



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 03:09 PM EDT

PDB ID : 6MZE / pdb_00006mze
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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

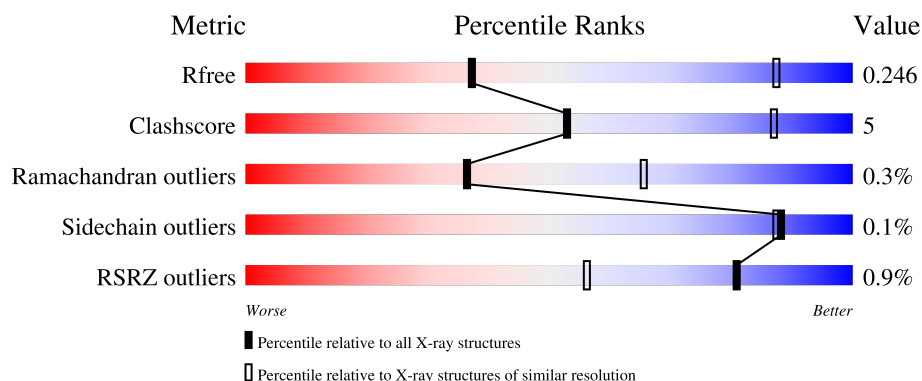
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



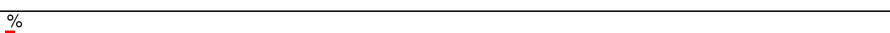
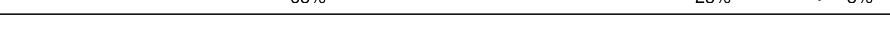
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	2% 88% 6% 6%
1	C	451	88% 5% 6%
1	H	451	87% 6% 6%
1	J	451	89% 5% 6%
1	O	451	2% 87% 7% 6%

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Mol	Chain	Length	Quality of chain
1	Q	451	
1	V	451	
1	X	451	
2	B	445	
2	D	445	
2	I	445	
2	K	445	
2	P	445	
2	R	445	
2	W	445	
2	Y	445	
3	E	536	
3	L	536	
3	S	536	
3	Z	536	
4	F	169	
4	G	169	
4	M	169	
4	N	169	
4	T	169	
4	U	169	
4	a	169	
4	b	169	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 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
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			

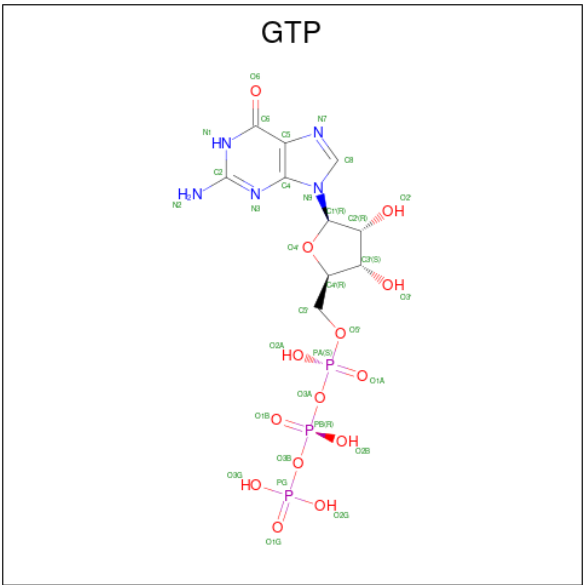
- Molecule 3 is a protein called Protein Stu2p/Alp14p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	492	Total	C	N	O	S	0	0	0
			3936	2521	665	734	16			
3	L	491	Total	C	N	O	S	0	0	0
			3924	2514	661	733	16			
3	S	490	Total	C	N	O	S	0	0	0
			3922	2513	662	731	16			
3	Z	492	Total	C	N	O	S	0	0	0
			3936	2521	665	734	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
			1135	713	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 (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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 (CCD ID: MG) (formula: Mg).

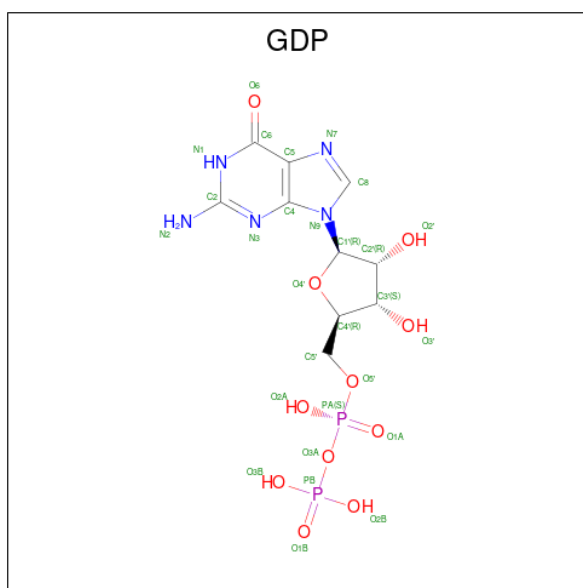
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		

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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 (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

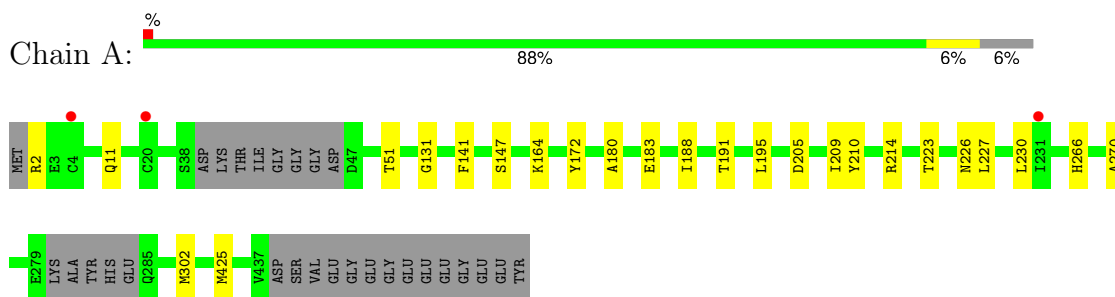


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
7	D	1	Total 28	C 10	N 5	O 11	P 2	0	0
7	I	1	Total 28	C 10	N 5	O 11	P 2	0	0
7	K	1	Total 28	C 10	N 5	O 11	P 2	0	0
7	P	1	Total 28	C 10	N 5	O 11	P 2	0	0
7	R	1	Total 28	C 10	N 5	O 11	P 2	0	0
7	W	1	Total 28	C 10	N 5	O 11	P 2	0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

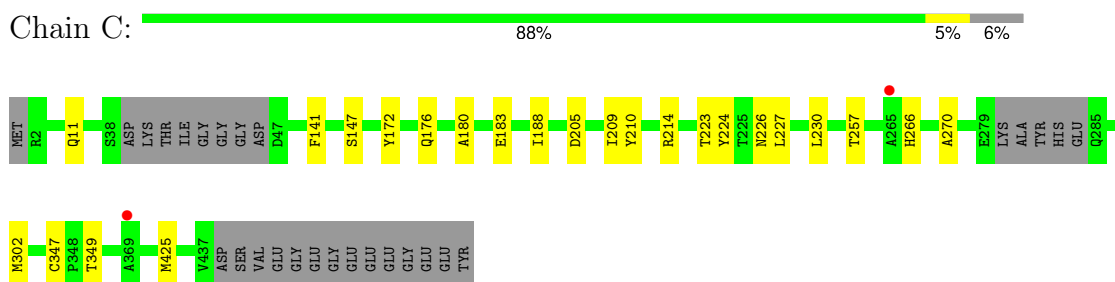
3 Residue-property plots [i](#)

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.

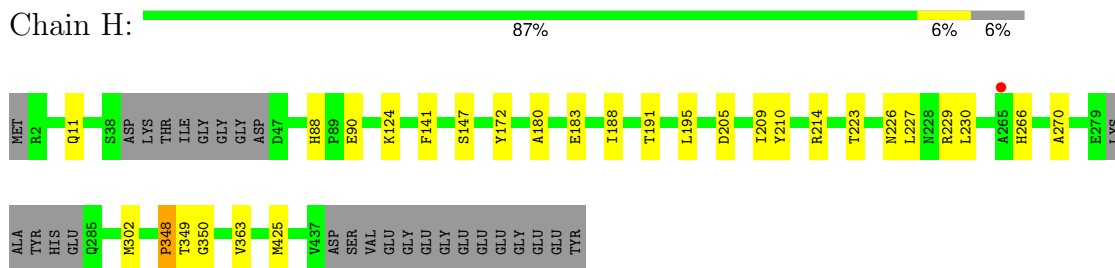
- Molecule 1: Tubulin alpha-1A chain



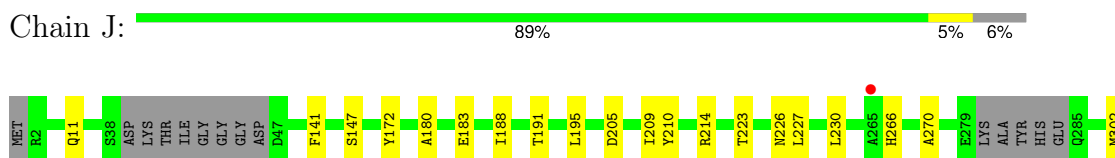
- Molecule 1: Tubulin alpha-1A chain

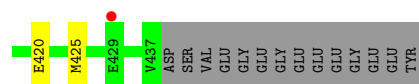


- Molecule 1: Tubulin alpha-1A chain

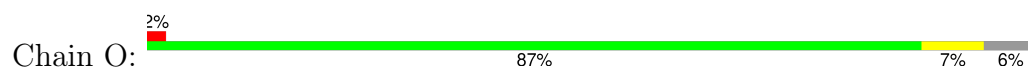


- Molecule 1: Tubulin alpha-1A chain

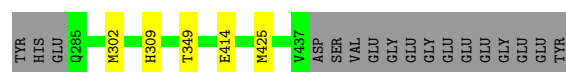
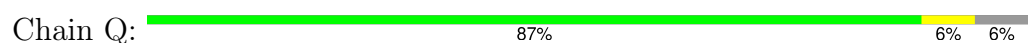




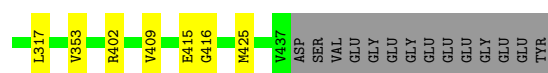
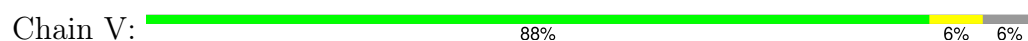
- Molecule 1: Tubulin alpha-1A chain



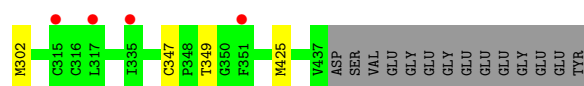
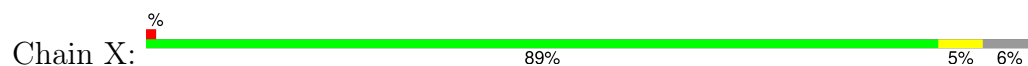
- Molecule 1: Tubulin alpha-1A chain



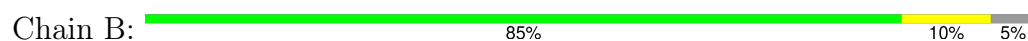
- Molecule 1: Tubulin alpha-1A chain

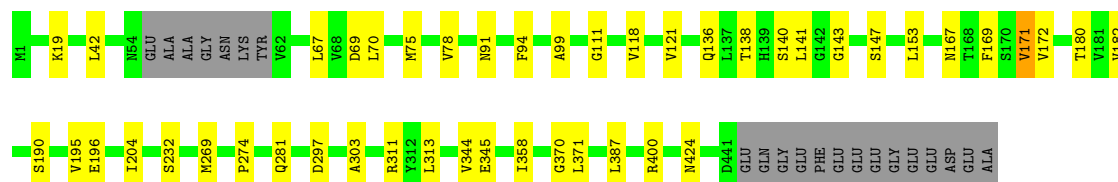


- Molecule 1: Tubulin alpha-1A chain



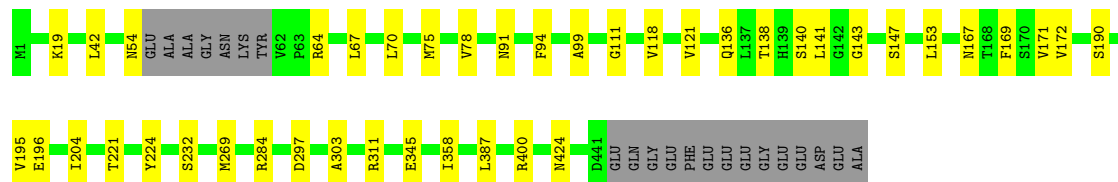
- Molecule 2: Tubulin beta chain





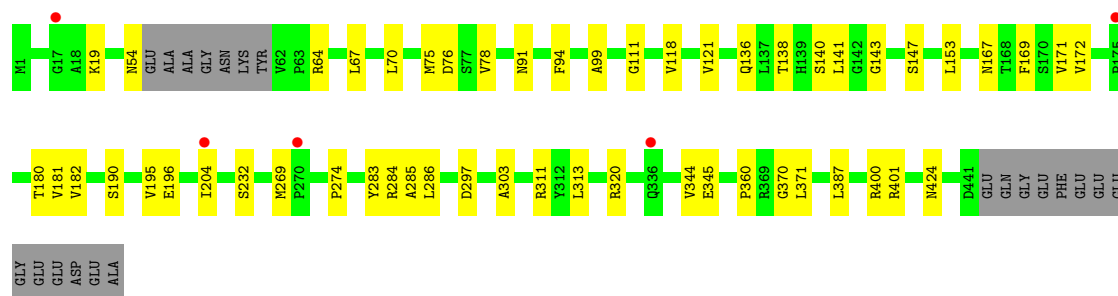
• Molecule 2: Tubulin beta chain

Chain D: 86% 9% 5%



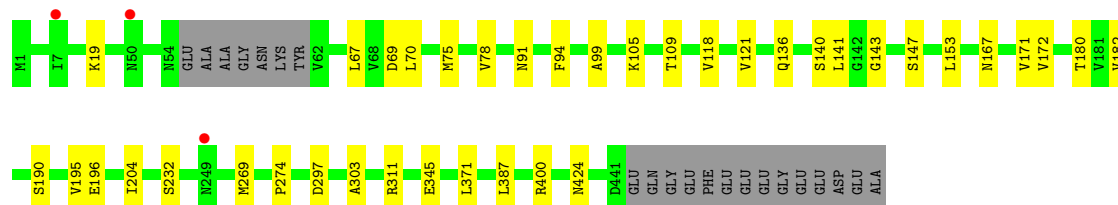
• Molecule 2: Tubulin beta chain

Chain I: 83% 12% 5%



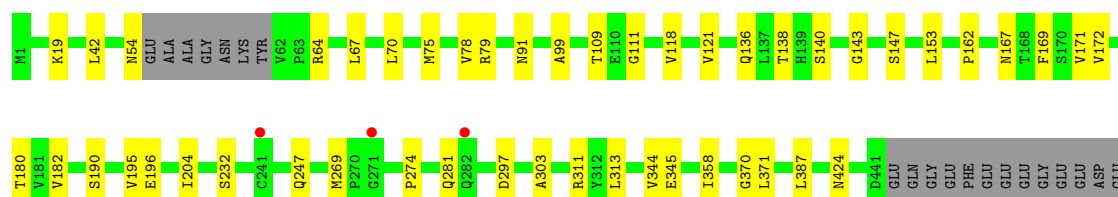
• Molecule 2: Tubulin beta chain

Chain K: 87% 9% 5%



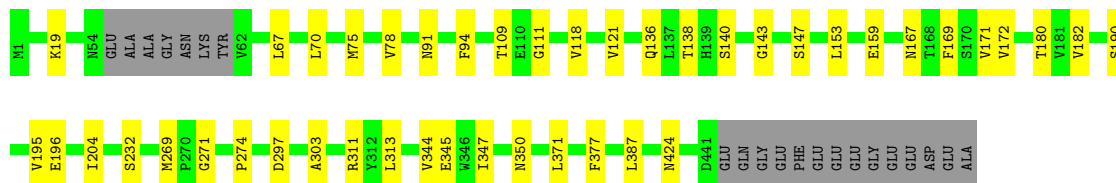
• Molecule 2: Tubulin beta chain

Chain P: 84% 11% 5%

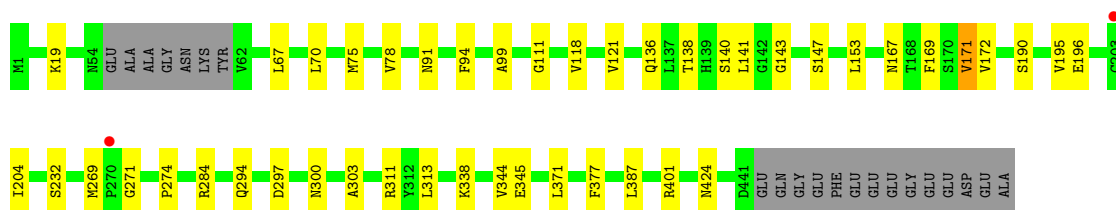


ALA

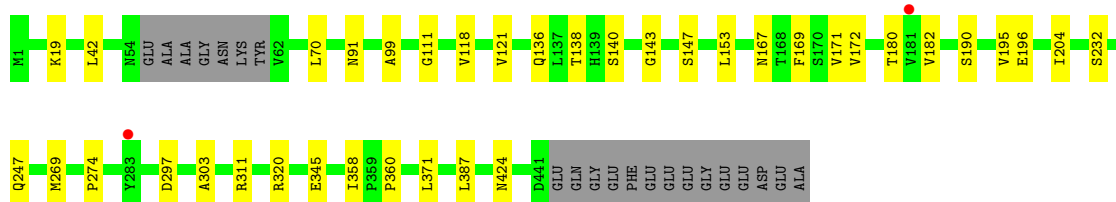
- Molecule 2: Tubulin beta chain

Chain R:  85% 10% 5%

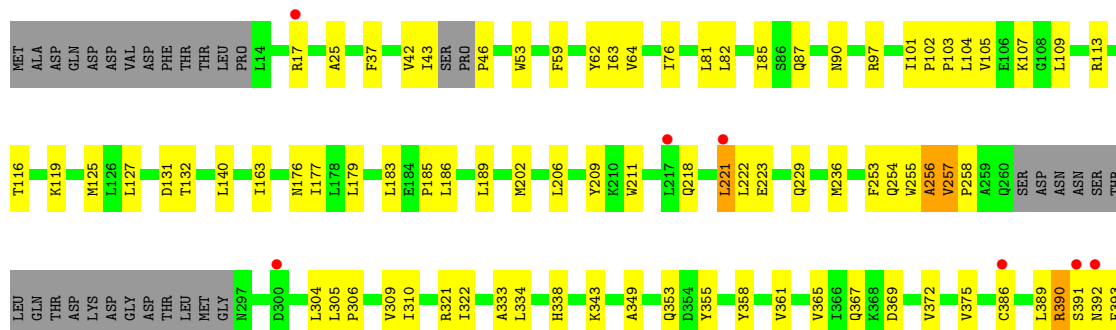
- Molecule 2: Tubulin beta chain

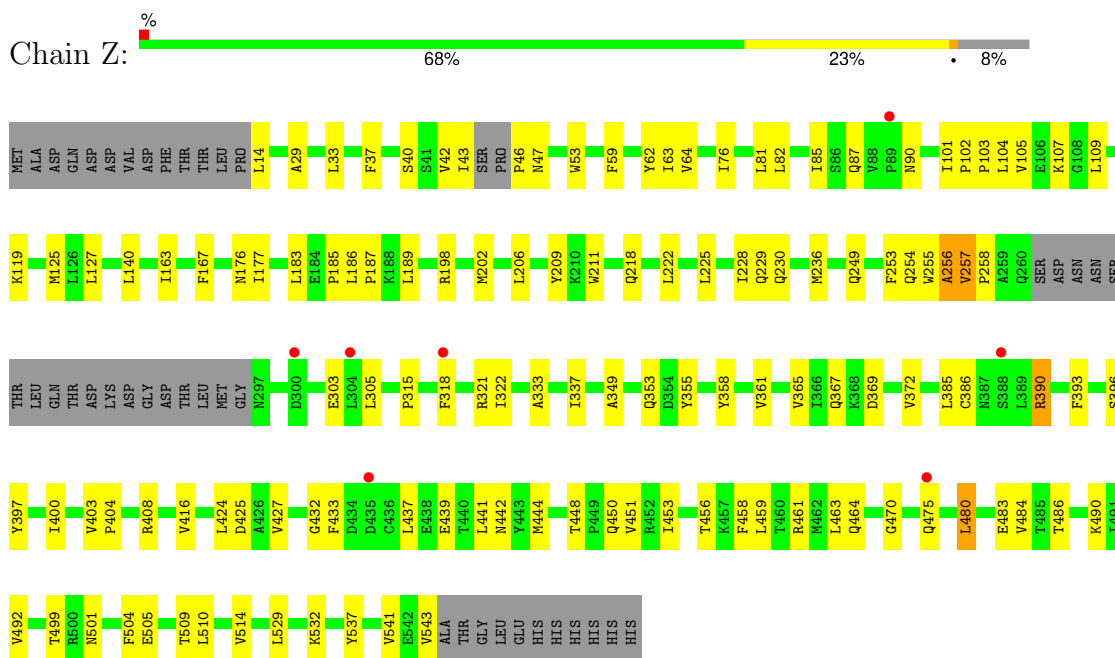
Chain W:  85% 10% 5%

- Molecule 2: Tubulin beta chain

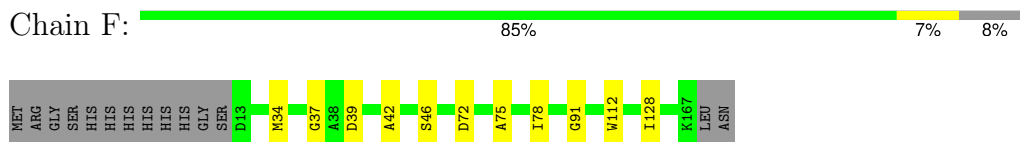
Chain Y:  87% 9% 5%

- Molecule 3: Protein Stu2p/Alp14p

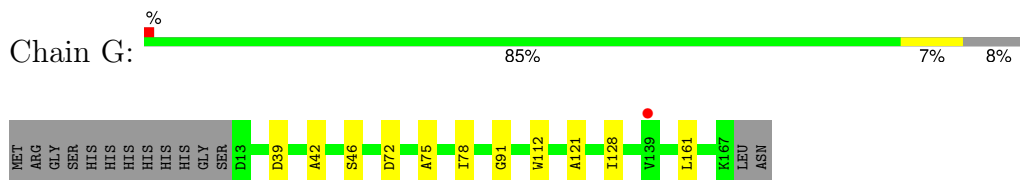
Chain E:  67% 24% 8%



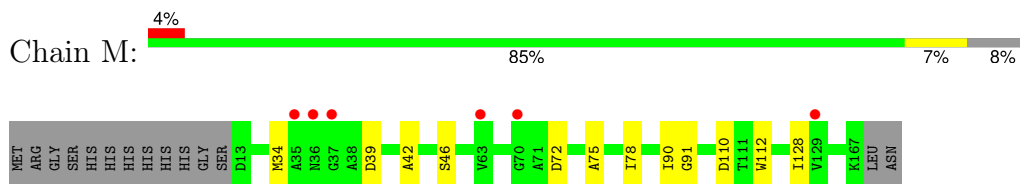
- Molecule 4: Designed ankyrin repeat protein (DARPIN) D1



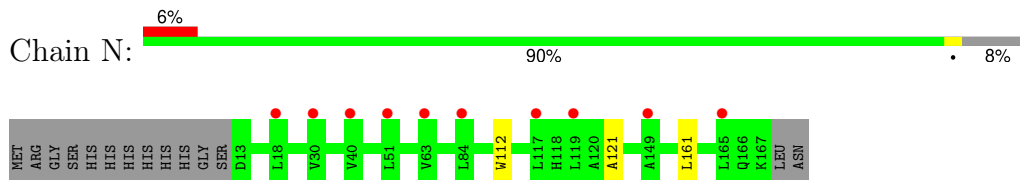
- Molecule 4: Designed ankyrin repeat protein (DARPIN) D1



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



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



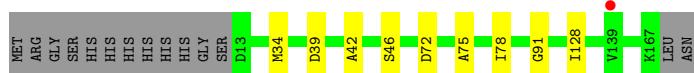
- Molecule 4: Designed ankyrin repeat protein (DARPIN) D1

Chain T:  86% 5% 8%



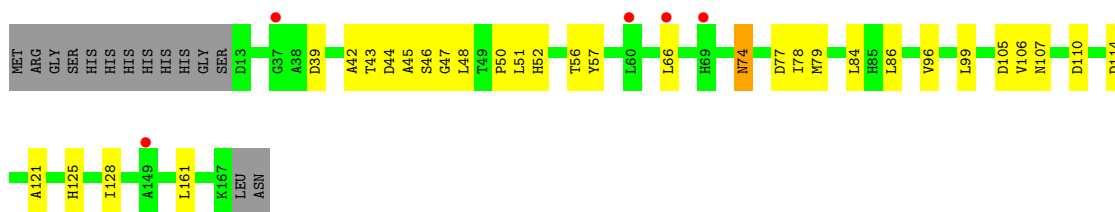
- Molecule 4: Designed ankyrin repeat protein (DARPIN) D1

Chain U:  86% 5% 8%



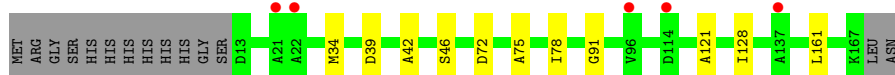
- Molecule 4: Designed ankyrin repeat protein (DARPIN) D1

Chain a:  73% 18% 8%



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

Chain b:  85% 7% 8%



4 Data and refinement statistics

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 – 3.60	Depositor EDS
% Data completeness (in resolution range)	79.4 (59.45-3.60) 80.9 (59.45-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 3.57Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.202 , 0.245 0.205 , 0.246	Depositor DCC
R_{free} test set	5975 reflections (3.89%)	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)	0.34 , 92.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.11	0/3339	0.33	0/4539
1	C	0.11	0/3339	0.32	0/4539
1	H	0.19	1/3339 (0.0%)	0.36	0/4539
1	J	0.11	0/3339	0.32	0/4539
1	O	0.12	0/3339	0.33	0/4539
1	Q	0.11	0/3339	0.33	0/4539
1	V	0.11	0/3339	0.33	0/4539
1	X	0.11	0/3339	0.32	0/4539
2	B	0.13	0/3380	0.35	0/4581
2	D	0.12	0/3380	0.34	0/4581
2	I	0.12	0/3380	0.35	0/4581
2	K	0.12	0/3380	0.35	0/4581
2	P	0.12	0/3380	0.34	0/4581
2	R	0.13	0/3380	0.36	0/4581
2	W	0.12	0/3380	0.35	0/4581
2	Y	0.12	0/3380	0.34	0/4581
3	E	0.22	0/4009	0.55	4/5438 (0.1%)
3	L	0.20	0/3997	0.53	3/5423 (0.1%)
3	S	0.18	0/3995	0.47	1/5419 (0.0%)
3	Z	0.20	0/4009	0.50	3/5438 (0.1%)
4	F	0.10	0/1150	0.28	0/1565
4	G	0.10	0/1150	0.29	0/1565
4	M	0.10	0/1150	0.28	0/1565
4	N	0.14	0/1150	0.36	0/1565
4	T	0.10	0/1150	0.28	0/1565
4	U	0.10	0/1150	0.28	0/1565
4	a	0.16	0/1150	0.44	1/1565 (0.1%)
4	b	0.10	0/1150	0.29	0/1565
All	All	0.14	1/78962 (0.0%)	0.38	12/107198 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	230	LEU	C-N	8.45	1.44	1.33

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Z	256	ALA	N-CA-C	8.30	120.41	111.36
4	a	57	TYR	N-CA-C	7.90	119.97	111.36
3	E	256	ALA	N-CA-C	7.89	119.96	111.36
3	Z	257	VAL	CB-CA-C	-5.64	108.37	114.35
3	L	218	GLN	N-CA-C	-5.53	105.65	112.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3265	0	3134	16	0
1	C	3265	0	3134	15	0
1	H	3265	0	3134	18	0
1	J	3265	0	3134	14	0
1	O	3265	0	3134	23	0
1	Q	3265	0	3134	19	0
1	V	3265	0	3134	16	0
1	X	3265	0	3134	15	0
2	B	3308	0	3180	28	0
2	D	3308	0	3180	26	0
2	I	3308	0	3180	33	0
2	K	3308	0	3180	23	0
2	P	3308	0	3180	31	0
2	R	3308	0	3180	25	0
2	W	3308	0	3180	24	0
2	Y	3308	0	3180	22	0
3	E	3936	0	4050	89	0
3	L	3924	0	4035	99	0
3	S	3922	0	4037	109	0
3	Z	3936	0	4050	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	1135	0	1125	7	0
4	G	1135	0	1125	6	0
4	M	1135	0	1125	9	0
4	N	1135	0	1125	2	0
4	T	1135	0	1125	5	0
4	U	1135	0	1125	5	0
4	a	1135	0	1125	23	0
4	b	1135	0	1125	6	0
5	A	32	0	12	1	0
5	C	32	0	12	2	0
5	H	32	0	12	1	0
5	J	32	0	12	1	0
5	O	32	0	12	2	0
5	Q	32	0	12	2	0
5	V	32	0	12	1	0
5	X	32	0	12	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	H	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
6	K	1	0	0	0	0
6	O	1	0	0	0	0
6	P	1	0	0	0	0
6	Q	1	0	0	0	0
6	R	1	0	0	0	0
6	V	1	0	0	0	0
6	W	1	0	0	0	0
6	X	1	0	0	0	0
6	Y	1	0	0	0	0
7	B	28	0	12	0	0
7	D	28	0	12	0	0
7	I	28	0	12	0	0
7	K	28	0	12	0	0
7	P	28	0	12	0	0
7	R	28	0	12	0	0
7	W	28	0	12	0	0
7	Y	28	0	12	0	0
All	All	77878	0	75876	766	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 766 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:218:GLN:HA	3:E:222:LEU:HB3	1.59	0.85
3:E:403:VAL:HG13	3:E:404:PRO:HD3	1.61	0.81
3:Z:403:VAL:HG13	3:Z:404:PRO:HD3	1.61	0.81
3:E:305:LEU:HD22	3:E:306:PRO:HD2	1.62	0.81
3:Z:218:GLN:HA	3:Z:222:LEU:HB2	1.62	0.81

There are no symmetry-related clashes.

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%)	24	57
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%)	43	72
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%)	43	72
2	D	420/445 (94%)	403 (96%)	15 (4%)	2 (0%)	24	57
2	I	420/445 (94%)	402 (96%)	16 (4%)	2 (0%)	24	57
2	K	420/445 (94%)	403 (96%)	16 (4%)	1 (0%)	43	72
2	P	420/445 (94%)	403 (96%)	16 (4%)	1 (0%)	43	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	R	420/445 (94%)	404 (96%)	15 (4%)	1 (0%)	43	72
2	W	420/445 (94%)	402 (96%)	16 (4%)	2 (0%)	24	57
2	Y	420/445 (94%)	404 (96%)	15 (4%)	1 (0%)	43	72
3	E	486/536 (91%)	448 (92%)	36 (7%)	2 (0%)	30	61
3	L	485/536 (90%)	448 (92%)	35 (7%)	2 (0%)	30	61
3	S	484/536 (90%)	449 (93%)	30 (6%)	5 (1%)	12	45
3	Z	486/536 (91%)	453 (93%)	29 (6%)	4 (1%)	16	49
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%)	18	51
4	b	153/169 (90%)	145 (95%)	8 (5%)	0	100	100
All	All	9861/10664 (92%)	9284 (94%)	549 (6%)	28 (0%)	36	65

5 of 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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/377 (92%)	346 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	346/377 (92%)	346 (100%)	0	100	100
1	H	346/377 (92%)	346 (100%)	0	100	100
1	J	346/377 (92%)	346 (100%)	0	100	100
1	O	346/377 (92%)	346 (100%)	0	100	100
1	Q	346/377 (92%)	346 (100%)	0	100	100
1	V	346/377 (92%)	346 (100%)	0	100	100
1	X	346/377 (92%)	346 (100%)	0	100	100
2	B	361/381 (95%)	360 (100%)	1 (0%)	86	83
2	D	361/381 (95%)	361 (100%)	0	100	100
2	I	361/381 (95%)	361 (100%)	0	100	100
2	K	361/381 (95%)	361 (100%)	0	100	100
2	P	361/381 (95%)	361 (100%)	0	100	100
2	R	361/381 (95%)	361 (100%)	0	100	100
2	W	361/381 (95%)	359 (99%)	2 (1%)	78	79
2	Y	361/381 (95%)	361 (100%)	0	100	100
3	E	448/488 (92%)	446 (100%)	2 (0%)	84	81
3	L	447/488 (92%)	446 (100%)	1 (0%)	87	85
3	S	447/488 (92%)	447 (100%)	0	100	100
3	Z	448/488 (92%)	447 (100%)	1 (0%)	87	85
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%)	8367 (100%)	7 (0%)	88	87

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	403	VAL

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Mol	Chain	Res	Type
2	W	171	VAL
3	Z	390	ARG
2	W	338	LYS
3	E	390	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
2	Y	385	GLN
3	Z	171	ASN
3	L	171	ASN
2	K	385	GLN
3	Z	340	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
5	GTP	C	600	6	33,34,34	1.02	4 (12%)	50,54,54	1.52	8 (16%)
5	GTP	H	600	6	33,34,34	1.03	2 (6%)	50,54,54	1.98	8 (16%)
7	GDP	R	600	6	29,30,30	1.17	2 (6%)	45,47,47	1.75	7 (15%)
7	GDP	D	600	6	29,30,30	1.17	2 (6%)	45,47,47	1.70	6 (13%)
5	GTP	Q	600	6	33,34,34	1.02	4 (12%)	50,54,54	1.54	8 (16%)
7	GDP	B	600	6	29,30,30	1.16	2 (6%)	45,47,47	1.71	6 (13%)
7	GDP	K	600	6	29,30,30	1.17	2 (6%)	45,47,47	1.72	6 (13%)
5	GTP	J	600	6	33,34,34	1.00	3 (9%)	50,54,54	1.55	8 (16%)
5	GTP	V	600	6	33,34,34	1.00	2 (6%)	50,54,54	1.52	8 (16%)
5	GTP	A	600	6	33,34,34	1.00	4 (12%)	50,54,54	1.56	8 (16%)
7	GDP	W	600	6	29,30,30	1.16	2 (6%)	45,47,47	1.70	6 (13%)
7	GDP	P	600	6	29,30,30	1.16	2 (6%)	45,47,47	1.75	6 (13%)
5	GTP	X	600	6	33,34,34	1.01	3 (9%)	50,54,54	1.54	8 (16%)
5	GTP	O	600	6	33,34,34	0.99	3 (9%)	50,54,54	1.56	8 (16%)
7	GDP	I	600	6	29,30,30	1.16	2 (6%)	45,47,47	1.73	7 (15%)
7	GDP	Y	600	6	29,30,30	1.17	2 (6%)	45,47,47	1.72	7 (15%)

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
5	GTP	C	600	6	-	2/22/38/38	0/3/3/3
5	GTP	H	600	6	-	2/22/38/38	0/3/3/3
7	GDP	R	600	6	-	5/16/32/32	0/3/3/3
7	GDP	D	600	6	-	5/16/32/32	0/3/3/3
5	GTP	Q	600	6	-	2/22/38/38	0/3/3/3
7	GDP	B	600	6	-	3/16/32/32	0/3/3/3
7	GDP	K	600	6	-	3/16/32/32	0/3/3/3
5	GTP	J	600	6	-	2/22/38/38	0/3/3/3
5	GTP	V	600	6	-	1/22/38/38	0/3/3/3
5	GTP	A	600	6	-	2/22/38/38	0/3/3/3
7	GDP	W	600	6	-	5/16/32/32	0/3/3/3
7	GDP	P	600	6	-	4/16/32/32	0/3/3/3
5	GTP	X	600	6	-	3/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	O	600	6	-	3/22/38/38	0/3/3/3
7	GDP	I	600	6	-	5/16/32/32	0/3/3/3
7	GDP	Y	600	6	-	4/16/32/32	0/3/3/3

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	K	600	GDP	C5-C4	3.18	1.47	1.38
7	P	600	GDP	C5-C4	3.17	1.47	1.38
7	R	600	GDP	C5-C4	3.16	1.47	1.38
7	I	600	GDP	C5-C4	3.16	1.47	1.38
7	W	600	GDP	C5-C4	3.16	1.47	1.38

The worst 5 of 115 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	600	GTP	C5-C4-N3	-6.71	117.72	128.39
7	P	600	GDP	C5-C4-N3	-5.96	118.91	128.39
7	R	600	GDP	C5-C4-N3	-5.95	118.92	128.39
7	I	600	GDP	C5-C4-N3	-5.95	118.92	128.39
7	W	600	GDP	C5-C4-N3	-5.94	118.94	128.39

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

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

There are no ring outliers.

8 monomers are involved in 11 short contacts:

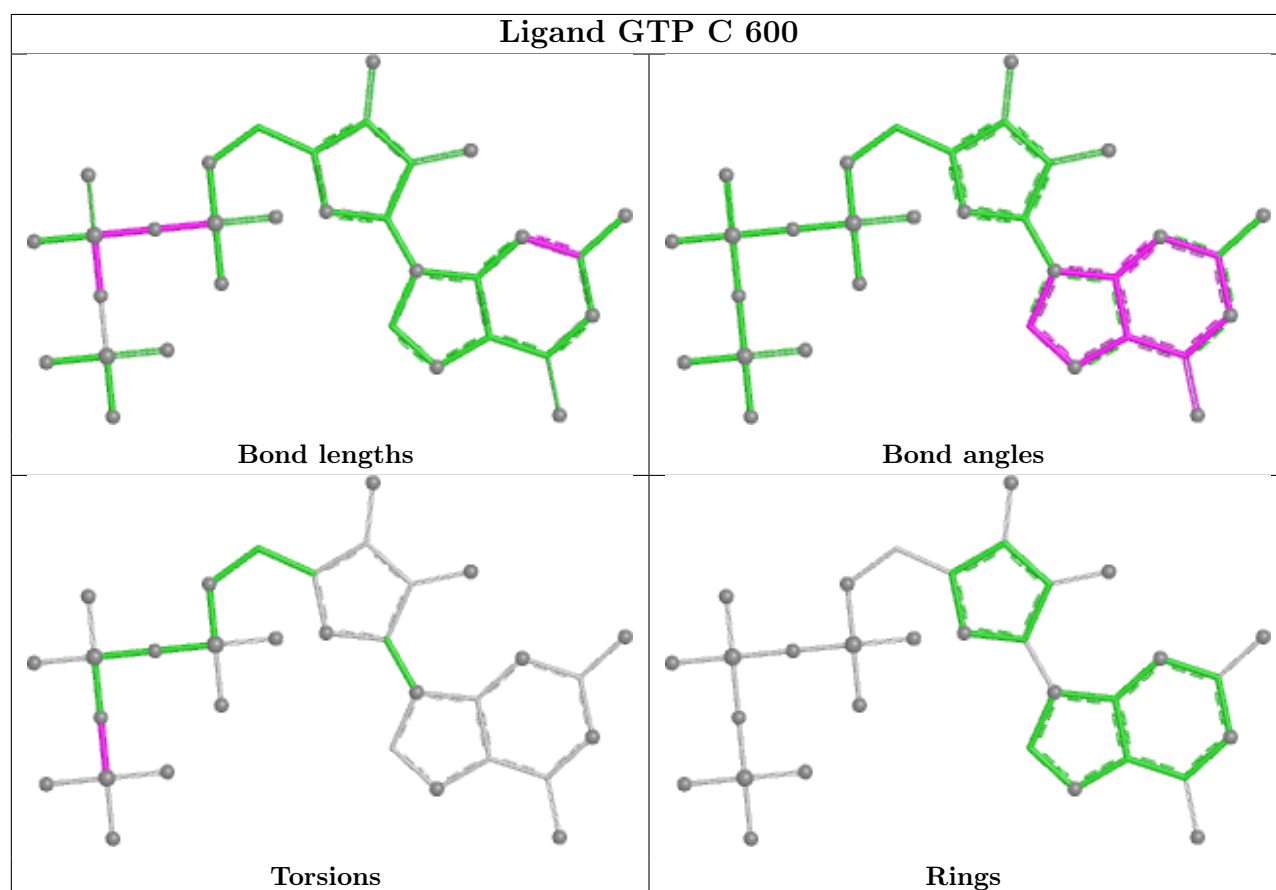
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	600	GTP	2	0
5	H	600	GTP	1	0
5	Q	600	GTP	2	0
5	J	600	GTP	1	0

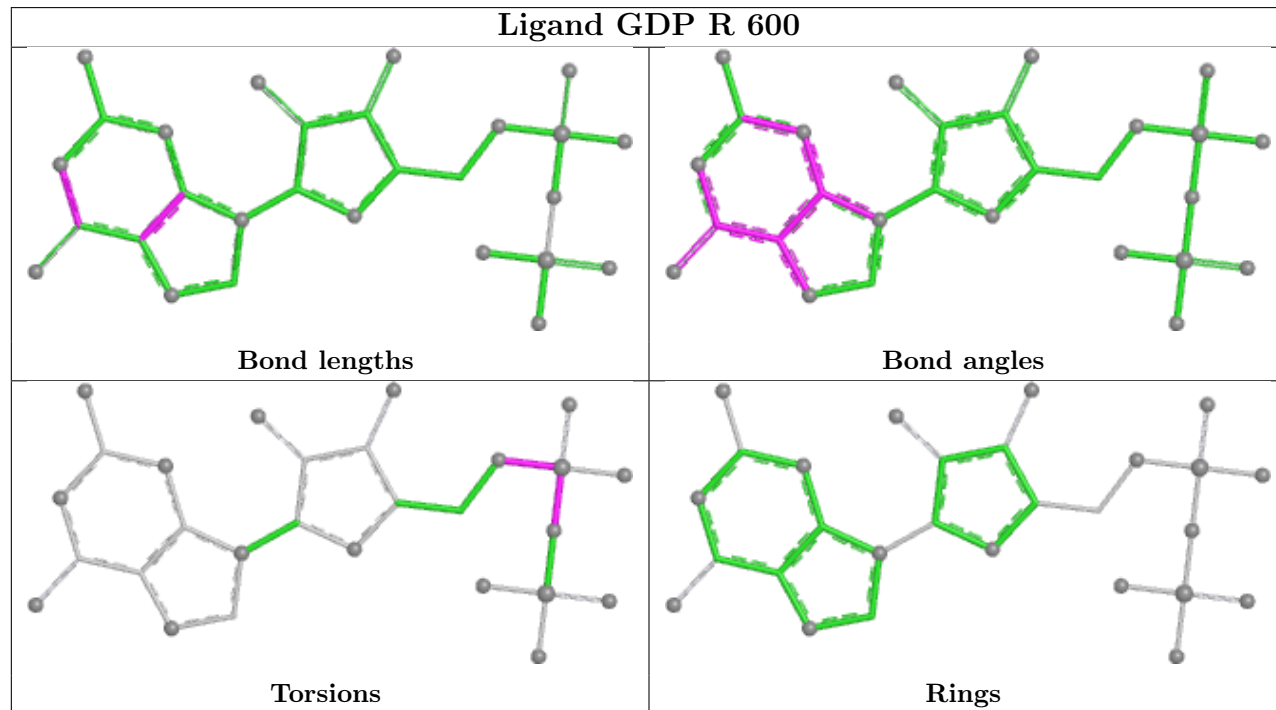
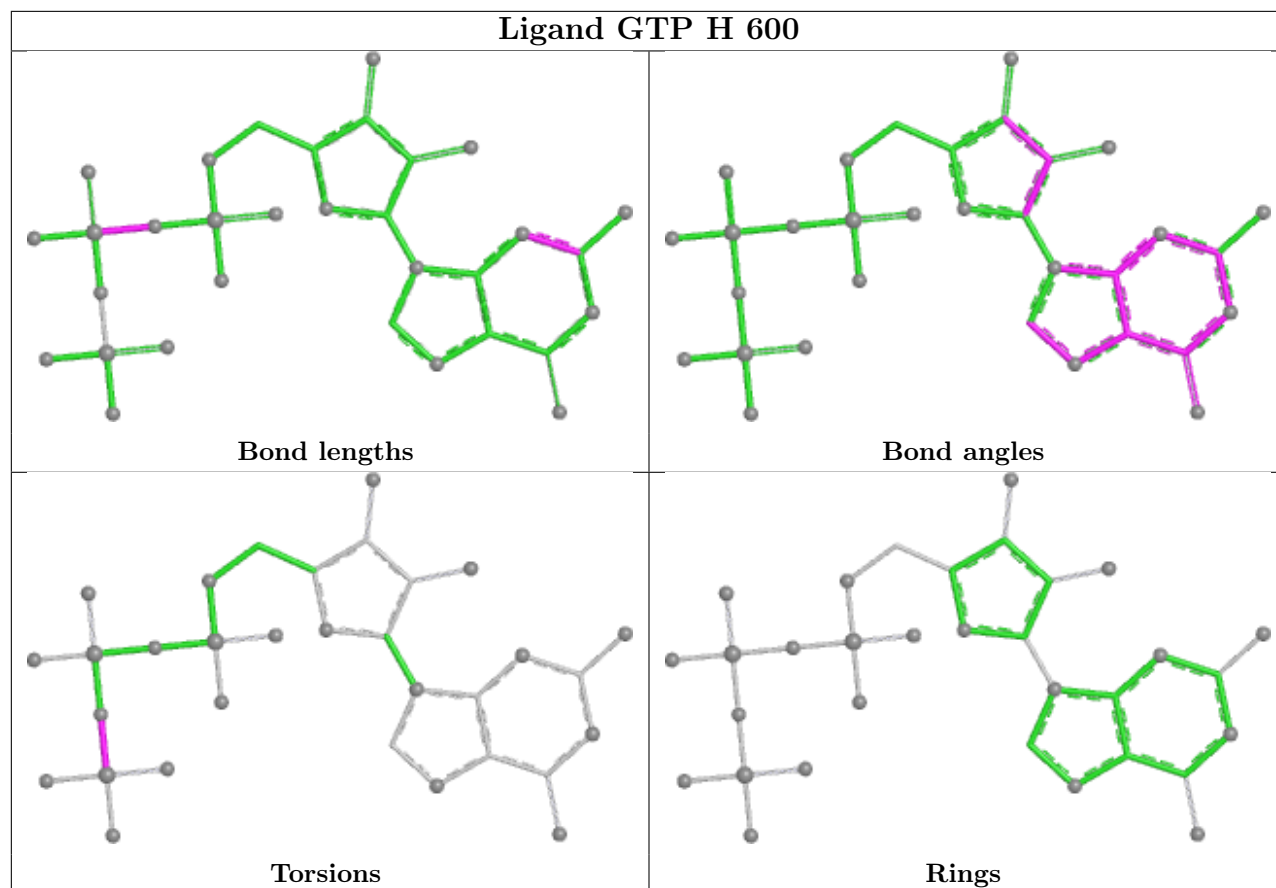
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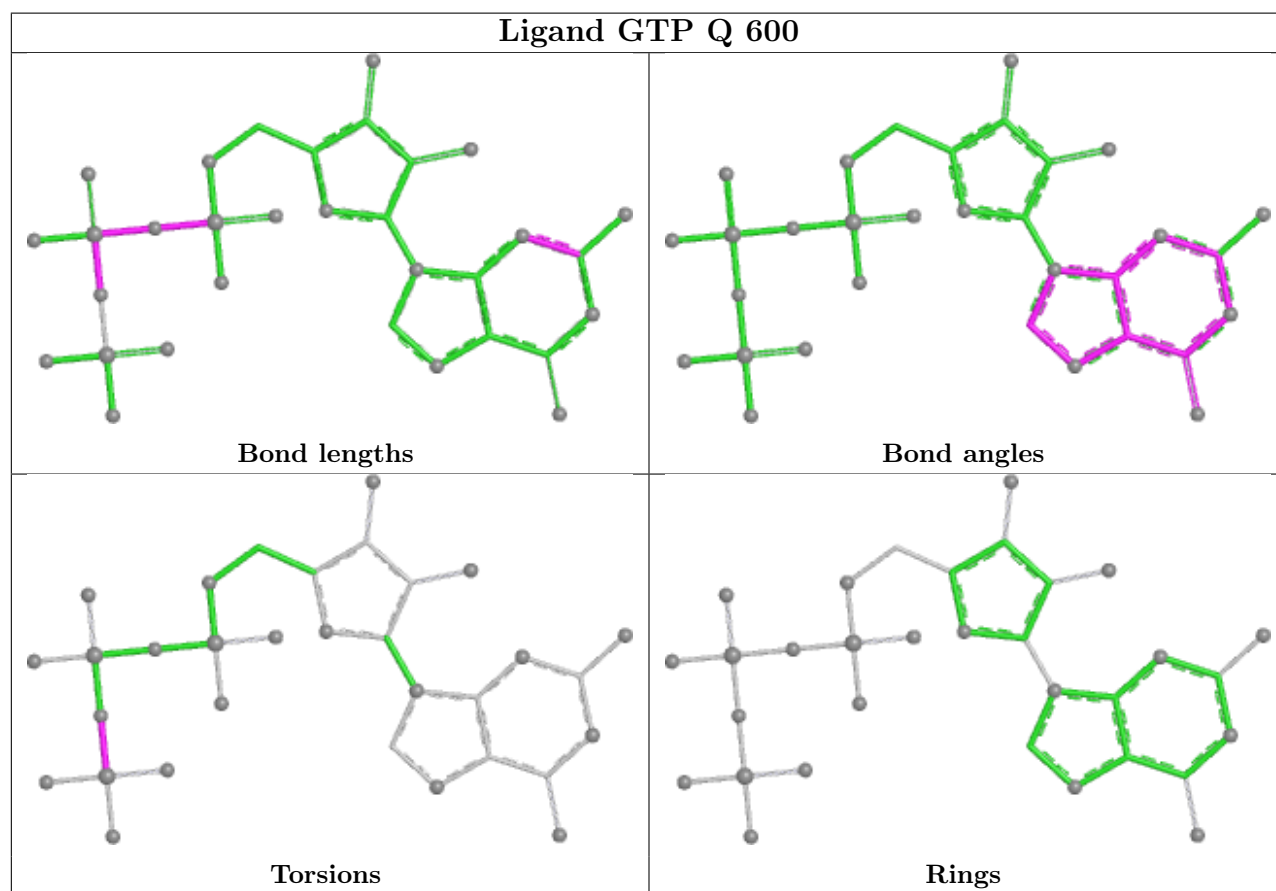
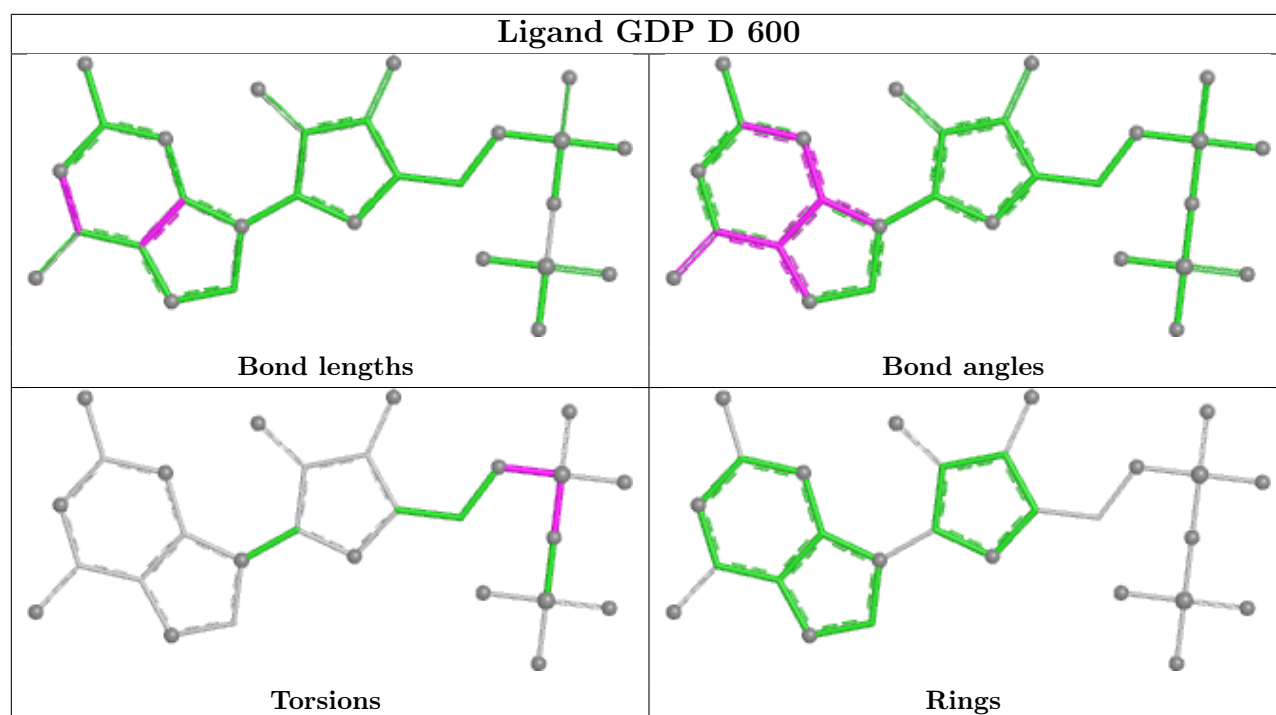
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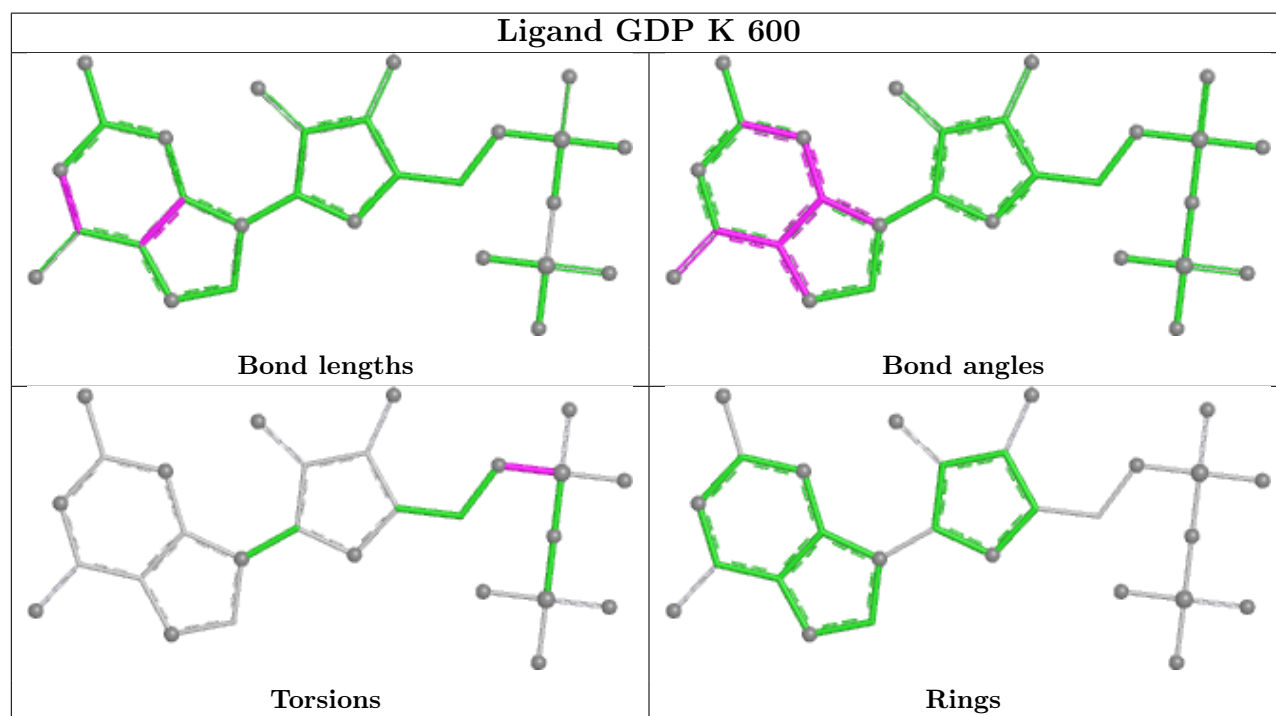
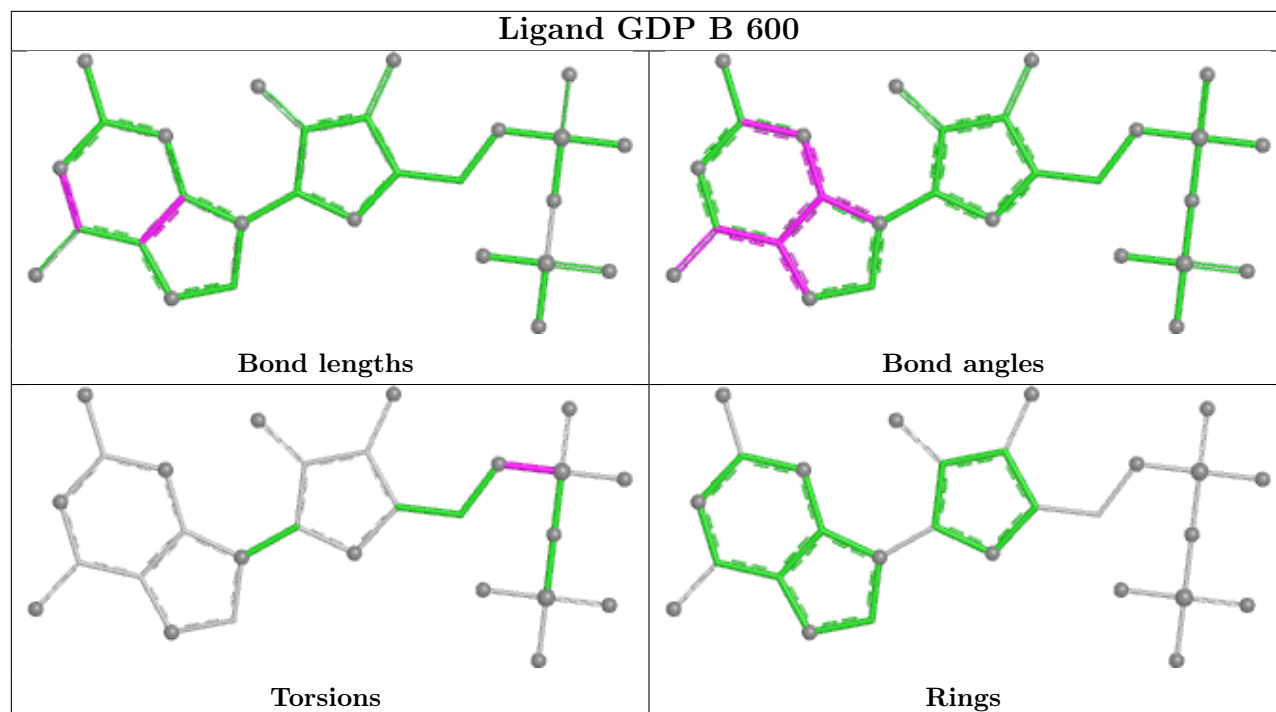
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	V	600	GTP	1	0
5	A	600	GTP	1	0
5	X	600	GTP	1	0
5	O	600	GTP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

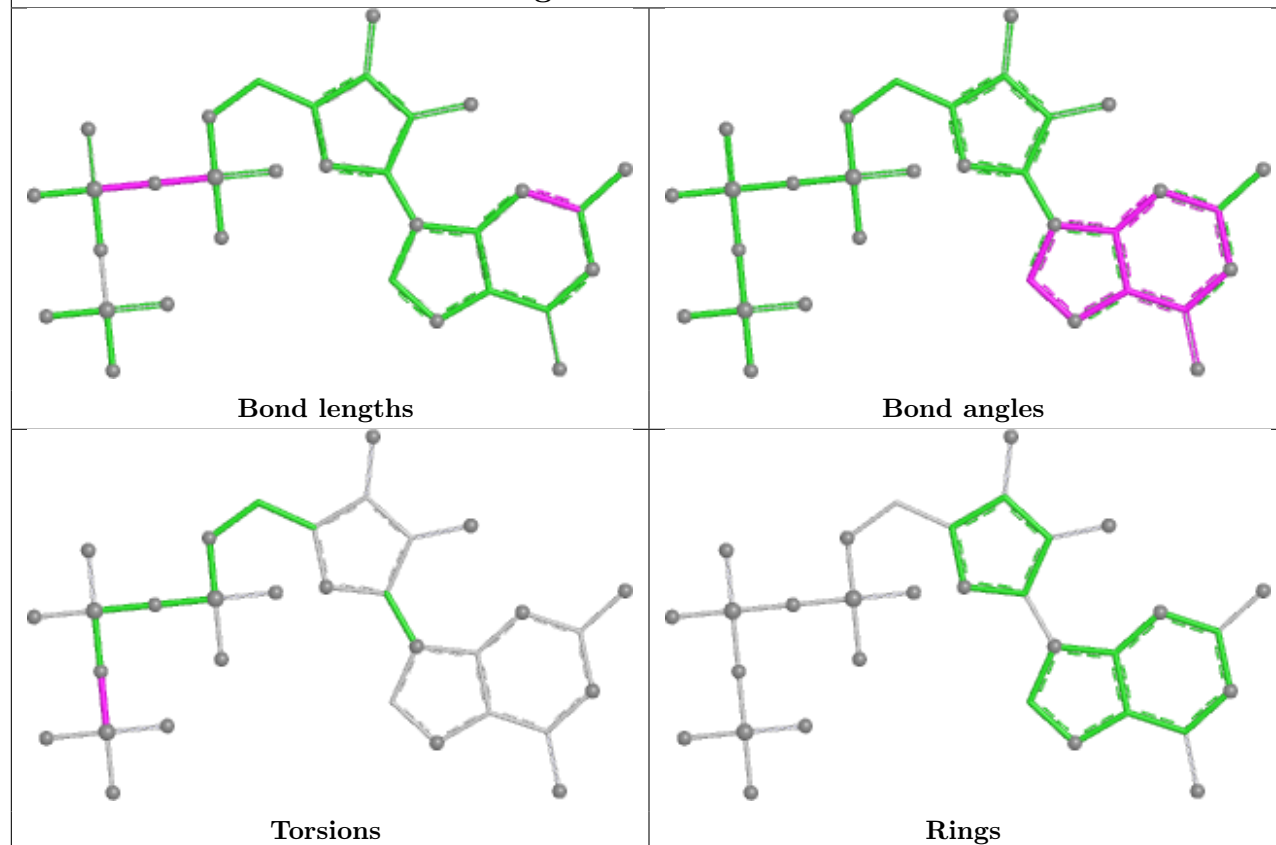




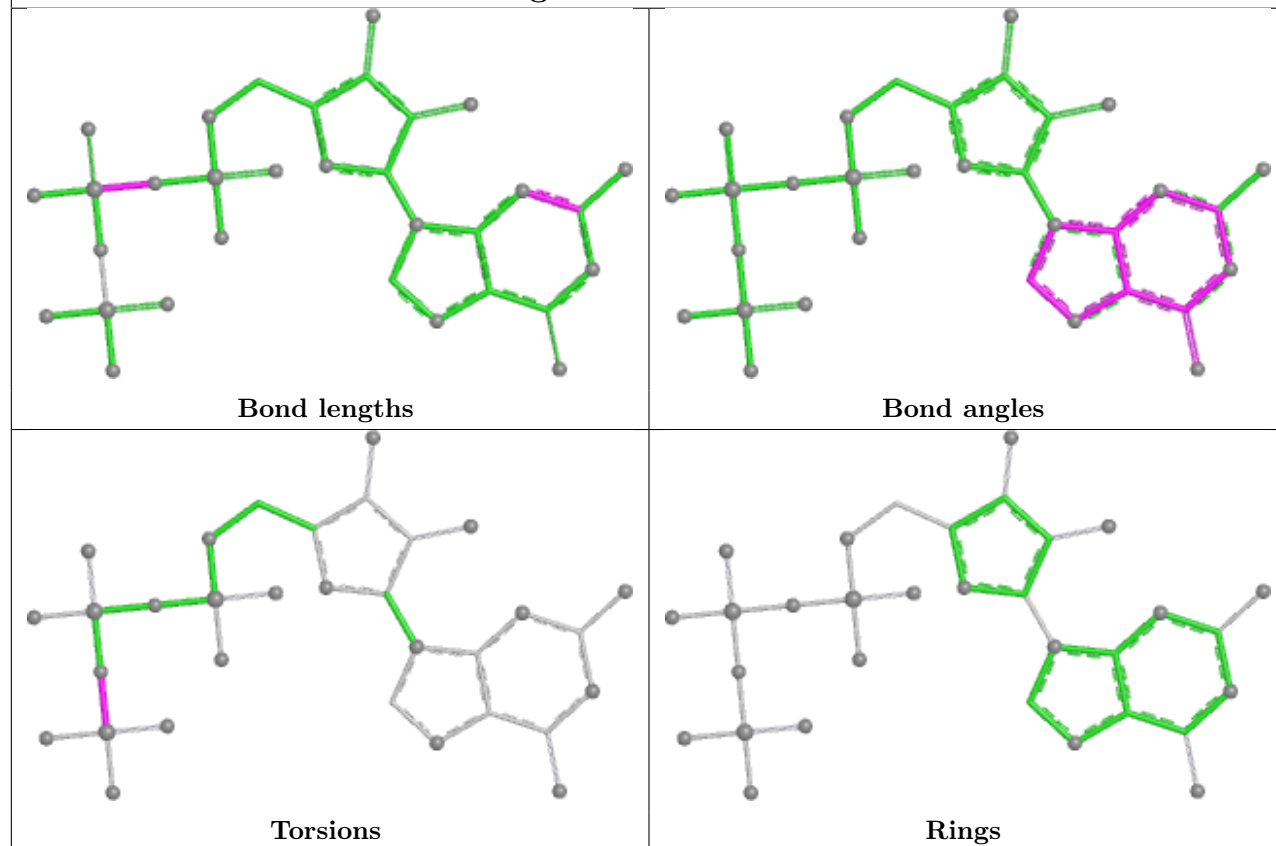


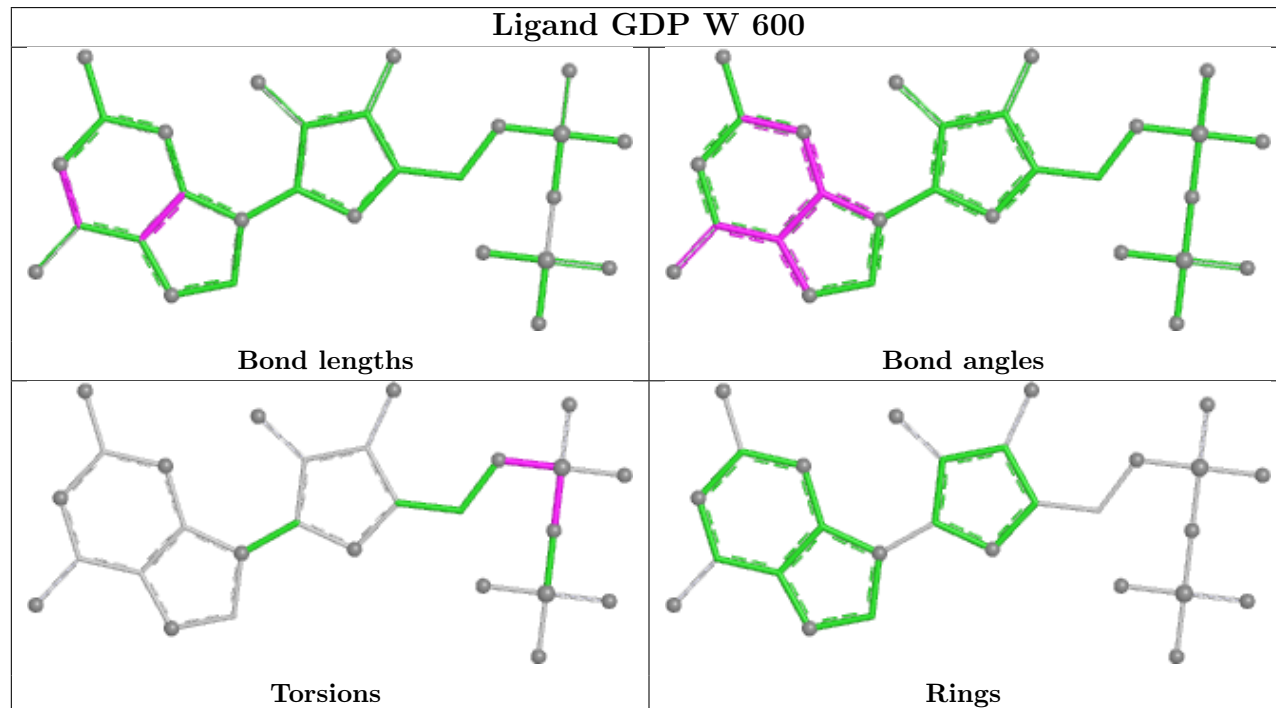
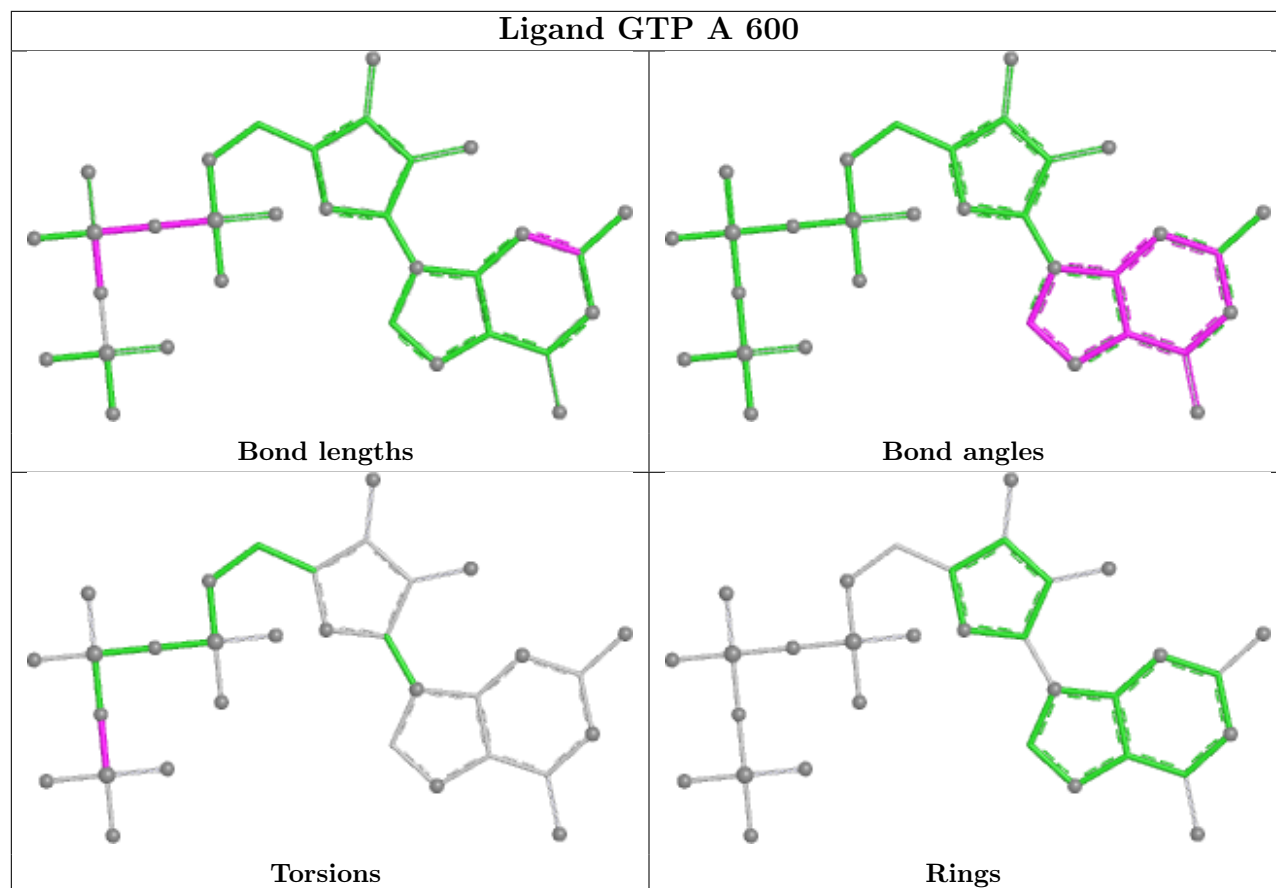


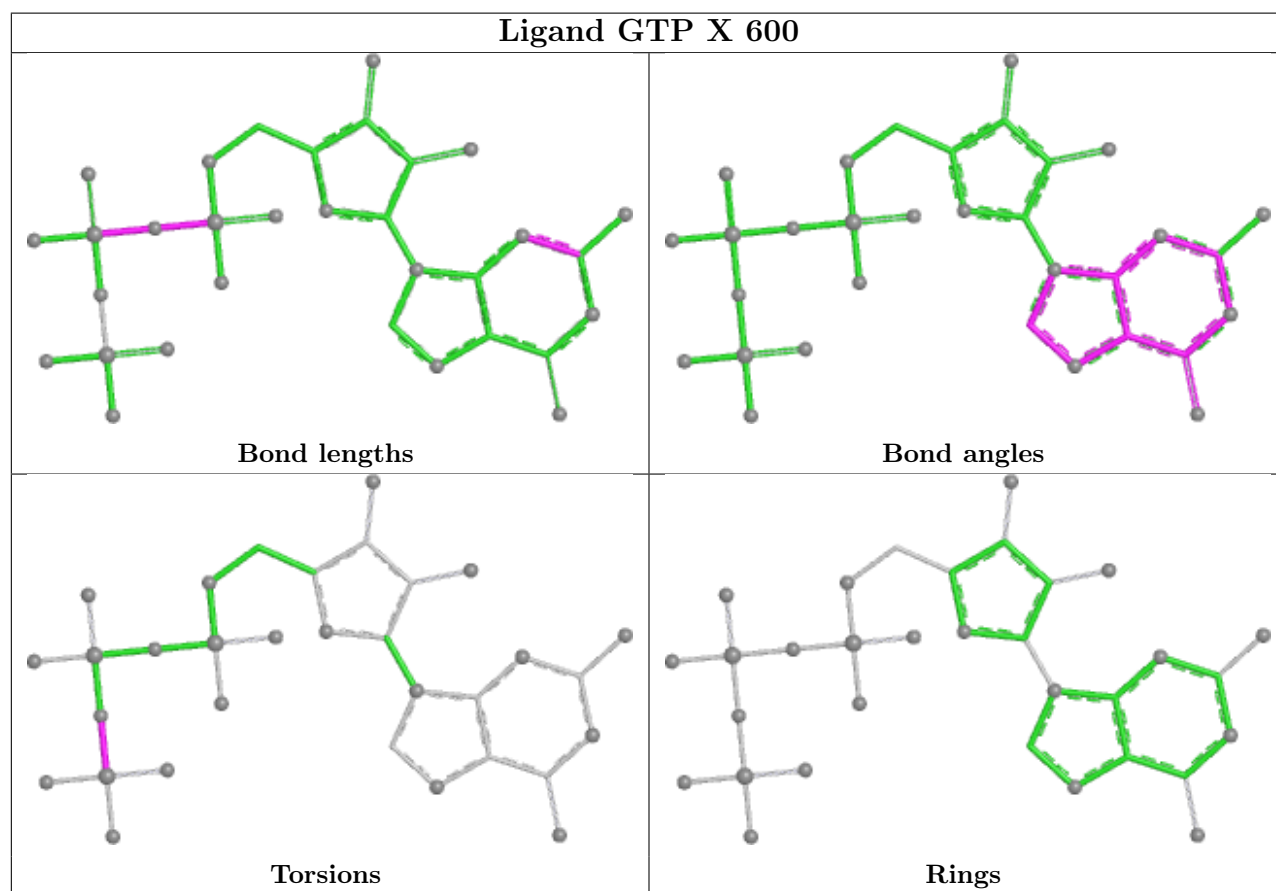
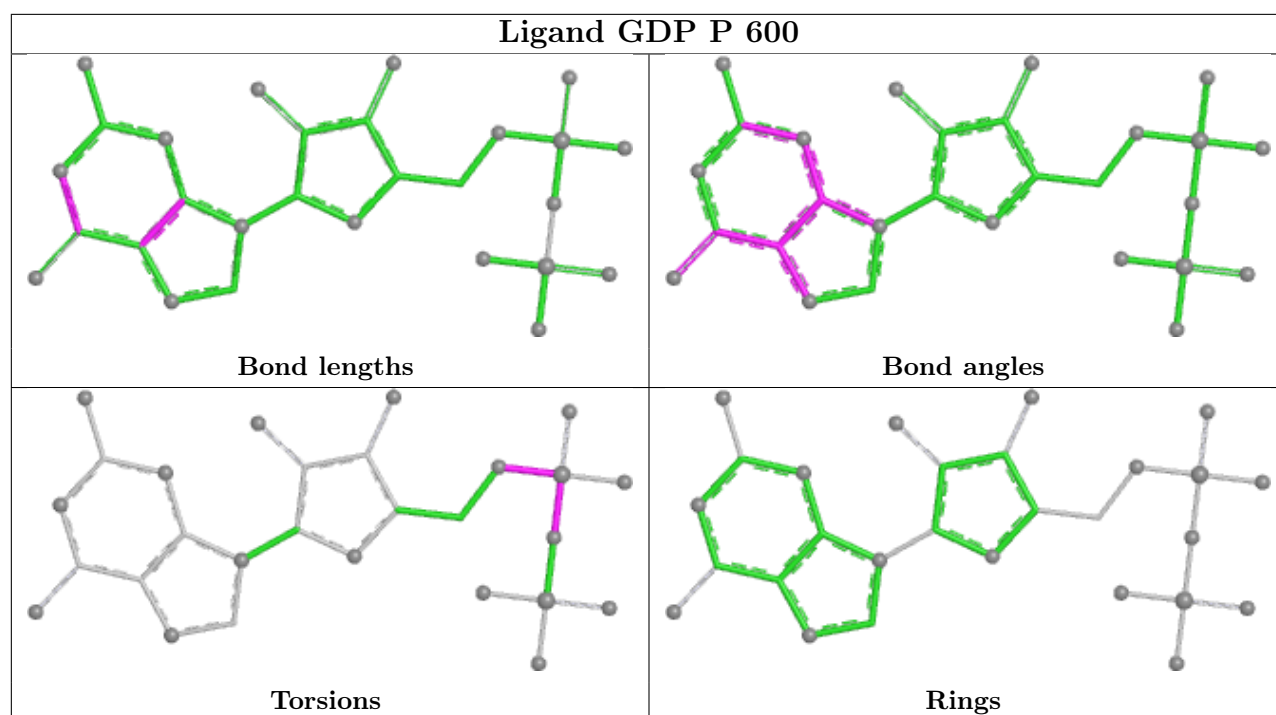
Ligand GTP J 600

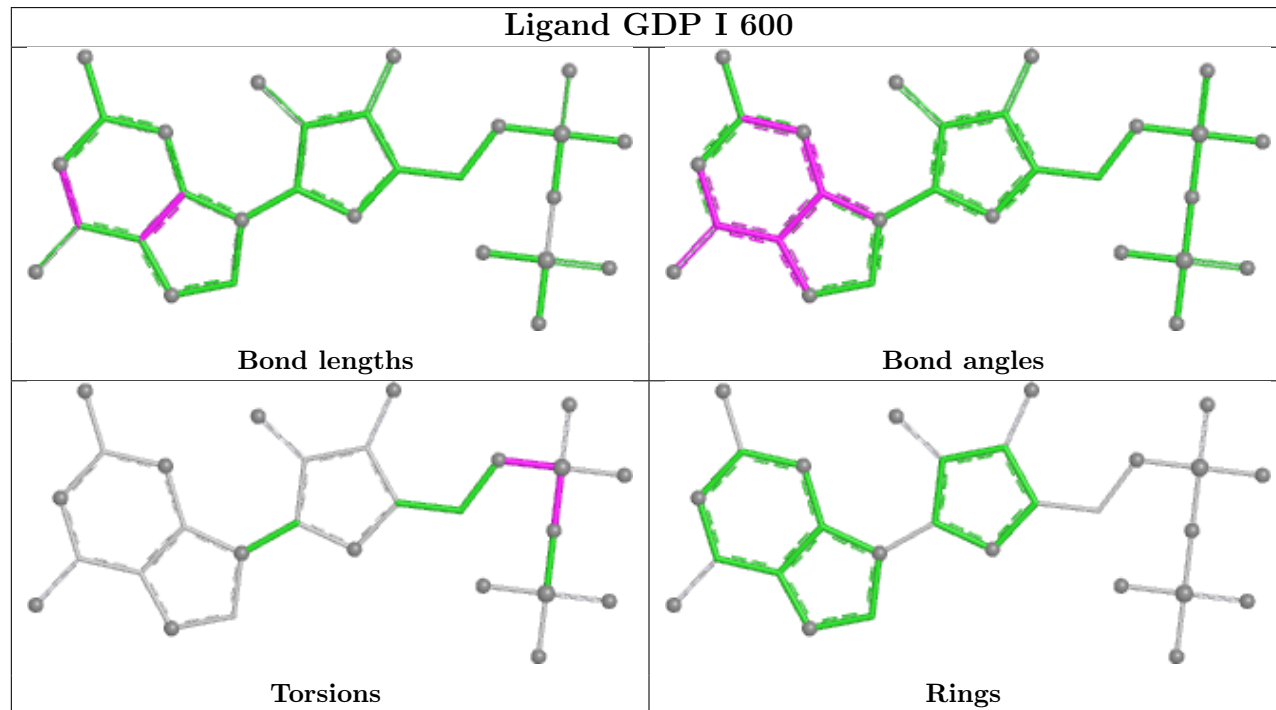
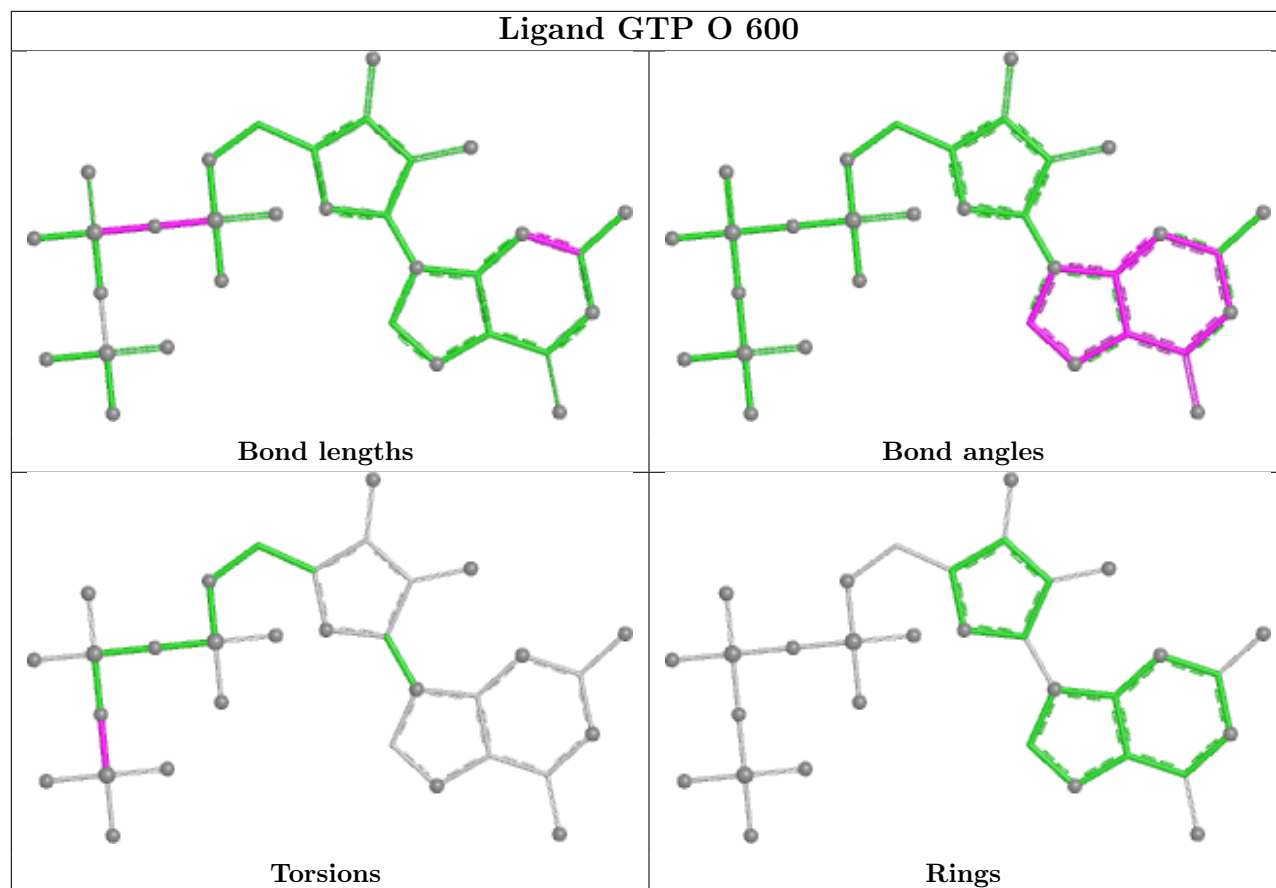


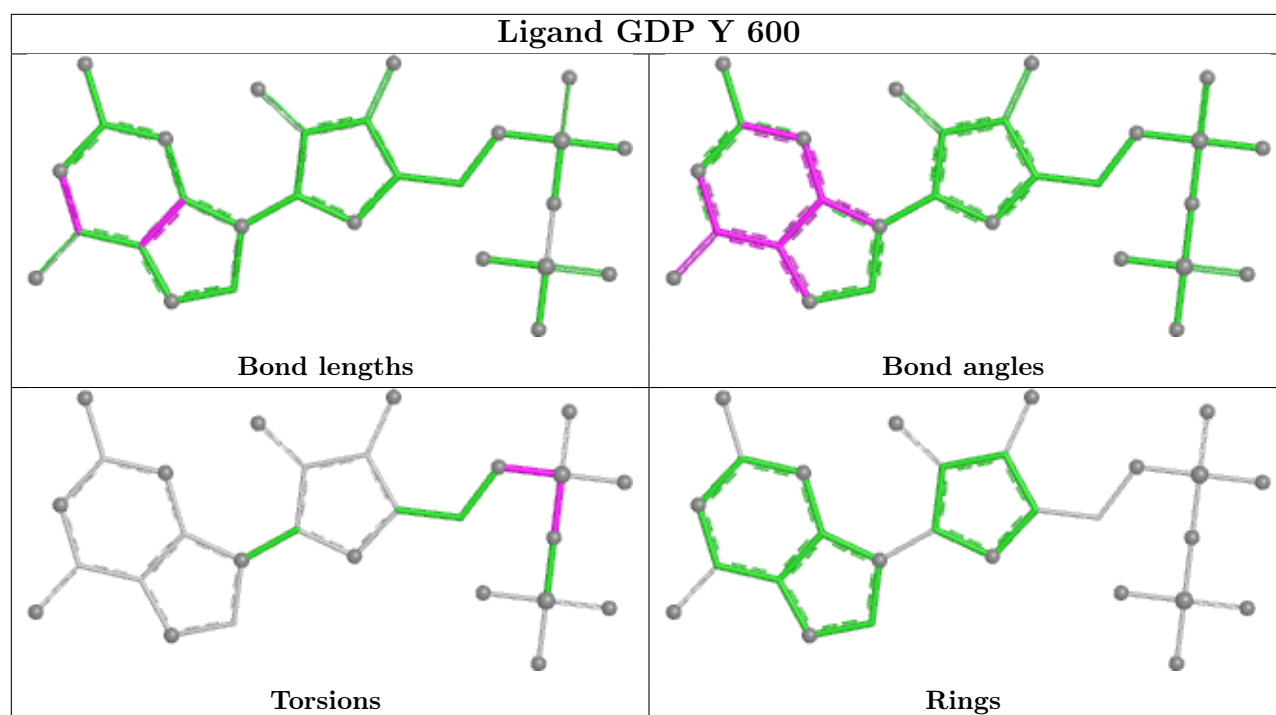
Ligand GTP V 600











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.02	3 (0%) 84 61	33, 103, 160, 243	0
1	C	423/451 (93%)	-0.20	2 (0%) 87 66	41, 86, 135, 174	0
1	H	423/451 (93%)	-0.16	1 (0%) 91 80	37, 89, 136, 211	0
1	J	423/451 (93%)	0.04	2 (0%) 87 66	55, 131, 206, 260	0
1	O	423/451 (93%)	0.11	10 (2%) 59 34	58, 133, 192, 267	0
1	Q	423/451 (93%)	-0.31	1 (0%) 91 80	29, 75, 133, 178	0
1	V	423/451 (93%)	-0.12	1 (0%) 91 80	37, 100, 150, 208	0
1	X	423/451 (93%)	0.06	6 (1%) 73 46	45, 116, 179, 304	0
2	B	424/445 (95%)	-0.39	0 100 100	18, 46, 85, 125	0
2	D	424/445 (95%)	-0.22	0 100 100	32, 69, 130, 173	0
2	I	424/445 (95%)	0.04	5 (1%) 76 50	50, 101, 146, 187	0
2	K	424/445 (95%)	0.14	3 (0%) 84 61	72, 122, 170, 283	0
2	P	424/445 (95%)	-0.22	3 (0%) 84 61	42, 82, 125, 176	0
2	R	424/445 (95%)	-0.28	0 100 100	24, 57, 119, 221	0
2	W	424/445 (95%)	0.06	2 (0%) 87 66	50, 98, 153, 177	0
2	Y	424/445 (95%)	-0.16	2 (0%) 87 66	45, 96, 149, 181	0
3	E	492/536 (91%)	-0.13	7 (1%) 73 46	27, 72, 123, 153	0
3	L	491/536 (91%)	-0.09	4 (0%) 82 58	45, 82, 133, 190	0
3	S	490/536 (91%)	-0.02	7 (1%) 73 46	26, 83, 136, 170	0
3	Z	492/536 (91%)	0.03	7 (1%) 73 46	38, 86, 144, 175	0
4	F	155/169 (91%)	-0.19	0 100 100	44, 75, 132, 171	0
4	G	155/169 (91%)	-0.26	1 (0%) 85 64	52, 90, 126, 170	0
4	M	155/169 (91%)	0.61	6 (3%) 43 24	121, 181, 223, 280	0
4	N	155/169 (91%)	0.73	10 (6%) 25 16	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%)	0.16	0 100 100	97, 156, 203, 265	0
4	U	155/169 (91%)	-0.31	1 (0%) 85 64	25, 64, 101, 126	0
4	a	155/169 (91%)	0.73	5 (3%) 50 29	120, 166, 215, 302	0
4	b	155/169 (91%)	0.38	5 (3%) 50 29	89, 148, 200, 245	0
All	All	9981/10664 (93%)	-0.05	94 (0%) 81 56	18, 93, 170, 304	0

The worst 5 of 94 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	b	22	ALA	4.0
1	O	274	PRO	3.8
4	N	63	VAL	3.4
1	O	351	PHE	3.4
4	b	96	VAL	3.3

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	I	601	1/1	0.59	0.24	89,89,89,89	0
6	MG	K	601	1/1	0.66	0.09	72,72,72,72	0
6	MG	O	601	1/1	0.66	0.25	56,56,56,56	0
6	MG	R	601	1/1	0.66	0.25	53,53,53,53	0
6	MG	Y	601	1/1	0.67	0.16	74,74,74,74	0
6	MG	C	601	1/1	0.69	0.30	74,74,74,74	0
6	MG	X	601	1/1	0.72	0.27	83,83,83,83	0

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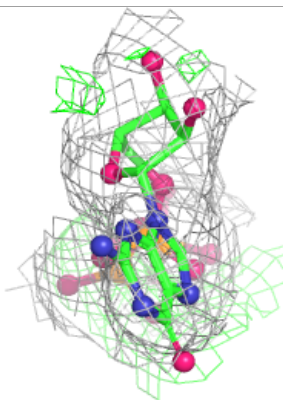
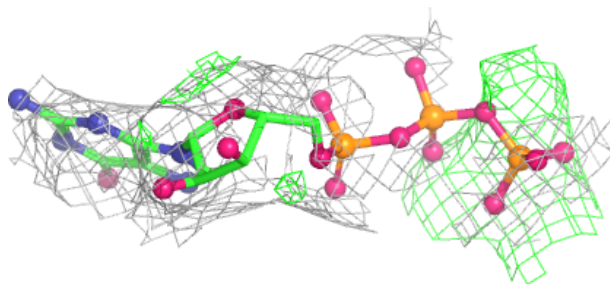
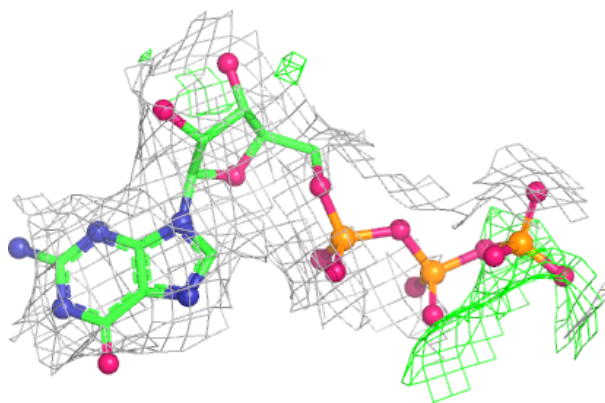
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	J	601	1/1	0.72	0.22	95,95,95,95	0
6	MG	P	601	1/1	0.74	0.27	83,83,83,83	0
6	MG	V	601	1/1	0.74	0.29	52,52,52,52	0
6	MG	W	601	1/1	0.80	0.17	71,71,71,71	0
6	MG	A	601	1/1	0.80	0.26	62,62,62,62	0
6	MG	B	601	1/1	0.80	0.28	30,30,30,30	0
6	MG	H	601	1/1	0.83	0.20	64,64,64,64	0
5	GTP	O	600	32/32	0.87	0.10	78,99,116,120	0
5	GTP	J	600	32/32	0.88	0.09	102,113,137,152	0
7	GDP	K	600	28/28	0.89	0.12	94,122,145,151	0
6	MG	D	601	1/1	0.91	0.20	85,85,85,85	0
6	MG	Q	601	1/1	0.91	0.20	27,27,27,27	0
5	GTP	X	600	32/32	0.91	0.10	58,94,107,113	0
5	GTP	C	600	32/32	0.91	0.10	64,88,100,104	0
7	GDP	P	600	28/28	0.91	0.12	72,97,119,129	0
7	GDP	B	600	28/28	0.93	0.12	38,62,78,89	0
7	GDP	I	600	28/28	0.93	0.10	70,99,114,116	0
5	GTP	H	600	32/32	0.93	0.11	58,89,113,117	0
5	GTP	A	600	32/32	0.93	0.10	68,86,100,107	0
7	GDP	Y	600	28/28	0.93	0.11	76,102,123,125	0
5	GTP	Q	600	32/32	0.94	0.10	51,77,95,97	0
5	GTP	V	600	32/32	0.95	0.10	55,88,102,107	0
7	GDP	W	600	28/28	0.95	0.07	81,99,113,120	0
7	GDP	D	600	28/28	0.95	0.10	59,69,102,108	0
7	GDP	R	600	28/28	0.97	0.08	51,72,85,89	0

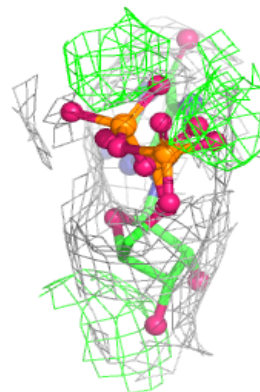
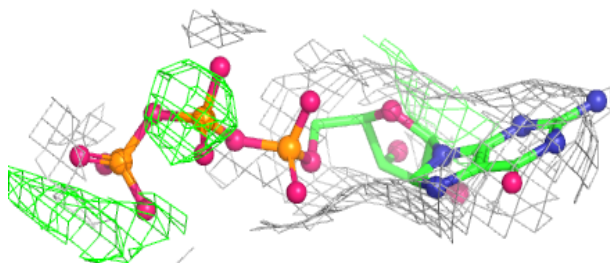
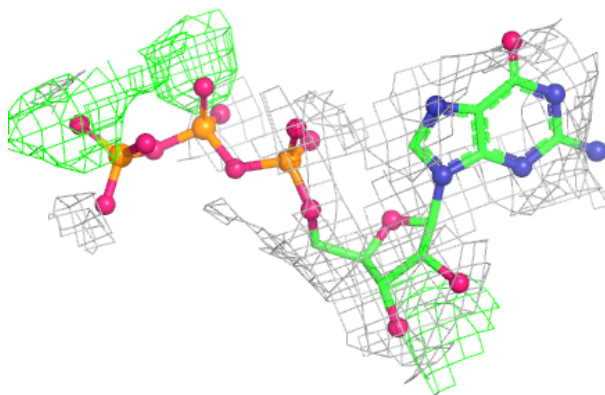
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

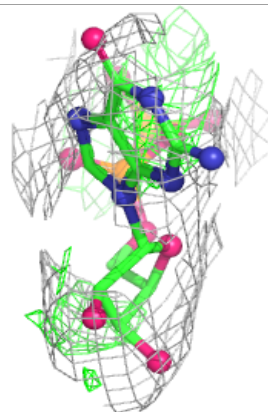
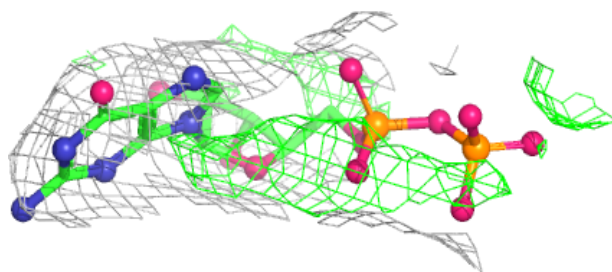
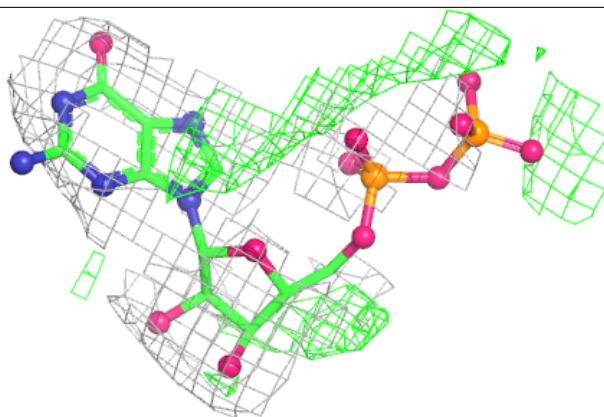
**Electron density around GTP J 600:**

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

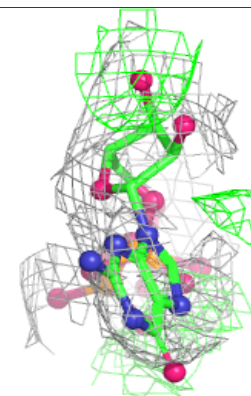
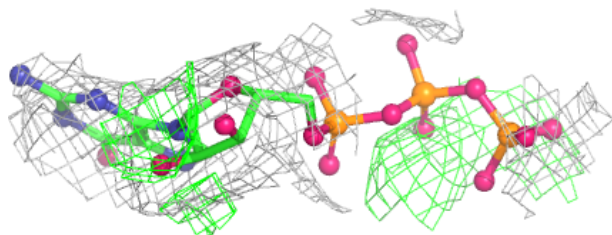
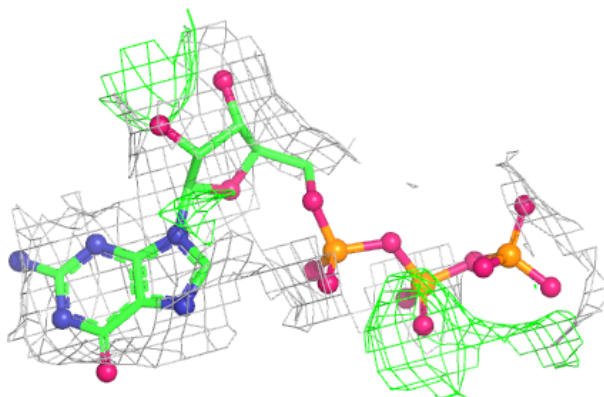


Electron density around GDP K 600:

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

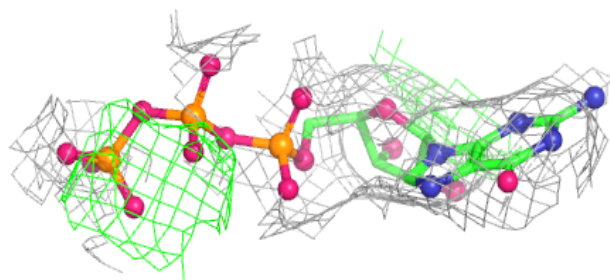
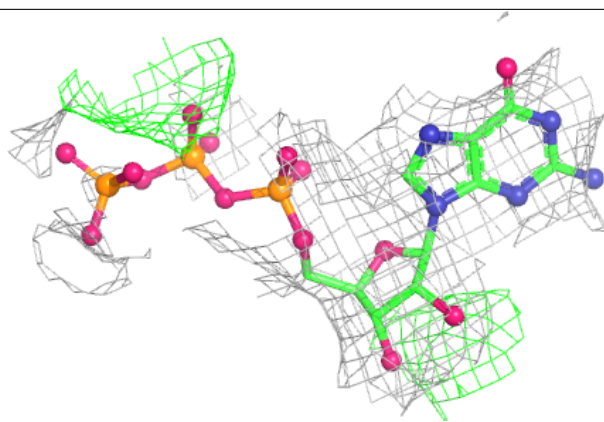
**Electron density around GTP X 600:**

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

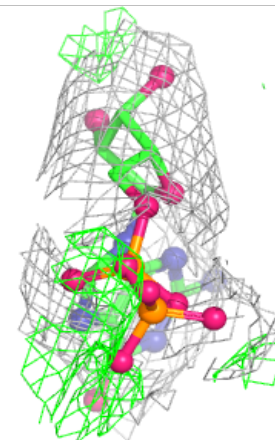
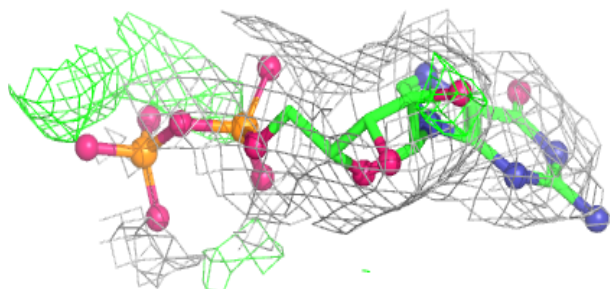
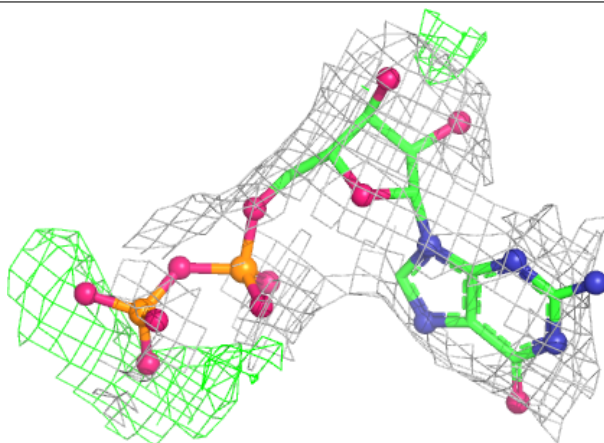


Electron density around GTP C 600:

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

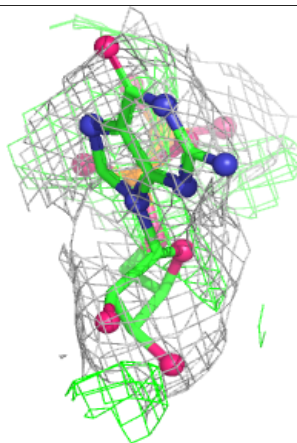
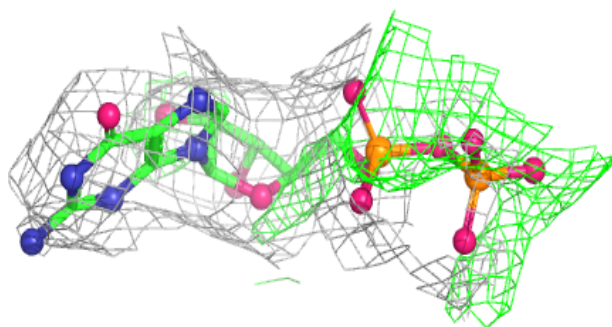
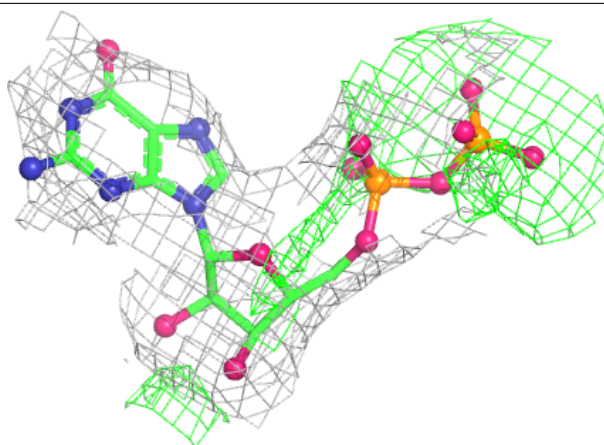
**Electron density around GDP P 600:**

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and green (positive)



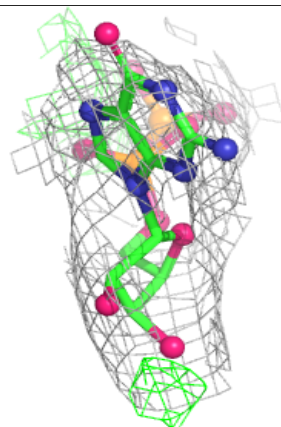
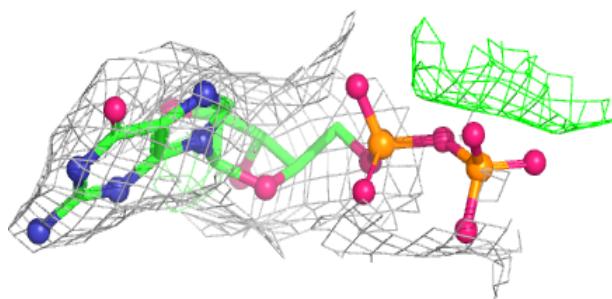
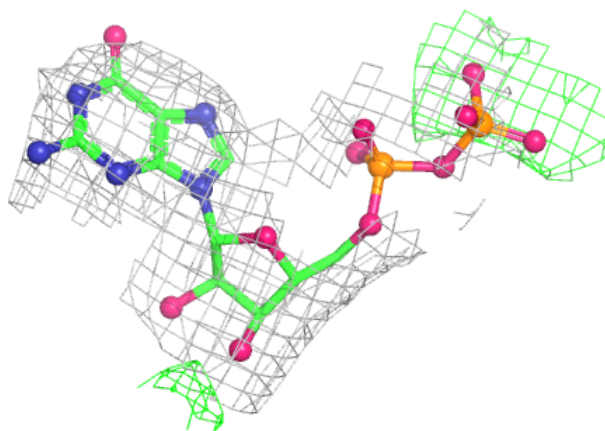
Electron density around GDP B 600:

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

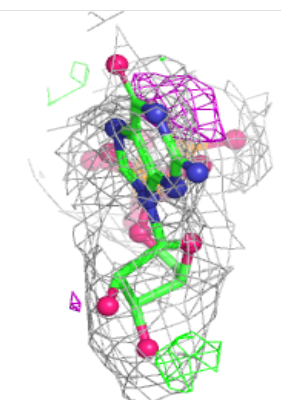
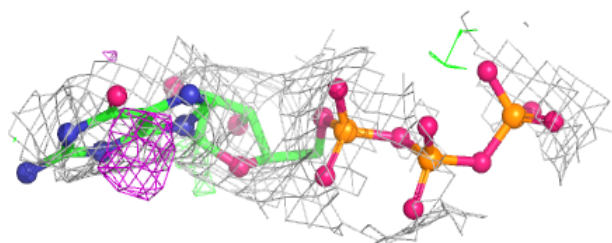
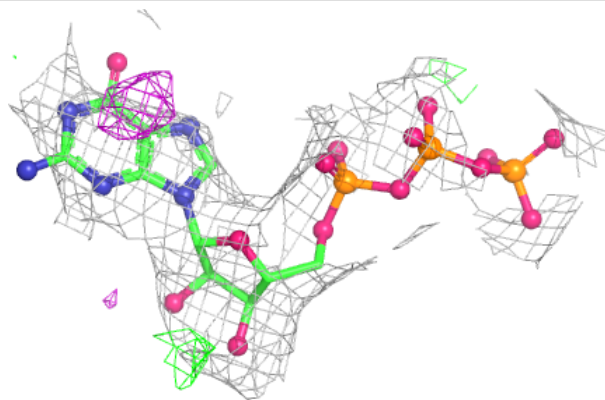


Electron density around GDP I 600:

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and green (positive)

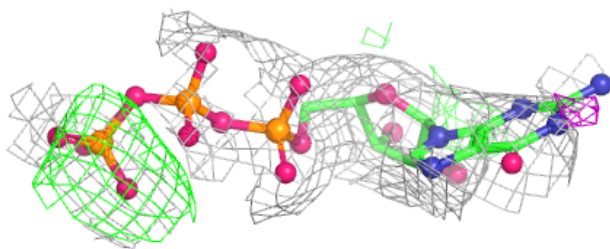
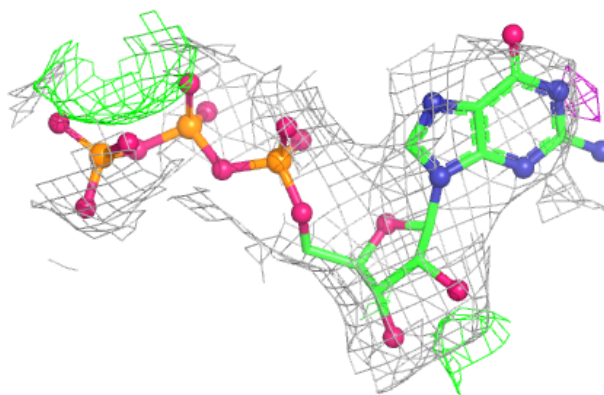
**Electron density around GTP H 600:**

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and green (positive)

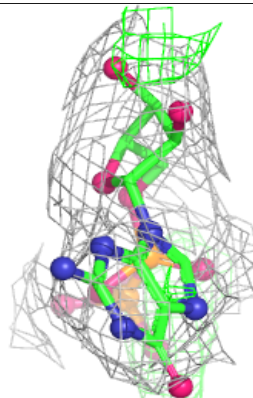
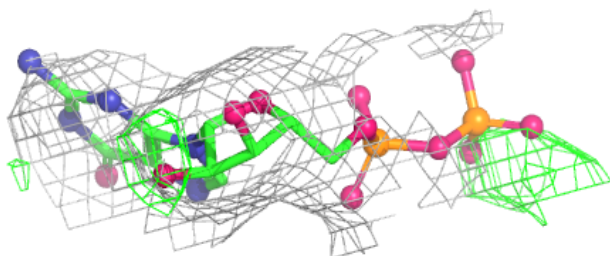
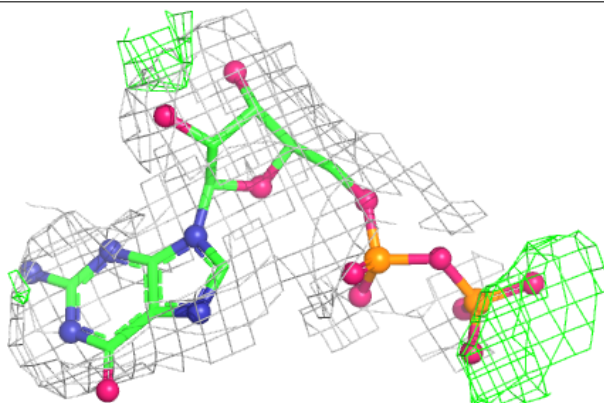


Electron density around GTP A 600:

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and green (positive)

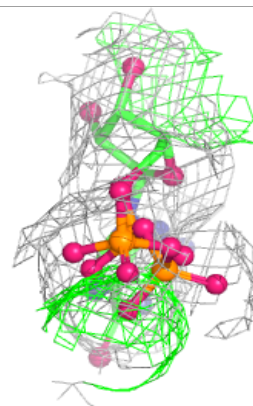
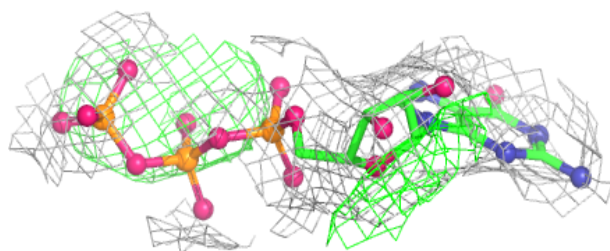
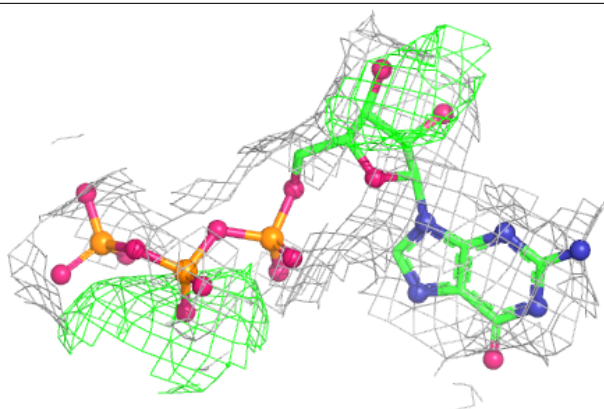
**Electron density around GDP Y 600:**

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

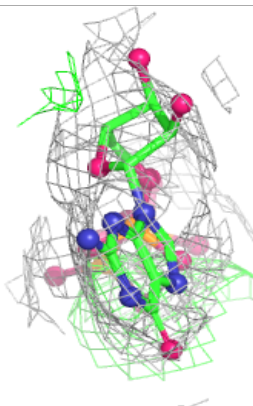
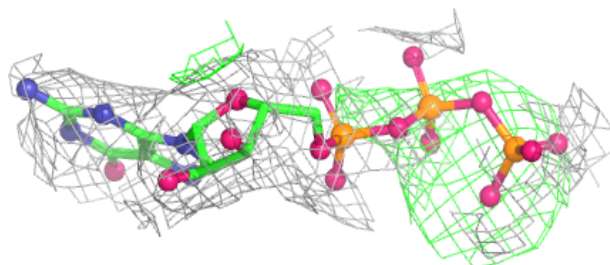
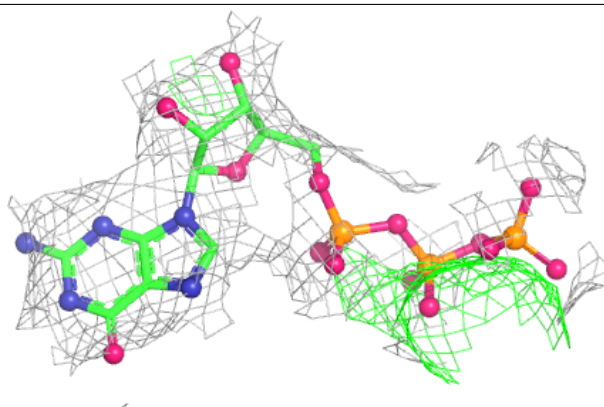


Electron density around GTP Q 600:

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and green (positive)

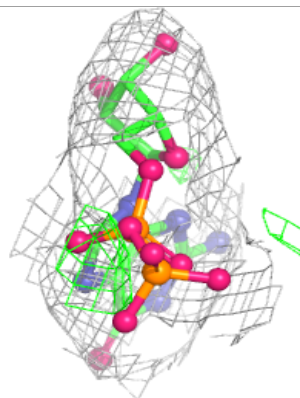
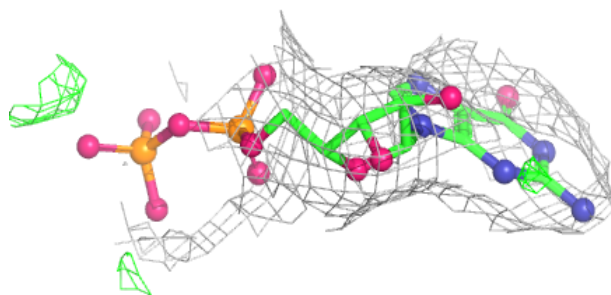
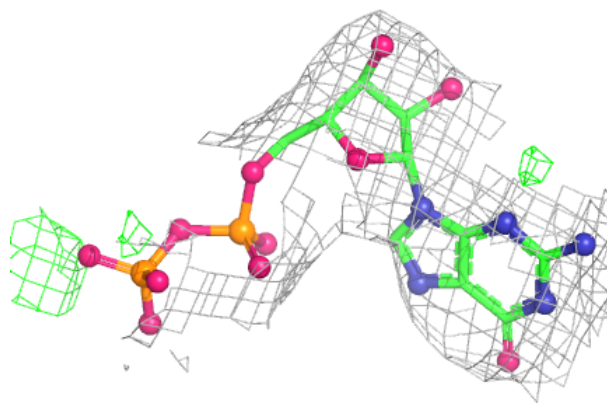
**Electron density around GTP V 600:**

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

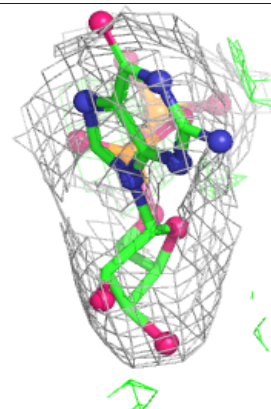
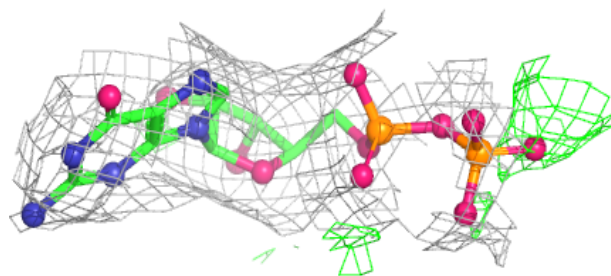
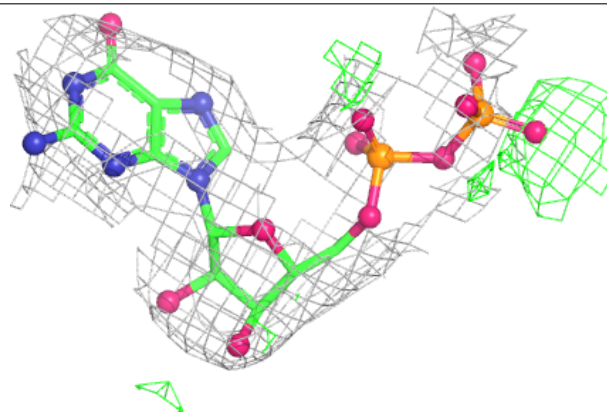


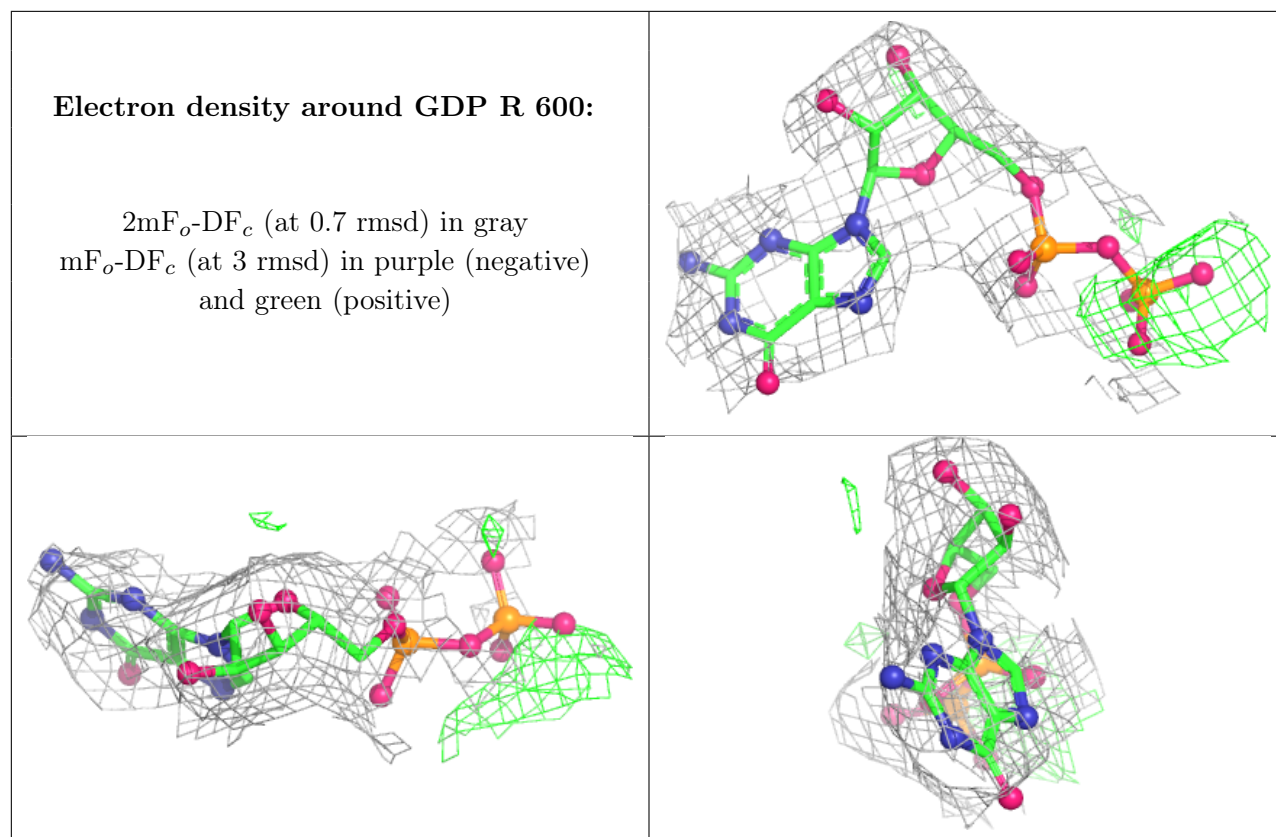
Electron density around GDP W 600:

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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)





6.5 Other polymers [i](#)

There are no such residues in this entry.