



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 6, 2026 – 04:22 pm BST

PDB ID : 9RTC / pdb_00009rtc
Title : Okeania NrnC bound to pGG
Authors : Mortensen, S.; Burnim, A.; Dufault-Thompson, K.; Jiang, X.; Lipka, A.E.;
Sondermann, H.
Deposited on : 2025-07-02
Resolution : 3.00 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 : 1.8.4, CSD as541be (2020)
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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

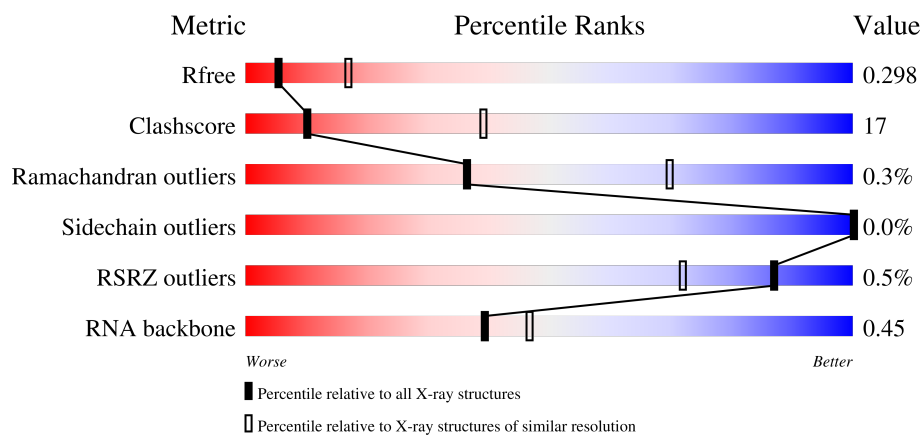
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.



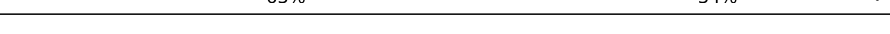
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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	208	
1	AA	208	
1	B	208	
1	BB	208	

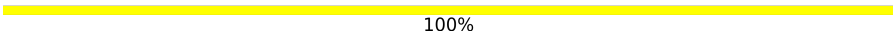
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Mol	Chain	Length	Quality of chain
1	C	208	
1	CC	208	
1	D	208	
1	DD	208	
1	E	208	
1	EE	208	
1	F	208	
1	FF	208	
1	G	208	
1	H	208	
1	I	208	
1	J	208	
1	K	208	
1	L	208	
1	M	208	
1	N	208	
1	O	208	
1	P	208	
1	Q	208	
1	R	208	
1	S	208	
1	T	208	
1	U	208	
1	V	208	
1	W	208	

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Mol	Chain	Length	Quality of chain
1	X	208	 63% 36%
1	Y	208	 59% 40%
1	Z	208	 59% 40%
2	bb	2	 50% 50%
2	cc	2	 50% 50%
2	ff	2	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CL	U	303	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 54470 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 nanoRNase C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1661	1058	279	314	10			
1	N	205	Total	C	N	O	S	0	0	0
			1655	1055	278	312	10			
1	B	205	Total	C	N	O	S	0	0	0
			1655	1055	278	312	10			
1	C	205	Total	C	N	O	S	0	0	0
			1655	1055	278	312	10			
1	D	205	Total	C	N	O	S	0	0	0
			1655	1055	278	312	10			
1	E	205	Total	C	N	O	S	0	0	0
			1655	1055	278	312	10			
1	F	205	Total	C	N	O	S	0	0	0
			1655	1055	278	312	10			
1	G	207	Total	C	N	O	S	0	0	0
			1671	1064	280	316	11			
1	H	205	Total	C	N	O	S	0	0	0
			1655	1055	278	312	10			
1	I	206	Total	C	N	O	S	0	0	0
			1661	1058	279	314	10			
1	J	207	Total	C	N	O	S	0	0	0
			1669	1063	280	315	11			
1	K	205	Total	C	N	O	S	0	0	0
			1655	1055	278	312	10			
1	L	205	Total	C	N	O	S	0	0	0
			1651	1053	278	310	10			
1	M	203	Total	C	N	O	S	0	0	0
			1641	1047	276	308	10			
1	O	205	Total	C	N	O	S	0	0	0
			1655	1055	278	312	10			
1	P	208	Total	C	N	O	S	0	0	0
			1675	1066	281	317	11			

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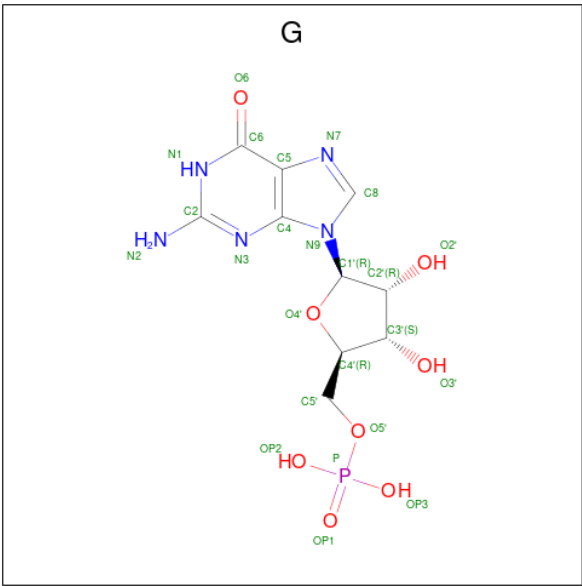
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	205	Total	C	N	O	S	0	0	0
			1651	1053	278	310	10			
1	R	205	Total	C	N	O	S	0	0	0
			1655	1055	278	312	10			
1	S	205	Total	C	N	O	S	0	0	0
			1655	1055	278	312	10			
1	T	205	Total	C	N	O	S	0	0	0
			1655	1055	278	312	10			
1	U	207	Total	C	N	O	S	0	0	0
			1669	1063	280	315	11			
1	V	205	Total	C	N	O	S	0	0	0
			1655	1055	278	312	10			
1	W	201	Total	C	N	O	S	0	0	0
			1622	1034	274	304	10			
1	X	205	Total	C	N	O	S	0	0	0
			1655	1055	278	312	10			
1	Y	205	Total	C	N	O	S	0	0	0
			1655	1055	278	312	10			
1	Z	205	Total	C	N	O	S	0	0	0
			1655	1055	278	312	10			
1	AA	202	Total	C	N	O	S	0	0	0
			1631	1039	275	307	10			
1	BB	205	Total	C	N	O	S	0	0	0
			1655	1055	278	312	10			
1	CC	205	Total	C	N	O	S	0	0	0
			1655	1055	278	312	10			
1	DD	199	Total	C	N	O	S	0	0	0
			1610	1030	271	299	10			
1	EE	205	Total	C	N	O	S	0	0	0
			1655	1055	278	312	10			
1	FF	205	Total	C	N	O	S	0	0	0
			1655	1055	278	312	10			

- Molecule 2 is a RNA chain called RNA (5'-R(P*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	bb	2	Total	C	N	O	P	0	0	0
			47	20	10	15	2			
2	cc	2	Total	C	N	O	P	0	0	0
			47	20	10	15	2			
2	ff	2	Total	C	N	O	P	0	0	0
			47	20	10	15	2			

- Molecule 3 is GUANOSINE-5'-MONOPHOSPHATE (CCD ID: G) (formula: C₁₀H₁₄N₅O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	A	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	N	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	N	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	B	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	B	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	B	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	C	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	D	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	D	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	E	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	E	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	F	1	Total	C	N	O	P	0	0
			24	10	5	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	G	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	G	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	H	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	H	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	H	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	I	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	J	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	J	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	K	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	K	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	L	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	L	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	L	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	M	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	O	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	O	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	P	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	P	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	Q	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	Q	1	Total 24	C 10	N 5	O 8	P 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	R	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	R	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	S	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	S	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	T	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	T	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	U	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	U	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	V	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	V	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	W	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	W	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	X	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	X	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	Y	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	Y	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	Y	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	Z	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	CC	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	CC	1	Total 24	C 10	N 5	O 8	P 1	0	0
3	DD	1	Total 24	C 10	N 5	O 8	P 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	DD	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	FF	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	FF	1	Total	C	N	O	P	0	0
			24	10	5	8	1		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Na	0	0
			2	2		
4	N	1	Total	Na	0	0
			1	1		
4	C	1	Total	Na	0	0
			1	1		
4	D	1	Total	Na	0	0
			1	1		
4	G	1	Total	Na	0	0
			1	1		
4	H	2	Total	Na	0	0
			2	2		
4	J	2	Total	Na	0	0
			2	2		
4	L	1	Total	Na	0	0
			1	1		
4	Q	2	Total	Na	0	0
			2	2		
4	R	2	Total	Na	0	0
			2	2		
4	V	2	Total	Na	0	0
			2	2		
4	W	2	Total	Na	0	0
			2	2		
4	X	1	Total	Na	0	0
			1	1		
4	EE	2	Total	Na	0	0
			2	2		
4	FF	2	Total	Na	0	0
			2	2		

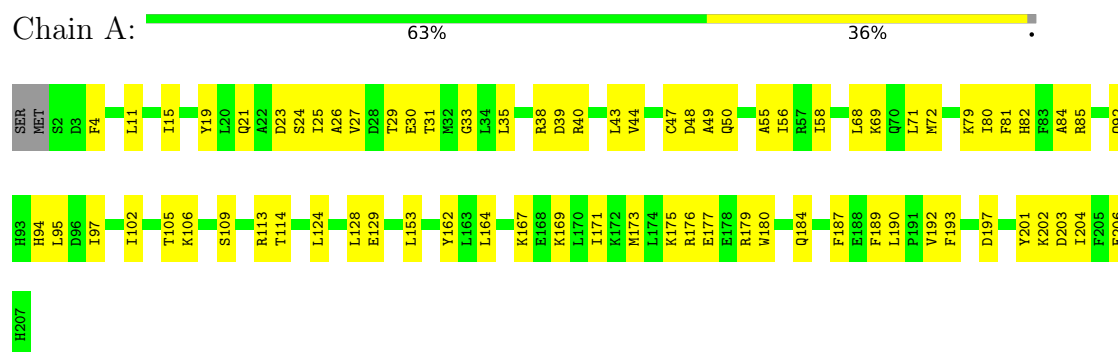
- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	U	1	Total	Cl	0	0
			1	1		

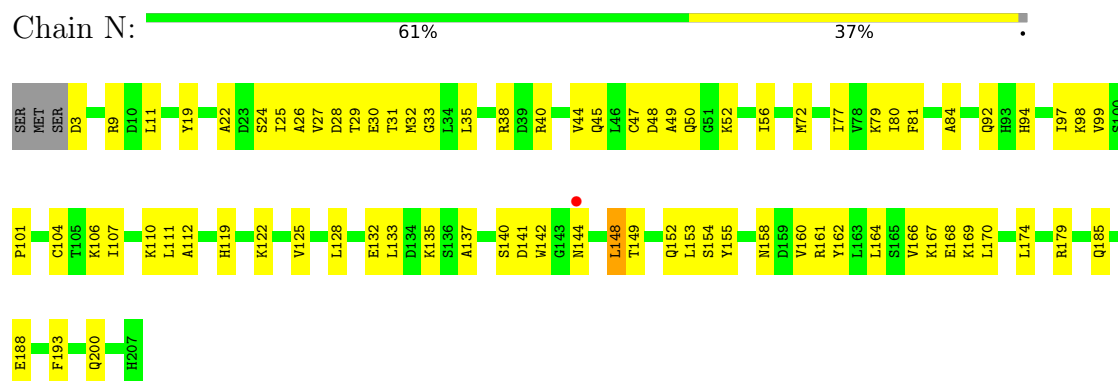
3 Residue-property plots [i](#)

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.

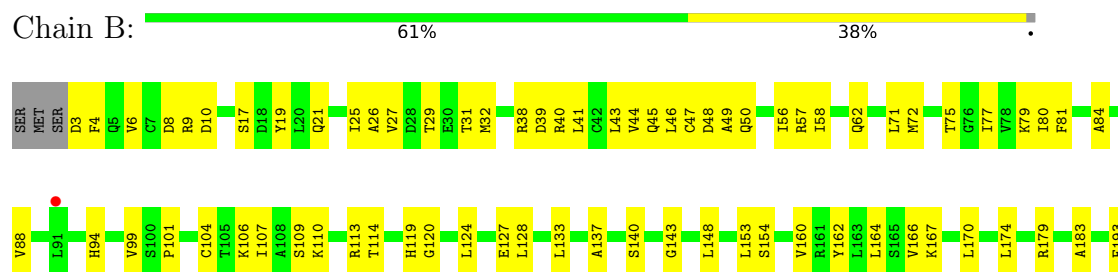
• Molecule 1: nanoRNase C



• Molecule 1: nanoRNase C



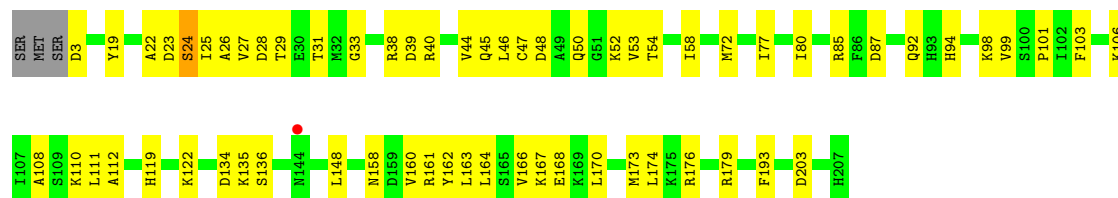
• Molecule 1: nanoRNase C





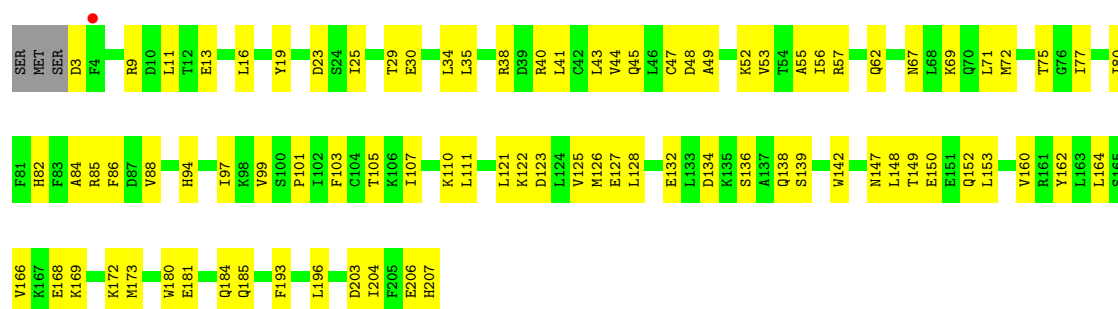
- Molecule 1: nanoRNase C

Chain C: 68% 30%



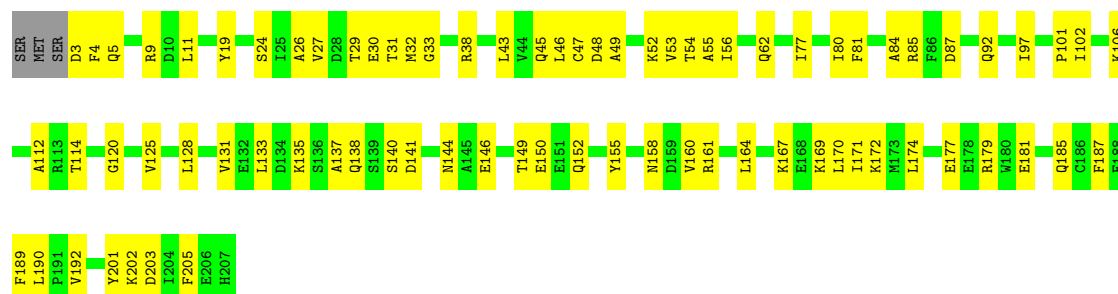
- Molecule 1: nanoRNase C

Chain D: 58% 41%



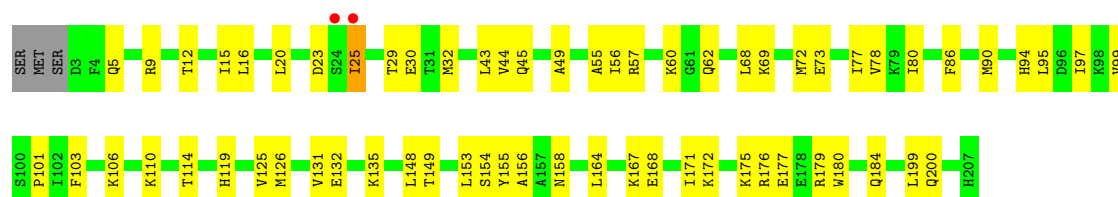
- Molecule 1: nanoRNase C

Chain E: 61% 38%

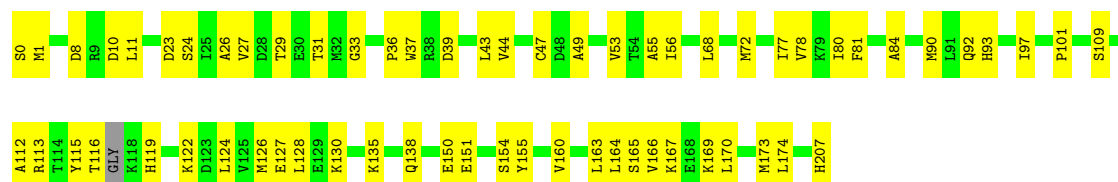


- Molecule 1: nanoRNase C

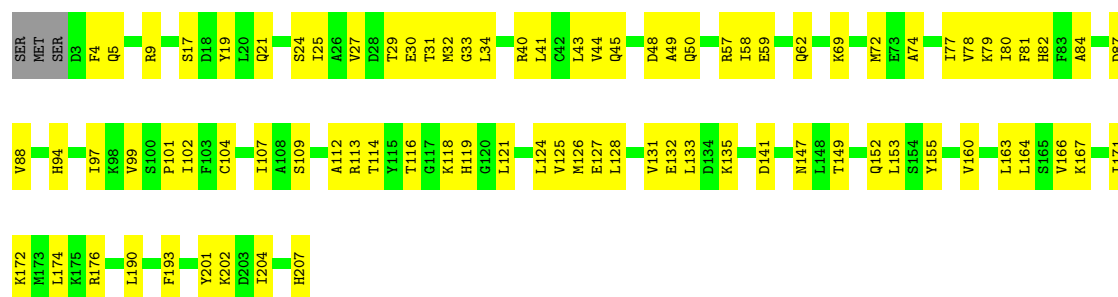
Chain F: 68% 30%



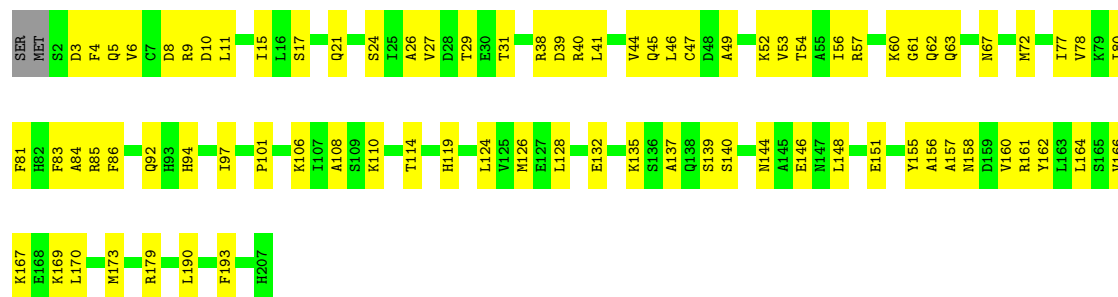
● Molecule 1: nanoRNase C

Chain G:  69% 30%

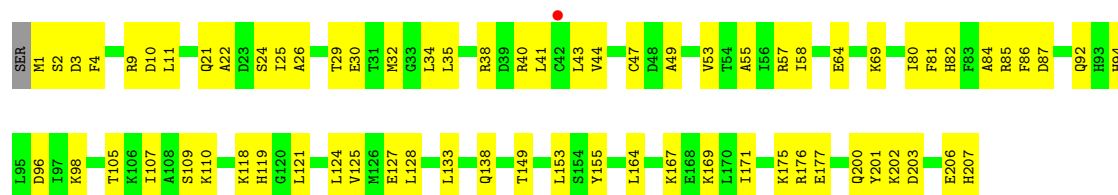
● Molecule 1: nanoRNase C

Chain H:  58% 40%

● Molecule 1: nanoRNase C

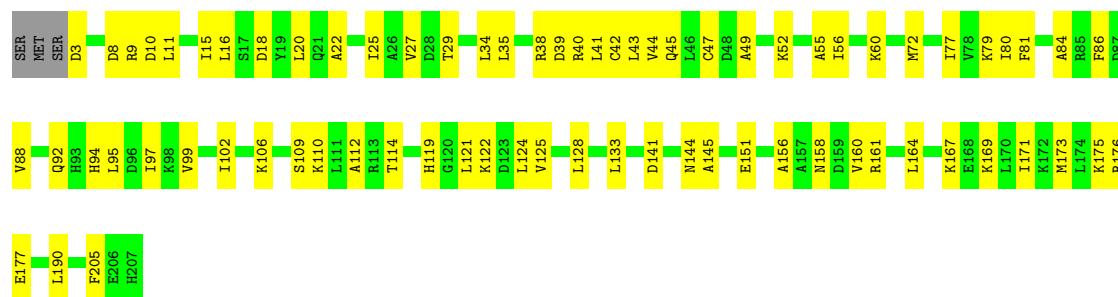
Chain I:  60% 39%

● Molecule 1: nanoRNase C

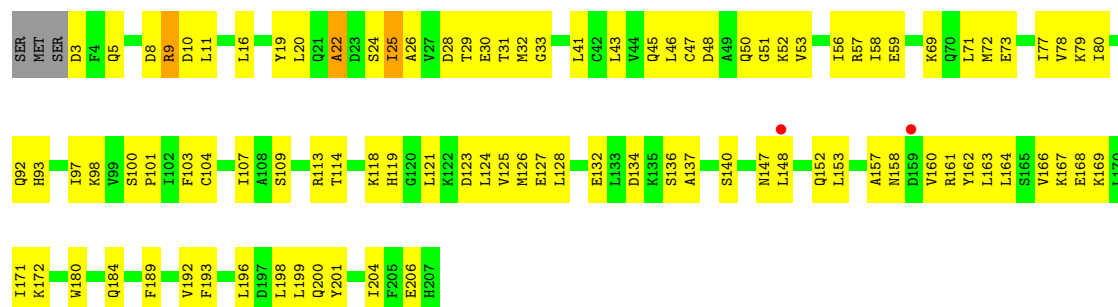
Chain J:  66% 34%

● Molecule 1: nanoRNase C

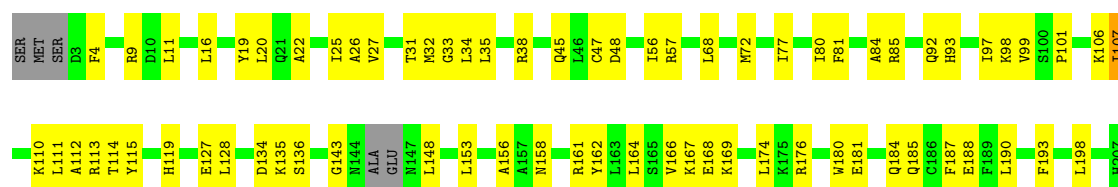
Chain K:  63% 35%



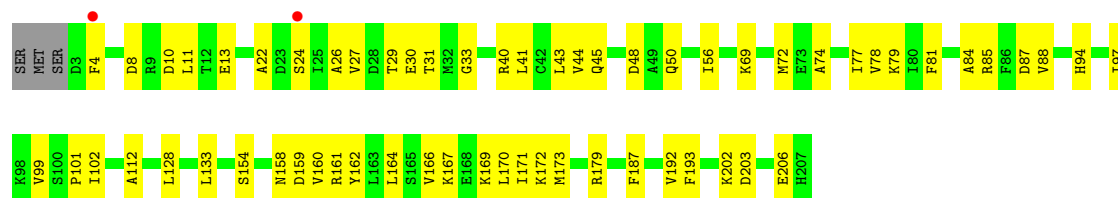
- Molecule 1: nanoRNase C



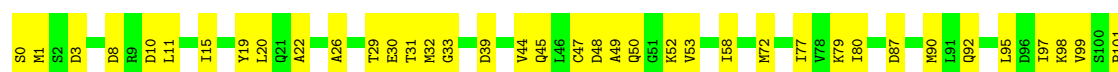
- Molecule 1: nanoRNase C

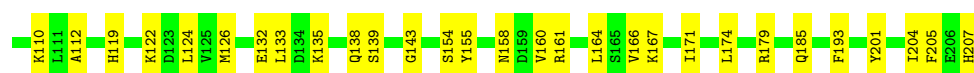


- Molecule 1: nanoRNase C

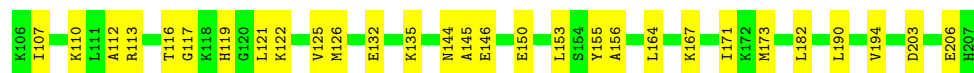
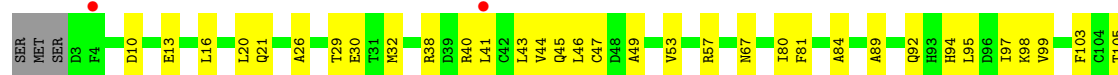


- Molecule 1: nanoRNase C

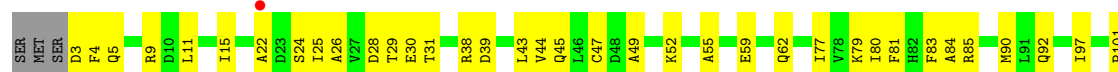




• Molecule 1: nanoRNase C



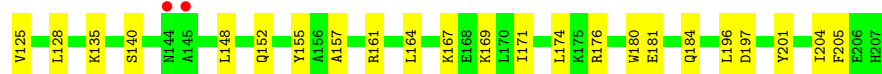
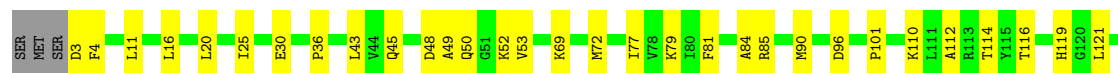
• Molecule 1: nanoRNase C



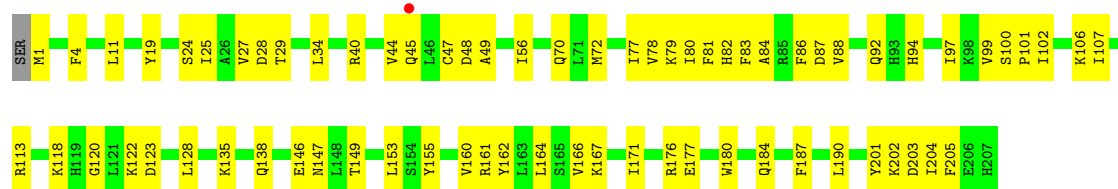
• Molecule 1: nanoRNase C



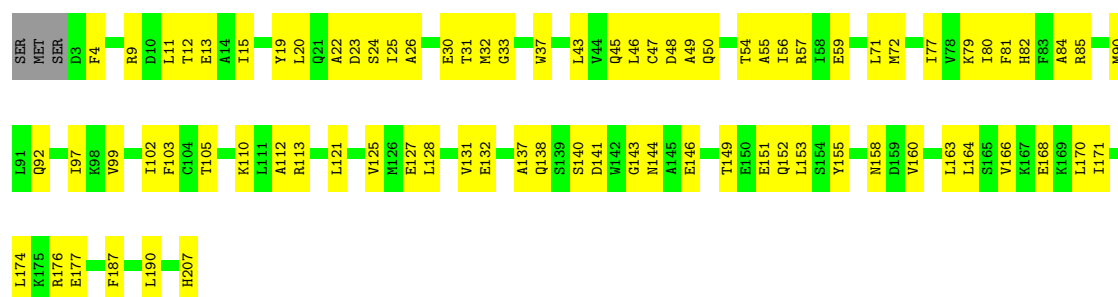
• Molecule 1: nanoRNase C



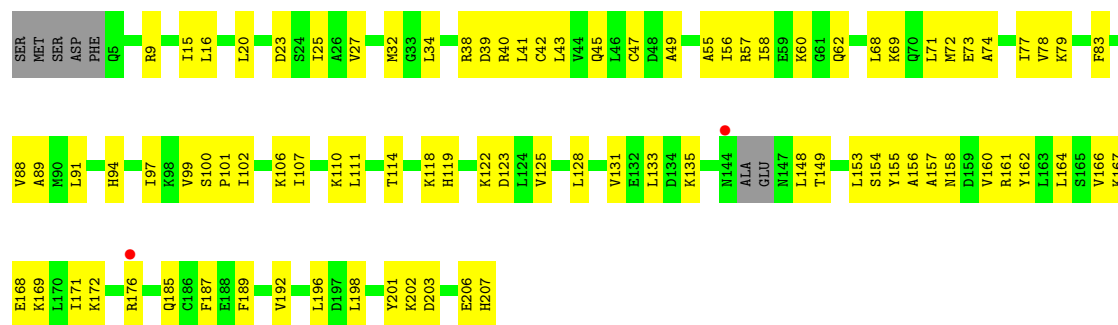
• Molecule 1: nanoRNase C

Chain U:  66% 34%

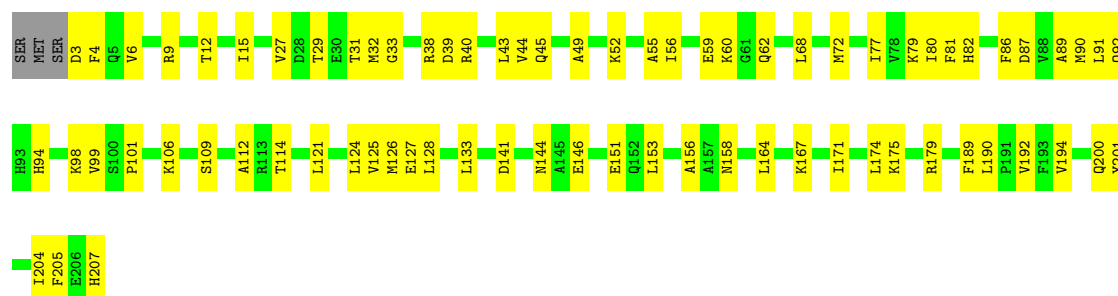
• Molecule 1: nanoRNase C

Chain V:  60% 39%

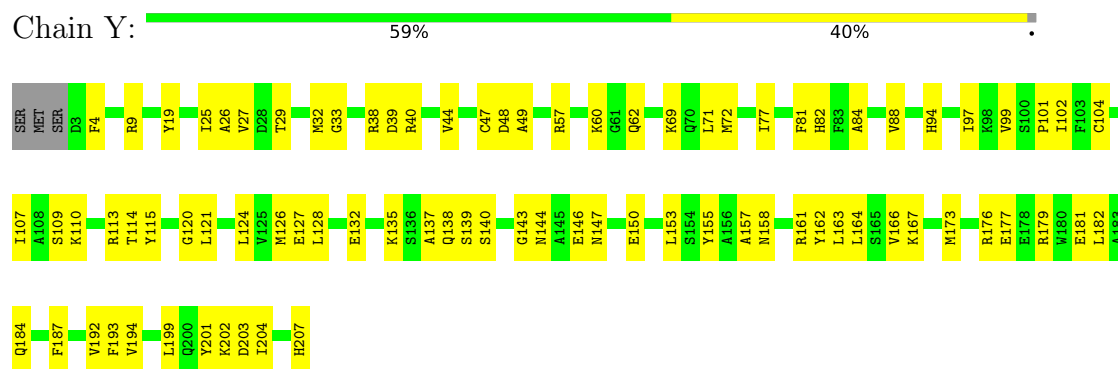
• Molecule 1: nanoRNase C

Chain W:  55% 42%

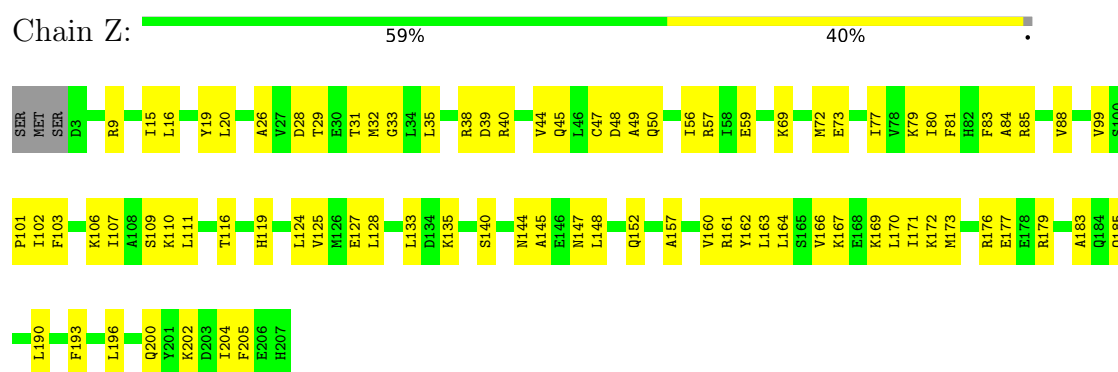
• Molecule 1: nanoRNase C

Chain X:  63% 36%

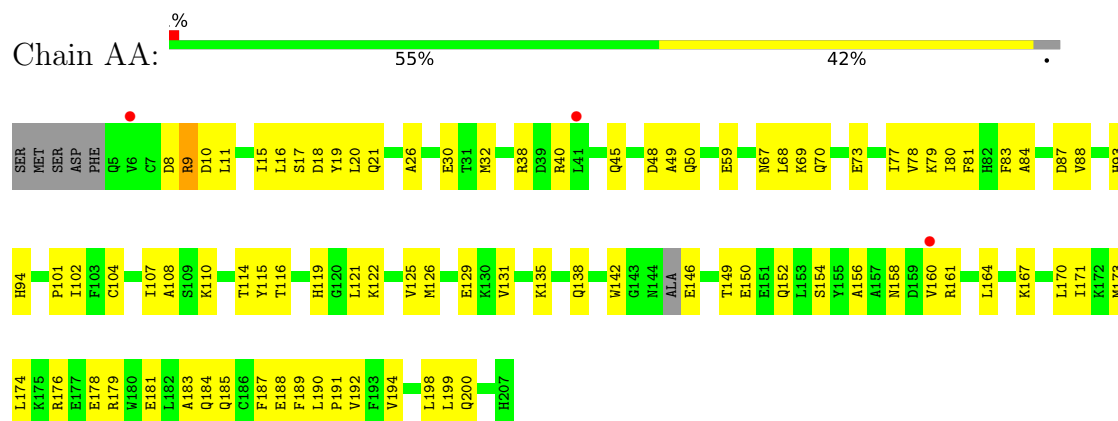
• Molecule 1: nanoRNase C



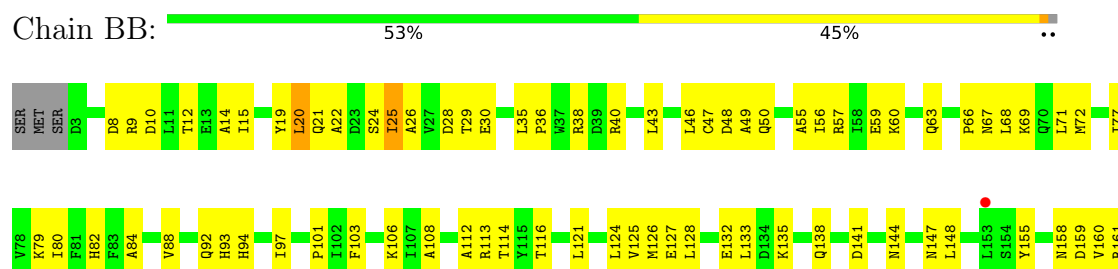
• Molecule 1: nanoRNase C



• Molecule 1: nanoRNase C



• Molecule 1: nanoRNase C





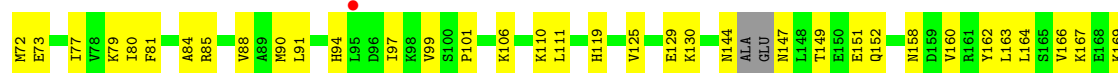
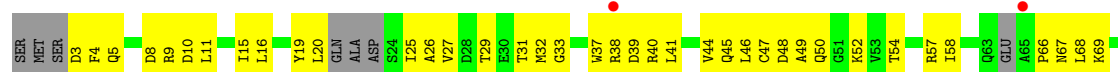
• Molecule 1: nanoRNase C

Chain CC: 55% 42% ..



• Molecule 1: nanoRNase C

Chain DD: 52% 44% .



• Molecule 1: nanoRNase C

Chain EE: 59% 39% ..



• Molecule 1: nanoRNase C

Chain FF: 65% 33% .





• Molecule 2: RNA (5'-R(P*GP*G)-3')



• Molecule 2: RNA (5'-R(P*GP*G)-3')



• Molecule 2: RNA (5'-R(P*GP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	142.48Å 176.18Å 159.67Å 90.00° 94.85° 90.00°	Depositor
Resolution (Å)	49.09 – 3.00 49.09 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.09-3.00) 98.7 (49.09-3.00)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.235 , 0.298 0.234 , 0.298	Depositor DCC
R_{free} test set	1998 reflections (0.59%)	wwPDB-VP
Wilson B-factor (Å ²)	71.5	Xtriage
Anisotropy	0.567	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 23.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	54470	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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: NA, CL

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	0.14	0/1689	0.35	0/2276
1	AA	0.15	0/1657	0.41	0/2231
1	B	0.19	0/1683	0.38	0/2268
1	BB	0.18	0/1683	0.44	0/2268
1	C	0.12	0/1683	0.38	0/2268
1	CC	0.14	0/1683	0.41	0/2268
1	D	0.14	0/1683	0.38	0/2268
1	DD	0.17	0/1635	0.44	0/2198
1	E	0.13	0/1683	0.37	0/2268
1	EE	0.12	0/1683	0.35	0/2268
1	F	0.14	0/1683	0.40	0/2268
1	FF	0.19	0/1683	0.41	0/2268
1	G	0.13	0/1698	0.36	0/2286
1	H	0.12	0/1683	0.36	0/2268
1	I	0.12	0/1689	0.34	0/2276
1	J	0.12	0/1697	0.34	0/2286
1	K	0.12	0/1683	0.31	0/2268
1	L	0.21	0/1679	0.44	0/2263
1	M	0.12	0/1668	0.37	0/2246
1	N	0.13	0/1683	0.40	0/2268
1	O	0.13	0/1683	0.37	0/2268
1	P	0.15	0/1703	0.38	0/2294
1	Q	0.14	0/1679	0.40	0/2263
1	R	0.12	0/1683	0.34	0/2268
1	S	0.15	0/1683	0.37	0/2268
1	T	0.13	0/1683	0.38	0/2268
1	U	0.12	0/1697	0.30	0/2286
1	V	0.13	0/1683	0.35	0/2268
1	W	0.18	0/1648	0.40	0/2219
1	X	0.13	0/1683	0.37	0/2268
1	Y	0.19	0/1683	0.47	0/2268
1	Z	0.14	0/1683	0.39	0/2268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	bb	0.12	0/52	0.35	0/78
2	cc	0.11	0/52	0.35	0/78
2	ff	0.08	0/52	0.25	0/78
All	All	0.15	0/53955	0.38	0/72718

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1661	0	1670	57	1
1	AA	1631	0	1646	75	0
1	B	1655	0	1665	61	1
1	BB	1655	0	1665	87	0
1	C	1655	0	1665	54	1
1	CC	1655	0	1665	86	0
1	D	1655	0	1665	65	0
1	DD	1610	0	1628	96	0
1	E	1655	0	1665	68	1
1	EE	1655	0	1665	75	0
1	F	1655	0	1665	46	0
1	FF	1655	0	1665	52	0
1	G	1671	0	1683	46	0
1	H	1655	0	1665	68	0
1	I	1661	0	1670	64	0
1	J	1669	0	1682	50	0
1	K	1655	0	1665	56	1
1	L	1651	0	1661	86	0
1	M	1641	0	1653	61	0
1	N	1655	0	1665	62	0
1	O	1655	0	1665	49	0
1	P	1675	0	1687	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Q	1651	0	1661	52	0
1	R	1655	0	1665	52	0
1	S	1655	0	1665	58	0
1	T	1655	0	1665	40	1
1	U	1669	0	1682	58	0
1	V	1655	0	1665	63	0
1	W	1622	0	1640	69	0
1	X	1655	0	1665	69	0
1	Y	1655	0	1665	74	0
1	Z	1655	0	1665	70	0
2	bb	47	0	23	1	0
2	cc	47	0	23	1	0
2	ff	47	0	23	2	0
3	A	48	0	24	1	0
3	B	72	0	36	2	0
3	C	24	0	12	1	0
3	CC	48	0	24	1	0
3	D	48	0	24	2	0
3	DD	48	0	24	1	0
3	E	48	0	24	2	0
3	F	48	0	24	0	0
3	FF	48	0	24	2	0
3	G	48	0	24	4	0
3	H	72	0	36	3	0
3	I	24	0	12	0	0
3	J	48	0	24	2	0
3	K	48	0	24	0	0
3	L	72	0	36	0	0
3	M	24	0	12	2	0
3	N	48	0	24	1	0
3	O	48	0	24	0	0
3	P	48	0	24	0	0
3	Q	48	0	24	1	0
3	R	48	0	24	1	0
3	S	48	0	24	1	0
3	T	48	0	24	0	0
3	U	48	0	24	4	0
3	V	48	0	23	1	0
3	W	48	0	24	2	0
3	X	48	0	24	2	0
3	Y	72	0	36	2	0
3	Z	24	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	EE	2	0	0	0	0
4	FF	2	0	0	0	0
4	G	1	0	0	0	0
4	H	2	0	0	0	0
4	J	2	0	0	0	0
4	L	1	0	0	0	0
4	N	1	0	0	0	0
4	Q	2	0	0	0	0
4	R	2	0	0	0	0
4	V	2	0	0	0	0
4	W	2	0	0	0	0
4	X	1	0	0	0	0
5	U	1	0	0	2	0
All	All	54470	0	54027	1864	3

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 17.

The worst 5 of 1864 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:D:150:GLU:HA	1:D:153:LEU:HD21	1.28	1.15
1:I:45:GLN:NE2	1:I:156:ALA:O	1.82	1.12
1:X:45:GLN:NE2	1:X:156:ALA:O	1.84	1.10
1:L:28:ASP:HB3	1:L:45:GLN:HE21	0.94	1.10
1:Q:150:GLU:HA	1:Q:153:LEU:CD2	1.82	1.08

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:ASP:OD2	1:T:4:PHE:O[2_455]	1.90	0.30
1:A:38:ARG:NH1	1:E:114:THR:OG1[2_545]	2.15	0.05
1:C:176:ARG:O	1:K:60:LYS:NZ[2_555]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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	204/208 (98%)	194 (95%)	10 (5%)	0	100	100
1	AA	198/208 (95%)	187 (94%)	10 (5%)	1 (0%)	24	60
1	B	203/208 (98%)	191 (94%)	12 (6%)	0	100	100
1	BB	203/208 (98%)	187 (92%)	14 (7%)	2 (1%)	12	45
1	C	203/208 (98%)	189 (93%)	13 (6%)	1 (0%)	24	60
1	CC	203/208 (98%)	187 (92%)	13 (6%)	3 (2%)	8	35
1	D	203/208 (98%)	186 (92%)	17 (8%)	0	100	100
1	DD	191/208 (92%)	177 (93%)	14 (7%)	0	100	100
1	E	203/208 (98%)	192 (95%)	11 (5%)	0	100	100
1	EE	203/208 (98%)	185 (91%)	15 (7%)	3 (2%)	8	35
1	F	203/208 (98%)	186 (92%)	16 (8%)	1 (0%)	24	60
1	FF	203/208 (98%)	196 (97%)	7 (3%)	0	100	100
1	G	203/208 (98%)	190 (94%)	13 (6%)	0	100	100
1	H	203/208 (98%)	193 (95%)	10 (5%)	0	100	100
1	I	204/208 (98%)	196 (96%)	8 (4%)	0	100	100
1	J	205/208 (99%)	194 (95%)	10 (5%)	1 (0%)	24	60
1	K	203/208 (98%)	196 (97%)	6 (3%)	1 (0%)	24	60
1	L	203/208 (98%)	186 (92%)	14 (7%)	3 (2%)	8	35
1	M	199/208 (96%)	188 (94%)	10 (5%)	1 (0%)	24	60
1	N	203/208 (98%)	188 (93%)	13 (6%)	2 (1%)	12	45
1	O	203/208 (98%)	189 (93%)	14 (7%)	0	100	100
1	P	206/208 (99%)	195 (95%)	11 (5%)	0	100	100
1	Q	203/208 (98%)	188 (93%)	15 (7%)	0	100	100
1	R	203/208 (98%)	192 (95%)	11 (5%)	0	100	100
1	S	203/208 (98%)	192 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	T	203/208 (98%)	192 (95%)	11 (5%)	0	100	100
1	U	205/208 (99%)	197 (96%)	8 (4%)	0	100	100
1	V	203/208 (98%)	194 (96%)	9 (4%)	0	100	100
1	W	197/208 (95%)	183 (93%)	14 (7%)	0	100	100
1	X	203/208 (98%)	192 (95%)	11 (5%)	0	100	100
1	Y	203/208 (98%)	189 (93%)	14 (7%)	0	100	100
1	Z	203/208 (98%)	195 (96%)	7 (3%)	1 (0%)	24	60
All	All	6478/6656 (97%)	6086 (94%)	372 (6%)	20 (0%)	36	70

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	25	ILE
1	L	25	ILE
1	BB	20	LEU
1	EE	25	ILE
1	N	22	ALA

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	182/184 (99%)	182 (100%)	0	100	100
1	AA	179/184 (97%)	179 (100%)	0	100	100
1	B	181/184 (98%)	181 (100%)	0	100	100
1	BB	181/184 (98%)	181 (100%)	0	100	100
1	C	181/184 (98%)	181 (100%)	0	100	100
1	CC	181/184 (98%)	181 (100%)	0	100	100
1	D	181/184 (98%)	181 (100%)	0	100	100
1	DD	177/184 (96%)	177 (100%)	0	100	100
1	E	181/184 (98%)	181 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	EE	181/184 (98%)	181 (100%)	0	100	100
1	F	181/184 (98%)	181 (100%)	0	100	100
1	FF	181/184 (98%)	181 (100%)	0	100	100
1	G	184/184 (100%)	184 (100%)	0	100	100
1	H	181/184 (98%)	181 (100%)	0	100	100
1	I	182/184 (99%)	182 (100%)	0	100	100
1	J	183/184 (100%)	182 (100%)	1 (0%)	81	89
1	K	181/184 (98%)	181 (100%)	0	100	100
1	L	180/184 (98%)	180 (100%)	0	100	100
1	M	180/184 (98%)	180 (100%)	0	100	100
1	N	181/184 (98%)	181 (100%)	0	100	100
1	O	181/184 (98%)	181 (100%)	0	100	100
1	P	184/184 (100%)	184 (100%)	0	100	100
1	Q	180/184 (98%)	180 (100%)	0	100	100
1	R	181/184 (98%)	181 (100%)	0	100	100
1	S	181/184 (98%)	181 (100%)	0	100	100
1	T	181/184 (98%)	180 (99%)	1 (1%)	78	88
1	U	183/184 (100%)	183 (100%)	0	100	100
1	V	181/184 (98%)	181 (100%)	0	100	100
1	W	178/184 (97%)	178 (100%)	0	100	100
1	X	181/184 (98%)	181 (100%)	0	100	100
1	Y	181/184 (98%)	181 (100%)	0	100	100
1	Z	181/184 (98%)	181 (100%)	0	100	100
All	All	5792/5888 (98%)	5790 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	64	GLU
1	T	53	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	207	HIS
1	CC	82	HIS
1	EE	184	GLN
1	L	207	HIS
1	L	45	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	bb	1/2 (50%)	0	0
2	cc	1/2 (50%)	0	0
2	ff	1/2 (50%)	0	0
All	All	3/6 (50%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 83 ligands modelled in this entry, 25 are monoatomic - leaving 58 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	$\# Z > 2$
3	G	J	302	-	26,26,26	0.54	0	40,40,40	0.52	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	G	H	303	-	26,26,26	0.55	0	40,40,40	0.52	1 (2%)
3	G	I	301	-	26,26,26	0.54	0	40,40,40	0.49	1 (2%)
3	G	W	301	4	26,26,26	0.54	0	40,40,40	0.50	1 (2%)
3	G	A	301	4	26,26,26	0.54	0	40,40,40	0.50	1 (2%)
3	G	CC	302	-	26,26,26	0.54	0	40,40,40	0.53	1 (2%)
3	G	E	302	-	26,26,26	0.54	0	40,40,40	0.54	1 (2%)
3	G	Y	303	-	26,26,26	0.55	0	40,40,40	0.49	0
3	G	D	301	-	26,26,26	0.55	0	40,40,40	0.50	1 (2%)
3	G	H	302	4	26,26,26	0.54	0	40,40,40	0.50	1 (2%)
3	G	F	302	-	26,26,26	0.54	0	40,40,40	0.48	0
3	G	X	302	4	26,26,26	0.53	0	40,40,40	0.51	1 (2%)
3	G	G	301	-	26,26,26	0.54	0	40,40,40	0.51	1 (2%)
3	G	L	302	4	26,26,26	0.54	0	40,40,40	0.49	1 (2%)
3	G	B	302	-	26,26,26	0.54	0	40,40,40	0.48	1 (2%)
3	G	V	301	4	26,26,26	0.54	0	40,40,40	0.52	1 (2%)
3	G	H	301	-	26,26,26	0.54	0	40,40,40	0.51	1 (2%)
3	G	T	302	-	26,26,26	0.54	0	40,40,40	0.48	0
3	G	U	302	-	26,26,26	0.54	0	40,40,40	0.53	1 (2%)
3	G	P	302	-	26,26,26	0.54	0	40,40,40	0.50	1 (2%)
3	G	FF	302	4	26,26,26	0.57	0	40,40,40	0.51	1 (2%)
3	G	N	302	4	26,26,26	0.54	0	40,40,40	0.48	0
3	G	DD	301	-	26,26,26	0.54	0	40,40,40	0.51	1 (2%)
3	G	U	301	-	26,26,26	0.55	0	40,40,40	0.51	1 (2%)
3	G	X	301	-	26,26,26	0.55	0	40,40,40	0.54	1 (2%)
3	G	D	302	4	26,26,26	0.54	0	40,40,40	0.49	1 (2%)
3	G	J	301	4	26,26,26	0.54	0	40,40,40	0.49	0
3	G	R	301	-	26,26,26	0.54	0	40,40,40	0.51	1 (2%)
3	G	L	303	-	26,26,26	0.54	0	40,40,40	0.53	1 (2%)
3	G	Z	301	-	26,26,26	0.57	0	40,40,40	0.62	1 (2%)
3	G	C	301	4	26,26,26	0.54	0	40,40,40	0.55	1 (2%)
3	G	G	302	4	26,26,26	0.58	0	40,40,40	0.69	1 (2%)
3	G	S	301	-	26,26,26	0.55	0	40,40,40	0.54	1 (2%)
3	G	P	301	-	26,26,26	0.54	0	40,40,40	0.52	1 (2%)
3	G	V	302	4	26,26,26	0.54	0	40,40,40	0.49	0
3	G	Q	301	-	26,26,26	0.54	0	40,40,40	0.51	1 (2%)
3	G	N	301	4	26,26,26	0.54	0	40,40,40	0.53	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	G	K	302	-	26,26,26	0.54	0	40,40,40	0.50	0
3	G	Y	302	-	26,26,26	0.54	0	40,40,40	0.50	1 (2%)
3	G	FF	301	4	26,26,26	0.54	0	40,40,40	0.52	1 (2%)
3	G	B	303	-	26,26,26	0.54	0	40,40,40	0.53	1 (2%)
3	G	T	301	-	26,26,26	0.55	0	40,40,40	0.51	1 (2%)
3	G	E	301	-	26,26,26	0.55	0	40,40,40	0.53	1 (2%)
3	G	O	302	-	26,26,26	0.54	0	40,40,40	0.50	1 (2%)
3	G	R	302	4	26,26,26	0.54	0	40,40,40	0.50	1 (2%)
3	G	M	301	-	26,26,26	0.53	0	40,40,40	0.48	0
3	G	L	301	-	26,26,26	0.55	0	40,40,40	0.51	1 (2%)
3	G	A	302	-	26,26,26	0.54	0	40,40,40	0.51	1 (2%)
3	G	Y	301	-	26,26,26	0.55	0	40,40,40	0.52	1 (2%)
3	G	DD	302	-	26,26,26	0.53	0	40,40,40	0.49	0
3	G	K	301	4	26,26,26	0.54	0	40,40,40	0.51	1 (2%)
3	G	F	301	-	26,26,26	0.55	0	40,40,40	0.49	0
3	G	O	301	-	26,26,26	0.54	0	40,40,40	0.52	1 (2%)
3	G	B	301	-	26,26,26	0.55	0	40,40,40	0.52	1 (2%)
3	G	W	302	4	26,26,26	0.54	0	40,40,40	0.56	1 (2%)
3	G	S	302	-	26,26,26	0.54	0	40,40,40	0.51	1 (2%)
3	G	Q	302	4	26,26,26	0.53	0	40,40,40	0.50	0
3	G	CC	301	-	26,26,26	0.55	0	40,40,40	0.50	1 (2%)

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
3	G	J	302	-	-	0/10/26/26	0/3/3/3
3	G	H	303	-	-	2/10/26/26	0/3/3/3
3	G	I	301	-	-	0/10/26/26	0/3/3/3
3	G	W	301	4	-	3/10/26/26	0/3/3/3
3	G	A	301	4	-	0/10/26/26	0/3/3/3
3	G	CC	302	-	-	3/10/26/26	0/3/3/3
3	G	E	302	-	-	1/10/26/26	0/3/3/3
3	G	Y	303	-	-	2/10/26/26	0/3/3/3
3	G	D	301	-	-	0/10/26/26	0/3/3/3
3	G	H	302	4	-	2/10/26/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	G	F	302	-	-	3/10/26/26	0/3/3/3
3	G	X	302	4	-	3/10/26/26	0/3/3/3
3	G	G	301	-	-	5/10/26/26	0/3/3/3
3	G	L	302	4	-	0/10/26/26	0/3/3/3
3	G	B	302	-	-	3/10/26/26	0/3/3/3
3	G	V	301	4	-	0/10/26/26	0/3/3/3
3	G	H	301	-	-	3/10/26/26	0/3/3/3
3	G	T	302	-	-	2/10/26/26	0/3/3/3
3	G	U	302	-	-	3/10/26/26	0/3/3/3
3	G	P	302	-	-	2/10/26/26	0/3/3/3
3	G	FF	302	4	-	2/10/26/26	0/3/3/3
3	G	N	302	4	-	2/10/26/26	0/3/3/3
3	G	DD	301	-	-	2/10/26/26	0/3/3/3
3	G	U	301	-	-	0/10/26/26	0/3/3/3
3	G	X	301	-	-	4/10/26/26	0/3/3/3
3	G	D	302	4	-	0/10/26/26	0/3/3/3
3	G	J	301	4	-	3/10/26/26	0/3/3/3
3	G	R	301	-	-	0/10/26/26	0/3/3/3
3	G	L	303	-	-	0/10/26/26	0/3/3/3
3	G	Z	301	-	-	1/10/26/26	0/3/3/3
3	G	C	301	4	-	6/10/26/26	0/3/3/3
3	G	G	302	4	-	3/10/26/26	0/3/3/3
3	G	S	301	-	-	0/10/26/26	0/3/3/3
3	G	P	301	-	-	0/10/26/26	0/3/3/3
3	G	V	302	4	-	0/10/26/26	0/3/3/3
3	G	Q	301	-	-	2/10/26/26	0/3/3/3
3	G	N	301	4	-	4/10/26/26	0/3/3/3
3	G	K	302	-	-	4/10/26/26	0/3/3/3
3	G	Y	302	-	-	0/10/26/26	0/3/3/3
3	G	FF	301	4	-	3/10/26/26	0/3/3/3
3	G	B	303	-	-	5/10/26/26	0/3/3/3
3	G	T	301	-	-	0/10/26/26	0/3/3/3
3	G	E	301	-	-	0/10/26/26	0/3/3/3
3	G	O	302	-	-	4/10/26/26	0/3/3/3
3	G	R	302	4	-	0/10/26/26	0/3/3/3
3	G	M	301	-	-	3/10/26/26	0/3/3/3
3	G	L	301	-	-	0/10/26/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	G	A	302	-	-	0/10/26/26	0/3/3/3
3	G	Y	301	-	-	0/10/26/26	0/3/3/3
3	G	DD	302	-	-	3/10/26/26	0/3/3/3
3	G	K	301	4	-	0/10/26/26	0/3/3/3
3	G	F	301	-	-	1/10/26/26	0/3/3/3
3	G	O	301	-	-	2/10/26/26	0/3/3/3
3	G	B	301	-	-	0/10/26/26	0/3/3/3
3	G	W	302	4	-	6/10/26/26	0/3/3/3
3	G	S	302	-	-	2/10/26/26	0/3/3/3
3	G	Q	302	4	-	5/10/26/26	0/3/3/3
3	G	CC	301	-	-	2/10/26/26	0/3/3/3

There are no bond length outliers.

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Z	301	G	OP2-P-OP1	2.33	119.78	110.68
3	W	302	G	OP3-P-OP1	2.27	119.56	110.68
3	FF	301	G	OP2-P-OP1	2.21	119.34	110.68
3	B	301	G	OP2-P-OP1	2.15	119.11	110.68
3	X	301	G	OP2-P-OP1	2.15	119.11	110.68

There are no chirality outliers.

5 of 106 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	N	301	G	C5'-O5'-P-OP3
3	N	301	G	C5'-O5'-P-OP2
3	B	302	G	C5'-O5'-P-OP1
3	B	302	G	C5'-O5'-P-OP2
3	B	303	G	C5'-O5'-P-OP3

There are no ring outliers.

29 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	303	G	1	0
3	W	301	G	1	0
3	CC	302	G	1	0

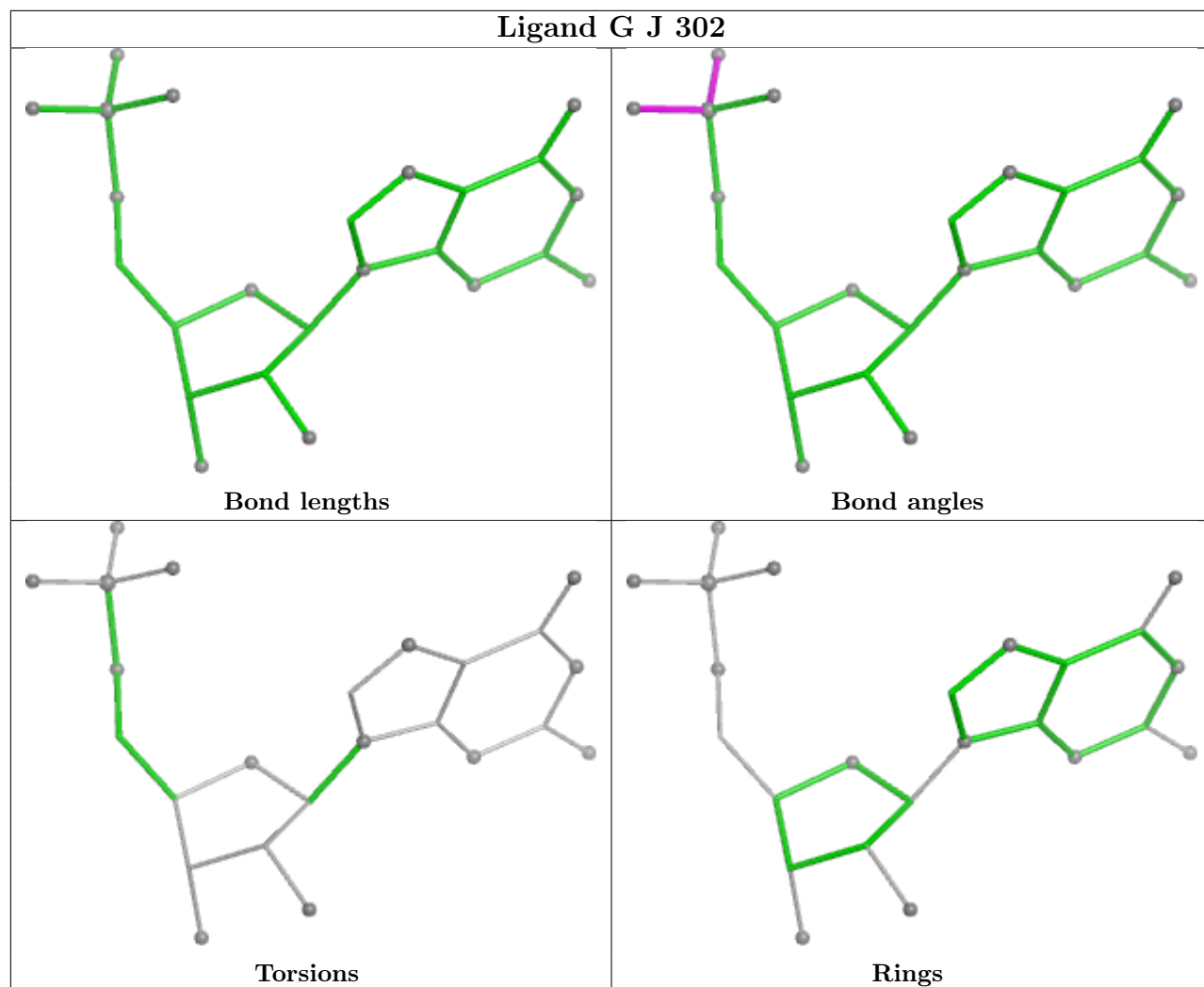
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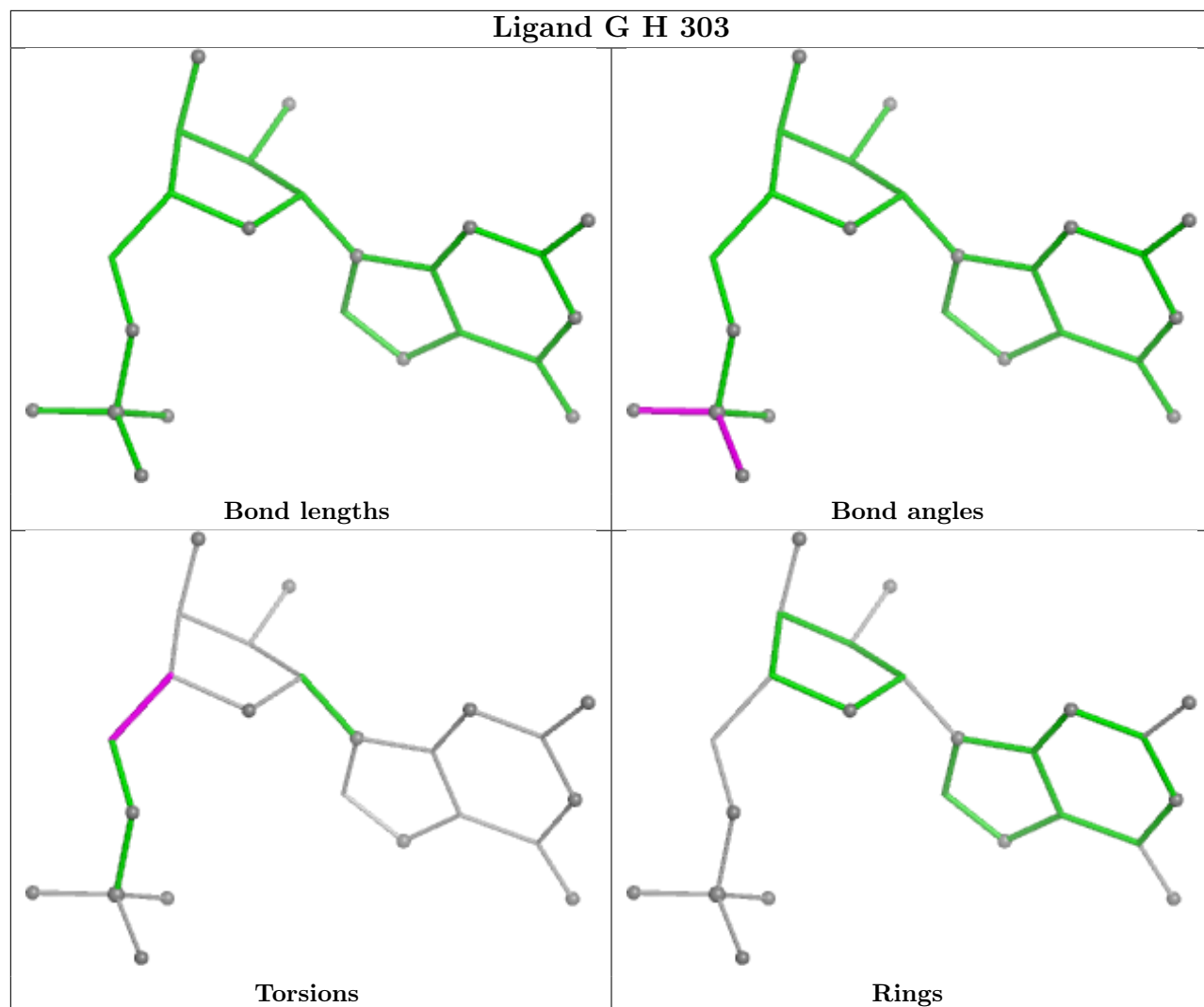
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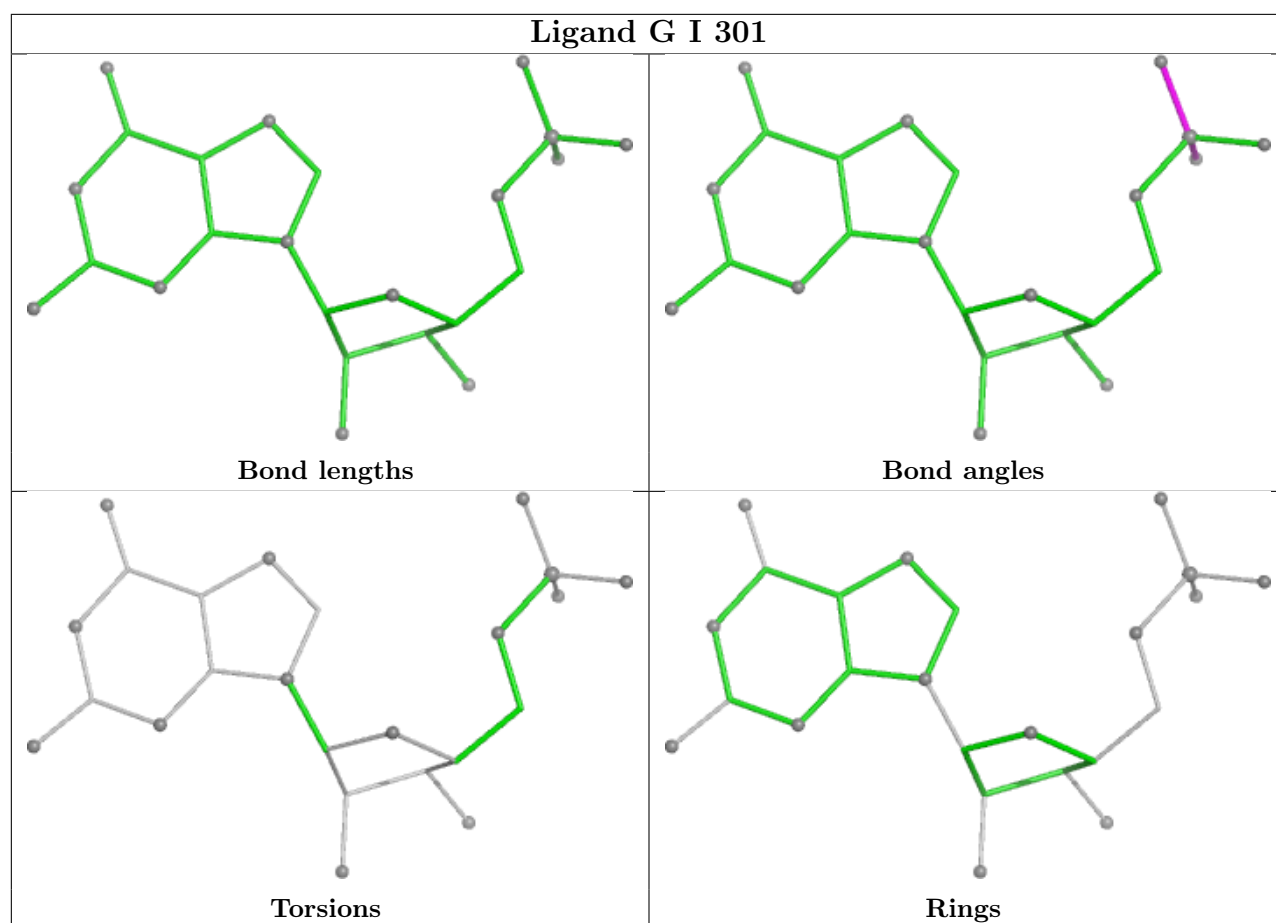
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	302	G	1	0
3	Y	303	G	1	0
3	D	301	G	1	0
3	H	302	G	2	0
3	U	302	G	2	0
3	FF	302	G	2	0
3	DD	301	G	1	0
3	U	301	G	2	0
3	X	301	G	2	0
3	D	302	G	1	0
3	J	301	G	2	0
3	R	301	G	1	0
3	C	301	G	1	0
3	G	302	G	4	0
3	V	302	G	1	0
3	N	301	G	1	0
3	B	303	G	1	0
3	E	301	G	1	0
3	M	301	G	2	0
3	A	302	G	1	0
3	Y	301	G	1	0
3	DD	302	G	1	0
3	B	301	G	1	0
3	W	302	G	1	0
3	S	302	G	1	0
3	Q	302	G	1	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.

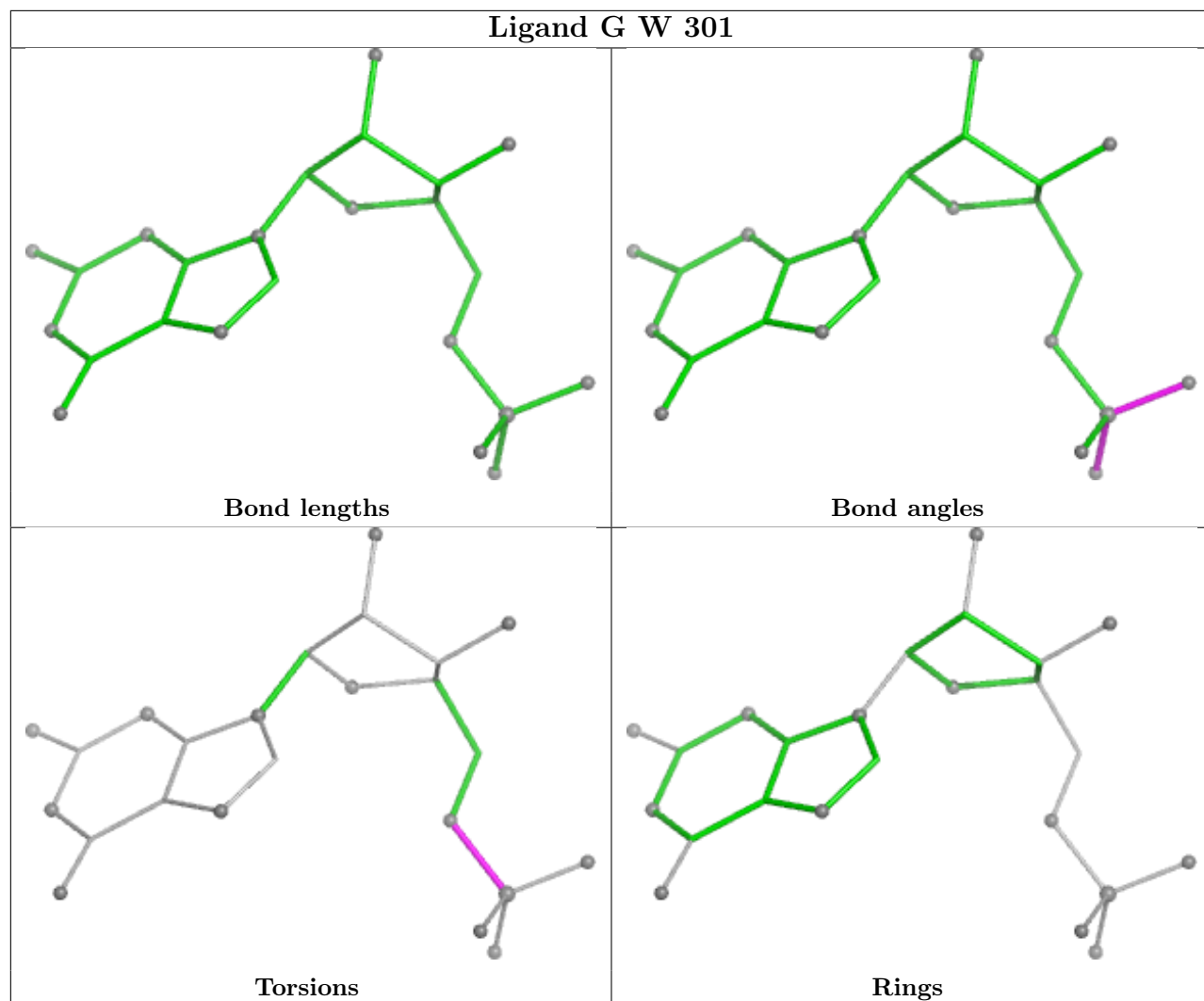
Ligand G J 302



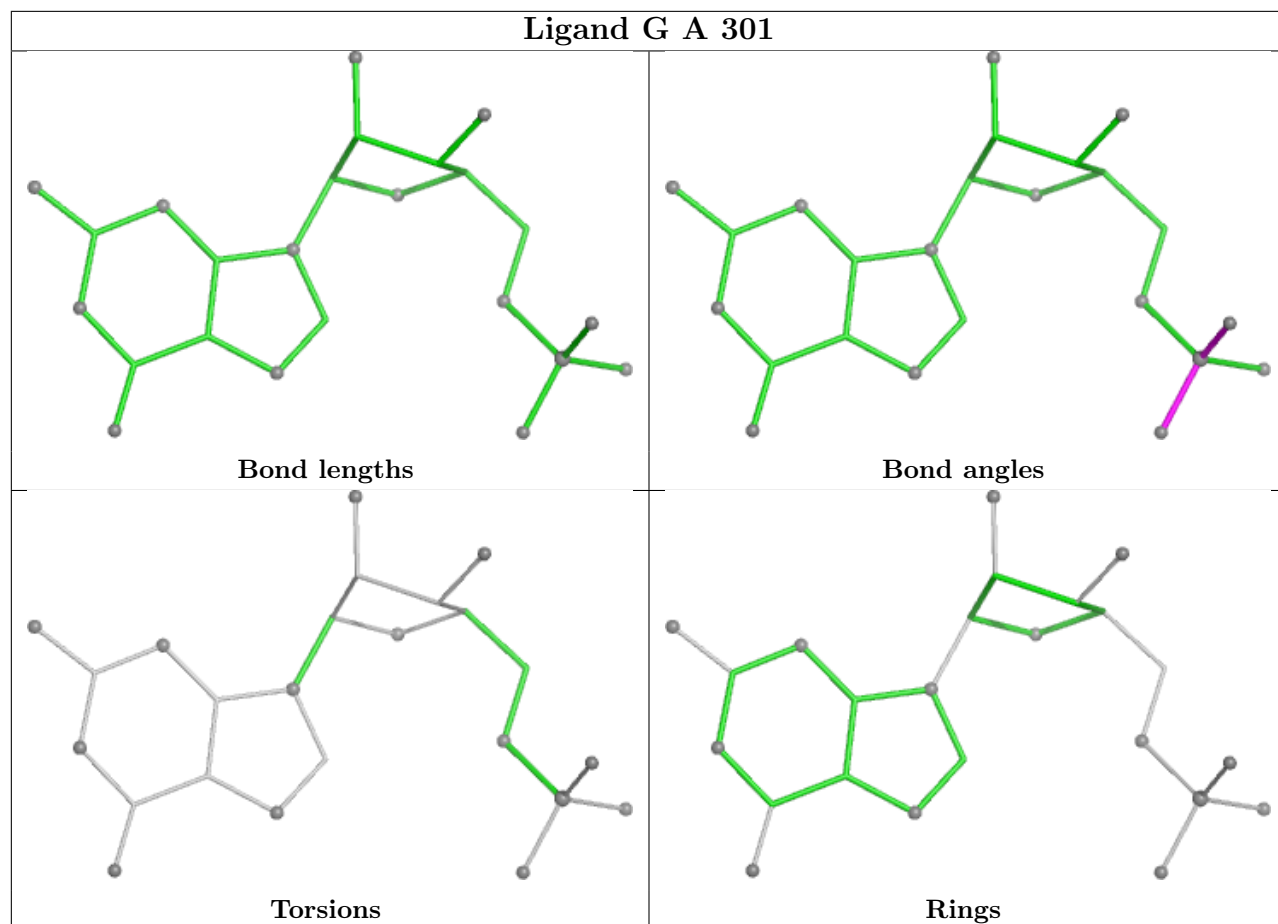




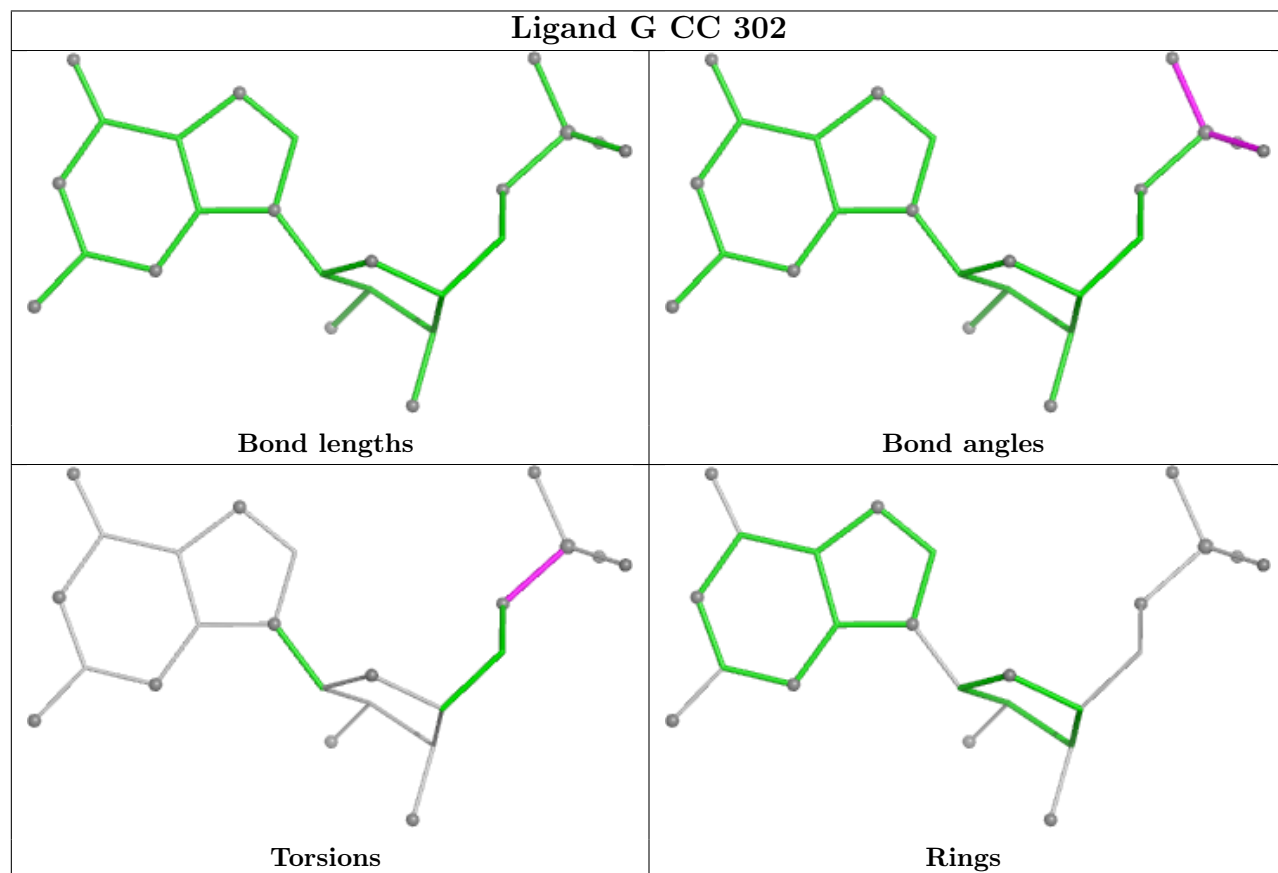
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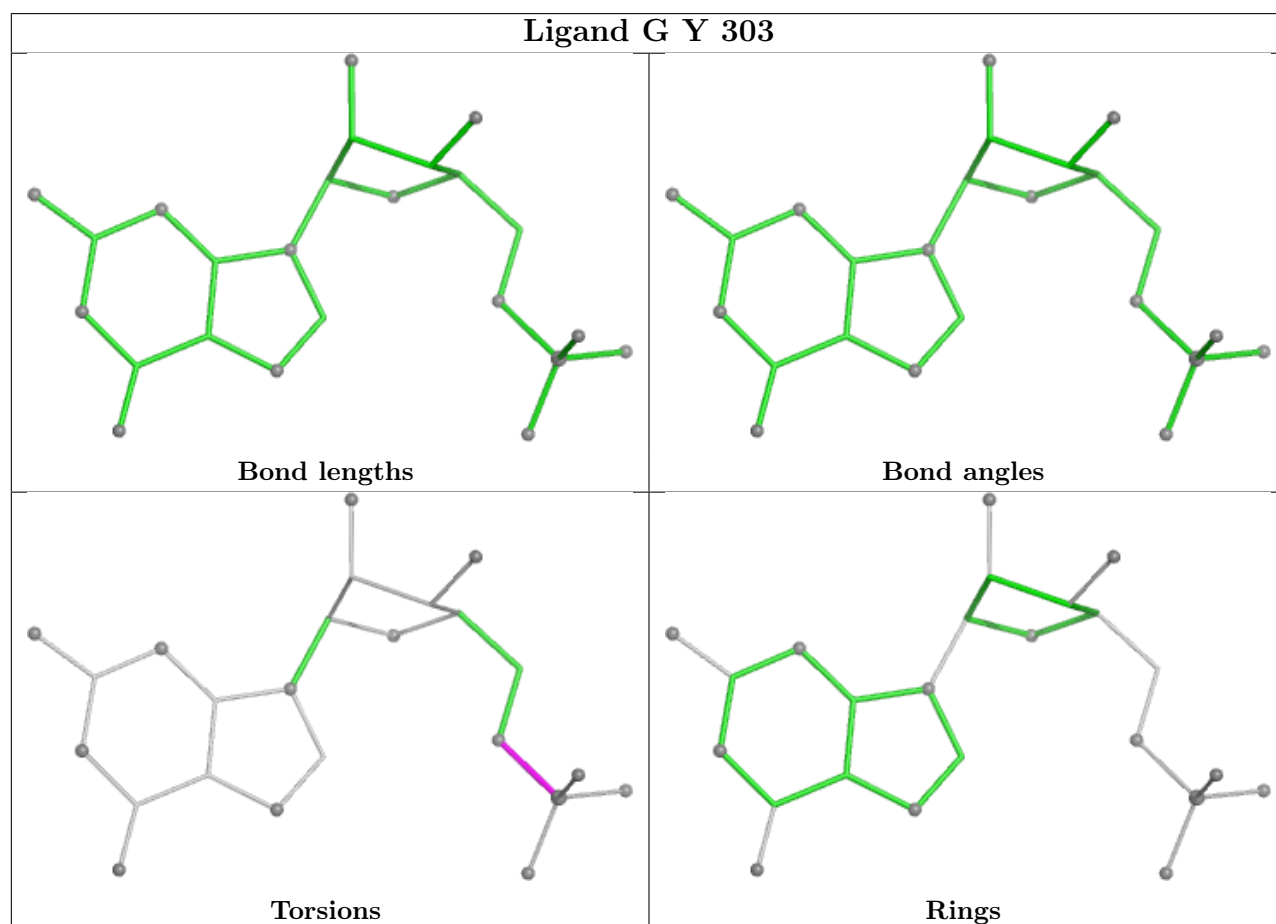
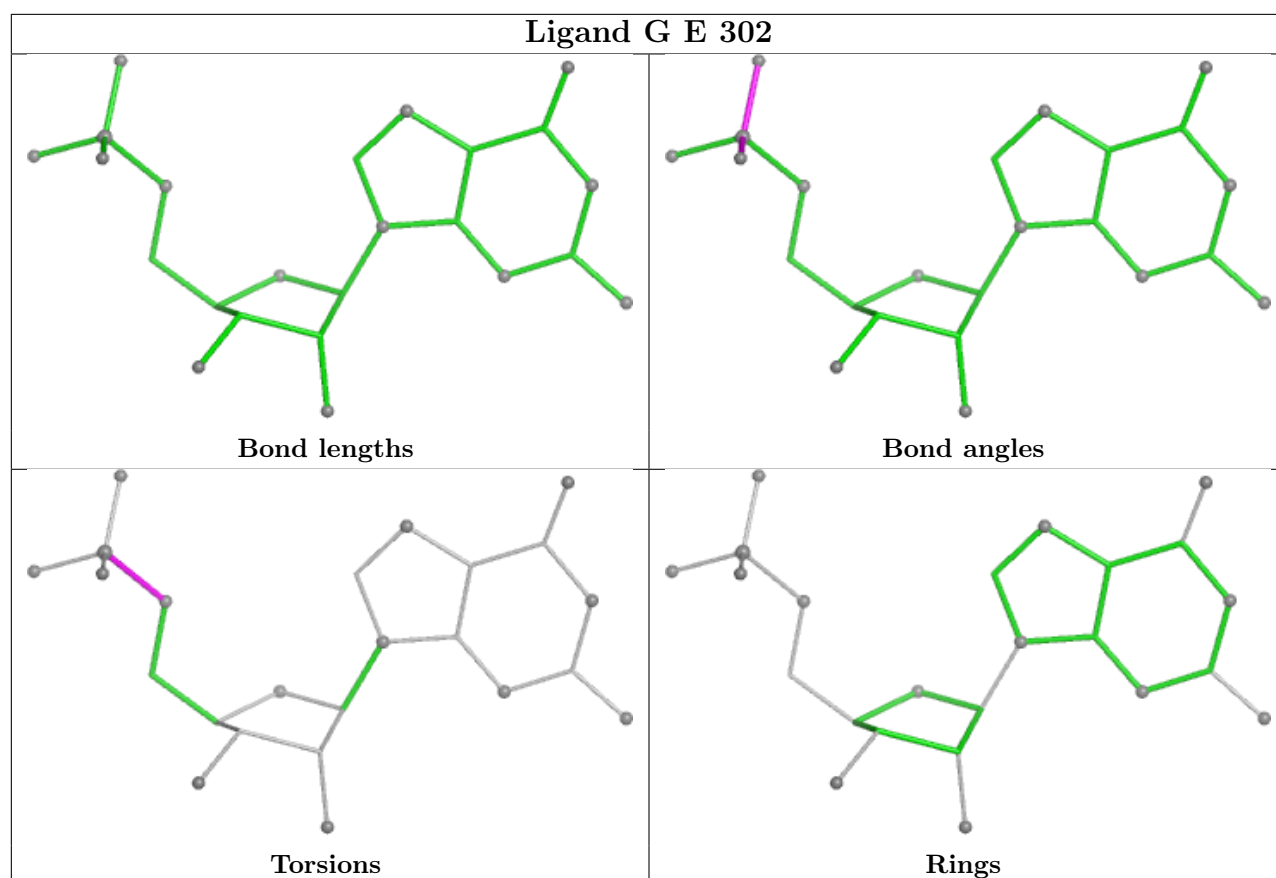


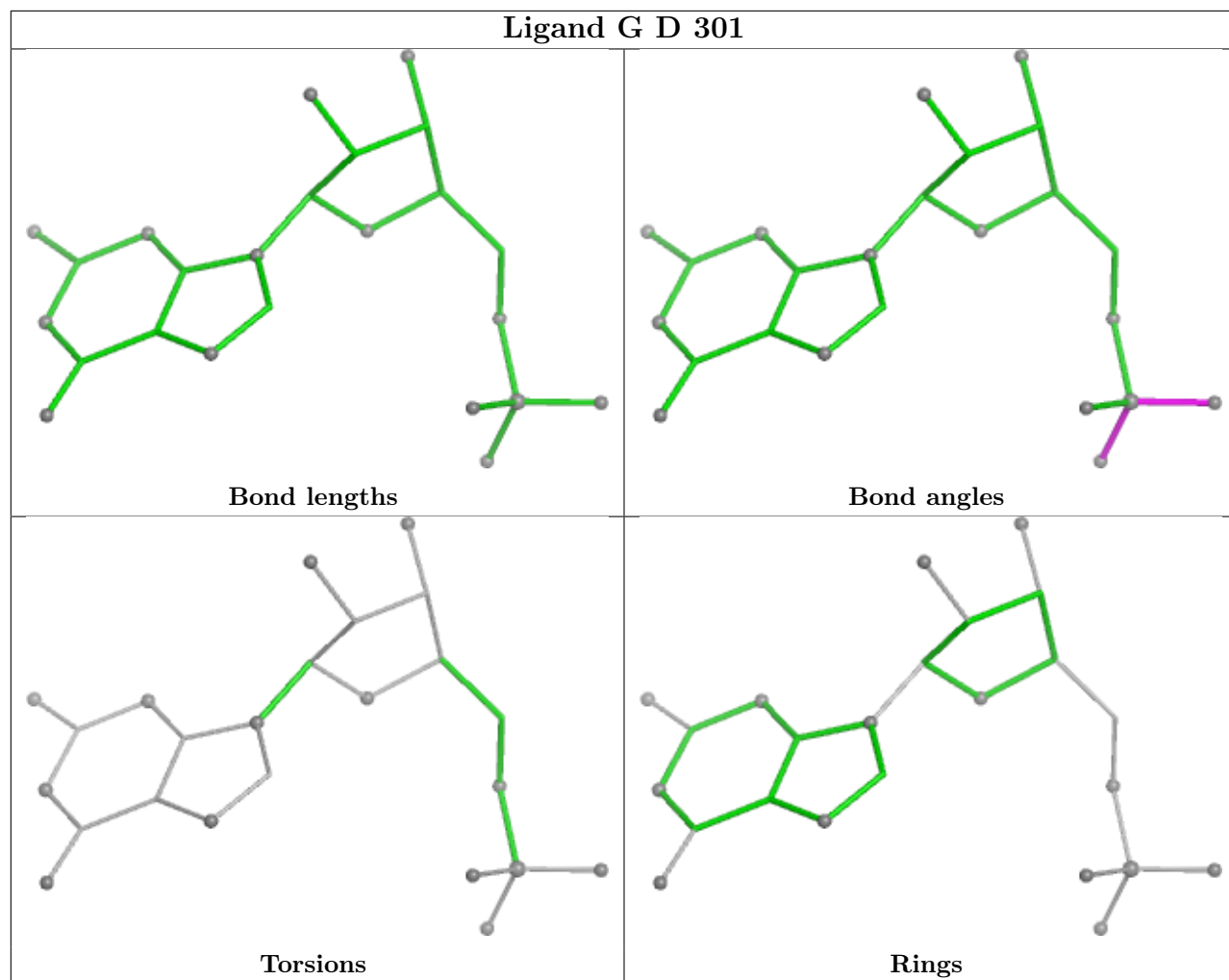
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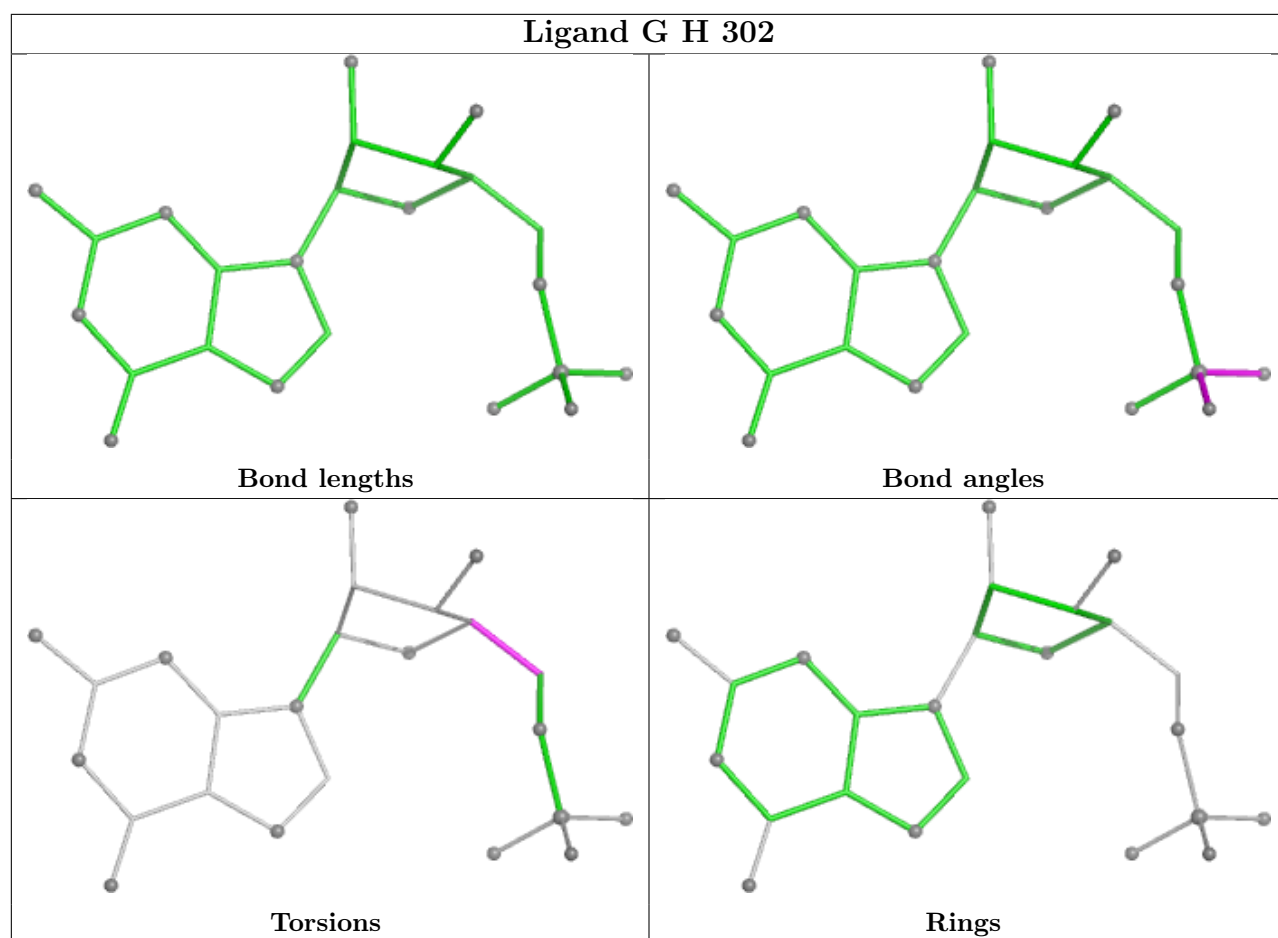


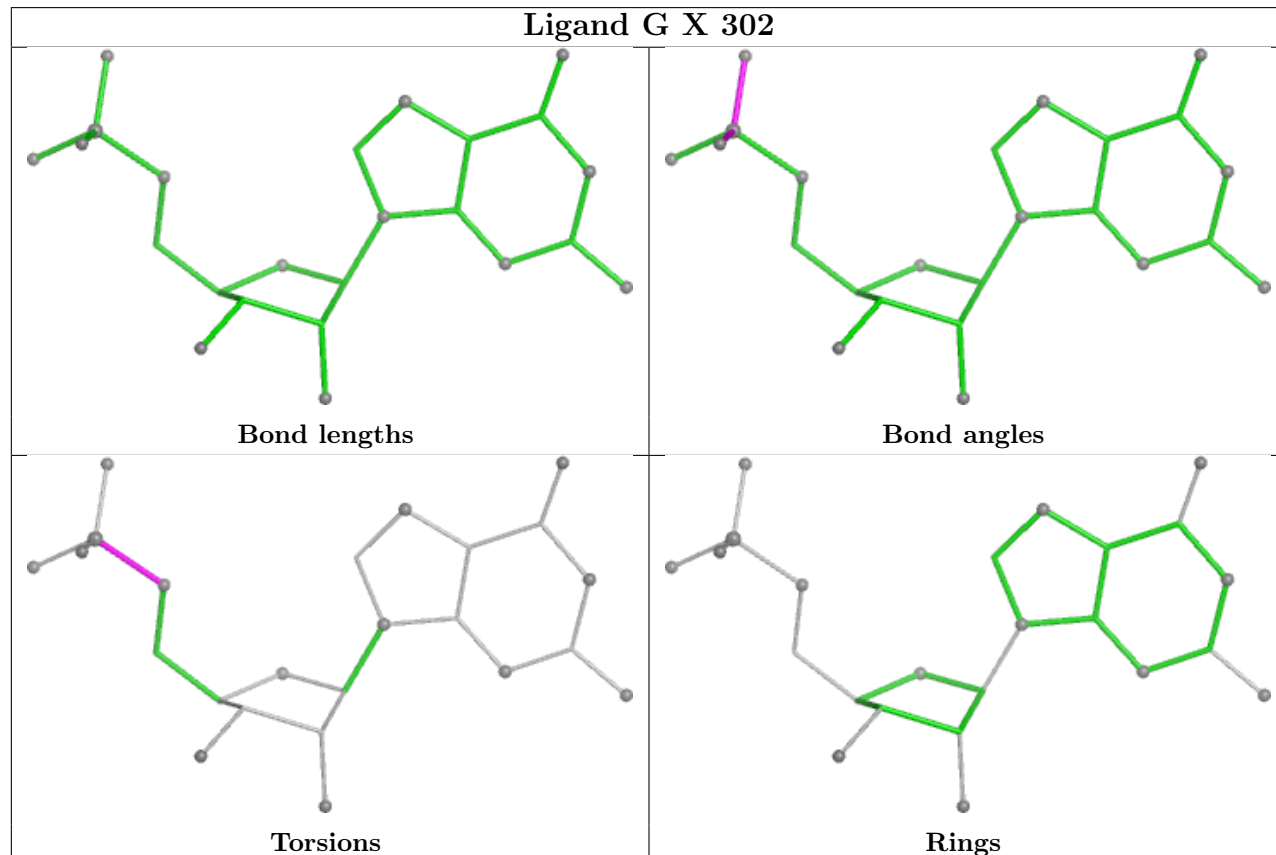
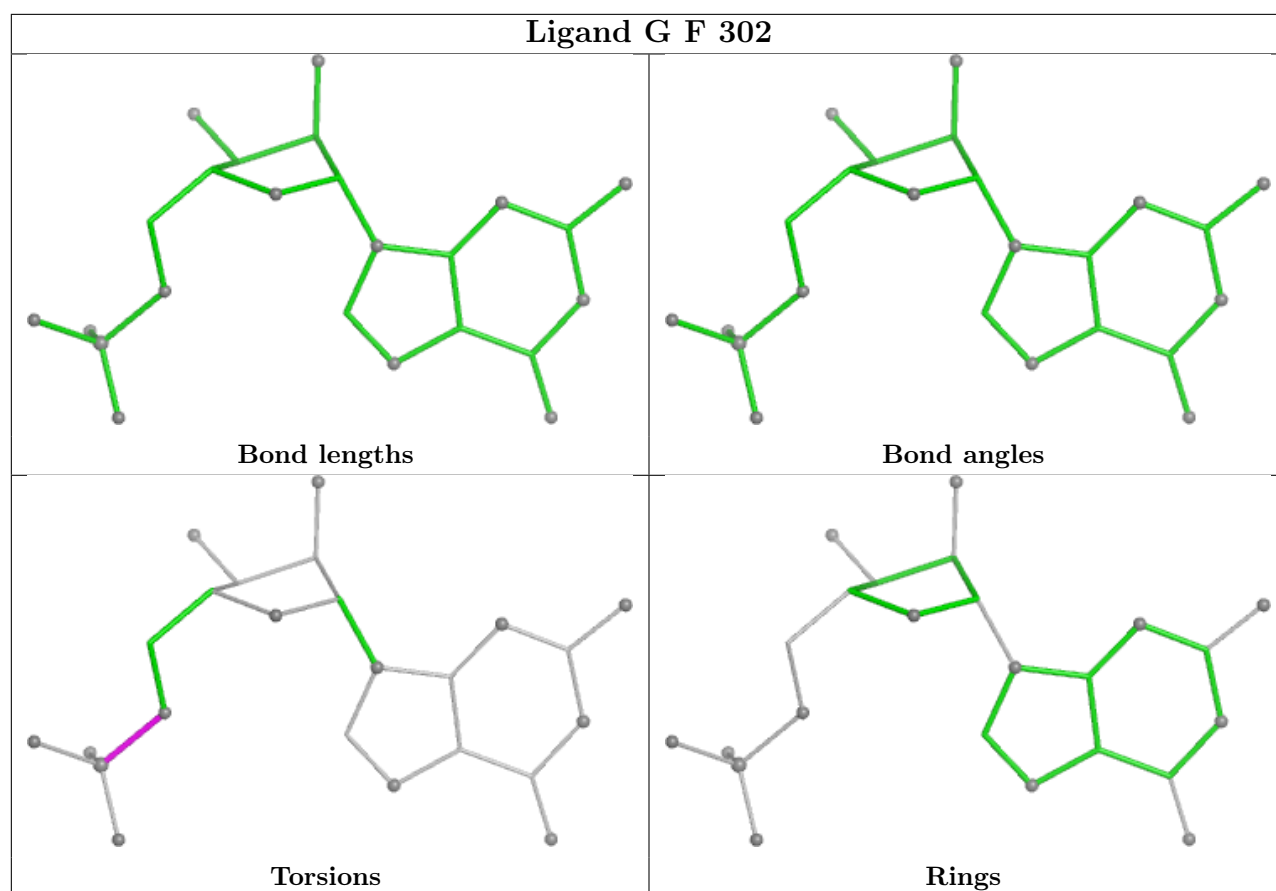
Ligand G CC 302

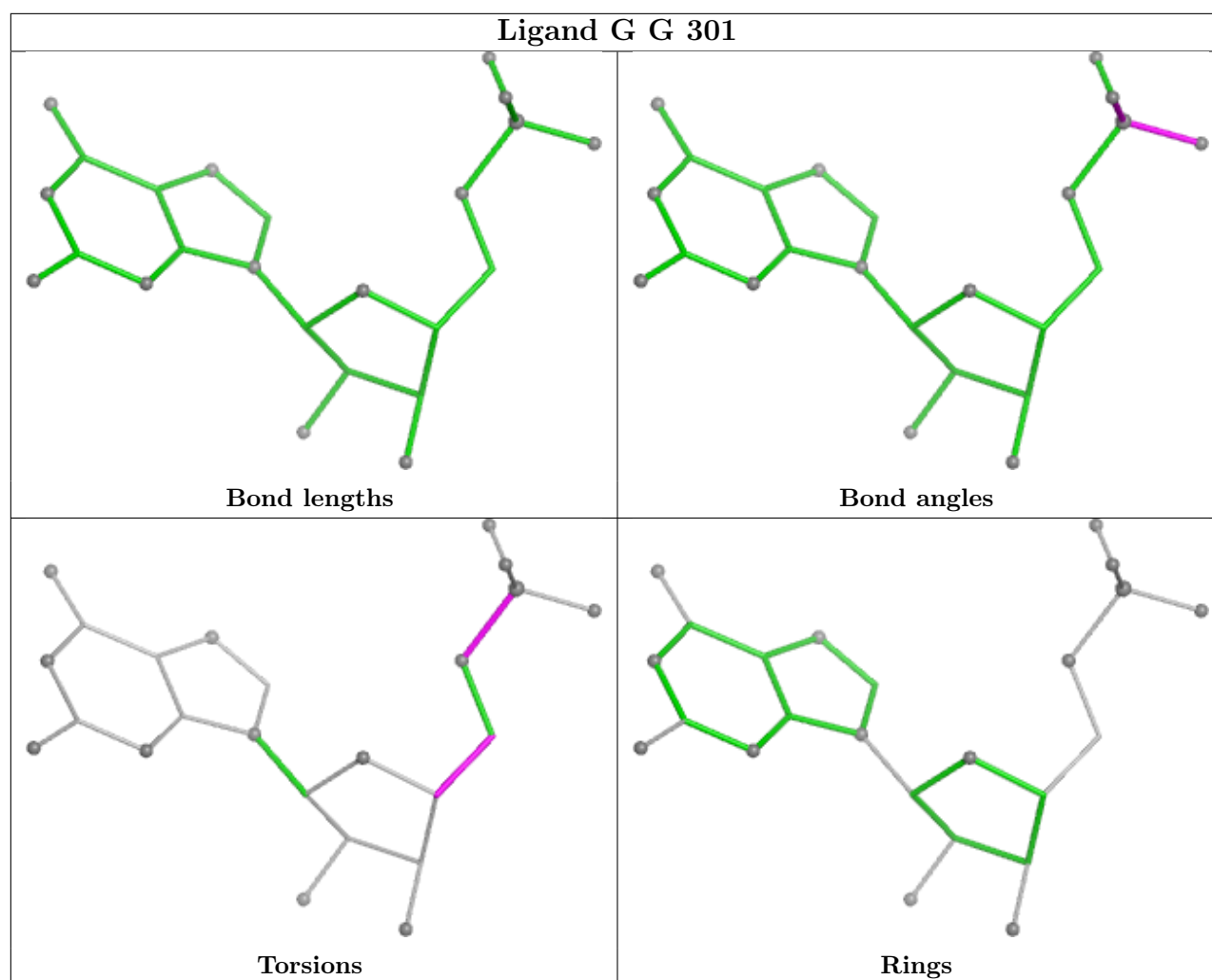


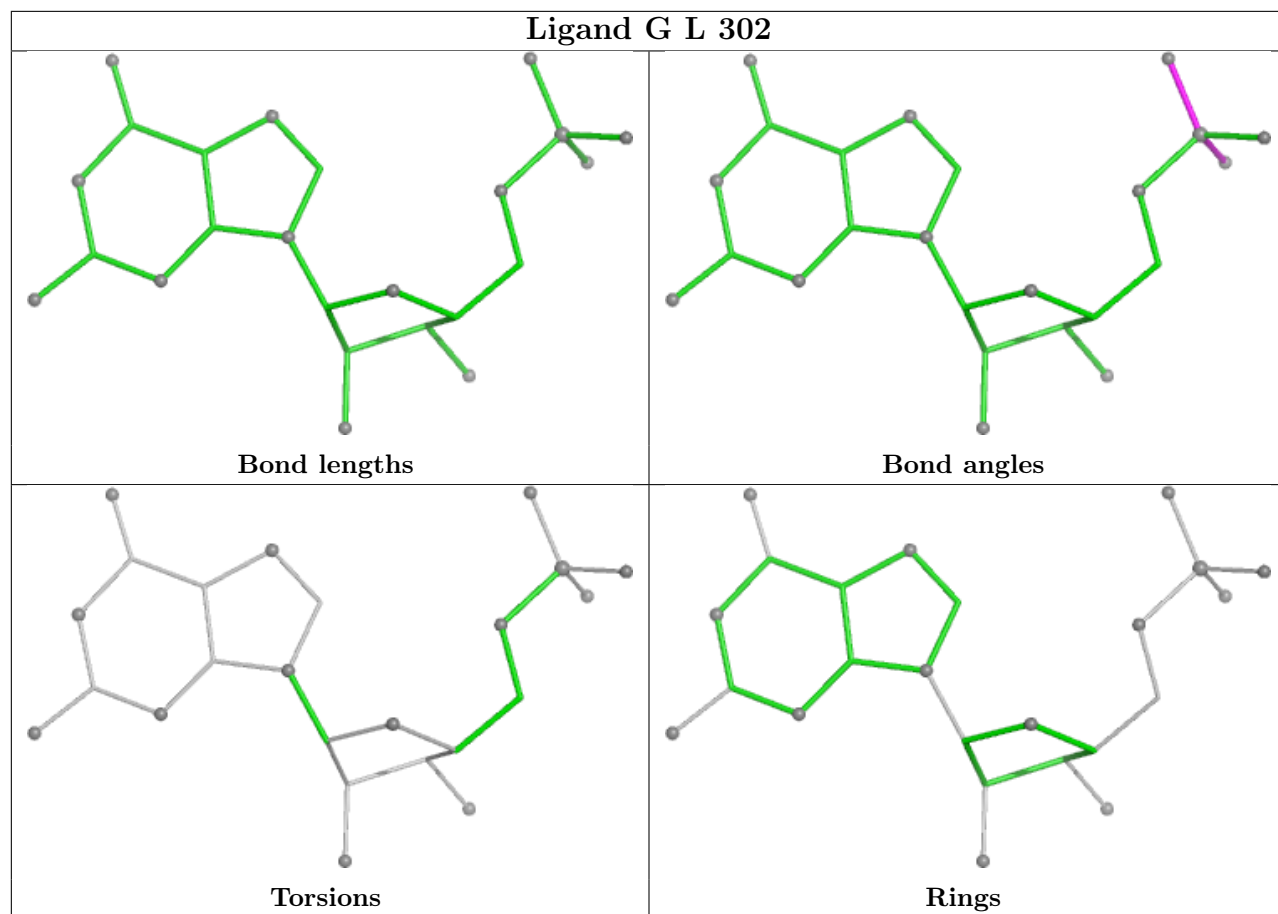


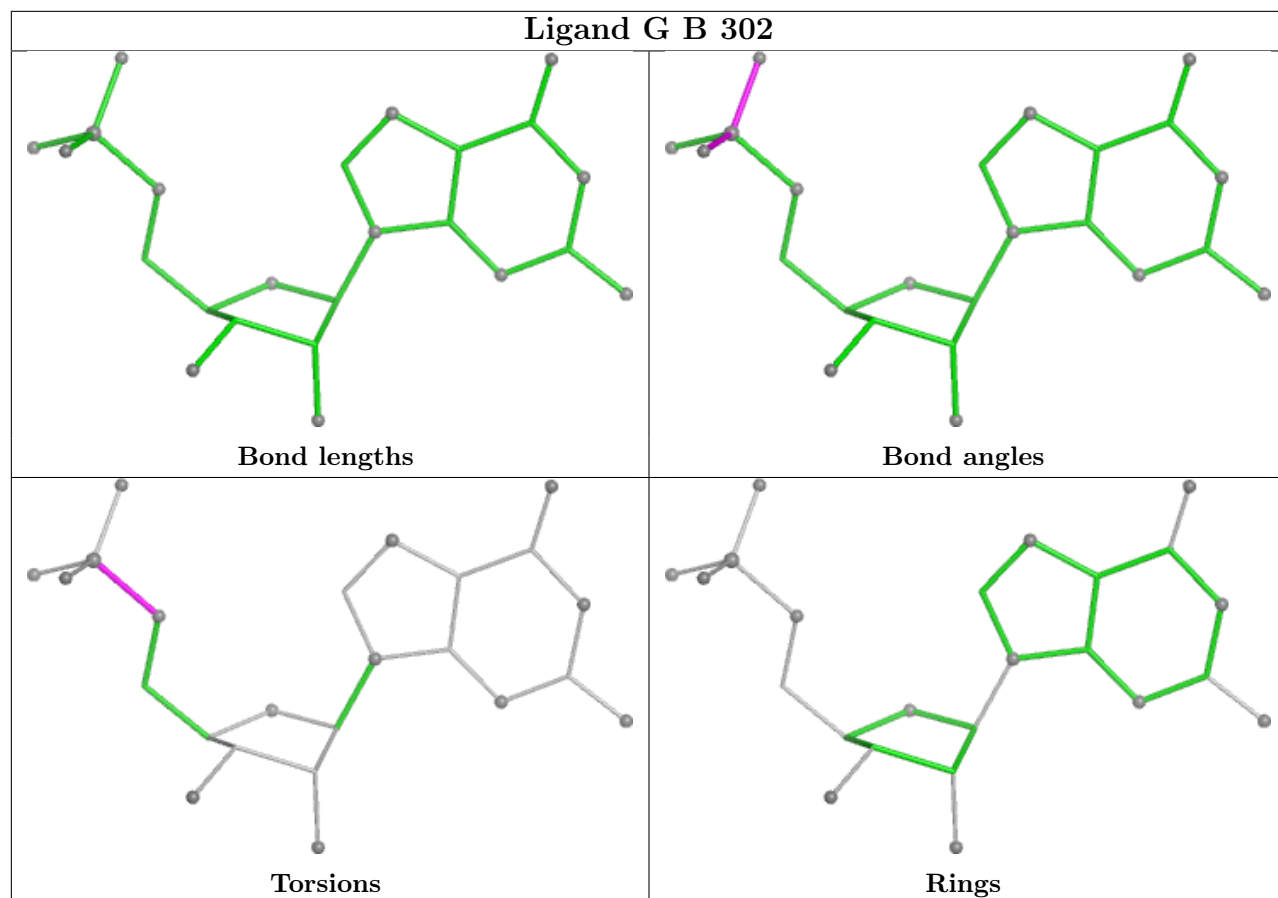


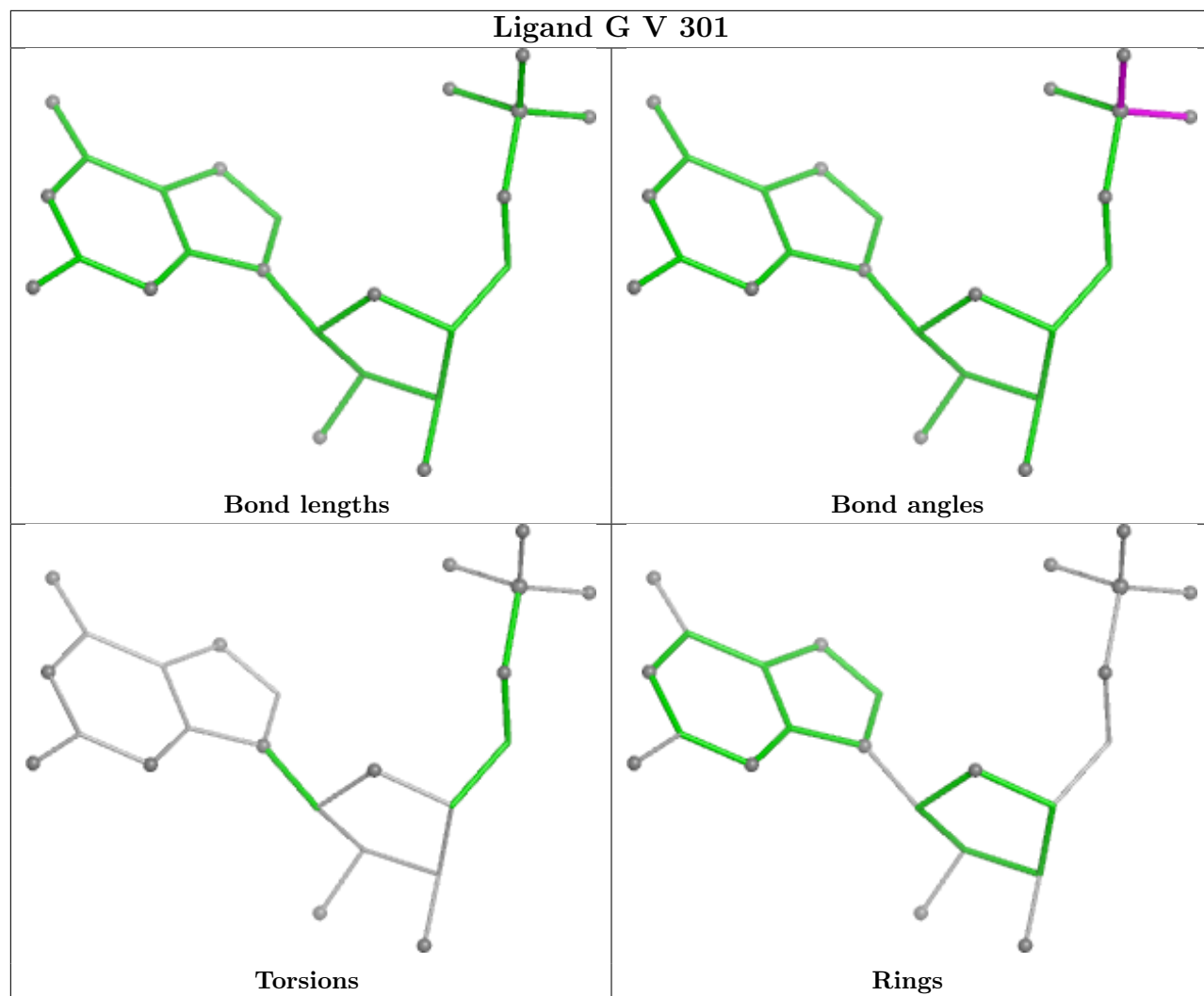


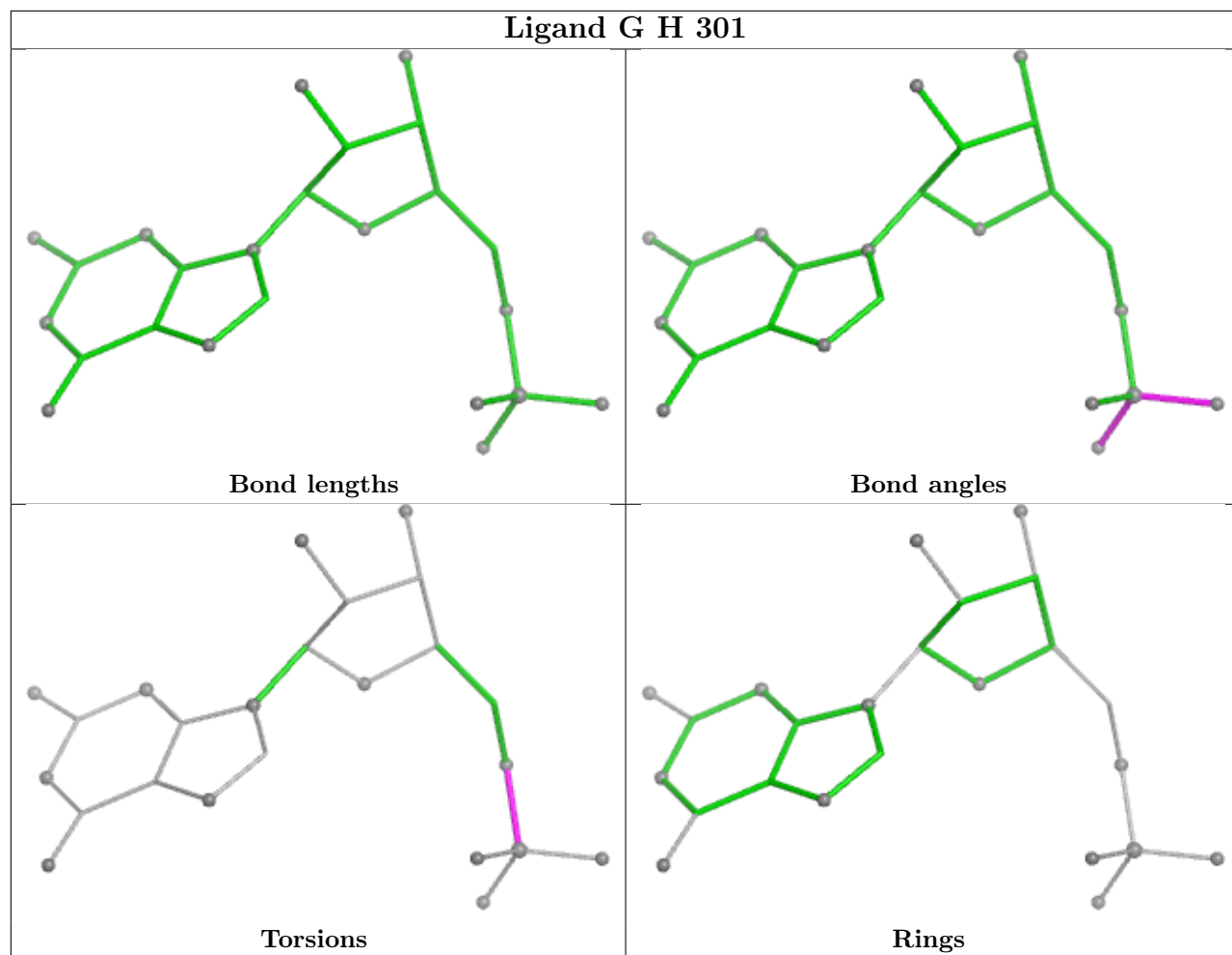




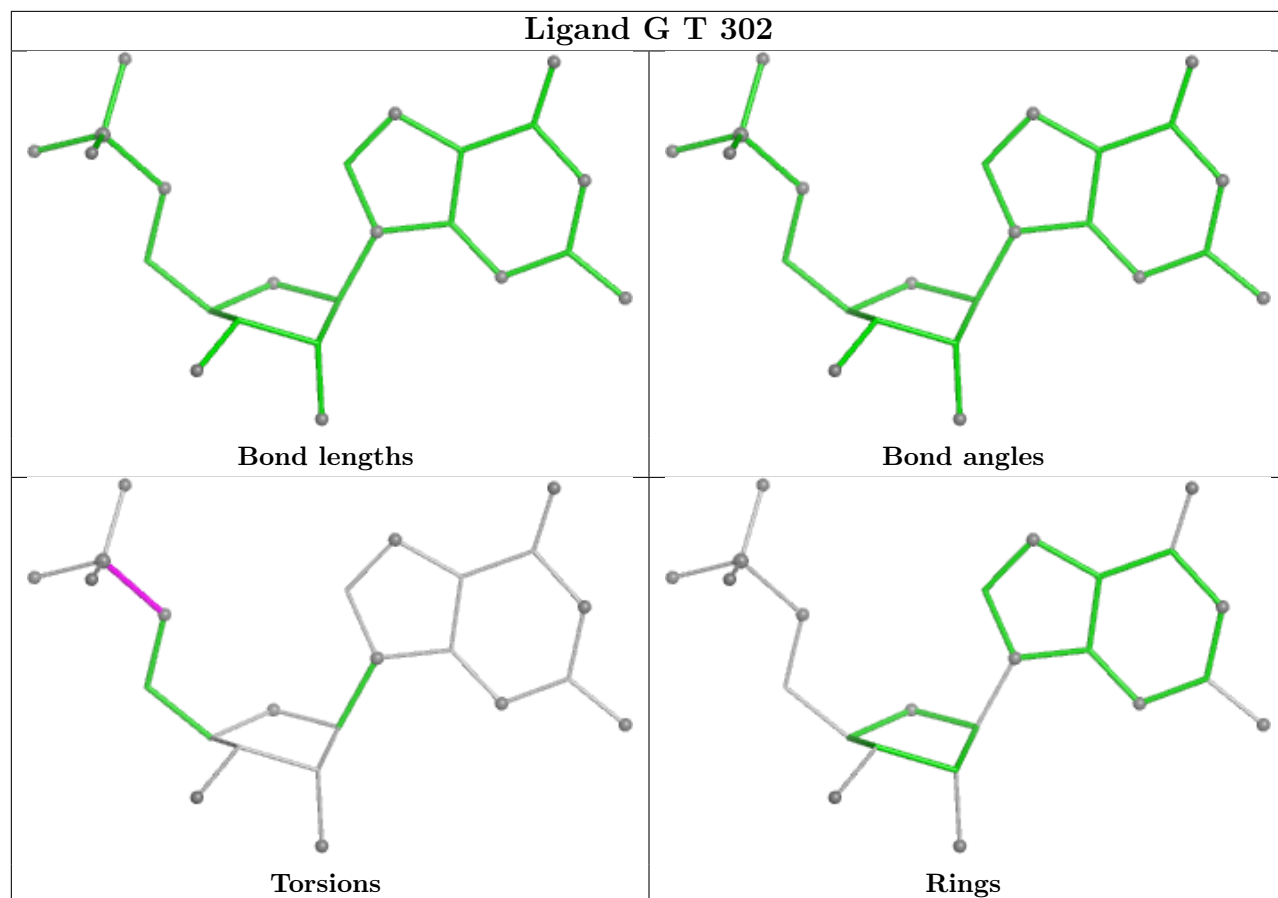




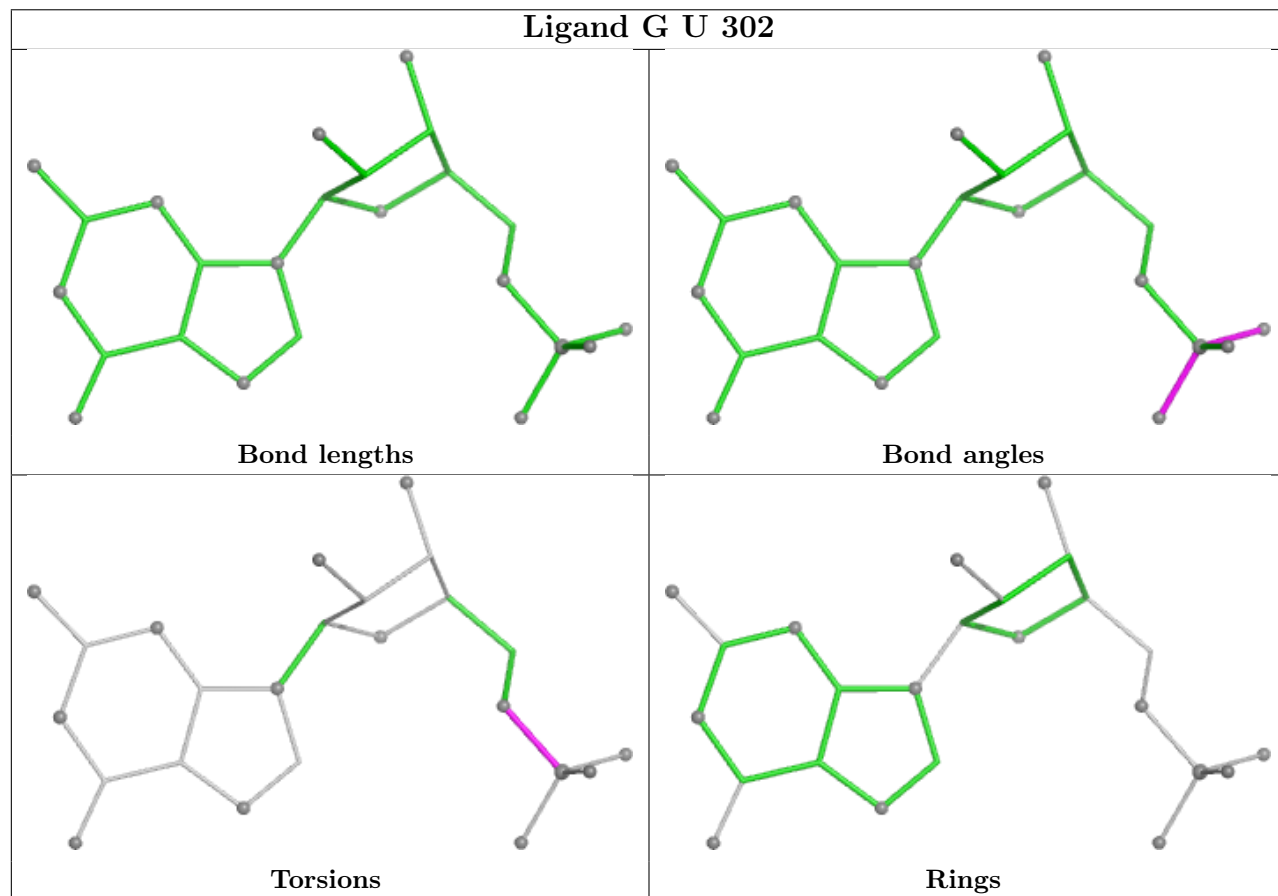


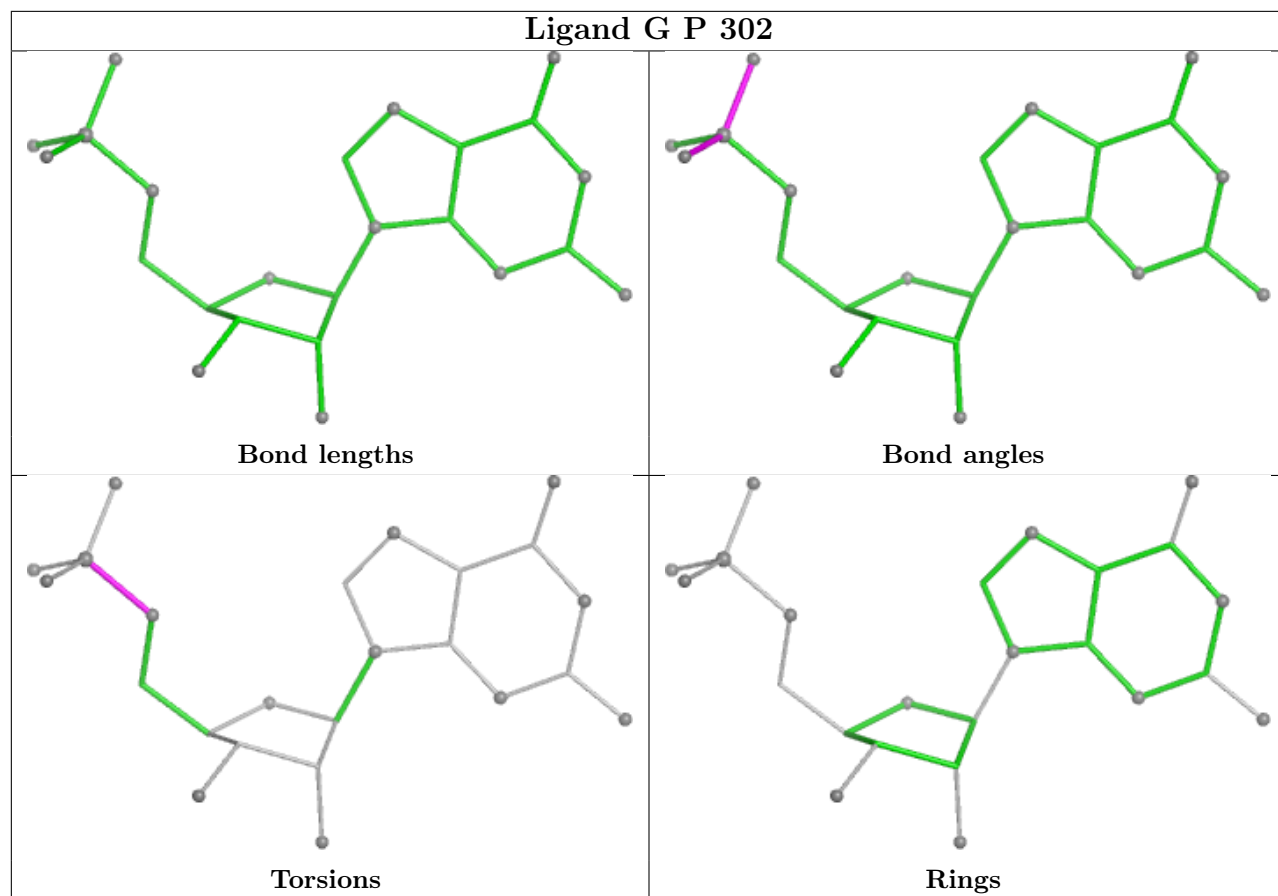


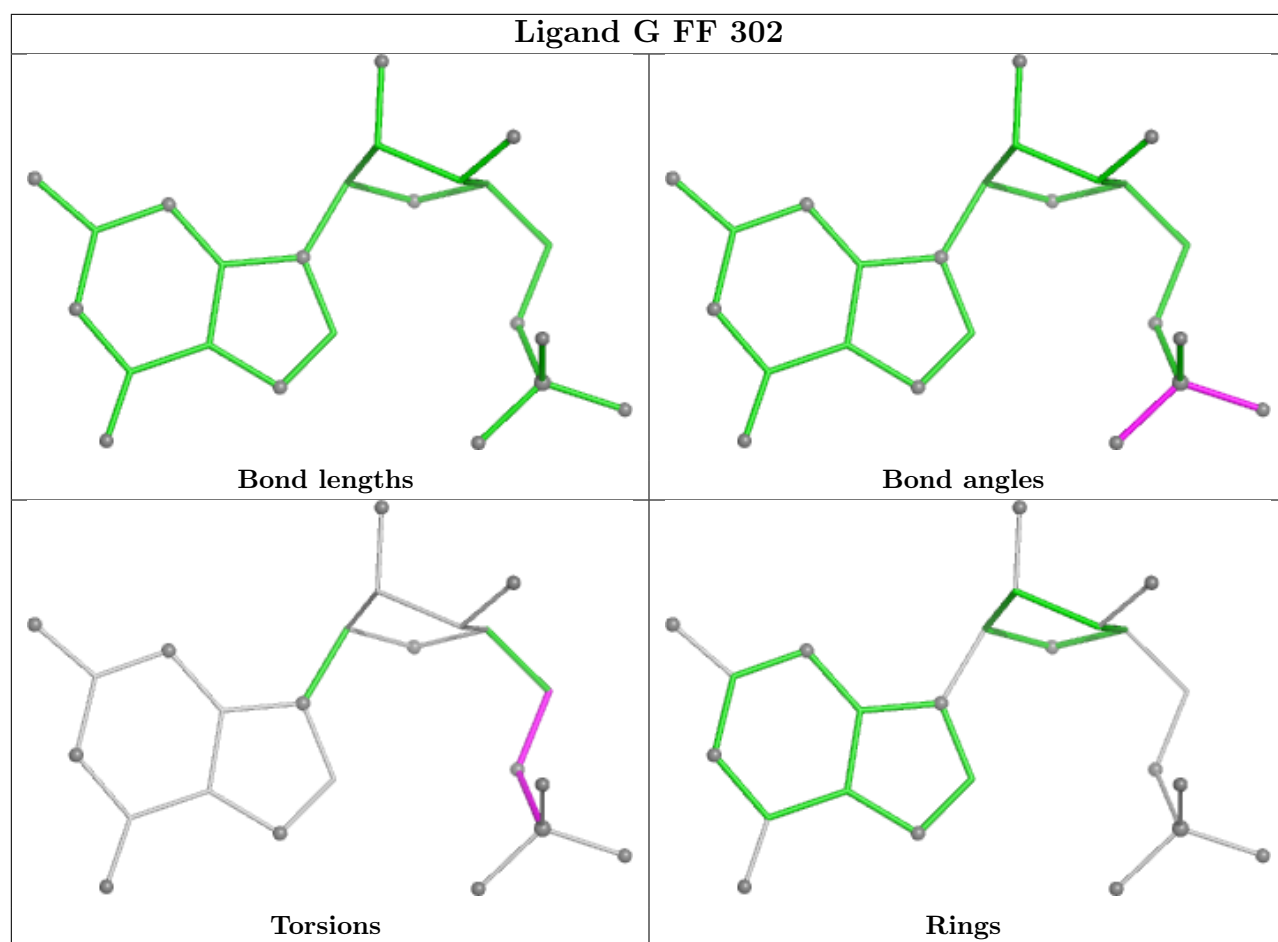
Ligand G T 302

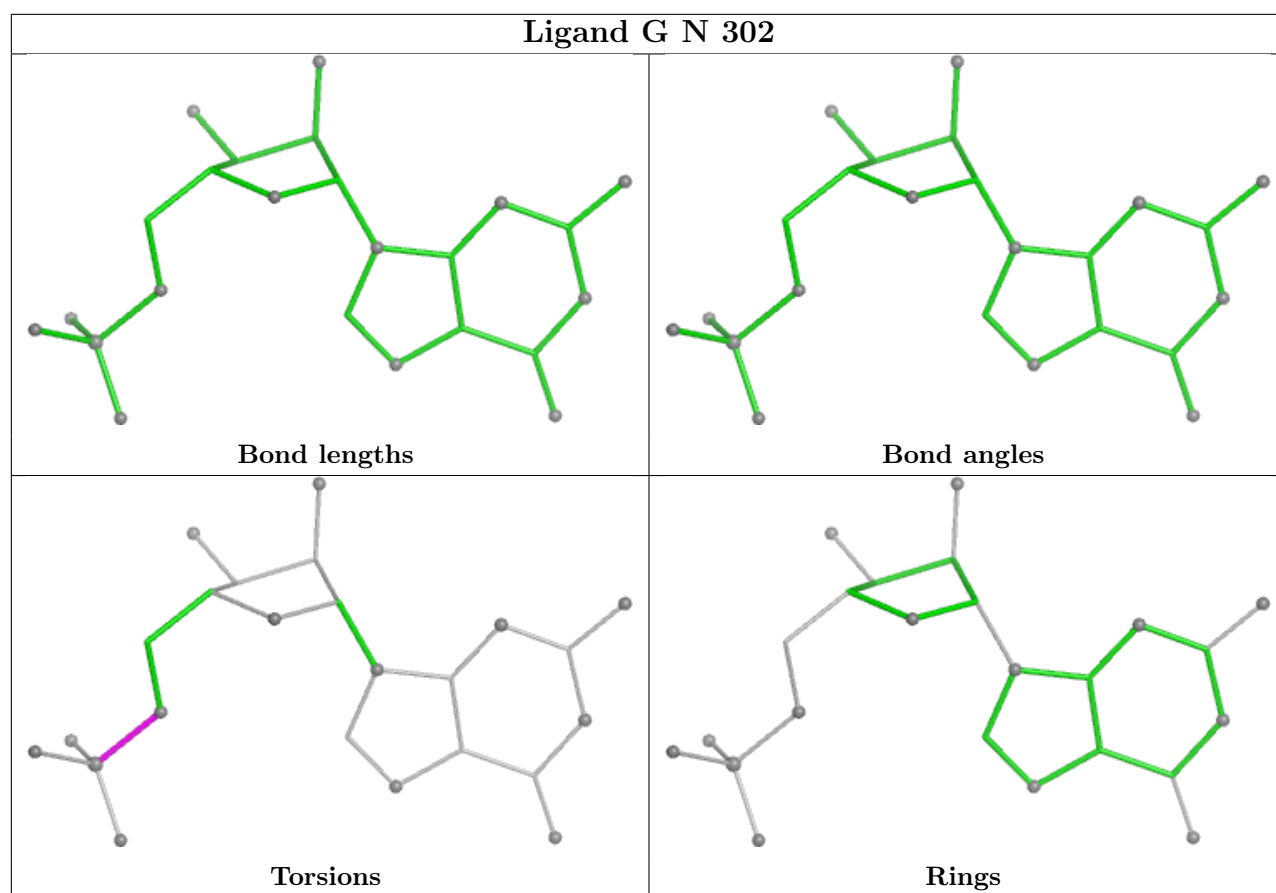


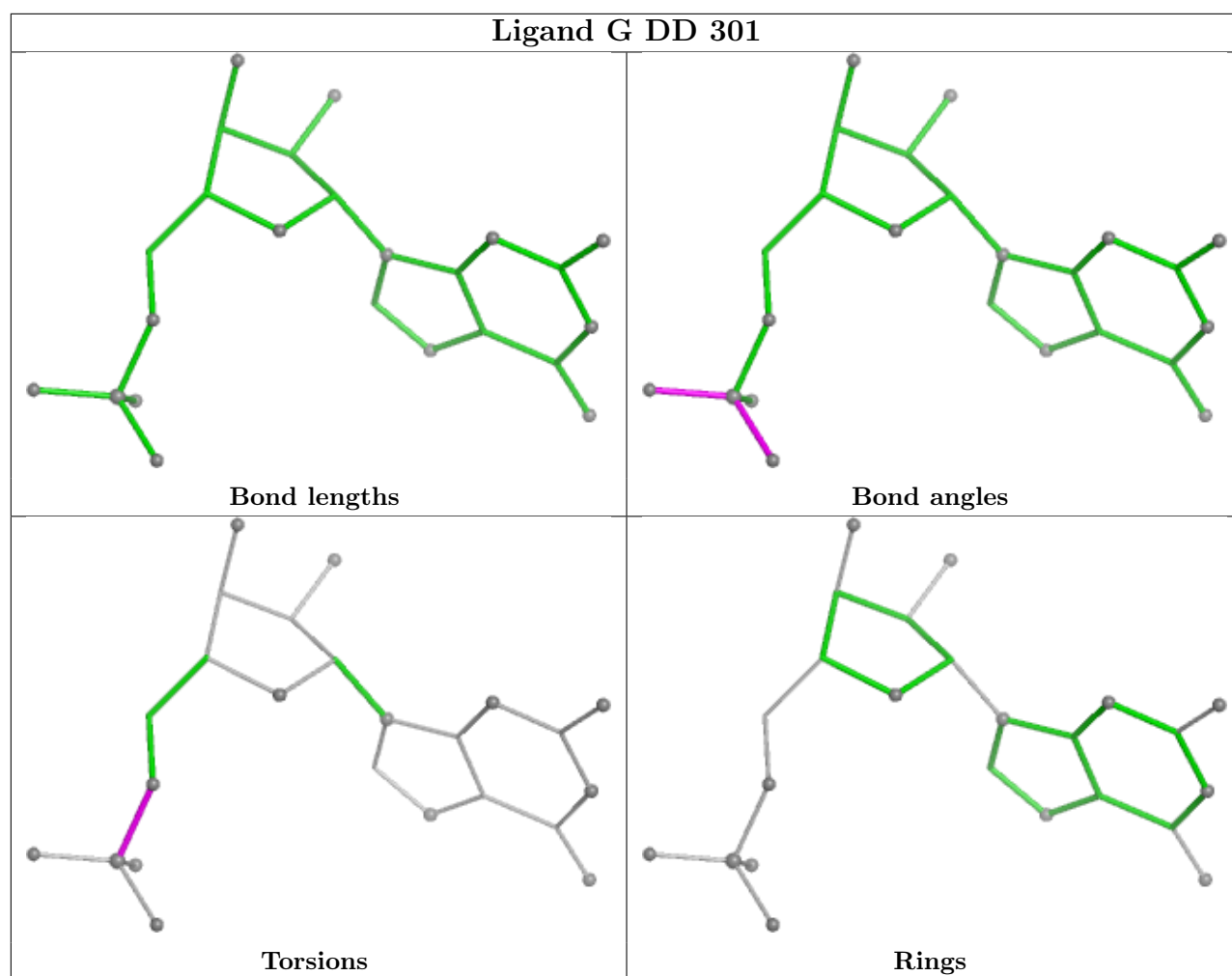
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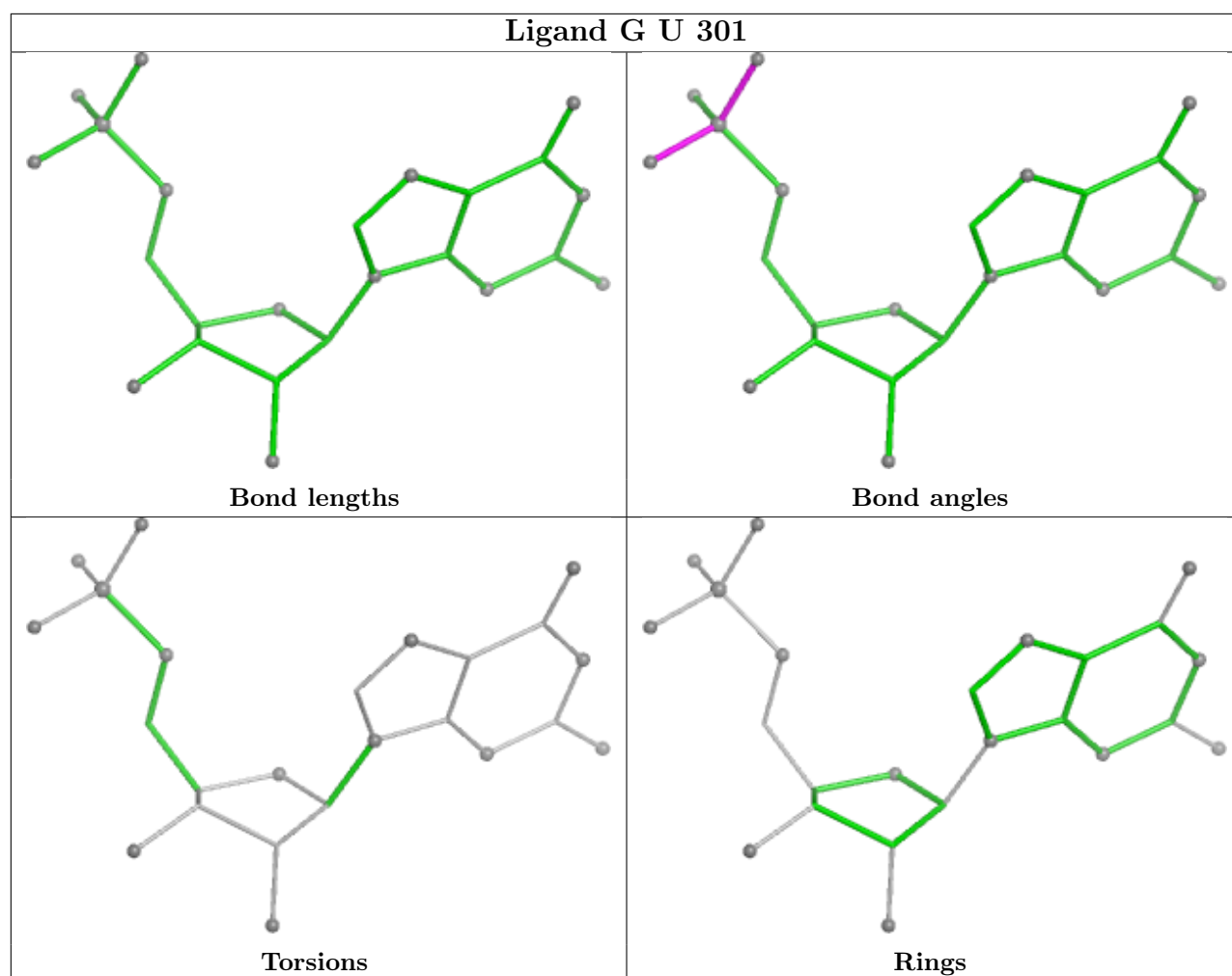


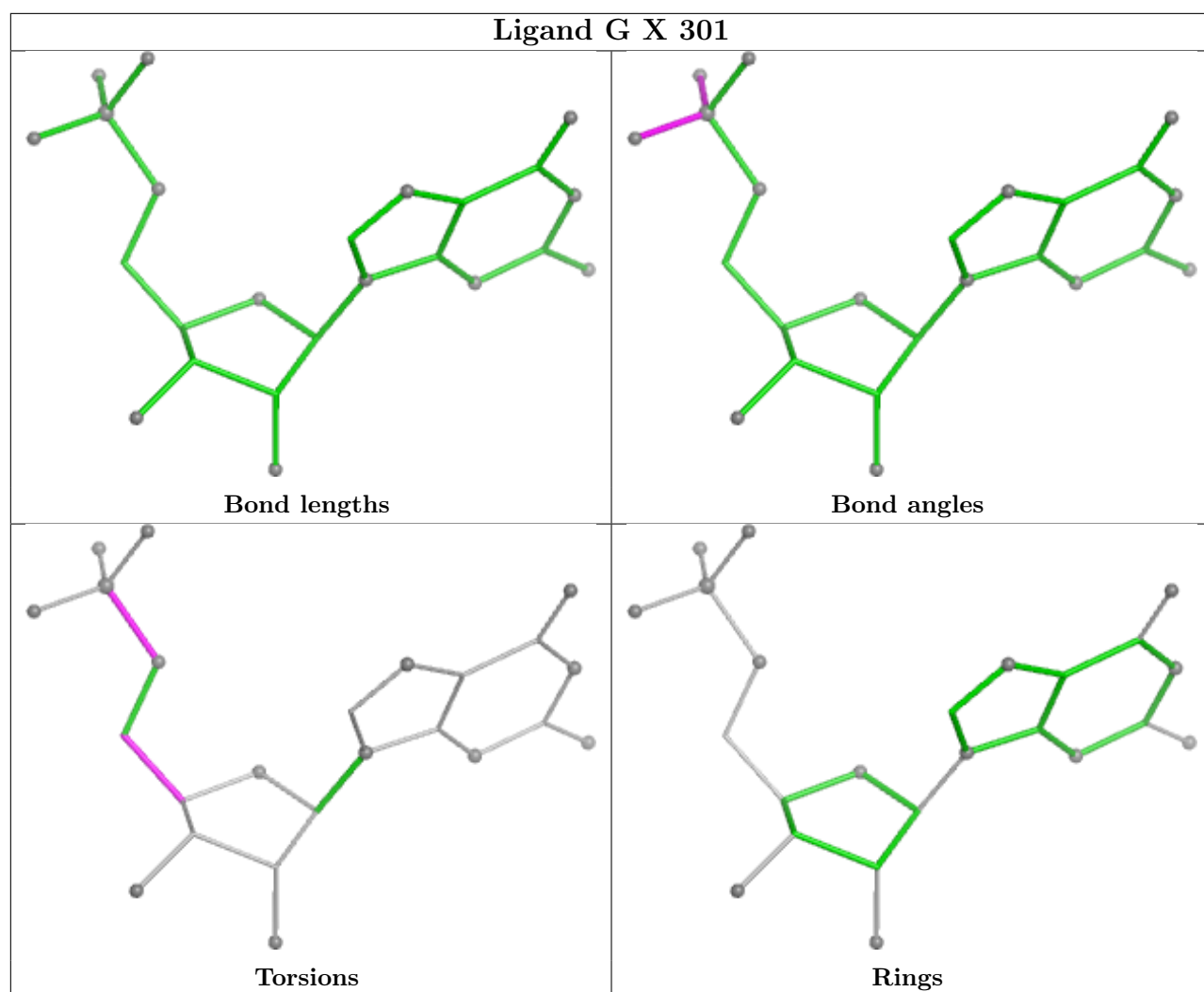


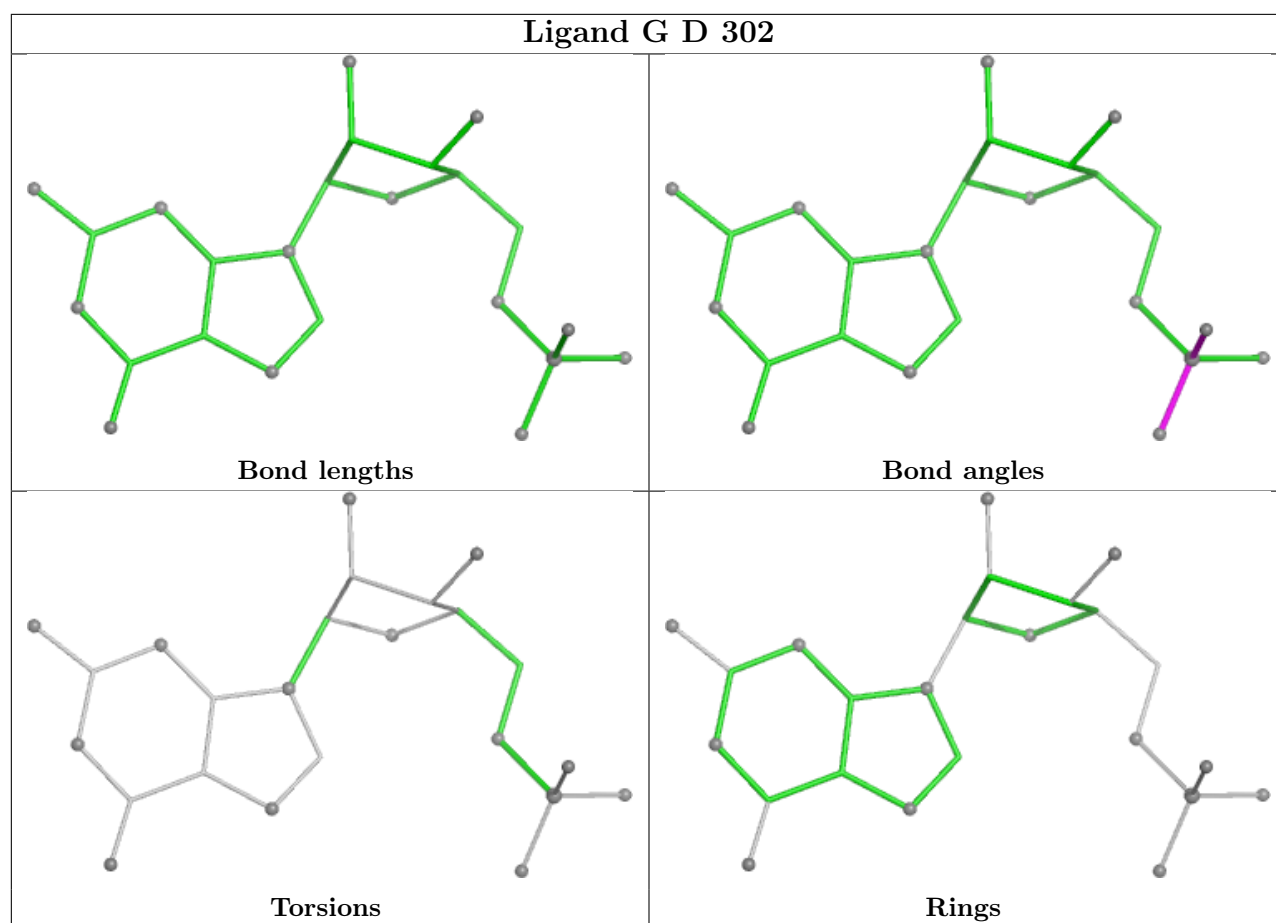


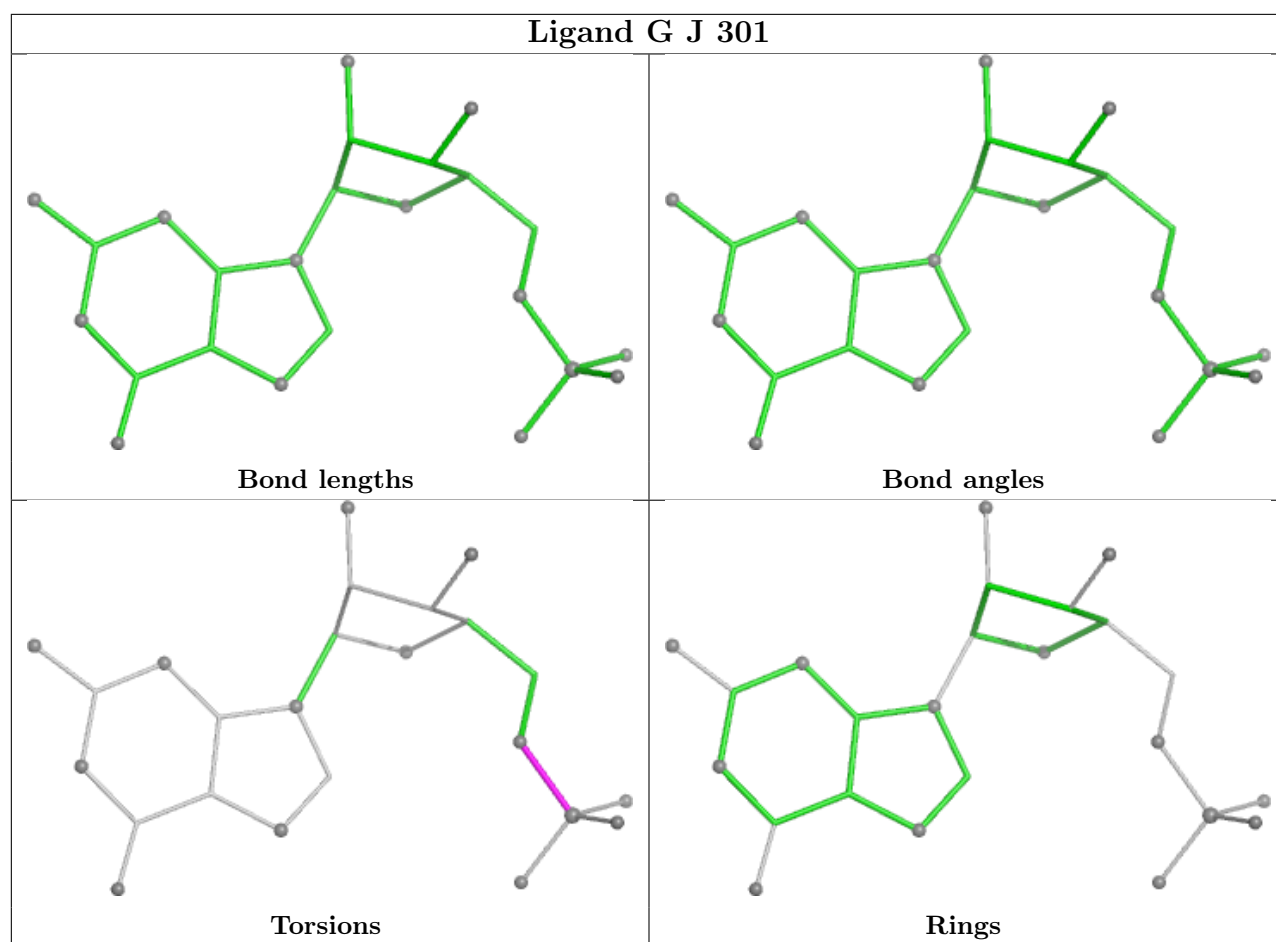


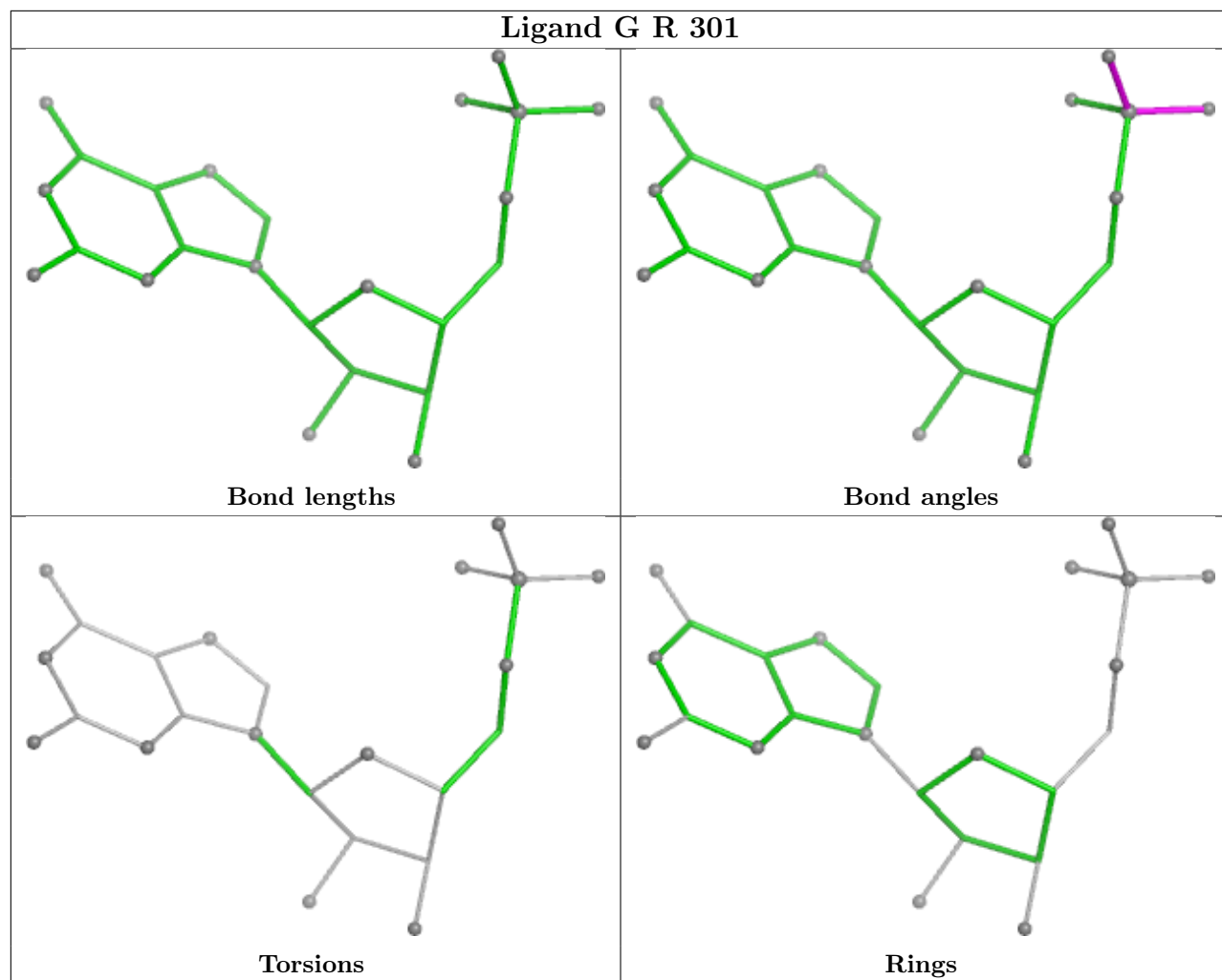


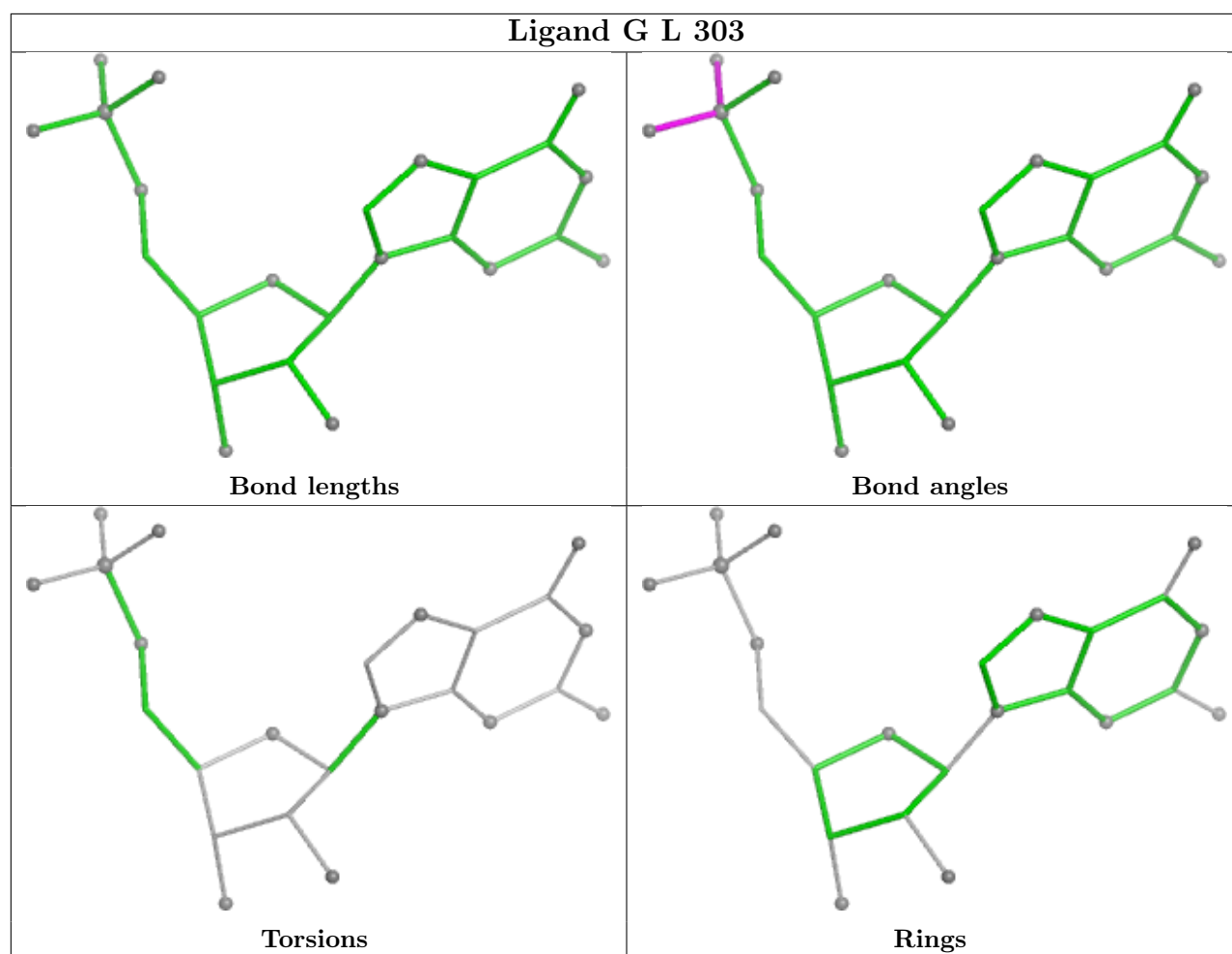


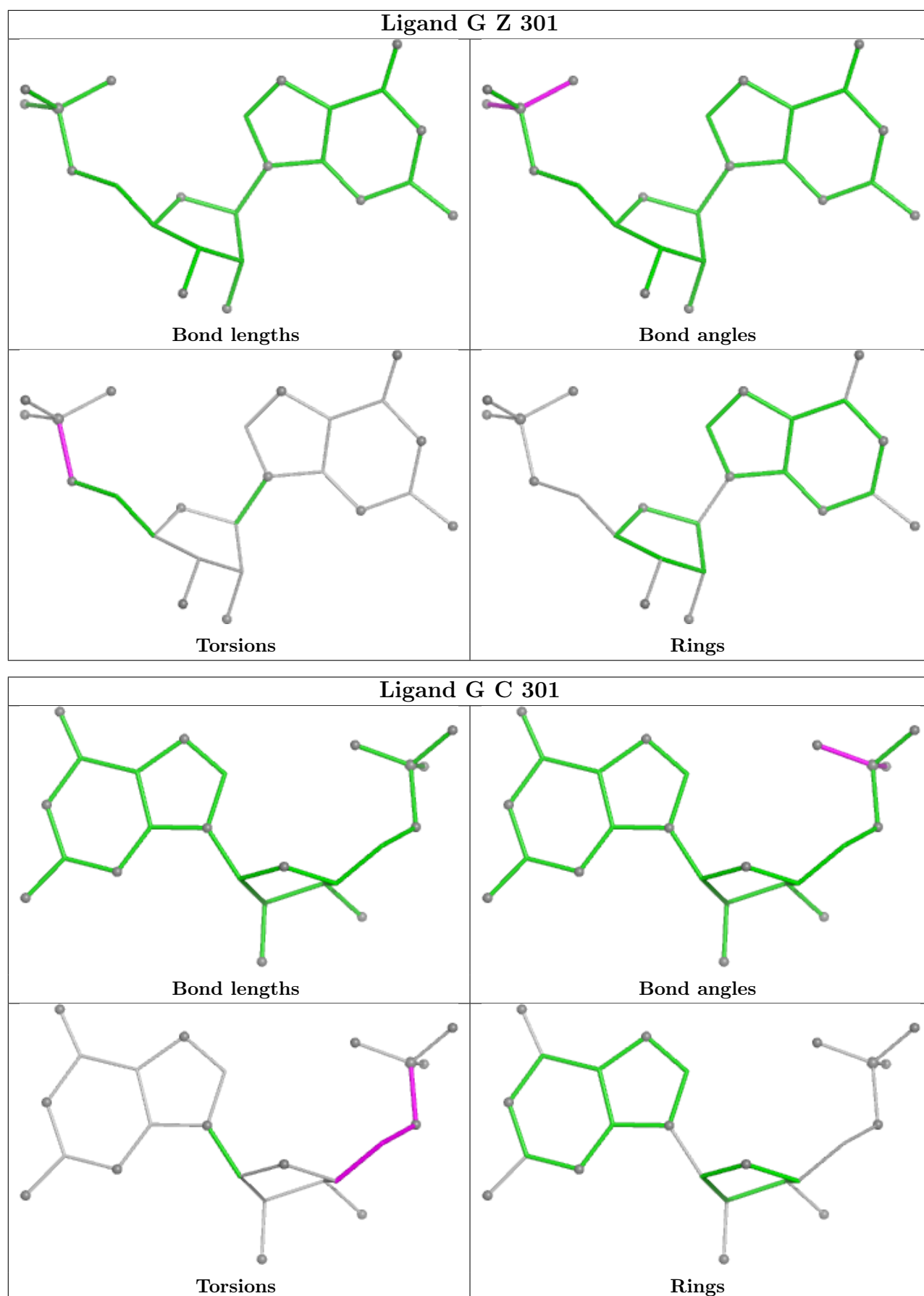


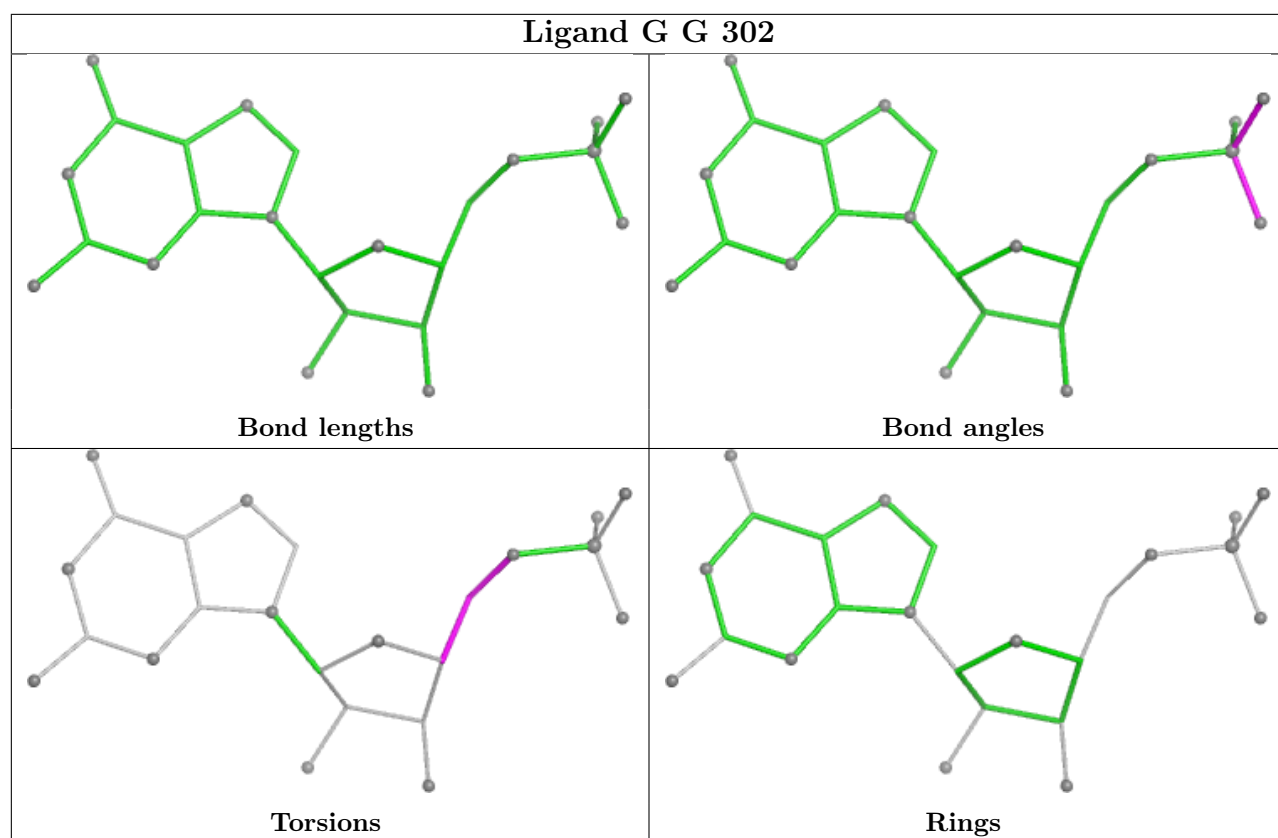


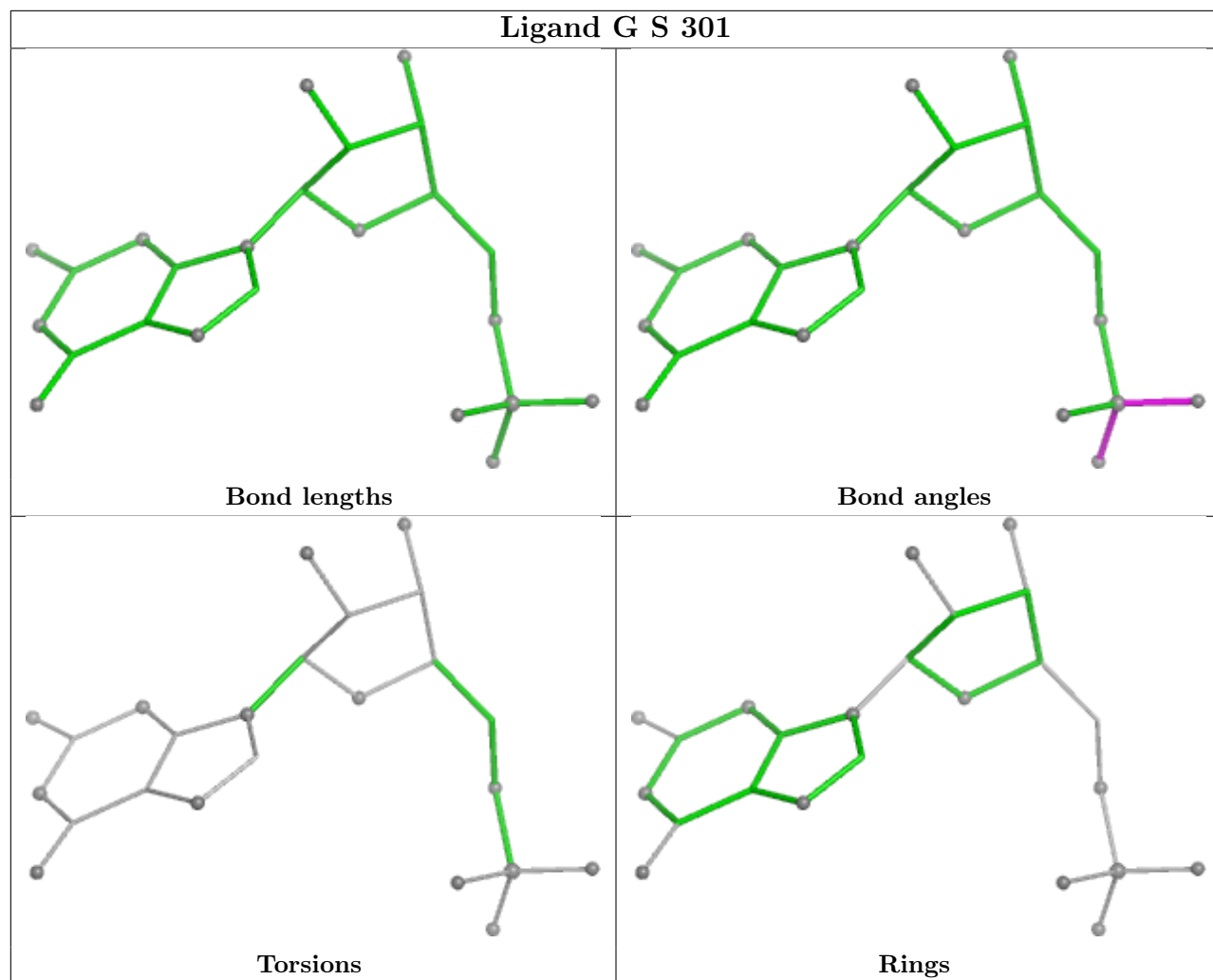


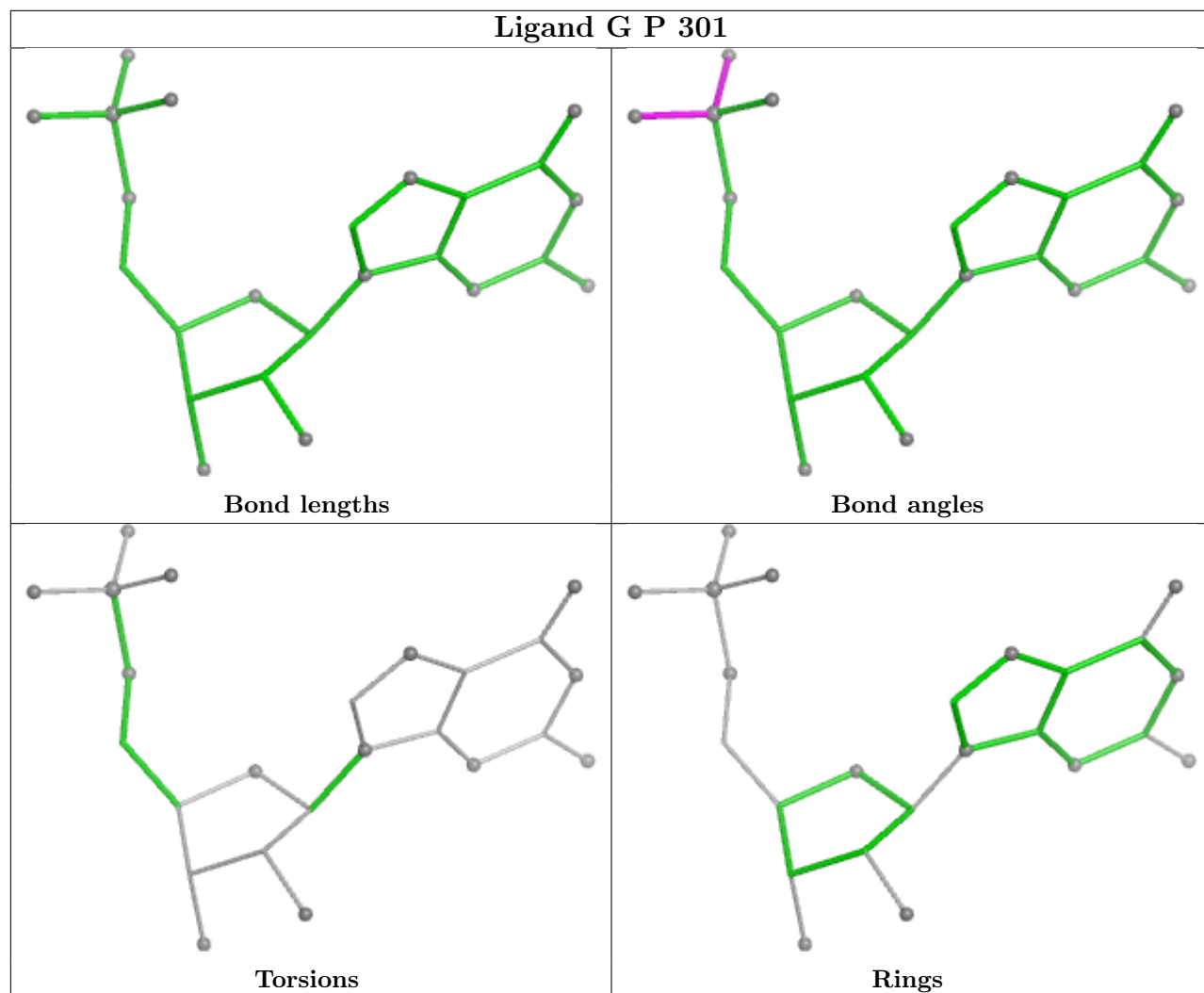


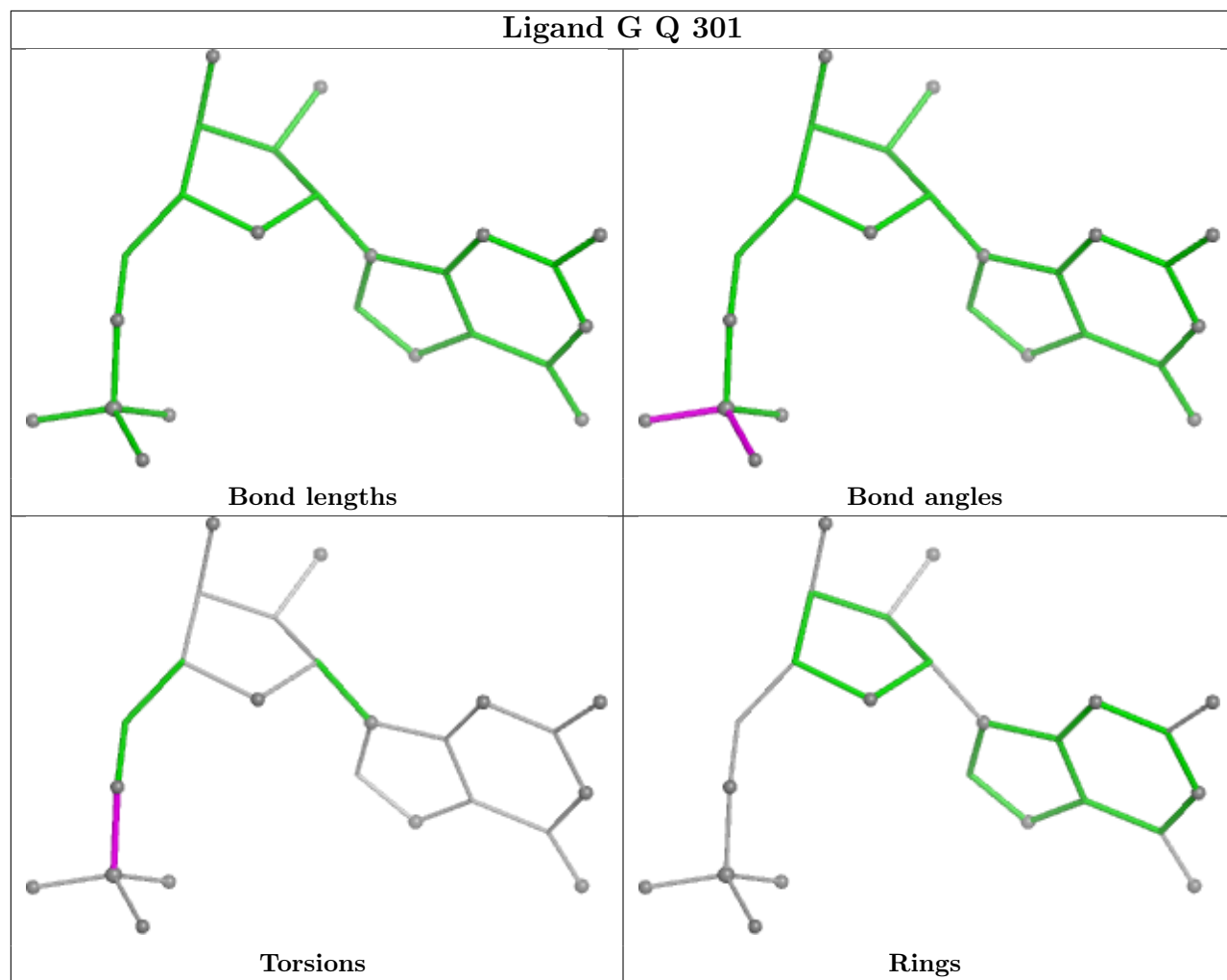


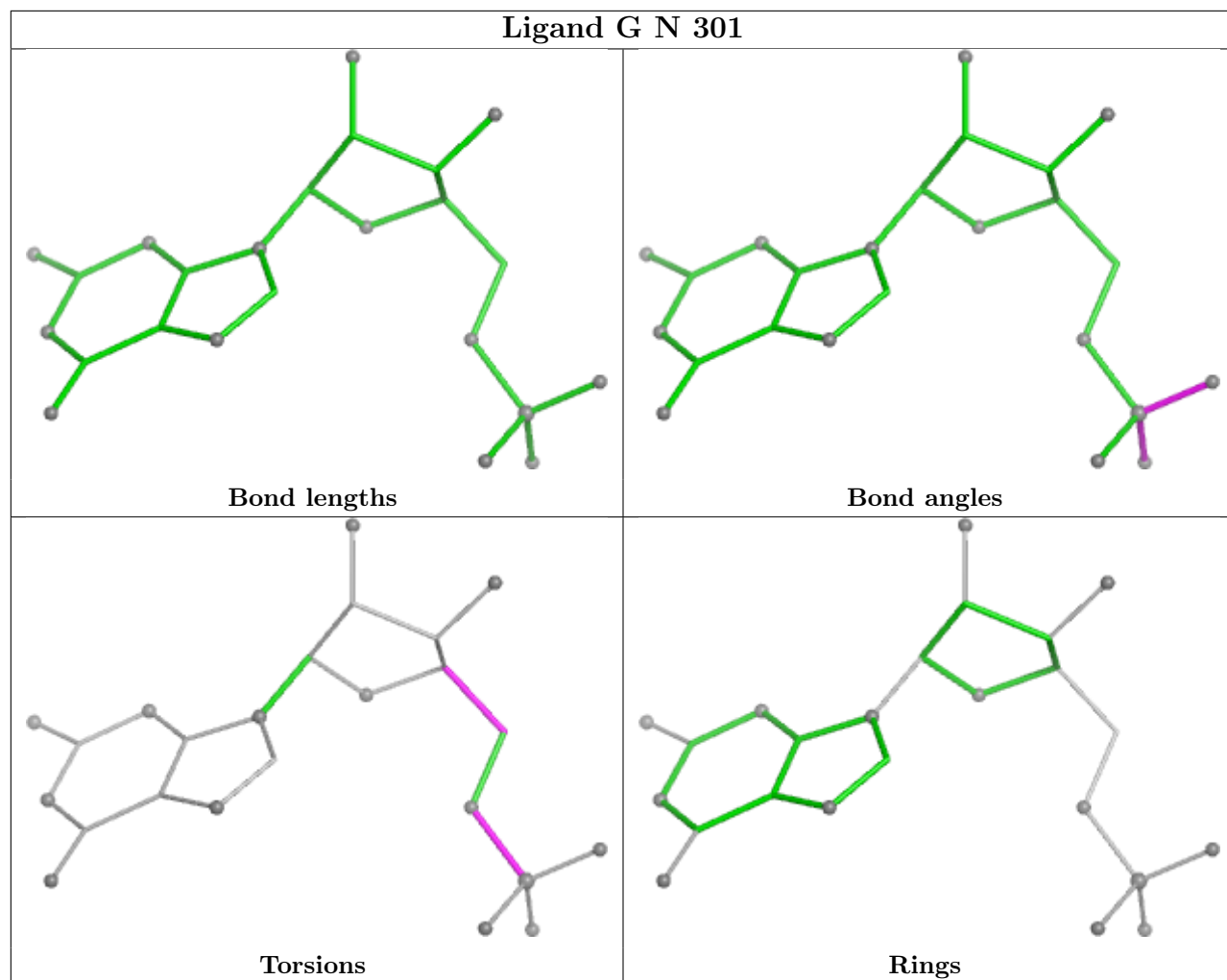


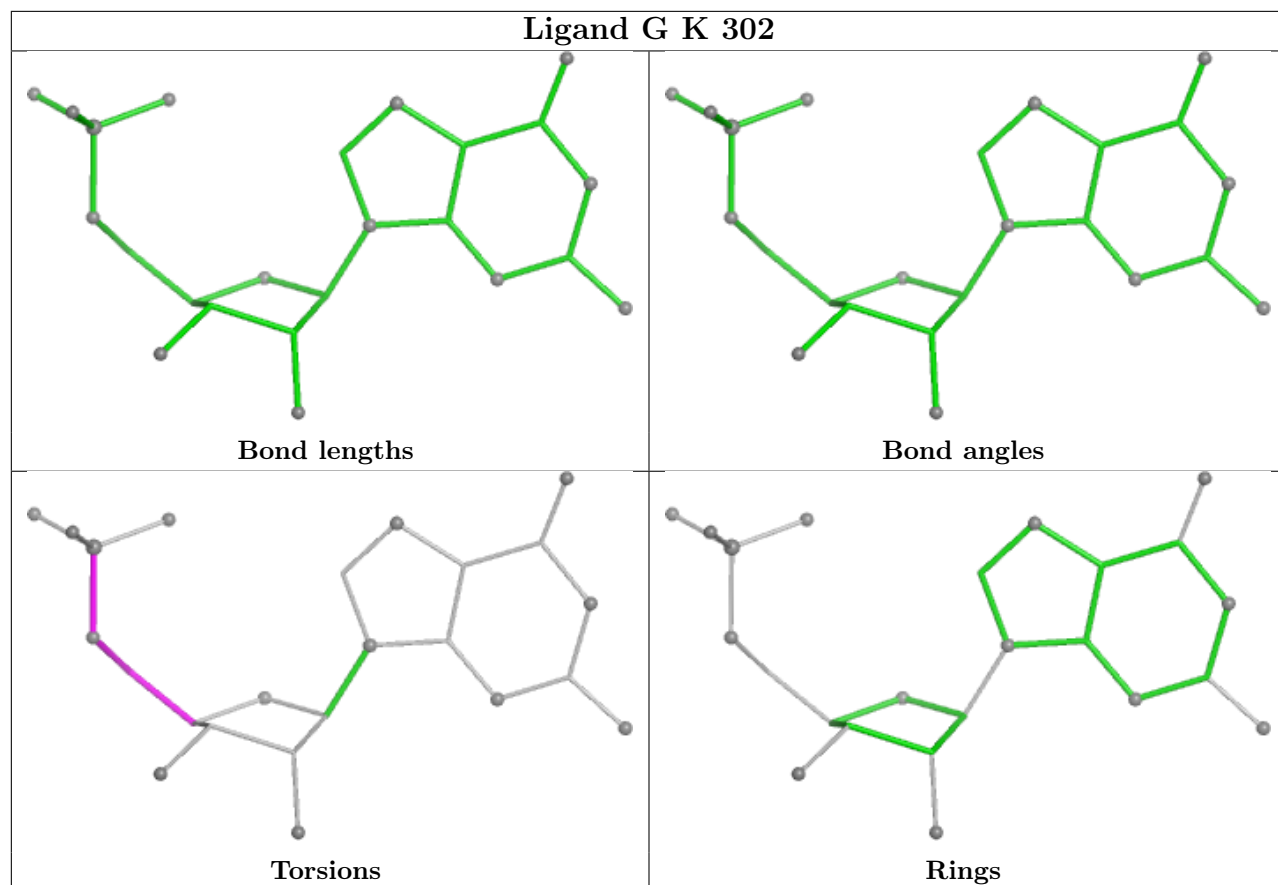


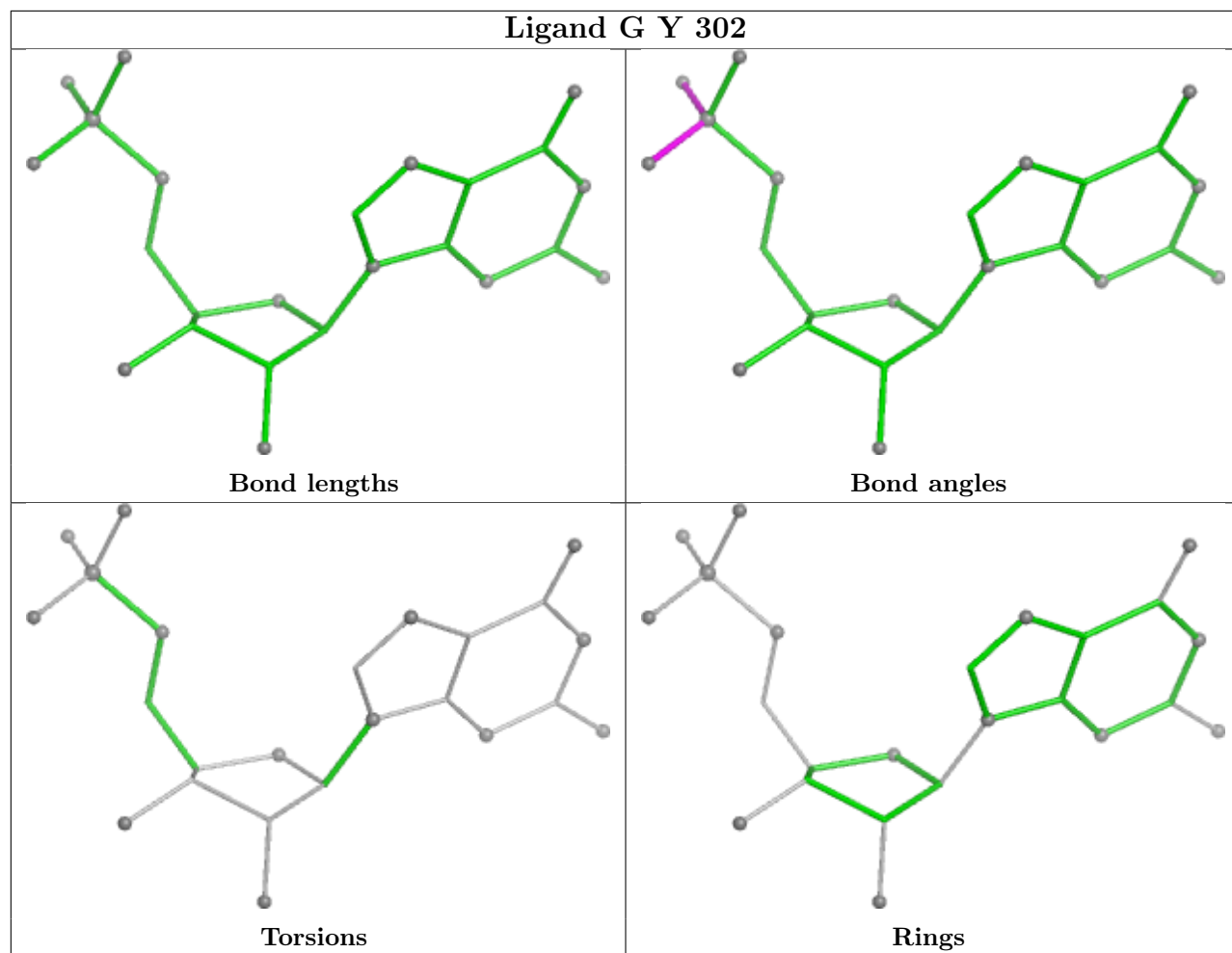


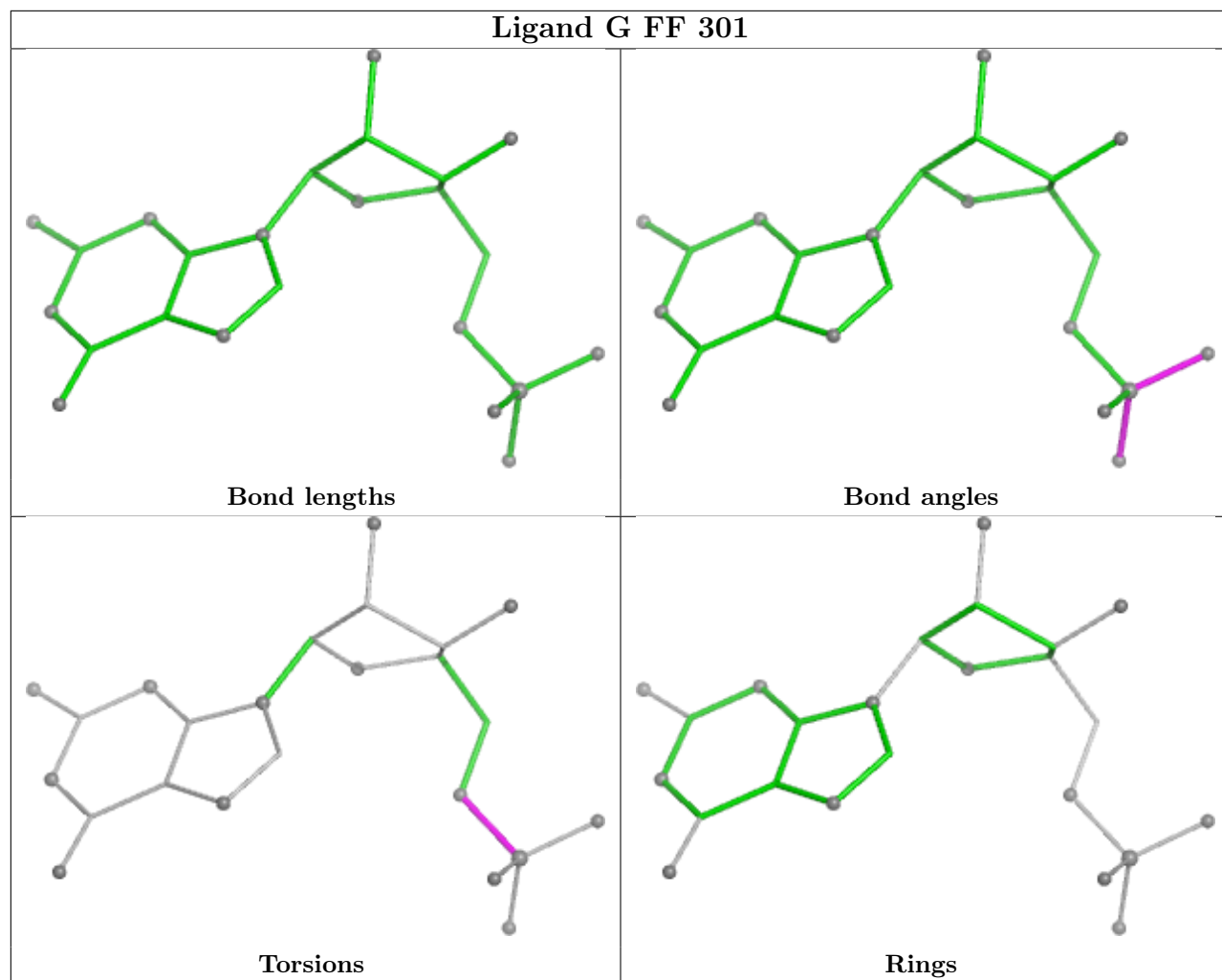


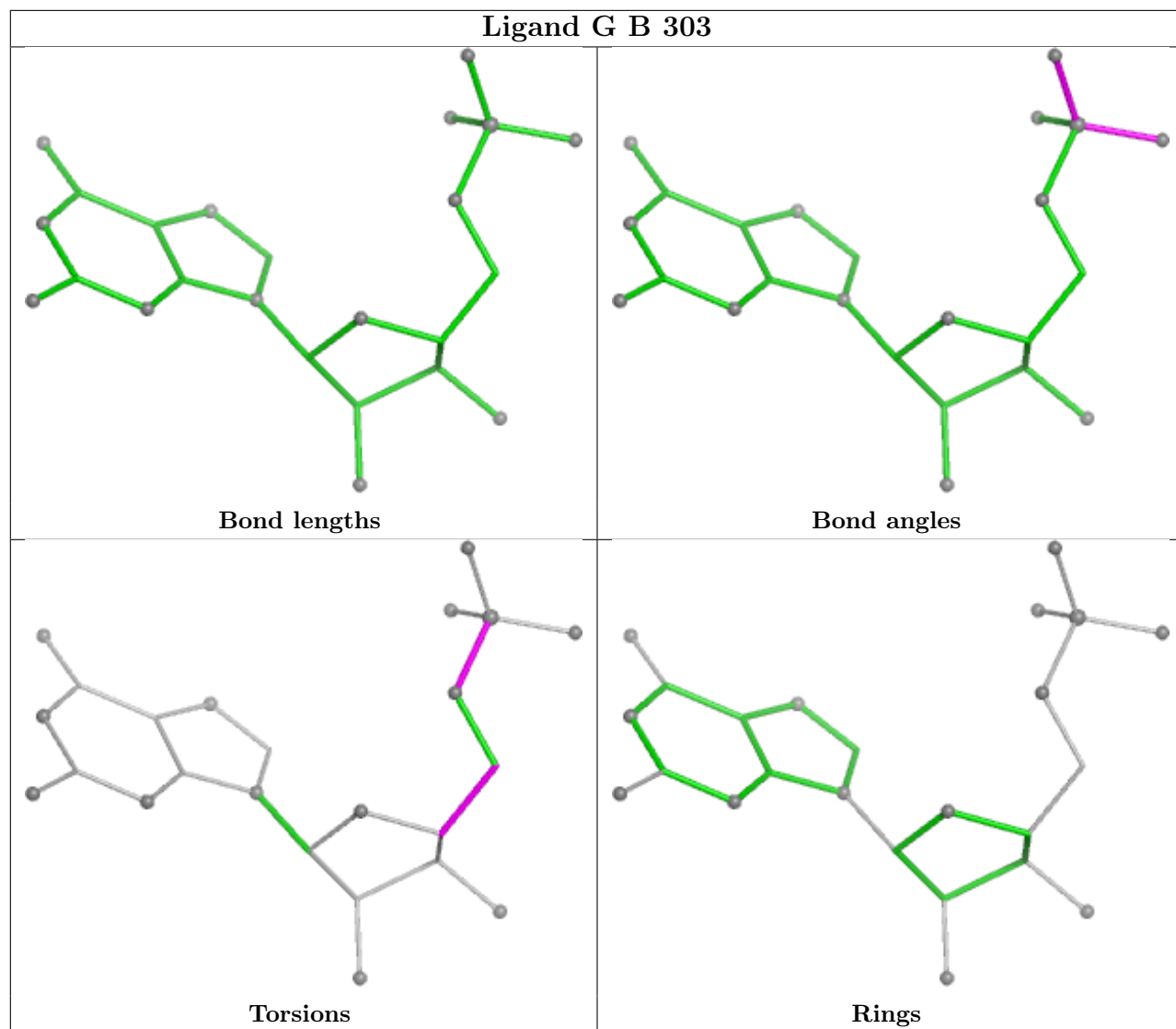


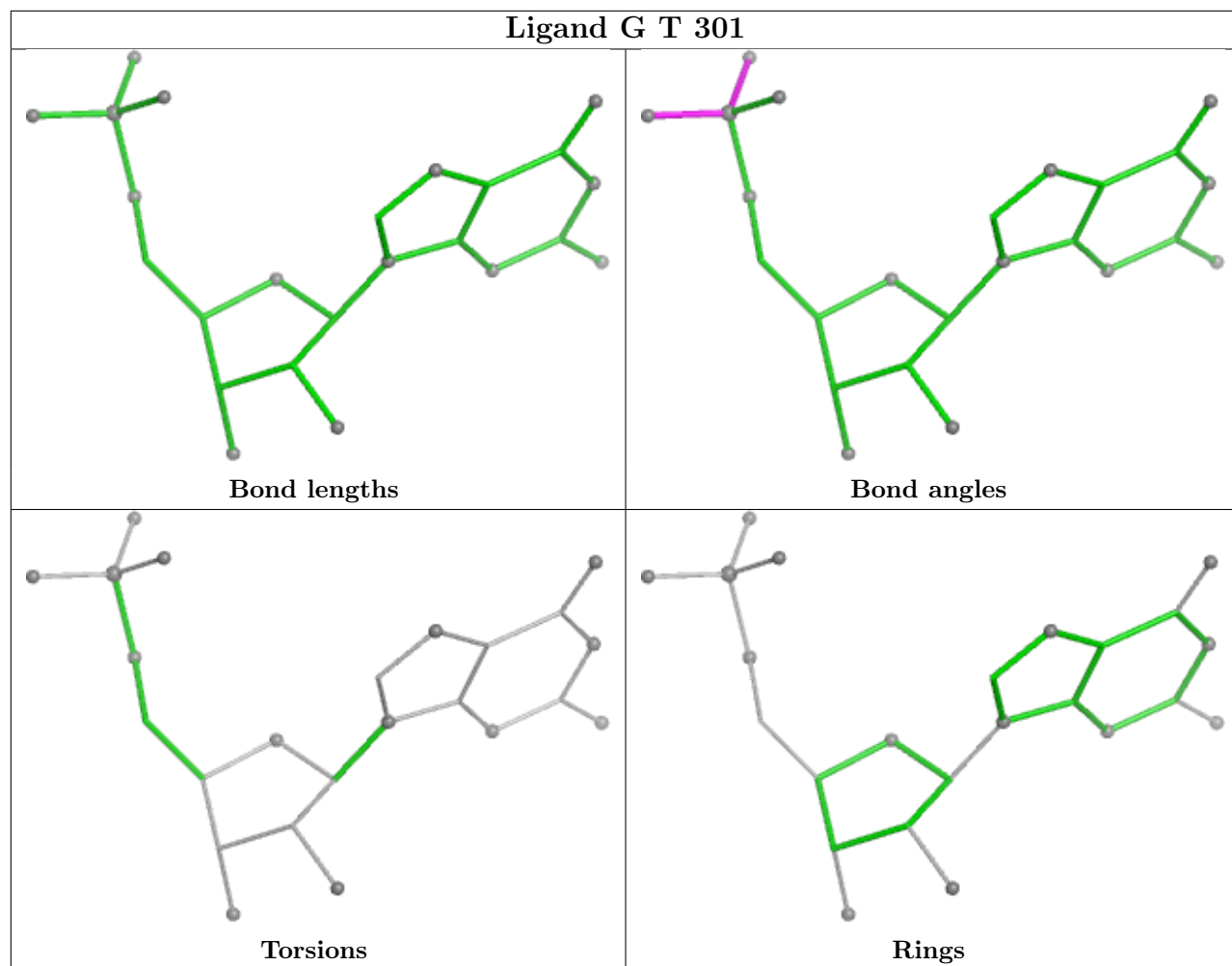


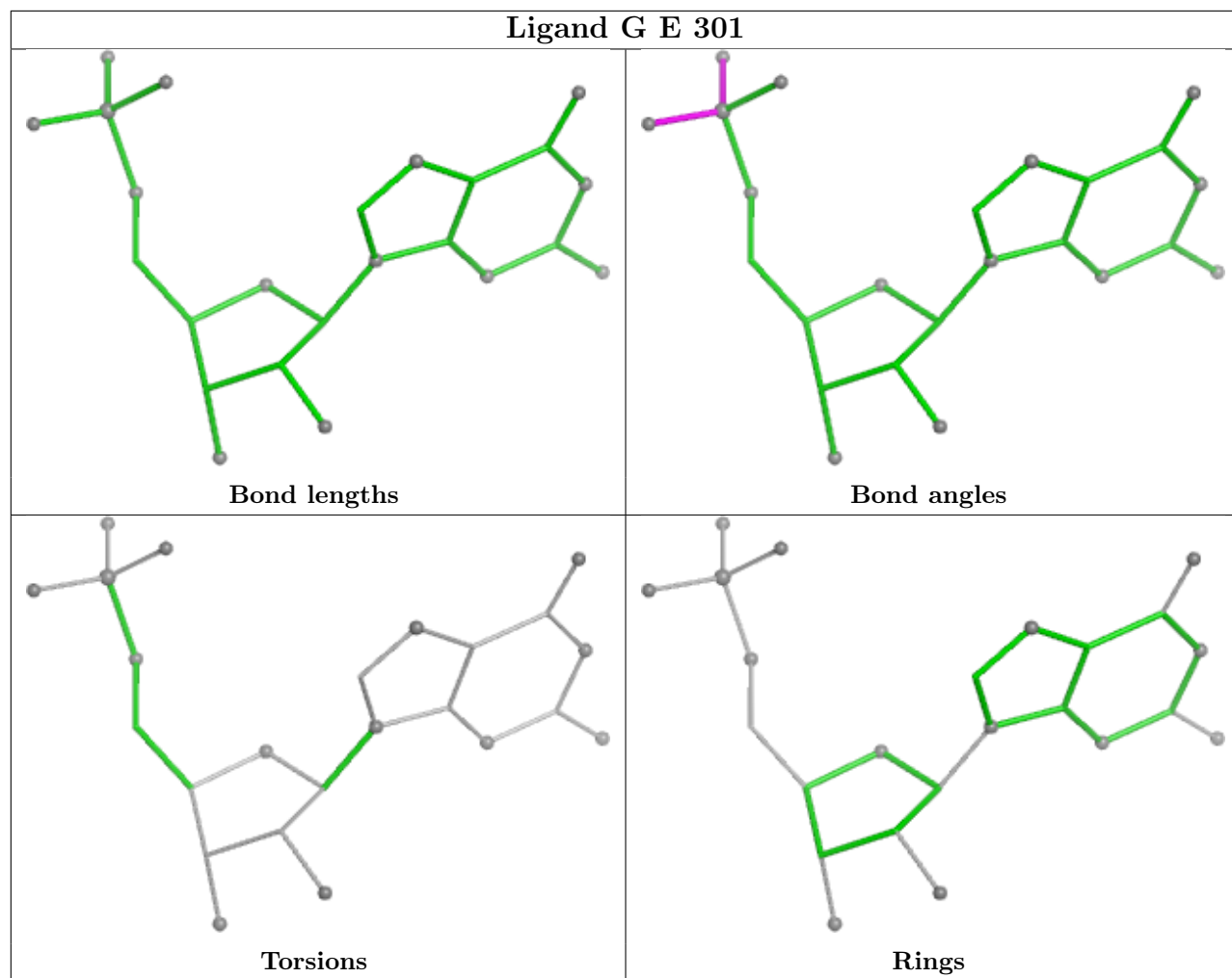


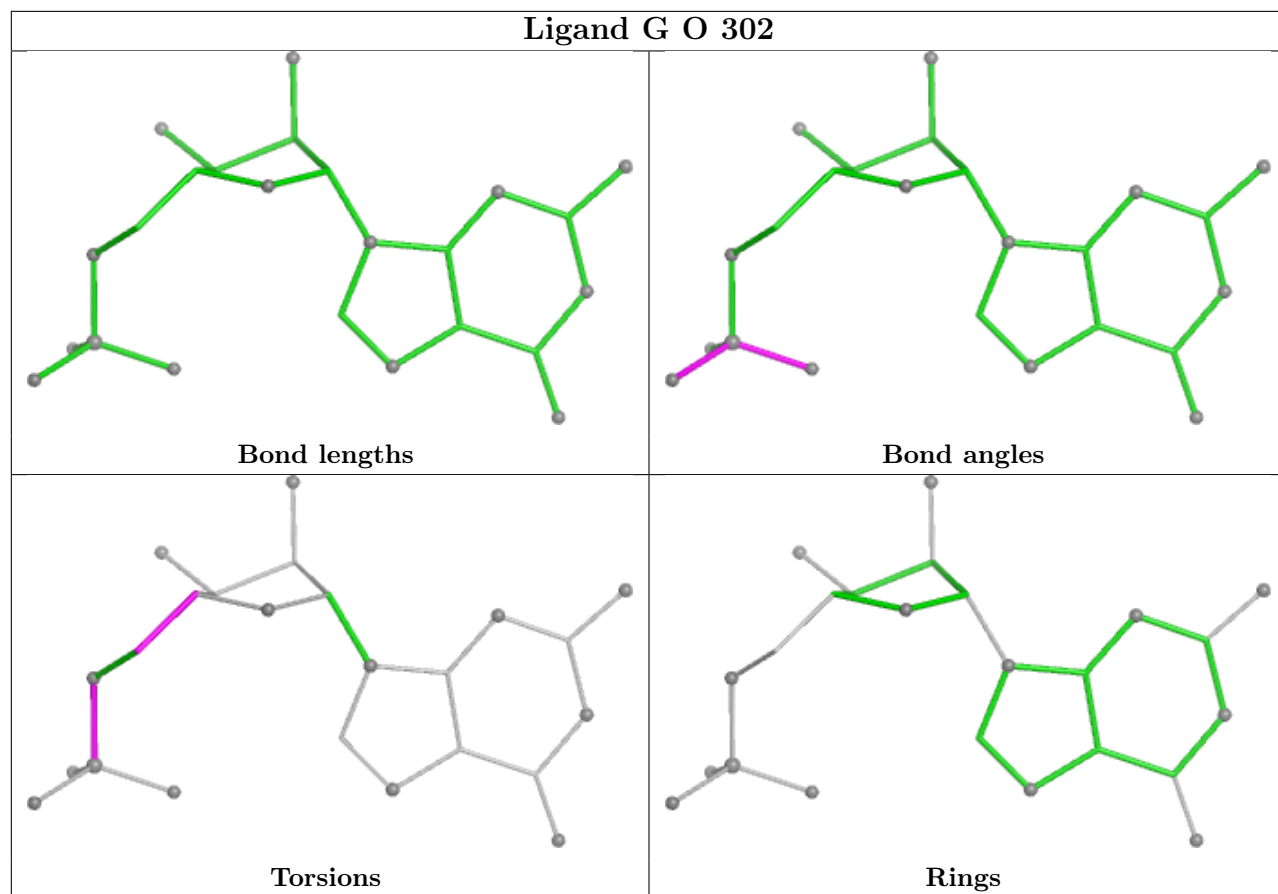


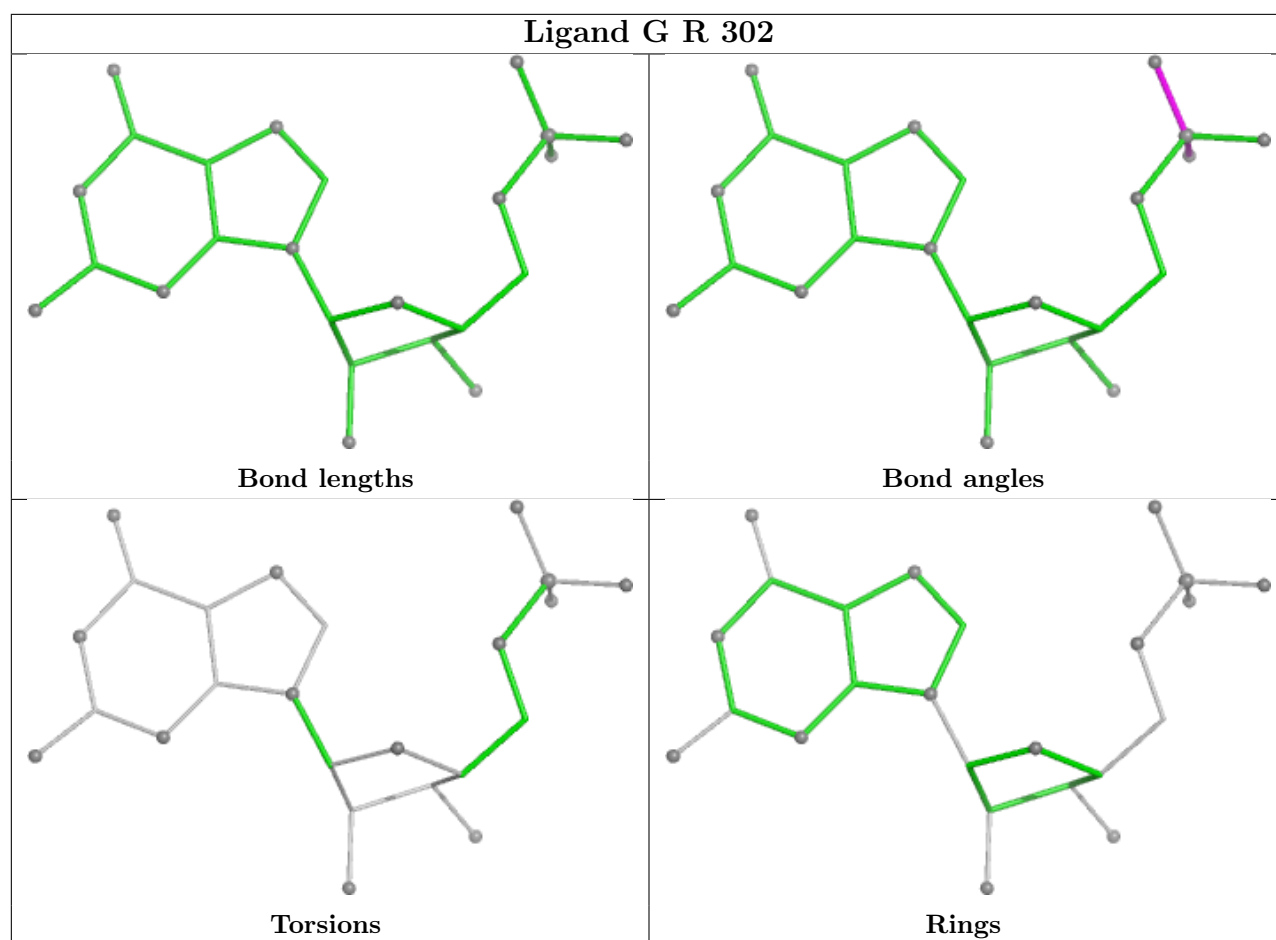


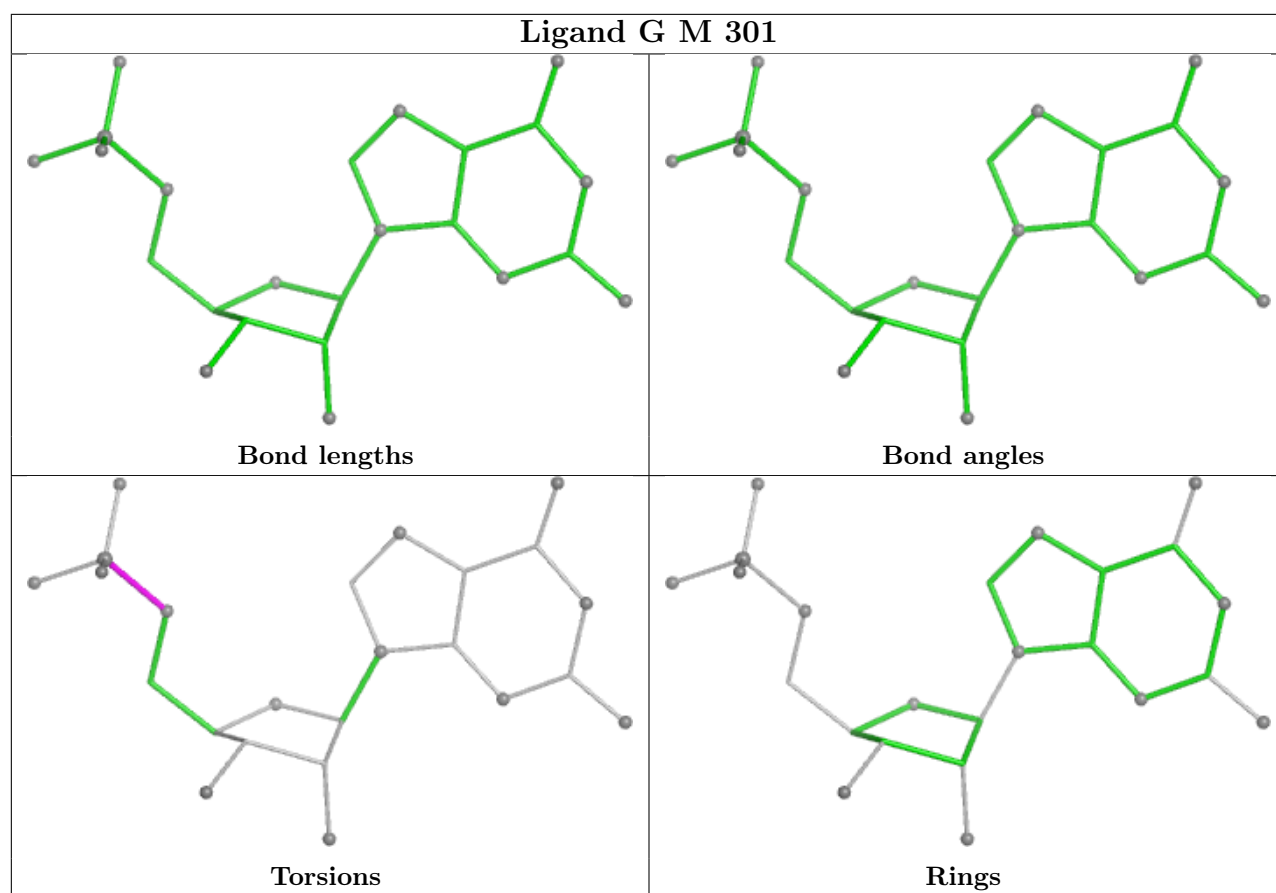


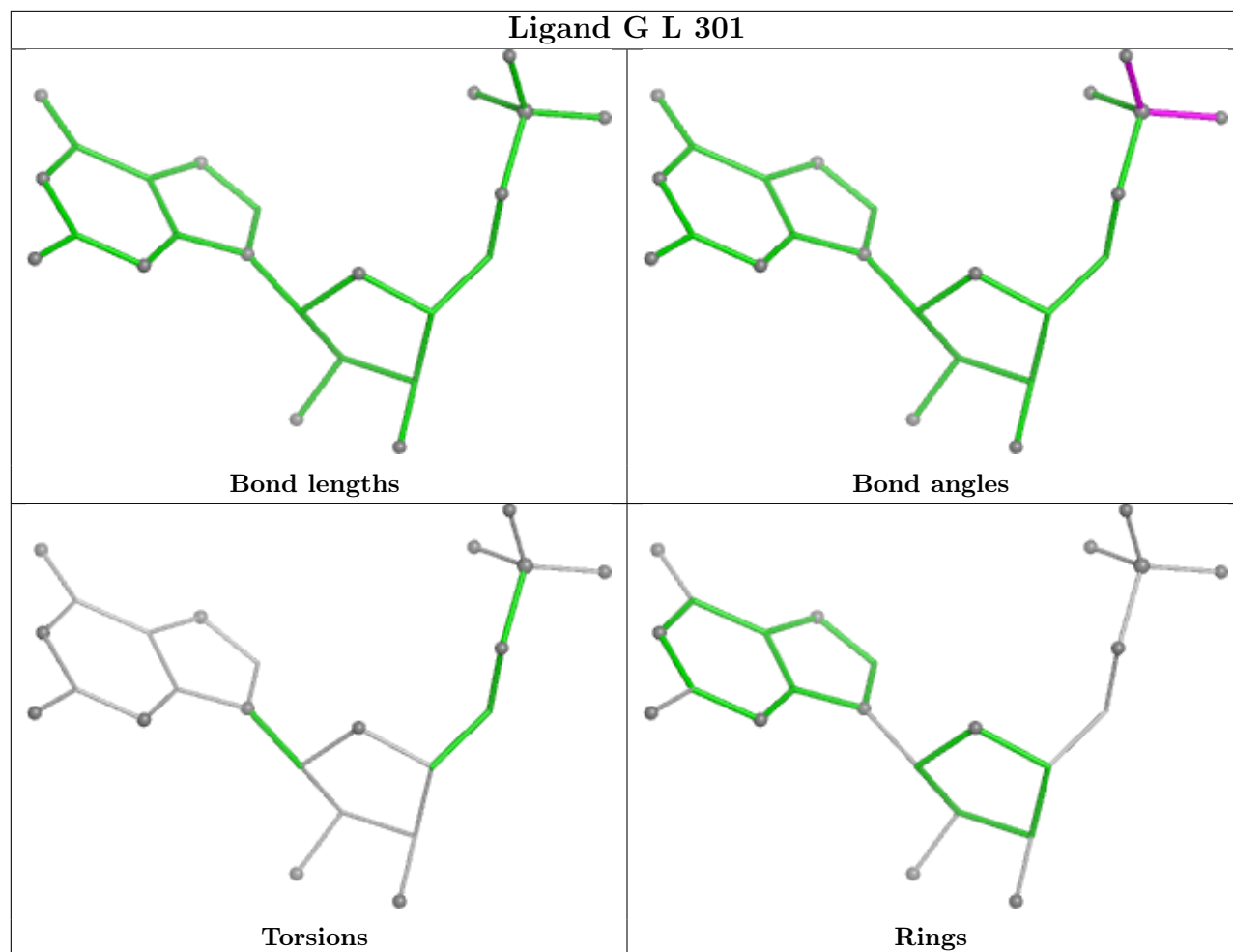




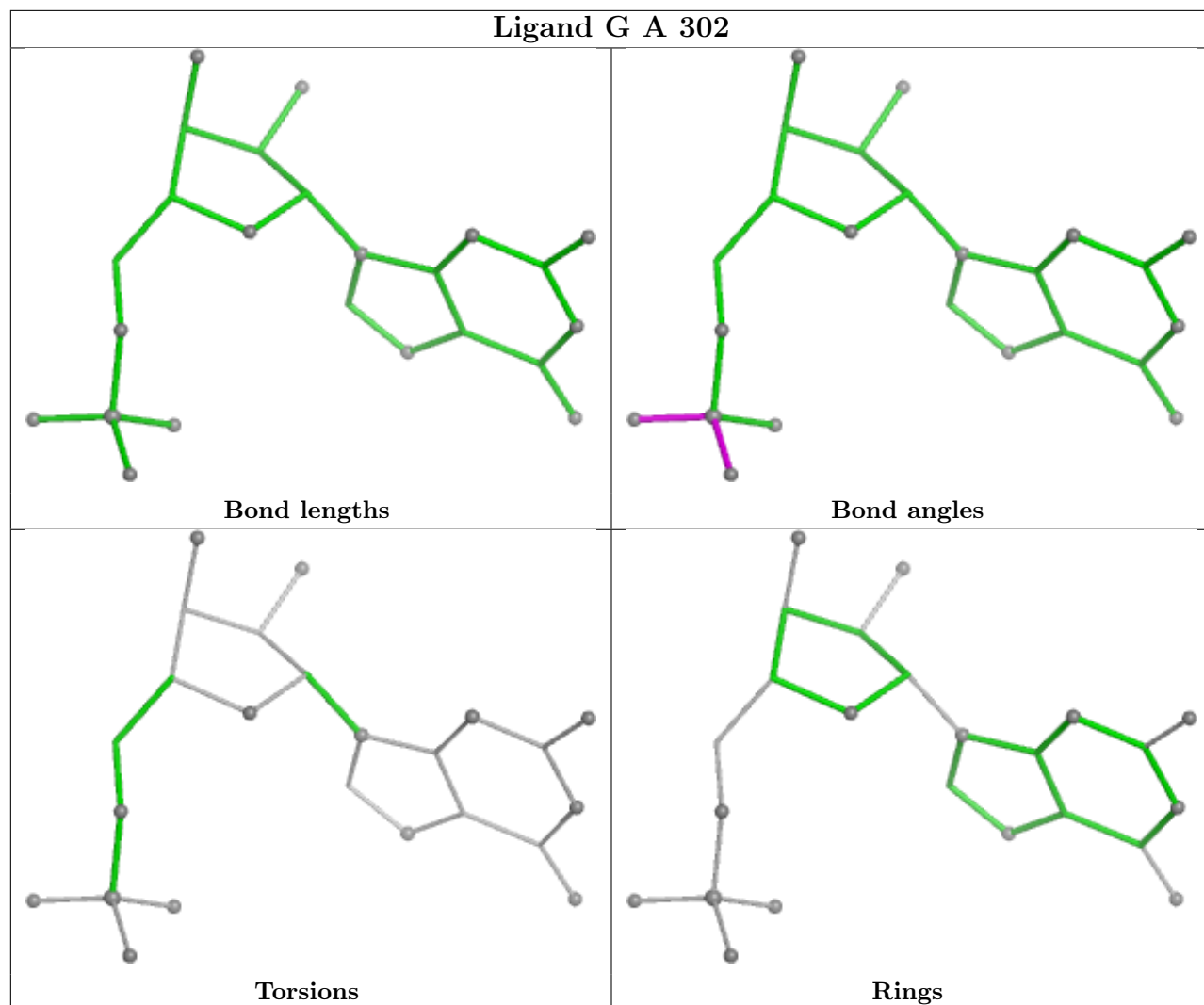


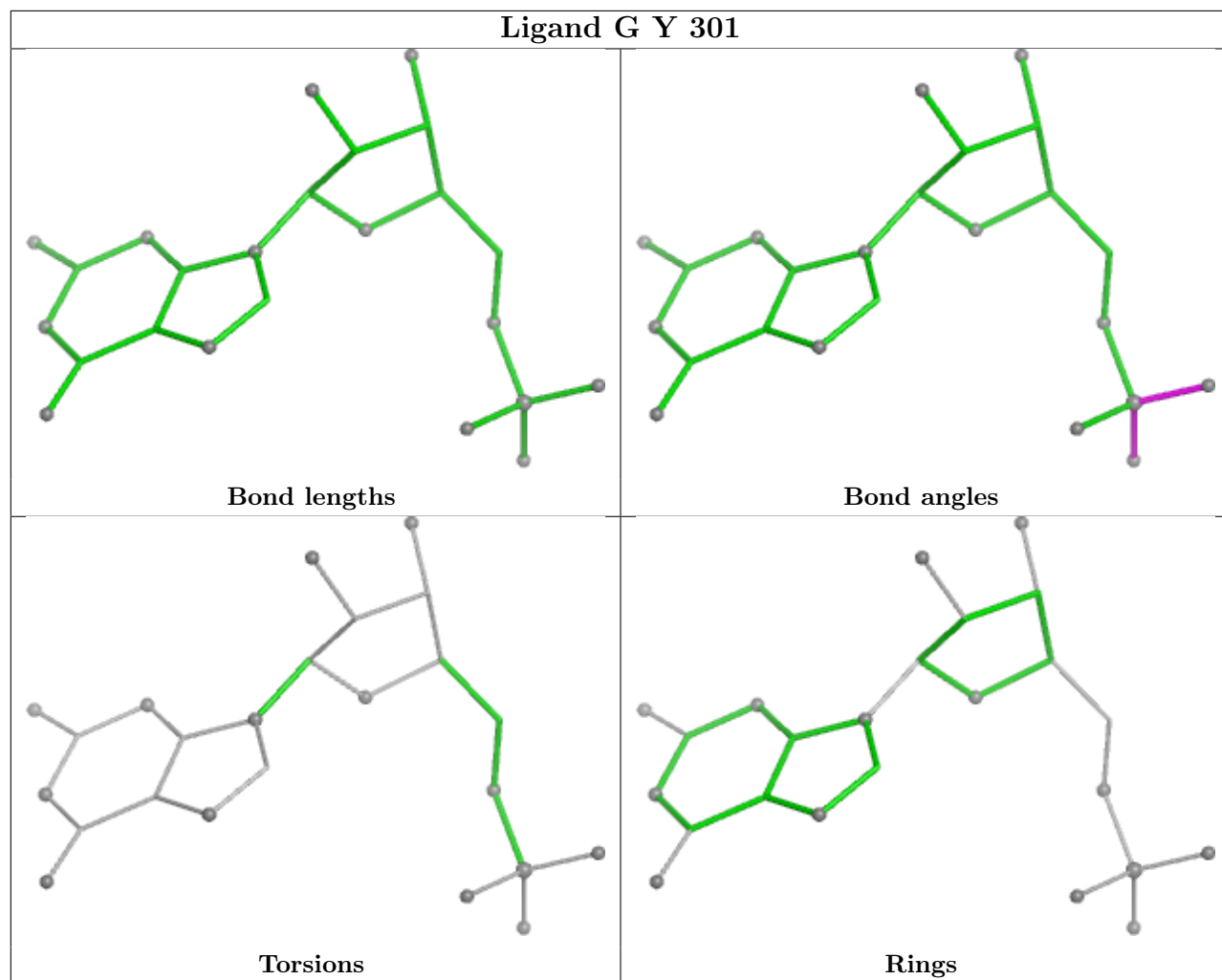


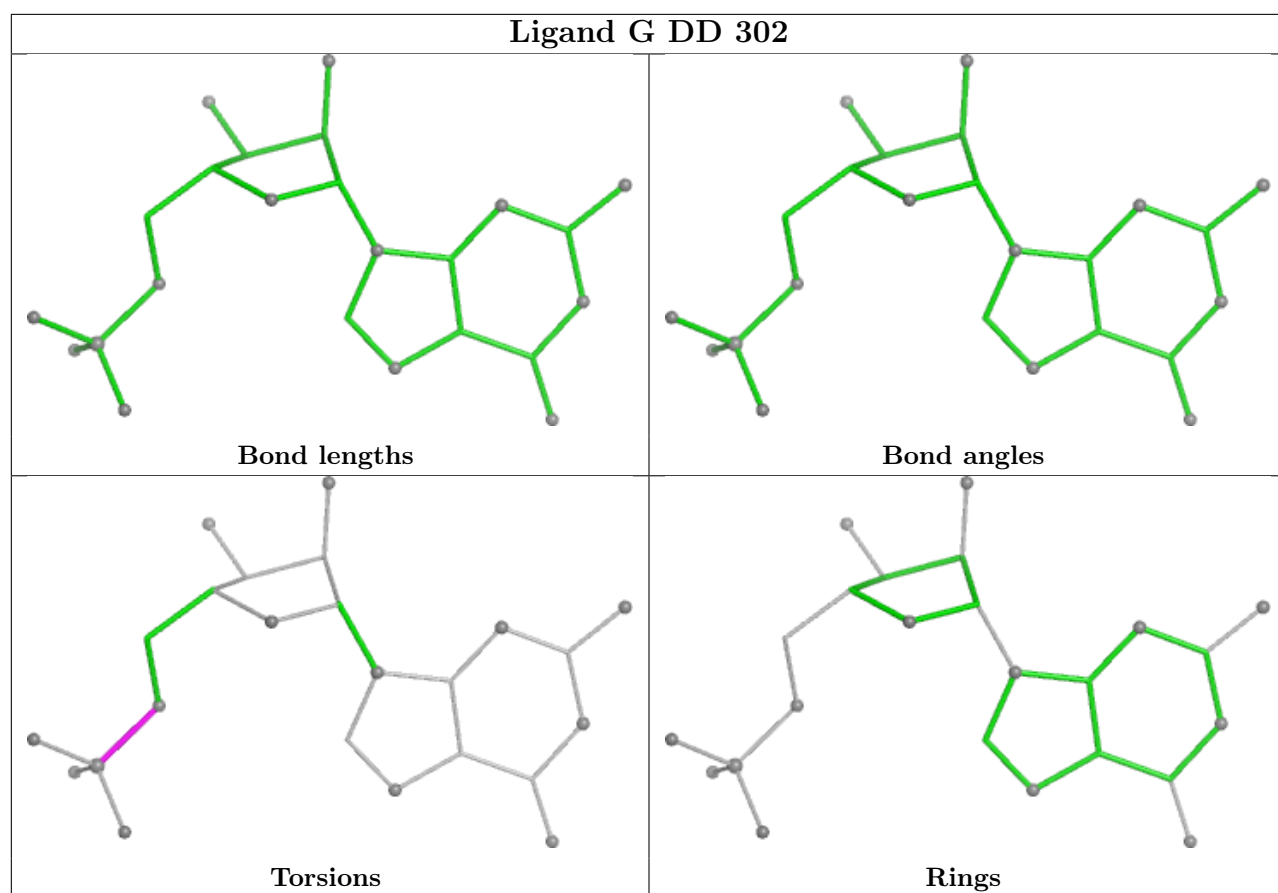


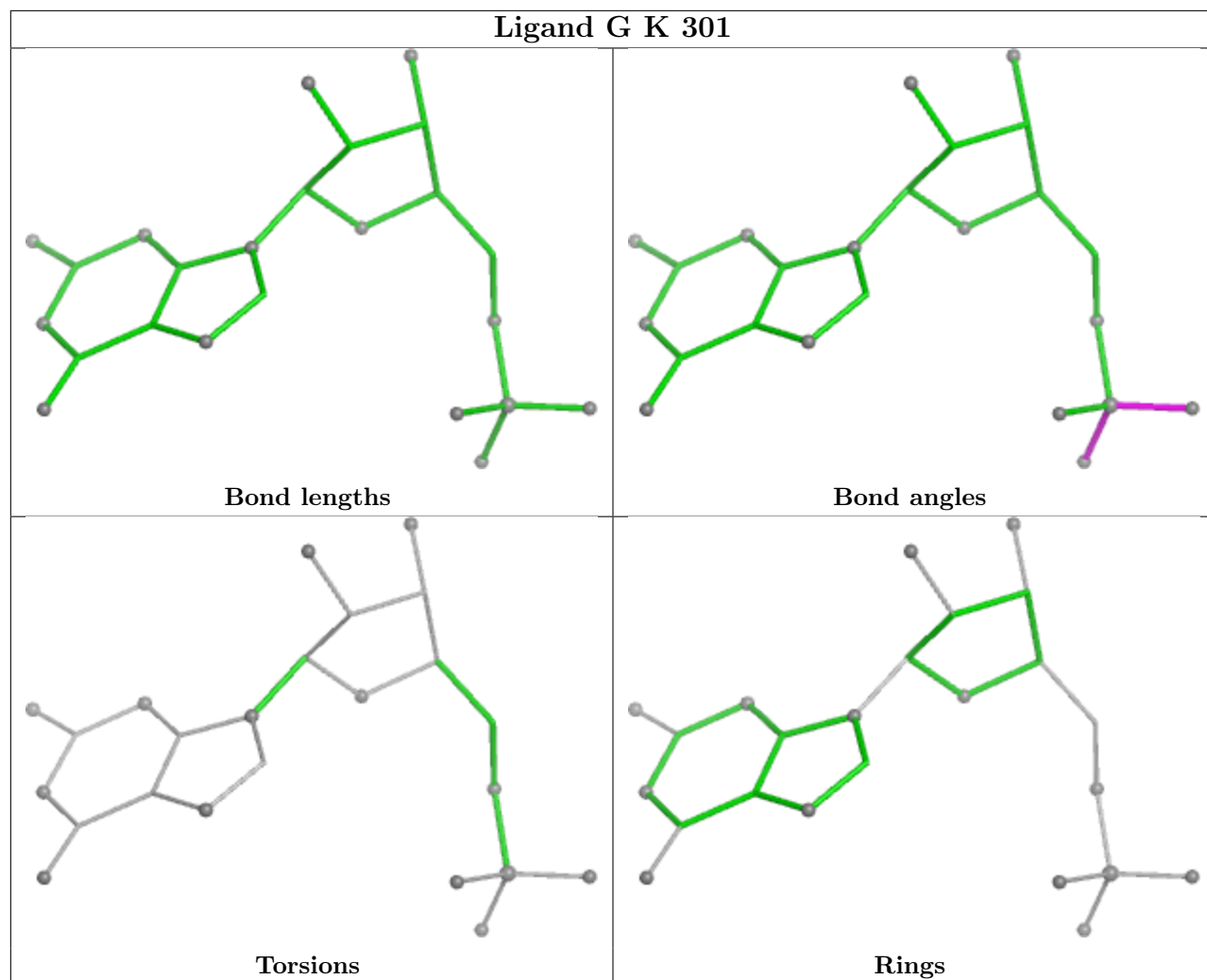


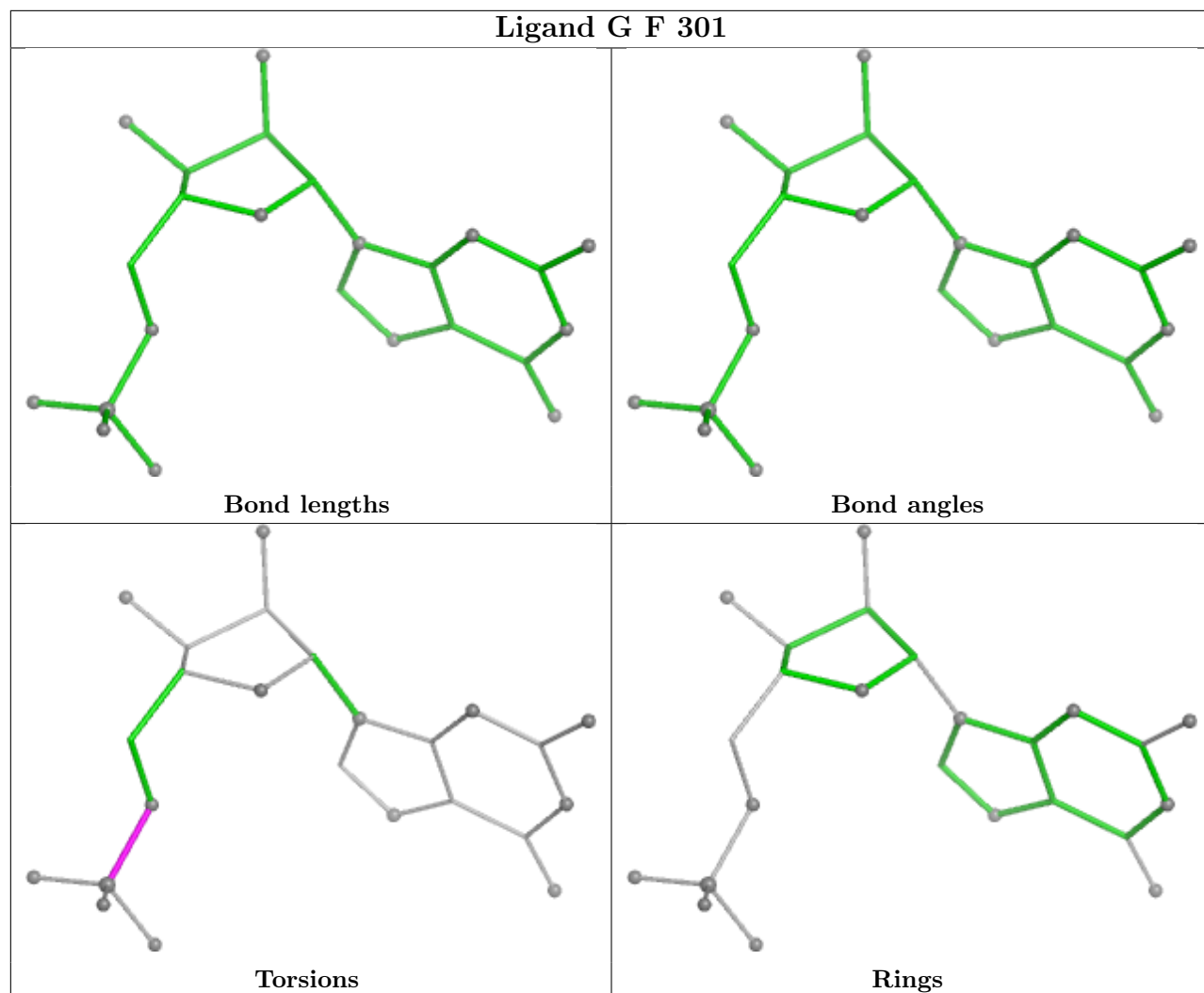
Ligand G A 302

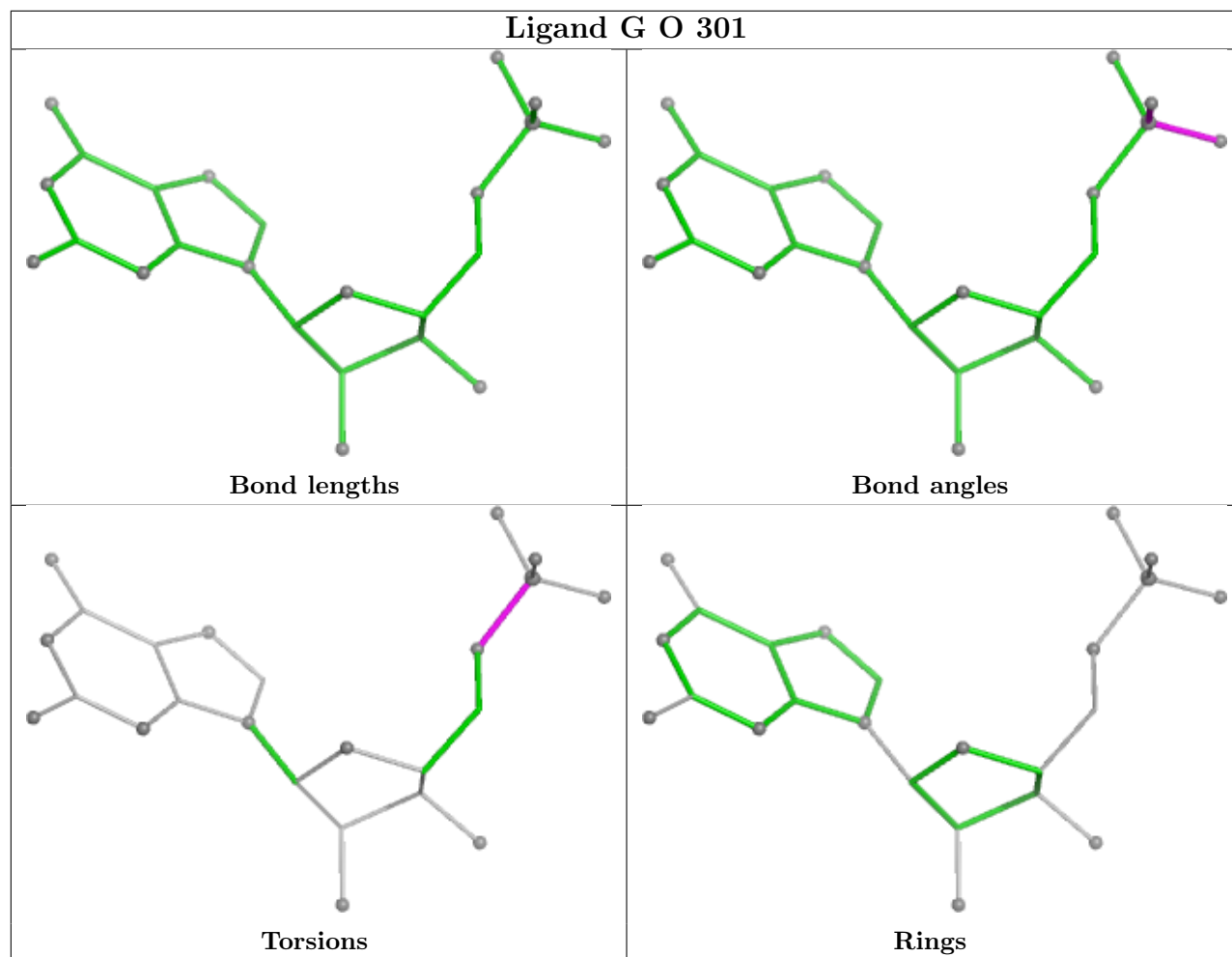


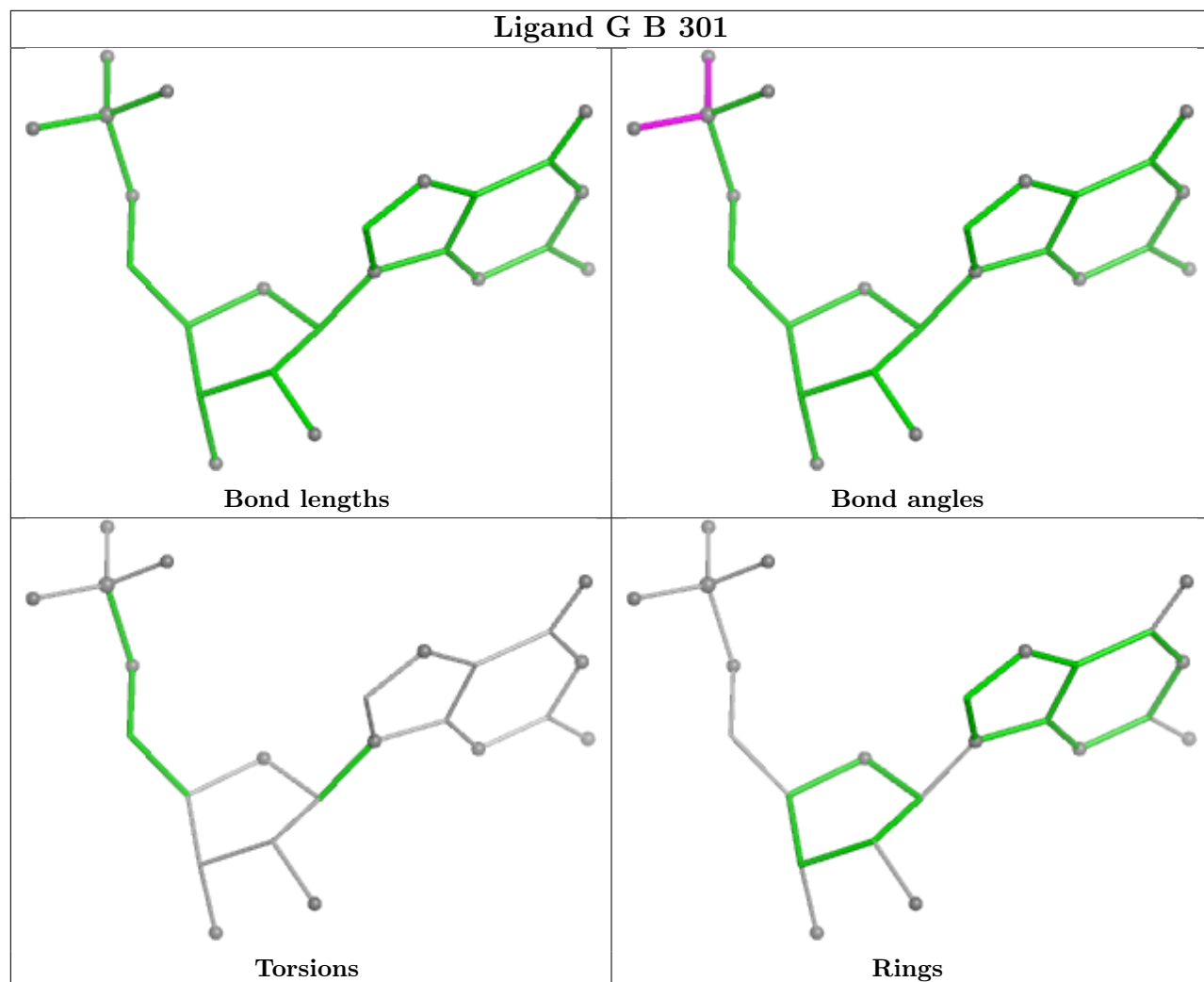




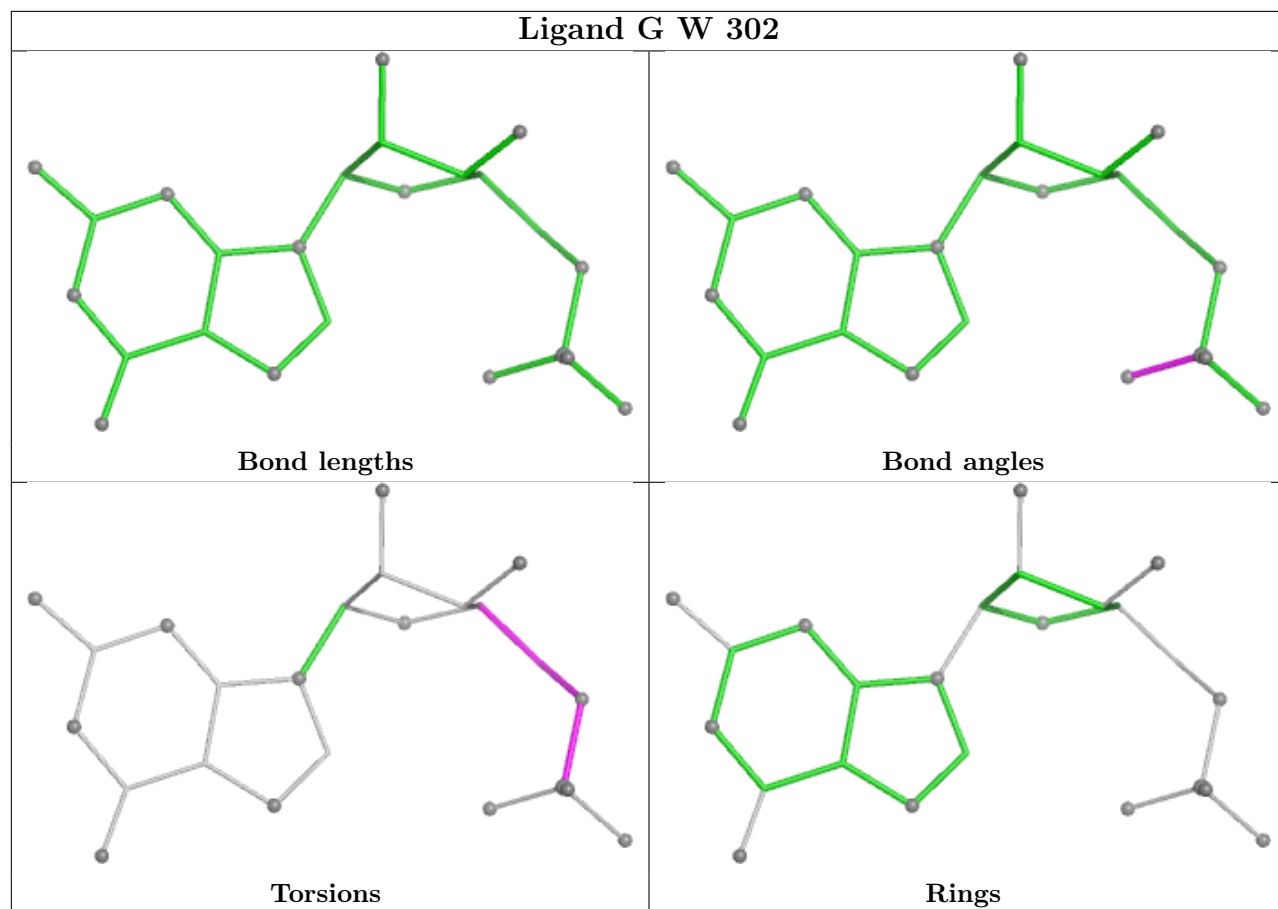




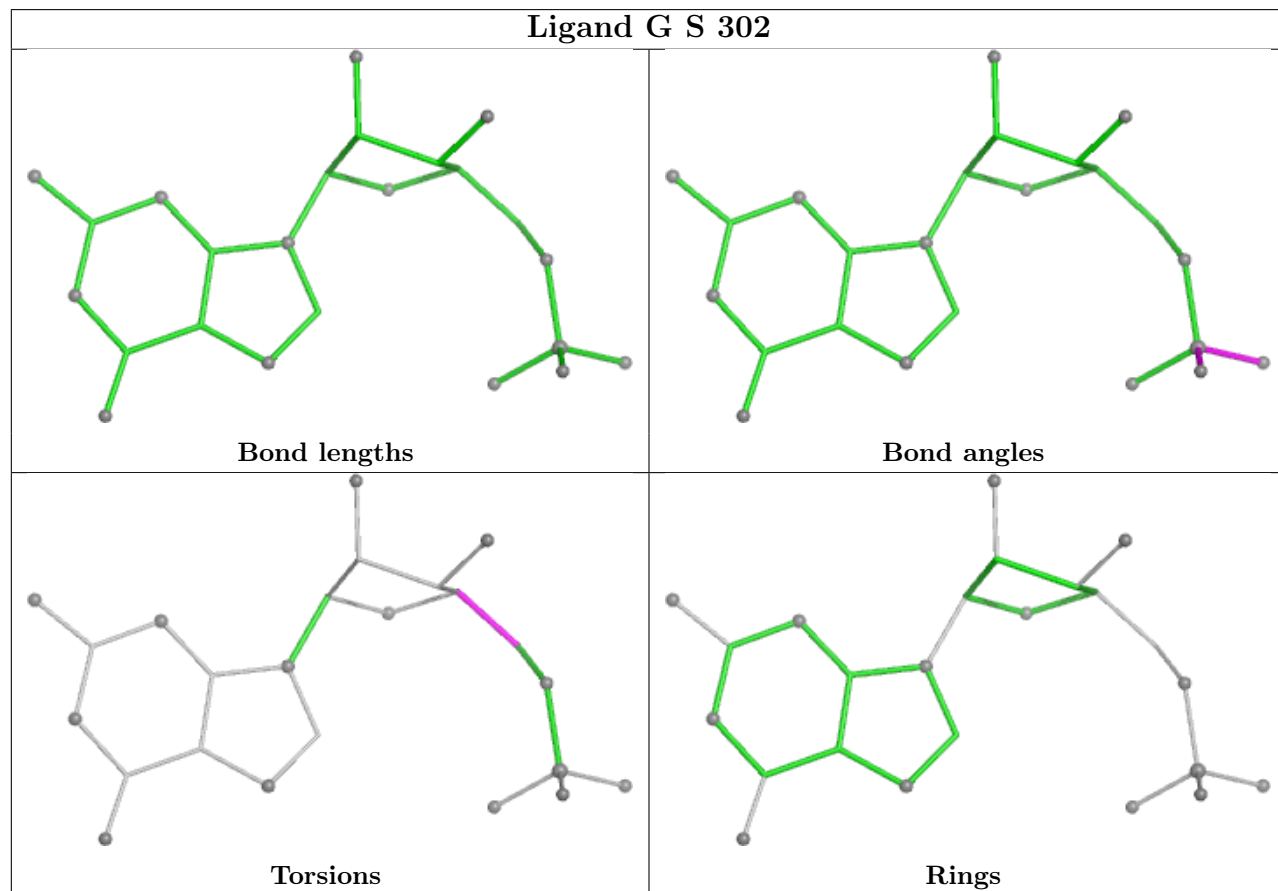


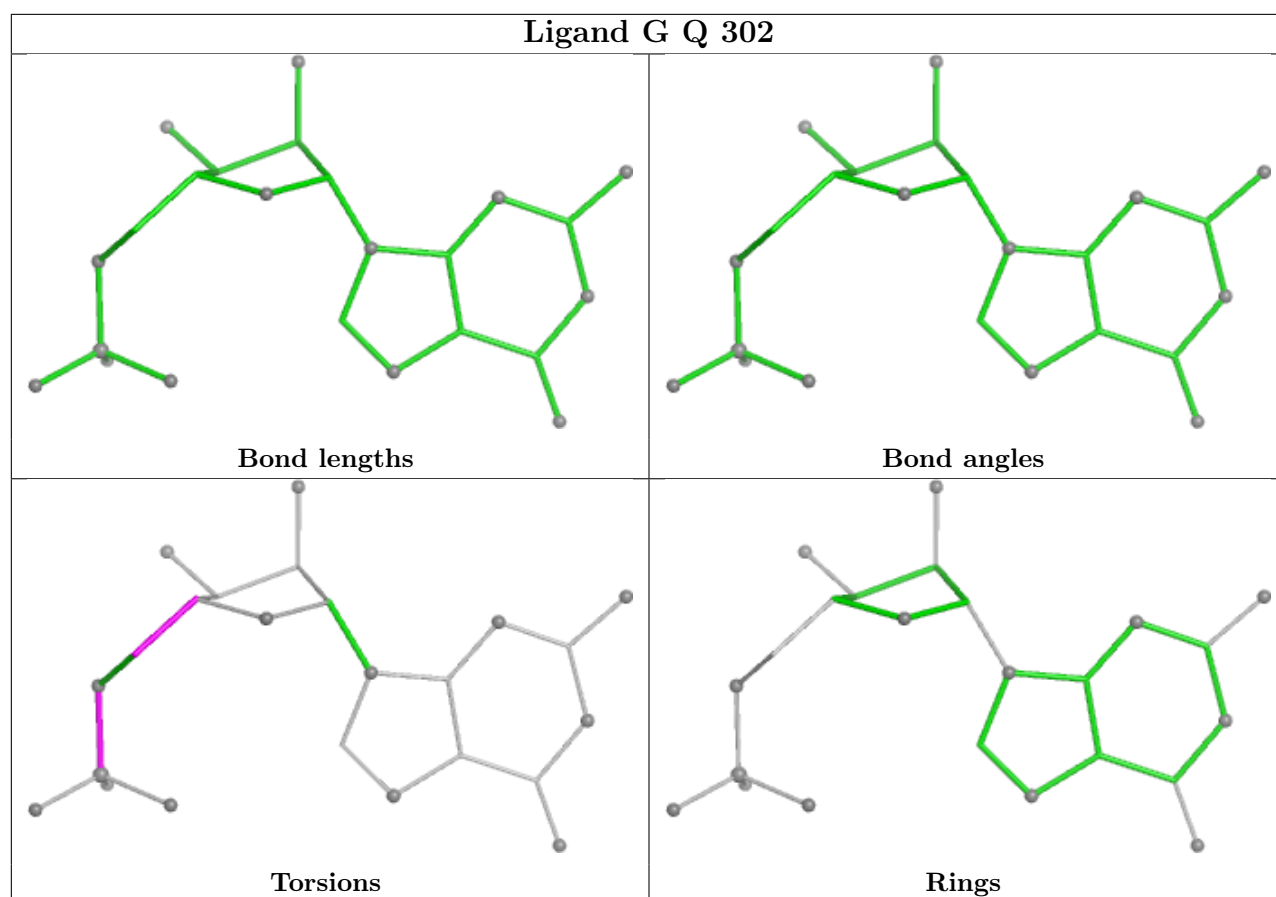


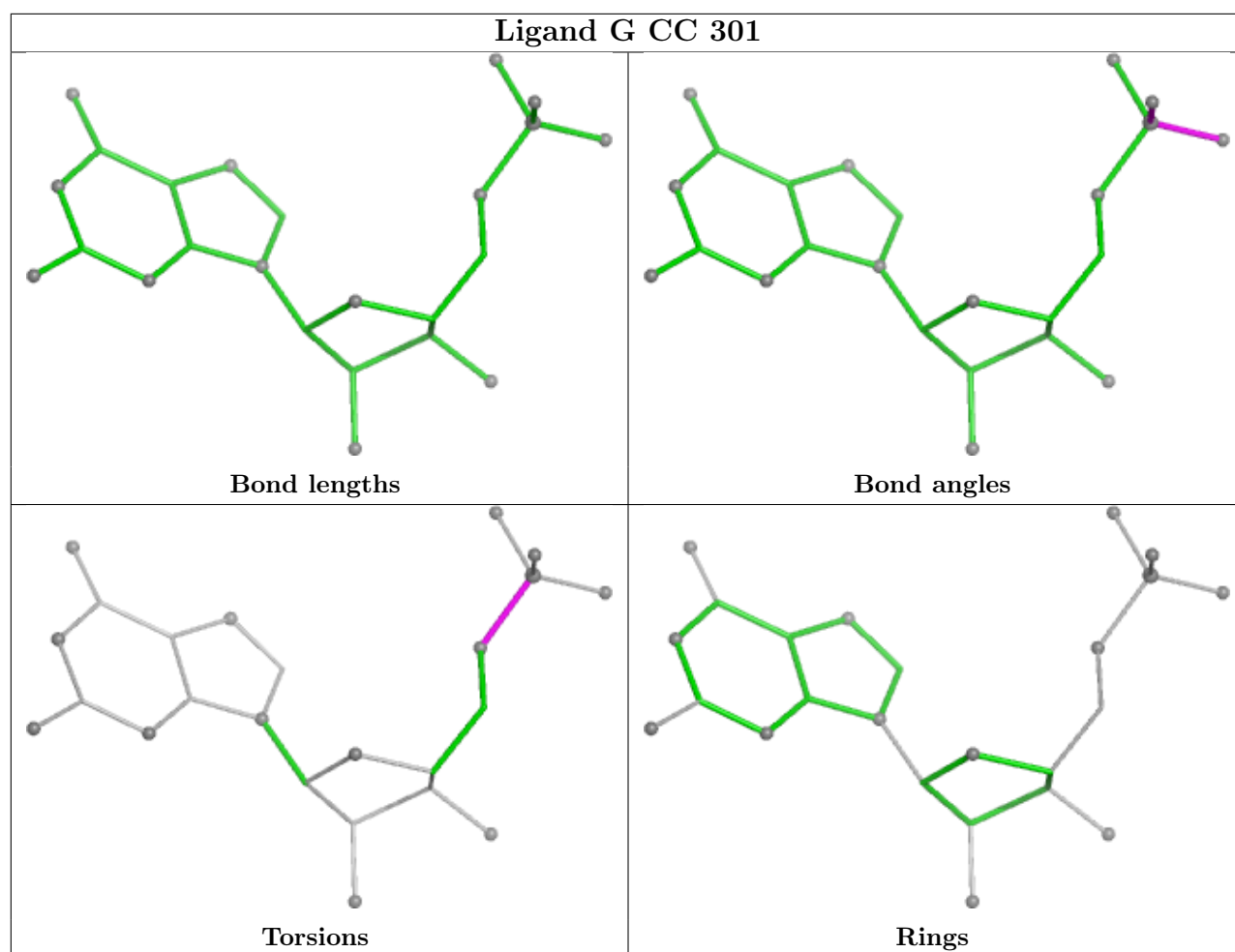
Ligand G W 302



Ligand G S 302







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	206/208 (99%)	-0.26	0 100 100	53, 67, 92, 102	0
1	AA	202/208 (97%)	0.09	3 (1%) 72 49	69, 101, 146, 163	0
1	B	205/208 (98%)	-0.28	1 (0%) 87 72	61, 74, 98, 113	0
1	BB	205/208 (98%)	-0.07	1 (0%) 87 72	75, 103, 131, 148	0
1	C	205/208 (98%)	-0.17	1 (0%) 87 72	60, 79, 104, 125	0
1	CC	205/208 (98%)	0.04	0 100 100	75, 103, 141, 165	0
1	D	205/208 (98%)	-0.23	1 (0%) 87 72	62, 78, 102, 137	0
1	DD	199/208 (95%)	0.03	3 (1%) 72 49	69, 103, 131, 149	0
1	E	205/208 (98%)	-0.24	0 100 100	51, 71, 96, 122	0
1	EE	205/208 (98%)	-0.14	0 100 100	65, 88, 122, 147	0
1	F	205/208 (98%)	-0.27	2 (0%) 79 59	50, 74, 99, 138	0
1	FF	205/208 (98%)	-0.15	1 (0%) 87 72	60, 74, 91, 126	0
1	G	207/208 (99%)	-0.36	0 100 100	51, 66, 88, 108	0
1	H	205/208 (98%)	-0.27	0 100 100	54, 69, 86, 107	0
1	I	206/208 (99%)	-0.32	0 100 100	55, 68, 85, 104	0
1	J	207/208 (99%)	-0.22	1 (0%) 87 72	55, 74, 96, 109	0
1	K	205/208 (98%)	-0.25	0 100 100	61, 75, 104, 130	0
1	L	205/208 (98%)	-0.06	2 (0%) 79 59	60, 80, 111, 133	0
1	M	203/208 (97%)	-0.33	0 100 100	54, 69, 88, 127	0
1	N	205/208 (98%)	-0.26	1 (0%) 87 72	54, 72, 97, 119	0
1	O	205/208 (98%)	-0.27	2 (0%) 79 59	58, 72, 97, 132	0
1	P	208/208 (100%)	-0.17	0 100 100	65, 81, 122, 174	0
1	Q	205/208 (98%)	-0.19	2 (0%) 79 59	58, 74, 93, 113	0
1	R	205/208 (98%)	-0.25	1 (0%) 87 72	60, 75, 97, 123	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	S	205/208 (98%)	-0.21	3 (1%) 72 49	59, 79, 104, 141	0
1	T	205/208 (98%)	-0.24	2 (0%) 79 59	57, 73, 93, 119	0
1	U	207/208 (99%)	-0.22	1 (0%) 87 72	54, 73, 89, 124	0
1	V	205/208 (98%)	-0.18	0 100 100	63, 80, 110, 133	0
1	W	201/208 (96%)	-0.05	2 (0%) 79 59	67, 88, 111, 130	0
1	X	205/208 (98%)	-0.15	0 100 100	64, 81, 100, 116	0
1	Y	205/208 (98%)	-0.19	0 100 100	60, 78, 100, 117	0
1	Z	205/208 (98%)	-0.13	0 100 100	67, 87, 126, 158	0
2	bb	2/2 (100%)	-0.55	0 100 100	103, 103, 103, 104	0
2	cc	2/2 (100%)	0.01	0 100 100	104, 104, 104, 112	0
2	ff	2/2 (100%)	-0.48	0 100 100	92, 92, 92, 99	0
All	All	6562/6662 (98%)	-0.19	30 (0%) 87 72	50, 78, 114, 174	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	144	ASN	3.9
1	DD	38	ARG	3.7
1	S	46	LEU	3.4
1	N	144	ASN	3.4
1	Q	4	PHE	3.2

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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($\text{\AA}^2$)	Q<0.9
4	NA	H	305	1/1	0.24	0.21	75,75,75,75	0
4	NA	FF	304	1/1	0.56	0.17	70,70,70,70	0
4	NA	V	304	1/1	0.65	0.10	71,71,71,71	0
4	NA	J	304	1/1	0.69	0.14	78,78,78,78	0
4	NA	G	303	1/1	0.73	0.17	83,83,83,83	0
4	NA	R	303	1/1	0.74	0.16	73,73,73,73	0
4	NA	EE	302	1/1	0.77	0.09	79,79,79,79	0
4	NA	FF	303	1/1	0.77	0.07	85,85,85,85	0
4	NA	C	302	1/1	0.77	0.08	91,91,91,91	0
3	G	B	303	24/24	0.78	0.11	128,133,141,143	0
4	NA	N	303	1/1	0.79	0.11	73,73,73,73	0
3	G	Y	302	24/24	0.80	0.12	102,109,114,119	0
3	G	FF	301	24/24	0.80	0.10	81,86,92,93	0
3	G	DD	302	24/24	0.81	0.10	108,111,117,127	0
4	NA	X	303	1/1	0.83	0.09	81,81,81,81	0
4	NA	A	304	1/1	0.84	0.07	62,62,62,62	0
3	G	Z	301	24/24	0.84	0.12	102,104,107,114	0
3	G	H	301	24/24	0.86	0.10	81,99,105,112	0
4	NA	L	304	1/1	0.86	0.09	91,91,91,91	0
3	G	W	301	24/24	0.86	0.08	119,121,123,125	0
3	G	Y	301	24/24	0.86	0.09	96,105,113,115	0
3	G	CC	301	24/24	0.87	0.08	114,117,119,121	0
4	NA	D	303	1/1	0.87	0.07	80,80,80,80	0
3	G	W	302	24/24	0.87	0.09	100,104,108,113	0
3	G	F	301	24/24	0.87	0.10	98,105,108,109	0
3	G	B	301	24/24	0.87	0.11	93,109,115,121	0
3	G	E	301	24/24	0.87	0.09	89,102,107,111	0
4	NA	V	303	1/1	0.88	0.07	75,75,75,75	0
3	G	H	303	24/24	0.88	0.10	102,106,114,116	0
3	G	L	301	24/24	0.88	0.09	69,81,87,88	0
3	G	CC	302	24/24	0.88	0.09	82,93,100,108	0
3	G	DD	301	24/24	0.88	0.09	104,119,123,123	0
3	G	N	301	24/24	0.88	0.09	98,100,103,107	0
3	G	T	302	24/24	0.89	0.09	67,77,81,83	0
3	G	U	301	24/24	0.89	0.09	78,91,97,98	0
3	G	U	302	24/24	0.89	0.09	71,75,81,87	0
3	G	D	301	24/24	0.89	0.09	97,100,105,106	0
3	G	FF	302	24/24	0.89	0.08	75,87,94,99	0
3	G	J	301	24/24	0.89	0.10	83,89,95,99	0
3	G	J	302	24/24	0.89	0.09	87,99,111,113	0
3	G	B	302	24/24	0.89	0.10	106,110,113,115	0
3	G	P	302	24/24	0.89	0.09	93,98,111,115	0
3	G	Q	301	24/24	0.89	0.09	89,120,130,134	0

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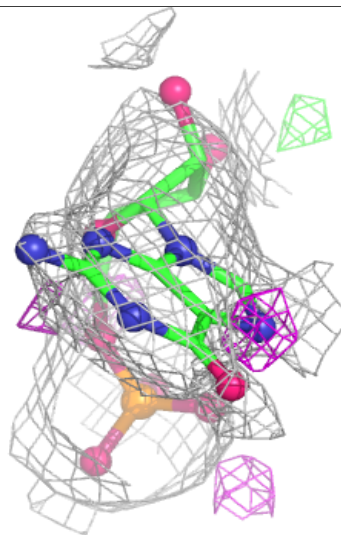
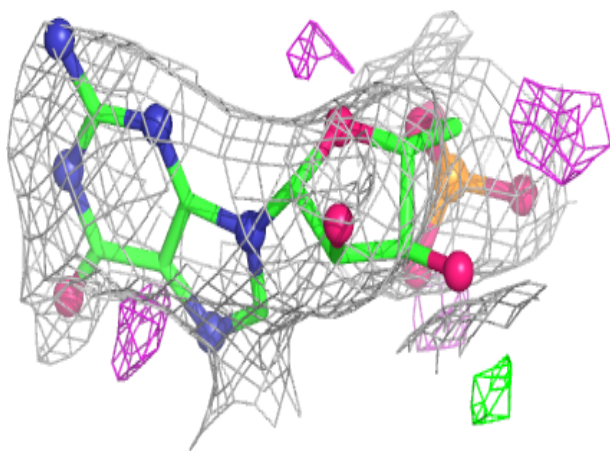
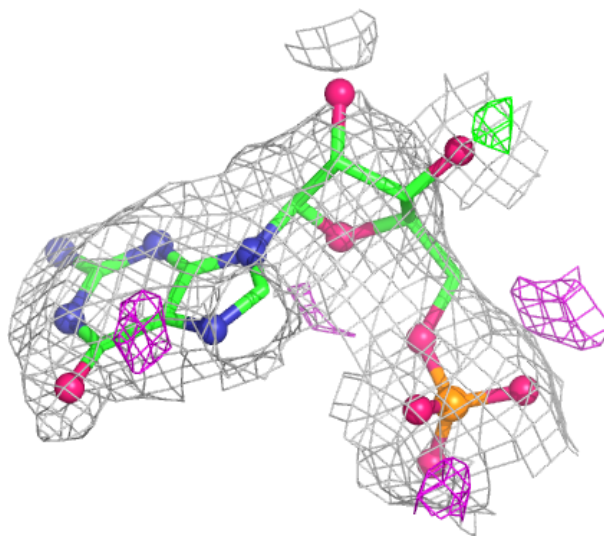
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	G	P	301	24/24	0.90	0.09	93,98,104,108	0
3	G	Y	303	24/24	0.90	0.07	76,84,88,89	0
3	G	S	301	24/24	0.90	0.08	100,107,110,112	0
3	G	T	301	24/24	0.90	0.09	98,99,106,109	0
3	G	F	302	24/24	0.91	0.08	78,84,91,93	0
3	G	G	301	24/24	0.91	0.08	76,87,93,99	0
3	G	X	301	24/24	0.91	0.09	83,104,108,112	0
4	NA	Q	304	1/1	0.91	0.07	69,69,69,69	0
3	G	R	301	24/24	0.91	0.08	88,100,107,109	0
3	G	K	301	24/24	0.91	0.08	78,84,94,98	0
3	G	E	302	24/24	0.91	0.07	71,74,78,80	0
3	G	L	302	24/24	0.91	0.08	73,82,86,89	0
4	NA	EE	301	1/1	0.91	0.07	100,100,100,100	0
3	G	L	303	24/24	0.91	0.09	61,76,83,87	0
3	G	A	302	24/24	0.91	0.08	78,88,94,96	0
4	NA	H	304	1/1	0.91	0.05	81,81,81,81	0
3	G	G	302	24/24	0.92	0.08	70,73,79,84	0
3	G	X	302	24/24	0.92	0.07	59,71,81,86	0
3	G	Q	302	24/24	0.92	0.08	72,79,89,97	0
3	G	O	301	24/24	0.92	0.09	84,89,97,107	0
3	G	V	302	24/24	0.92	0.08	70,76,79,82	0
4	NA	J	303	1/1	0.92	0.08	78,78,78,78	0
3	G	A	301	24/24	0.92	0.09	67,71,80,85	0
3	G	H	302	24/24	0.92	0.08	83,85,91,99	0
4	NA	Q	303	1/1	0.92	0.05	74,74,74,74	0
4	NA	A	303	1/1	0.93	0.08	70,70,70,70	0
3	G	R	302	24/24	0.93	0.07	60,68,77,78	0
4	NA	W	303	1/1	0.93	0.06	87,87,87,87	0
3	G	O	302	24/24	0.93	0.07	64,73,80,85	0
3	G	V	301	24/24	0.93	0.07	59,74,81,84	0
3	G	S	302	24/24	0.93	0.07	79,84,90,93	0
3	G	C	301	24/24	0.93	0.07	92,94,100,103	0
3	G	K	302	24/24	0.93	0.07	74,83,87,89	0
5	CL	U	303	1/1	0.93	0.07	79,79,79,79	0
3	G	M	301	24/24	0.94	0.07	55,61,67,74	0
3	G	N	302	24/24	0.94	0.07	71,76,83,85	0
3	G	D	302	24/24	0.94	0.07	58,73,76,80	0
4	NA	W	304	1/1	0.95	0.05	93,93,93,93	0
3	G	I	301	24/24	0.96	0.06	41,67,73,75	0
4	NA	R	304	1/1	0.96	0.04	76,76,76,76	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.

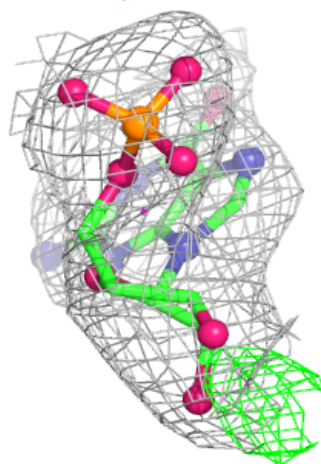
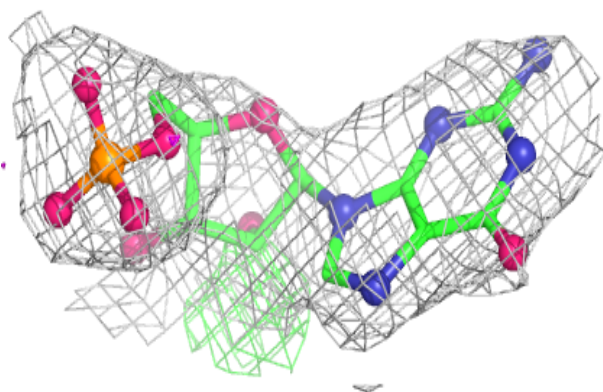
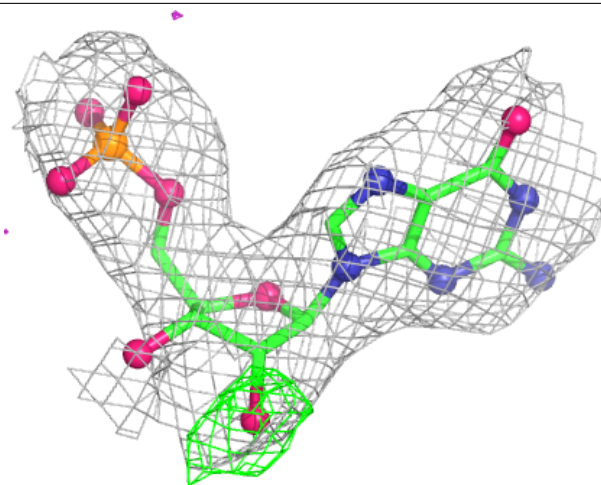
Electron density around G B 303:

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



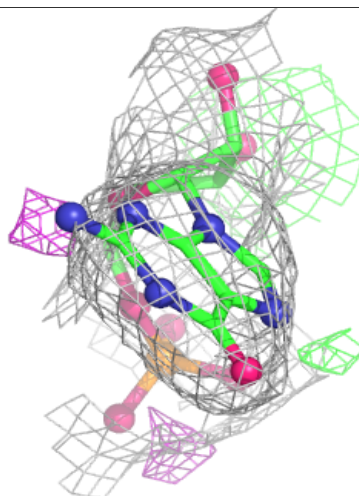
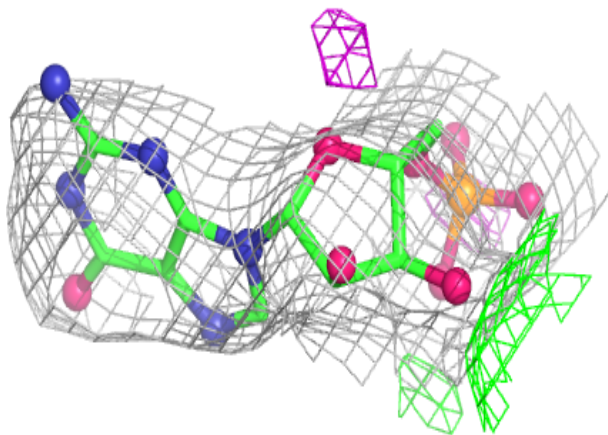
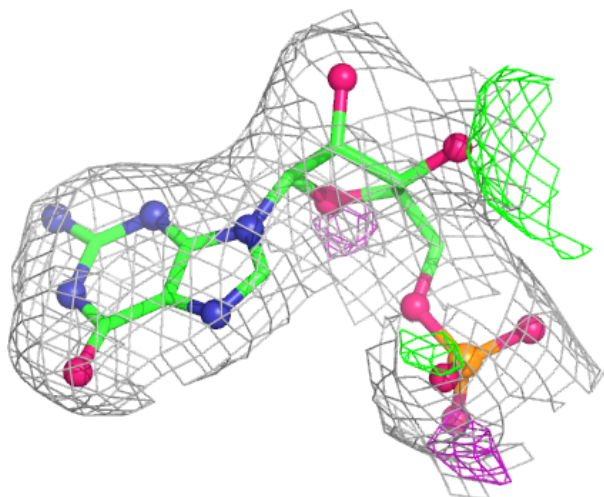
Electron density around G Y 302:

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



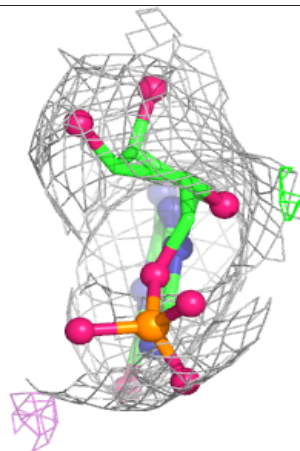
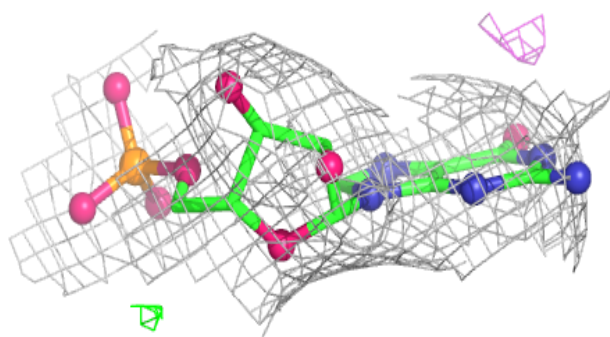
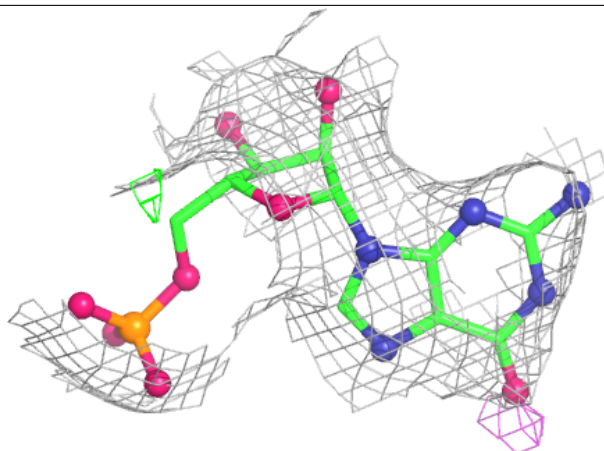
Electron density around G FF 301:

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and green (positive)



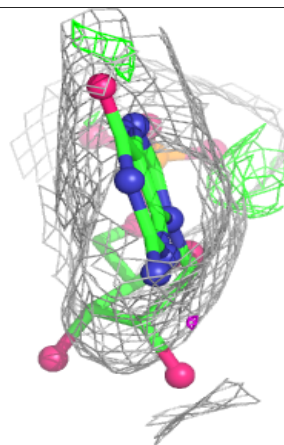
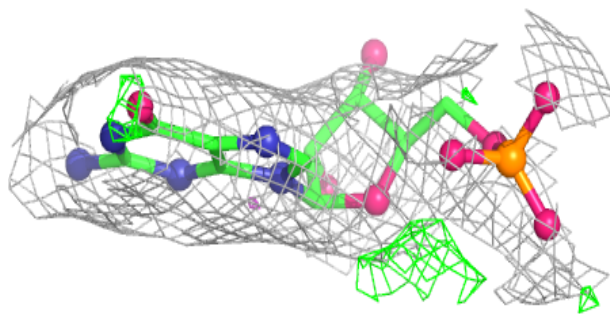
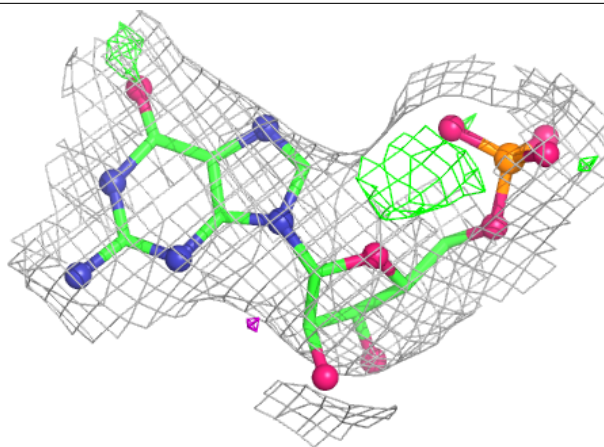
Electron density around G DD 302:

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and green (positive)



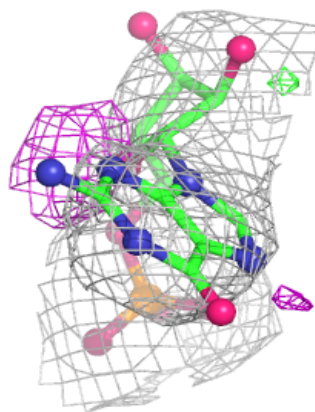
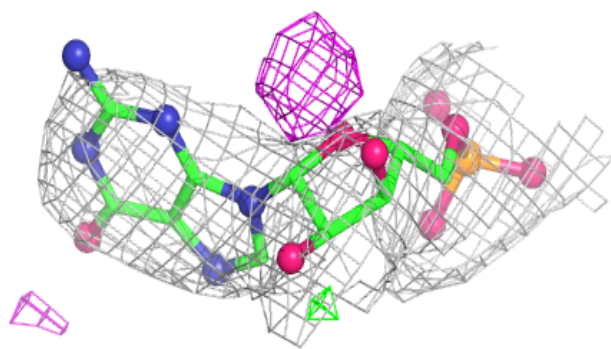
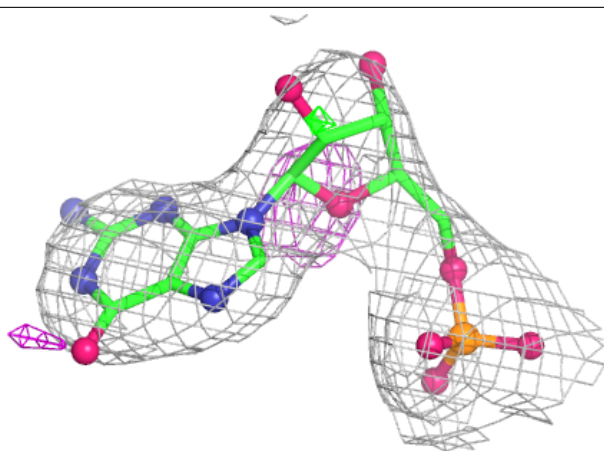
Electron density around G Z 301:

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



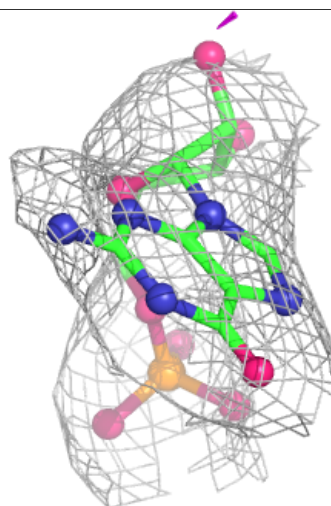
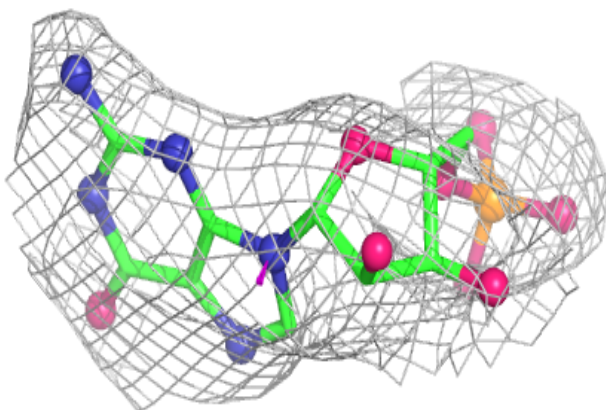
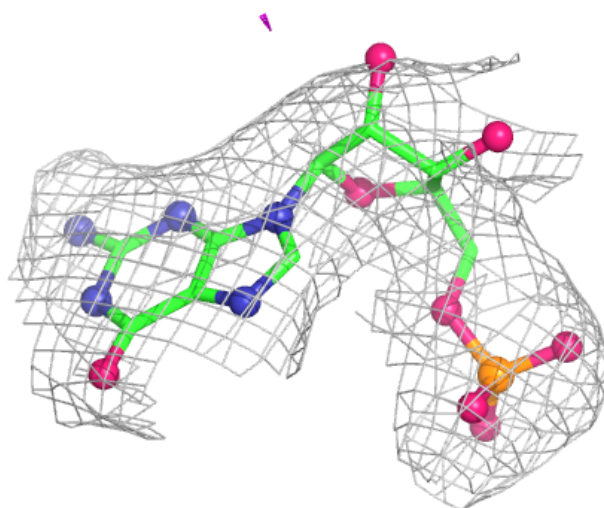
Electron density around G H 301:

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and green (positive)



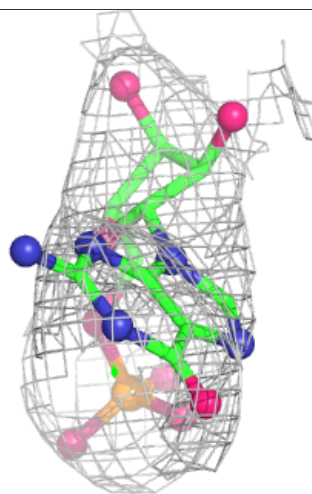
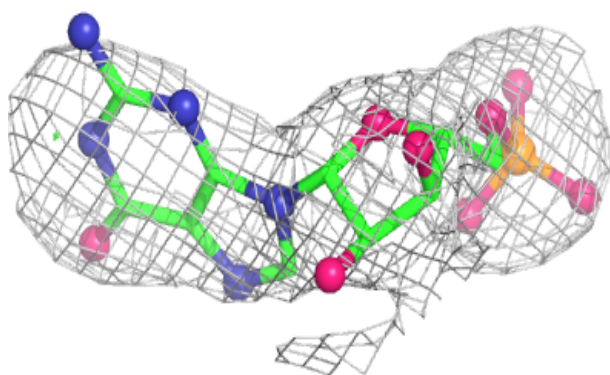
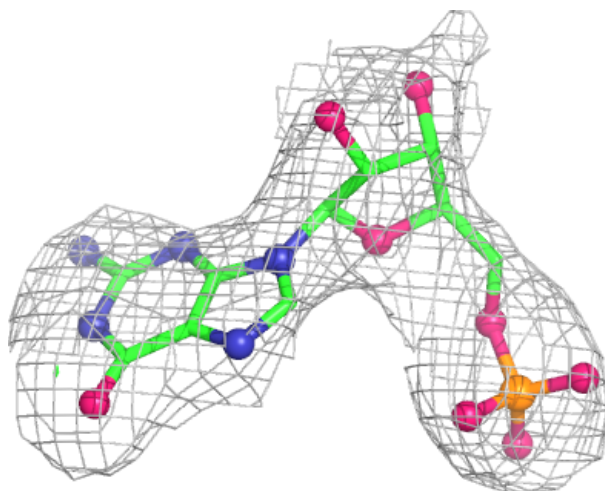
Electron density around G W 301:

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and green (positive)



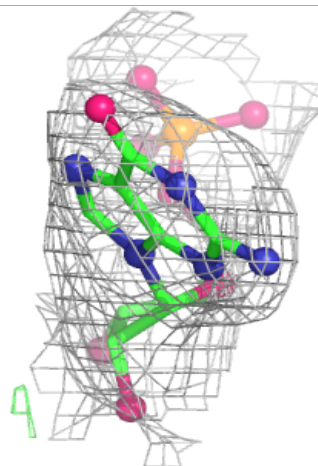
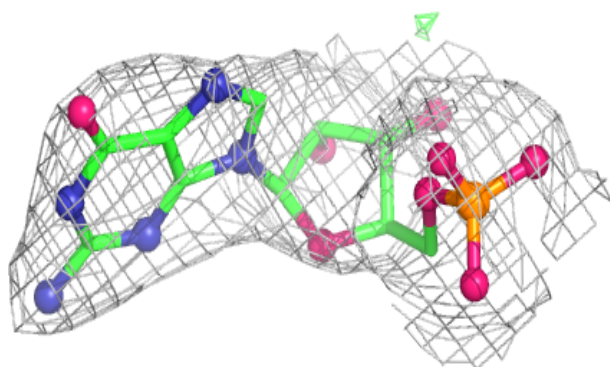
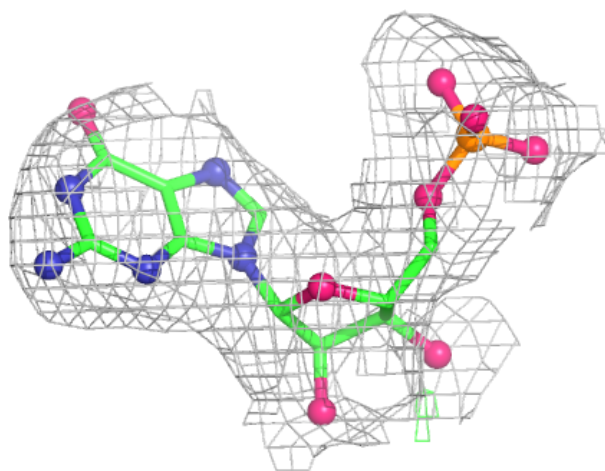
Electron density around G Y 301:

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



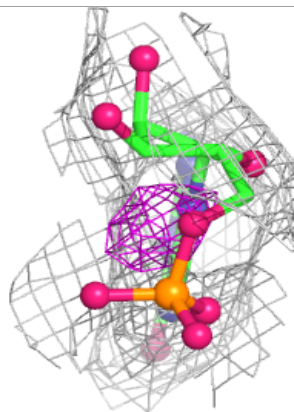
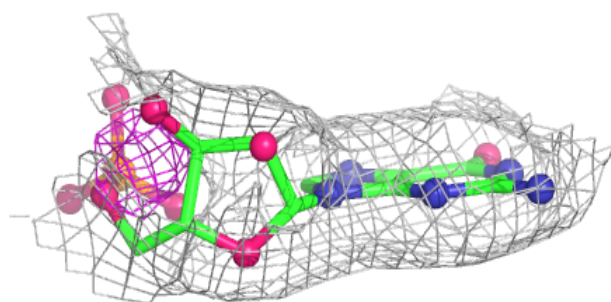
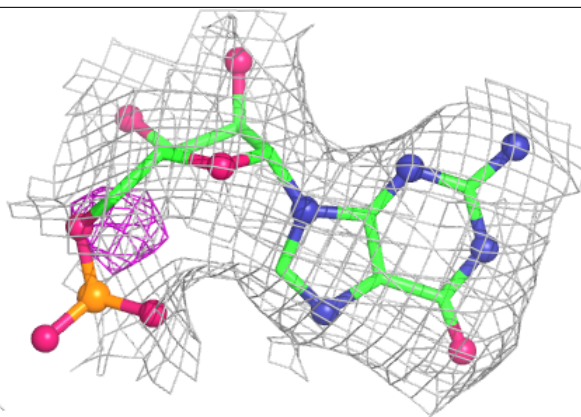
Electron density around G CC 301:

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



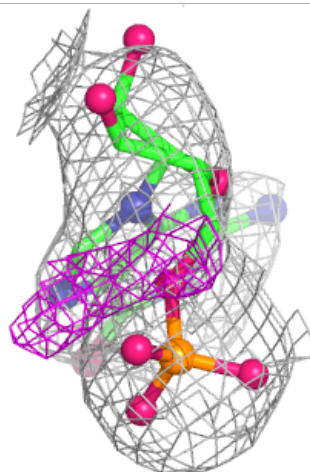
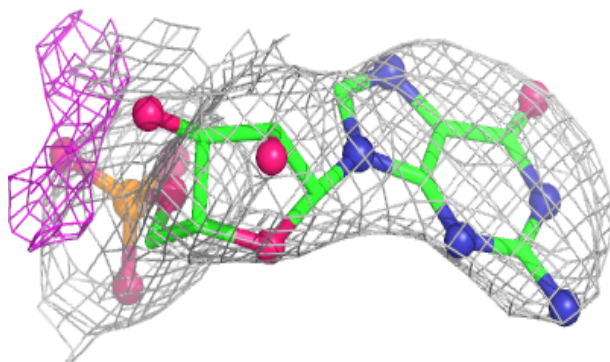
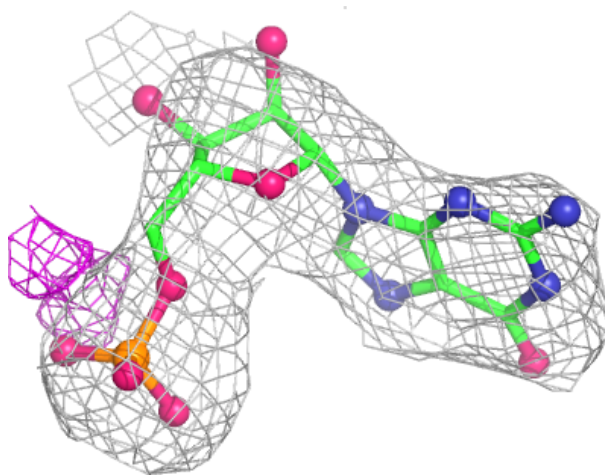
Electron density around G W 302:

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



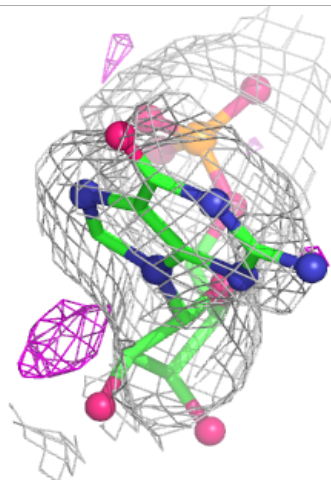
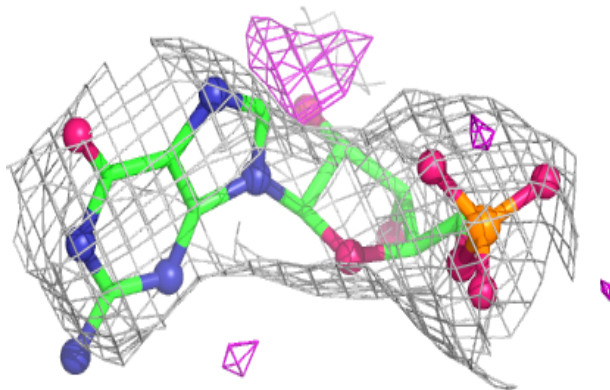
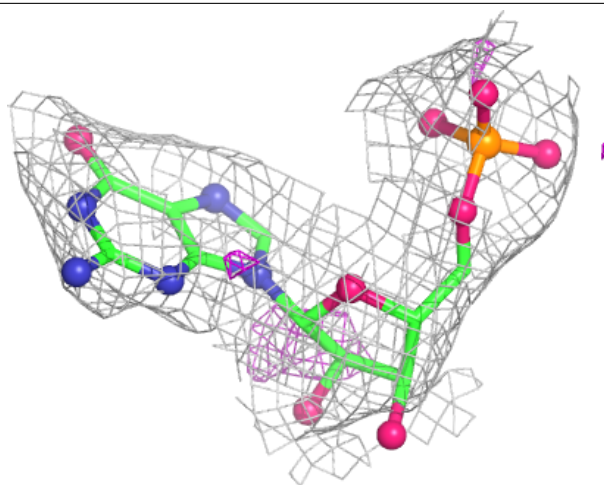
Electron density around G F 301:

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



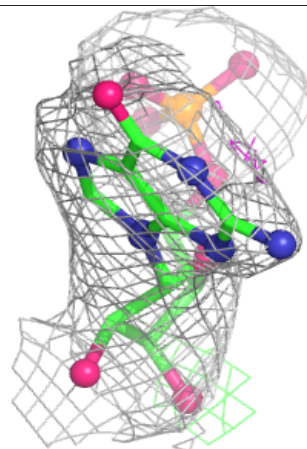
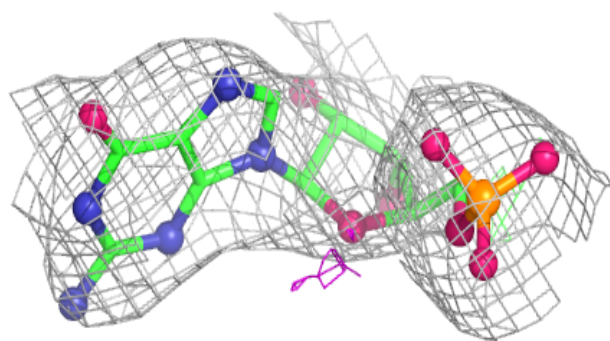
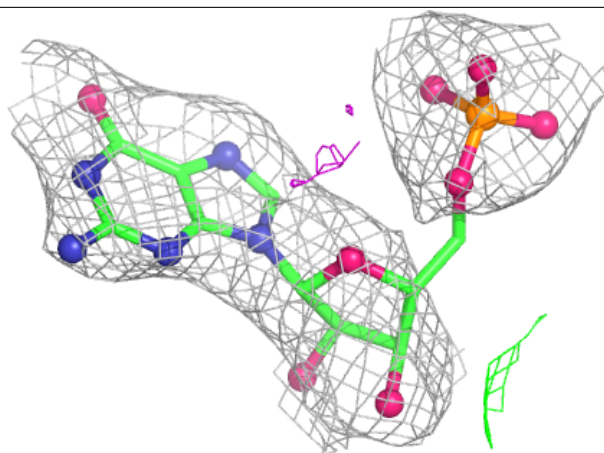
Electron density around G B 301:

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



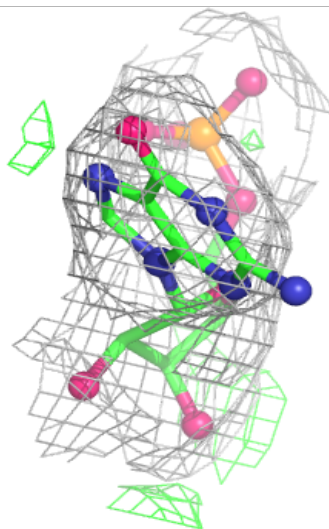
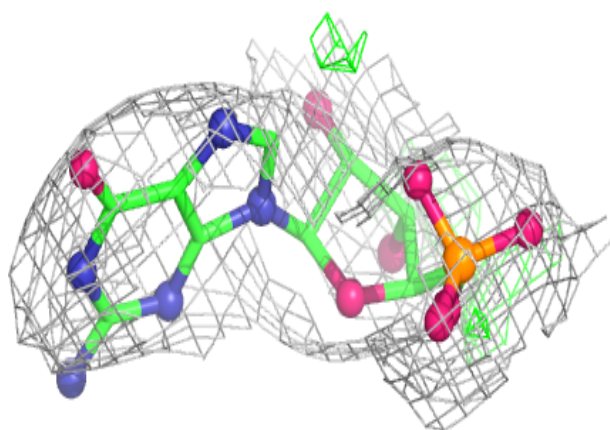
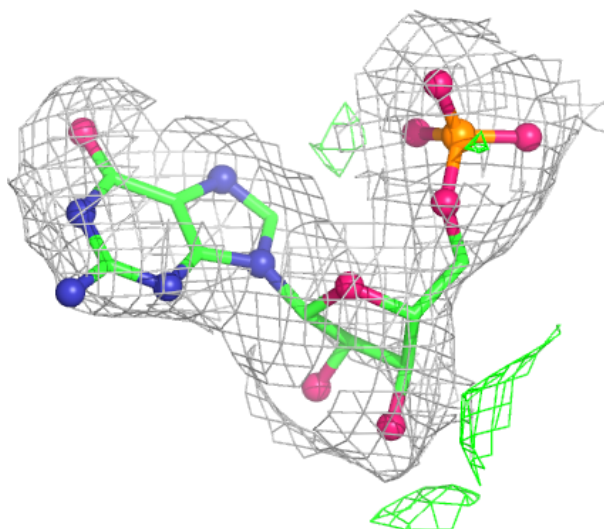
Electron density around G E 301:

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



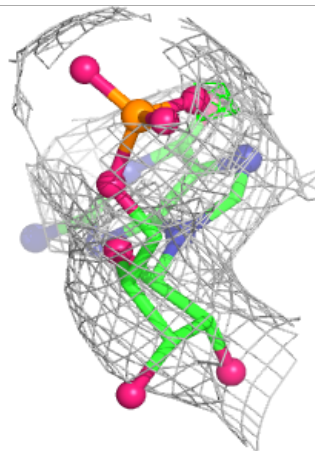
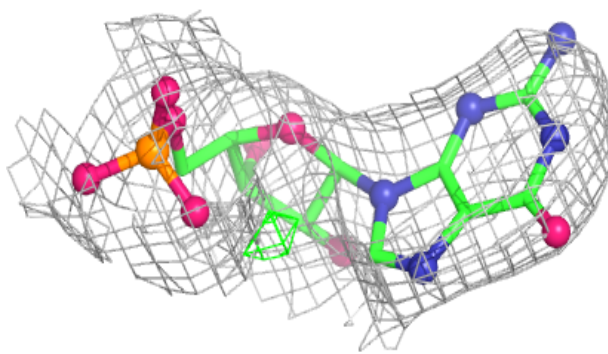
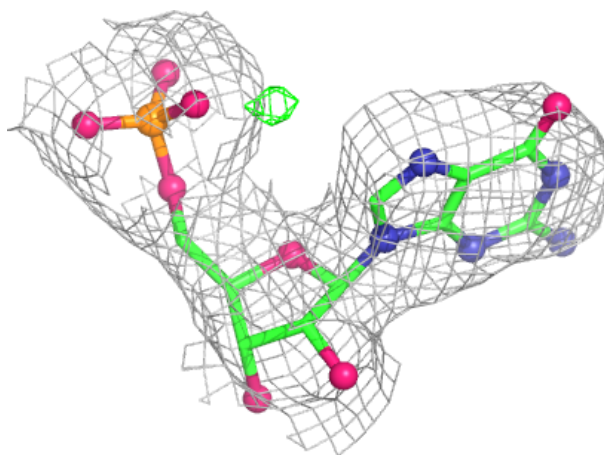
Electron density around G H 303:

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



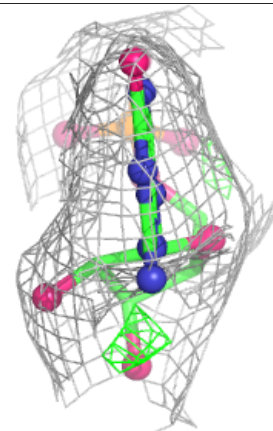
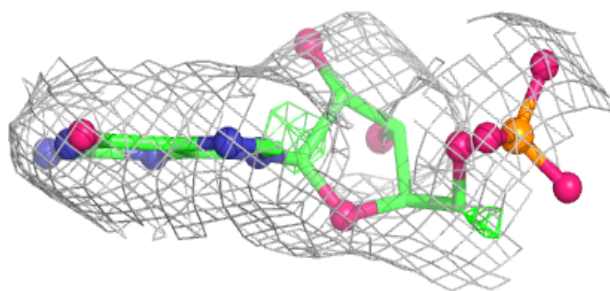
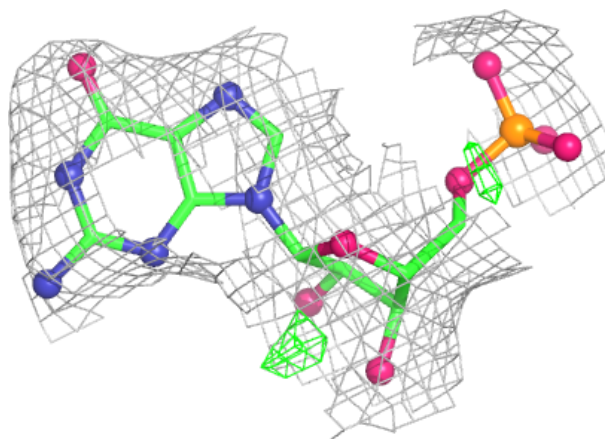
Electron density around G L 301:

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



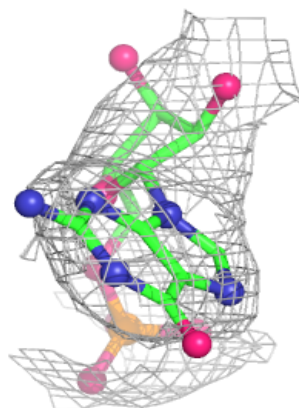
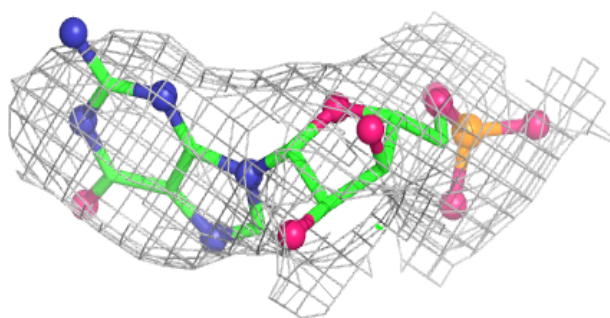
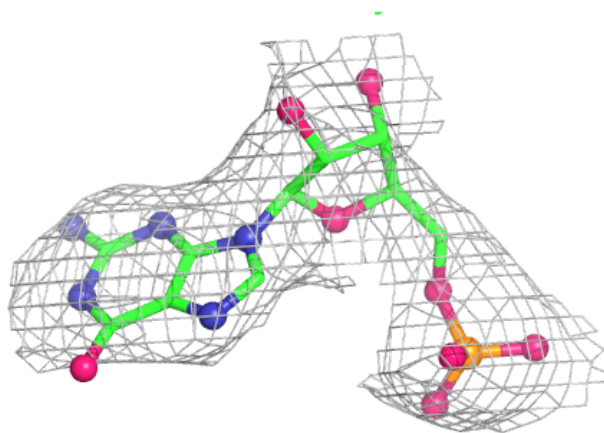
Electron density around G CC 302:

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



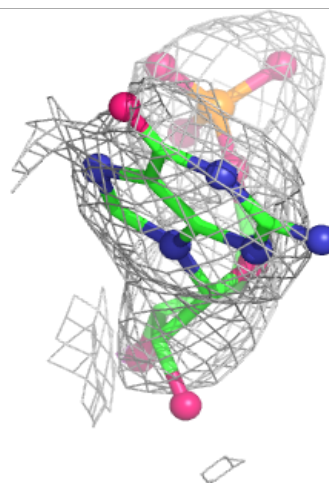
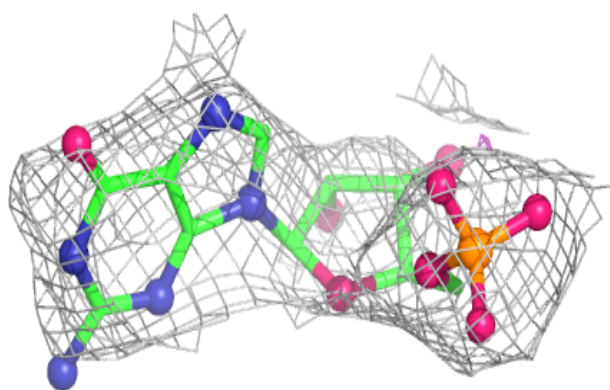
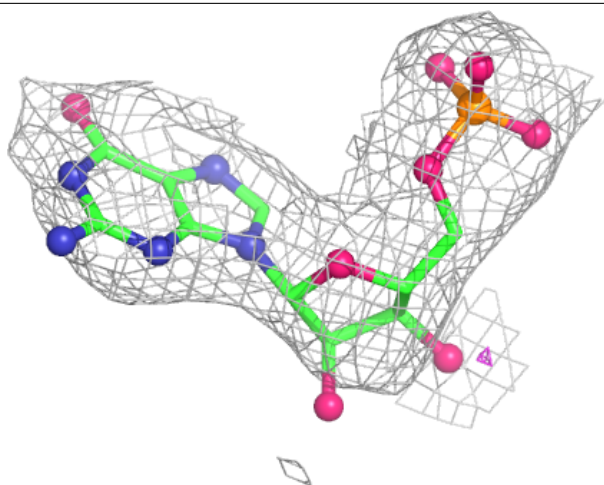
Electron density around G DD 301:

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



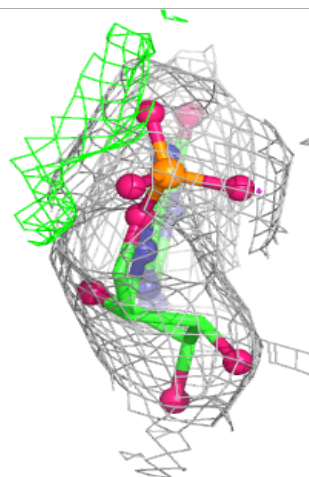
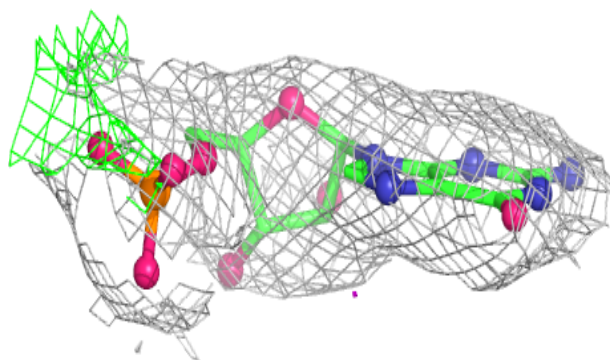
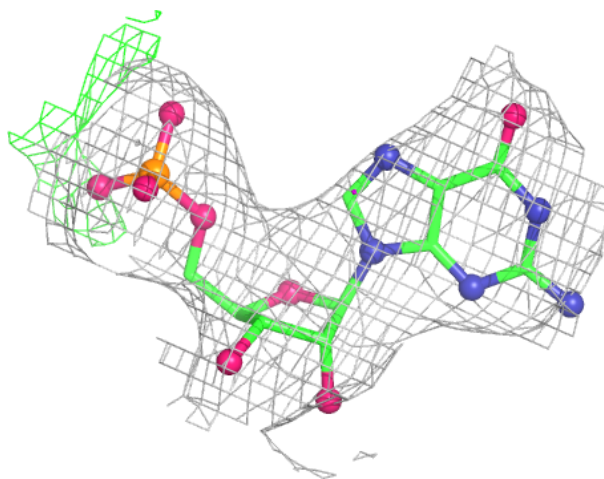
Electron density around G N 301:

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



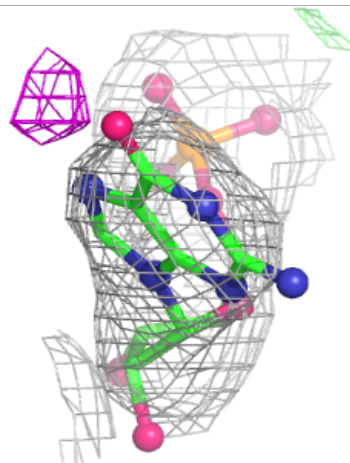
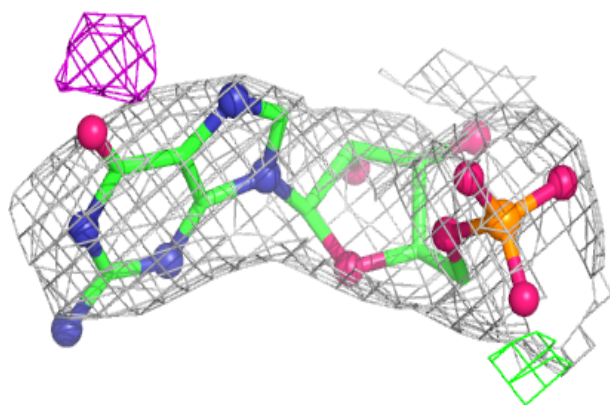
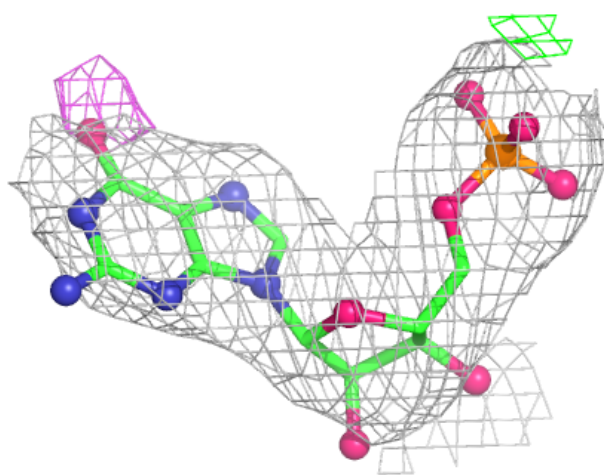
Electron density around G T 302:

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



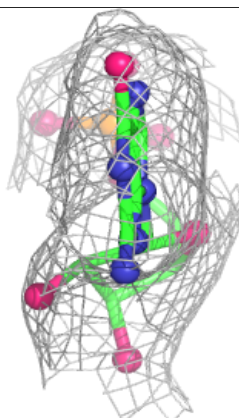
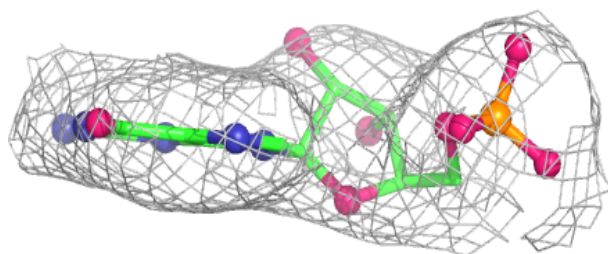
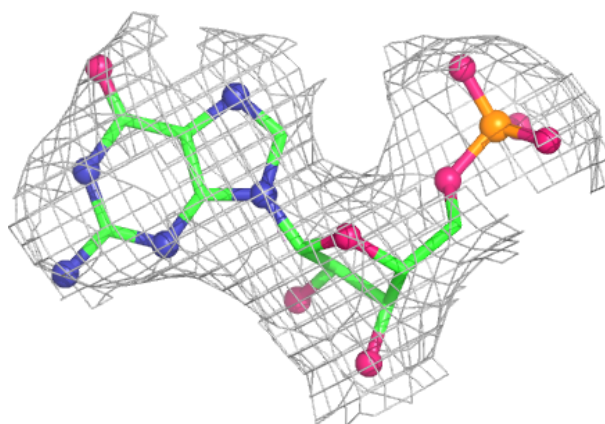
Electron density around G U 301:

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



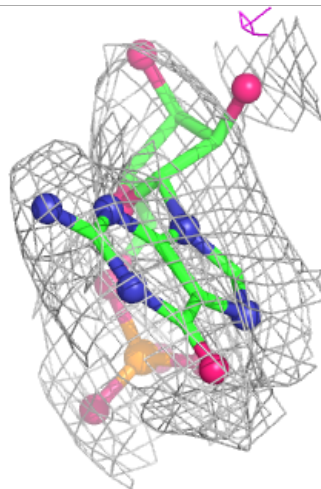
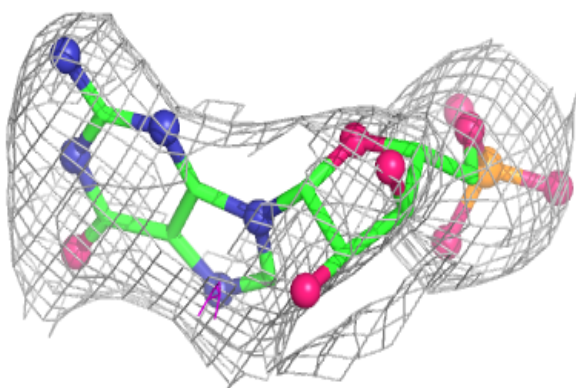
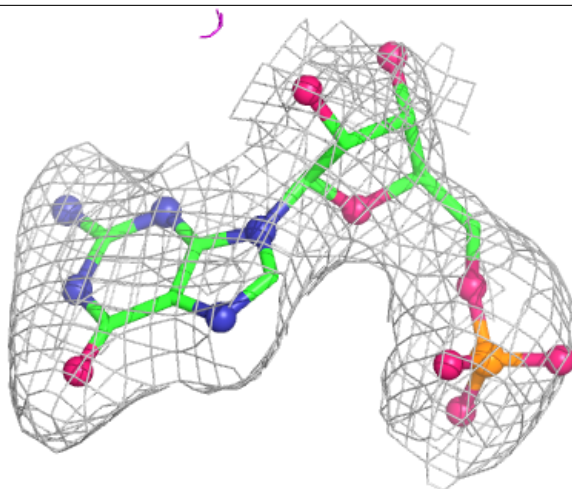
Electron density around G U 302:

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



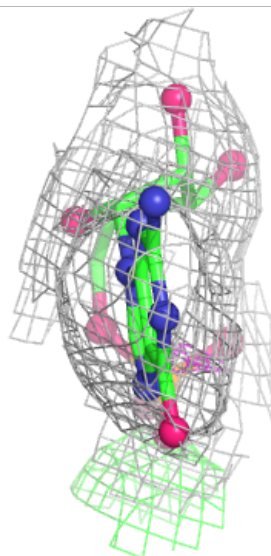
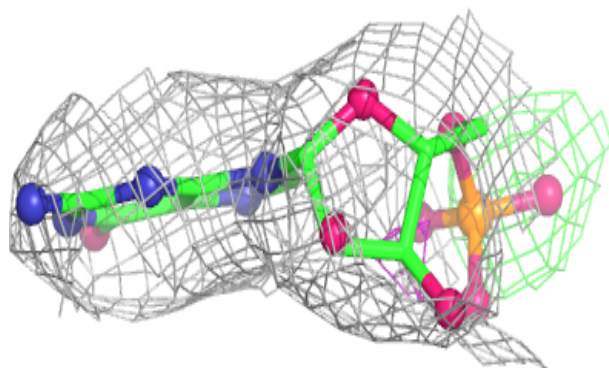
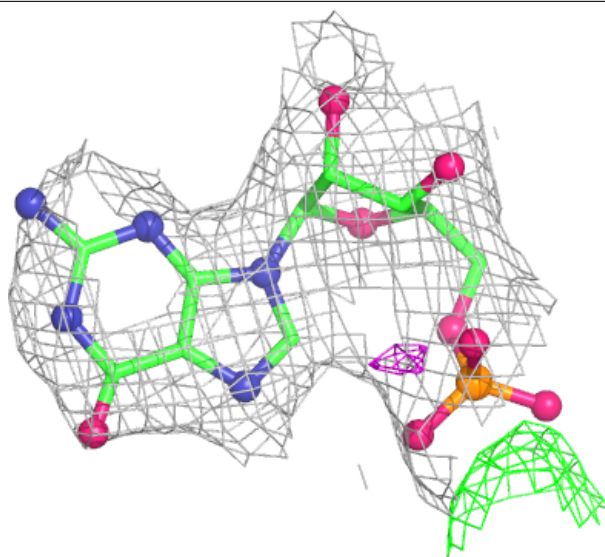
Electron density around G D 301:

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



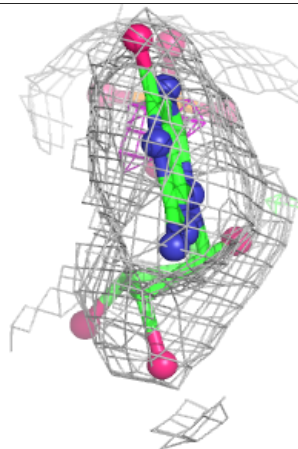
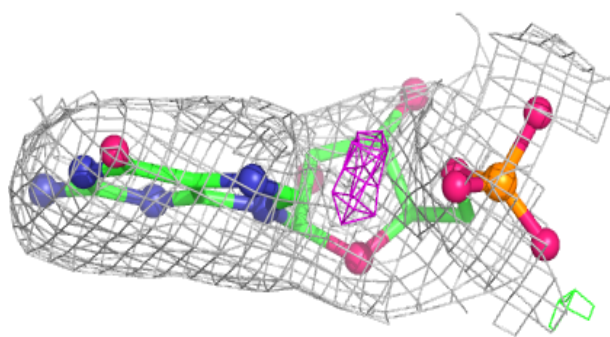
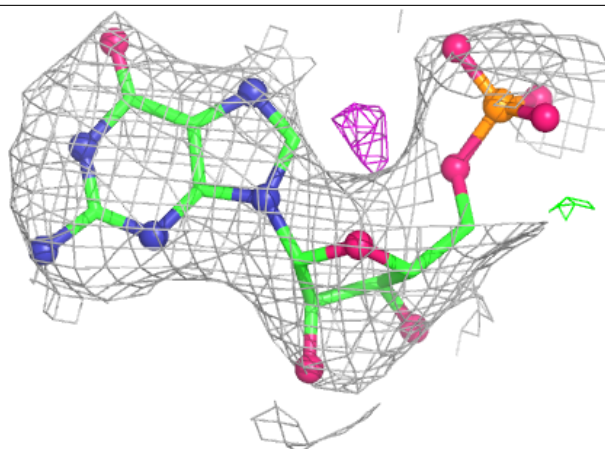
Electron density around G FF 302:

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



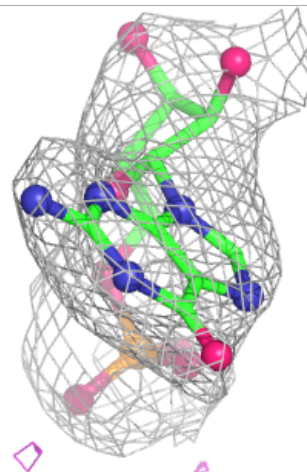
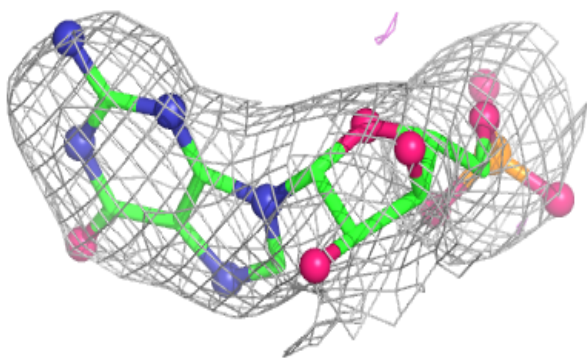
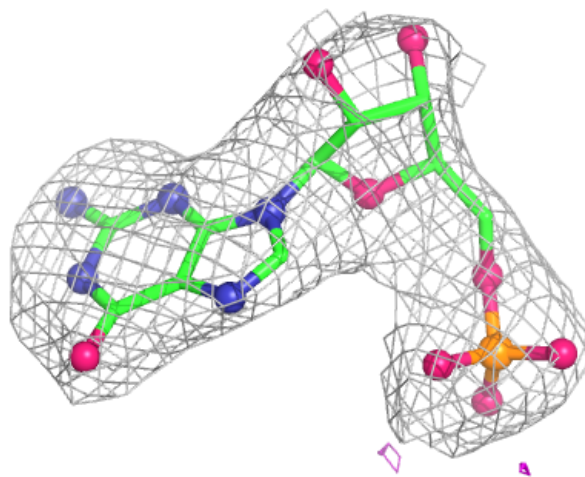
Electron density around G J 301:

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



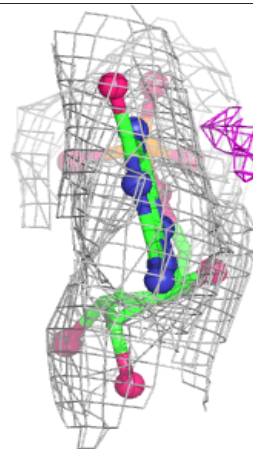
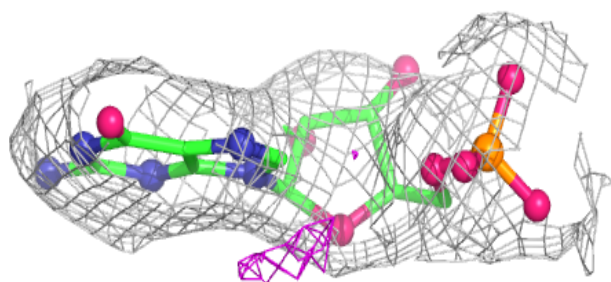
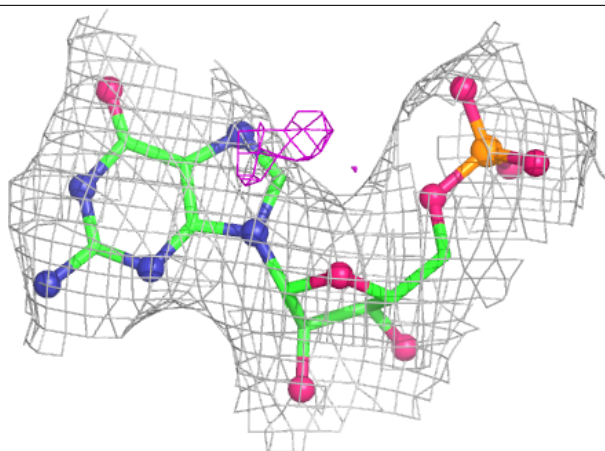
Electron density around G J 302:

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

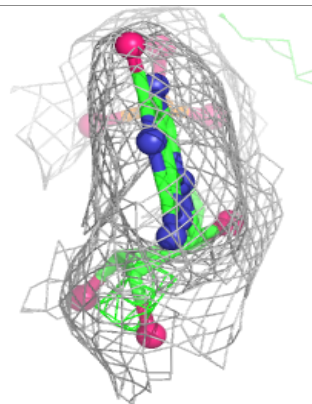
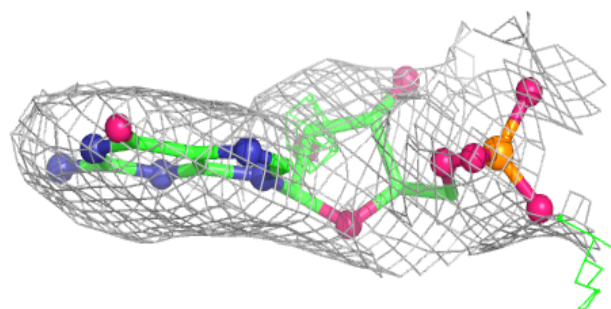
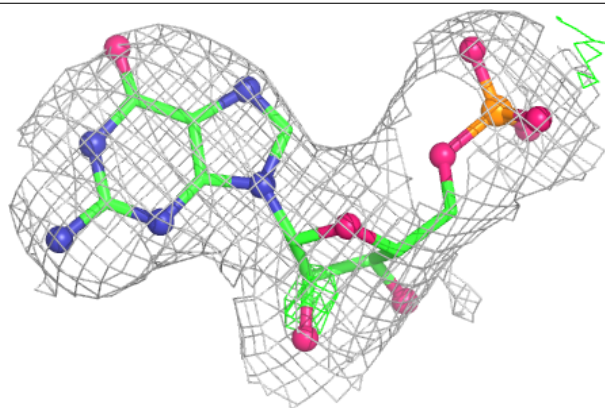


Electron density around G B 302:

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

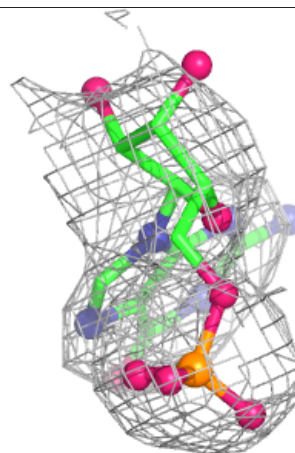
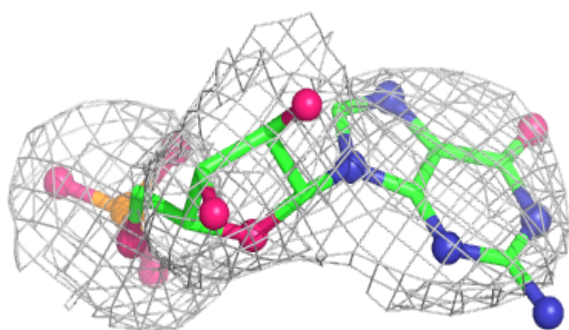
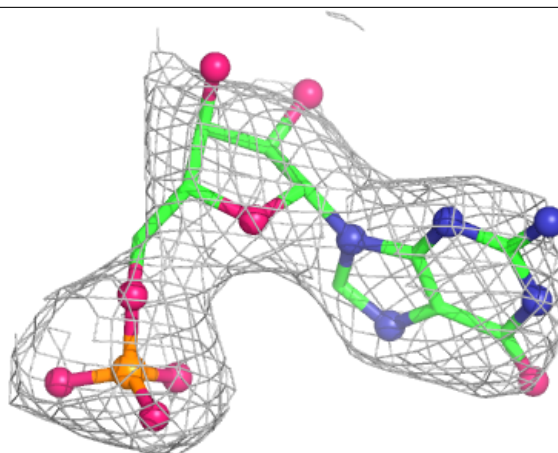
**Electron density around G P 302:**

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



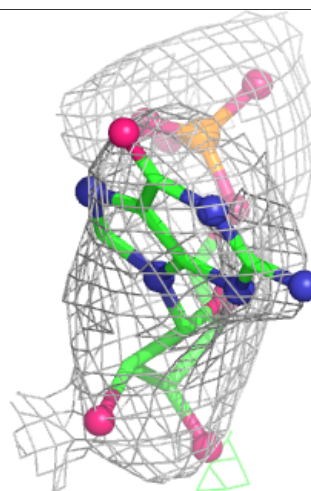
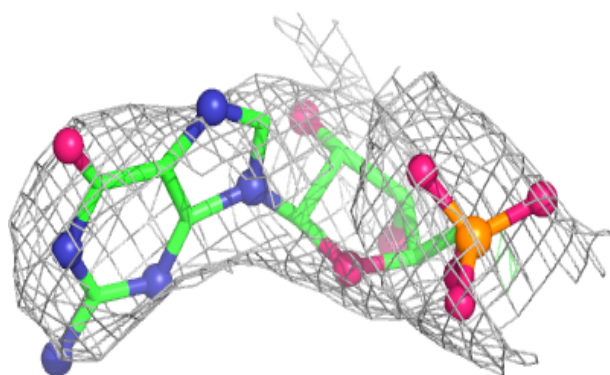
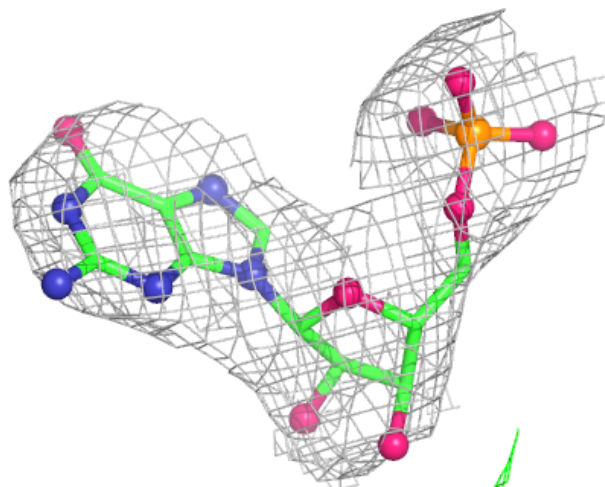
Electron density around G Q 301:

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



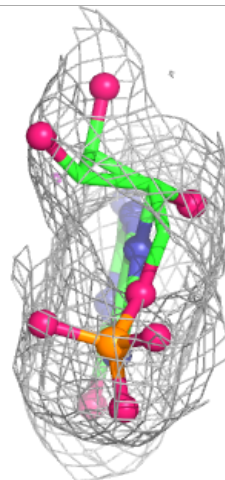
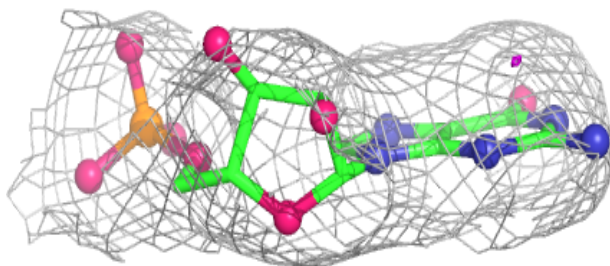
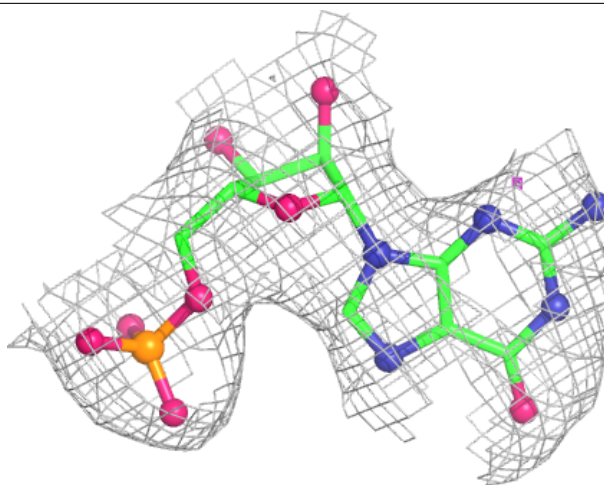
Electron density around G P 301:

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



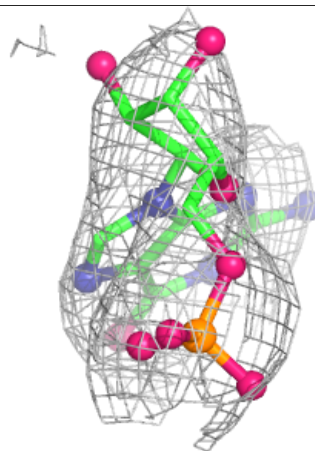
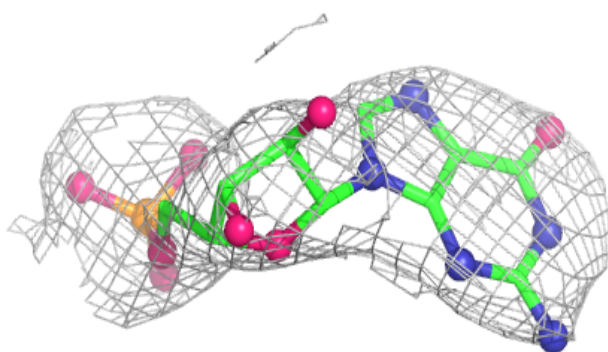
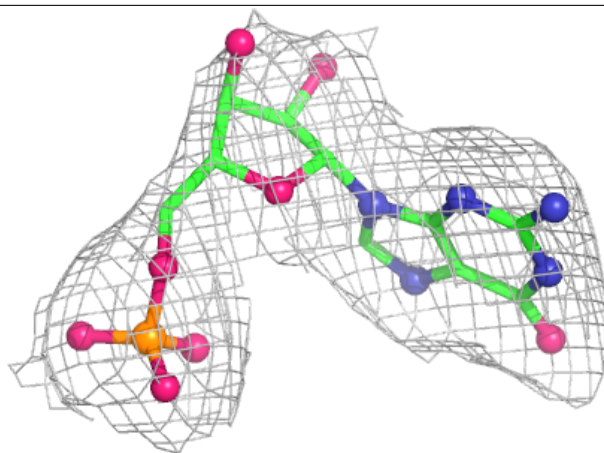
Electron density around G Y 303:

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



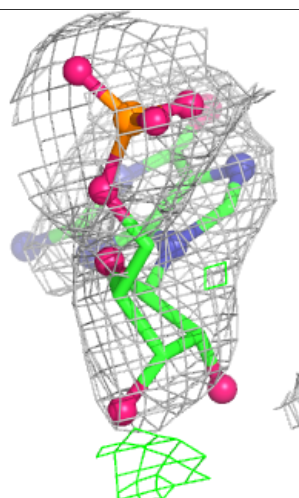
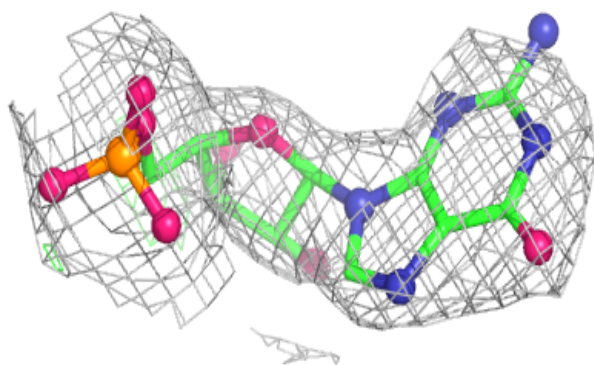
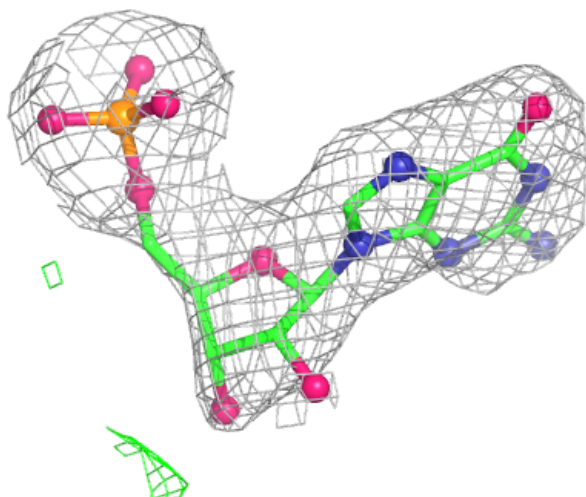
Electron density around G S 301:

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



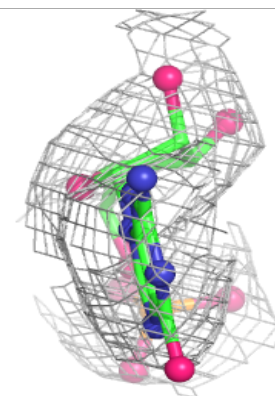
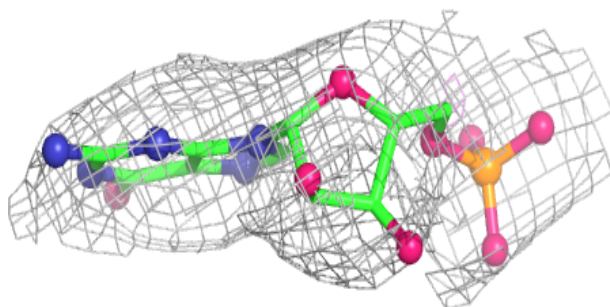
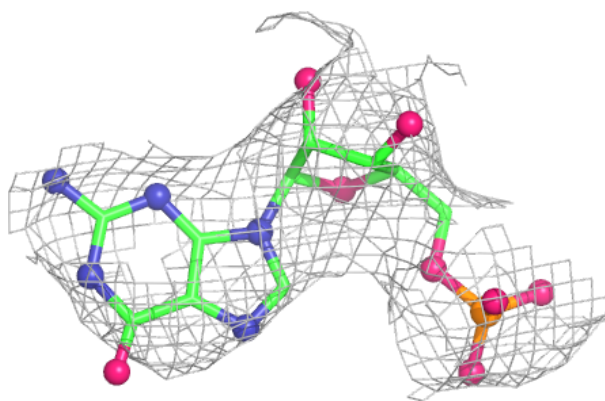
Electron density around G T 301:

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



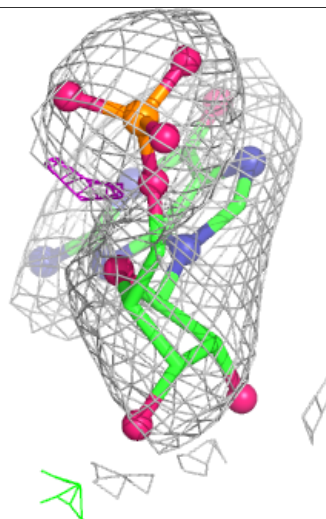
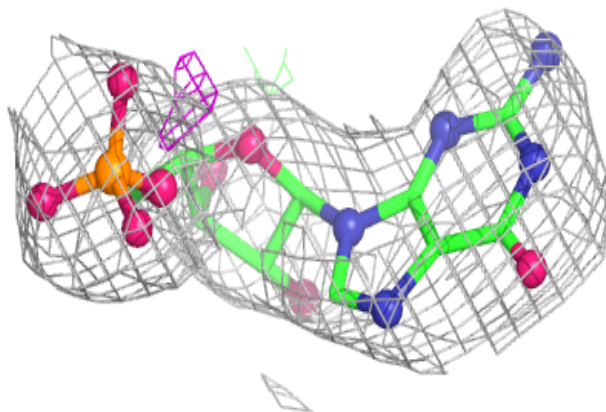
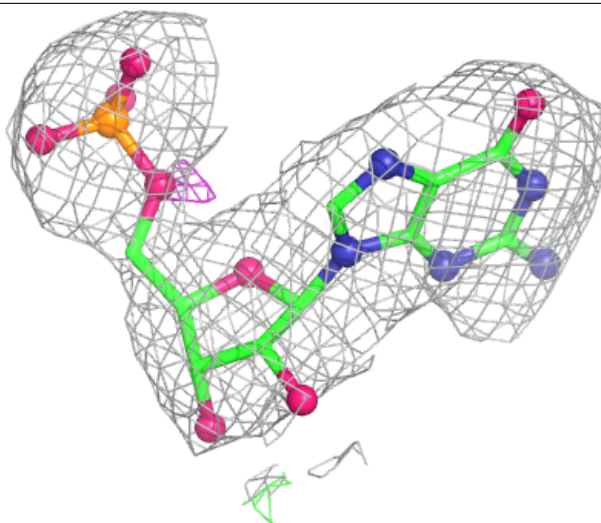
Electron density around G F 302:

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



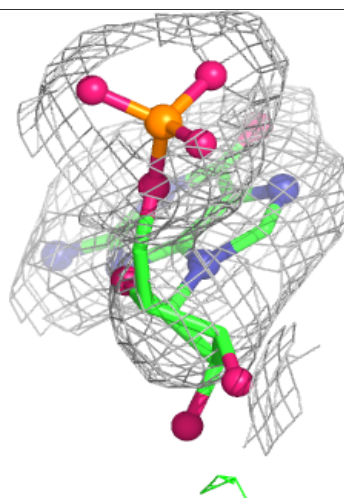
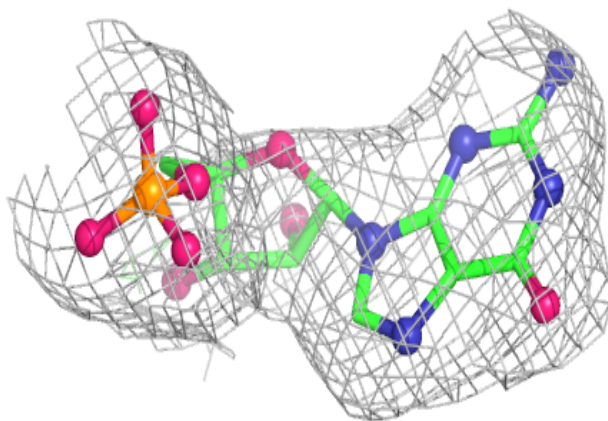
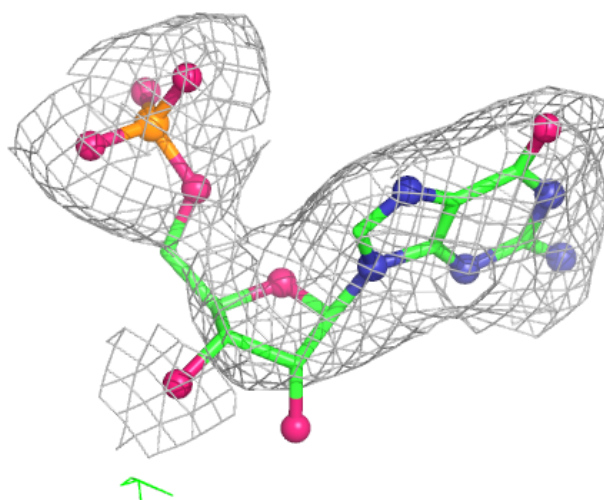
Electron density around G G 301:

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



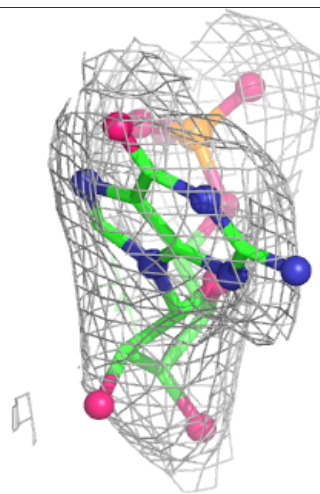
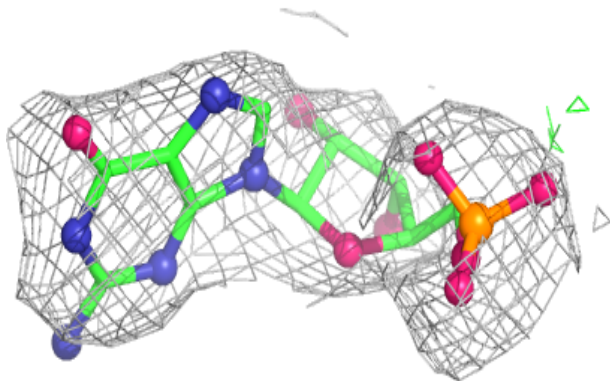
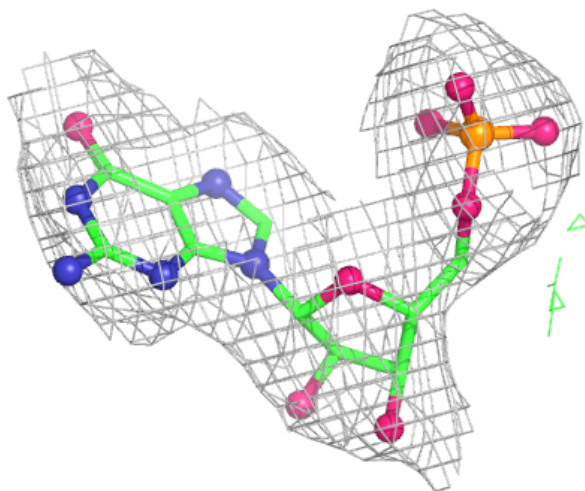
Electron density around G X 301:

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



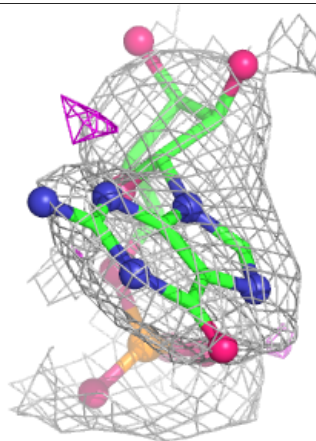
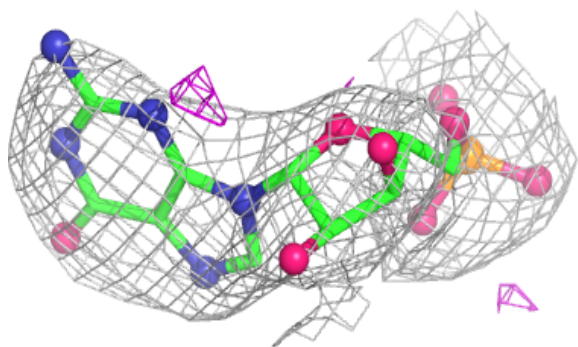
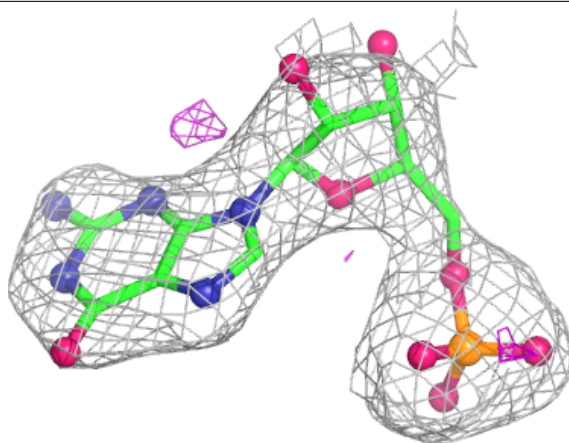
Electron density around G R 301:

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



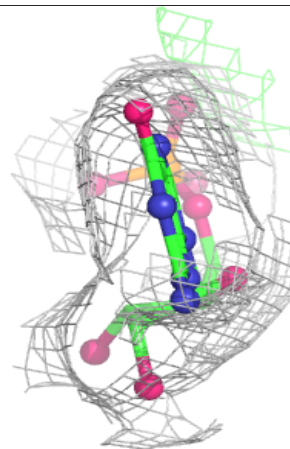
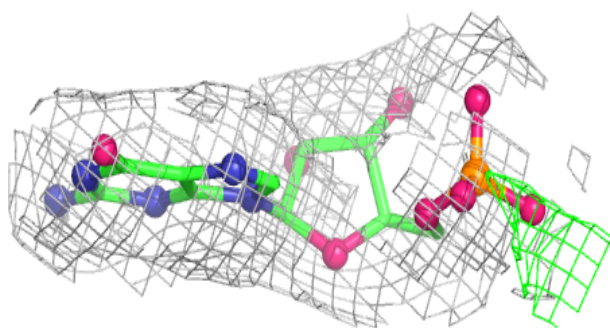
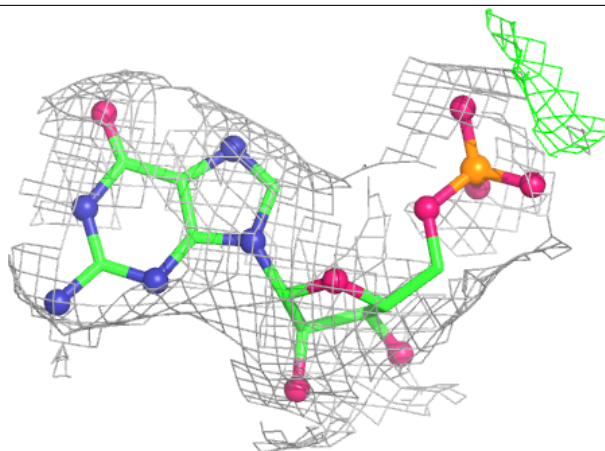
Electron density around G K 301:

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



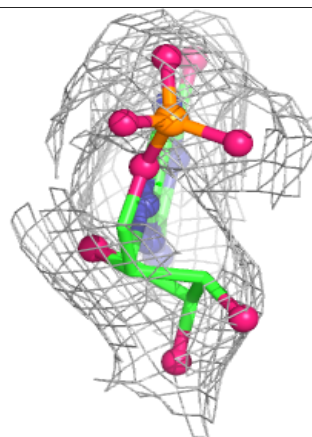
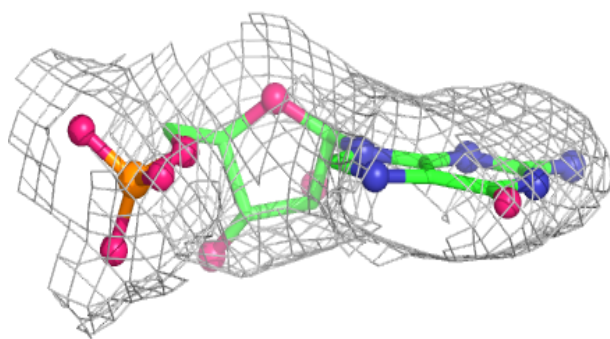
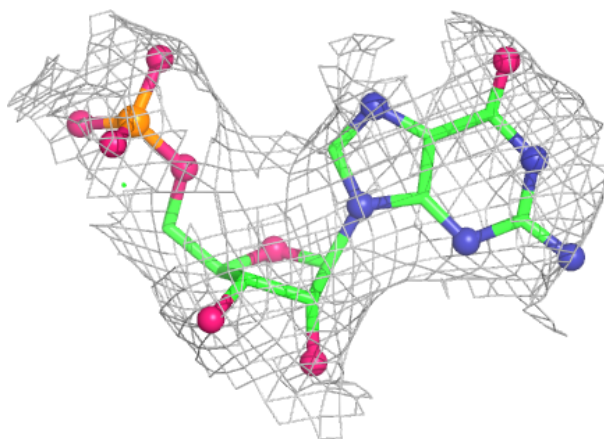
Electron density around G E 302:

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



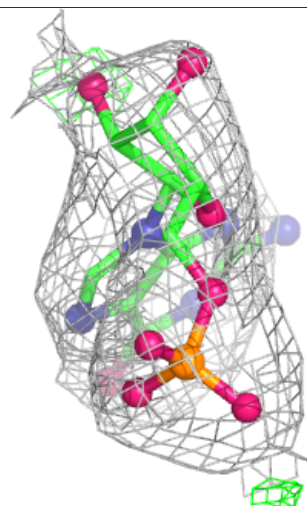
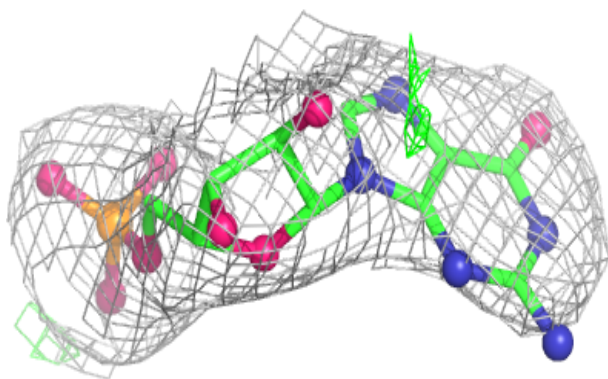
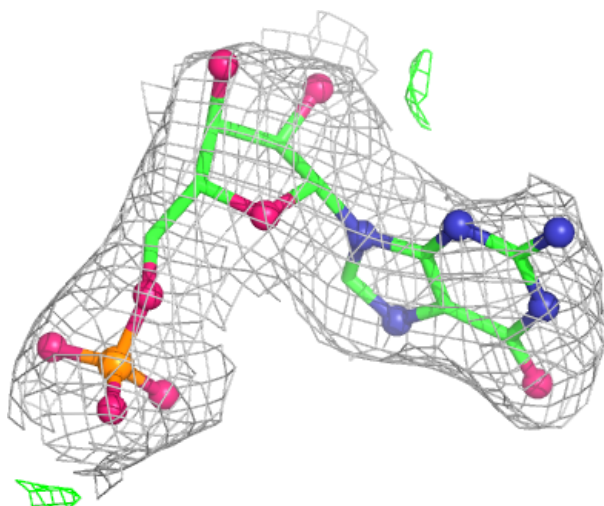
Electron density around G L 302:

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



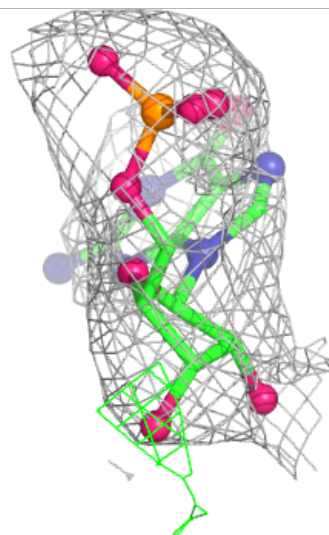
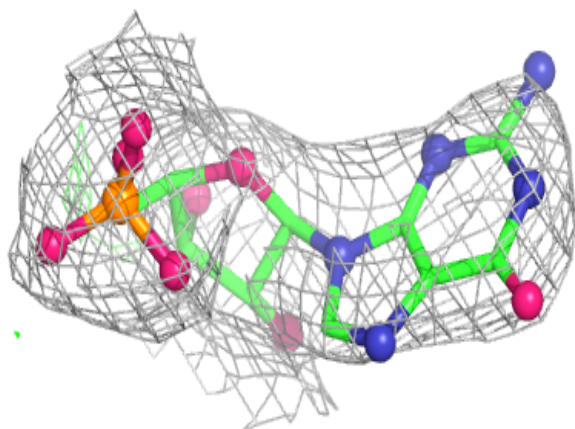
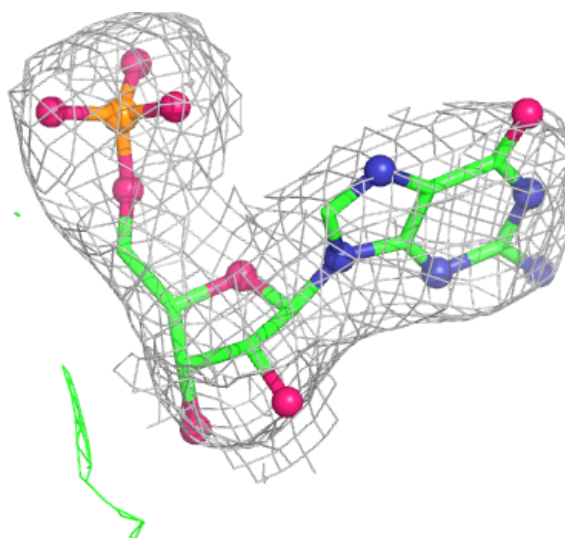
Electron density around G L 303:

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



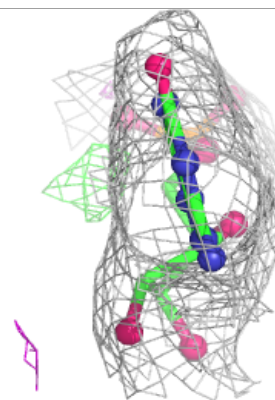
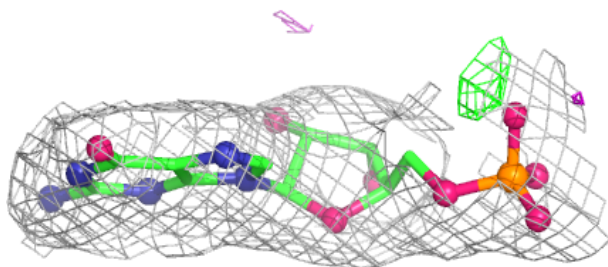
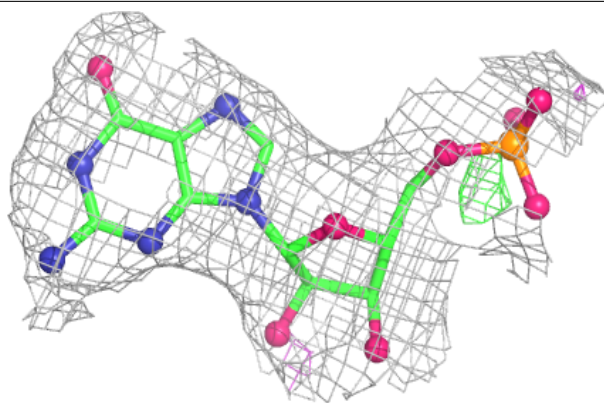
Electron density around G A 302:

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



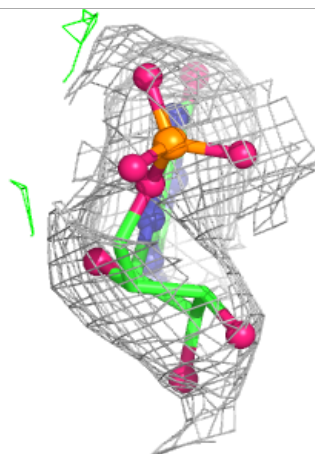
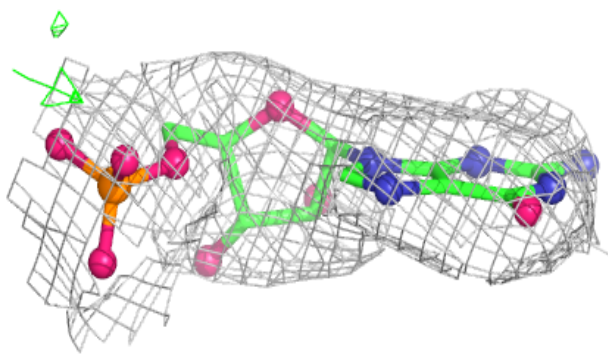
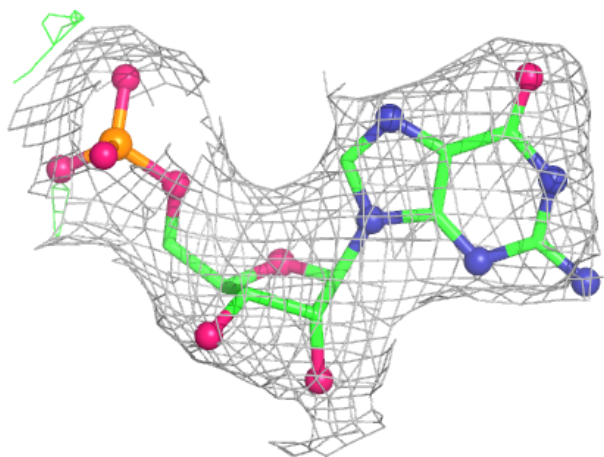
Electron density around G G 302:

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



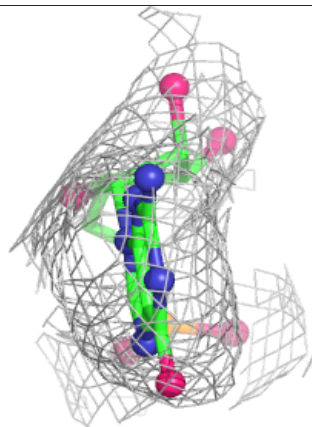
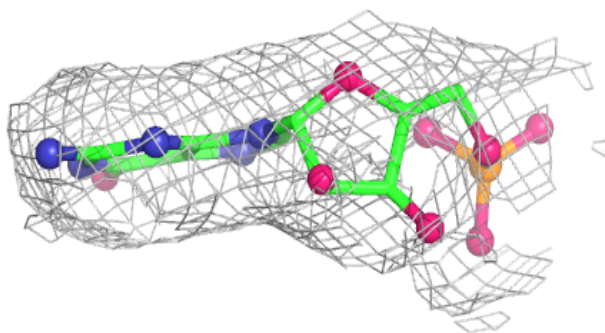
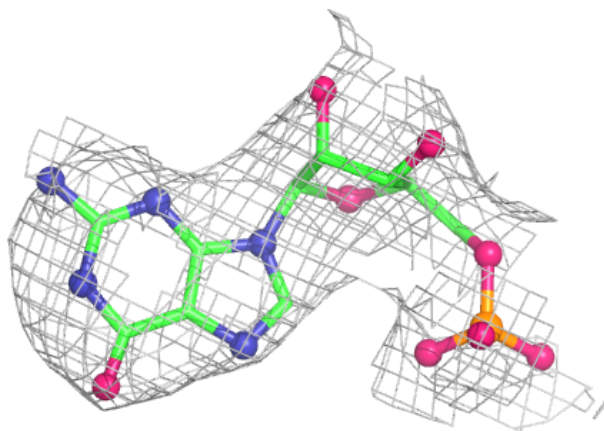
Electron density around G X 302:

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



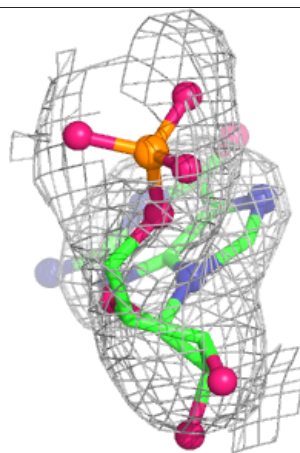
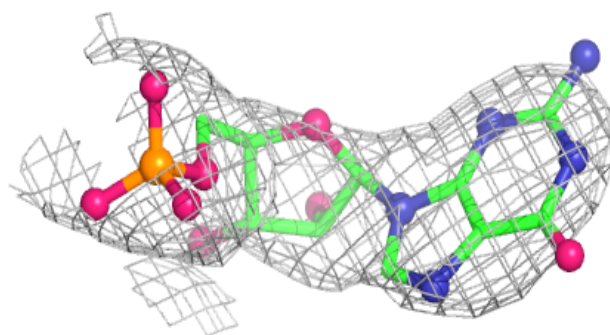
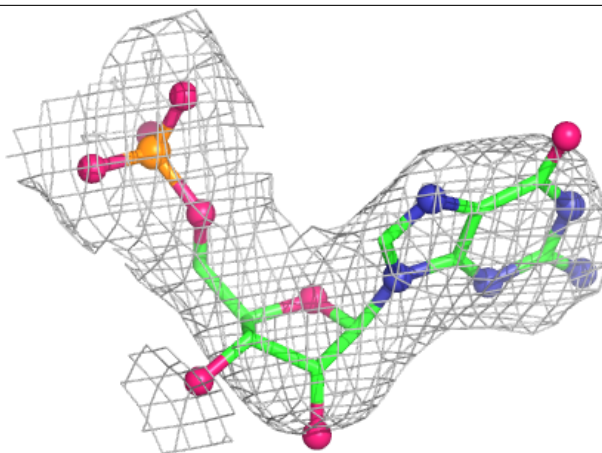
Electron density around G Q 302:

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



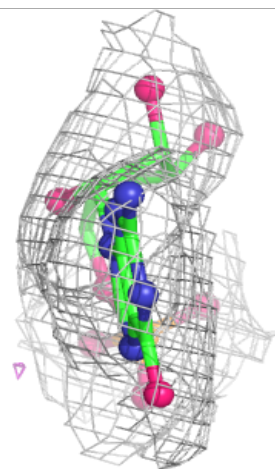
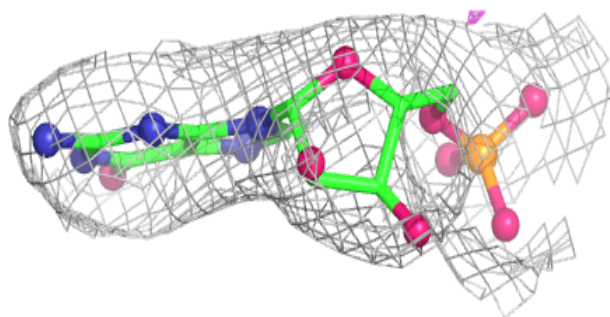
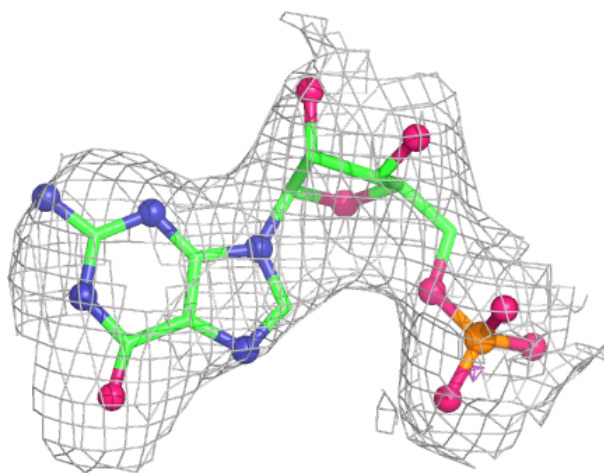
Electron density around G O 301:

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



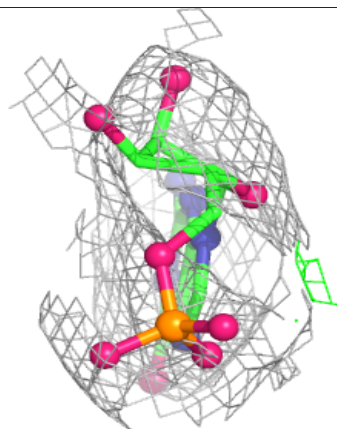
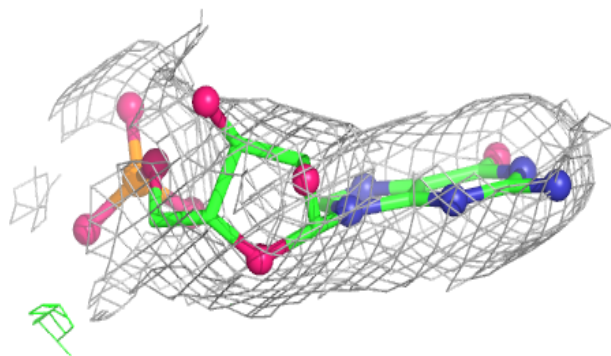
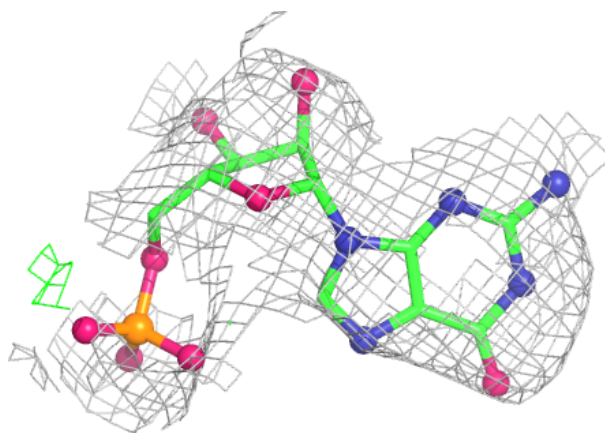
Electron density around G A 301:

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



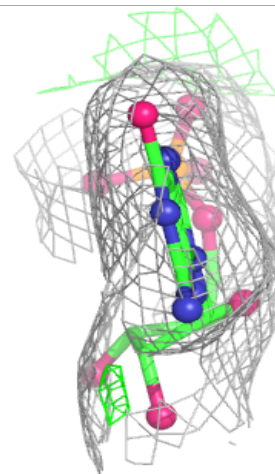
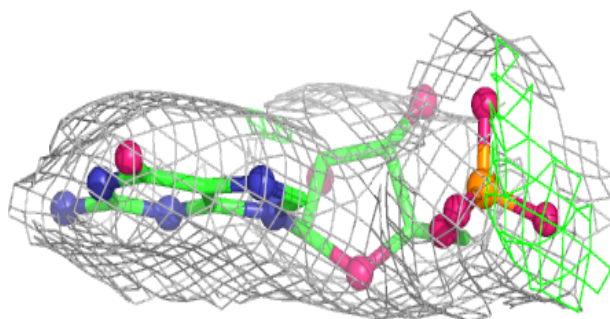
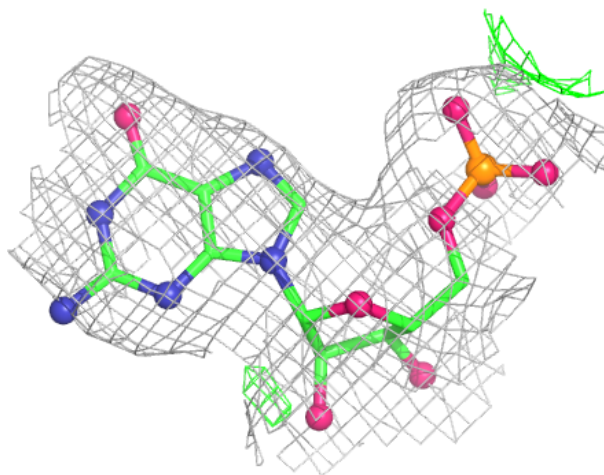
Electron density around G H 302:

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



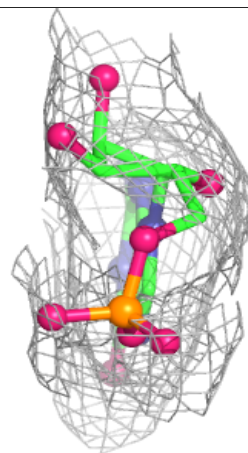
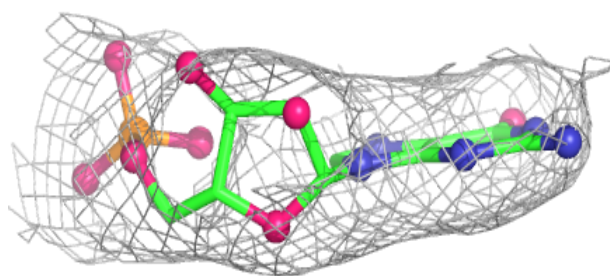
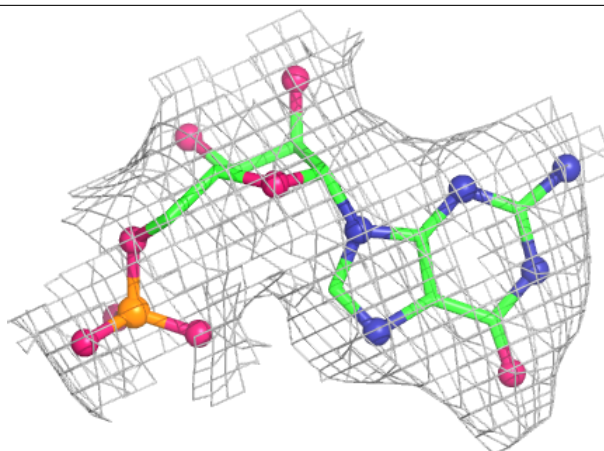
Electron density around G R 302:

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



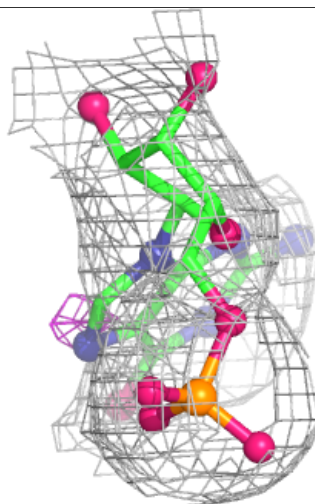
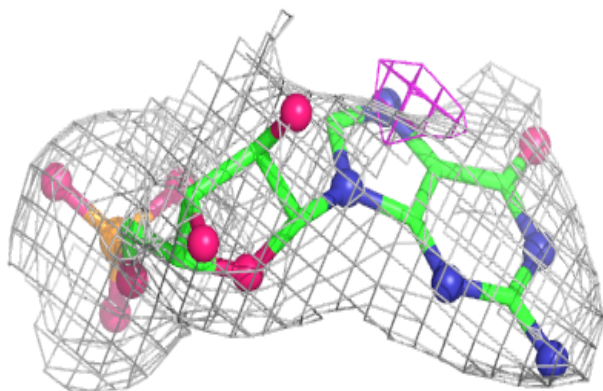
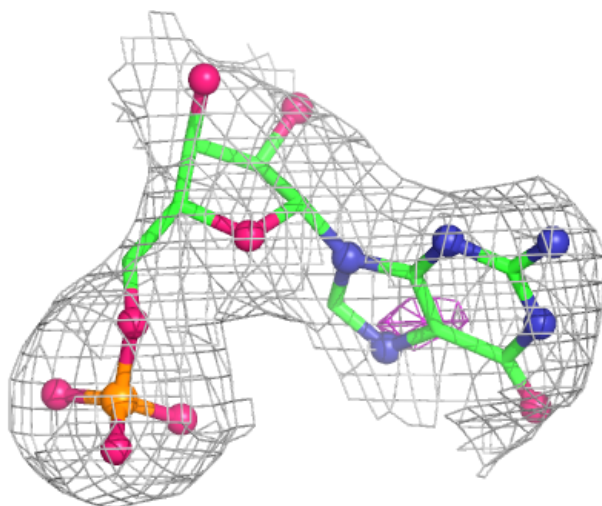
Electron density around G O 302:

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



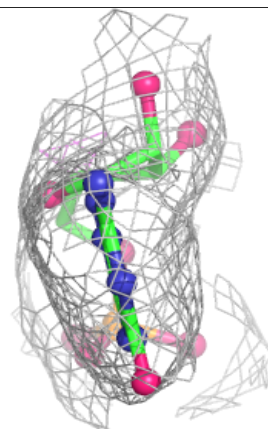
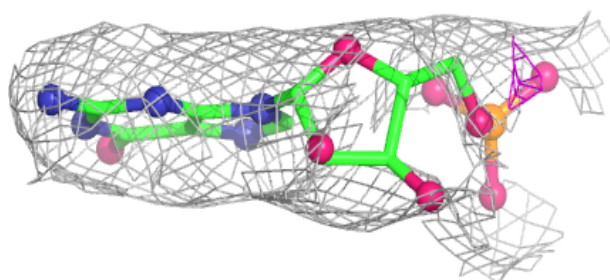
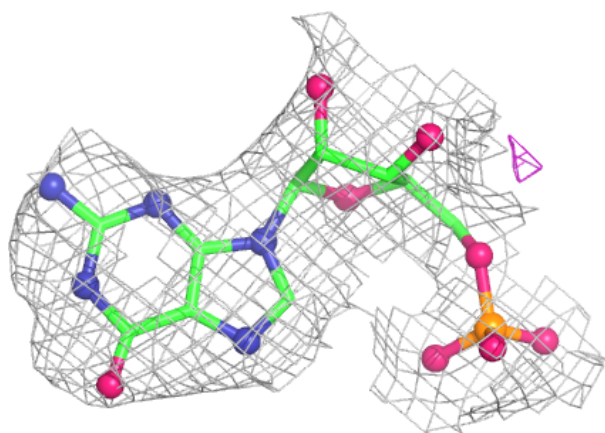
Electron density around G V 301:

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



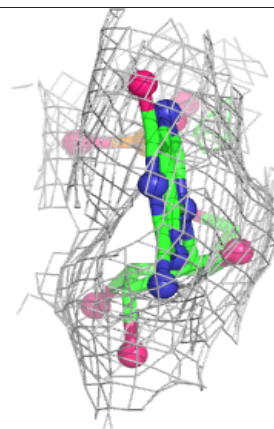
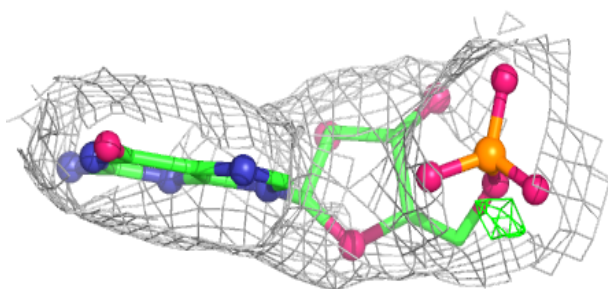
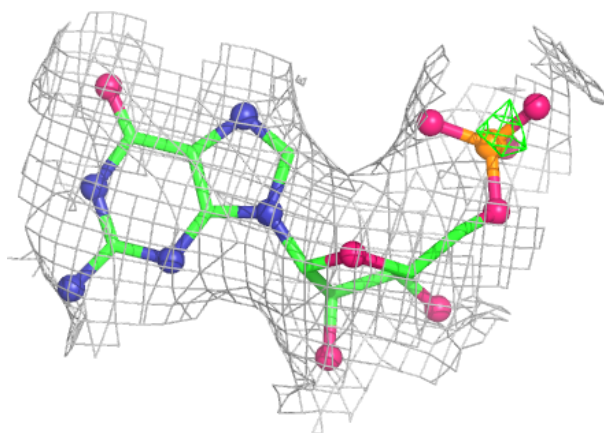
Electron density around G S 302:

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



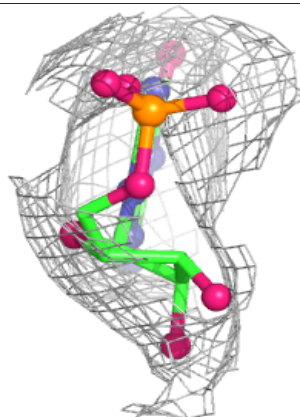
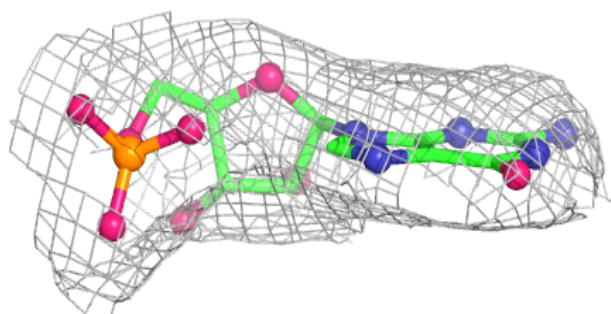
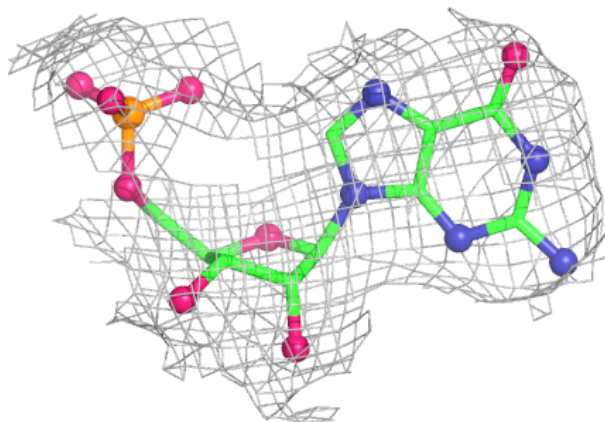
Electron density around G C 301:

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

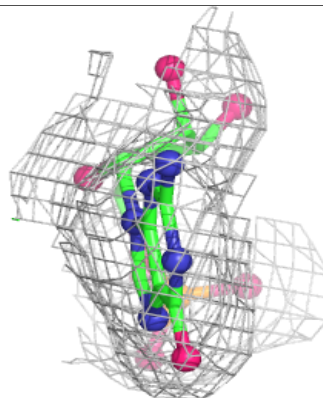
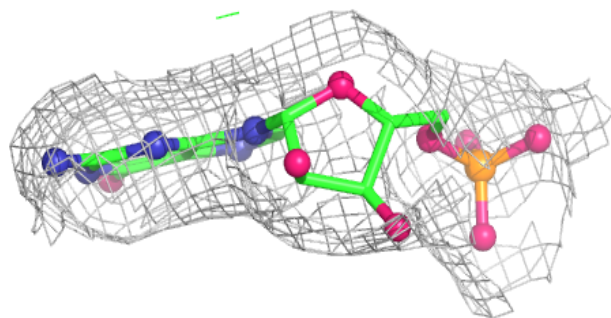
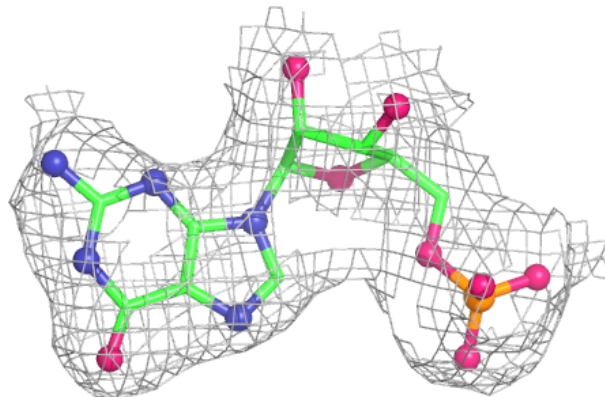


Electron density around G K 302:

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

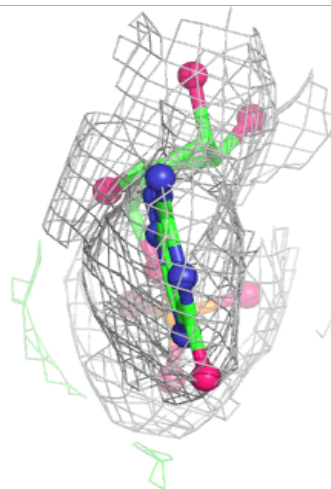
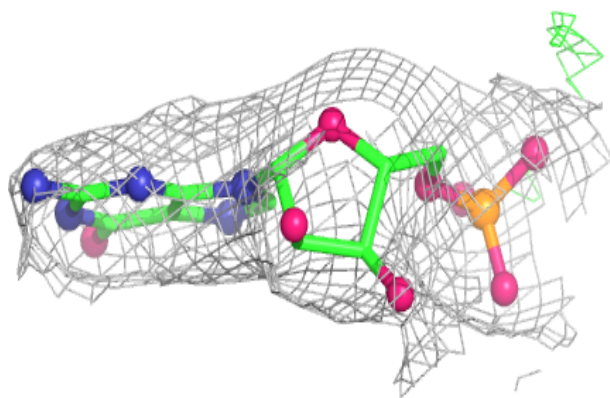
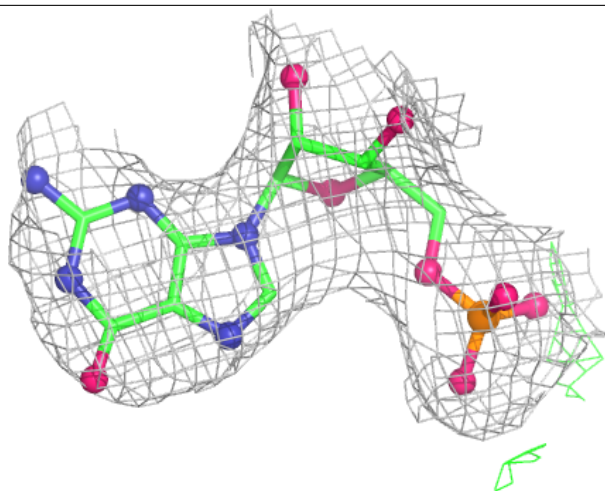
**Electron density around G M 301:**

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



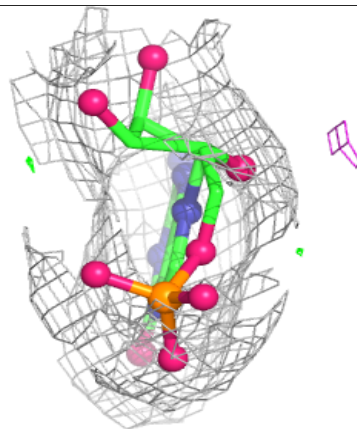
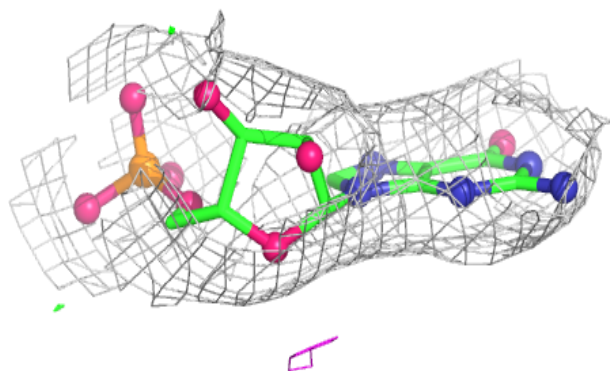
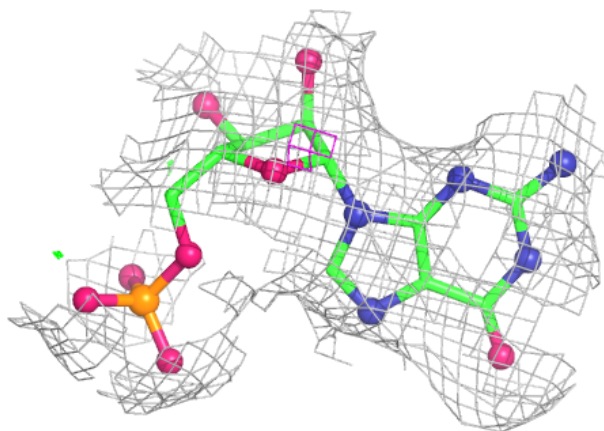
Electron density around G N 302:

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



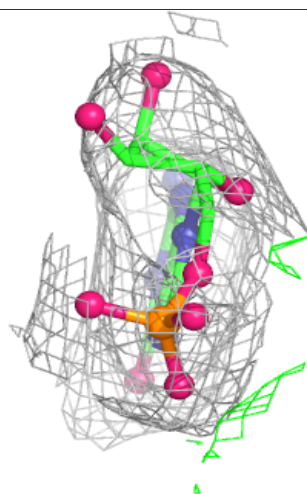
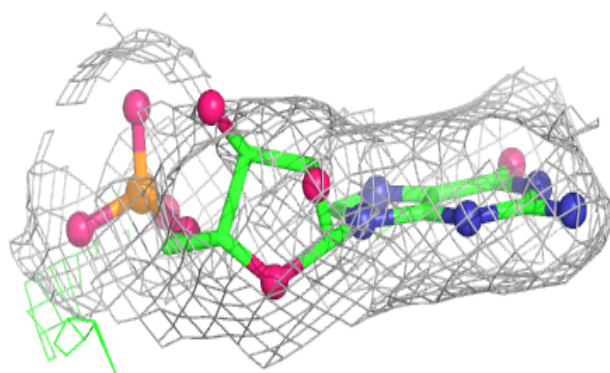
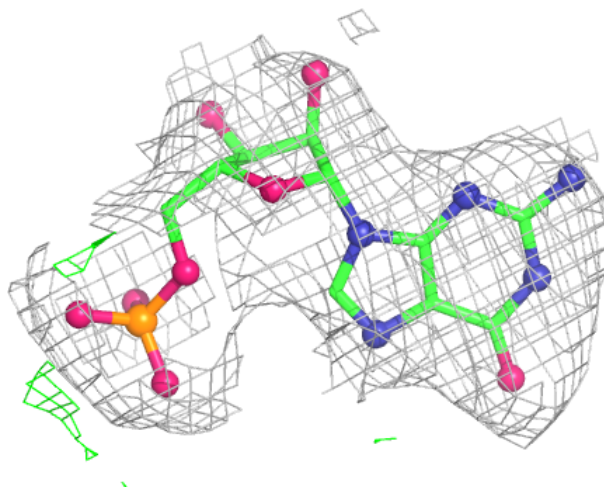
Electron density around G D 302:

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



Electron density around G I 301:

$2mF_o-DF_c$ (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.