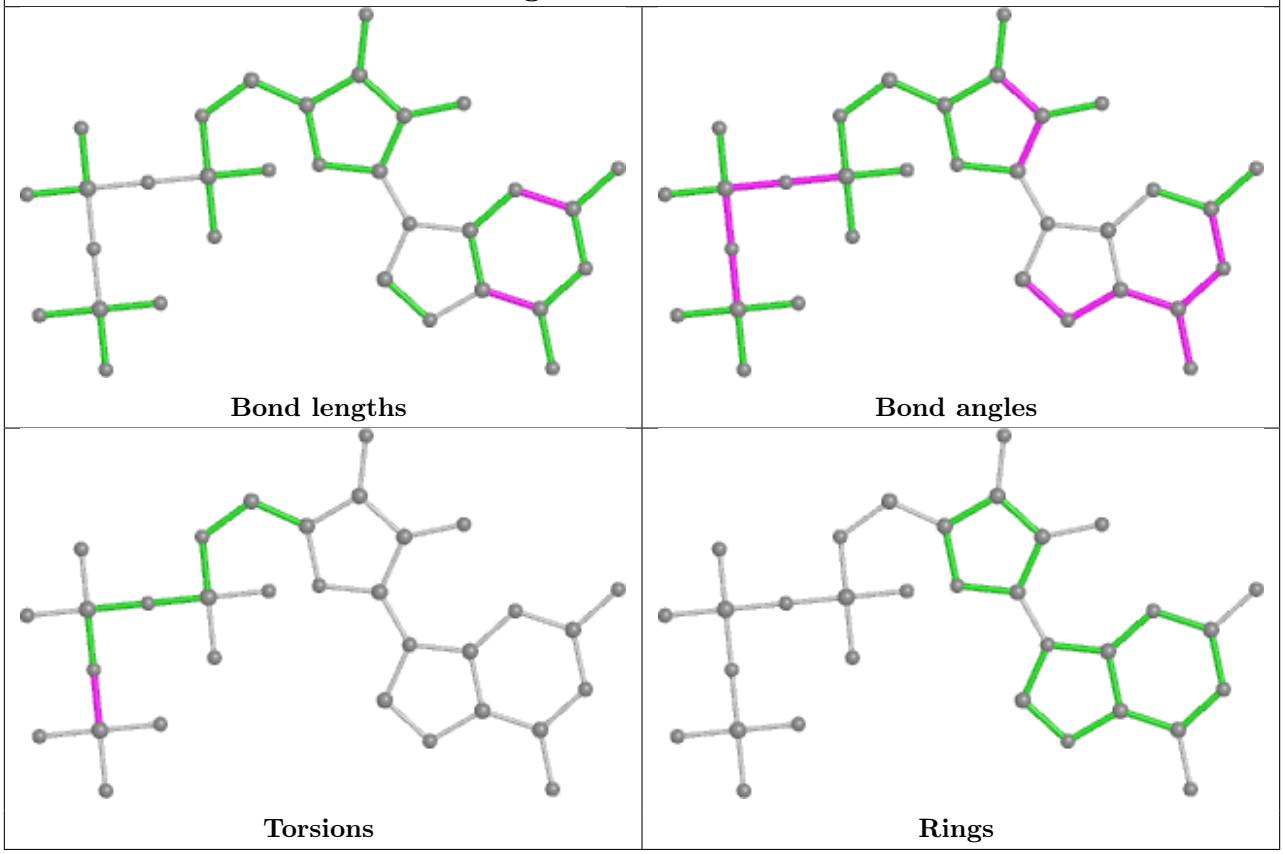


Rings

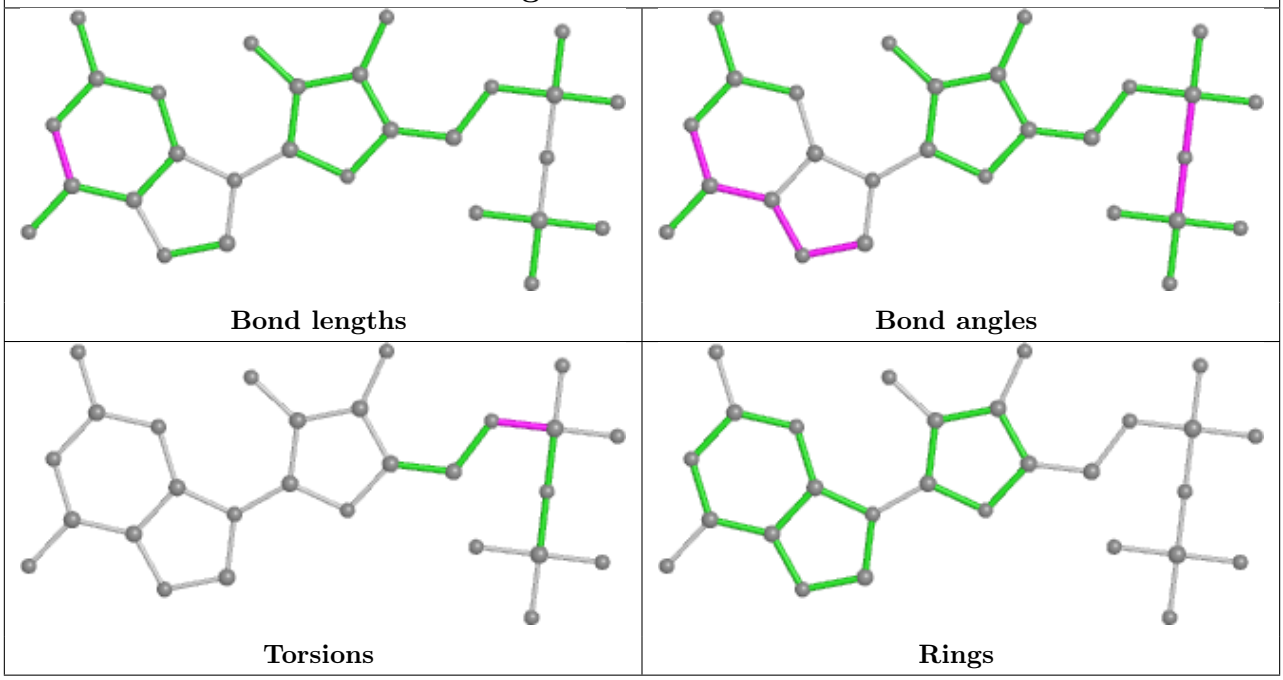
Ligand GDP W 600



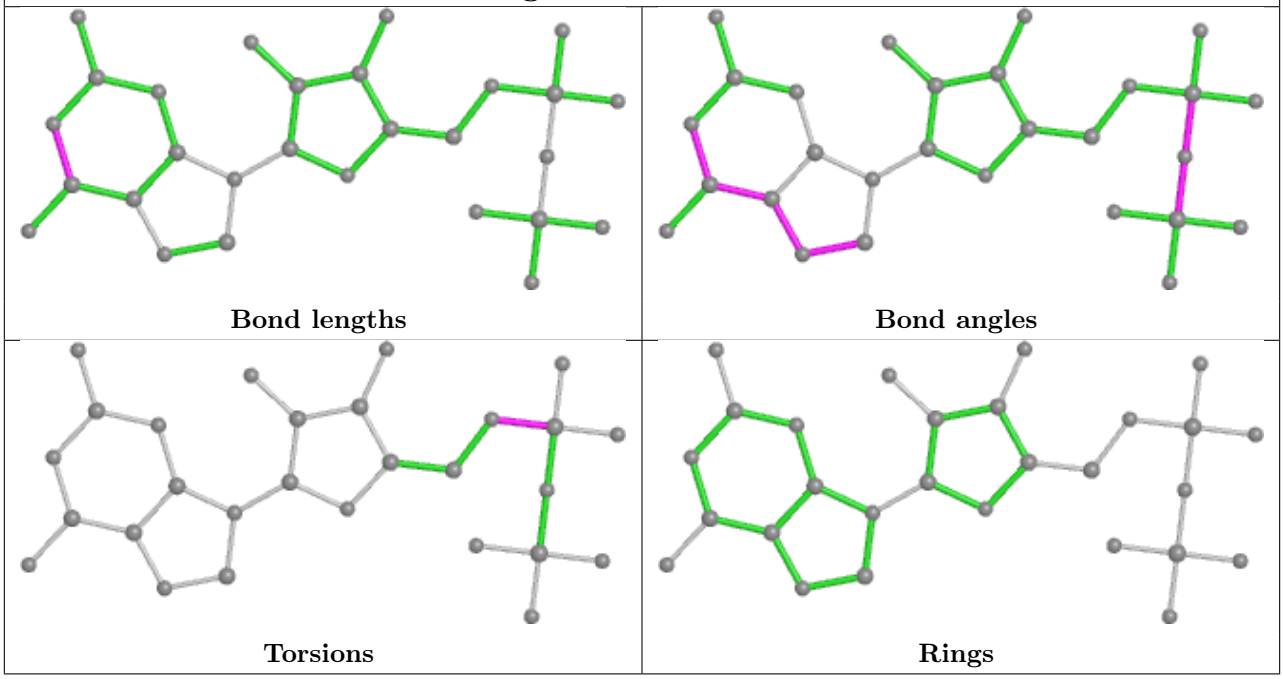
Ligand GTP V 600



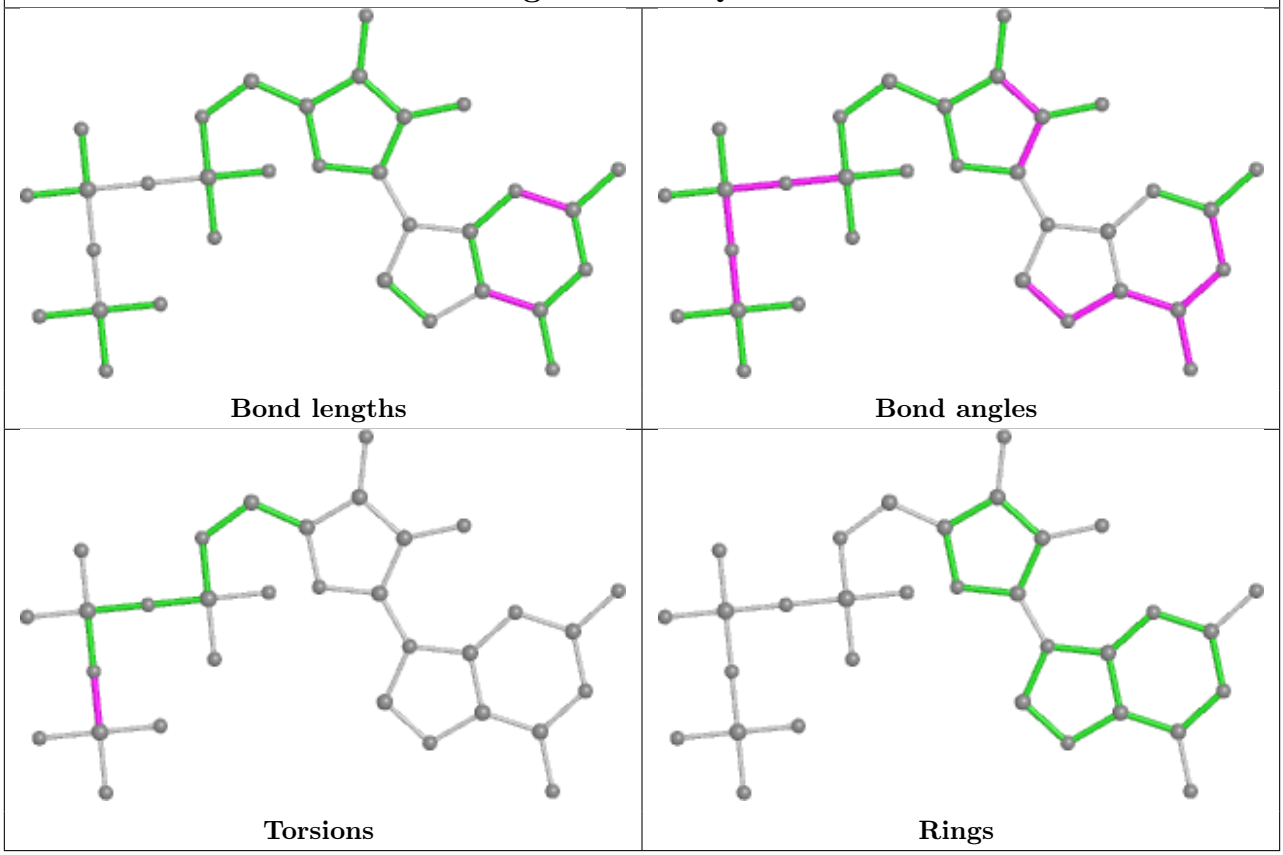
Ligand GDP Y 600



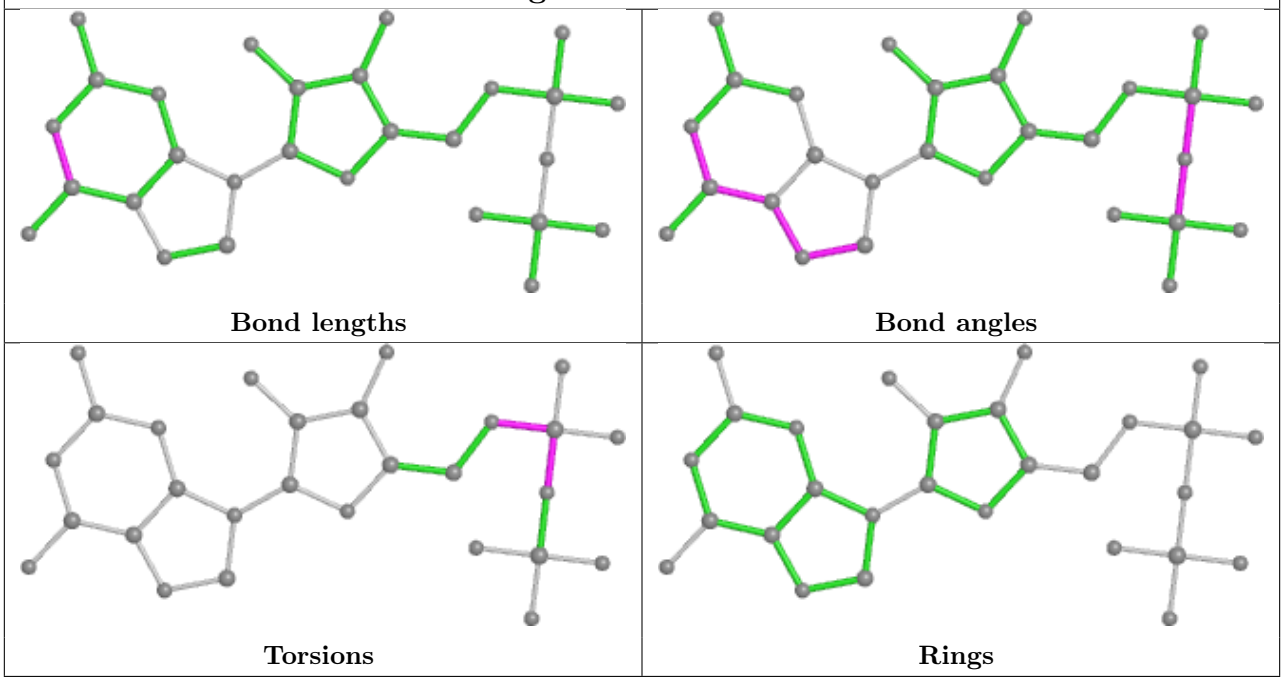
Ligand GDP R 600

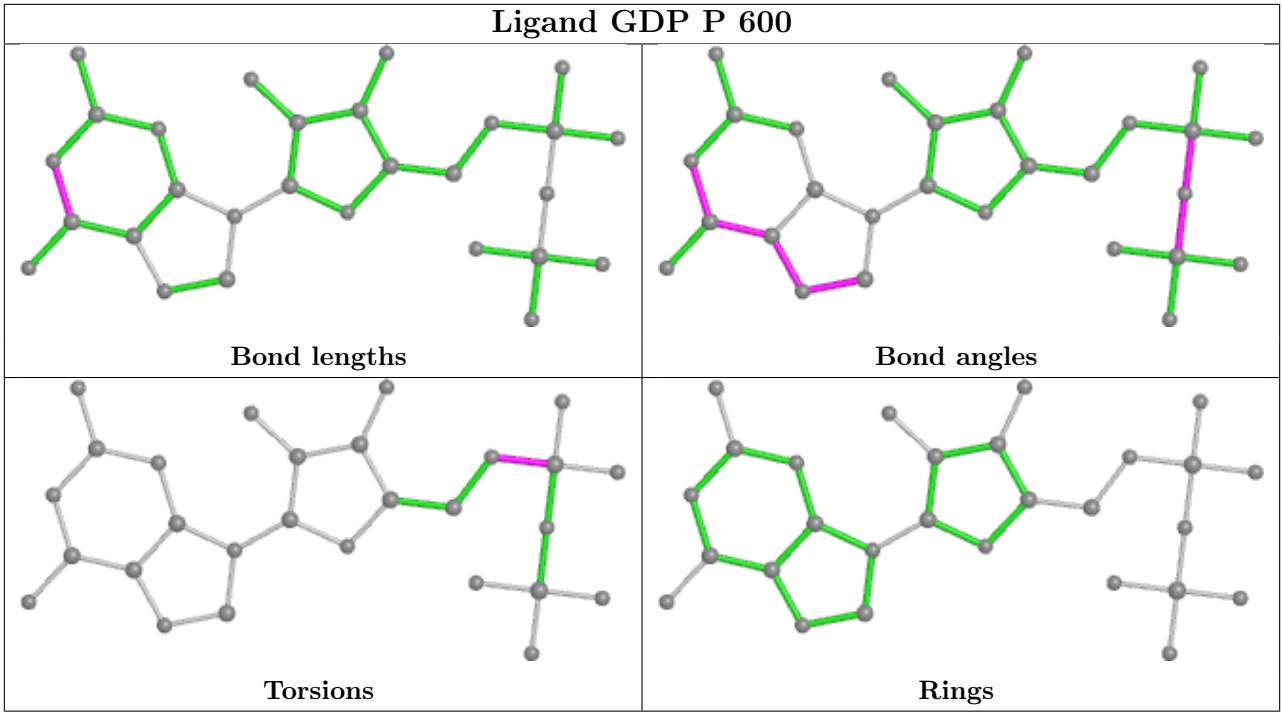


Ligand GTP Q 600



Ligand GDP I 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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	423/451 (93%)	0.19	14 (3%)	46	31	33, 103, 160, 243	0
1	C	423/451 (93%)	0.15	11 (2%)	56	40	41, 86, 135, 174	0
1	H	423/451 (93%)	-0.08	4 (0%)	84	73	37, 89, 136, 211	0
1	J	423/451 (93%)	0.43	36 (8%)	10	6	55, 131, 206, 260	0
1	O	423/451 (93%)	0.72	56 (13%)	3	2	58, 133, 192, 267	0
1	Q	423/451 (93%)	0.01	2 (0%)	91	83	29, 75, 133, 178	0
1	V	423/451 (93%)	0.14	19 (4%)	33	21	37, 100, 150, 208	0
1	X	423/451 (93%)	0.54	42 (9%)	7	4	45, 116, 179, 304	0
2	B	424/445 (95%)	-0.35	0	100	100	18, 46, 85, 125	0
2	D	424/445 (95%)	-0.03	7 (1%)	70	55	32, 69, 130, 173	0
2	I	424/445 (95%)	0.13	8 (1%)	66	51	50, 101, 146, 187	0
2	K	424/445 (95%)	0.39	25 (5%)	22	13	72, 122, 170, 283	0
2	P	424/445 (95%)	-0.20	1 (0%)	95	91	42, 82, 125, 176	0
2	R	424/445 (95%)	-0.16	3 (0%)	87	78	24, 57, 119, 221	0
2	W	424/445 (95%)	0.11	5 (1%)	79	66	50, 98, 153, 177	0
2	Y	424/445 (95%)	0.16	12 (2%)	53	37	45, 96, 149, 181	0
3	E	492/536 (91%)	0.00	7 (1%)	75	61	27, 72, 123, 153	0
3	L	491/536 (91%)	0.09	10 (2%)	65	49	45, 82, 133, 190	0
3	S	490/536 (91%)	0.10	16 (3%)	46	31	26, 83, 136, 170	0
3	Z	492/536 (91%)	0.16	11 (2%)	62	45	38, 86, 144, 175	0
4	F	155/169 (91%)	0.17	5 (3%)	47	32	44, 75, 132, 171	0
4	G	155/169 (91%)	0.06	6 (3%)	39	25	52, 90, 126, 170	0
4	M	155/169 (91%)	1.50	49 (31%)	0	0	121, 181, 223, 280	0
4	N	155/169 (91%)	1.70	53 (34%)	0	0	103, 129, 145, 158	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
4	T	155/169 (91%)	1.46	49 (31%)	0	0	97, 156, 203, 265	0
4	U	155/169 (91%)	-0.17	0	100	100	25, 64, 101, 126	0
4	a	155/169 (91%)	1.67	54 (34%)	0	0	120, 166, 215, 302	0
4	b	155/169 (91%)	0.74	20 (12%)	3	2	89, 148, 200, 245	0
All	All	9981/10664 (93%)	0.22	525 (5%)	26	16	18, 93, 170, 304	0

All (525) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	a	75	ALA	11.0
4	a	76	ILE	9.2
1	X	317	LEU	9.1
4	a	64	GLU	8.3
1	J	59	GLY	6.8
4	M	153	SER	6.4
4	M	134	LYS	6.2
1	J	374	ALA	6.2
4	M	139	VAL	6.1
1	X	335	ILE	6.0
1	O	296	PHE	5.9
4	a	68	LYS	5.8
4	T	139	VAL	5.7
4	a	33	LEU	5.6
4	N	63	VAL	5.5
1	O	351	PHE	5.5
4	T	37	GLY	5.5
4	N	76	ILE	5.4
2	I	179	ASP	5.3
4	T	126	LEU	5.2
1	X	347	CYS	5.2
1	A	4	CYS	5.2
4	a	74	ASN	5.2
1	O	335	ILE	5.1
3	S	297	ASN	5.1
1	V	342	GLN	5.0
4	b	22	ALA	4.9
4	N	43	THR	4.7
1	X	315	CYS	4.7
4	M	36	ASN	4.7
4	M	16	LYS	4.6
4	N	84	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
4	a	158	ASN	4.6
4	M	33	LEU	4.6
4	N	49	THR	4.5
2	K	276	THR	4.5
1	A	437	VAL	4.5
4	a	15	GLY	4.5
2	K	249	ASN	4.4
4	M	37	GLY	4.4
4	a	41	ASN	4.4
4	M	133	LEU	4.4
1	O	4	CYS	4.4
4	a	37	GLY	4.4
1	O	269	LEU	4.4
4	N	93	LEU	4.4
1	J	319	TYR	4.4
4	M	140	ASN	4.3
3	Z	300	ASP	4.3
4	N	102	HIS	4.3
4	T	101	LYS	4.3
4	a	137	ALA	4.3
4	a	36	ASN	4.3
4	a	165	LEU	4.2
4	T	106	VAL	4.2
1	X	348	PRO	4.2
4	F	15	GLY	4.2
1	X	4	CYS	4.2
4	N	26	GLN	4.2
1	O	271	THR	4.2
3	S	258	PRO	4.2
4	N	67	LEU	4.2
1	J	351	PHE	4.2
4	N	80	GLY	4.1
2	K	1	MET	4.1
4	M	67	LEU	4.1
3	Z	260	GLN	4.1
4	a	167	LYS	4.1
4	a	26	GLN	4.1
1	X	38	SER	4.0
1	O	317	LEU	4.0
4	a	18	LEU	4.0
4	M	70	GLY	4.0
1	O	306	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
4	T	18	LEU	4.0
1	X	351	PHE	4.0
4	T	134	LYS	3.9
1	O	302	MET	3.9
4	a	39	ASP	3.9
4	M	15	GLY	3.9
4	b	15	GLY	3.9
4	b	18	LEU	3.9
4	a	97	GLU	3.9
1	X	376	CYS	3.9
4	M	124	GLY	3.8
1	J	64	ARG	3.8
1	O	379	SER	3.8
4	a	43	THR	3.8
4	T	165	LEU	3.8
1	C	47	ASP	3.7
2	I	270	PRO	3.7
1	O	378	LEU	3.7
4	N	51	LEU	3.7
1	V	352	LYS	3.7
4	M	101	LYS	3.7
1	X	316	CYS	3.6
4	a	150	PHE	3.6
1	X	271	THR	3.6
2	K	286	LEU	3.6
1	O	52	PHE	3.6
4	a	29	GLU	3.6
4	a	153	SER	3.6
1	H	350	GLY	3.6
4	T	107	ASN	3.6
1	X	355	ILE	3.6
1	X	134	GLY	3.6
3	E	259	ALA	3.5
4	N	41	ASN	3.5
3	L	207	GLN	3.5
4	a	51	LEU	3.5
3	E	300	ASP	3.5
4	a	140	ASN	3.5
4	N	96	VAL	3.5
4	N	46	SER	3.5
3	S	435	ASP	3.5
3	L	259	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
4	M	106	VAL	3.5
2	Y	277	SER	3.5
3	E	249	GLN	3.5
4	N	135	HIS	3.5
1	V	343	PHE	3.5
4	N	109	VAL	3.5
4	M	130	GLU	3.4
4	N	164	ILE	3.4
1	O	204	VAL	3.4
2	Y	1	MET	3.4
4	b	96	VAL	3.4
4	G	27	ASP	3.4
4	N	30	VAL	3.4
2	K	270	PRO	3.4
1	X	311	LYS	3.4
4	a	160	ASP	3.4
3	S	90	ASN	3.4
4	N	81	SER	3.4
3	Z	298	ALA	3.4
1	J	65	ALA	3.4
1	O	353	VAL	3.3
4	M	51	LEU	3.3
1	O	315	CYS	3.3
4	N	100	LEU	3.3
3	Z	18	ALA	3.3
4	M	129	VAL	3.3
2	K	203	CYS	3.3
4	M	100	LEU	3.3
4	T	36	ASN	3.3
2	K	285	ALA	3.3
1	O	369	ALA	3.2
4	F	35	ALA	3.2
2	K	42	LEU	3.2
2	K	271	GLY	3.2
4	N	42	ALA	3.2
2	K	281	GLN	3.2
1	O	165	SER	3.2
1	V	351	PHE	3.2
4	T	98	VAL	3.2
4	b	35	ALA	3.2
4	N	114	ASP	3.2
4	T	117	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
4	T	102	HIS	3.2
1	O	374	ALA	3.2
4	T	30	VAL	3.2
4	a	117	LEU	3.1
4	a	161	LEU	3.1
4	a	107	ASN	3.1
4	a	38	ALA	3.1
4	M	126	LEU	3.1
4	T	142	GLN	3.1
1	A	165	SER	3.1
4	N	22	ALA	3.1
4	T	135	HIS	3.1
1	O	309	HIS	3.1
1	O	323	VAL	3.1
3	S	176	ASN	3.1
4	T	149	ALA	3.1
4	M	75	ALA	3.1
3	E	217	LEU	3.1
4	N	149	ALA	3.1
1	O	230	LEU	3.0
1	X	378	LEU	3.0
4	b	26	GLN	3.0
2	W	270	PRO	3.0
4	N	48	LEU	3.0
4	a	60	LEU	3.0
4	T	164	ILE	3.0
4	M	132	LEU	3.0
4	T	160	ASP	3.0
1	C	302	MET	3.0
4	M	61	GLU	3.0
4	a	159	GLU	3.0
1	J	91	GLN	3.0
1	O	334	THR	3.0
2	I	404	PHE	3.0
4	b	42	ALA	3.0
2	Y	283	TYR	3.0
1	O	337	THR	3.0
4	M	71	ALA	3.0
4	b	120	ALA	3.0
1	O	249	ASN	3.0
1	O	388	TRP	2.9
3	Z	82	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	K	277	SER	2.9
4	M	117	LEU	2.9
4	N	77	ASP	2.9
4	M	125	HIS	2.9
4	M	150	PHE	2.9
1	X	437	VAL	2.9
4	a	141	ALA	2.9
3	E	248	GLN	2.9
4	N	92	HIS	2.9
4	M	137	ALA	2.9
1	J	258	ASN	2.9
3	L	435	ASP	2.9
3	S	300	ASP	2.9
4	M	43	THR	2.9
1	V	347	CYS	2.9
2	P	179	ASP	2.9
1	J	335	ILE	2.9
4	T	52	HIS	2.9
3	Z	259	ALA	2.9
4	T	76	ILE	2.9
1	X	168	GLU	2.9
3	S	255	TRP	2.9
1	O	128	GLN	2.9
1	V	319	TYR	2.9
4	a	108	ALA	2.9
2	Y	42	LEU	2.9
1	V	273	ALA	2.9
2	K	396	THR	2.8
1	A	249	ASN	2.8
4	N	121	ALA	2.8
4	T	66	LEU	2.8
1	O	273	ALA	2.8
1	V	61	HIS	2.8
4	a	69	HIS	2.8
4	N	104	ALA	2.8
4	T	55	ALA	2.8
4	N	62	ILE	2.8
1	J	38	SER	2.8
1	O	27	GLU	2.8
3	E	260	GLN	2.8
4	M	141	ALA	2.8
4	a	162	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
4	N	138	ASP	2.8
1	J	334	THR	2.7
1	J	320	ARG	2.7
4	M	154	ILE	2.7
4	T	109	VAL	2.7
4	a	130	GLU	2.7
1	J	47	ASP	2.7
1	O	292	THR	2.7
4	N	47	GLY	2.7
4	a	34	MET	2.7
1	A	85	GLN	2.7
1	X	379	SER	2.7
1	X	260	VAL	2.7
4	M	55	ALA	2.7
1	H	38	SER	2.7
1	O	133	GLN	2.7
1	J	24	TYR	2.7
1	Q	38	SER	2.7
1	X	302	MET	2.7
4	M	136	GLY	2.7
1	X	319	TYR	2.7
3	Z	37	PHE	2.7
4	a	66	LEU	2.7
4	M	68	LYS	2.7
1	V	38	SER	2.7
1	O	361	THR	2.7
4	T	71	ALA	2.7
4	N	16	LYS	2.7
1	J	272	TYR	2.6
2	K	136	GLN	2.6
4	N	55	ALA	2.6
2	Y	350	ASN	2.6
1	O	134	GLY	2.6
4	M	76	ILE	2.6
4	M	23	ARG	2.6
4	a	136	GLY	2.6
4	T	156	ASN	2.6
1	A	61	HIS	2.6
4	T	67	LEU	2.6
4	T	70	GLY	2.6
1	V	353	VAL	2.6
4	T	131	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	J	273	ALA	2.6
4	N	88	ALA	2.6
2	Y	292	THR	2.6
1	X	342	GLN	2.6
1	C	4	CYS	2.6
1	J	357	TYR	2.6
1	X	336	LYS	2.6
3	S	257	VAL	2.6
1	J	316	CYS	2.6
4	a	114	ASP	2.6
1	O	345	ASP	2.5
4	M	97	GLU	2.5
4	T	114	ASP	2.5
2	D	220	THR	2.5
2	D	278	ARG	2.5
4	T	84	LEU	2.5
2	K	170	SER	2.5
4	F	101	LYS	2.5
1	O	87	PHE	2.5
4	T	43	THR	2.5
3	L	475	GLN	2.5
1	X	318	LEU	2.5
4	N	117	LEU	2.5
2	Y	80	SER	2.5
2	K	6	HIS	2.5
4	T	51	LEU	2.5
1	V	248	LEU	2.5
4	M	35	ALA	2.5
2	W	299	LYS	2.5
1	X	202	PHE	2.5
4	N	110	ASP	2.5
2	I	336	GLN	2.5
4	a	40	VAL	2.5
4	b	114	ASP	2.5
1	X	432	TYR	2.5
1	A	313	MET	2.5
1	V	380	ASN	2.5
4	a	42	ALA	2.5
2	K	28	HIS	2.5
2	Y	296	PHE	2.5
1	X	248	LEU	2.4
4	T	127	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
4	b	64	GLU	2.4
4	G	26	GLN	2.4
4	a	142	GLN	2.4
1	J	25	CYS	2.4
1	J	37	PRO	2.4
4	N	79	MET	2.4
4	b	41	ASN	2.4
2	I	271	GLY	2.4
4	N	15	GLY	2.4
1	C	271	THR	2.4
1	C	338	LYS	2.4
3	L	519	LEU	2.4
4	a	84	LEU	2.4
2	K	53	TYR	2.4
4	N	27	ASP	2.4
4	N	25	GLY	2.4
4	T	144	LYS	2.4
2	Y	48	ARG	2.4
3	S	298	ALA	2.4
1	V	357	TYR	2.4
1	O	293	ASN	2.4
4	a	67	LEU	2.4
4	b	117	LEU	2.4
1	J	375	VAL	2.4
4	b	100	LEU	2.4
4	T	81	SER	2.4
4	N	13	ASP	2.4
2	W	394	GLN	2.3
2	K	279	GLY	2.3
2	K	282	GLN	2.3
4	T	161	LEU	2.3
4	N	158	ASN	2.3
1	O	214	ARG	2.3
1	J	248	LEU	2.3
1	O	63	PRO	2.3
2	D	285	ALA	2.3
4	F	22	ALA	2.3
4	M	14	LEU	2.3
1	J	202	PHE	2.3
1	J	331	ALA	2.3
1	O	268	PRO	2.3
1	C	357	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	X	357	TYR	2.3
1	X	305	CYS	2.3
4	N	118	HIS	2.3
1	O	53	PHE	2.3
4	a	96	VAL	2.3
1	H	351	PHE	2.3
1	X	388	TRP	2.3
4	T	41	ASN	2.3
1	X	167	LEU	2.3
2	D	355	VAL	2.3
2	W	275	LEU	2.3
1	J	373	ARG	2.3
4	M	84	LEU	2.3
4	b	127	GLU	2.3
1	X	331	ALA	2.3
1	A	342	GLN	2.3
1	O	291	ILE	2.3
4	N	74	ASN	2.3
1	A	239	THR	2.3
1	A	235	VAL	2.3
2	K	319	PHE	2.3
4	b	59	HIS	2.3
4	M	41	ASN	2.3
1	V	375	VAL	2.3
1	A	231	ILE	2.3
3	S	175	ILE	2.3
4	G	38	ALA	2.3
1	O	24	TYR	2.3
1	J	342	GLN	2.2
1	O	360	PRO	2.2
3	Z	180	SER	2.2
1	O	167	LEU	2.2
1	O	270	ALA	2.2
4	M	163	GLU	2.2
4	T	167	LYS	2.2
1	J	295	CYS	2.2
1	V	341	ILE	2.2
1	O	258	ASN	2.2
4	M	120	ALA	2.2
2	D	275	LEU	2.2
3	L	541	VAL	2.2
4	T	141	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	X	435	VAL	2.2
4	a	32	ILE	2.2
4	M	160	ASP	2.2
4	b	146	GLY	2.2
1	V	374	ALA	2.2
4	N	45	ALA	2.2
4	a	23	ARG	2.2
4	T	118	HIS	2.2
4	N	70	GLY	2.2
4	G	22	ALA	2.2
3	Z	299	VAL	2.2
3	S	82	LEU	2.2
4	N	154	ILE	2.2
4	a	22	ALA	2.2
1	X	274	PRO	2.2
2	R	42	LEU	2.2
1	O	295	CYS	2.2
4	T	99	LEU	2.2
4	N	52	HIS	2.2
1	X	353	VAL	2.2
4	a	166	GLN	2.2
1	O	234	ILE	2.2
2	I	279	GLY	2.2
2	R	220	THR	2.2
1	V	317	LEU	2.2
3	S	217	LEU	2.2
3	Z	30	TYR	2.2
4	b	126	LEU	2.2
2	W	179	ASP	2.2
2	Y	280	SER	2.2
4	F	28	ASP	2.2
3	S	91	VAL	2.2
1	C	342	GLN	2.2
1	V	35	GLN	2.2
4	G	15	GLY	2.1
4	N	130	GLU	2.2
4	a	21	ALA	2.1
4	a	163	GLU	2.1
2	I	269	MET	2.1
2	I	102	ASN	2.1
1	X	128	GLN	2.1
2	K	137	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	271	THR	2.1
1	A	360	PRO	2.1
1	J	275	VAL	2.1
3	L	91	VAL	2.1
1	A	351	PHE	2.1
1	O	244	PHE	2.1
2	D	1	MET	2.1
4	N	101	LYS	2.1
2	K	52	TYR	2.1
4	b	25	GLY	2.1
1	J	288	VAL	2.1
1	O	303	VAL	2.1
1	X	203	MET	2.1
2	R	281	GLN	2.1
3	L	258	PRO	2.1
1	O	412	GLY	2.1
1	C	270	ALA	2.1
1	O	20	CYS	2.1
3	S	254	GLN	2.1
3	Z	25	ALA	2.1
4	T	87	ALA	2.1
4	b	27	ASP	2.1
1	C	179	THR	2.1
4	a	52	HIS	2.1
1	J	315	CYS	2.1
4	M	29	GLU	2.1
1	O	36	MET	2.1
1	H	357	TYR	2.1
1	A	248	LEU	2.1
1	Q	165	SER	2.1
4	N	82	THR	2.1
1	J	87	PHE	2.1
1	V	372	GLN	2.1
1	O	371	VAL	2.1
1	O	382	THR	2.1
4	T	19	LEU	2.1
1	J	60	LYS	2.1
1	X	346	TRP	2.1
4	N	139	VAL	2.1
4	M	34	MET	2.0
2	K	320	ARG	2.0
3	S	183	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
4	a	139	VAL	2.0
1	C	57	GLY	2.0
4	M	149	ALA	2.0
2	Y	319	PHE	2.0
4	T	15	GLY	2.0
1	O	21	TRP	2.0
2	D	360	PRO	2.0
4	T	116	PRO	2.0
1	C	351	PHE	2.0
1	J	347	CYS	2.0
3	L	108	GLY	2.0
1	J	313	MET	2.0
1	X	341	ILE	2.0
1	X	170	SER	2.0
1	X	350	GLY	2.0
4	b	28	ASP	2.0
2	K	302	MET	2.0
3	E	258	PRO	2.0
4	G	106	VAL	2.0
1	X	88	HIS	2.0
1	O	320	ARG	2.0
3	S	511	MET	2.0
2	K	222	PRO	2.0
3	L	252	LEU	2.0
4	T	150	PHE	2.0
4	M	135	HIS	2.0
2	Y	284	ARG	2.0
4	T	108	ALA	2.0
4	T	100	LEU	2.0
1	J	380	ASN	2.0
4	M	158	ASN	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)

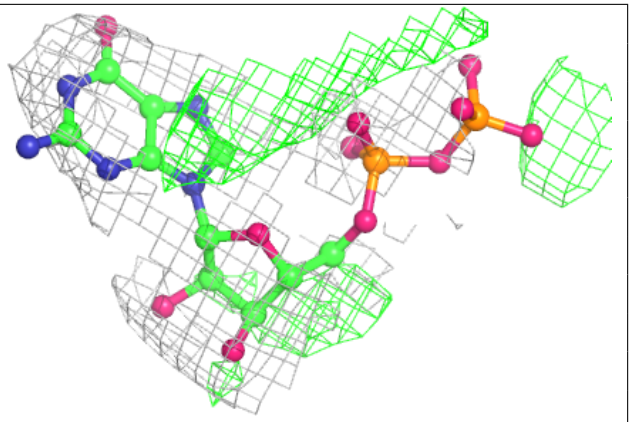
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

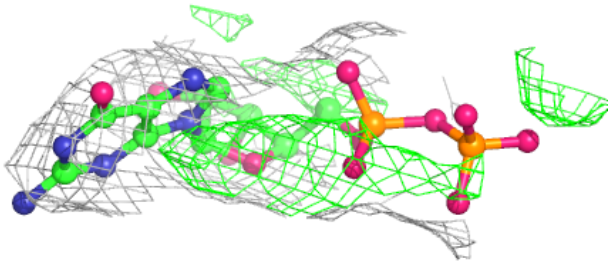
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	W	601	1/1	0.47	0.20	71,71,71,71	0
6	MG	K	601	1/1	0.48	0.20	72,72,72,72	0
6	MG	R	601	1/1	0.59	0.44	53,53,53,53	0
6	MG	B	601	1/1	0.66	0.54	30,30,30,30	0
6	MG	I	601	1/1	0.70	0.39	89,89,89,89	0
6	MG	D	601	1/1	0.87	0.47	85,85,85,85	0
7	GDP	K	600	28/28	0.87	0.21	94,122,145,151	0
7	GDP	I	600	28/28	0.90	0.25	70,99,114,116	0
7	GDP	B	600	28/28	0.91	0.31	38,62,78,89	0
5	GTP	O	600	32/32	0.91	0.24	78,99,116,120	0
5	GTP	X	600	32/32	0.91	0.24	58,94,107,113	0
7	GDP	P	600	28/28	0.91	0.25	72,97,119,129	0
6	MG	H	601	1/1	0.92	0.33	64,64,64,64	0
5	GTP	C	600	32/32	0.92	0.24	64,88,100,104	0
5	GTP	J	600	32/32	0.92	0.20	102,113,137,152	0
7	GDP	W	600	28/28	0.92	0.22	81,99,113,120	0
7	GDP	Y	600	28/28	0.92	0.22	76,102,123,125	0
5	GTP	A	600	32/32	0.93	0.24	68,86,100,107	0
6	MG	P	601	1/1	0.93	0.39	83,83,83,83	0
6	MG	Y	601	1/1	0.93	0.17	74,74,74,74	0
5	GTP	Q	600	32/32	0.94	0.23	51,77,95,97	0
5	GTP	V	600	32/32	0.94	0.25	55,88,102,107	0
5	GTP	H	600	32/32	0.94	0.24	58,89,113,117	0
7	GDP	D	600	28/28	0.95	0.23	59,69,102,108	0
7	GDP	R	600	28/28	0.95	0.24	51,72,85,89	0
6	MG	O	601	1/1	0.96	0.30	56,56,56,56	0
6	MG	J	601	1/1	0.97	0.29	95,95,95,95	0
6	MG	C	601	1/1	0.97	0.37	74,74,74,74	0
6	MG	X	601	1/1	0.97	0.33	83,83,83,83	0
6	MG	V	601	1/1	0.98	0.45	52,52,52,52	0
6	MG	Q	601	1/1	0.98	0.32	27,27,27,27	0
6	MG	A	601	1/1	0.98	0.33	62,62,62,62	0

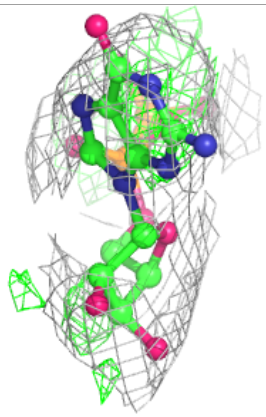
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

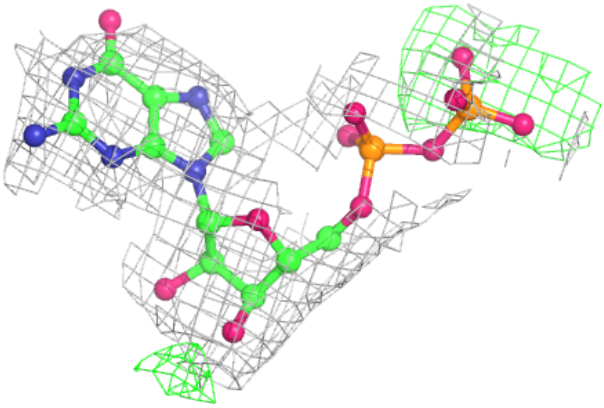


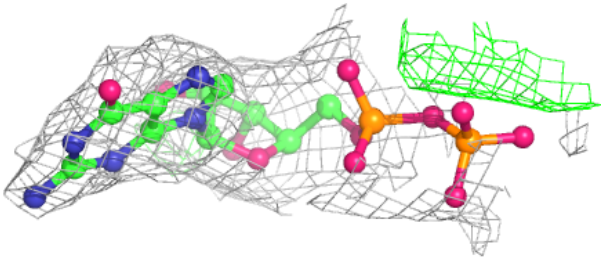


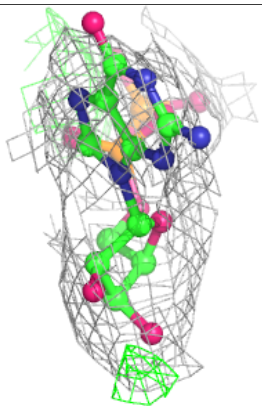


Electron density around GDP I 600:

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

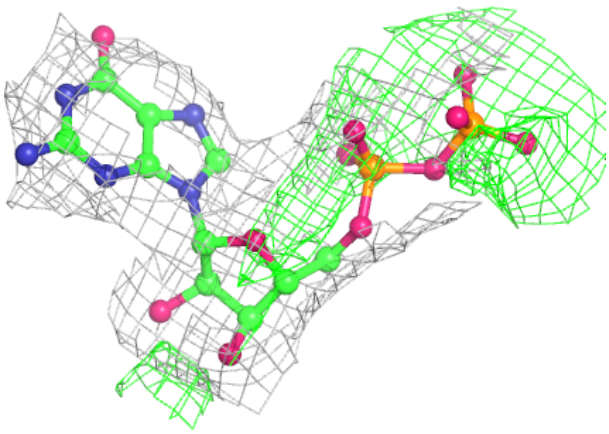


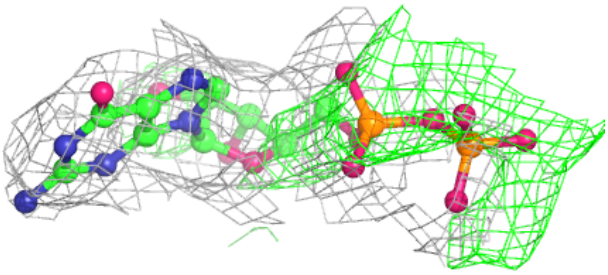


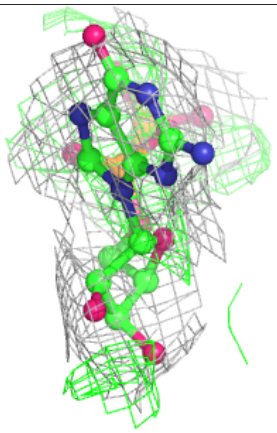


Electron density around GDP B 600:

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

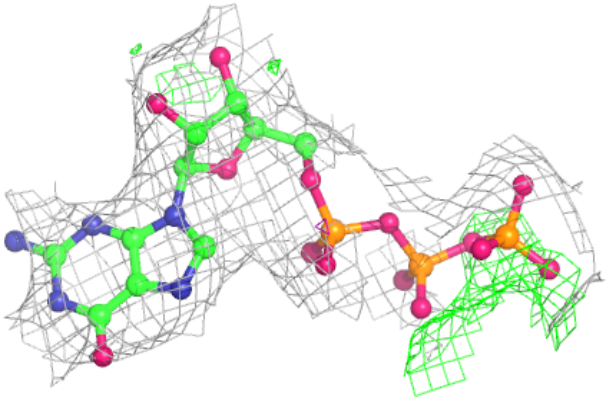


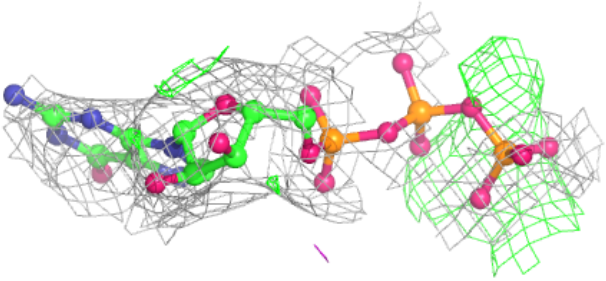


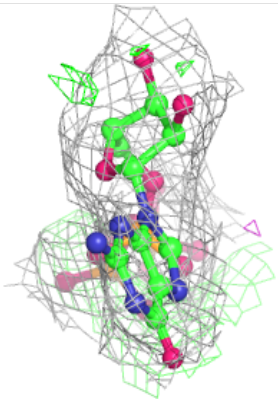


Electron density around GTP O 600:

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

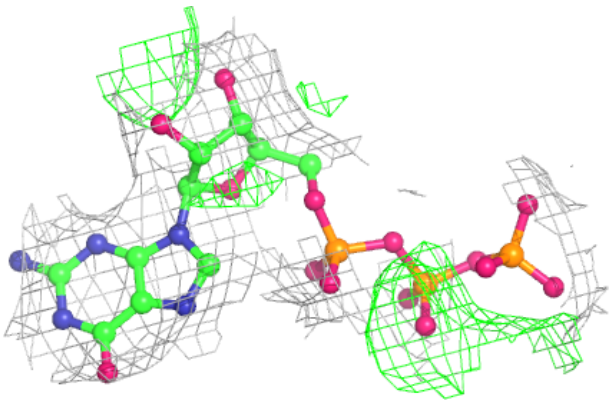


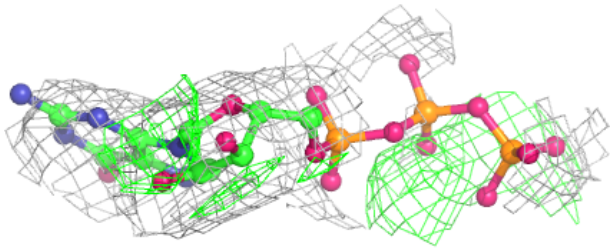


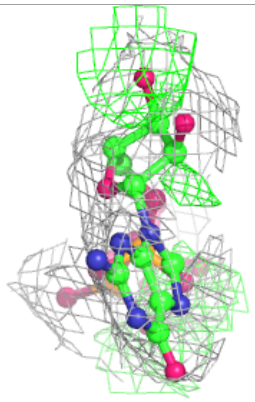


Electron density around GTP X 600:

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

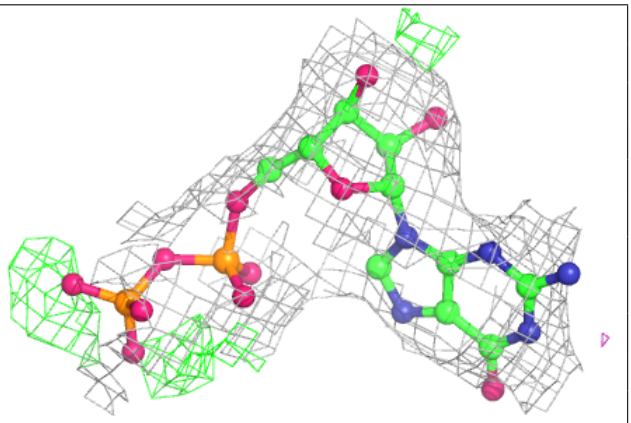


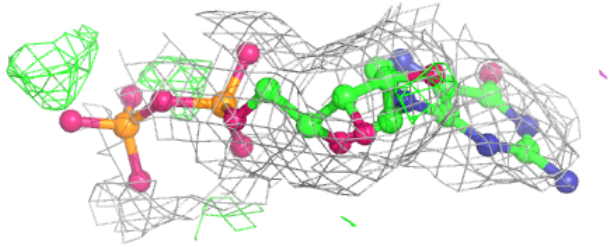


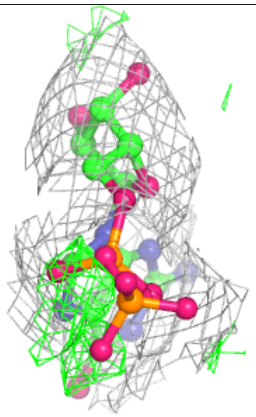


Electron density around GDP P 600:

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

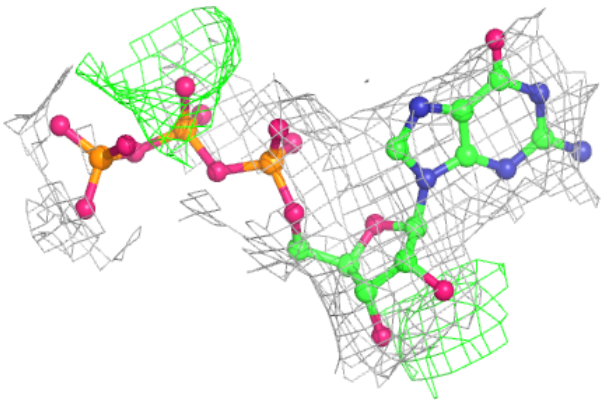


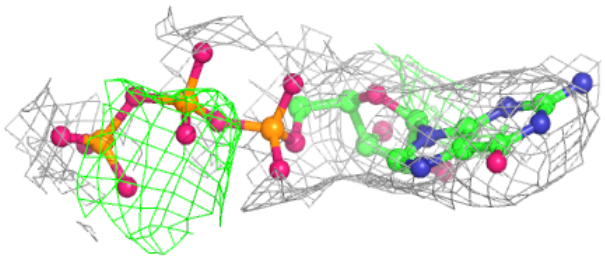


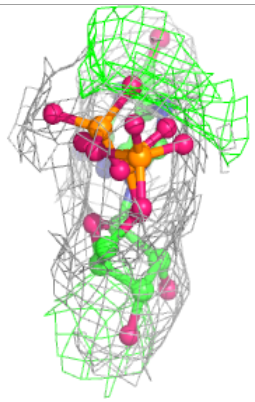


Electron density around GTP C 600:

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

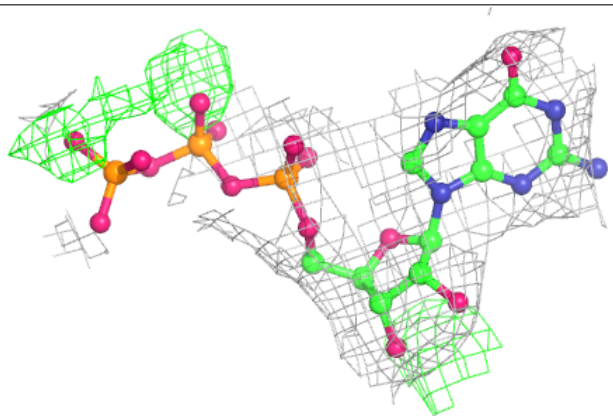


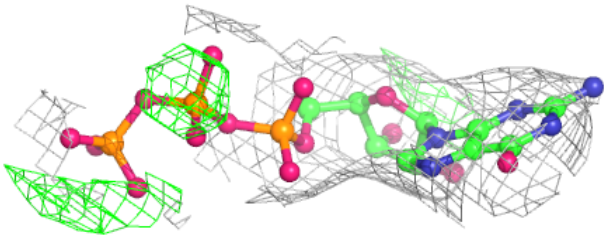


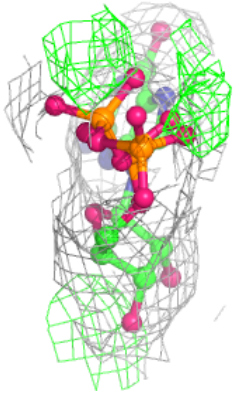


Electron density around GTP J 600:

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

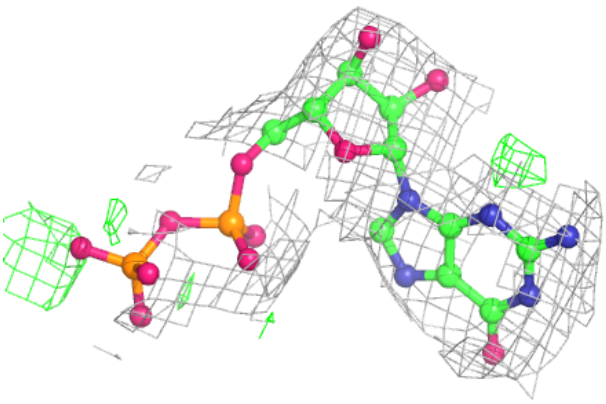


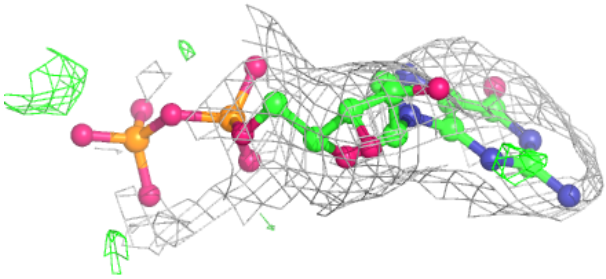


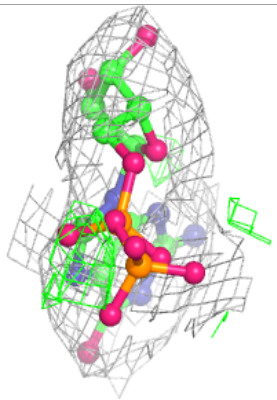


Electron density around GDP W 600:

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

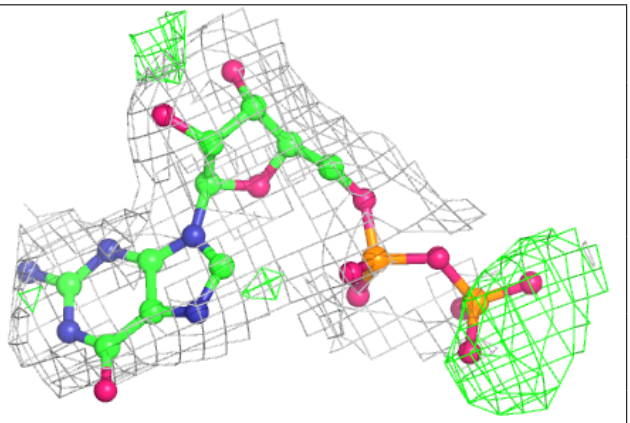


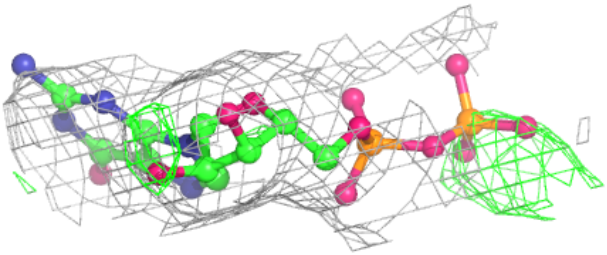


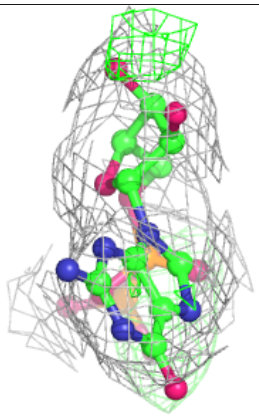


Electron density around GDP Y 600:

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

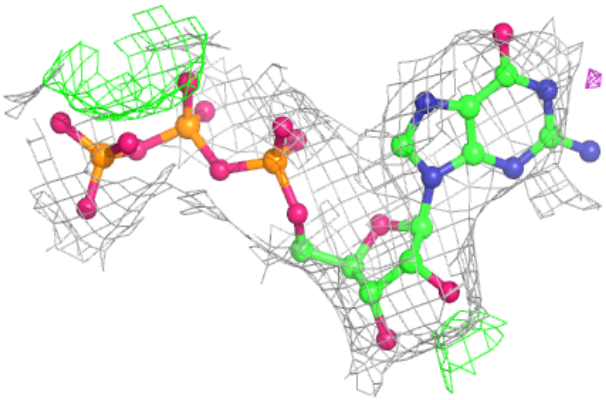


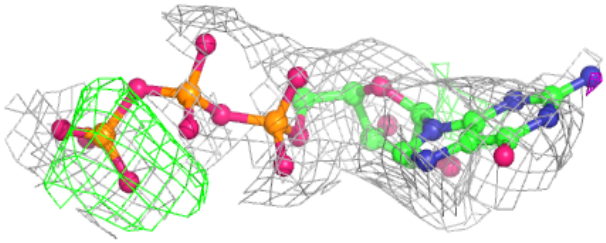


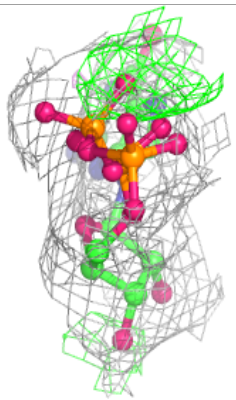


Electron density around GTP A 600:

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

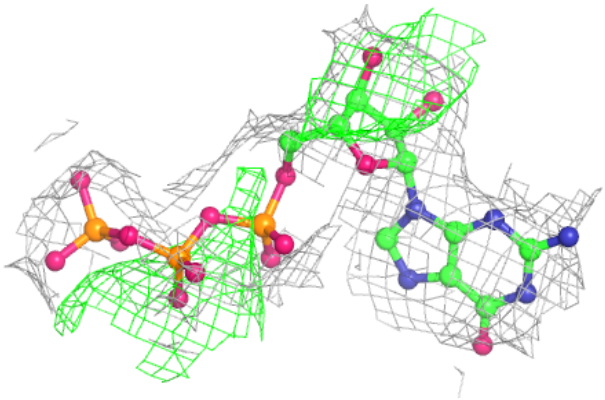


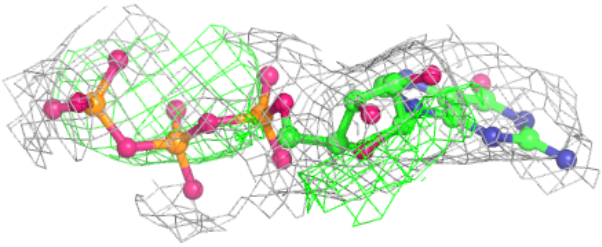


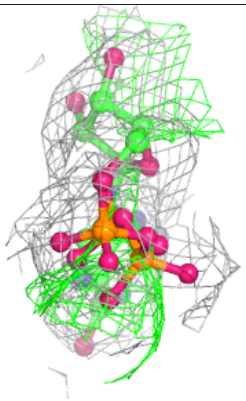


Electron density around GTP Q 600:

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

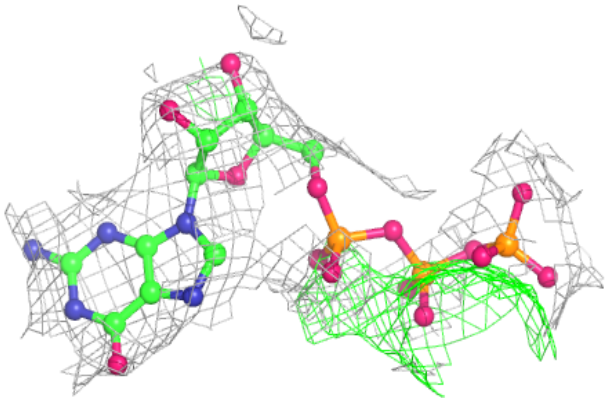


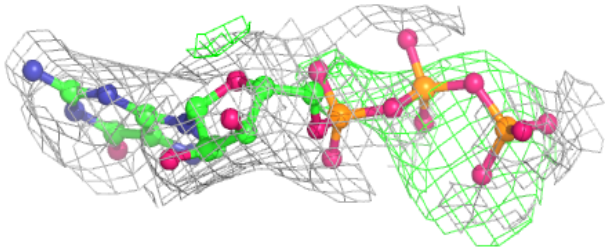




Electron density around GTP V 600:

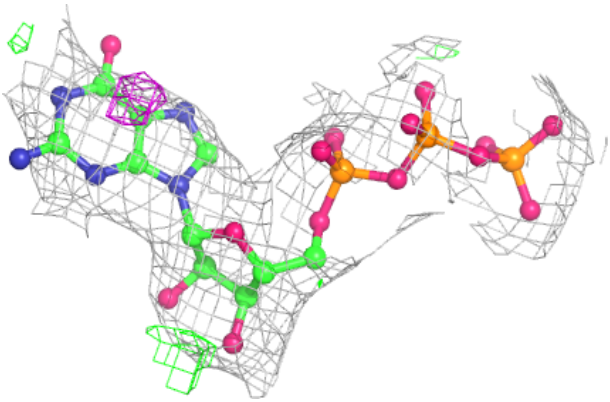
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

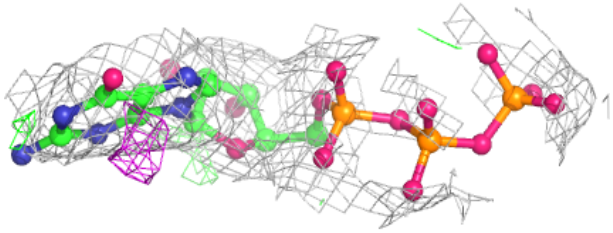


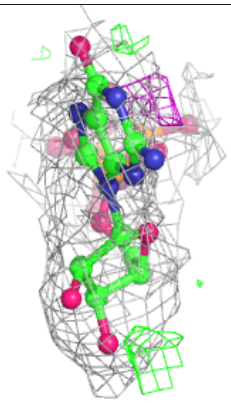


Electron density around GTP H 600:

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

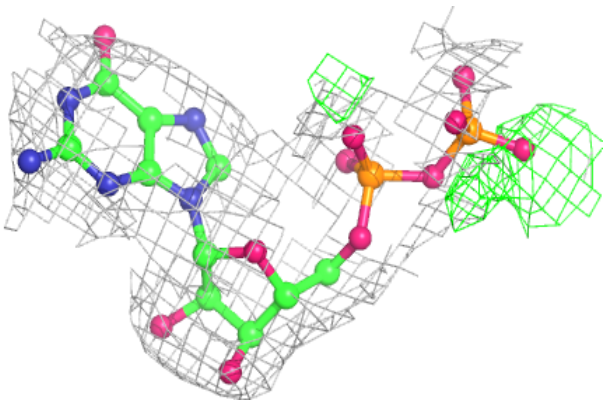


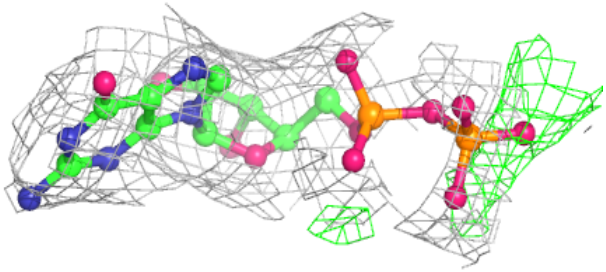


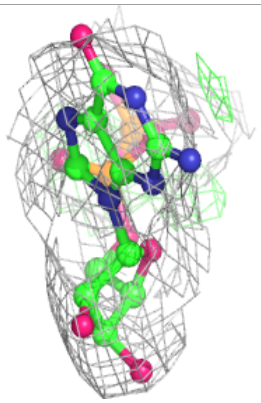


Electron density around GDP D 600:

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

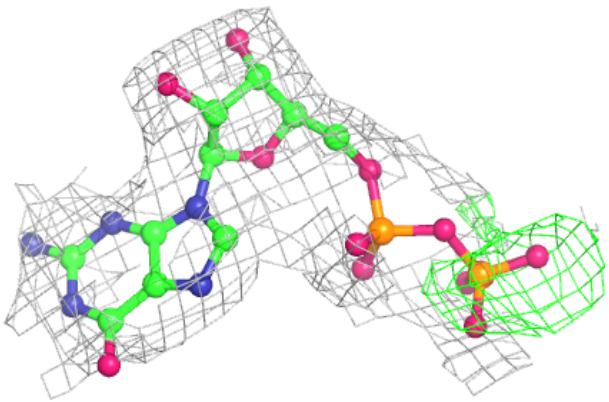


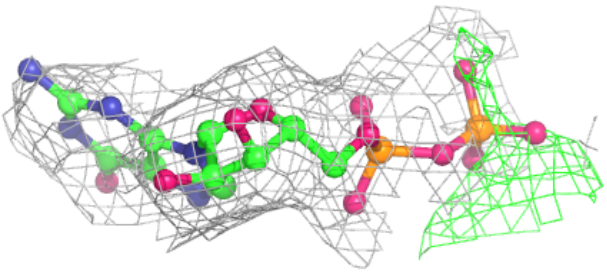


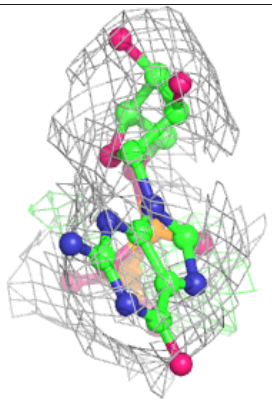


Electron density around GDP R 600:

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







6.5 Other polymers (i)

There are no such residues in this entry.