



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 04:48 AM UTC

PDB ID : 6MZF / pdb_00006mzf
Title : Structural Basis of Tubulin Recruitment and Assembly by Microtubule Polymerases with Tumor Overexpressed Gene (TOG) Domain Arrays
Authors : Nithianantham, S.; Al-Bassam, J.
Deposited on : 2018-11-05
Resolution : 4.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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

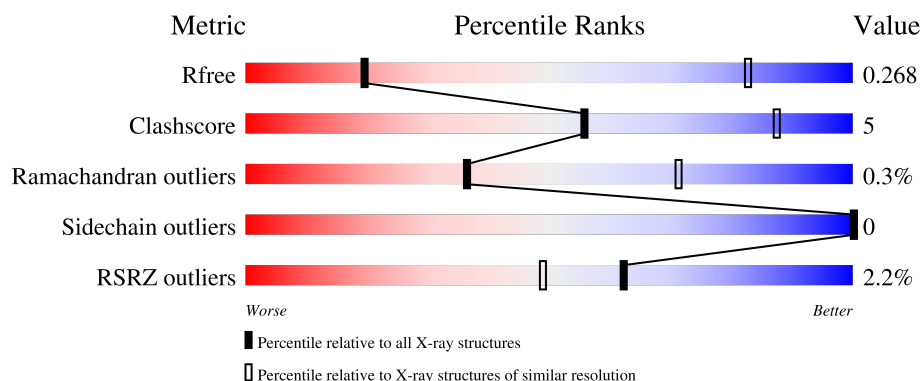
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1088 (4.90-3.90)
Clashscore	190562	1135 (4.90-3.90)
Ramachandran outliers	187476	1026 (4.90-3.90)
Sidechain outliers	187428	1010 (4.90-3.90)
RSRZ outliers	180081	1084 (4.90-3.90)

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	89% 6%
1	C	451	87% 6% 6%
1	H	451	88% 6% 6%
1	J	451	89% 6%
1	O	451	88% 5% 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	554	
3	L	554	
3	S	554	
3	Z	554	
4	F	169	
4	G	169	
4	M	169	
4	N	169	
4	T	169	
4	U	169	
4	a	169	
4	b	169	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 78030 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1A chain.

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

- Molecule 2 is a protein called Tubulin beta chain.

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

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

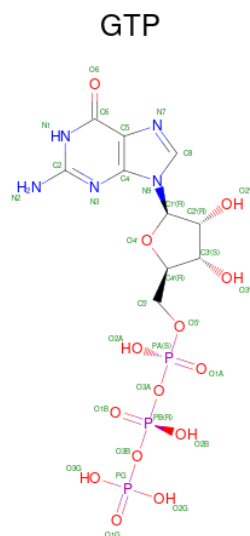
- Molecule 3 is a protein called Protein Stu2p/Alp14p.

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

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

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

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

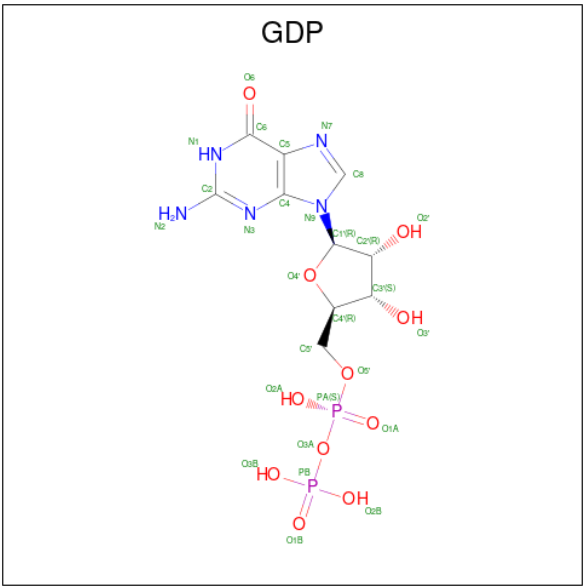
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Mg 1 1	0	0
6	B	1	Total Mg 1 1	0	0
6	C	1	Total Mg 1 1	0	0
6	D	1	Total Mg 1 1	0	0

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

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

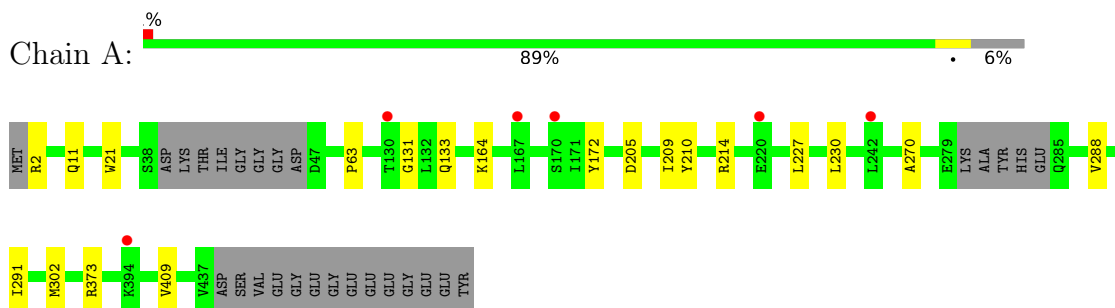


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
7	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
7	I	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
7	K	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
7	P	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
7	R	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
7	W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

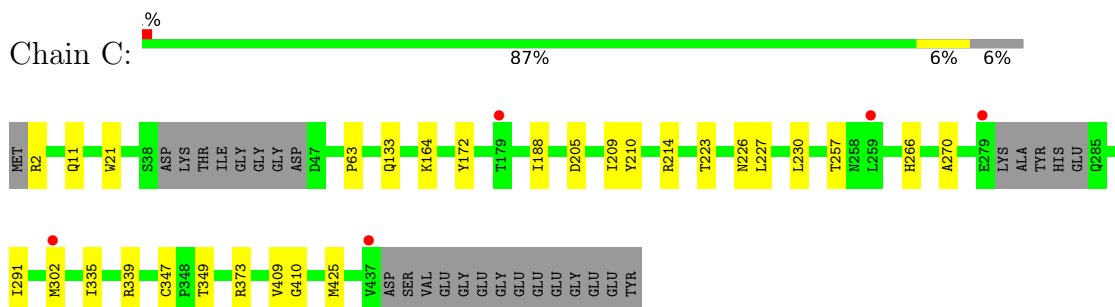
3 Residue-property plots [i](#)

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

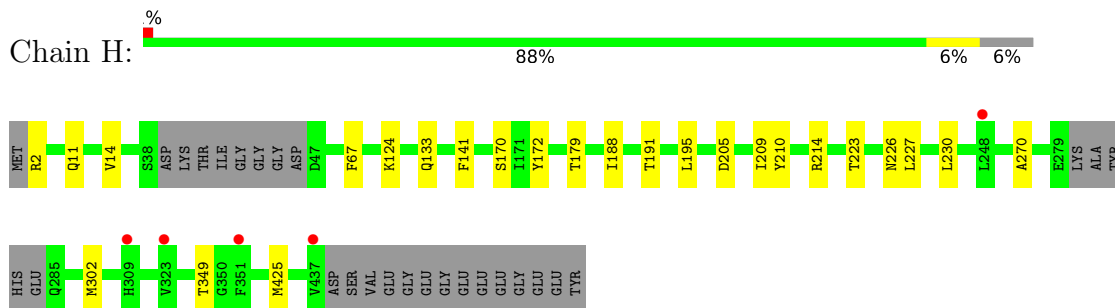
- Molecule 1: Tubulin alpha-1A chain



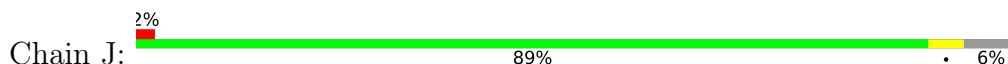
- Molecule 1: Tubulin alpha-1A chain

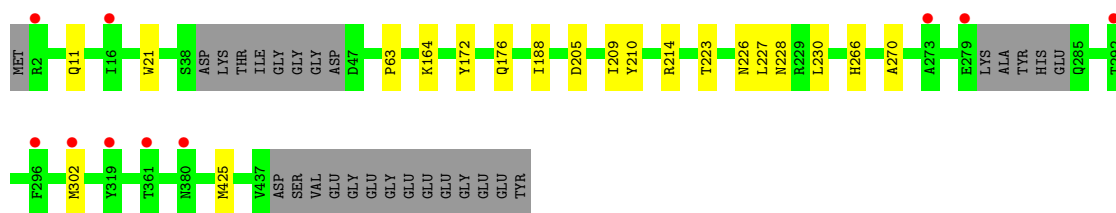


- Molecule 1: Tubulin alpha-1A chain

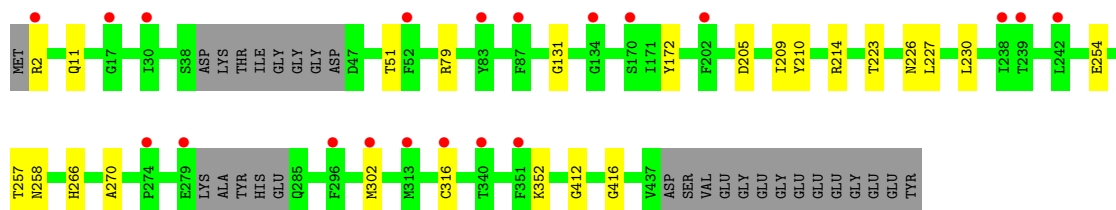
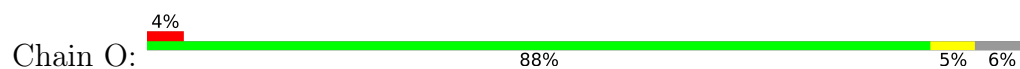


- Molecule 1: Tubulin alpha-1A chain

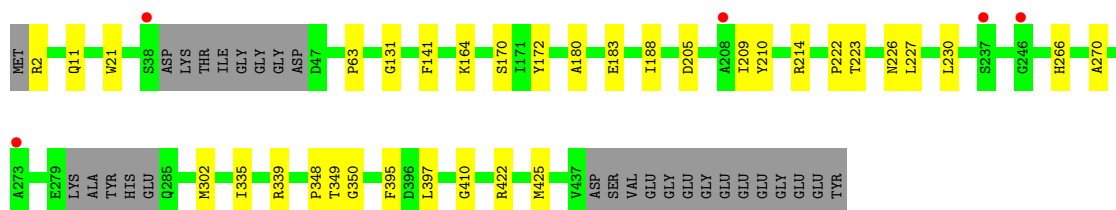
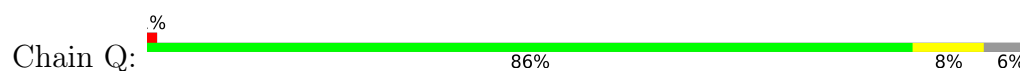




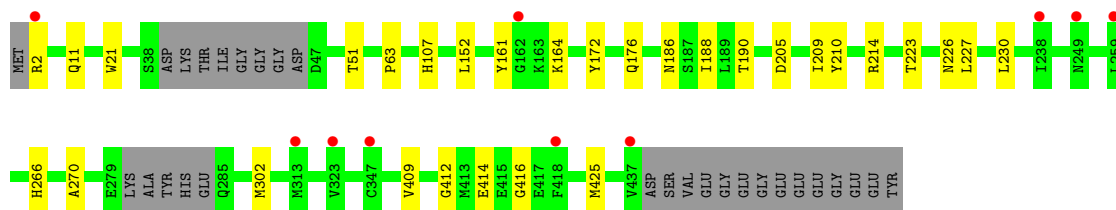
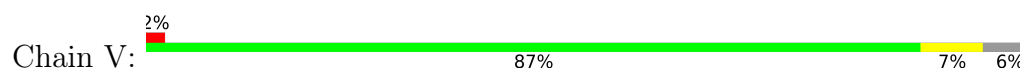
• Molecule 1: Tubulin alpha-1A chain



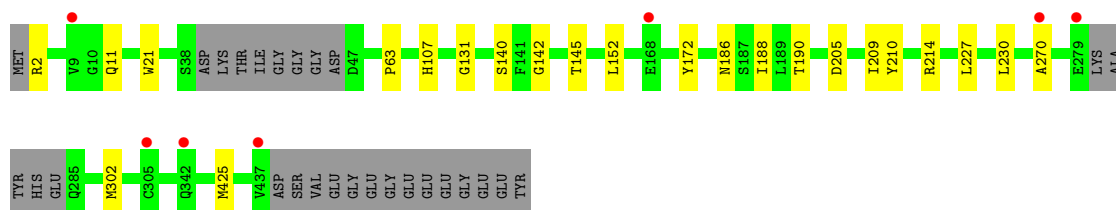
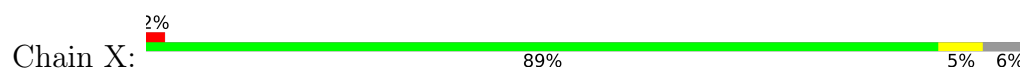
• Molecule 1: Tubulin alpha-1A chain



• Molecule 1: Tubulin alpha-1A chain

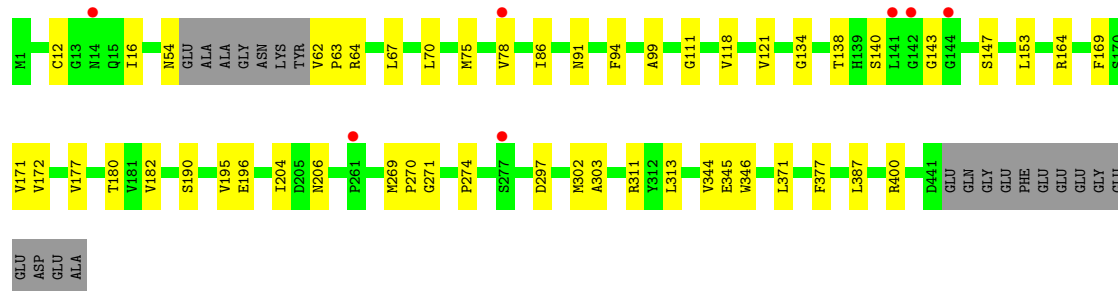


• Molecule 1: Tubulin alpha-1A chain



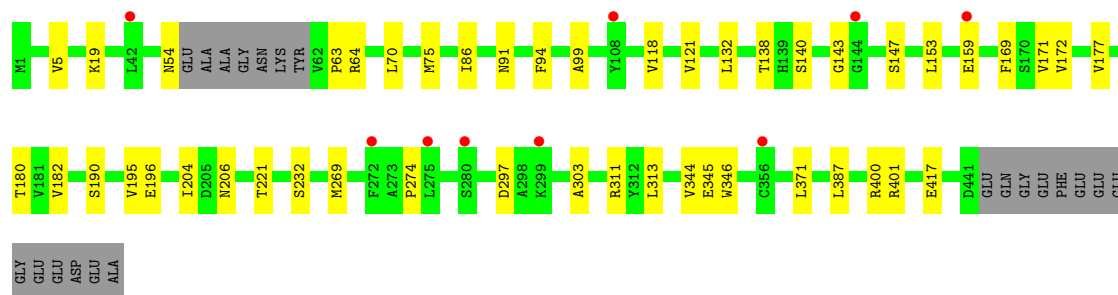
● Molecule 2: Tubulin beta chain

Chain B:  2% 84% 11% 5%



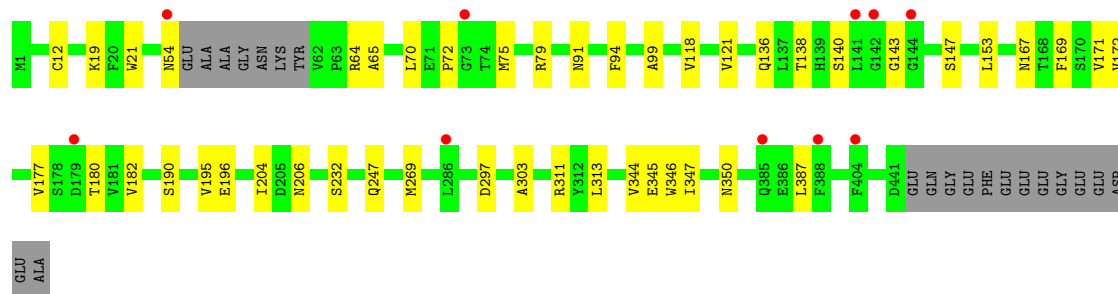
● Molecule 2: Tubulin beta chain

Chain D:  2% 85% 11% 5%



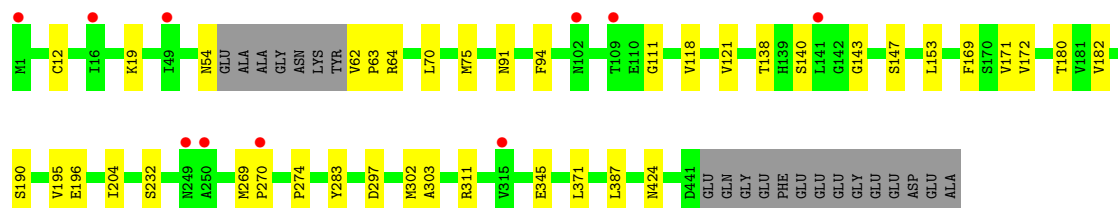
● Molecule 2: Tubulin beta chain

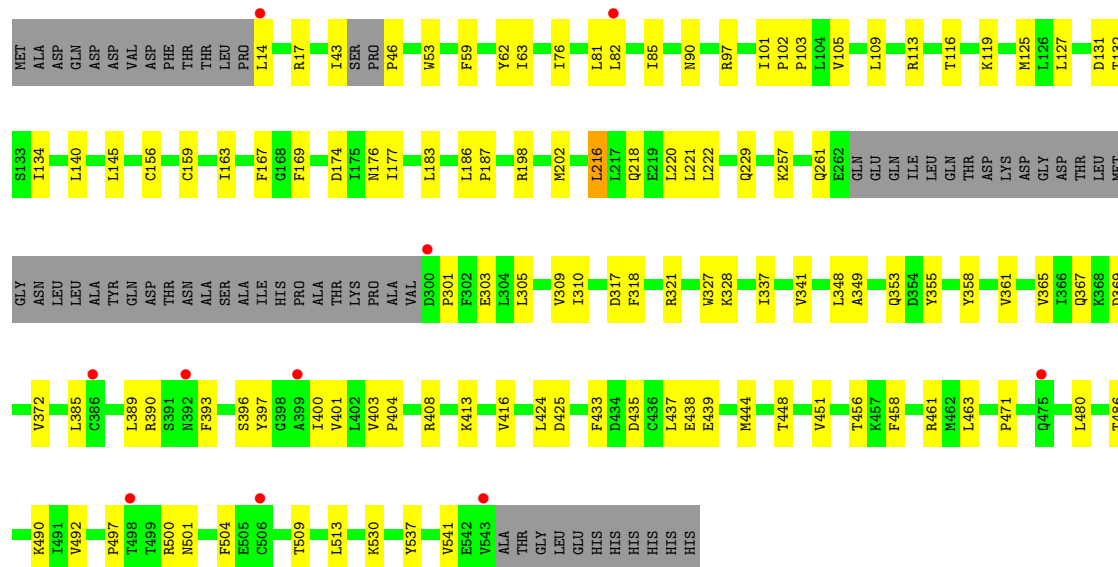
Chain I:  2% 85% 10% 5%



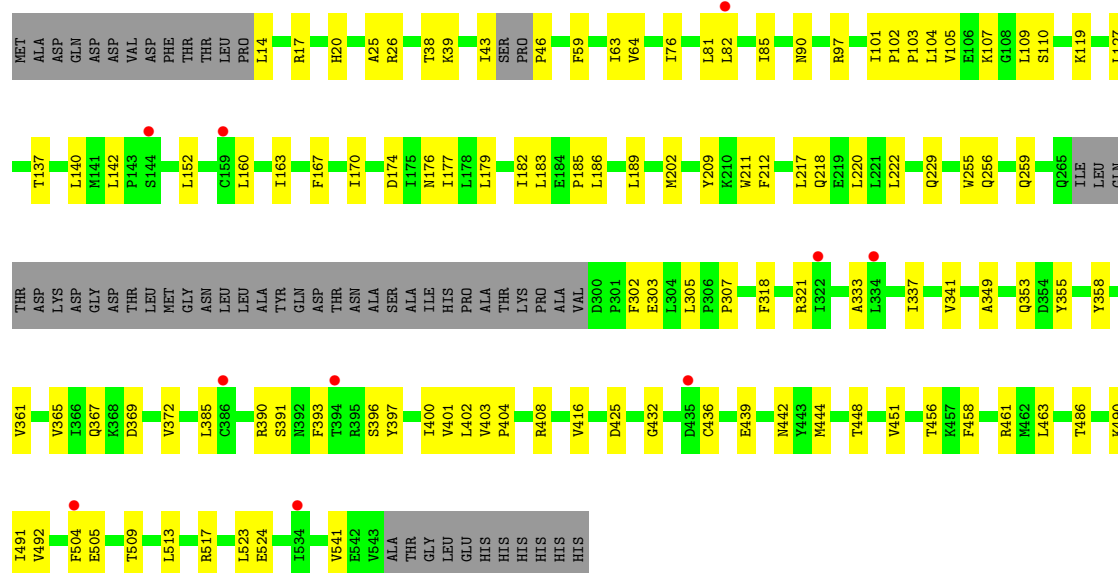
● Molecule 2: Tubulin beta chain

Chain K:  2% 86% 9% 5%

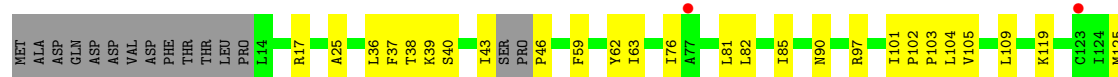


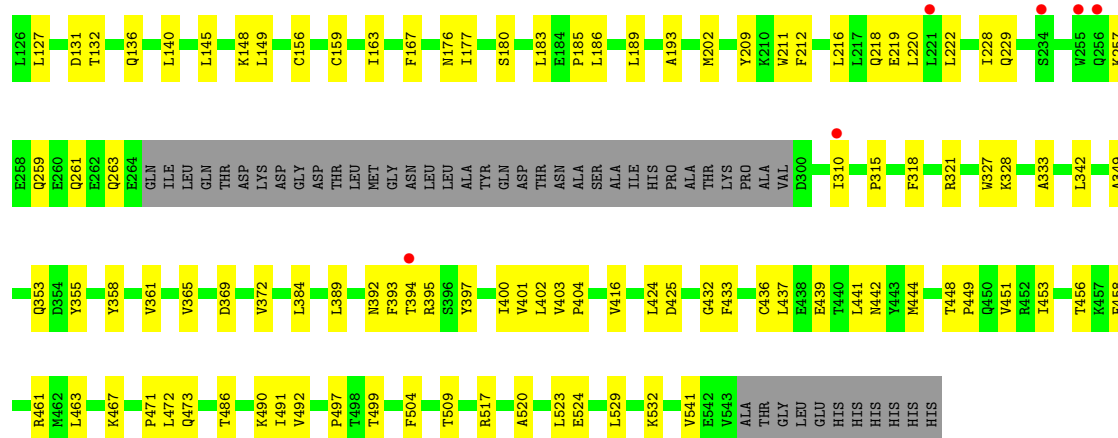


• Molecule 3: Protein Stu2p/Alp14p

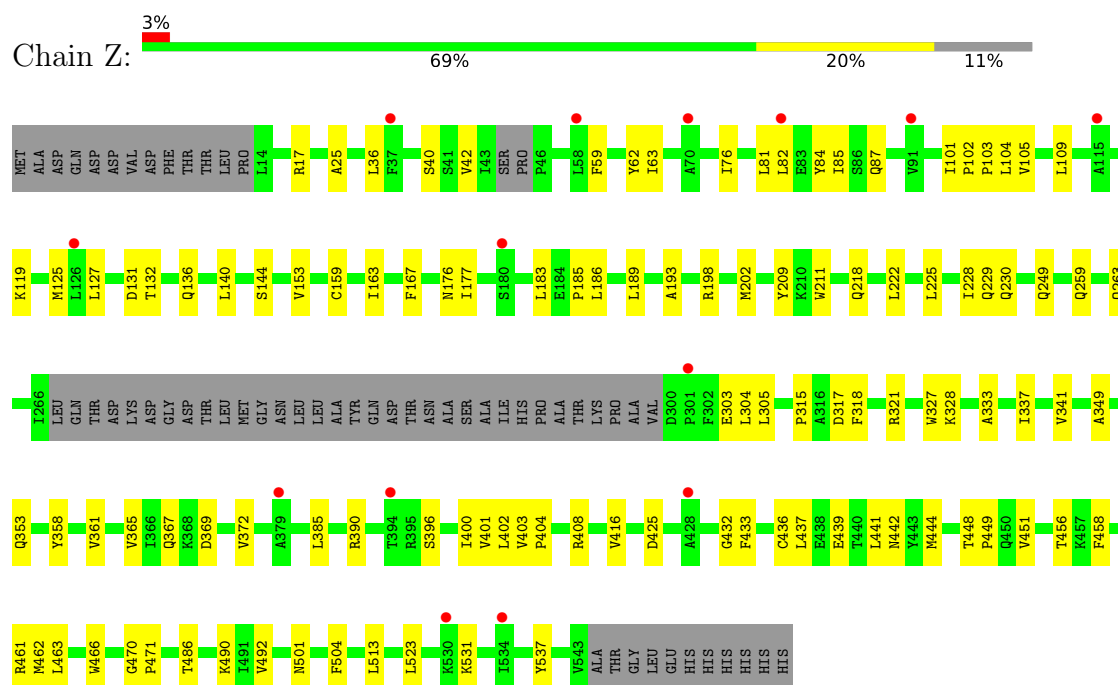


• Molecule 3: Protein Stu2p/Alp14p

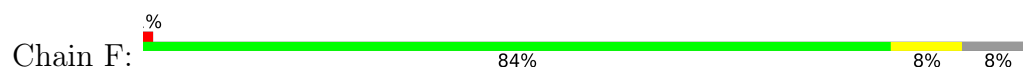




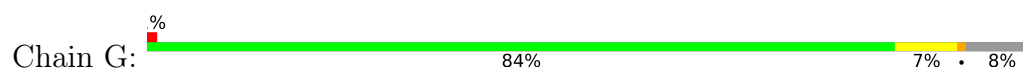
• Molecule 3: Protein Stu2p/Alp14p



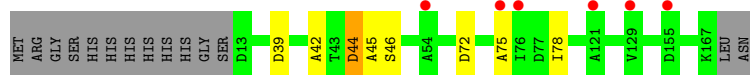
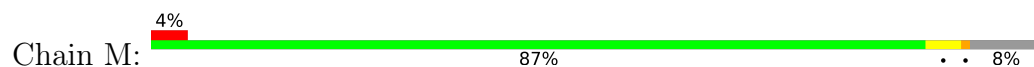
• Molecule 4: Designed ankyrin repeat protein (DARPIN) D1



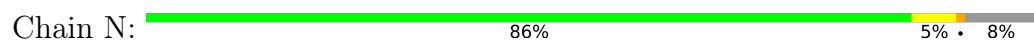
• Molecule 4: Designed ankyrin repeat protein (DARPIN) D1



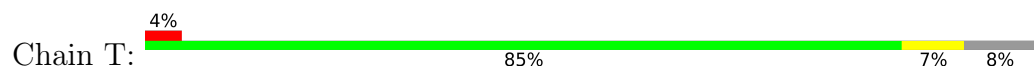
- Molecule 4: Designed ankyrin repeat protein (DARPIN) D1



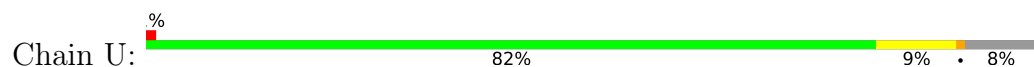
- Molecule 4: Designed ankyrin repeat protein (DARPIN) D1



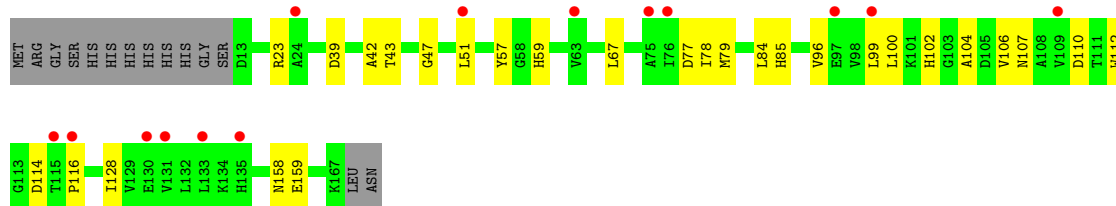
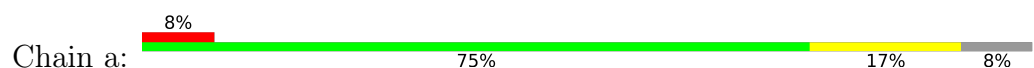
- Molecule 4: Designed ankyrin repeat protein (DARPIN) D1



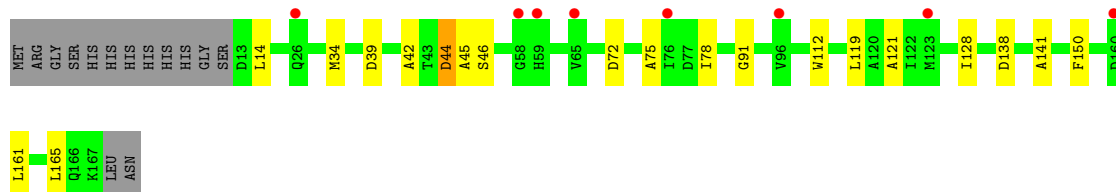
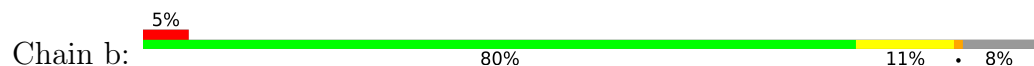
- Molecule 4: Designed ankyrin repeat protein (DARPIN) D1



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	218.80Å 107.65Å 282.74Å 90.00° 90.38° 90.00°	Depositor
Resolution (Å)	96.59 – 4.40 96.59 – 4.40	Depositor EDS
% Data completeness (in resolution range)	80.6 (96.59-4.40) 80.6 (96.59-4.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 4.47Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.225 , 0.252 0.240 , 0.268	Depositor DCC
R_{free} test set	3426 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	82.7	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 92.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.086 for h,-k,-l	Xtriage
Reported twinning fraction	0.120 for h,-k,-l	Depositor
Outliers	1 of 68039 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	78030	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.30	0/4539
1	C	0.11	0/3339	0.30	0/4539
1	H	0.11	0/3339	0.30	0/4539
1	J	0.11	0/3339	0.30	0/4539
1	O	0.11	0/3339	0.30	0/4539
1	Q	0.11	0/3339	0.31	0/4539
1	V	0.11	0/3339	0.31	0/4539
1	X	0.11	0/3339	0.30	0/4539
2	B	0.12	0/3380	0.33	0/4581
2	D	0.11	0/3380	0.31	0/4581
2	I	0.11	0/3380	0.31	0/4581
2	K	0.11	0/3380	0.32	0/4581
2	P	0.11	0/3380	0.32	0/4581
2	R	0.11	0/3380	0.32	0/4581
2	W	0.11	0/3380	0.32	0/4581
2	Y	0.10	0/3380	0.30	0/4581
3	E	0.15	0/4021	0.43	1/5449 (0.0%)
3	L	0.14	0/4048	0.43	0/5485
3	S	0.14	0/4039	0.39	0/5473
3	Z	0.14	0/4056	0.39	0/5496
4	F	0.11	0/1150	0.28	0/1565
4	G	0.11	0/1150	0.28	0/1565
4	M	0.11	0/1150	0.28	0/1565
4	N	0.11	0/1150	0.28	0/1565
4	T	0.10	0/1150	0.28	0/1565
4	U	0.12	0/1150	0.29	0/1565
4	a	0.13	0/1143	0.37	0/1556
4	b	0.12	0/1150	0.29	0/1565
All	All	0.12	0/79109	0.33	1/107374 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	216	LEU	N-CA-C	5.07	116.81	111.28

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	18	0
1	C	3265	0	3134	19	0
1	H	3265	0	3134	14	0
1	J	3265	0	3134	13	0
1	O	3265	0	3134	21	0
1	Q	3265	0	3134	20	0
1	V	3265	0	3134	20	0
1	X	3265	0	3134	14	0
2	B	3308	0	3180	33	0
2	D	3308	0	3180	30	0
2	I	3308	0	3180	29	0
2	K	3308	0	3180	22	0
2	P	3308	0	3180	36	0
2	R	3308	0	3180	37	0
2	W	3308	0	3180	27	0
2	Y	3308	0	3180	25	0
3	E	3949	0	4055	84	0
3	L	3976	0	4077	77	0
3	S	3967	0	4069	85	0
3	Z	3984	0	4088	71	0
4	F	1135	0	1125	8	0
4	G	1135	0	1125	9	0
4	M	1135	0	1125	4	0
4	N	1135	0	1125	6	0
4	T	1135	0	1125	8	0
4	U	1135	0	1125	10	0
4	a	1129	0	1118	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	b	1135	0	1125	12	0
5	A	32	0	12	1	0
5	C	32	0	12	1	0
5	H	32	0	12	1	0
5	J	32	0	12	2	0
5	O	32	0	12	1	0
5	Q	32	0	12	1	0
5	V	32	0	12	1	0
5	X	32	0	12	3	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	78030	0	75986	726	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 726 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)
1:O:258:ASN:HB3	1:O:352:LYS:HE3	1.53	0.88
1:O:257:THR:HG23	4:b:14:LEU:HD11	1.64	0.79
3:S:17:ARG:HD3	3:S:25:ALA:HB1	1.68	0.76
3:S:180:SER:HB2	3:Z:304:LEU:HD21	1.70	0.74
3:S:403:VAL:HG12	3:S:439:GLU:HG2	1.71	0.72

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%)	390 (94%)	27 (6%)	0	100	100
1	C	417/451 (92%)	389 (93%)	28 (7%)	0	100	100
1	H	417/451 (92%)	389 (93%)	27 (6%)	1 (0%)	43	77
1	J	417/451 (92%)	389 (93%)	28 (7%)	0	100	100
1	O	417/451 (92%)	390 (94%)	27 (6%)	0	100	100
1	Q	417/451 (92%)	388 (93%)	28 (7%)	1 (0%)	43	77
1	V	417/451 (92%)	391 (94%)	26 (6%)	0	100	100
1	X	417/451 (92%)	389 (93%)	28 (7%)	0	100	100
2	B	420/445 (94%)	406 (97%)	13 (3%)	1 (0%)	43	77
2	D	420/445 (94%)	406 (97%)	13 (3%)	1 (0%)	43	77
2	I	420/445 (94%)	406 (97%)	13 (3%)	1 (0%)	43	77
2	K	420/445 (94%)	404 (96%)	14 (3%)	2 (0%)	24	62
2	P	420/445 (94%)	406 (97%)	13 (3%)	1 (0%)	43	77
2	R	420/445 (94%)	406 (97%)	13 (3%)	1 (0%)	43	77
2	W	420/445 (94%)	406 (97%)	13 (3%)	1 (0%)	43	77
2	Y	420/445 (94%)	406 (97%)	13 (3%)	1 (0%)	43	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	485/554 (88%)	450 (93%)	32 (7%)	3 (1%)	21	58
3	L	488/554 (88%)	450 (92%)	37 (8%)	1 (0%)	43	77
3	S	487/554 (88%)	452 (93%)	31 (6%)	4 (1%)	16	52
3	Z	489/554 (88%)	451 (92%)	35 (7%)	3 (1%)	21	58
4	F	153/169 (90%)	143 (94%)	9 (6%)	1 (1%)	18	55
4	G	153/169 (90%)	145 (95%)	7 (5%)	1 (1%)	18	55
4	M	153/169 (90%)	144 (94%)	8 (5%)	1 (1%)	18	55
4	N	153/169 (90%)	144 (94%)	8 (5%)	1 (1%)	18	55
4	T	153/169 (90%)	144 (94%)	8 (5%)	1 (1%)	18	55
4	U	153/169 (90%)	145 (95%)	7 (5%)	1 (1%)	18	55
4	a	153/169 (90%)	138 (90%)	15 (10%)	0	100	100
4	b	153/169 (90%)	144 (94%)	8 (5%)	1 (1%)	18	55
All	All	9869/10736 (92%)	9311 (94%)	529 (5%)	29 (0%)	36	71

5 of 29 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	361 (100%)	0	100	100
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%)	361 (100%)	0	100	100
2	Y	361/381 (95%)	361 (100%)	0	100	100
3	E	451/504 (90%)	451 (100%)	0	100	100
3	L	454/504 (90%)	454 (100%)	0	100	100
3	S	453/504 (90%)	453 (100%)	0	100	100
3	Z	455/504 (90%)	455 (100%)	0	100	100
4	F	116/132 (88%)	116 (100%)	0	100	100
4	G	116/132 (88%)	116 (100%)	0	100	100
4	M	116/132 (88%)	116 (100%)	0	100	100
4	N	116/132 (88%)	116 (100%)	0	100	100
4	T	116/132 (88%)	116 (100%)	0	100	100
4	U	116/132 (88%)	116 (100%)	0	100	100
4	a	115/132 (87%)	115 (100%)	0	100	100
4	b	116/132 (88%)	116 (100%)	0	100	100
All	All	8396/9136 (92%)	8396 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
4	N	135	HIS
2	Y	167	ASN

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Mol	Chain	Res	Type
1	Q	61	HIS
1	X	393	HIS
3	Z	256	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 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	O	600	6	33,34,34	1.00	3 (9%)	50,54,54	1.56	8 (16%)
7	GDP	P	600	6	29,30,30	1.16	3 (10%)	45,47,47	1.71	6 (13%)
5	GTP	A	600	6	33,34,34	0.98	3 (9%)	50,54,54	1.58	8 (16%)
7	GDP	K	600	6	29,30,30	1.19	4 (13%)	45,47,47	1.70	6 (13%)
7	GDP	W	600	-	29,30,30	1.17	3 (10%)	45,47,47	1.67	6 (13%)
5	GTP	C	600	6	33,34,34	0.99	3 (9%)	50,54,54	1.52	8 (16%)
5	GTP	X	600	6	33,34,34	1.00	3 (9%)	50,54,54	1.55	8 (16%)
5	GTP	Q	600	6	33,34,34	0.99	2 (6%)	50,54,54	1.52	8 (16%)
7	GDP	B	600	6	29,30,30	1.18	4 (13%)	45,47,47	1.69	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GDP	D	600	6	29,30,30	1.19	4 (13%)	45,47,47	1.69	6 (13%)
7	GDP	I	600	6	29,30,30	1.18	3 (10%)	45,47,47	1.70	6 (13%)
7	GDP	R	600	6	29,30,30	1.18	3 (10%)	45,47,47	1.69	6 (13%)
7	GDP	Y	600	6	29,30,30	1.19	4 (13%)	45,47,47	1.70	6 (13%)
5	GTP	V	600	6	33,34,34	1.01	4 (12%)	50,54,54	1.52	8 (16%)
5	GTP	H	600	6	33,34,34	0.97	1 (3%)	50,54,54	1.48	8 (16%)
5	GTP	J	600	6	33,34,34	1.01	3 (9%)	50,54,54	1.55	8 (16%)

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

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Y	600	GDP	C5-C4	3.25	1.47	1.38
7	W	600	GDP	C5-C4	3.22	1.47	1.38
7	R	600	GDP	C5-C4	3.22	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	P	600	GDP	C5-C4	3.20	1.47	1.38
7	I	600	GDP	C5-C4	3.19	1.47	1.38

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	600	GDP	C5-C4-N3	-6.11	118.66	128.39
7	Y	600	GDP	C5-C4-N3	-6.10	118.69	128.39
7	I	600	GDP	C5-C4-N3	-6.09	118.69	128.39
7	W	600	GDP	C5-C4-N3	-6.00	118.84	128.39
7	D	600	GDP	C5-C4-N3	-5.98	118.87	128.39

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

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

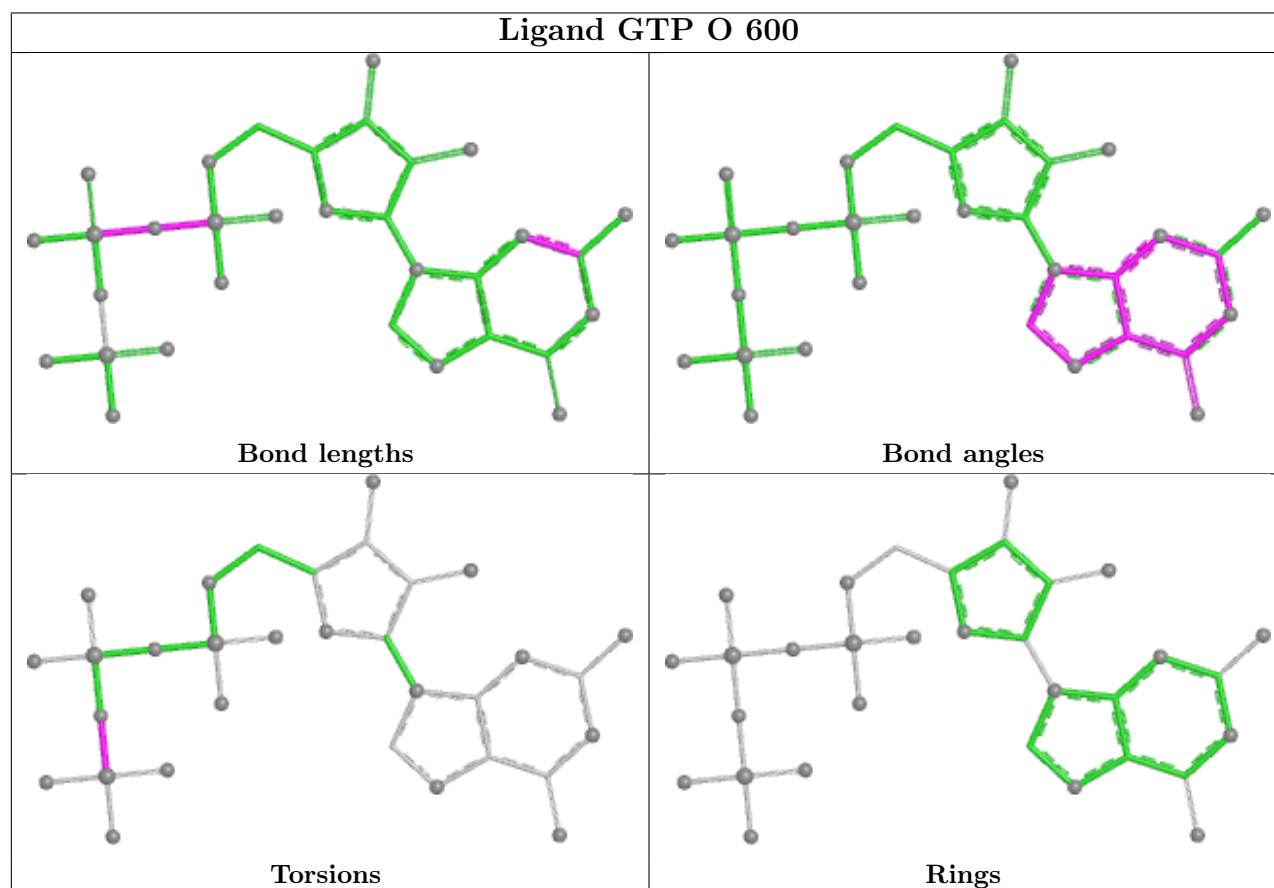
There are no ring outliers.

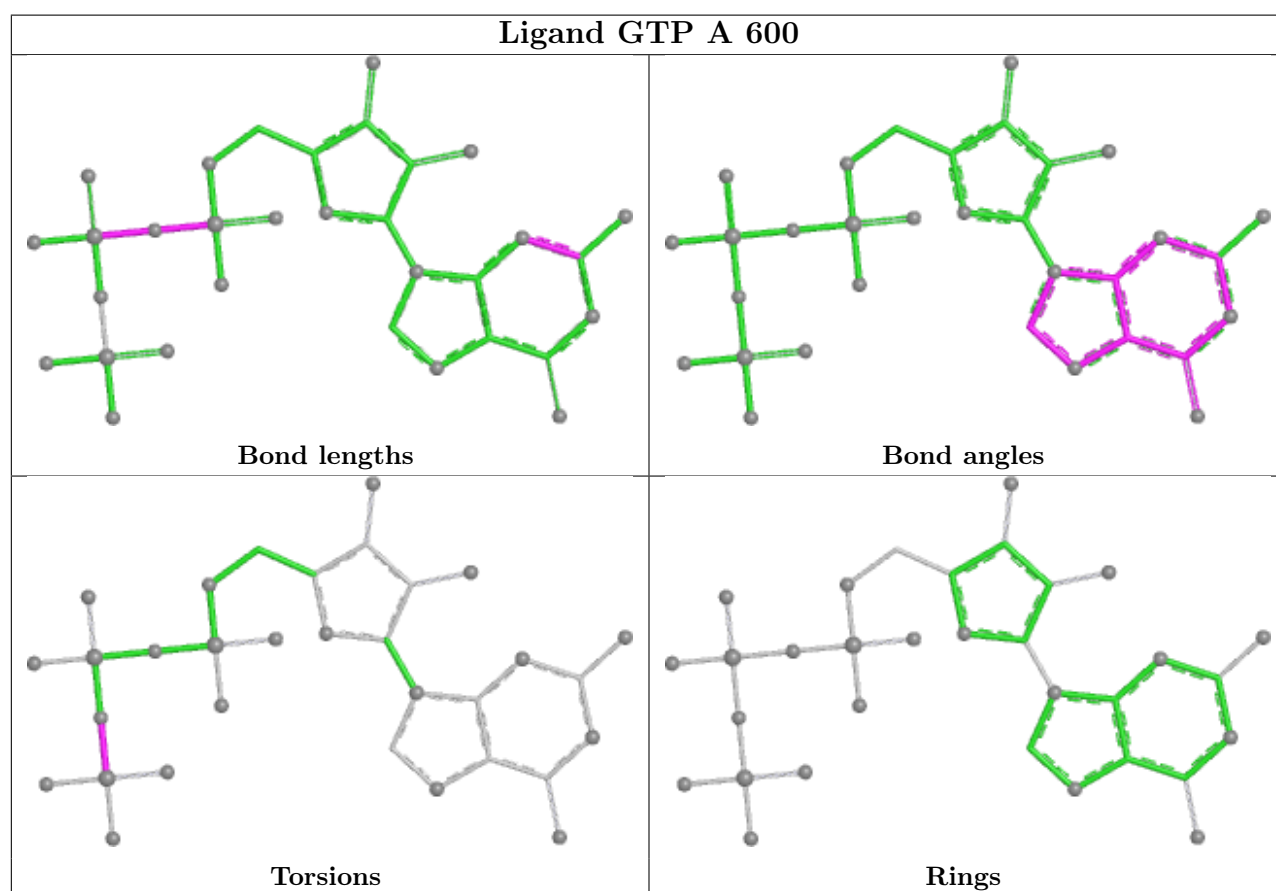
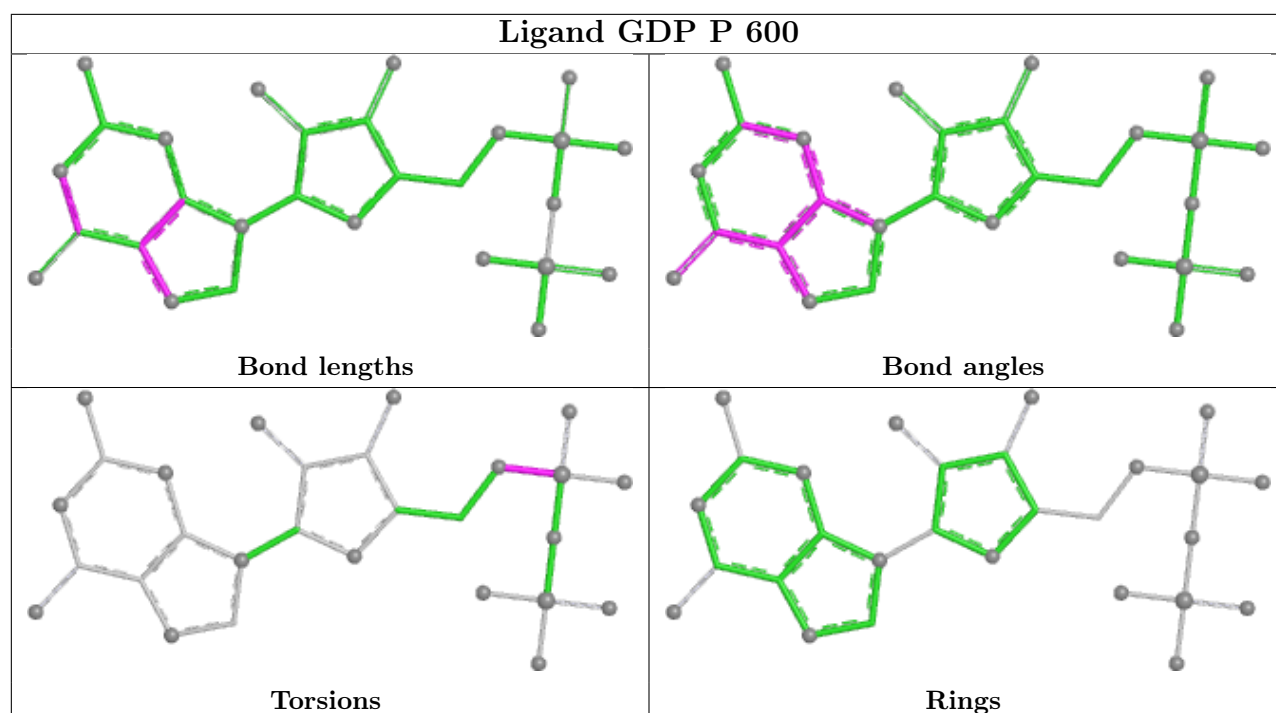
8 monomers are involved in 11 short contacts:

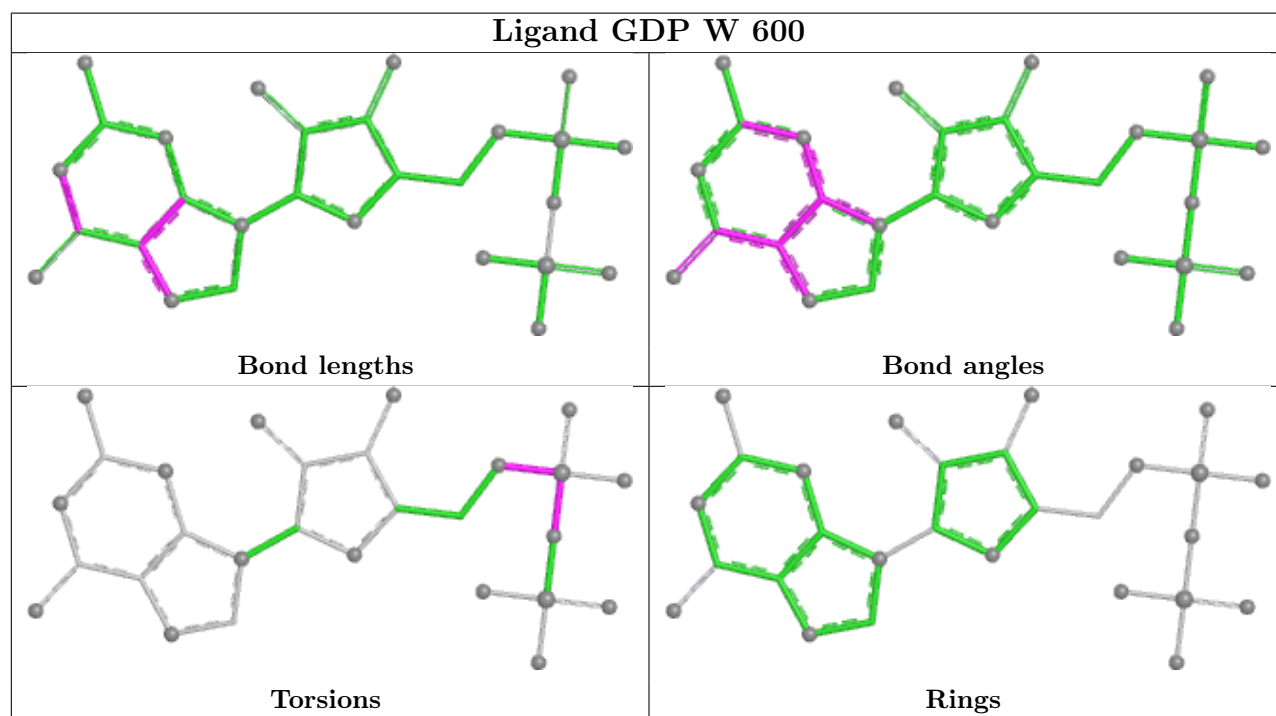
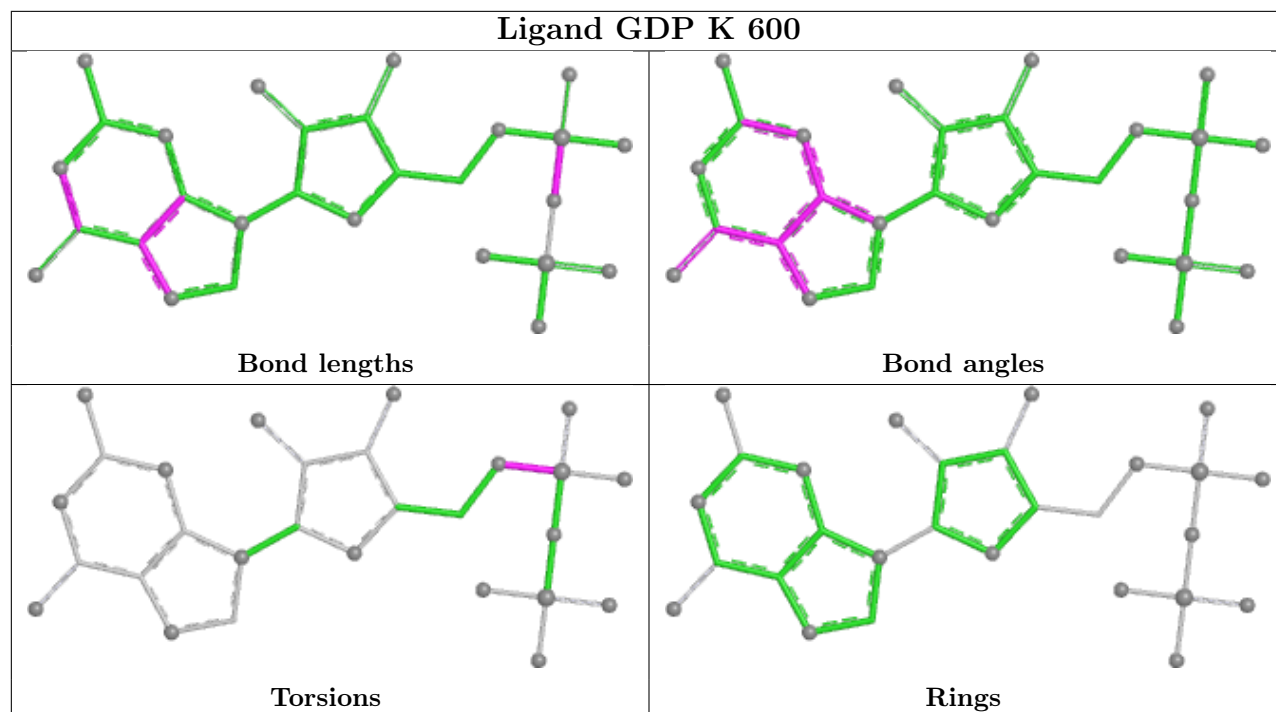
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	O	600	GTP	1	0
5	A	600	GTP	1	0
5	C	600	GTP	1	0
5	X	600	GTP	3	0
5	Q	600	GTP	1	0
5	V	600	GTP	1	0
5	H	600	GTP	1	0
5	J	600	GTP	2	0

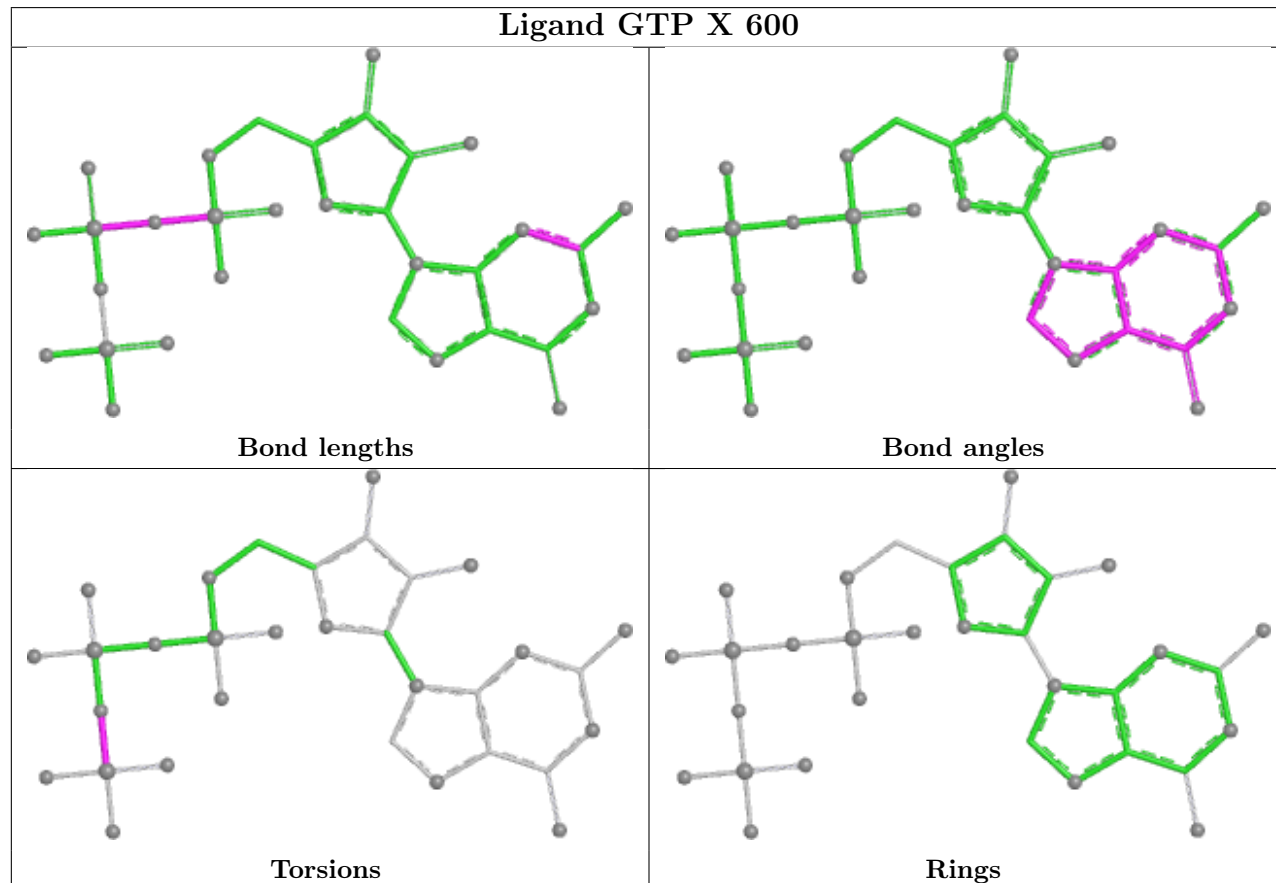
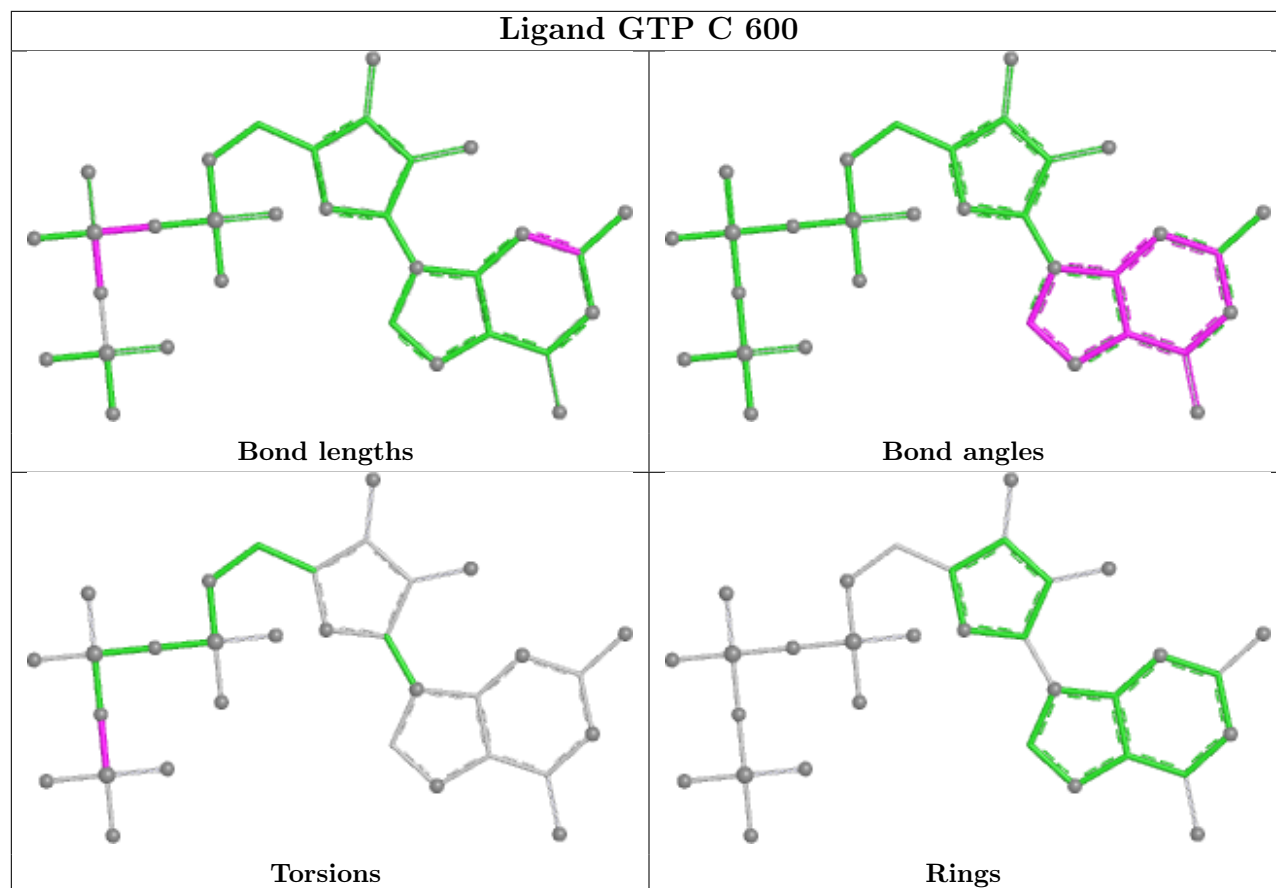
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

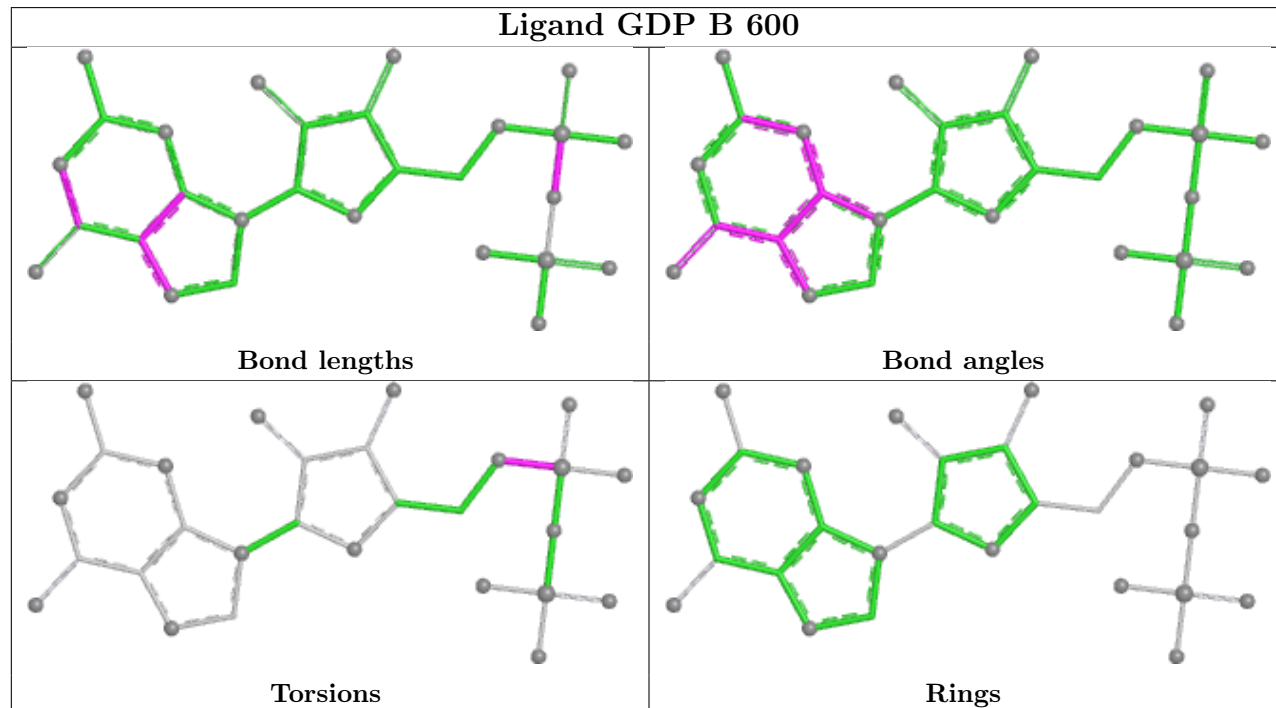
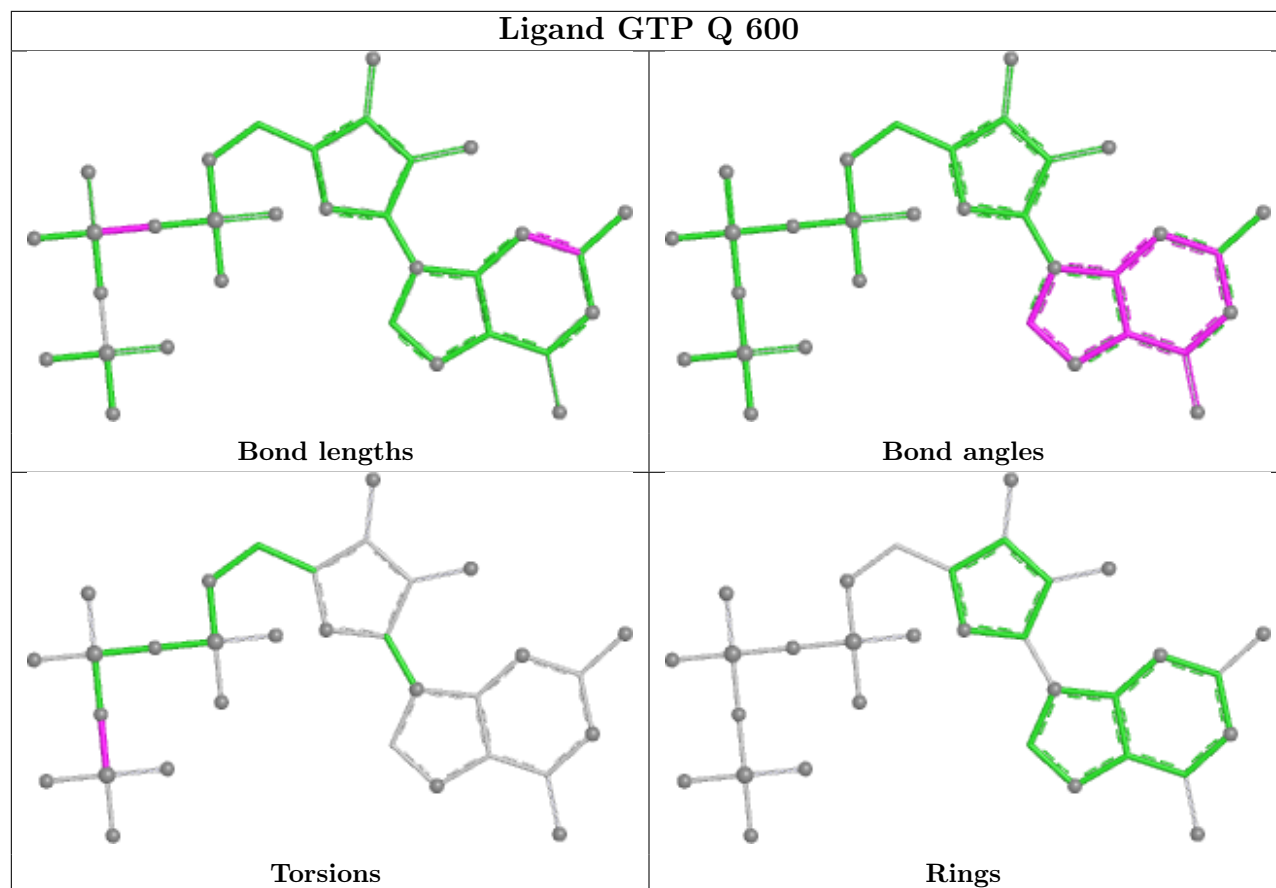
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

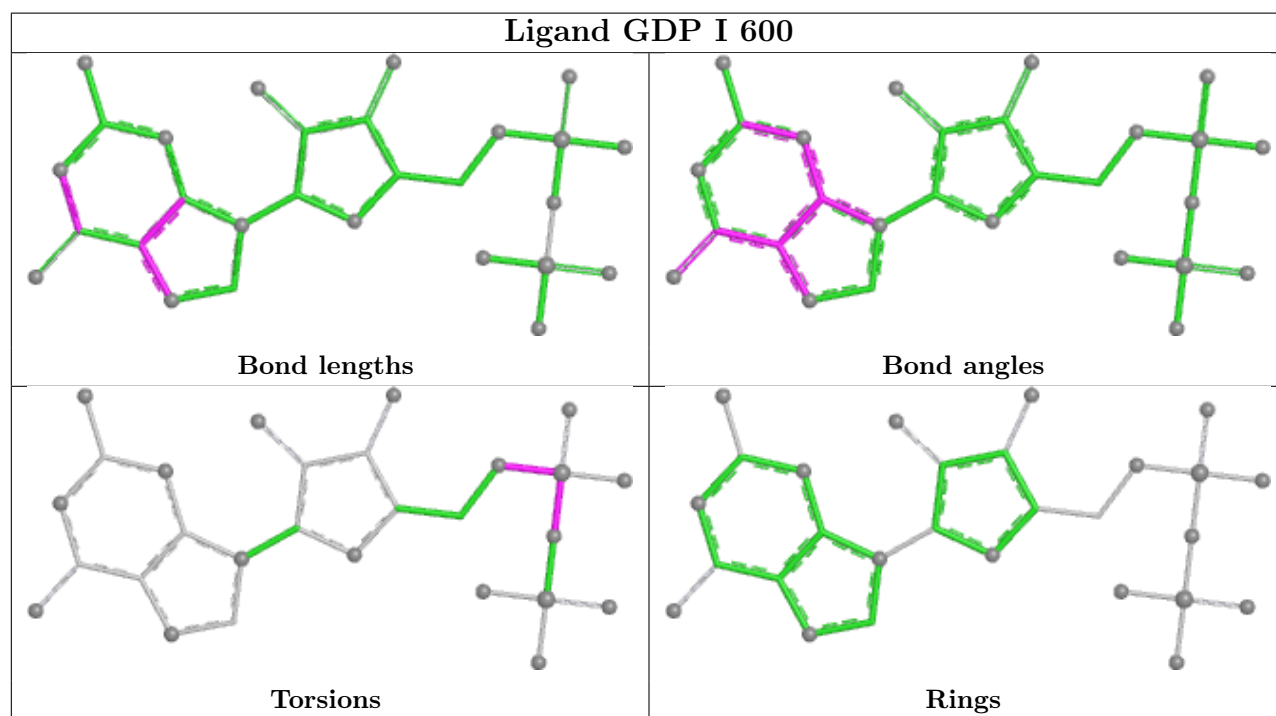
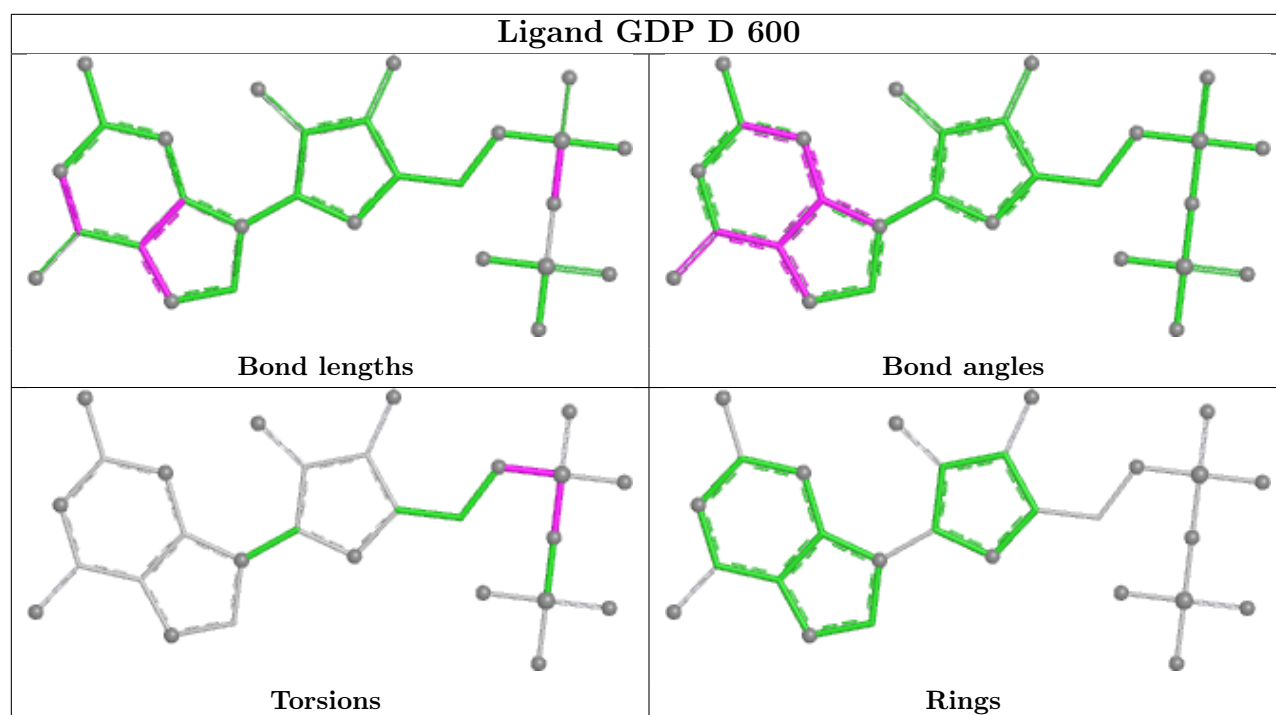


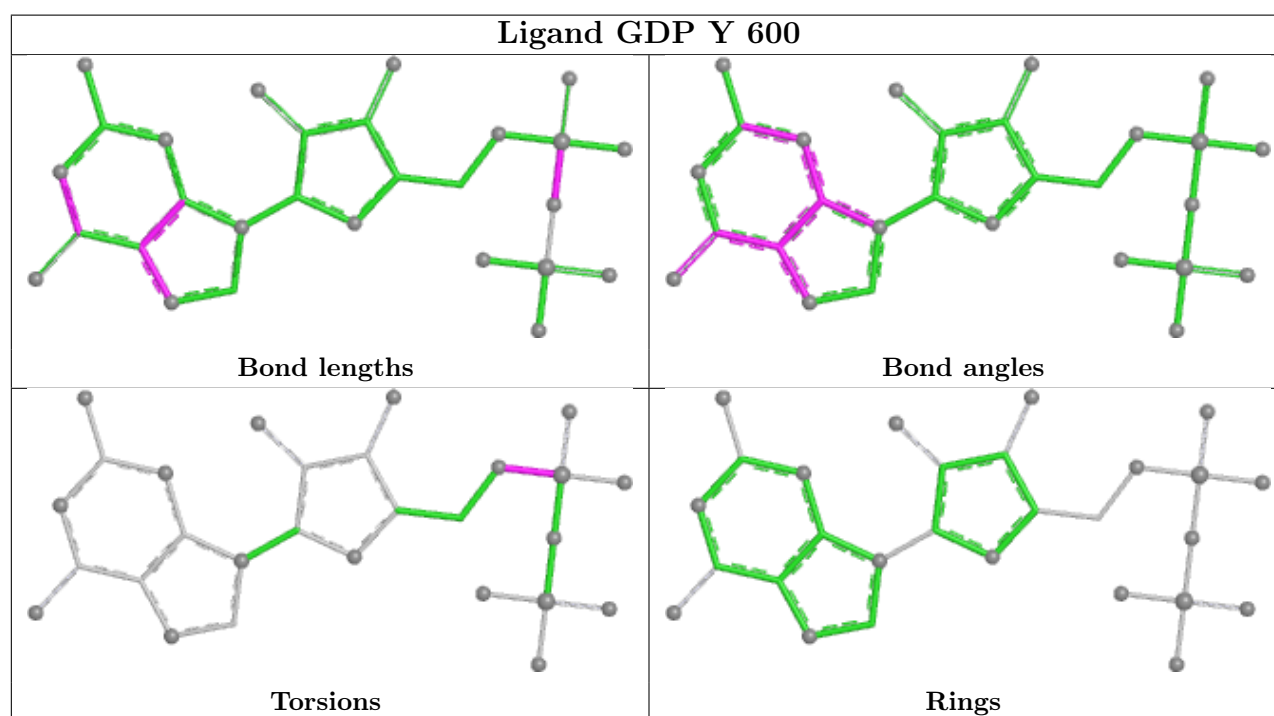
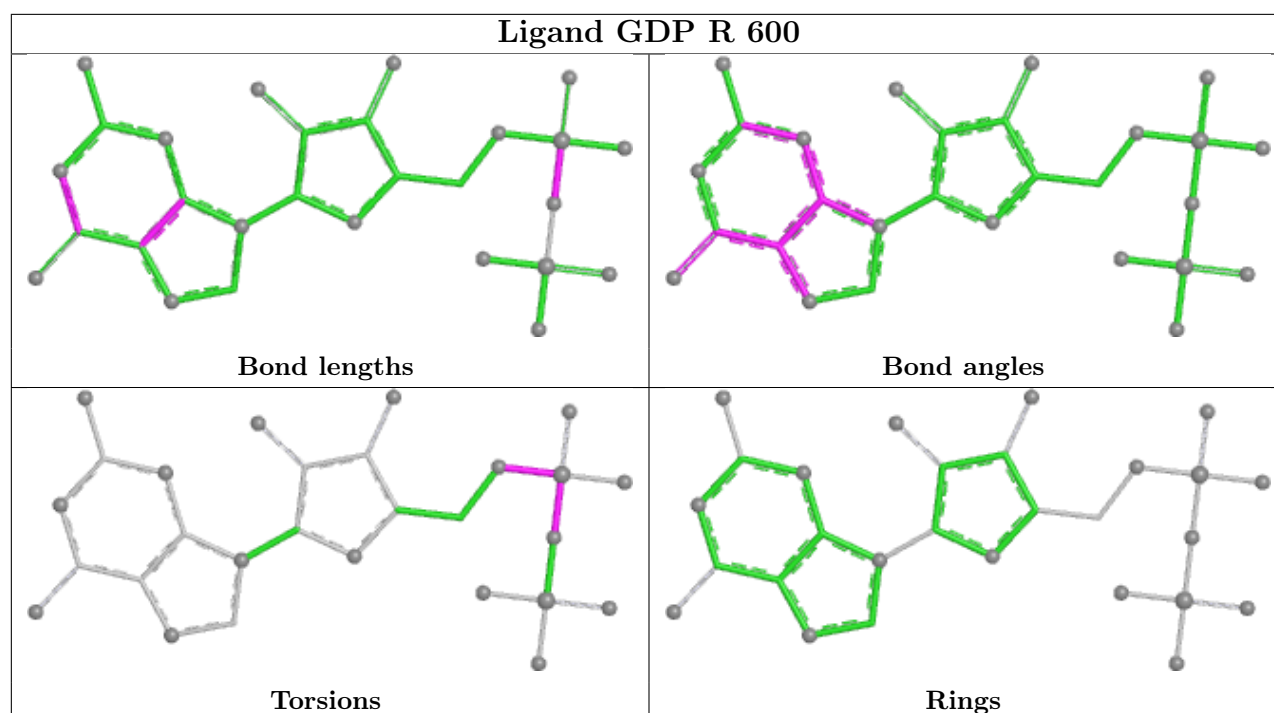


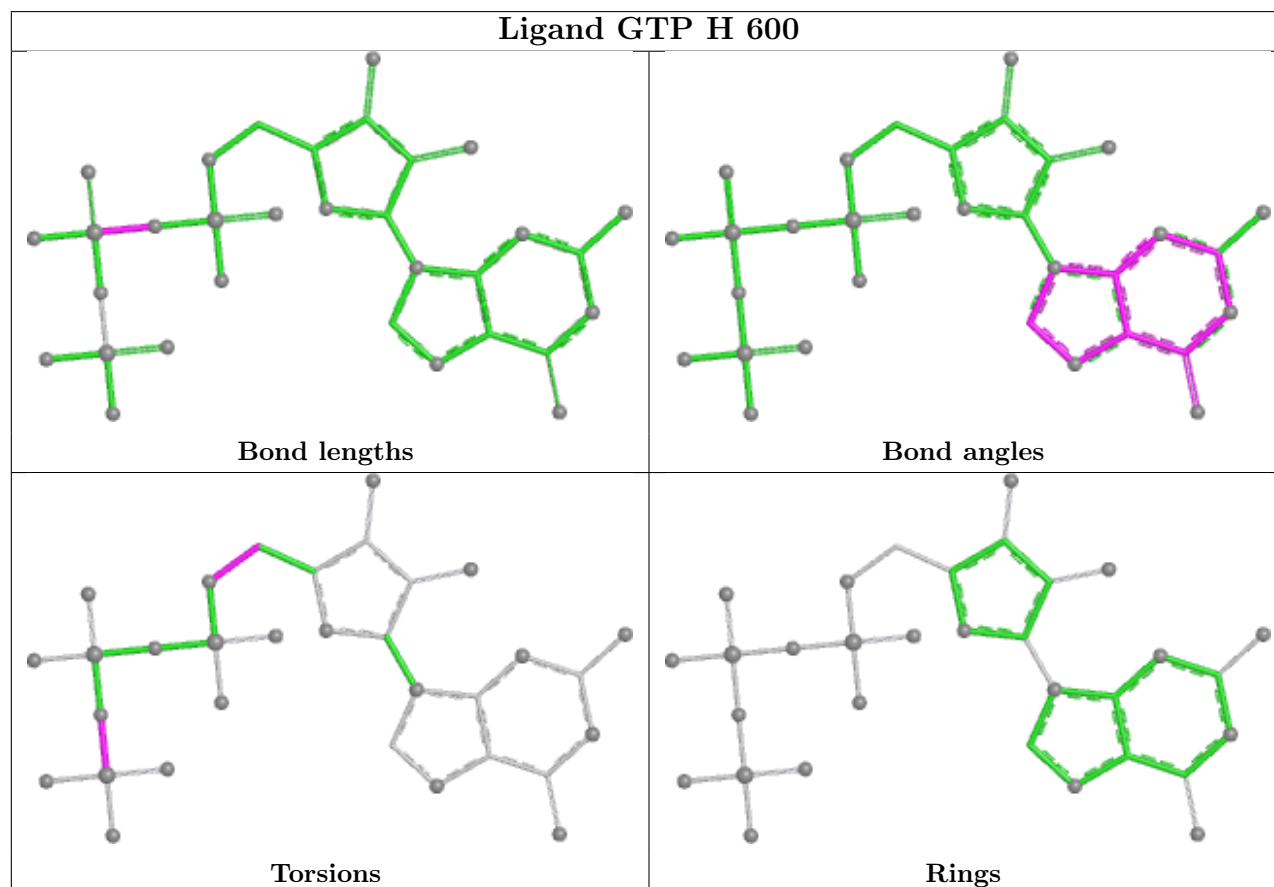
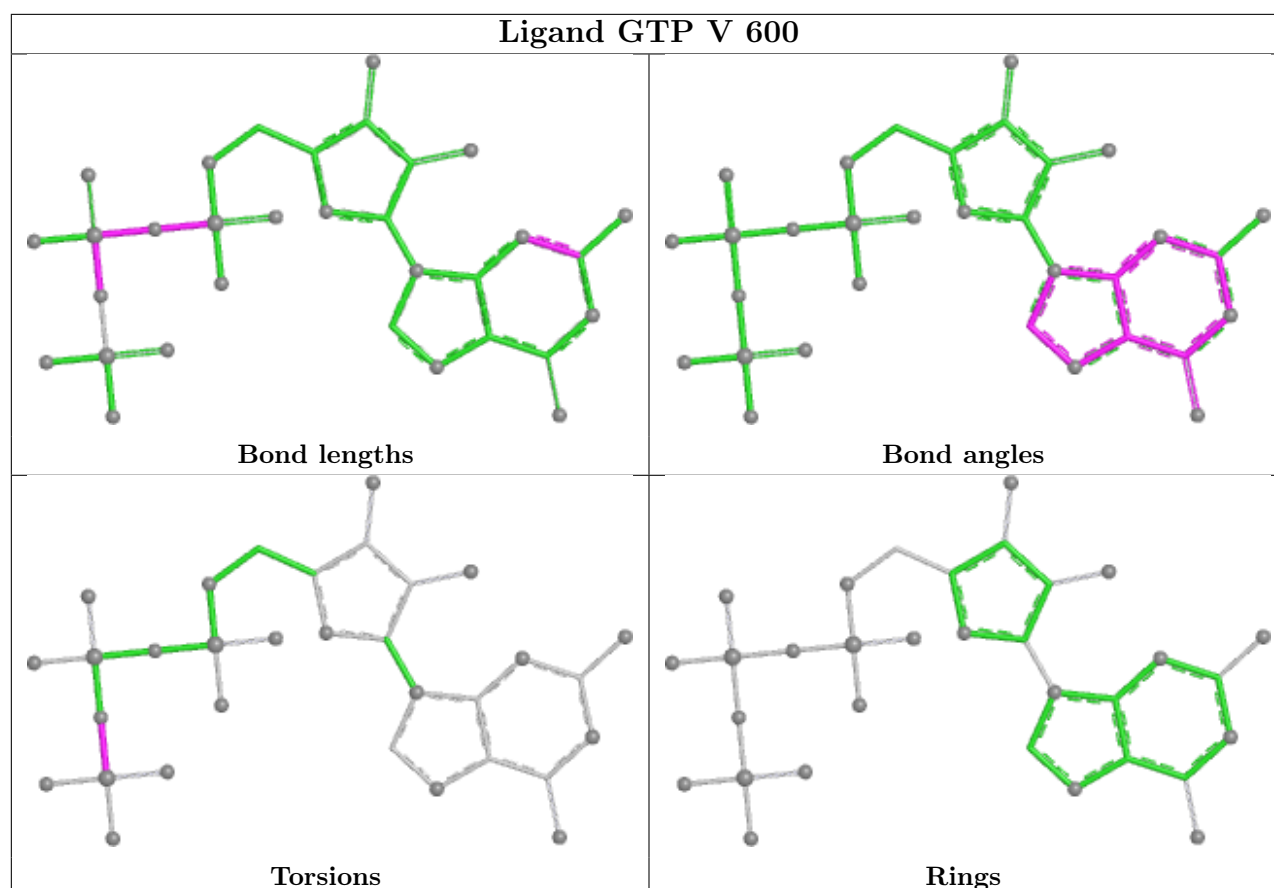


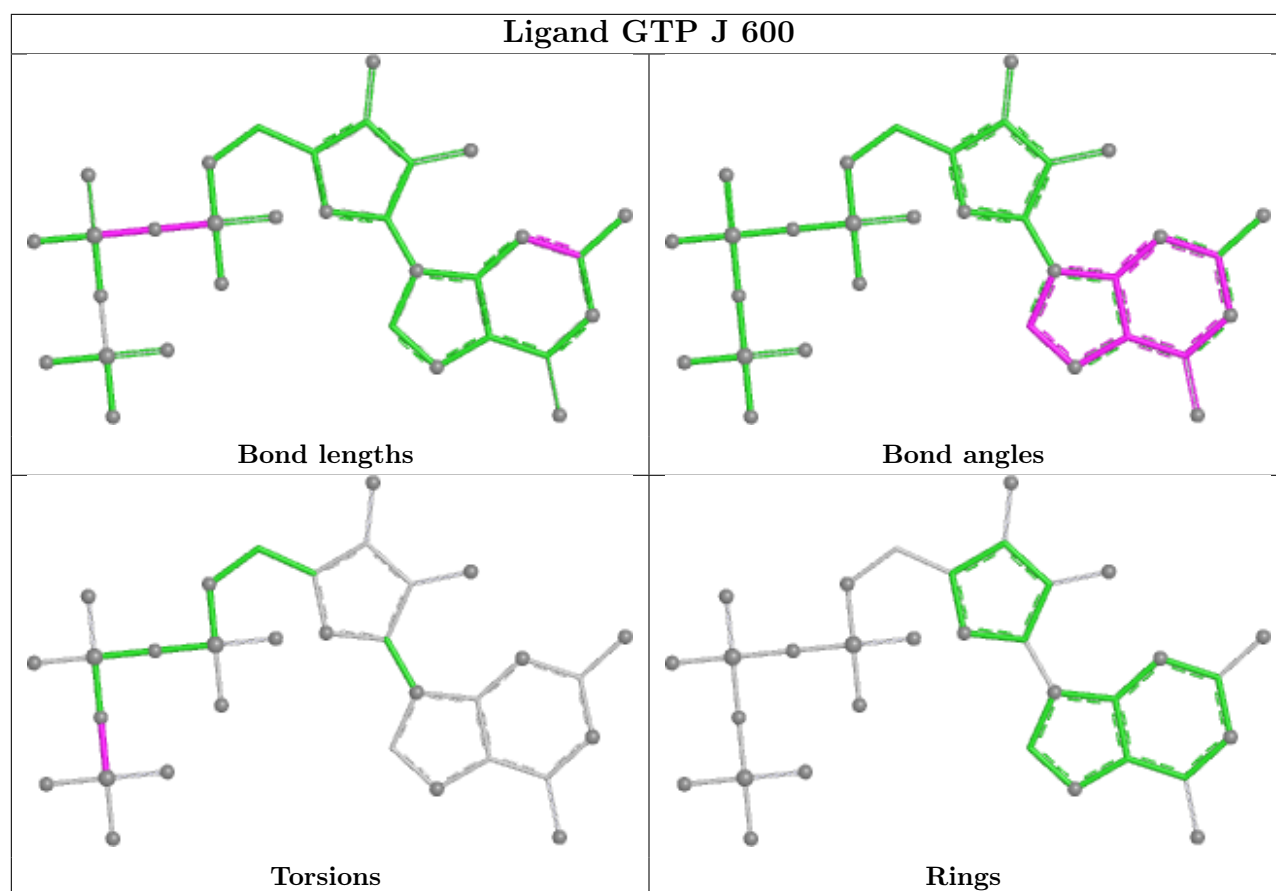












5.7 Other polymers [i](#)

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%)	0.27	6 (1%) 73 58	49, 113, 165, 235	0
1	C	423/451 (93%)	0.20	5 (1%) 76 62	54, 97, 139, 163	0
1	H	423/451 (93%)	0.24	5 (1%) 76 62	39, 97, 143, 207	0
1	J	423/451 (93%)	0.40	10 (2%) 59 47	77, 139, 203, 248	0
1	O	423/451 (93%)	0.55	20 (4%) 36 32	71, 139, 198, 263	0
1	Q	423/451 (93%)	0.15	5 (1%) 76 62	41, 87, 135, 176	0
1	V	423/451 (93%)	0.35	10 (2%) 59 47	50, 108, 156, 196	0
1	X	423/451 (93%)	0.40	7 (1%) 69 55	62, 124, 183, 294	0
2	B	424/445 (95%)	0.25	7 (1%) 69 55	32, 58, 92, 130	0
2	D	424/445 (95%)	0.31	9 (2%) 63 50	43, 82, 130, 182	0
2	I	424/445 (95%)	0.34	10 (2%) 59 47	66, 107, 148, 188	0
2	K	424/445 (95%)	0.43	10 (2%) 59 47	85, 131, 174, 274	0
2	P	424/445 (95%)	0.25	9 (2%) 63 50	54, 91, 130, 177	0
2	R	424/445 (95%)	0.29	6 (1%) 73 58	27, 69, 118, 210	0
2	W	424/445 (95%)	0.33	6 (1%) 73 58	62, 109, 152, 173	0
2	Y	424/445 (95%)	0.31	9 (2%) 63 50	57, 105, 152, 188	0
3	E	491/554 (88%)	0.28	10 (2%) 65 51	45, 81, 123, 158	0
3	L	494/554 (89%)	0.31	10 (2%) 65 51	63, 93, 133, 187	0
3	S	493/554 (88%)	0.33	8 (1%) 70 55	40, 92, 139, 165	0
3	Z	495/554 (89%)	0.40	14 (2%) 55 43	58, 96, 144, 179	0
4	F	155/169 (91%)	0.16	2 (1%) 75 60	52, 89, 133, 164	0
4	G	155/169 (91%)	0.23	1 (0%) 85 73	64, 98, 133, 170	0
4	M	155/169 (91%)	0.64	6 (3%) 43 36	136, 186, 227, 275	0
4	N	155/169 (91%)	0.32	0 100 100	150, 222, 280, 383	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
4	T	155/169 (91%)	0.47	7 (4%) 38 33	105, 166, 204, 251	0
4	U	155/169 (91%)	0.13	2 (1%) 75 60	44, 78, 111, 127	0
4	a	155/169 (91%)	1.01	14 (9%) 15 18	129, 173, 228, 294	0
4	b	155/169 (91%)	0.72	8 (5%) 33 30	110, 159, 205, 248	0
All	All	9989/10736 (93%)	0.34	216 (2%) 62 49	27, 102, 184, 383	0

The worst 5 of 216 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	534	ILE	4.8
1	O	302	MET	4.7
2	B	142	GLY	4.7
2	I	144	GLY	4.4
2	K	49	ILE	4.0

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 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	K	601	1/1	0.12	0.39	74,74,74,74	0
6	MG	I	601	1/1	0.54	0.26	70,70,70,70	0
6	MG	P	601	1/1	0.63	0.28	48,48,48,48	0
6	MG	X	601	1/1	0.68	0.31	62,62,62,62	0
6	MG	R	601	1/1	0.73	0.28	38,38,38,38	0
6	MG	H	601	1/1	0.73	0.29	37,37,37,37	0
6	MG	W	601	1/1	0.74	0.23	68,68,68,68	0

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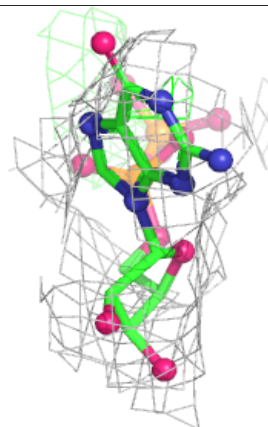
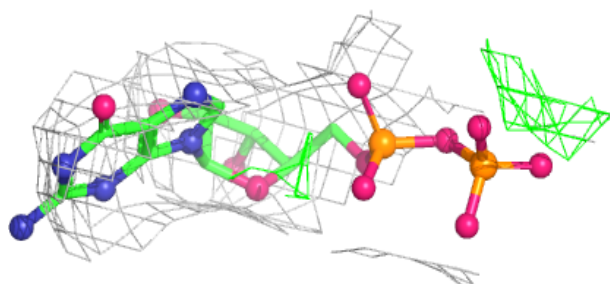
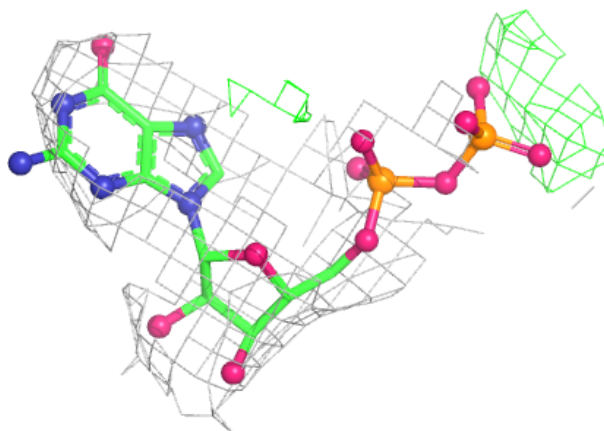
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	O	601	1/1	0.77	0.31	51,51,51,51	0
6	MG	V	601	1/1	0.80	0.26	36,36,36,36	0
6	MG	Y	601	1/1	0.80	0.22	69,69,69,69	0
6	MG	C	601	1/1	0.82	0.32	46,46,46,46	0
6	MG	Q	601	1/1	0.84	0.30	63,63,63,63	0
6	MG	A	601	1/1	0.84	0.26	47,47,47,47	0
6	MG	D	601	1/1	0.87	0.30	25,25,25,25	0
7	GDP	K	600	28/28	0.88	0.13	90,114,123,134	0
7	GDP	Y	600	28/28	0.88	0.16	63,80,101,103	0
5	GTP	J	600	32/32	0.89	0.11	84,109,117,126	0
7	GDP	D	600	28/28	0.89	0.12	37,66,79,89	0
7	GDP	W	600	28/28	0.90	0.12	70,100,108,108	0
5	GTP	X	600	32/32	0.90	0.12	67,87,98,102	0
7	GDP	I	600	28/28	0.91	0.12	69,81,89,94	0
7	GDP	R	600	28/28	0.91	0.13	41,63,74,74	0
6	MG	J	601	1/1	0.92	0.19	54,54,54,54	0
5	GTP	C	600	32/32	0.92	0.12	53,75,91,102	0
5	GTP	O	600	32/32	0.92	0.13	56,95,114,116	0
5	GTP	Q	600	32/32	0.92	0.11	50,70,82,86	0
5	GTP	A	600	32/32	0.93	0.13	54,79,89,93	0
5	GTP	H	600	32/32	0.94	0.11	45,66,81,84	0
7	GDP	B	600	28/28	0.94	0.13	36,47,61,87	0
7	GDP	P	600	28/28	0.95	0.09	55,68,79,84	0
5	GTP	V	600	32/32	0.95	0.12	46,70,80,81	0
6	MG	B	601	1/1	0.96	0.32	22,22,22,22	0

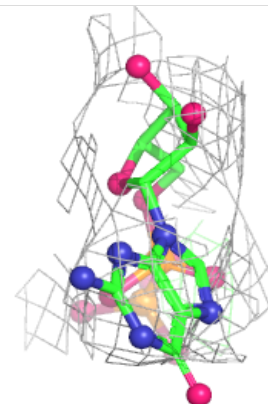
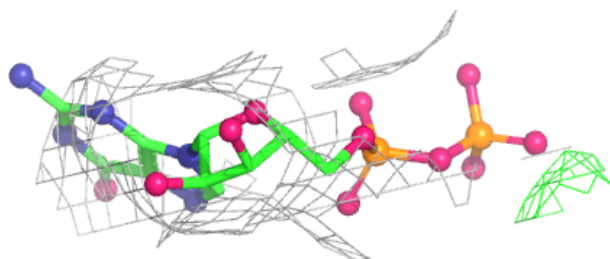
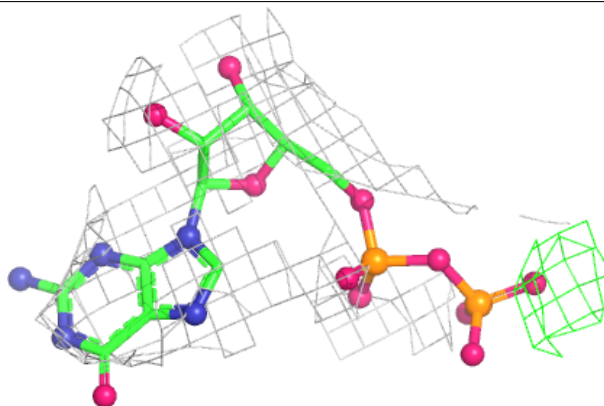
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

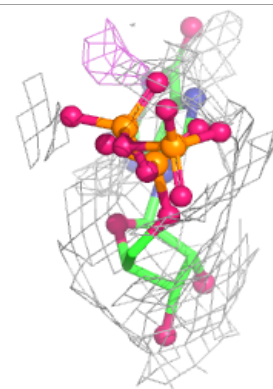
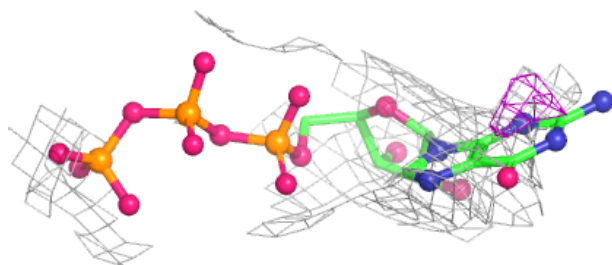
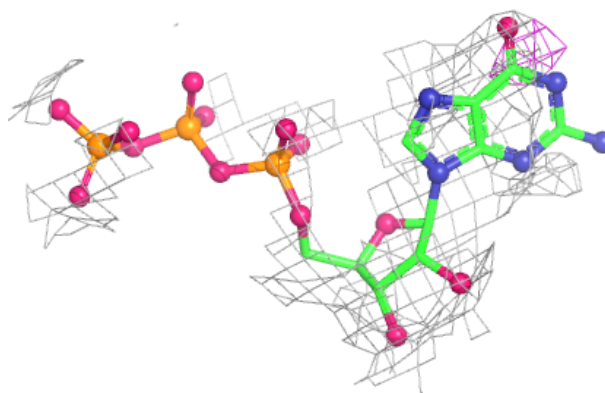
**Electron density around GDP Y 600:**

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



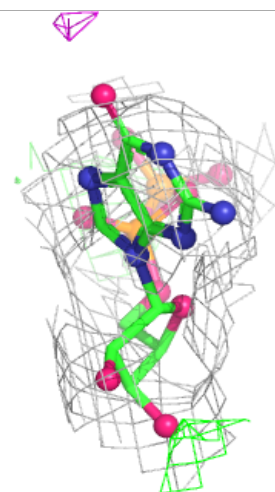
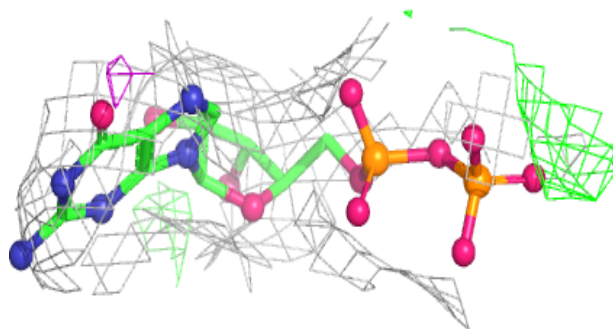
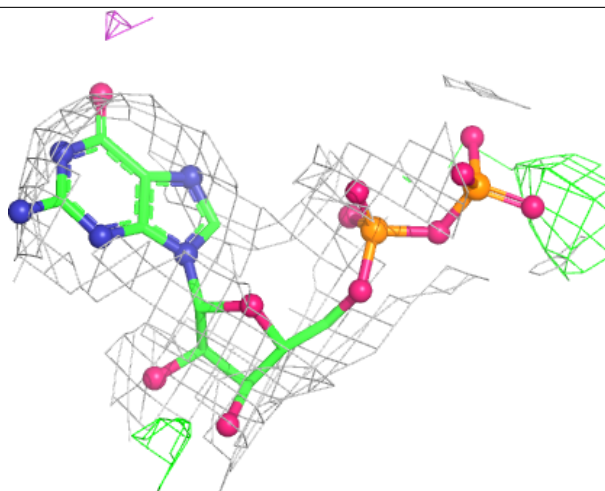
Electron density around GTP J 600:

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



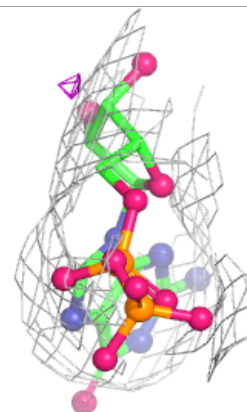
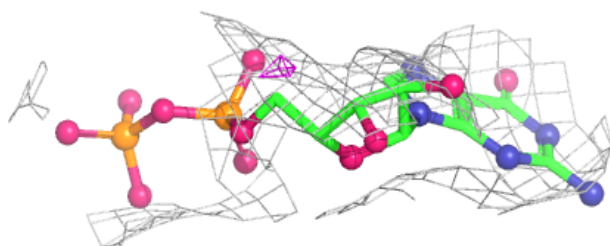
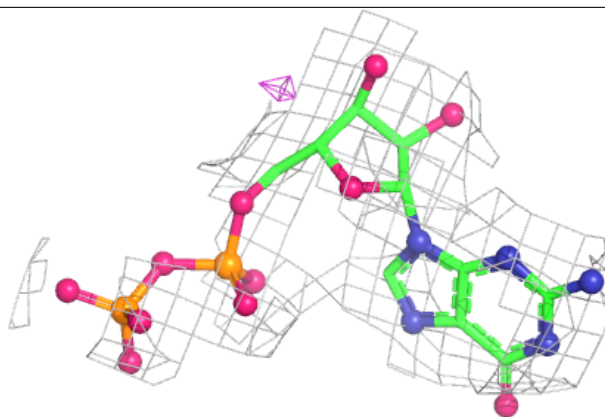
Electron density around GDP D 600:

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

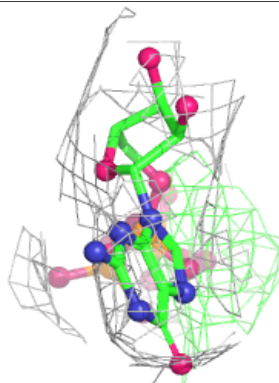
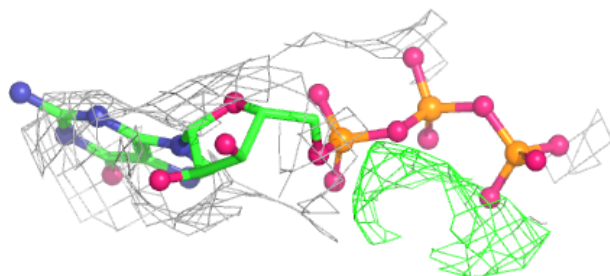
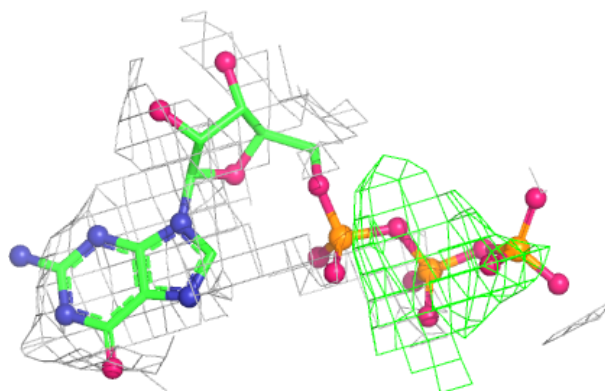


Electron density around GDP W 600:

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

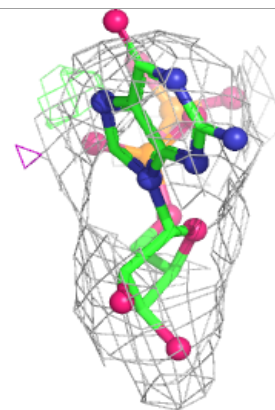
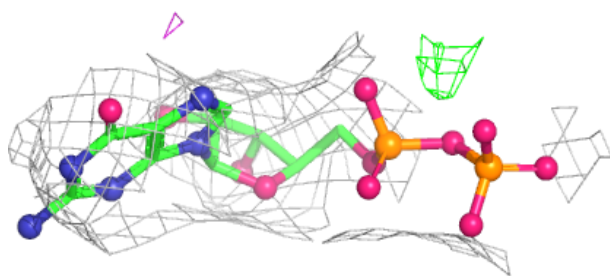
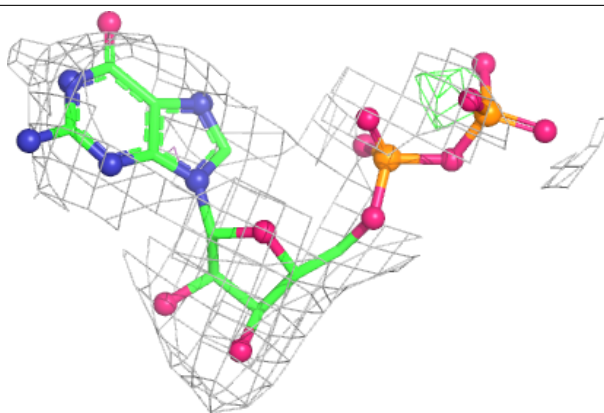
**Electron density around GTP X 600:**

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and green (positive)

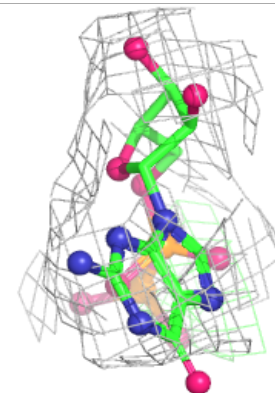
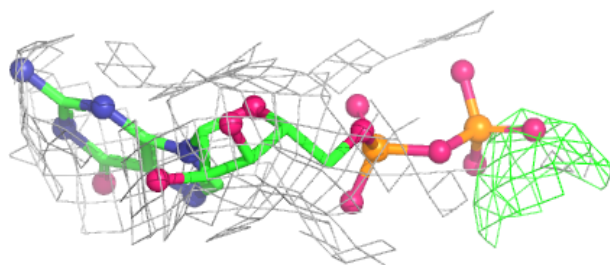
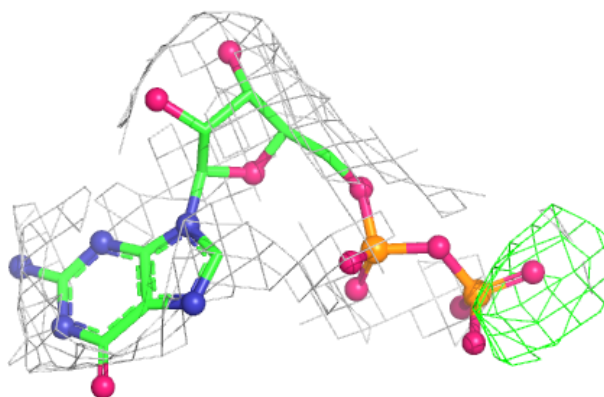


Electron density around GDP I 600:

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

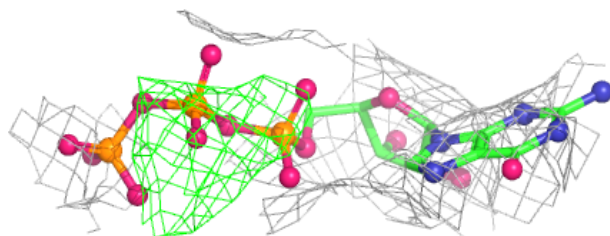
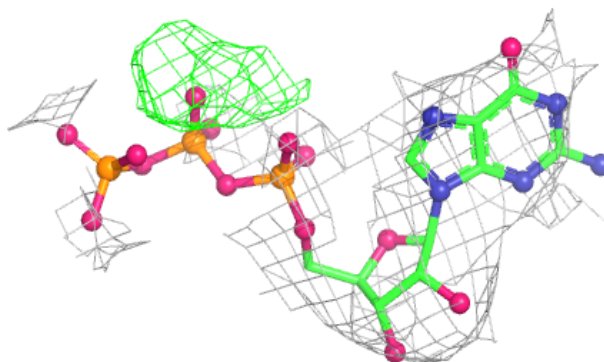
**Electron density around GDP R 600:**

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and green (positive)

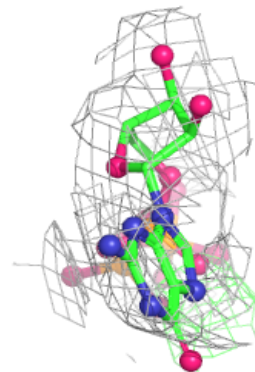
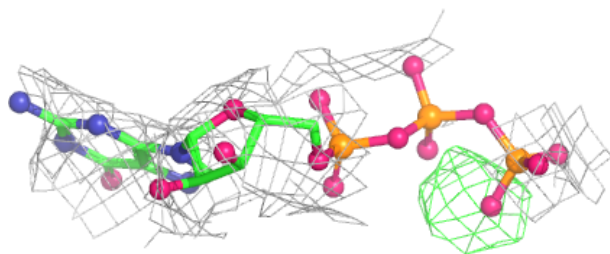
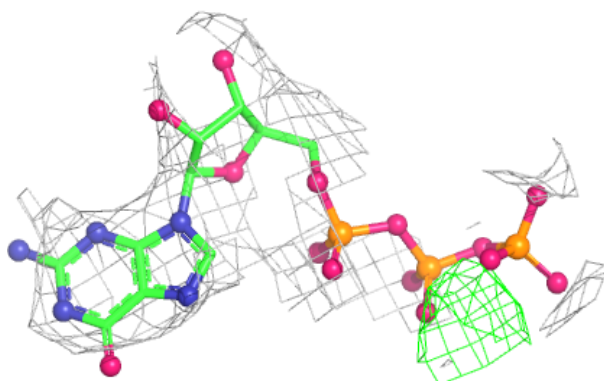


Electron density around GTP C 600:

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and green (positive)

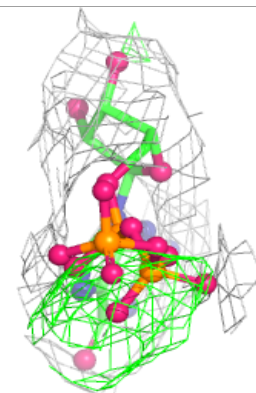
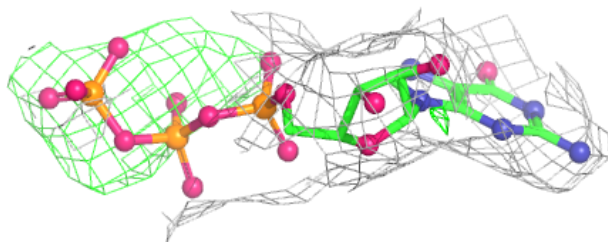
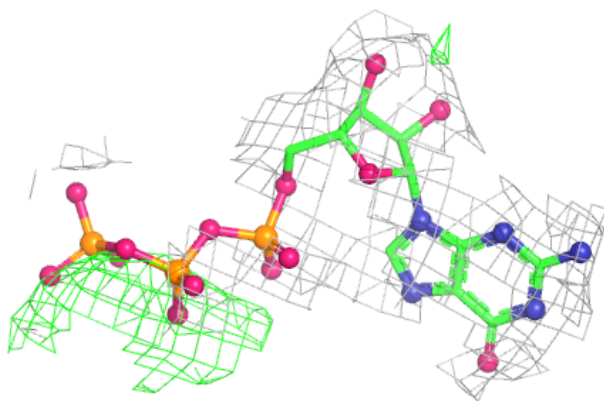
**Electron density around GTP O 600:**

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

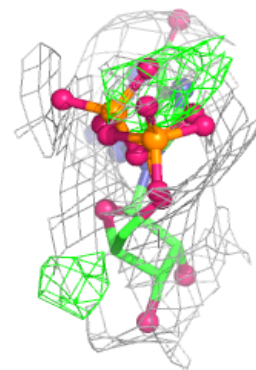
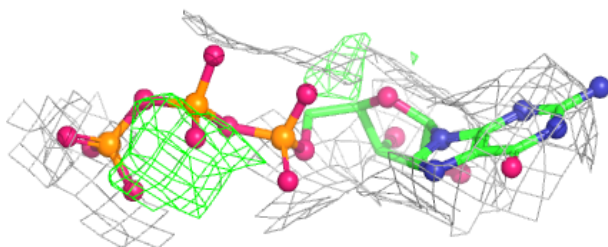
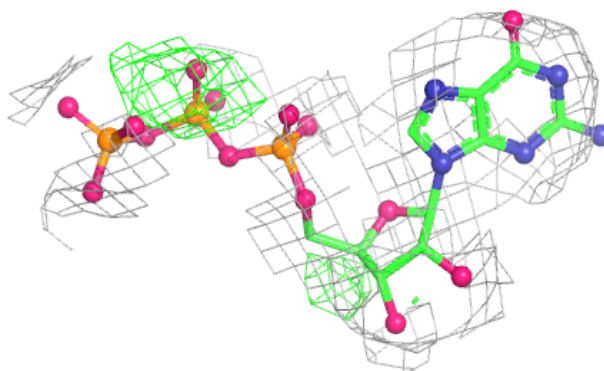


Electron density around GTP Q 600:

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and green (positive)

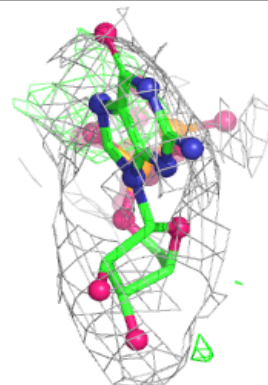
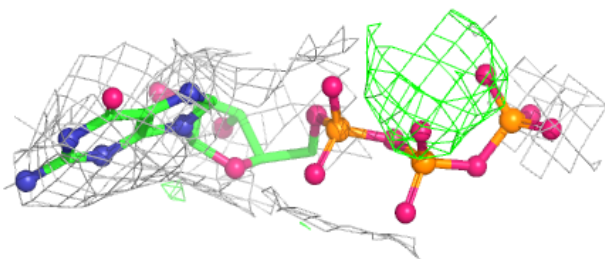
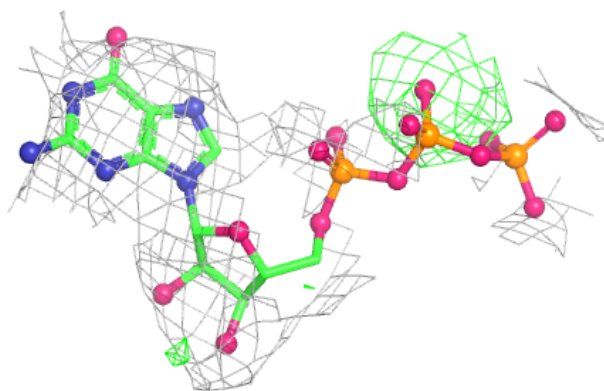
**Electron density around GTP A 600:**

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and green (positive)

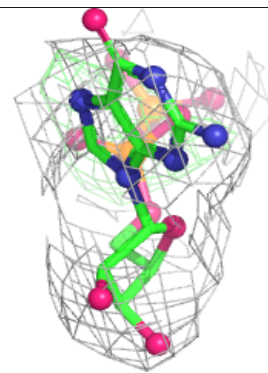
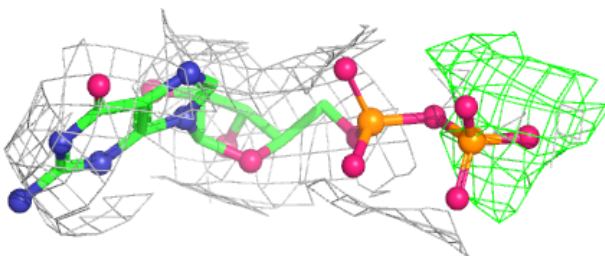
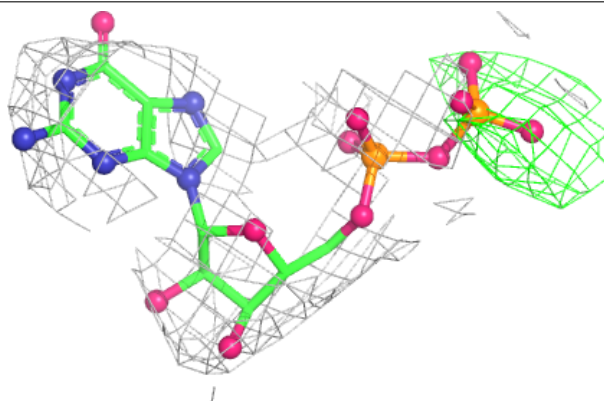


Electron density around GTP H 600:

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and green (positive)

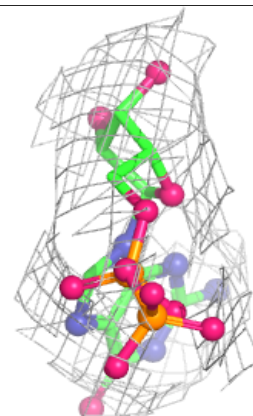
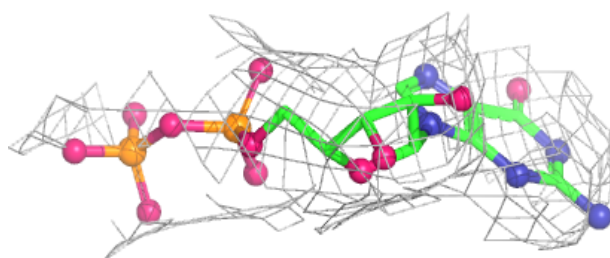
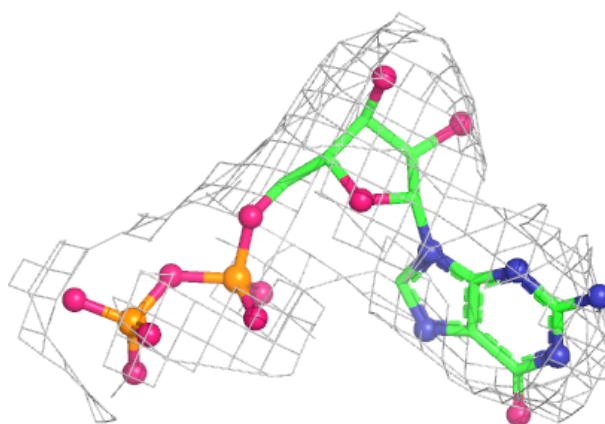
**Electron density around GDP B 600:**

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and green (positive)

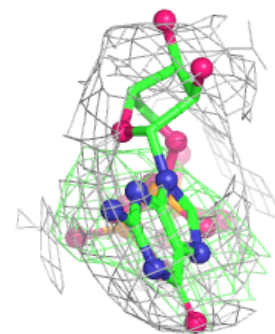
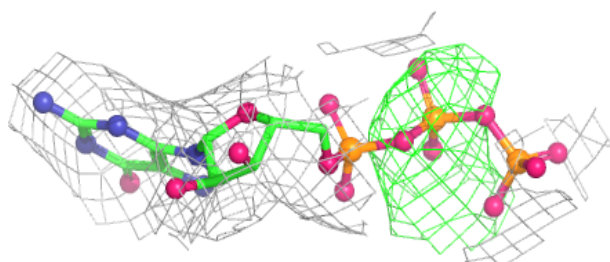
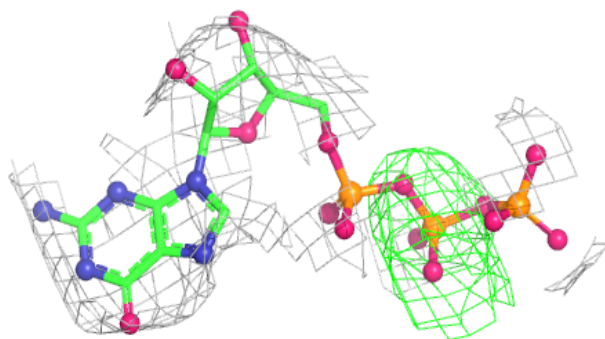


Electron density around GDP P 600:

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

**Electron density around GTP V 600:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.