



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2026 – 06:07 PM EDT

PDB ID : 9YRE / pdb_00009yre
Title : RNA oligonucleotides containing 4'-(R)-methyl-alpha-(L)-threofuranosyl nucleic acid.
Authors : Harp, J.M.; Egli, M.
Deposited on : 2025-10-16
Resolution : 1.54 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
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)	:	2.51

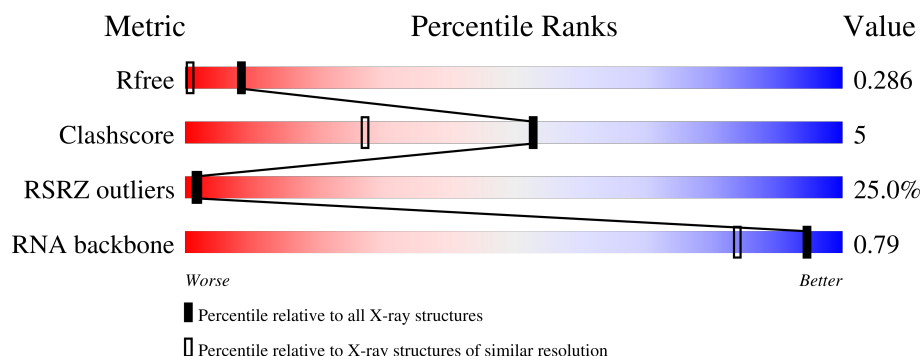
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.54 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	1003 (1.54-1.54)
Clashscore	190562	1025 (1.54-1.54)
RSRZ outliers	180081	1002 (1.54-1.54)
RNA backbone	3983	1008 (2.10-0.98)

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	12	
1	B	12	
1	C	12	
1	D	12	
1	E	12	
1	F	12	

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Mol	Chain	Length	Quality of chain
1	G	12	8%33%8%50%
1	H	12	17%8%33%8%50%

2 Entry composition

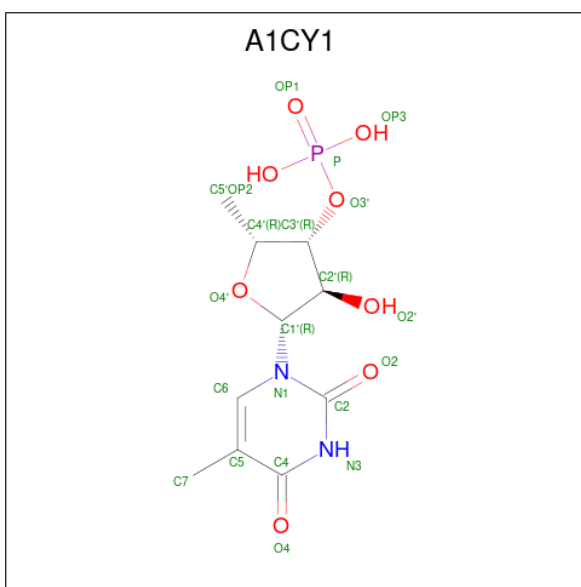
There are 7 unique types of molecules in this entry. The entry contains 3244 atoms, of which 966 are hydrogens and 0 are deuteriums.

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 RNA chain called Chains: A,B,C,D,E,F,G,H.

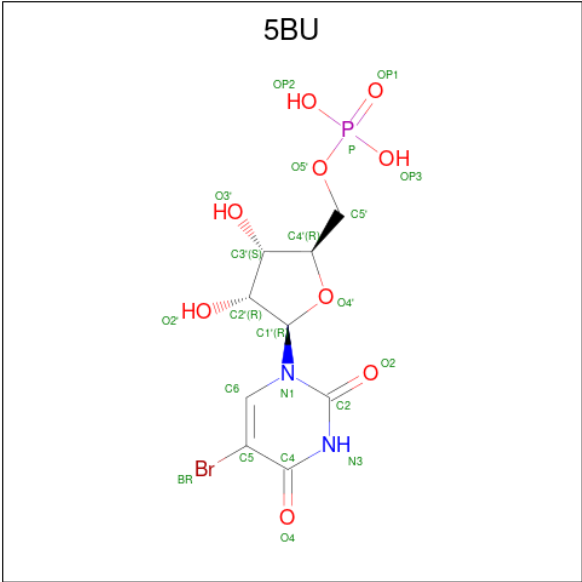
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	6	Total	C	H	N	O	P	0	0	0
			194	58	67	26	38	5			
1	B	6	Total	C	H	N	O	P	0	0	0
			194	58	67	26	38	5			
1	C	6	Total	C	H	N	O	P	0	0	0
			196	58	66	26	40	6			
1	D	6	Total	C	H	N	O	P	0	0	0
			194	58	67	26	38	5			
1	E	6	Total	C	H	N	O	P	0	0	0
			194	58	67	26	38	5			
1	F	6	Total	C	H	N	O	P	0	0	0
			194	58	67	26	38	5			
1	G	6	Total	C	H	N	O	P	0	0	0
			194	58	67	26	38	5			
1	H	6	Total	C	H	N	O	P	0	0	0
			194	58	67	26	38	5			

- Molecule 2 is 1-(5-deoxy-3-O-phosphono-beta-D-xylofuranosyl)-5-methylpyrimidine-2,4(1H, 3H)-dione (CCD ID: A1CY1) (formula: C₁₀H₁₅N₂O₈P) (labeled as "Ligand of Interest" by depositor).



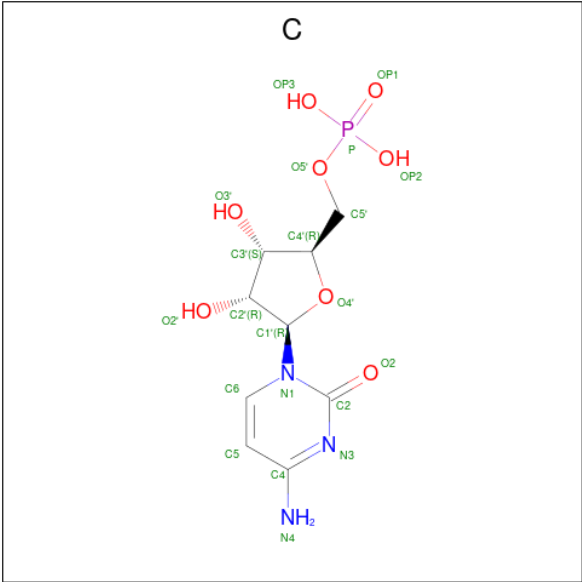
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	B	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	C	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	D	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	E	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	F	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	G	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	H	1	Total	C	N	O	P	0	0
			20	10	2	7	1		

- Molecule 3 is 5-BROMO-URIDINE-5'-MONOPHOSPHATE (CCD ID: 5BU) (formula: $C_9H_{12}BrN_2O_9P$).



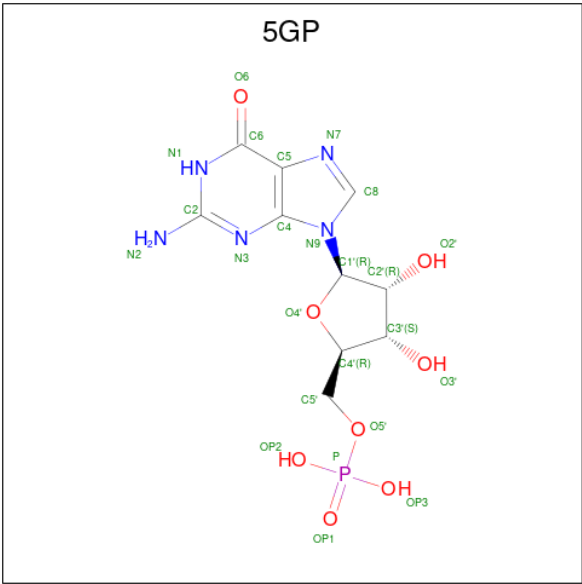
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	Br	C	H	N	O	P	0	0
			30	1	9	9	2	8	1		
3	A	1	Total	Br	C	H	N	O	P	0	0
			30	1	9	9	2	8	1		
3	C	1	Total	Br	C	H	N	O	P	0	0
			30	1	9	9	2	8	1		
3	D	1	Total	Br	C	H	N	O	P	0	0
			30	1	9	9	2	8	1		
3	E	1	Total	Br	C	H	N	O	P	0	0
			30	1	9	9	2	8	1		
3	F	1	Total	Br	C	H	N	O	P	0	0
			30	1	9	9	2	8	1		
3	G	1	Total	Br	C	H	N	O	P	0	0
			30	1	9	9	2	8	1		
3	G	1	Total	Br	C	H	N	O	P	0	0
			30	1	9	9	2	8	1		

- Molecule 4 is CYTIDINE-5'-MONOPHOSPHATE (CCD ID: C) (formula: C₉H₁₄N₃O₈P).



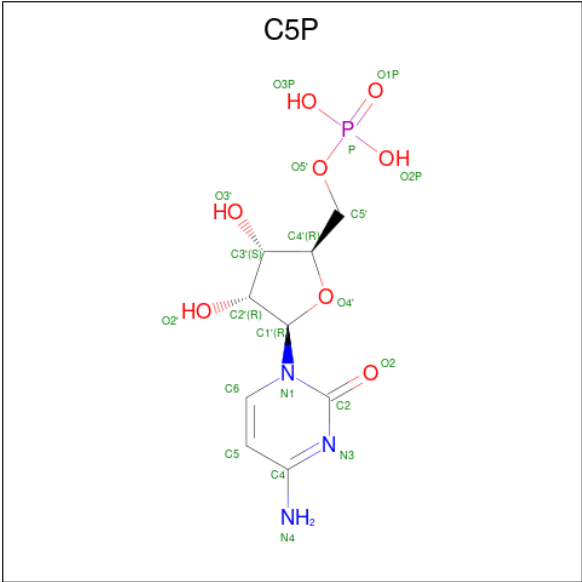
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	P	0	0
			31	9	11	3	7	1		
4	C	1	Total	C	H	N	O	P	0	0
			31	9	11	3	7	1		
4	E	1	Total	C	H	N	O	P	0	0
			31	9	11	3	7	1		
4	G	1	Total	C	H	N	O	P	0	0
			31	9	11	3	7	1		

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total 34	C 10	H 11	N 5	O 7	P 1	0	0
5	A	1	Total 35	C 10	H 12	N 5	O 7	P 1	0	0
5	B	1	Total 33	C 10	H 10	N 5	O 7	P 1	0	0
5	B	1	Total 35	C 10	H 12	N 5	O 7	P 1	0	0
5	C	1	Total 34	C 10	H 11	N 5	O 7	P 1	0	0
5	C	1	Total 35	C 10	H 12	N 5	O 7	P 1	0	0
5	D	1	Total 34	C 10	H 11	N 5	O 7	P 1	0	0
5	D	1	Total 35	C 10	H 12	N 5	O 7	P 1	0	0
5	E	1	Total 34	C 10	H 11	N 5	O 7	P 1	0	0
5	E	1	Total 35	C 10	H 12	N 5	O 7	P 1	0	0
5	F	1	Total 34	C 10	H 11	N 5	O 7	P 1	0	0
5	F	1	Total 35	C 10	H 12	N 5	O 7	P 1	0	0
5	G	1	Total 34	C 10	H 11	N 5	O 7	P 1	0	0
5	G	1	Total 35	C 10	H 12	N 5	O 7	P 1	0	0
5	H	1	Total 34	C 10	H 11	N 5	O 7	P 1	0	0
5	H	1	Total 35	C 10	H 12	N 5	O 7	P 1	0	0

- Molecule 6 is CYTIDINE-5'-MONOPHOSPHATE (CCD ID: C5P) (formula: $C_9H_{14}N_3O_8P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	P	0	0
			31	9	11	3	7	1		
6	B	1	Total	C	H	N	O	P	0	0
			31	9	11	3	7	1		
6	B	1	Total	C	H	N	O	P	0	0
			31	9	11	3	7	1		
6	C	1	Total	C	H	N	O	P	0	0
			31	9	11	3	7	1		
6	D	1	Total	C	H	N	O	P	0	0
			31	9	11	3	7	1		
6	D	1	Total	C	H	N	O	P	0	0
			31	9	11	3	7	1		
6	E	1	Total	C	H	N	O	P	0	0
			31	9	11	3	7	1		
6	F	1	Total	C	H	N	O	P	0	0
			31	9	11	3	7	1		
6	F	1	Total	C	H	N	O	P	0	0
			31	9	11	3	7	1		
6	G	1	Total	C	H	N	O	P	0	0
			31	9	11	3	7	1		
6	H	1	Total	C	H	N	O	P	0	0
			31	9	11	3	7	1		
6	H	1	Total	C	H	N	O	P	0	0
			31	9	11	3	7	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	35	Total 35	O 35	0	0
7	B	22	Total 22	O 22	0	0
7	C	35	Total 35	O 35	0	0
7	D	29	Total 29	O 29	0	0
7	E	24	Total 24	O 24	0	0
7	F	26	Total 26	O 26	0	0
7	G	39	Total 39	O 39	0	0
7	H	33	Total 33	O 33	0	0

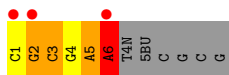
3 Residue-property plots [i](#)

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

- Molecule 1: Chains: A,B,C,D,E,F,G,H



- Molecule 1: Chains: A,B,C,D,E,F,G,H



- Molecule 1: Chains: A,B,C,D,E,F,G,H



- Molecule 1: Chains: A,B,C,D,E,F,G,H



- Molecule 1: Chains: A,B,C,D,E,F,G,H

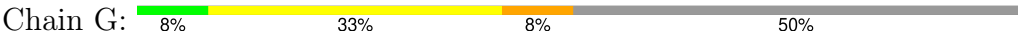


- Molecule 1: Chains: A,B,C,D,E,F,G,H

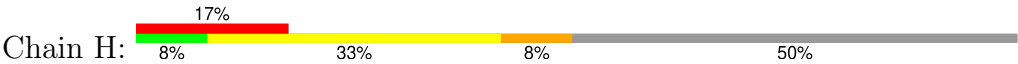




● Molecule 1: Chains: A,B,C,D,E,F,G,H



● Molecule 1: Chains: A,B,C,D,E,F,G,H



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	30.79Å 90.82Å 48.95Å 90.00° 98.72° 90.00°	Depositor
Resolution (Å)	30.43 – 1.54 30.43 – 1.54	Depositor EDS
% Data completeness (in resolution range)	91.8 (30.43-1.54) 92.3 (30.43-1.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 1.54Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.243 , 0.283 0.244 , 0.286	Depositor DCC
R_{free} test set	1800 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 61.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3244	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.24 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.3095e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 5BU, 5GP, A1CY1, C5P

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	2.06	5/142 (3.5%)	2.02	6/220 (2.7%)
1	B	1.83	5/142 (3.5%)	2.23	12/220 (5.5%)
1	C	1.95	3/145 (2.1%)	1.88	5/224 (2.2%)
1	D	1.76	2/142 (1.4%)	2.29	13/220 (5.9%)
1	E	1.87	2/142 (1.4%)	2.24	10/220 (4.5%)
1	F	2.00	4/142 (2.8%)	1.98	8/220 (3.6%)
1	G	1.77	1/142 (0.7%)	2.18	9/220 (4.1%)
1	H	2.09	6/142 (4.2%)	2.14	5/220 (2.3%)
All	All	1.92	28/1139 (2.5%)	2.12	68/1764 (3.9%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	G	N9-C8	-10.46	1.30	1.37
1	H	6	A	C6-N1	-9.57	1.28	1.35
1	H	4	G	N9-C4	-7.51	1.31	1.38
1	C	4	G	N9-C4	-7.23	1.32	1.38
1	F	4	G	C6-O6	7.17	1.30	1.24
1	C	2	G	N3-C4	-7.08	1.30	1.35
1	A	2	G	N3-C4	-6.95	1.30	1.35
1	B	2	G	N9-C4	-6.50	1.32	1.38
1	G	3	C	N1-C6	-6.22	1.33	1.37
1	F	2	G	N9-C8	-6.15	1.33	1.37
1	D	2	G	P-OP2	-6.11	1.36	1.49
1	H	4	G	N7-C5	-6.07	1.35	1.39
1	A	2	G	C5-C4	-5.82	1.34	1.38
1	B	1	C	N3-C4	-5.72	1.29	1.33
1	H	2	G	N7-C5	5.70	1.42	1.39
1	B	4	G	C8-N7	5.68	1.34	1.30
1	H	4	G	P-O5'	-5.68	1.54	1.59
1	B	1	C	C2-N3	-5.66	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	1	C	N1-C6	-5.63	1.33	1.37
1	F	1	C	N1-C6	-5.48	1.33	1.37
1	A	4	G	N7-C5	-5.46	1.35	1.39
1	F	5	A	N9-C8	-5.38	1.33	1.37
1	E	2	G	P-O5'	-5.33	1.54	1.59
1	D	2	G	N1-C2	-5.32	1.33	1.37
1	A	1	C	C5'-C4'	-5.18	1.47	1.51
1	B	3	C	N1-C6	-5.18	1.34	1.37
1	C	1	C	N3-C4	-5.08	1.30	1.33
1	E	5	A	C6-N1	-5.03	1.32	1.35

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	2	G	N1-C6-O6	-10.37	113.68	119.90
1	E	5	A	C6-N1-C2	9.39	124.24	118.60
1	B	1	C	C2-N3-C4	9.08	124.44	119.90
1	H	5	A	C6-N1-C2	8.87	123.92	118.60
1	D	4	G	C2-N3-C4	-8.82	107.49	111.90
1	D	5	A	C5-N7-C8	-8.80	99.50	103.90
1	H	2	G	C5-C6-O6	8.68	133.81	128.60
1	F	3	C	C5-C6-N1	-8.60	116.70	121.00
1	H	5	A	C5-C6-N1	-8.39	113.51	117.70
1	B	4	G	C5-N7-C8	-8.12	100.24	104.30
1	C	2	G	C2-N3-C4	7.81	115.81	111.90
1	G	5	A	C6-N1-C2	7.79	123.27	118.60
1	D	5	A	C6-N1-C2	7.59	123.15	118.60
1	G	6	A	N1-C2-N3	-7.59	125.51	129.30
1	D	1	C	N3-C4-C5	-7.56	118.88	121.90
1	B	4	G	C5-C6-O6	-7.38	124.17	128.60
1	B	5	A	C5-C6-N1	-7.33	114.03	117.70
1	C	1	C	C6-N1-C2	-7.33	117.37	120.30
1	F	2	G	C4-C5-N7	-7.32	107.87	110.80
1	E	2	G	C5-C6-N1	-7.26	107.87	111.50
1	F	3	C	N3-C2-O2	-7.14	116.90	121.90
1	B	4	G	N7-C8-N9	7.09	116.64	113.10
1	A	5	A	C5-C6-N1	-6.91	114.25	117.70
1	B	2	G	C2-N3-C4	-6.90	108.45	111.90
1	B	6	A	O5'-C5'-C4'	6.81	114.85	109.40
1	D	1	C	C6-N1-C2	-6.80	117.58	120.30
1	G	5	A	C5-C6-N1	-6.78	114.31	117.70
1	D	4	G	N3-C2-N2	-6.77	115.16	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	G	N1-C6-O6	6.71	123.92	119.90
1	B	4	G	C4-C5-N7	6.67	113.47	110.80
1	E	5	A	N3-C4-C5	6.55	131.39	126.80
1	G	5	A	N1-C2-N3	-6.46	126.07	129.30
1	A	5	A	C6-N1-C2	6.43	122.46	118.60
1	H	5	A	N1-C6-N6	6.26	122.36	118.60
1	F	3	C	C6-N1-C2	6.18	122.77	120.30
1	D	4	G	N1-C2-N3	6.17	127.60	123.90
1	E	5	A	C5-N7-C8	-6.11	100.84	103.90
1	F	3	C	N1-C2-O2	6.09	122.55	118.90
1	E	5	A	C2-N3-C4	-6.08	107.56	110.60
1	G	1	C	C6-N1-C2	-6.07	117.87	120.30
1	D	5	A	N3-C4-C5	6.04	131.03	126.80
1	E	2	G	C8-N9-C4	-6.04	103.98	106.40
1	F	3	C	C4-C5-C6	5.99	120.40	117.40
1	B	5	A	C6-N1-C2	5.98	122.19	118.60
1	G	4	G	N1-C6-O6	-5.96	116.33	119.90
1	D	5	A	C4-C5-N7	5.93	113.67	110.70
1	B	2	G	N3-C4-C5	5.89	131.55	128.60
1	E	5	A	C5-C6-N1	-5.79	114.81	117.70
1	A	5	A	C2-N3-C4	-5.72	107.74	110.60
1	C	4	G	C8-N9-C4	5.69	108.68	106.40
1	D	2	G	N1-C6-O6	5.69	123.31	119.90
1	D	5	A	N1-C2-N3	-5.59	126.50	129.30
1	E	1	C	C4-C5-C6	-5.59	114.60	117.40
1	E	1	C	N1-C2-O2	5.53	122.22	118.90
1	D	2	G	C5-C6-O6	-5.52	125.29	128.60
1	A	5	A	N1-C6-N6	5.50	121.90	118.60
1	G	6	A	C2-N3-C4	5.37	113.29	110.60
1	F	2	G	N3-C4-C5	-5.36	125.92	128.60
1	G	6	A	C4-C5-C6	-5.32	114.34	117.00
1	F	3	C	C2-N3-C4	-5.26	117.27	119.90
1	A	4	G	N7-C8-N9	5.26	115.73	113.10
1	C	3	C	N3-C4-C5	-5.24	119.80	121.90
1	D	5	A	N1-C6-N6	5.20	121.72	118.60
1	G	6	A	O5'-C5'-C4'	5.18	113.54	109.40
1	C	2	G	C6-N1-C2	-5.09	122.05	125.10
1	B	5	A	C2-N3-C4	-5.08	108.06	110.60
1	A	2	G	C4-C5-C6	5.05	121.83	118.80
1	E	5	A	N7-C8-N9	5.02	116.31	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	127	67	67	0	0
1	B	127	67	67	4	0
1	C	130	66	66	2	0
1	D	127	67	67	0	0
1	E	127	67	67	1	0
1	F	127	67	67	0	0
1	G	127	67	67	1	0
1	H	127	67	67	1	0
2	A	20	0	0	0	0
2	B	20	0	0	0	0
2	C	20	0	0	0	0
2	D	20	0	0	0	0
2	E	20	0	0	0	0
2	F	20	0	0	1	0
2	G	20	0	0	0	0
2	H	20	0	0	0	0
3	A	42	18	18	0	0
3	C	21	9	9	0	0
3	D	21	9	9	0	0
3	E	21	9	9	0	0
3	F	21	9	9	0	0
3	G	42	18	18	0	0
4	A	20	11	11	0	0
4	C	20	11	11	0	0
4	E	20	11	11	0	0
4	G	20	11	11	0	0
5	A	46	23	23	0	0
5	B	46	22	23	1	0
5	C	46	23	23	1	0
5	D	46	23	23	0	0
5	E	46	23	23	0	0
5	F	46	23	23	1	0
5	G	46	23	23	0	0
5	H	46	23	23	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	20	11	11	0	0
6	B	40	22	22	1	0
6	C	20	11	11	0	0
6	D	40	22	22	0	0
6	E	20	11	11	0	0
6	F	40	22	22	1	0
6	G	20	11	11	0	0
6	H	40	22	22	2	0
7	A	35	0	0	0	0
7	B	22	0	0	2	0
7	C	35	0	0	2	0
7	D	29	0	0	0	0
7	E	24	0	0	0	0
7	F	26	0	0	2	0
7	G	39	0	0	1	0
7	H	33	0	0	1	0
All	All	2278	966	967	15	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (15) 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:C:5:A:N3	7:C:202:HOH:O	2.07	0.88
1:B:5:A:O2'	7:B:201:HOH:O	1.93	0.86
5:C:104:5GP:OP1	7:C:201:HOH:O	2.04	0.75
6:H:101:C5P:H5'2	6:H:101:C5P:H6	1.72	0.71
6:H:101:C5P:H6	6:H:101:C5P:C5'	2.23	0.68
1:G:3:C:N4	7:G:202:HOH:O	2.37	0.56
1:H:4:G:P	7:H:205:HOH:O	2.66	0.54
1:B:2:G:OP1	7:B:202:HOH:O	2.19	0.53
1:B:2:G:H2'	1:B:3:C:C6	2.51	0.46
6:F:102:C5P:H5	7:F:204:HOH:O	2.17	0.45
5:F:105:5GP:N7	7:F:202:HOH:O	2.35	0.43
5:B:102:5GP:H2'	6:B:103:C5P:H6	2.02	0.42
1:B:6:A:C4'	1:B:6:A:OP2	2.67	0.42
1:E:6:A:N1	2:F:106:A1CY1:N3	2.67	0.42
1:C:6:A:H8	1:C:6:A:O5'	2.02	0.42

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	5/12 (41%)	0	0
1	B	5/12 (41%)	1 (20%)	0
1	C	5/12 (41%)	0	0
1	D	5/12 (41%)	0	0
1	E	5/12 (41%)	0	0
1	F	5/12 (41%)	0	0
1	G	5/12 (41%)	0	0
1	H	5/12 (41%)	0	0
All	All	40/96 (41%)	1 (2%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	6	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

48 ligands are modelled in this entry.

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
4	C	E	103	5,3	18,21,22	0.88	1 (5%)	25,30,33	0.74	0
3	5BU	A	102	6,2	19,22,23	1.33	3 (15%)	27,32,35	2.56	7 (25%)
2	A1CY1	F	106	3,1	18,21,22	1.28	3 (16%)	26,31,34	2.60	12 (46%)
3	5BU	A	103	2,4	19,22,23	1.23	3 (15%)	27,32,35	2.28	6 (22%)
6	C5P	A	106	5	18,21,22	0.69	0	25,30,33	0.54	0
2	A1CY1	A	101	3,1	18,21,22	1.48	4 (22%)	26,31,34	1.97	7 (26%)
2	A1CY1	E	101	3,1	18,21,22	1.78	5 (27%)	26,31,34	2.29	11 (42%)
5	5GP	H	102	6	22,25,26	0.67	0	32,37,40	0.77	0
6	C5P	B	101	5,3	18,21,22	0.69	0	25,30,33	0.75	1 (4%)
4	C	C	103	5,3	18,21,22	0.47	0	25,30,33	0.64	0
6	C5P	C	105	5	18,21,22	0.90	1 (5%)	25,30,33	0.89	0
6	C5P	B	103	5	18,21,22	0.54	0	25,30,33	0.65	0
5	5GP	B	102	6	22,25,26	0.61	0	32,37,40	0.75	2 (6%)
5	5GP	E	106	6	22,25,26	0.83	0	32,37,40	0.56	0
5	5GP	H	104	6	22,25,26	0.67	0	32,37,40	0.72	1 (3%)
3	5BU	F	101	6,2	19,22,23	1.42	4 (21%)	27,32,35	2.31	6 (22%)
2	A1CY1	D	106	3,1	18,21,22	1.44	4 (22%)	26,31,34	2.46	8 (30%)
3	5BU	G	103	2,4	19,22,23	1.90	4 (21%)	27,32,35	1.91	6 (22%)
2	A1CY1	H	105	3,1	18,21,22	2.01	7 (38%)	26,31,34	2.54	9 (34%)
3	5BU	E	102	2,4	19,22,23	1.34	4 (21%)	27,32,35	2.04	7 (25%)
6	C5P	G	106	5	18,21,22	0.79	0	25,30,33	0.86	1 (4%)
2	A1CY1	C	101	3,1	18,21,22	1.71	5 (27%)	26,31,34	2.59	12 (46%)
6	C5P	E	105	5	18,21,22	0.66	0	25,30,33	0.73	0
5	5GP	A	105	6,4	22,25,26	0.83	1 (4%)	32,37,40	0.73	0
6	C5P	H	103	5	18,21,22	0.69	0	25,30,33	0.59	0
2	A1CY1	G	101	3,1	18,21,22	1.70	4 (22%)	26,31,34	2.38	6 (23%)
5	5GP	D	105	6	22,25,26	0.76	0	32,37,40	0.59	0
5	5GP	D	103	6	22,25,26	0.70	0	32,37,40	0.70	0
5	5GP	G	105	6,4	22,25,26	0.82	1 (4%)	32,37,40	0.92	1 (3%)
3	5BU	D	101	6,2	19,22,23	1.43	5 (26%)	27,32,35	1.84	5 (18%)
4	C	A	104	5,3	18,21,22	0.67	0	25,30,33	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	C5P	D	104	5	18,21,22	0.70	0	25,30,33	0.59	0
5	5GP	C	106	6	22,25,26	0.94	1 (4%)	32,37,40	0.63	0
5	5GP	G	107	6	22,25,26	0.95	0	32,37,40	0.67	0
6	C5P	D	102	5,3	18,21,22	0.70	0	25,30,33	0.68	0
3	5BU	C	102	2,4	19,22,23	1.28	3 (15%)	27,32,35	1.82	6 (22%)
5	5GP	F	103	6	22,25,26	0.67	0	32,37,40	0.53	0
6	C5P	F	104	5	18,21,22	0.43	0	25,30,33	0.77	0
2	A1CY1	B	105	3,1	18,21,22	1.40	4 (22%)	26,31,34	2.41	10 (38%)
5	5GP	A	107	6	22,25,26	0.51	0	32,37,40	0.77	0
4	C	G	104	5,3	18,21,22	0.58	0	25,30,33	0.71	0
5	5GP	E	104	6,4	22,25,26	0.69	0	32,37,40	0.78	1 (3%)
5	5GP	F	105	6	22,25,26	0.78	1 (4%)	32,37,40	0.79	0
6	C5P	F	102	5,3	18,21,22	0.60	0	25,30,33	0.87	0
6	C5P	H	101	5,3	18,21,22	0.71	1 (5%)	25,30,33	1.10	2 (8%)
5	5GP	C	104	6,4	22,25,26	0.71	0	32,37,40	0.63	0
3	5BU	G	102	6,2	19,22,23	1.58	3 (15%)	27,32,35	2.14	9 (33%)
5	5GP	B	104	6	22,25,26	0.65	0	32,37,40	0.71	0

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
4	C	E	103	5,3	-	0/7/25/26	0/2/2/2
3	5BU	A	102	6,2	-	0/7/25/26	0/2/2/2
2	A1CY1	F	106	3,1	-	6/6/24/25	0/2/2/2
3	5BU	A	103	2,4	-	0/7/25/26	0/2/2/2
6	C5P	A	106	5	-	0/7/25/26	0/2/2/2
2	A1CY1	A	101	3,1	-	0/6/24/25	0/2/2/2
2	A1CY1	E	101	3,1	-	5/6/24/25	0/2/2/2
5	5GP	H	102	6	-	0/7/25/26	0/3/3/3
6	C5P	B	101	5,3	-	0/7/25/26	0/2/2/2
4	C	C	103	5,3	-	0/7/25/26	0/2/2/2
6	C5P	C	105	5	-	0/7/25/26	0/2/2/2
6	C5P	B	103	5	-	0/7/25/26	0/2/2/2
5	5GP	B	102	6	-	0/7/25/26	0/3/3/3
5	5GP	E	106	6	-	0/7/25/26	0/3/3/3
5	5GP	H	104	6	-	2/7/25/26	0/3/3/3
3	5BU	F	101	6,2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1CY1	D	106	3,1	-	0/6/24/25	0/2/2/2
3	5BU	G	103	2,4	-	0/7/25/26	0/2/2/2
2	A1CY1	H	105	3,1	-	0/6/24/25	0/2/2/2
3	5BU	E	102	2,4	-	0/7/25/26	0/2/2/2
6	C5P	G	106	5	-	0/7/25/26	0/2/2/2
2	A1CY1	C	101	3,1	-	0/6/24/25	0/2/2/2
6	C5P	E	105	5	-	0/7/25/26	0/2/2/2
5	5GP	A	105	6,4	-	0/7/25/26	0/3/3/3
6	C5P	H	103	5	-	0/7/25/26	0/2/2/2
2	A1CY1	G	101	3,1	-	0/6/24/25	0/2/2/2
5	5GP	D	105	6	-	0/7/25/26	0/3/3/3
5	5GP	D	103	6	-	0/7/25/26	0/3/3/3
5	5GP	G	105	6,4	-	2/7/25/26	0/3/3/3
3	5BU	D	101	6,2	-	0/7/25/26	0/2/2/2
4	C	A	104	5,3	-	0/7/25/26	0/2/2/2
6	C5P	D	104	5	-	0/7/25/26	0/2/2/2
5	5GP	C	106	6	-	0/7/25/26	0/3/3/3
5	5GP	G	107	6	-	0/7/25/26	0/3/3/3
6	C5P	D	102	5,3	-	0/7/25/26	0/2/2/2
3	5BU	C	102	2,4	-	0/7/25/26	0/2/2/2
5	5GP	F	103	6	-	0/7/25/26	0/3/3/3
6	C5P	F	104	5	-	0/7/25/26	0/2/2/2
2	A1CY1	B	105	3,1	-	2/6/24/25	0/2/2/2
5	5GP	A	107	6	-	0/7/25/26	0/3/3/3
4	C	G	104	5,3	-	0/7/25/26	0/2/2/2
5	5GP	E	104	6,4	-	0/7/25/26	0/3/3/3
5	5GP	F	105	6	-	0/7/25/26	0/3/3/3
6	C5P	F	102	5,3	-	0/7/25/26	0/2/2/2
6	C5P	H	101	5,3	-	2/7/25/26	0/2/2/2
5	5GP	C	104	6,4	-	0/7/25/26	0/3/3/3
3	5BU	G	102	6,2	-	0/7/25/26	0/2/2/2
5	5GP	B	104	6	-	0/7/25/26	0/3/3/3

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	103	5BU	C4-N3	-4.83	1.29	1.38
3	G	103	5BU	O4-C4	4.56	1.32	1.23
2	H	105	A1CY1	O3'-C3'	4.52	1.53	1.45
2	G	101	A1CY1	C4-C5	-4.35	1.37	1.44
3	G	102	5BU	C4-N3	-4.11	1.31	1.38
2	C	101	A1CY1	C6-C5	3.52	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	101	A1CY1	C6-C5	3.47	1.40	1.34
3	F	101	5BU	C6-C5	3.43	1.41	1.34
2	E	101	A1CY1	C2-N3	3.41	1.43	1.38
2	G	101	A1CY1	C6-C5	3.30	1.40	1.34
2	H	105	A1CY1	C6-N1	3.28	1.43	1.38
2	H	105	A1CY1	C4-C5	-3.27	1.39	1.44
3	E	102	5BU	C4-N3	-3.26	1.32	1.38
2	D	106	A1CY1	C4-C5	-3.22	1.39	1.44
3	F	101	5BU	C2-N1	3.07	1.43	1.38
3	F	101	5BU	C4-N3	-3.06	1.33	1.38
2	A	101	A1CY1	C6-C5	3.02	1.39	1.34
2	A	101	A1CY1	C4-C5	-3.02	1.39	1.44
2	C	101	A1CY1	C2-N3	2.98	1.43	1.38
3	D	101	5BU	C4-N3	-2.98	1.33	1.38
3	D	101	5BU	C6-N1	-2.92	1.33	1.38
3	A	102	5BU	C4-N3	-2.87	1.33	1.38
2	B	105	A1CY1	C4-C5	-2.80	1.40	1.44
2	E	101	A1CY1	C4-C5	-2.79	1.40	1.44
2	F	106	A1CY1	O4'-C1'	2.67	1.48	1.42
2	H	105	A1CY1	O2'-C2'	2.63	1.49	1.43
3	C	102	5BU	C4-N3	-2.62	1.33	1.38
4	E	103	C	C2-N3	-2.62	1.31	1.36
2	H	105	A1CY1	C7-C5	2.55	1.56	1.50
3	A	103	5BU	C4-N3	-2.54	1.34	1.38
2	C	101	A1CY1	C3'-C4'	-2.53	1.48	1.53
3	G	103	5BU	C6-C5	2.51	1.39	1.34
3	G	102	5BU	C4-C5	2.51	1.50	1.45
3	A	103	5BU	C6-C5	2.50	1.39	1.34
3	G	102	5BU	O4-C4	2.47	1.28	1.23
2	C	101	A1CY1	C4-C5	-2.44	1.40	1.44
2	E	101	A1CY1	C2'-C3'	-2.44	1.47	1.53
5	A	105	5GP	O6-C6	-2.43	1.19	1.23
2	B	105	A1CY1	C2-N1	-2.43	1.34	1.38
2	A	101	A1CY1	C3'-C4'	-2.42	1.48	1.53
2	A	101	A1CY1	C6-N1	2.41	1.42	1.38
3	E	102	5BU	C6-N1	-2.40	1.33	1.38
2	B	105	A1CY1	C6-C5	2.38	1.38	1.34
2	D	106	A1CY1	C6-C5	2.38	1.38	1.34
2	D	106	A1CY1	O4'-C1'	2.37	1.47	1.42
6	C	105	C5P	C6-C5	-2.37	1.29	1.35
2	B	105	A1CY1	O2'-C2'	2.35	1.48	1.43
2	E	101	A1CY1	C2-N1	-2.35	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	105	5GP	C2-N2	-2.34	1.28	1.34
6	H	101	C5P	O5'-C5'	-2.32	1.37	1.44
2	C	101	A1CY1	C2-N1	-2.32	1.34	1.38
5	F	105	5GP	C5-N7	2.30	1.43	1.39
2	H	105	A1CY1	C6-C5	2.29	1.38	1.34
3	A	102	5BU	O2-C2	2.27	1.27	1.23
3	E	102	5BU	C2-N3	-2.25	1.34	1.38
3	D	101	5BU	C4-C5	2.24	1.49	1.45
3	C	102	5BU	C6-N1	-2.23	1.34	1.38
2	G	101	A1CY1	C2-N1	-2.23	1.35	1.38
2	D	106	A1CY1	C2-N1	-2.20	1.35	1.38
5	C	106	5GP	C6-N1	2.20	1.43	1.38
2	F	106	A1CY1	C6-C5	2.20	1.38	1.34
3	C	102	5BU	C6-C5	2.18	1.38	1.34
2	H	105	A1CY1	C5'-C4'	2.15	1.56	1.51
2	F	106	A1CY1	C4-C5	-2.15	1.41	1.44
3	G	103	5BU	C6-N1	-2.13	1.34	1.38
3	D	101	5BU	O4-C4	2.13	1.27	1.23
3	A	102	5BU	C4-C5	2.10	1.49	1.45
3	E	102	5BU	C6-C5	2.08	1.38	1.34
3	F	101	5BU	O2-C2	2.04	1.26	1.23
3	D	101	5BU	C2-N3	-2.03	1.34	1.38
3	A	103	5BU	C6-N1	-2.02	1.34	1.38
2	G	101	A1CY1	O3'-C3'	-2.02	1.42	1.45

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	106	A1CY1	C4-N3-C2	-7.05	118.09	127.34
3	A	102	5BU	C5-C4-N3	6.99	121.38	113.34
3	A	103	5BU	O4-C4-C5	-6.55	117.45	125.80
3	A	102	5BU	C4-N3-C2	-6.53	118.77	127.34
3	F	101	5BU	C5-C4-N3	6.24	120.51	113.34
2	G	101	A1CY1	C4-N3-C2	-6.21	119.20	127.34
2	C	101	A1CY1	C4-N3-C2	-6.19	119.23	127.34
3	E	102	5BU	O4-C4-C5	-5.98	118.17	125.80
2	D	106	A1CY1	C4-N3-C2	-5.95	119.55	127.34
2	G	101	A1CY1	C5-C4-N3	5.75	120.32	115.32
3	G	103	5BU	C5-C4-N3	5.71	119.91	113.34
2	E	101	A1CY1	C4-N3-C2	-5.63	119.96	127.34
2	H	105	A1CY1	C4-N3-C2	-5.60	119.99	127.34
3	F	101	5BU	C4-N3-C2	-5.60	120.00	127.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	106	A1CY1	N3-C2-N1	5.49	122.04	114.89
2	B	105	A1CY1	C5-C4-N3	5.31	119.94	115.32
3	F	101	5BU	N3-C2-N1	5.25	121.72	114.89
2	B	105	A1CY1	C4-N3-C2	-5.25	120.46	127.34
3	A	102	5BU	N3-C2-N1	5.22	121.69	114.89
3	A	103	5BU	N3-C2-N1	5.22	121.68	114.89
3	D	101	5BU	N3-C2-N1	5.12	121.56	114.89
2	F	106	A1CY1	C5-C4-N3	5.08	119.74	115.32
2	H	105	A1CY1	C5-C6-N1	-5.02	117.86	123.31
3	A	103	5BU	C4-N3-C2	-4.93	120.87	127.34
2	G	101	A1CY1	O4-C4-C5	-4.93	119.28	124.92
2	D	106	A1CY1	C5-C4-N3	4.84	119.53	115.32
3	G	102	5BU	C5-C4-N3	4.83	118.90	113.34
2	C	101	A1CY1	C5-C4-N3	4.81	119.51	115.32
2	D	106	A1CY1	N3-C2-N1	4.71	121.02	114.89
3	A	102	5BU	O4-C4-C5	-4.65	119.87	125.80
2	H	105	A1CY1	C5-C4-N3	4.59	119.32	115.32
3	D	101	5BU	C4-N3-C2	-4.57	121.35	127.34
3	E	102	5BU	N3-C2-N1	4.40	120.61	114.89
2	H	105	A1CY1	C5'-C4'-C3'	-4.39	107.80	115.93
3	C	102	5BU	C4-N3-C2	-4.37	121.61	127.34
3	F	101	5BU	O4-C4-C5	-4.37	120.23	125.80
2	C	101	A1CY1	N3-C2-N1	4.37	120.57	114.89
3	A	103	5BU	C5-C4-N3	4.33	118.33	113.34
3	C	102	5BU	N3-C2-N1	4.31	120.50	114.89
2	E	101	A1CY1	C5-C4-N3	4.26	119.03	115.32
3	G	102	5BU	N3-C2-N1	4.20	120.36	114.89
3	E	102	5BU	C4-N3-C2	-4.11	121.95	127.34
3	G	103	5BU	C4-N3-C2	-4.11	121.95	127.34
2	H	105	A1CY1	N3-C2-N1	4.11	120.25	114.89
2	C	101	A1CY1	C5'-C4'-C3'	-4.09	108.35	115.93
2	D	106	A1CY1	O4-C4-C5	-4.08	120.25	124.92
3	C	102	5BU	C5-C4-N3	4.05	118.00	113.34
2	A	101	A1CY1	C5-C4-N3	4.02	118.82	115.32
2	A	101	A1CY1	O4'-C4'-C3'	-4.01	97.99	104.02
2	H	105	A1CY1	C6-C5-C4	3.91	121.24	118.02
3	G	102	5BU	O4-C4-C5	-3.88	120.86	125.80
3	G	102	5BU	BR-C5-C6	3.84	126.01	120.64
2	B	105	A1CY1	N3-C2-N1	3.82	119.87	114.89
3	G	102	5BU	C6-C5-C4	-3.78	116.84	120.67
3	G	102	5BU	C4-N3-C2	-3.76	122.41	127.34
2	A	101	A1CY1	O4-C4-C5	-3.76	120.61	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	102	5BU	O4-C4-C5	-3.75	121.02	125.80
2	A	101	A1CY1	C4-N3-C2	-3.75	122.43	127.34
2	C	101	A1CY1	C5-C6-N1	-3.72	119.28	123.31
3	E	102	5BU	C5-C4-N3	3.68	117.58	113.34
2	G	101	A1CY1	N3-C2-N1	3.67	119.67	114.89
2	B	105	A1CY1	C5'-C4'-C3'	-3.65	109.16	115.93
2	E	101	A1CY1	N3-C2-N1	3.64	119.63	114.89
2	A	101	A1CY1	C5-C6-N1	-3.61	119.39	123.31
3	D	101	5BU	C5-C4-N3	3.59	117.47	113.34
3	A	103	5BU	O2-C2-N1	-3.54	118.19	122.80
2	C	101	A1CY1	O2-C2-N1	-3.54	118.19	122.80
2	D	106	A1CY1	O4'-C4'-C3'	-3.51	98.73	104.02
2	B	105	A1CY1	C2'-C3'-C4'	-3.51	97.09	103.26
3	G	103	5BU	O4-C4-C5	-3.50	121.34	125.80
2	G	101	A1CY1	C5-C6-N1	-3.50	119.51	123.31
2	E	101	A1CY1	O2-C2-N1	-3.47	118.28	122.80
3	G	103	5BU	N3-C2-N1	3.42	119.35	114.89
2	C	101	A1CY1	O4-C4-C5	-3.37	121.06	124.92
2	F	106	A1CY1	C5-C6-N1	-3.35	119.67	123.31
3	A	102	5BU	C6-C5-C4	-3.35	117.27	120.67
3	D	101	5BU	O2-C2-N1	-3.28	118.52	122.80
2	E	101	A1CY1	O4-C4-C5	-3.27	121.18	124.92
3	A	102	5BU	BR-C5-C6	3.25	125.19	120.64
3	G	102	5BU	O2-C2-N1	-3.25	118.57	122.80
2	E	101	A1CY1	C5-C6-N1	-3.20	119.84	123.31
2	F	106	A1CY1	C5'-C4'-C3'	-3.18	110.04	115.93
2	B	105	A1CY1	C7-C5-C4	3.16	122.16	118.78
6	H	101	C5P	O2-C2-N3	3.09	127.20	122.33
2	H	105	A1CY1	C2'-C3'-C4'	-3.09	97.83	103.26
2	C	101	A1CY1	C7-C5-C6	-3.05	118.72	122.85
2	D	106	A1CY1	C5-C6-N1	-3.05	120.00	123.31
2	A	101	A1CY1	N3-C2-N1	3.02	118.83	114.89
2	B	105	A1CY1	O4'-C4'-C3'	-2.98	99.53	104.02
2	F	106	A1CY1	C7-C5-C6	-2.94	118.87	122.85
2	E	101	A1CY1	C7-C5-C6	-2.88	118.96	122.85
2	H	105	A1CY1	O4-C4-C5	-2.86	121.64	124.92
3	F	101	5BU	BR-C5-C6	2.85	124.62	120.64
2	E	101	A1CY1	O4'-C4'-C3'	-2.78	99.83	104.02
3	E	102	5BU	O2-C2-N1	-2.76	119.21	122.80
2	D	106	A1CY1	C2'-C3'-C4'	-2.71	98.49	103.26
2	C	101	A1CY1	C6-C5-C4	2.71	120.25	118.02
3	D	101	5BU	BR-C5-C4	2.69	121.12	118.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	103	5BU	C6-C5-C4	-2.68	117.95	120.67
3	C	102	5BU	O2-C2-N1	-2.65	119.35	122.80
2	E	101	A1CY1	C6-C5-C4	2.65	120.20	118.02
2	F	106	A1CY1	C6-C5-C4	2.65	120.20	118.02
2	B	105	A1CY1	O4-C4-C5	-2.64	121.90	124.92
6	G	106	C5P	O2-C2-N3	-2.62	118.21	122.33
5	E	104	5GP	O6-C6-N1	2.61	125.02	120.11
3	G	103	5BU	BR-C5-C4	2.59	121.00	118.02
2	B	105	A1CY1	O2-C2-N1	-2.52	119.52	122.80
3	F	101	5BU	O2-C2-N3	-2.51	116.85	121.49
2	G	101	A1CY1	O4'-C4'-C3'	-2.50	100.26	104.02
5	G	105	5GP	N2-C2-N3	-2.49	114.82	119.67
2	H	105	A1CY1	O2-C2-N3	-2.44	116.99	121.49
2	F	106	A1CY1	C2'-C3'-C4'	-2.43	98.99	103.26
3	C	102	5BU	BR-C5-C4	2.42	120.80	118.02
2	E	101	A1CY1	C5'-C4'-C3'	-2.39	111.51	115.93
2	E	101	A1CY1	C2'-C3'-C4'	-2.37	99.10	103.26
5	H	104	5GP	O3'-C3'-C2'	-2.34	104.33	111.82
2	C	101	A1CY1	O4'-C4'-C3'	-2.31	100.54	104.02
3	E	102	5BU	BR-C5-C6	2.28	123.84	120.64
3	G	102	5BU	C6-N1-C2	-2.28	119.04	121.30
2	D	106	A1CY1	C5'-C4'-C3'	-2.24	111.77	115.93
6	B	101	C5P	N4-C4-N3	2.23	121.90	117.91
6	H	101	C5P	O2-C2-N1	-2.20	114.58	118.90
3	E	102	5BU	O4-C4-N3	2.20	124.25	120.11
2	B	105	A1CY1	C7-C5-C6	-2.18	119.90	122.85
3	A	103	5BU	O4-C4-N3	2.15	124.15	120.11
3	A	102	5BU	O2-C2-N3	-2.13	117.55	121.49
2	C	101	A1CY1	C2'-C3'-C4'	-2.12	99.53	103.26
2	F	106	A1CY1	O4'-C4'-C3'	-2.10	100.85	104.02
2	C	101	A1CY1	C7-C5-C4	2.10	121.02	118.78
2	F	106	A1CY1	O2-C2-N3	-2.06	117.69	121.49
5	B	102	5GP	O6-C6-N1	-2.05	116.26	120.11
5	B	102	5GP	O6-C6-C5	2.04	131.91	126.53
2	F	106	A1CY1	O2-C2-N1	-2.03	120.16	122.80
3	G	102	5BU	C1'-N1-C6	2.02	124.48	121.15
2	A	101	A1CY1	C5'-C4'-C3'	-2.01	112.20	115.93
2	F	106	A1CY1	C7-C5-C4	2.01	120.93	118.78

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	105	A1CY1	C2'-C3'-O3'-P
2	B	105	A1CY1	C4'-C3'-O3'-P
2	E	101	A1CY1	C2'-C1'-N1-C6
2	E	101	A1CY1	C4'-C3'-O3'-P
2	F	106	A1CY1	C2'-C3'-O3'-P
2	F	106	A1CY1	C4'-C3'-O3'-P
5	G	105	5GP	O4'-C4'-C5'-O5'
5	H	104	5GP	O4'-C4'-C5'-O5'
6	H	101	C5P	O4'-C4'-C5'-O5'
5	G	105	5GP	C3'-C4'-C5'-O5'
6	H	101	C5P	C3'-C4'-C5'-O5'
2	F	106	A1CY1	C2'-C1'-N1-C6
2	E	101	A1CY1	C2'-C1'-N1-C2
2	F	106	A1CY1	C2'-C1'-N1-C2
5	H	104	5GP	C3'-C4'-C5'-O5'
2	F	106	A1CY1	O4'-C1'-N1-C6
2	E	101	A1CY1	O4'-C1'-N1-C2
2	F	106	A1CY1	O4'-C1'-N1-C2
2	E	101	A1CY1	O4'-C1'-N1-C6

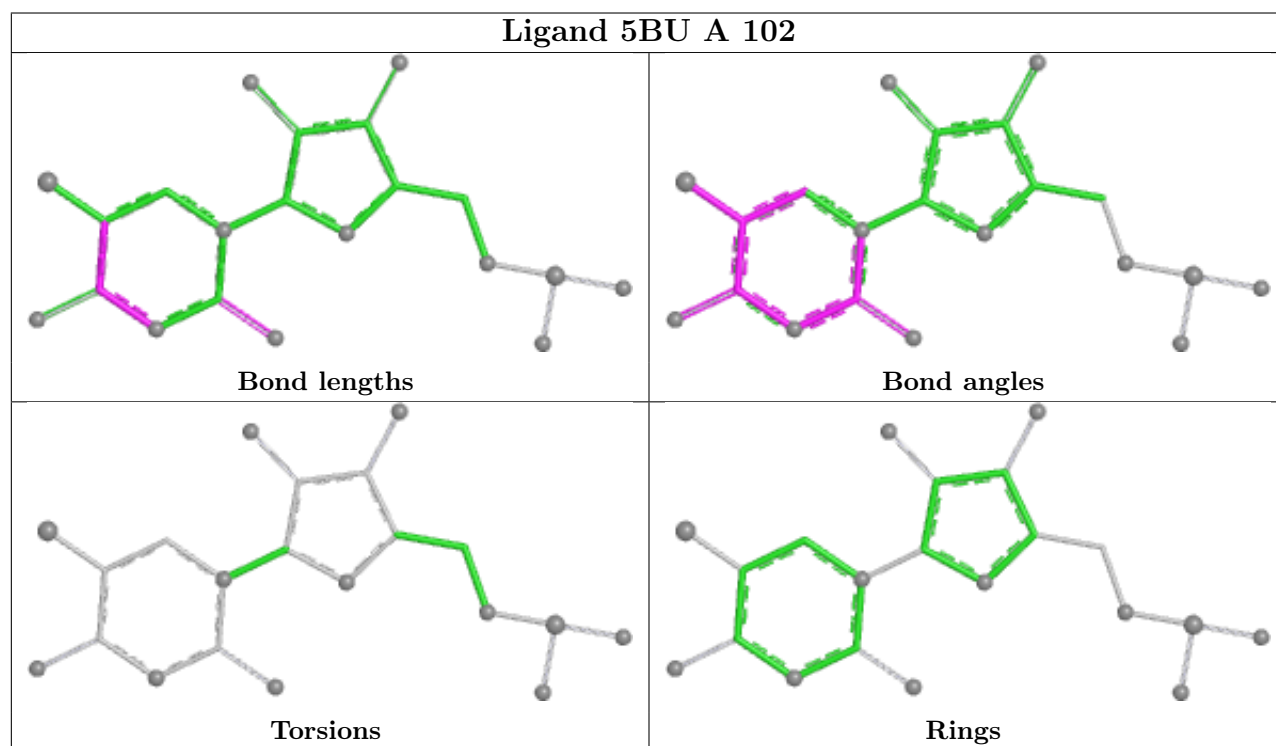
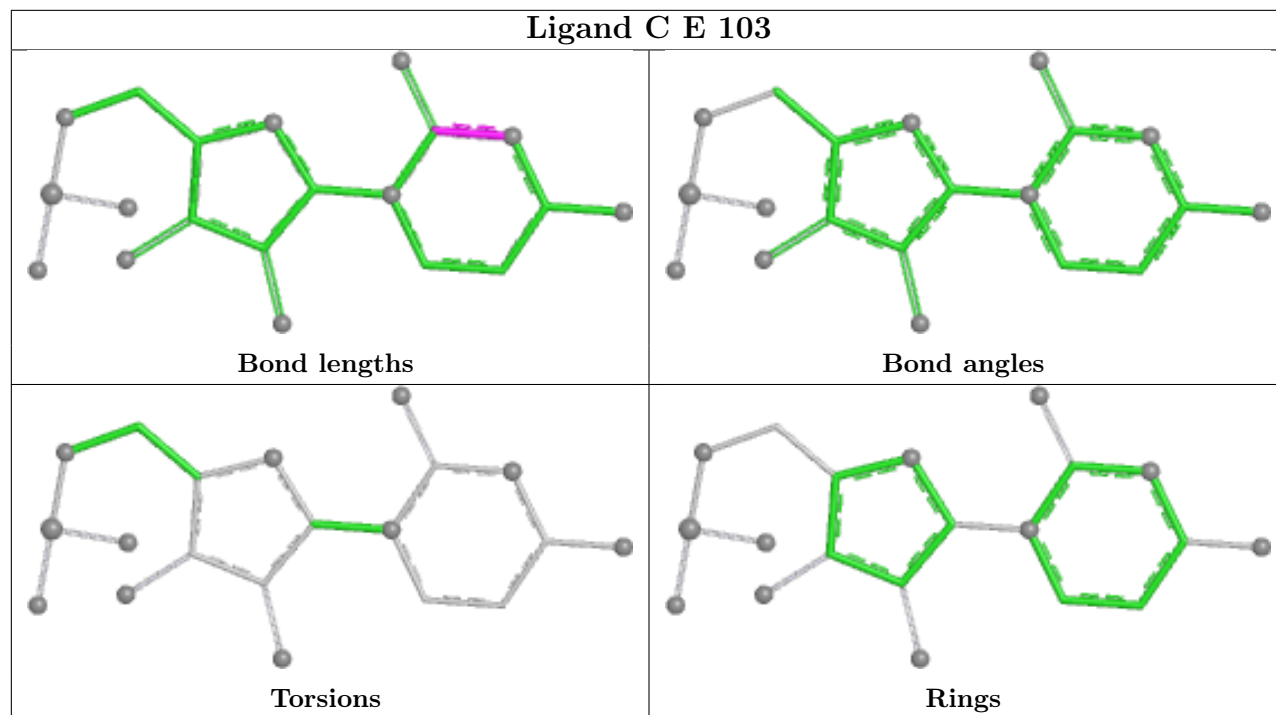
There are no ring outliers.

7 monomers are involved in 7 short contacts:

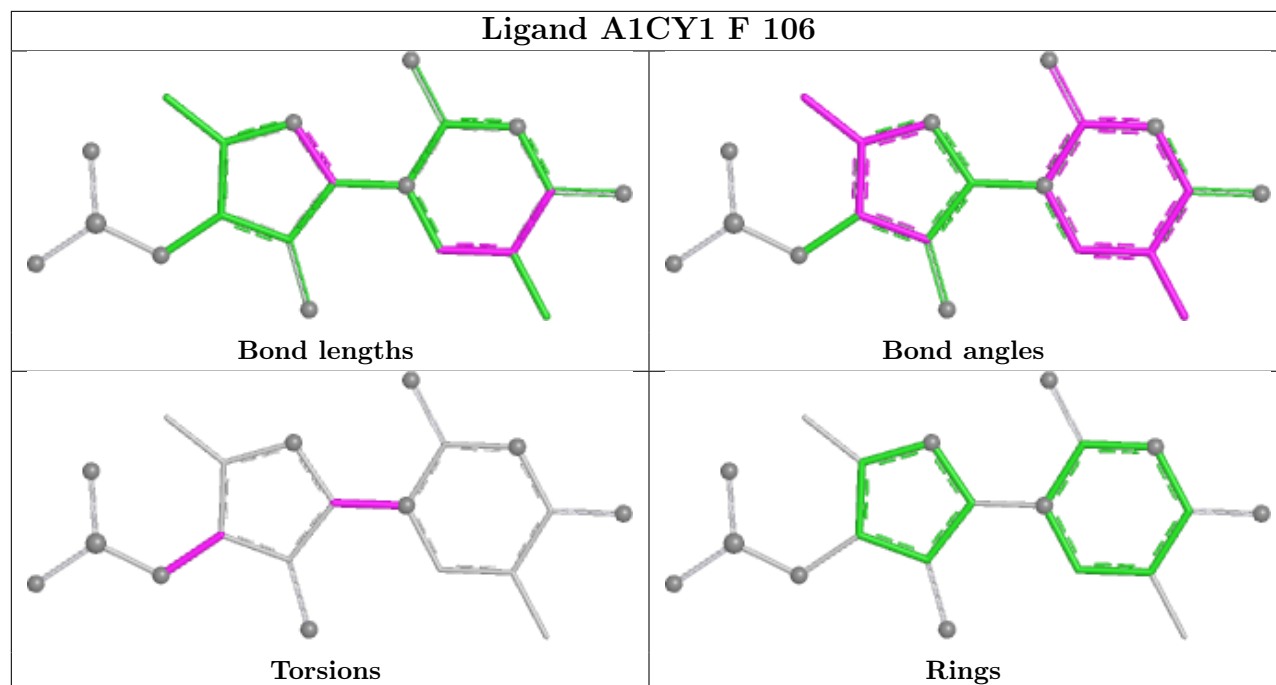
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	106	A1CY1	1	0
6	B	103	C5P	1	0
5	B	102	5GP	1	0
5	F	105	5GP	1	0
6	F	102	C5P	1	0
6	H	101	C5P	2	0
5	C	104	5GP	1	0

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

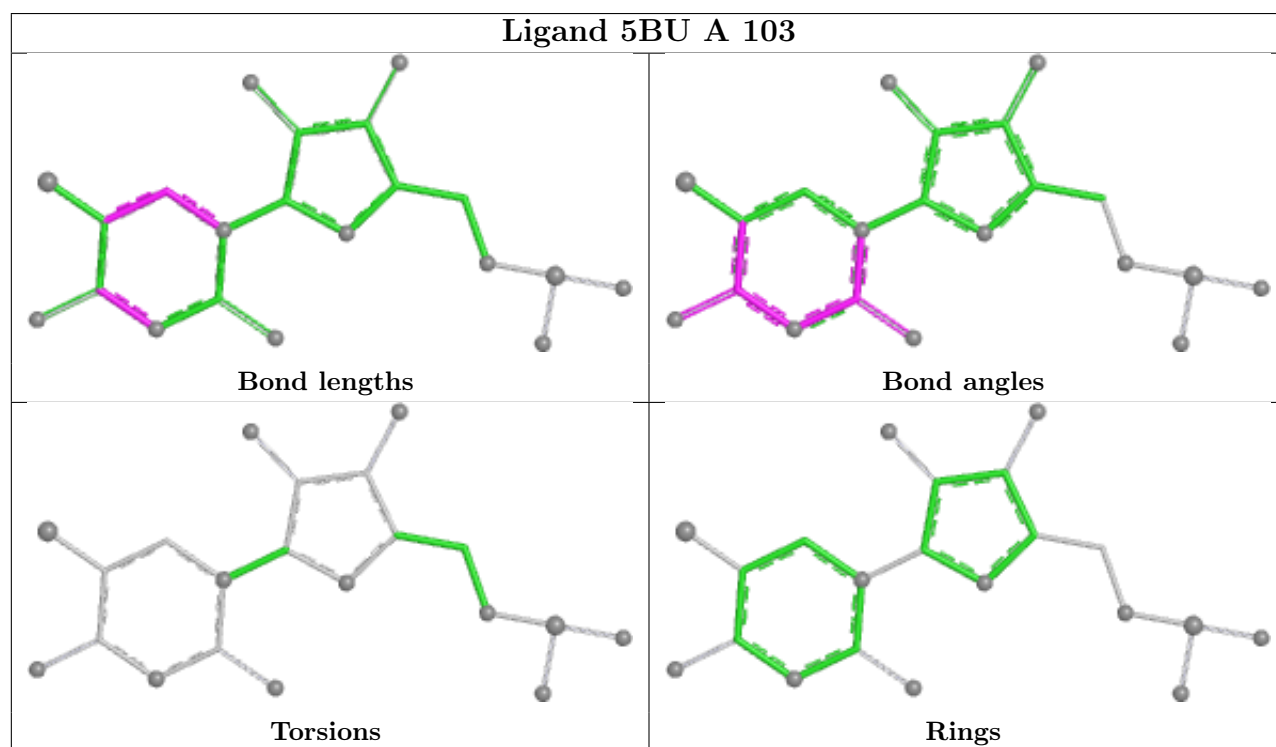
equivalents in the CSD to analyse the geometry.



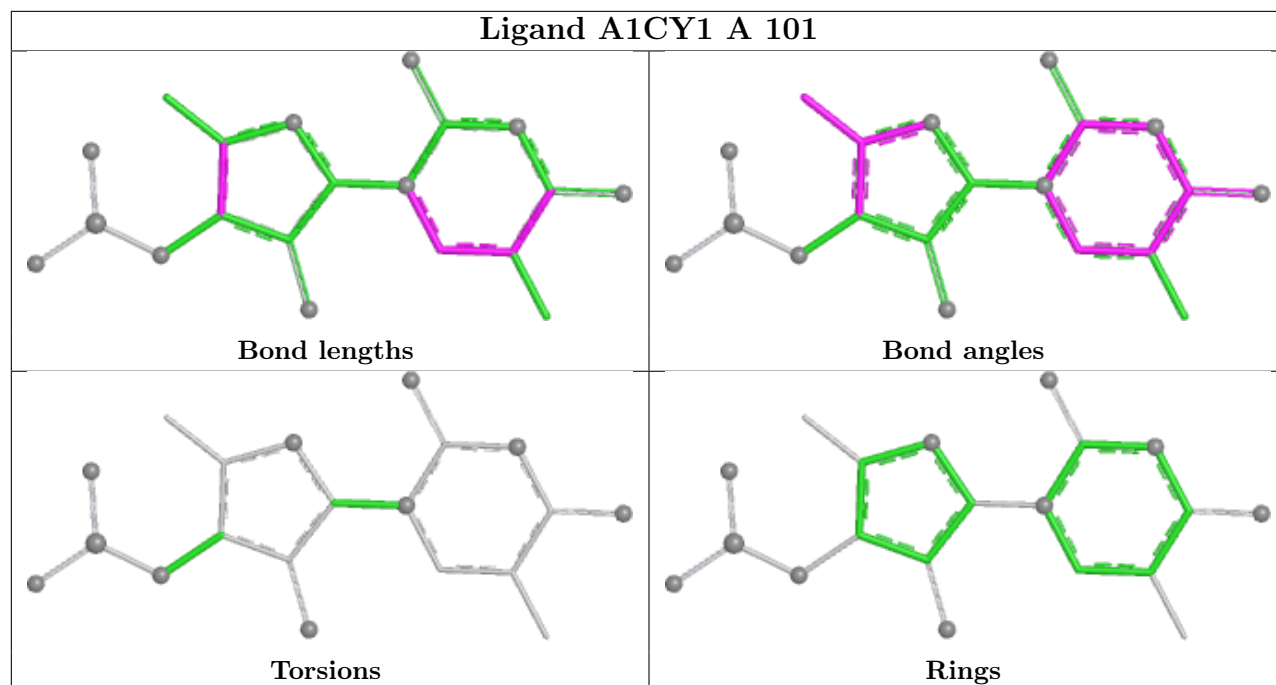
Ligand A1CY1 F 106



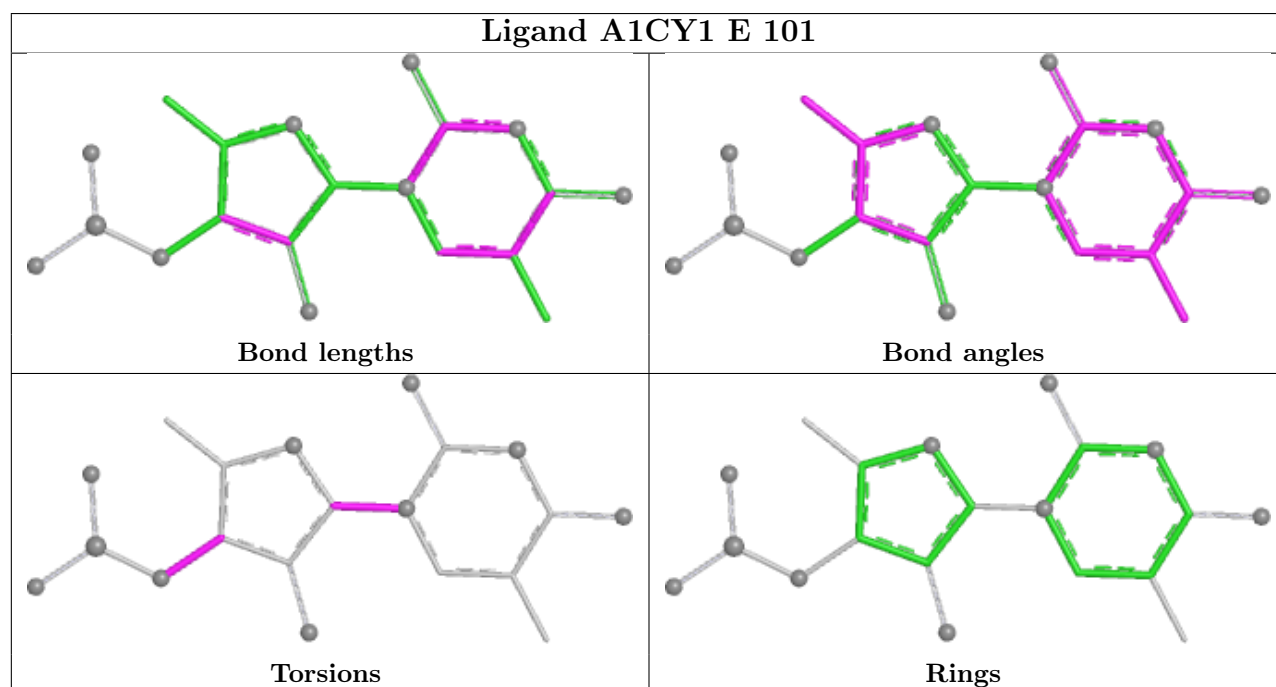
Ligand 5BU A 103



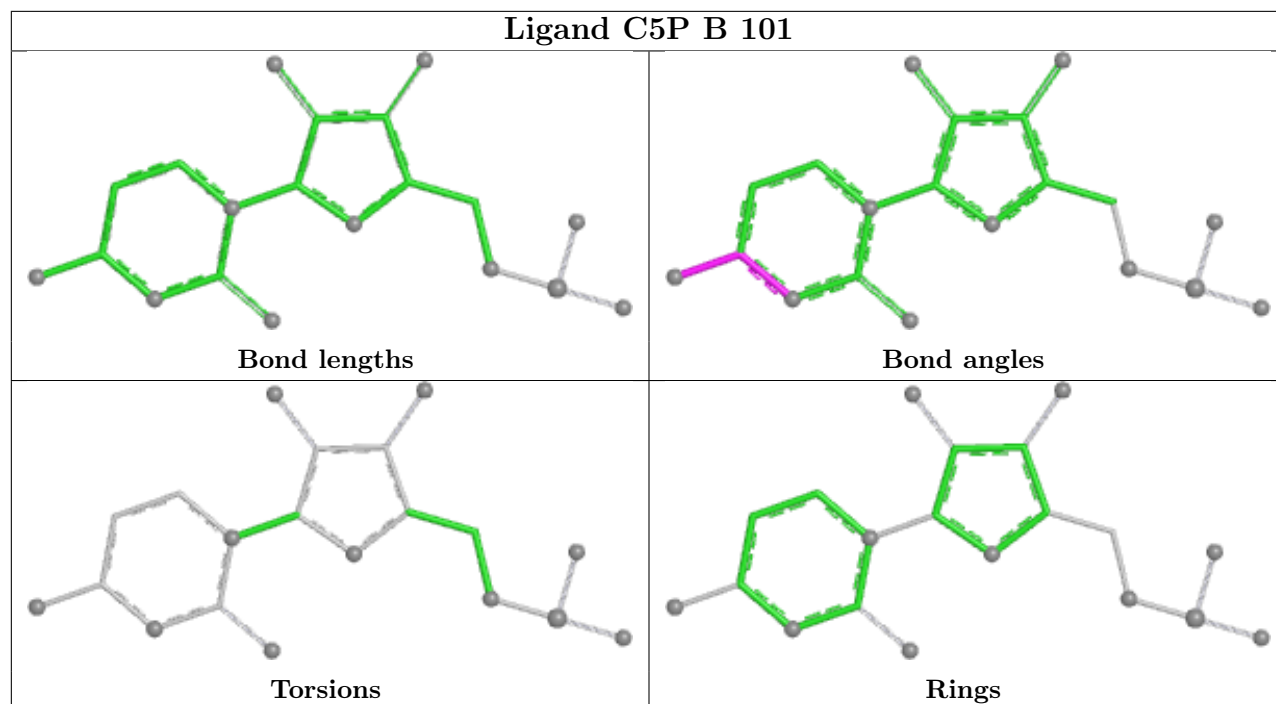
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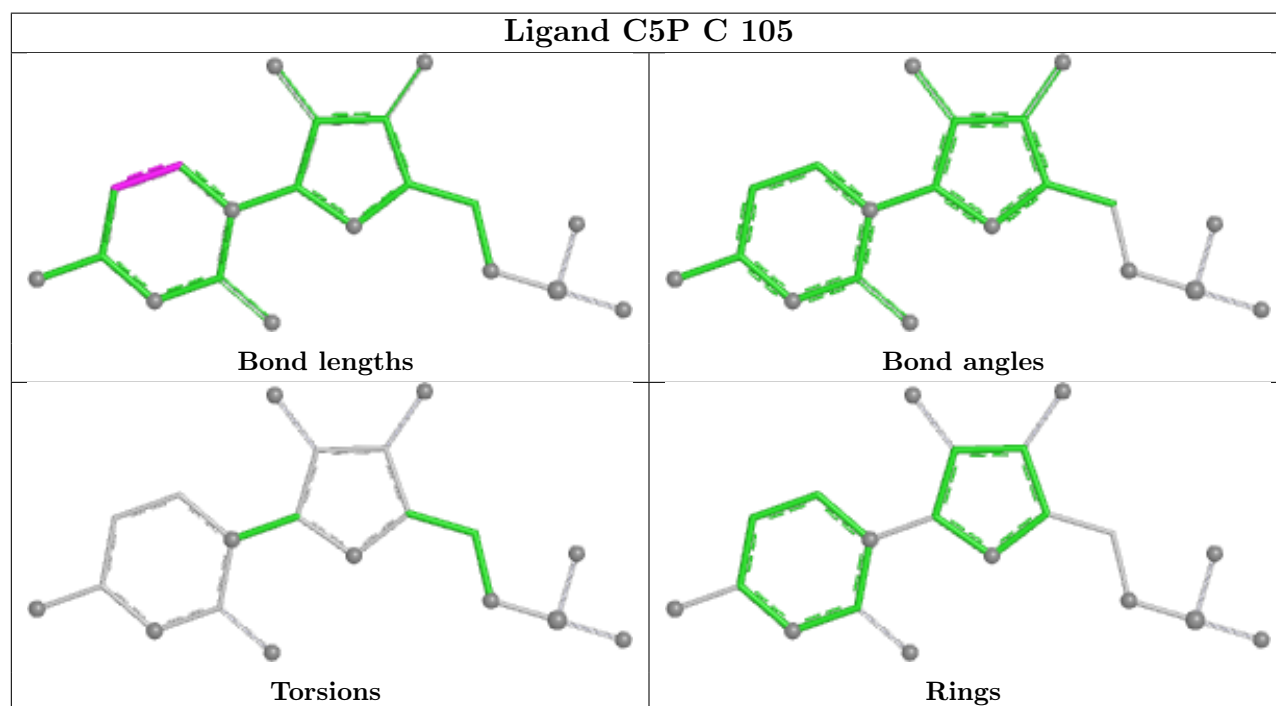
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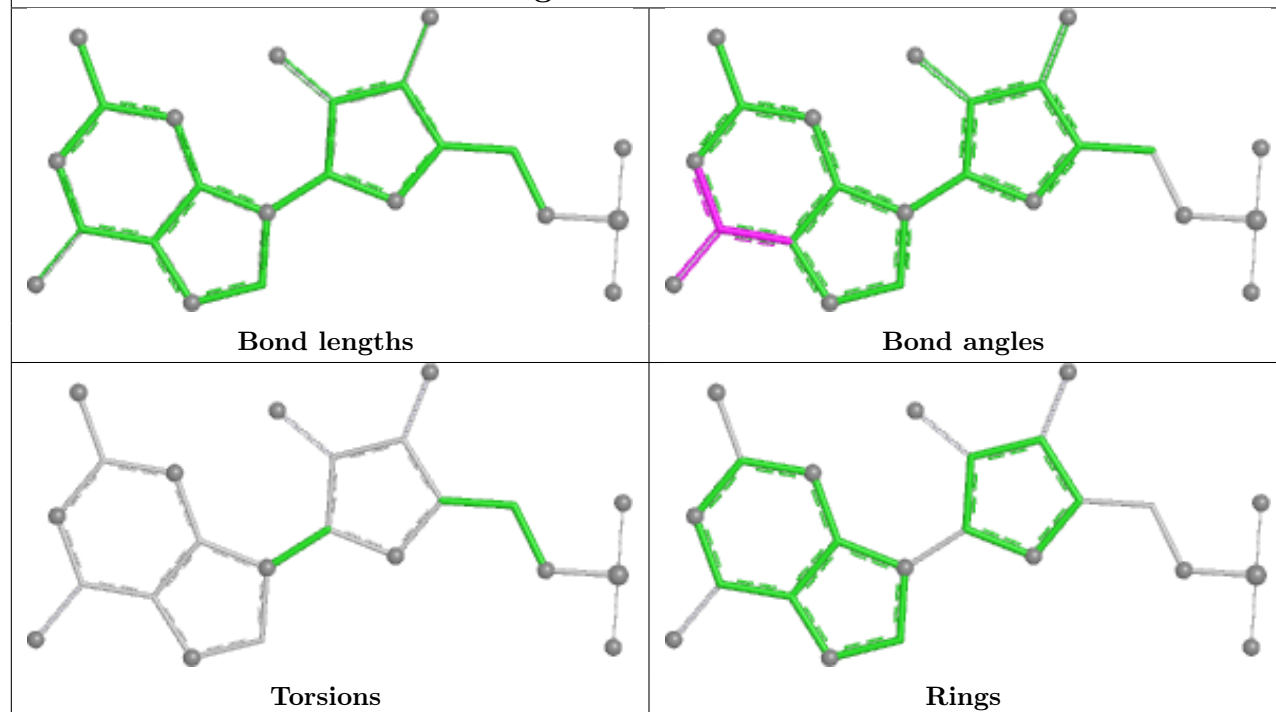
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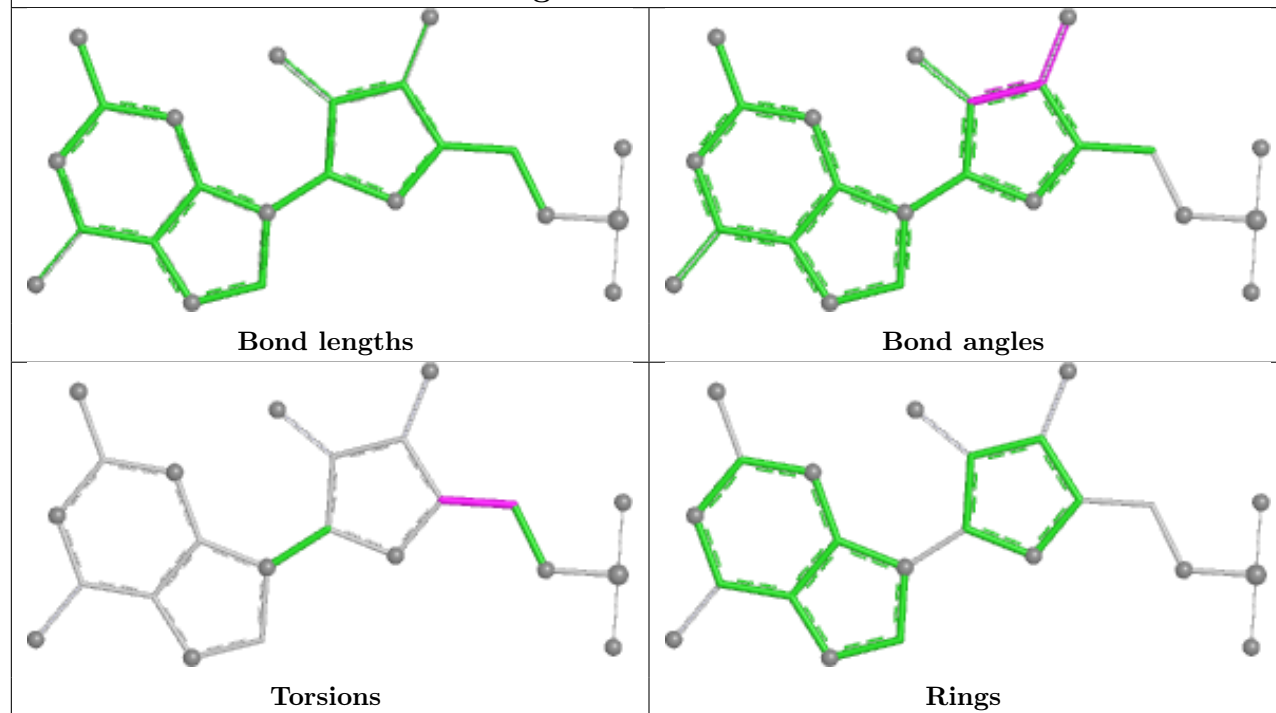
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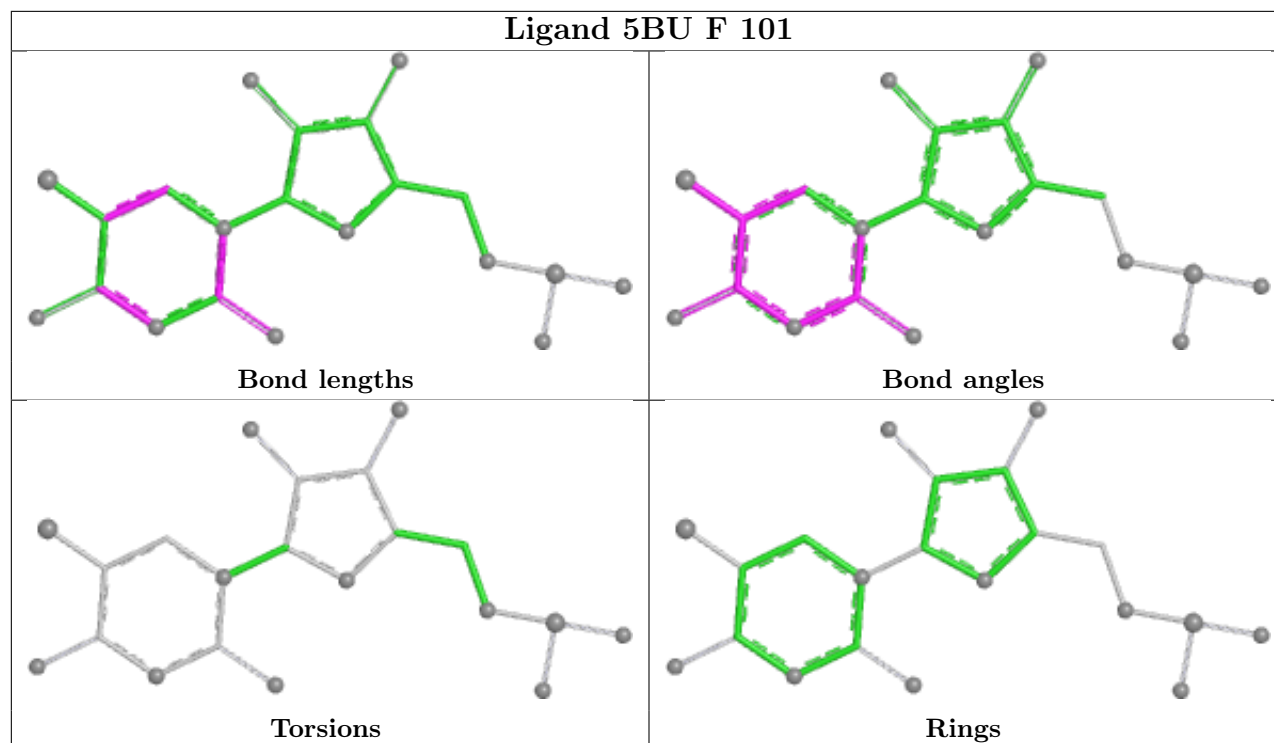
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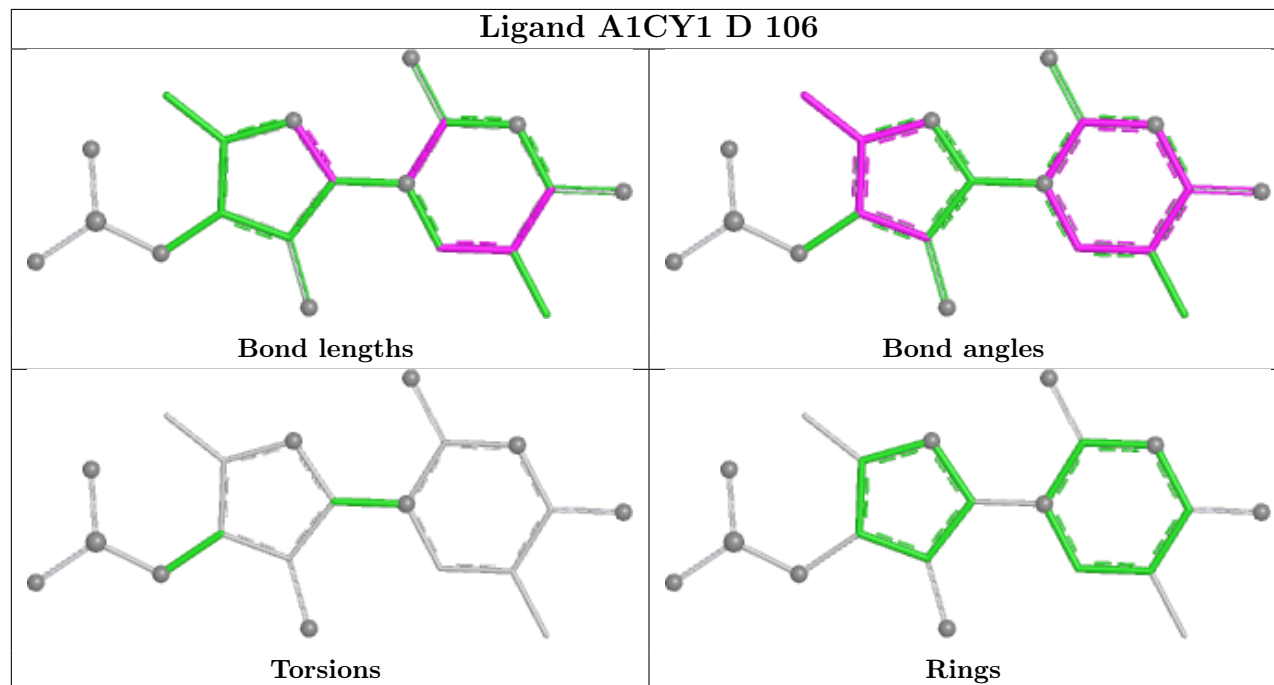
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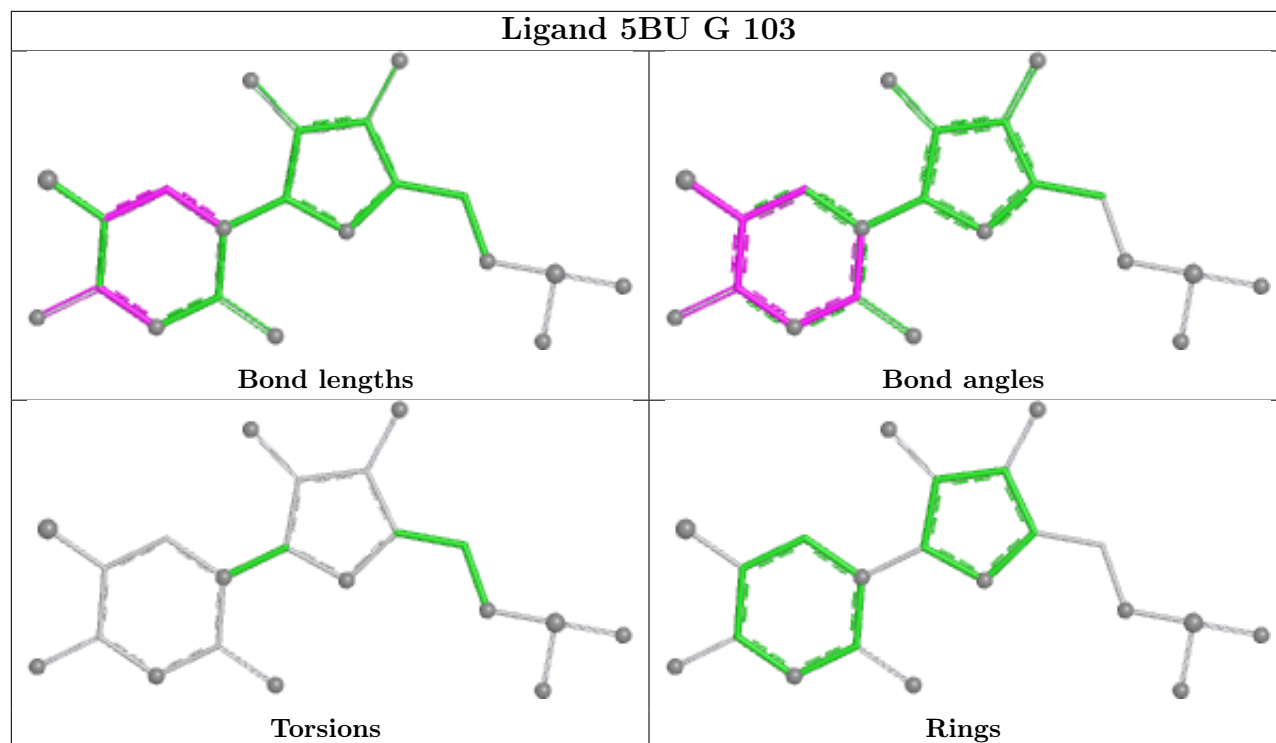
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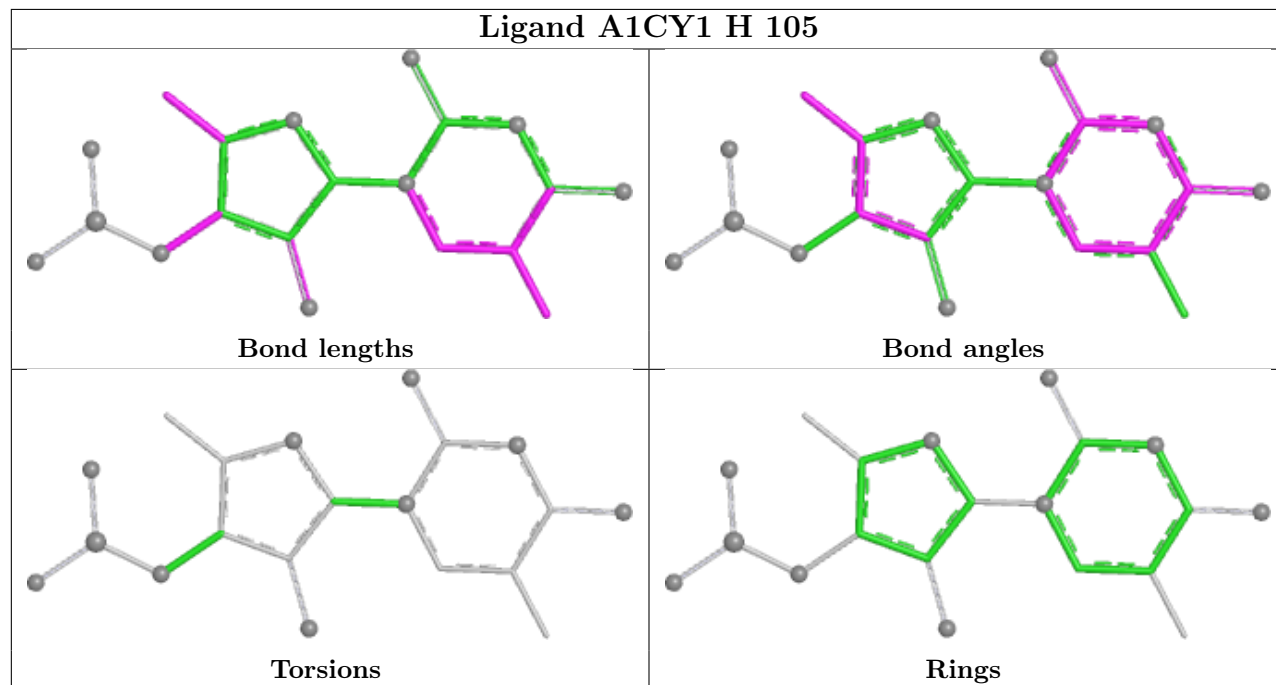
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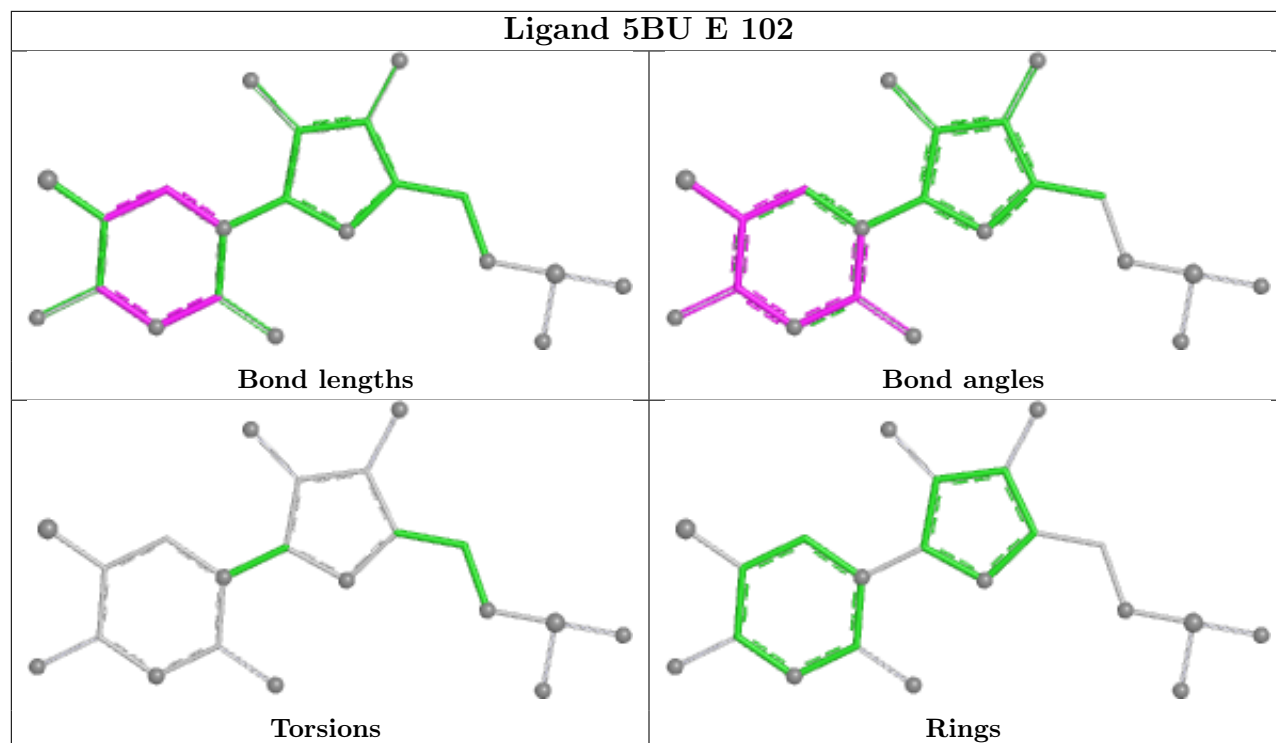
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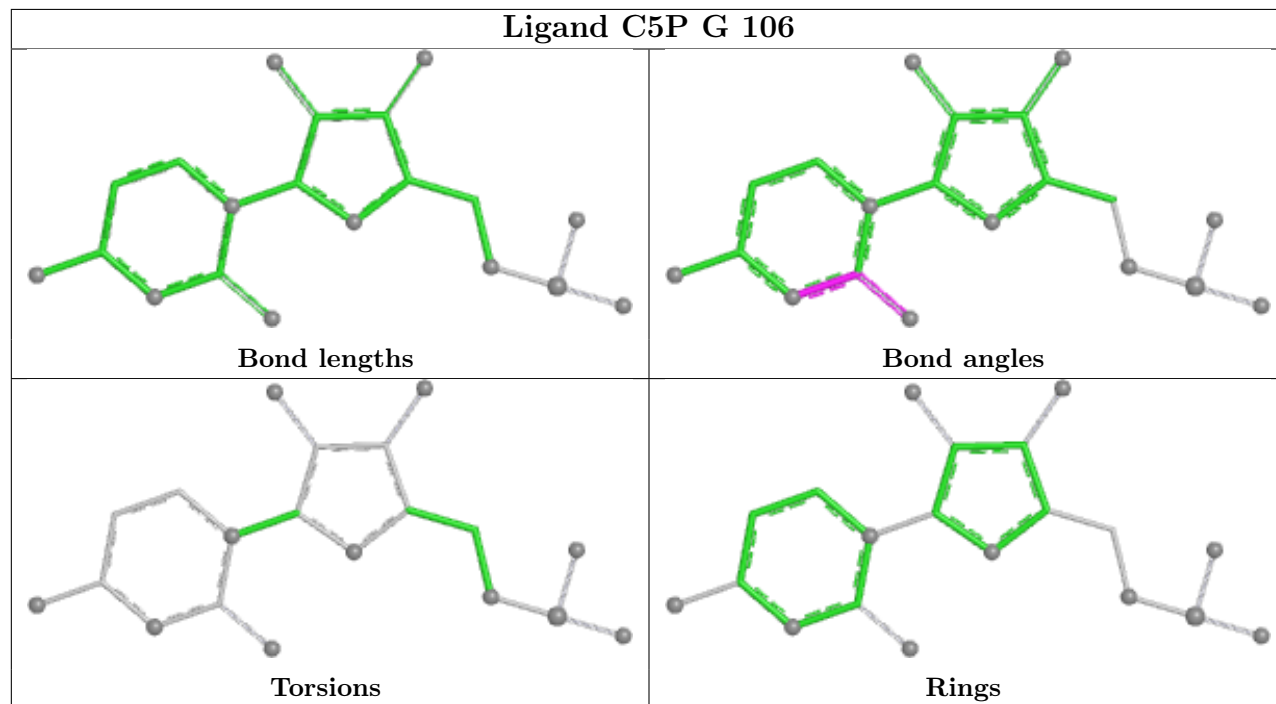
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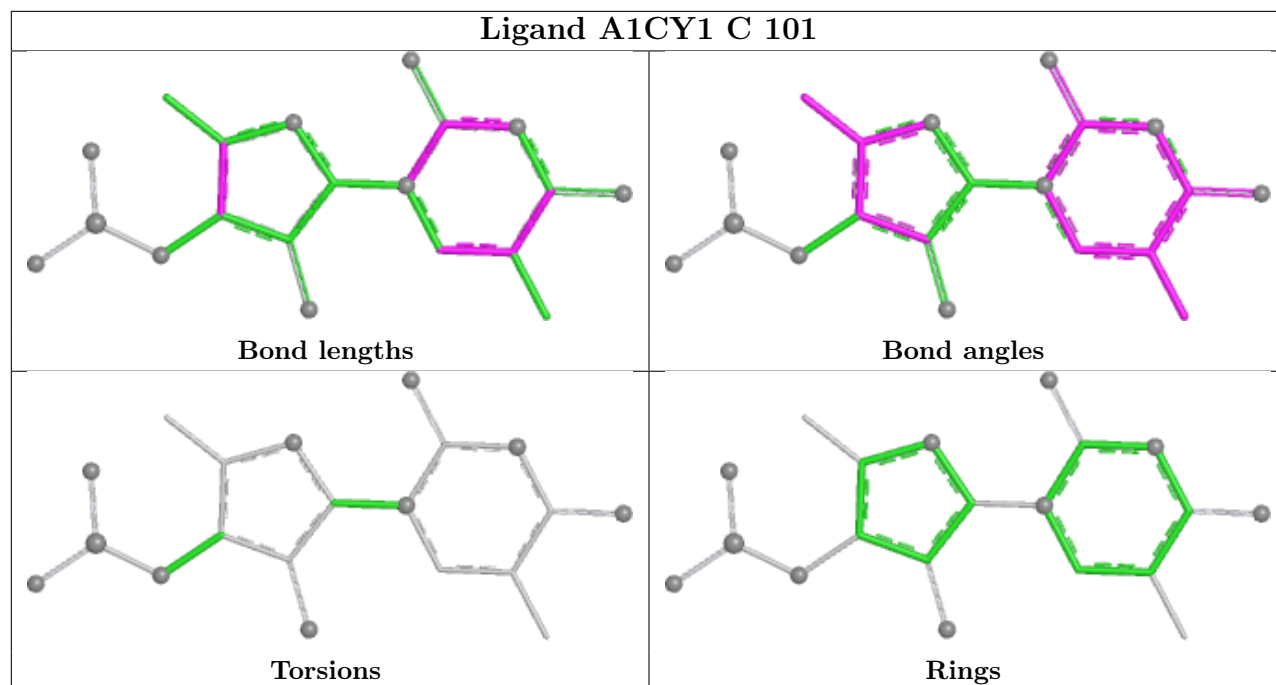
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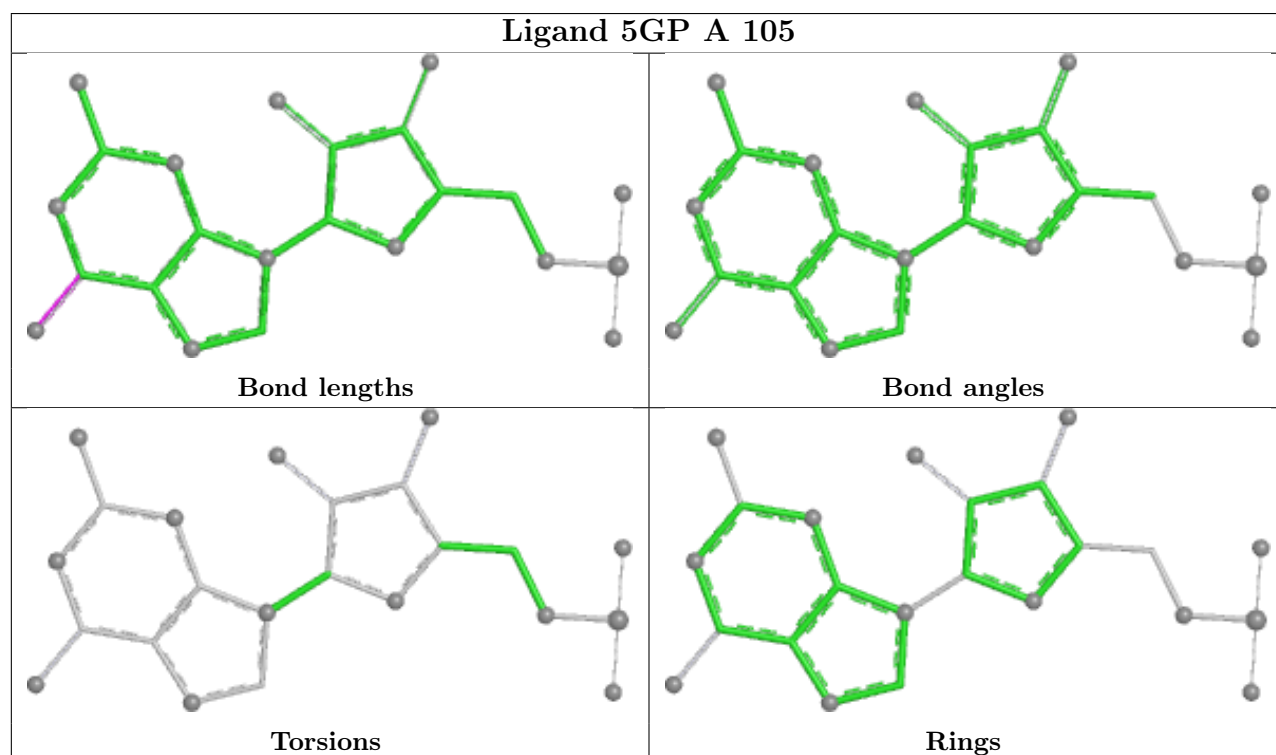
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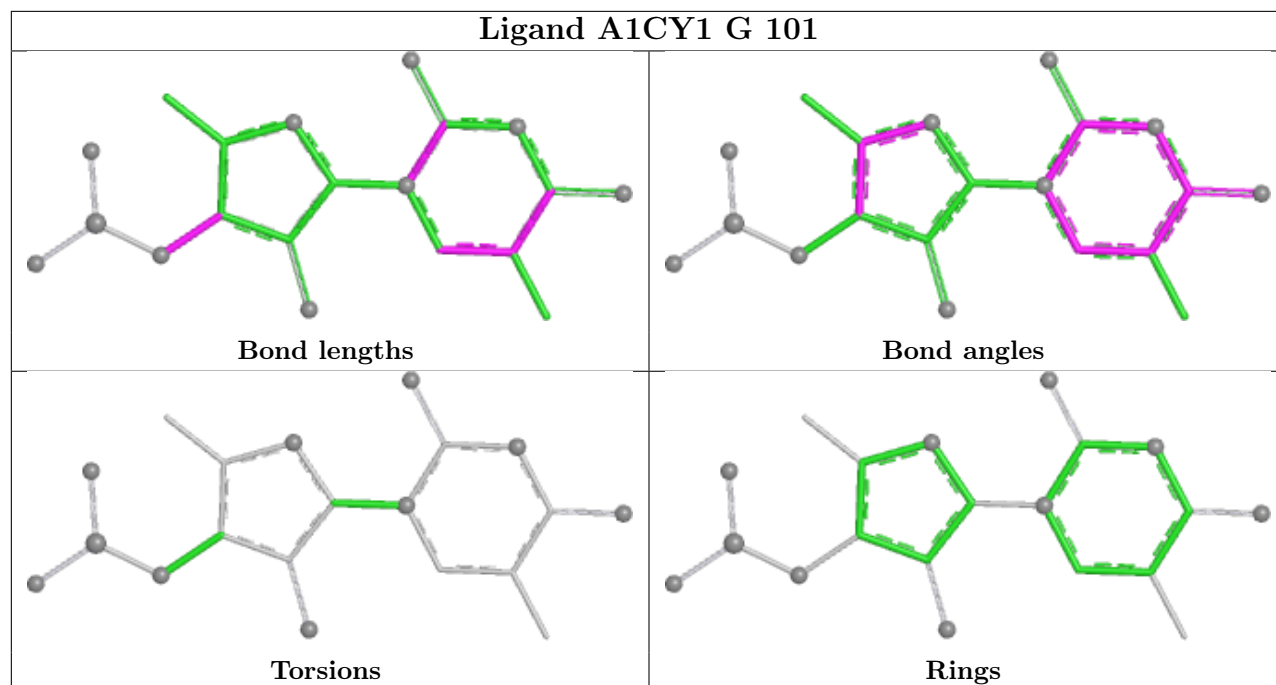
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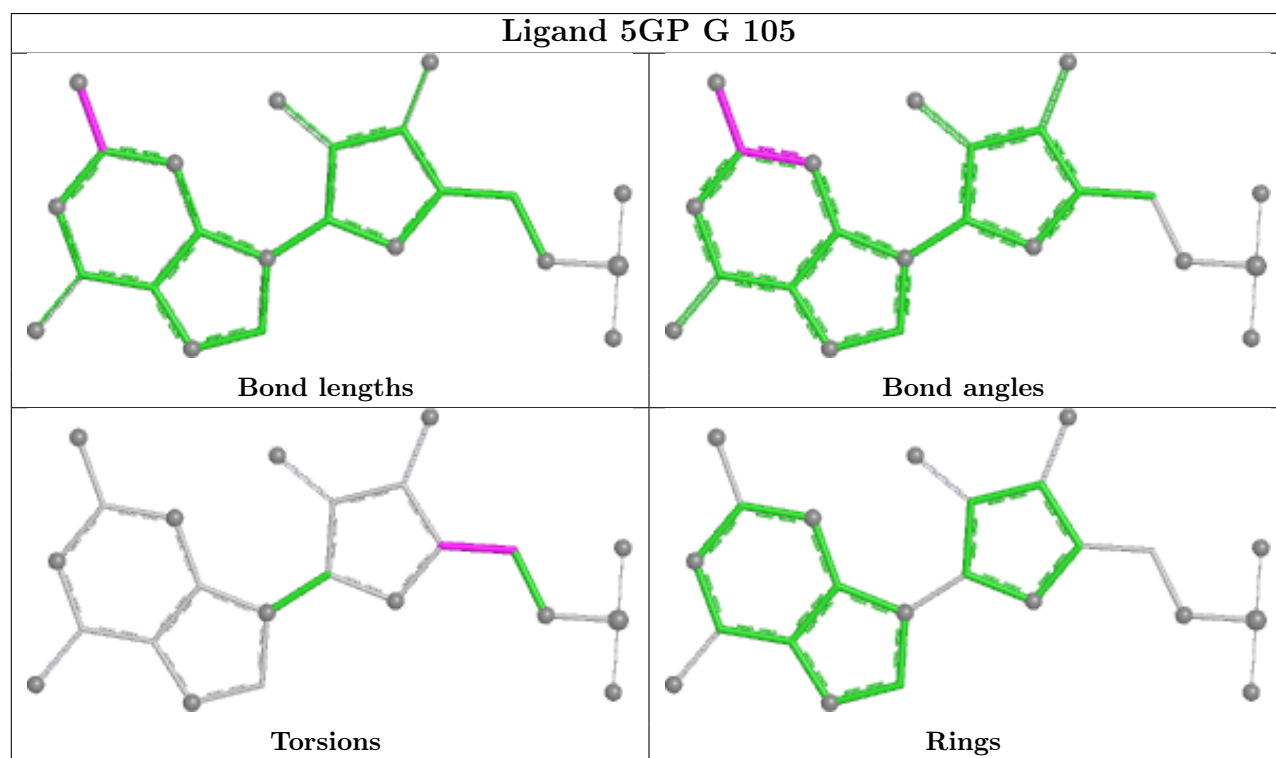
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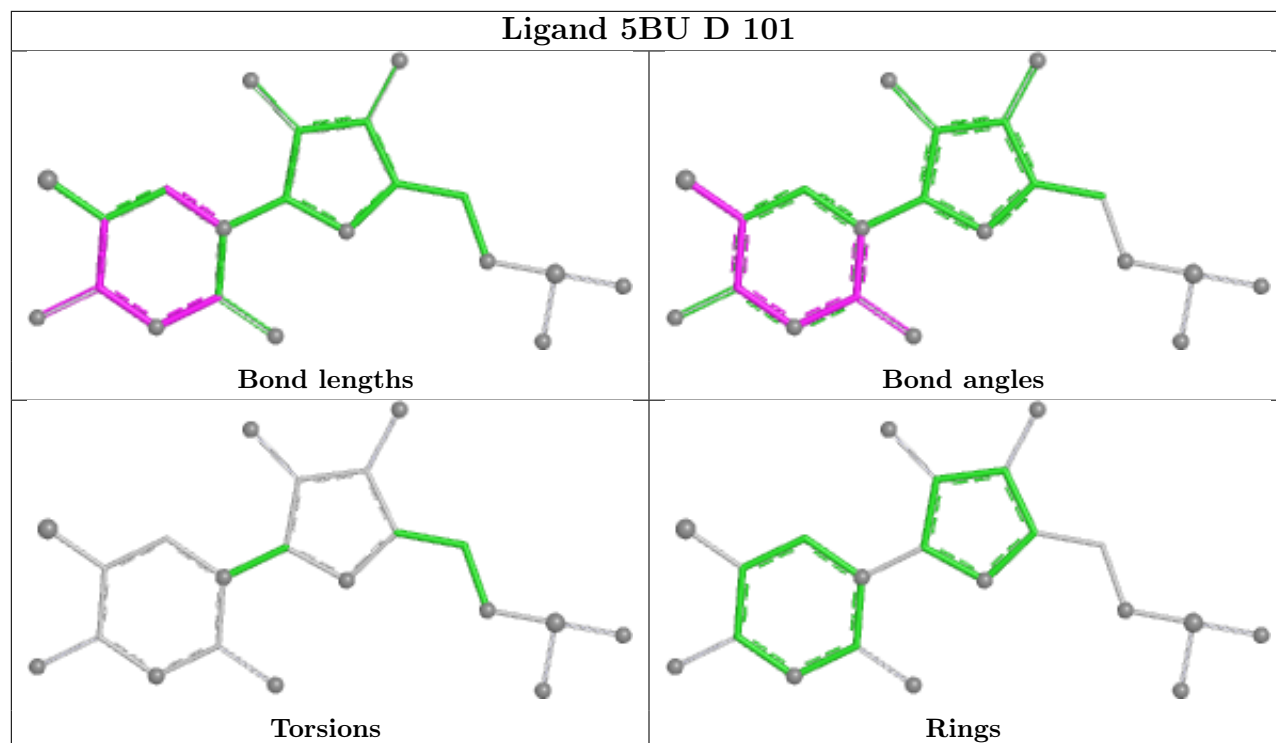
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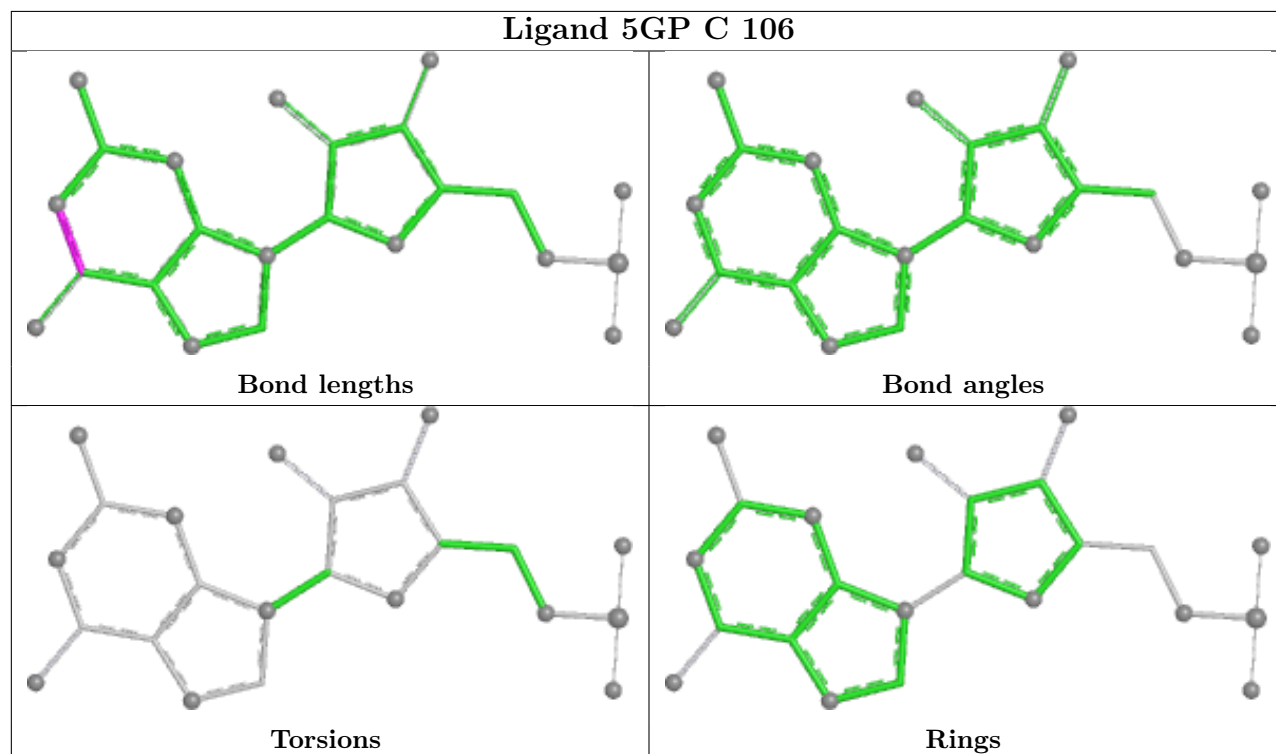
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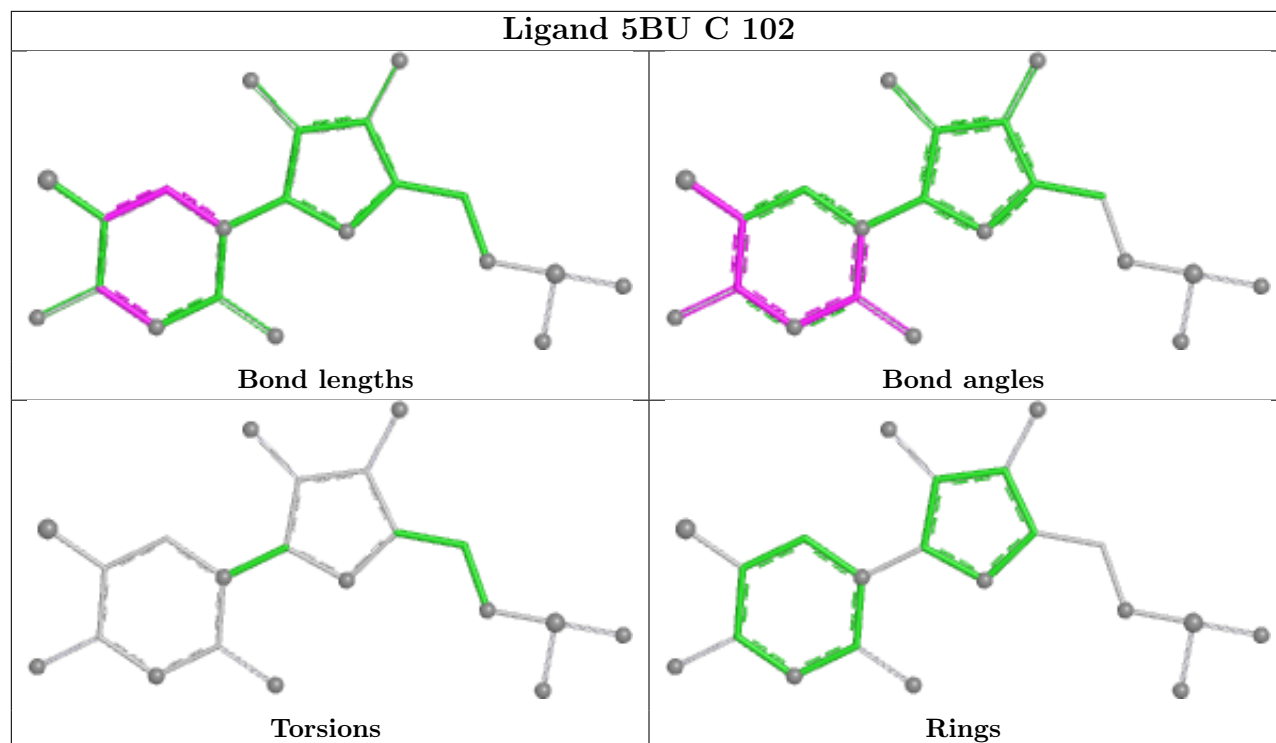
Ligand 5BU D 101



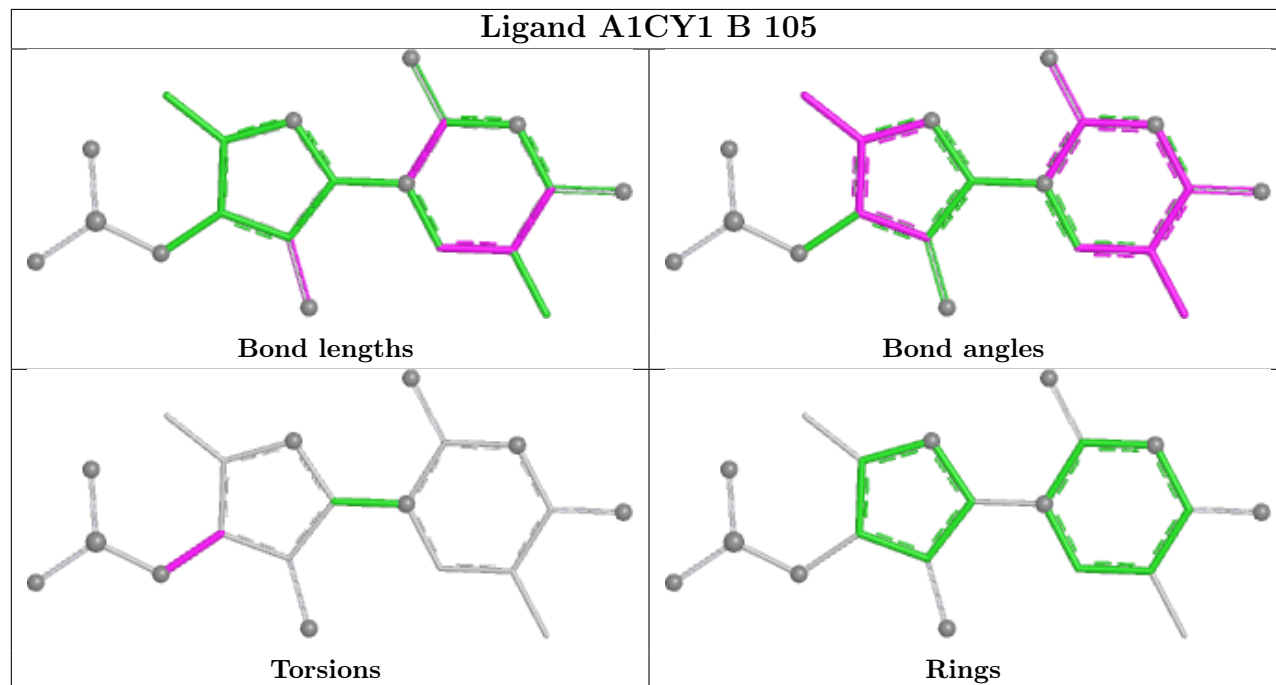
Ligand 5GP C 106



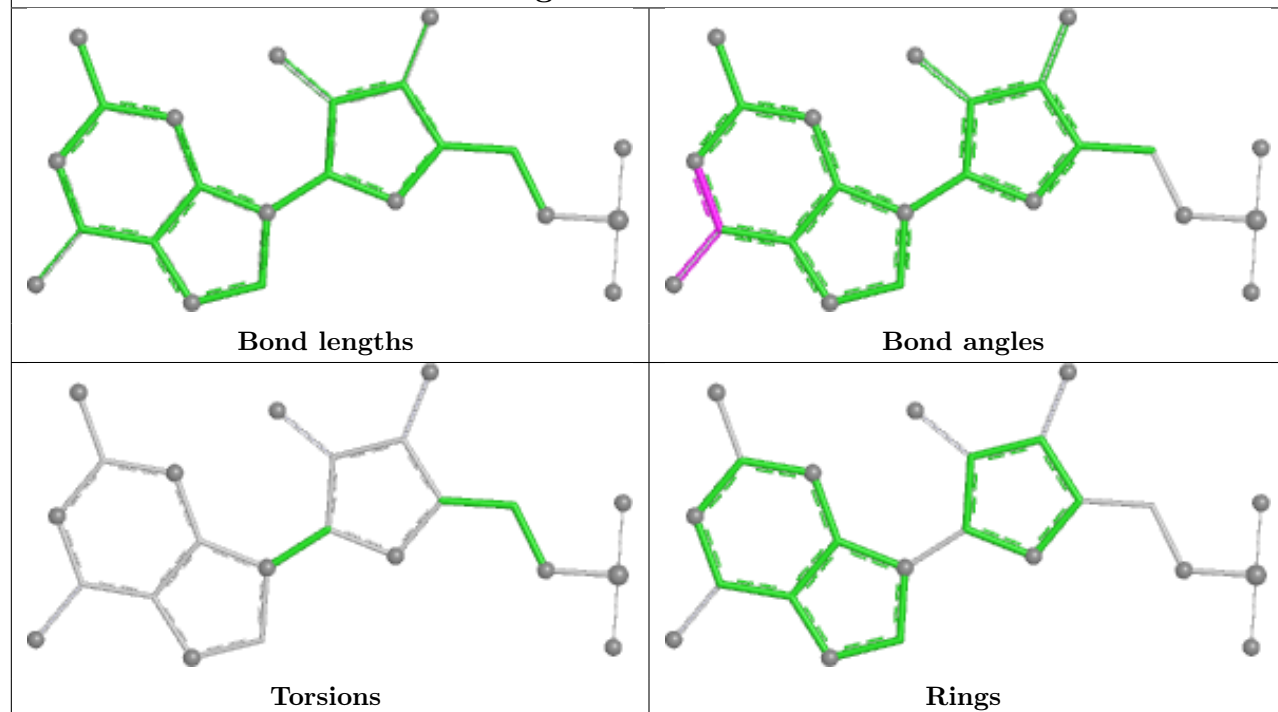
Ligand 5BU C 102



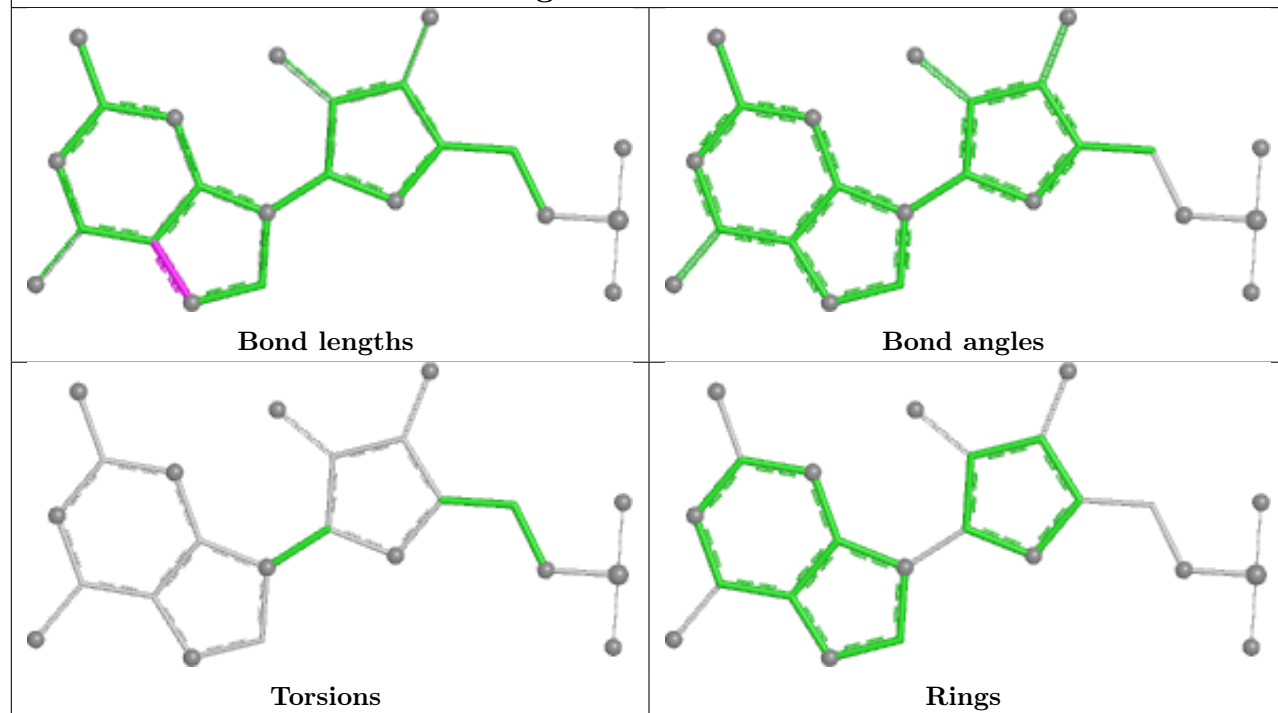
Ligand A1CY1 B 105

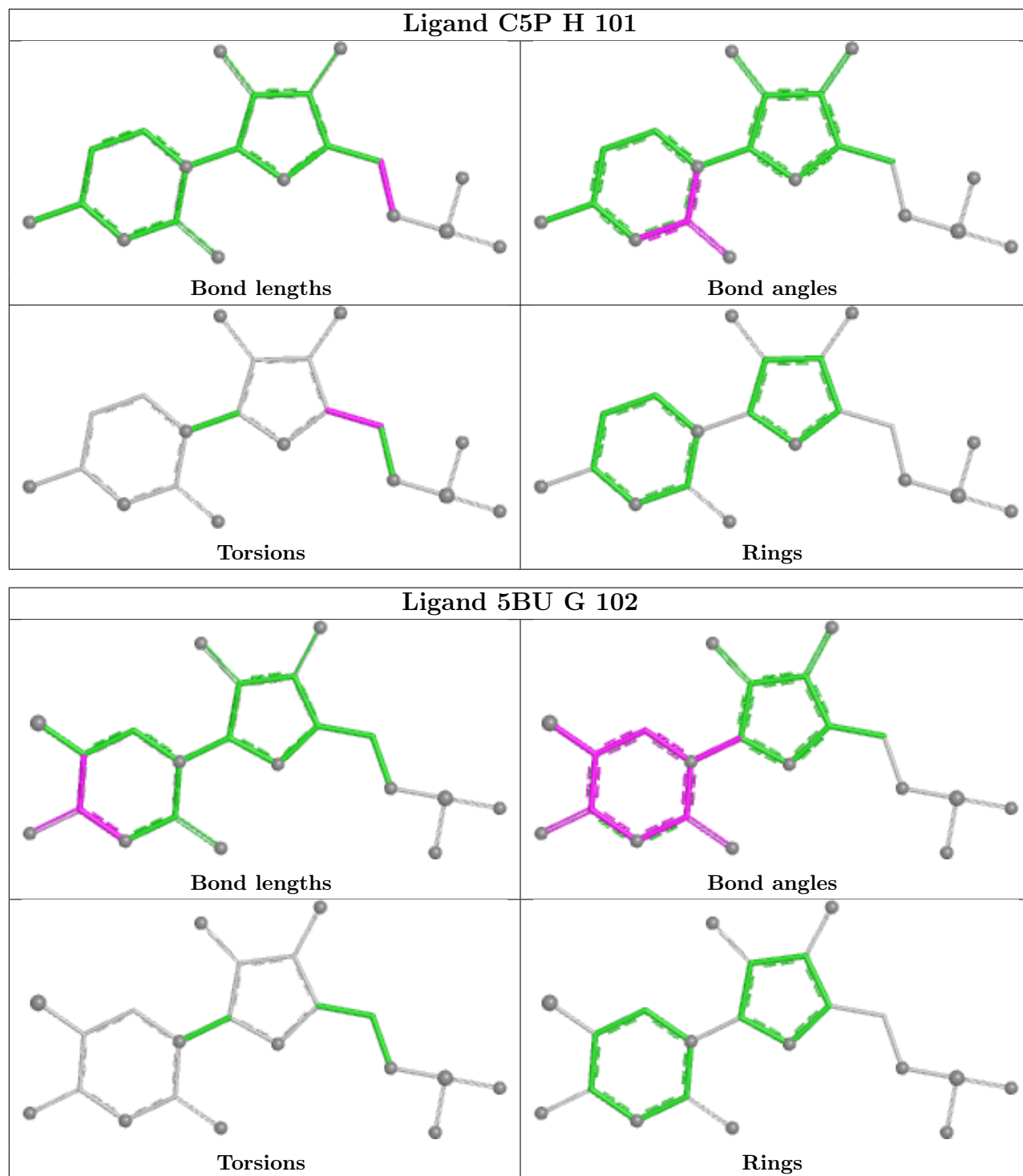


Ligand 5GP E 104



Ligand 5GP F 105





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	6/12 (50%)	0.90	1 (16%)  	23, 24, 31, 33	0
1	B	6/12 (50%)	2.14	3 (50%)  	31, 31, 35, 54	0
1	C	6/12 (50%)	1.87	3 (50%)  	27, 28, 32, 41	0
1	D	6/12 (50%)	1.10	0  	22, 24, 29, 42	0
1	E	6/12 (50%)	1.71	2 (33%)  	26, 29, 32, 37	0
1	F	6/12 (50%)	1.31	1 (16%)  	25, 27, 33, 34	0
1	G	6/12 (50%)	1.10	0  	26, 27, 28, 31	0
1	H	6/12 (50%)	1.78	2 (33%)  	23, 27, 33, 35	0
All	All	48/96 (50%)	1.49	12 (25%)  	22, 28, 37, 54	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	6	A	3.4
1	H	2	G	3.2
1	H	1	C	2.7
1	B	1	C	2.5
1	C	6	A	2.5
1	E	6	A	2.5
1	F	6	A	2.5
1	C	1	C	2.5
1	C	5	A	2.5
1	B	2	G	2.4
1	E	4	G	2.1
1	A	6	A	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	A1CY1	D	106	20/21	0.76	0.18	44,49,53,58	0
3	5BU	C	102	21/22	0.78	0.16	38,48,58,59	1
2	A1CY1	C	101	20/21	0.80	0.15	37,40,44,44	0
6	C5P	B	103	20/21	0.80	0.15	23,30,39,40	0
2	A1CY1	E	101	20/21	0.81	0.16	32,37,42,43	0
5	5GP	B	102	23/24	0.82	0.13	24,36,45,50	0
6	C5P	D	102	20/21	0.82	0.14	23,31,39,39	0
2	A1CY1	A	101	20/21	0.83	0.15	31,35,38,42	0
5	5GP	C	104	23/24	0.84	0.13	22,29,37,37	0
6	C5P	B	101	20/21	0.84	0.13	22,36,45,47	0
6	C5P	F	102	20/21	0.84	0.13	25,36,43,48	0
3	5BU	F	101	21/22	0.85	0.13	32,38,48,50	1
2	A1CY1	B	105	20/21	0.86	0.15	26,30,38,39	0
6	C5P	H	101	20/21	0.86	0.12	19,33,45,51	0
6	C5P	A	106	20/21	0.87	0.12	21,27,35,38	0
2	A1CY1	F	106	20/21	0.87	0.13	27,30,34,35	0
5	5GP	H	104	23/24	0.87	0.13	22,29,39,42	0
5	5GP	F	103	23/24	0.88	0.11	21,34,44,45	0
5	5GP	G	105	23/24	0.88	0.12	19,28,38,47	0
5	5GP	H	102	23/24	0.88	0.11	24,32,43,43	0
5	5GP	B	104	23/24	0.88	0.12	18,24,30,31	0
6	C5P	F	104	20/21	0.88	0.12	21,31,38,43	0
4	C	A	104	20/21	0.88	0.12	25,30,37,39	0
2	A1CY1	G	101	20/21	0.89	0.11	29,34,40,42	0
5	5GP	F	105	23/24	0.89	0.11	20,25,35,39	0
6	C5P	D	104	20/21	0.90	0.12	21,26,32,35	0
6	C5P	H	103	20/21	0.90	0.10	25,30,37,39	0

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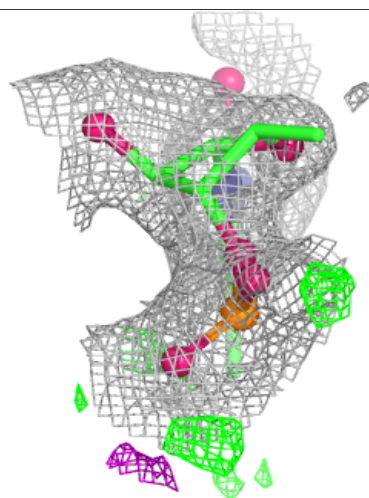
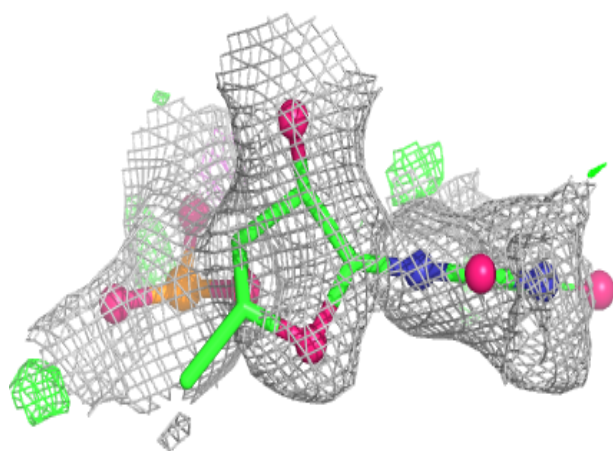
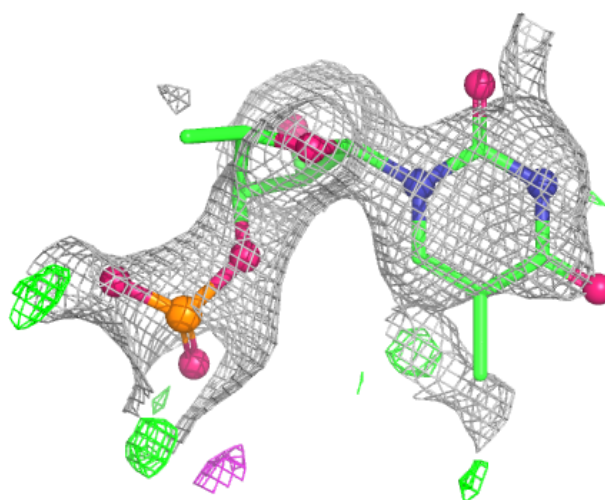
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	5BU	D	101	21/22	0.91	0.12	31,36,43,45	1
3	5BU	A	103	21/22	0.91	0.14	27,33,40,41	1
3	5BU	A	102	21/22	0.91	0.12	26,32,45,46	1
5	5GP	D	103	23/24	0.91	0.09	19,26,33,35	0
6	C5P	G	106	20/21	0.91	0.12	20,27,32,34	0
4	C	C	103	20/21	0.91	0.11	28,38,47,47	0
5	5GP	A	105	23/24	0.91	0.10	20,28,35,35	0
3	5BU	G	102	21/22	0.92	0.11	20,28,36,40	1
4	C	E	103	20/21	0.92	0.09	24,31,41,42	0
4	C	G	104	20/21	0.92	0.11	22,27,35,37	0
5	5GP	G	107	23/24	0.92	0.10	20,24,33,40	0
6	C5P	C	105	20/21	0.92	0.10	17,23,28,31	0
2	A1CY1	H	105	20/21	0.92	0.10	19,24,32,33	0
5	5GP	D	105	23/24	0.93	0.09	18,24,32,35	0
5	5GP	E	104	23/24	0.93	0.09	20,29,34,34	0
5	5GP	E	106	23/24	0.93	0.09	16,23,28,33	0
5	5GP	C	106	23/24	0.93	0.09	19,22,26,30	0
3	5BU	E	102	21/22	0.93	0.12	26,31,38,44	1
5	5GP	A	107	23/24	0.94	0.09	21,26,34,38	0
3	5BU	G	103	21/22	0.94	0.10	21,25,33,35	1
6	C5P	E	105	20/21	0.95	0.08	20,25,30,36	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.

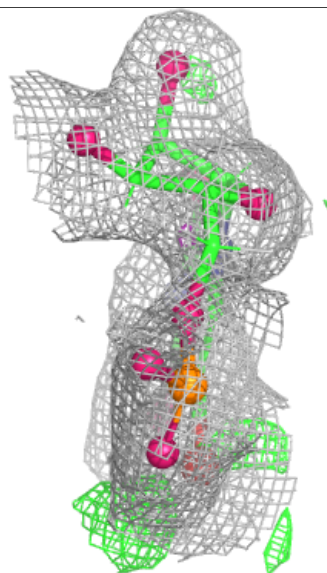
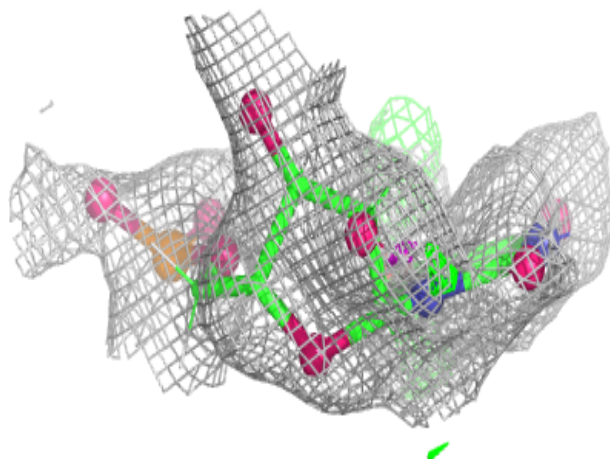
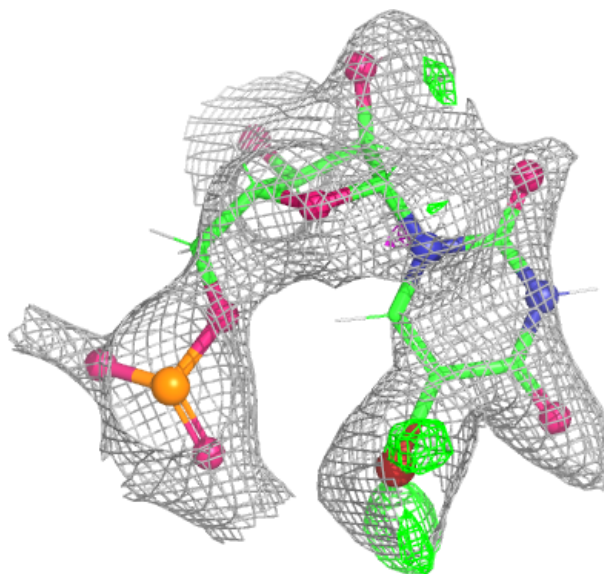
Electron density around A1CY1 D 106:

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



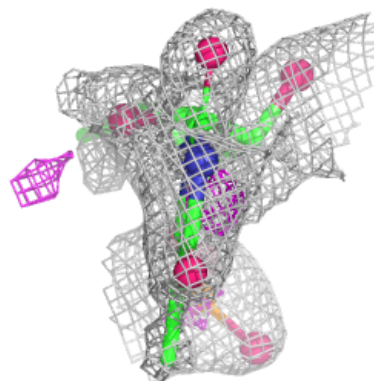
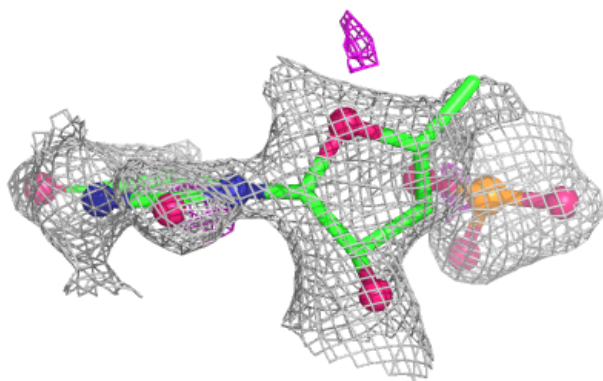
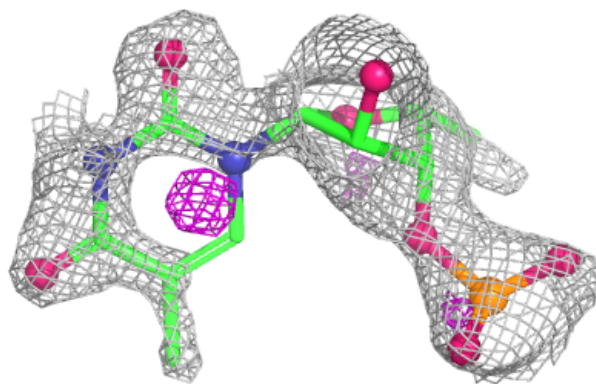
Electron density around 5BU C 102:

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



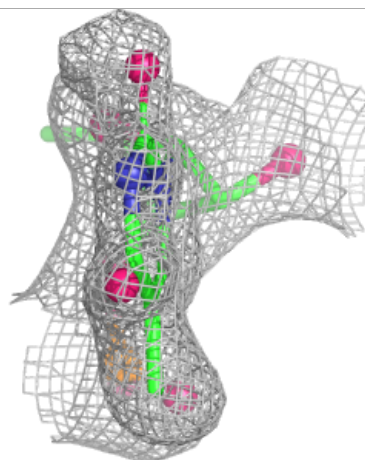
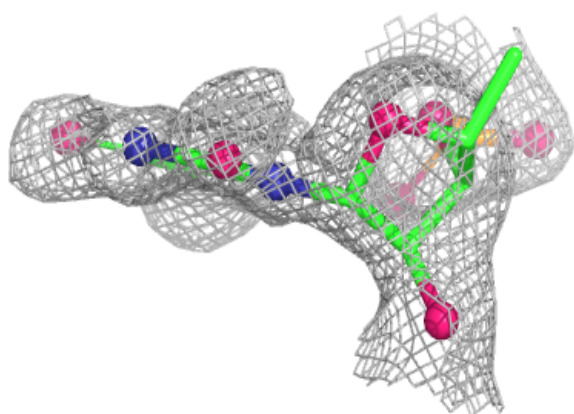
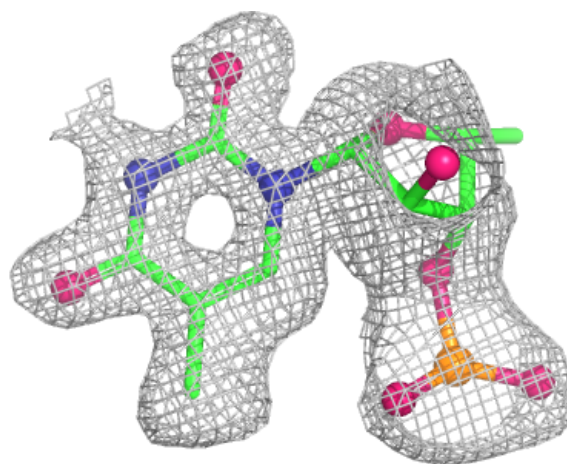
Electron density around A1CY1 C 101:

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



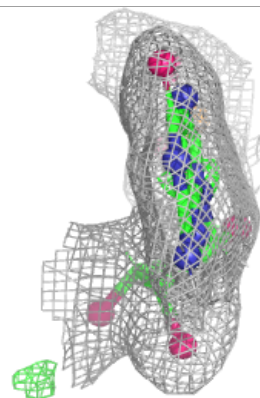
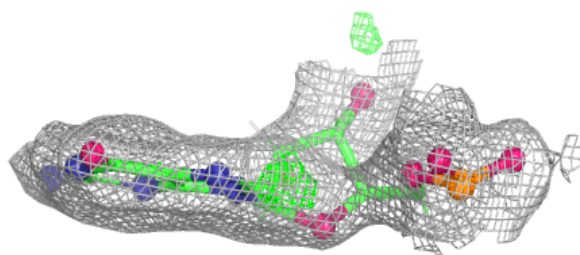
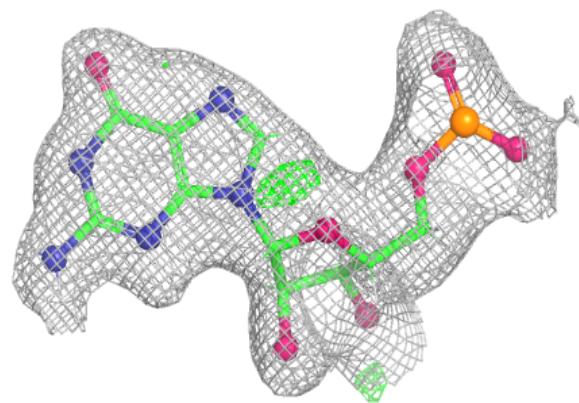
Electron density around A1CY1 E 101:

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and green (positive)

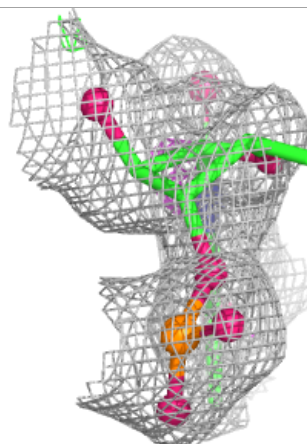
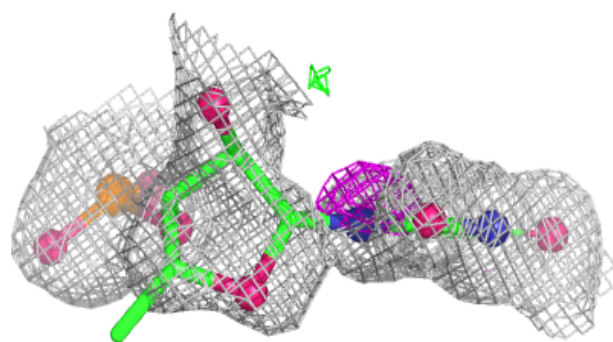
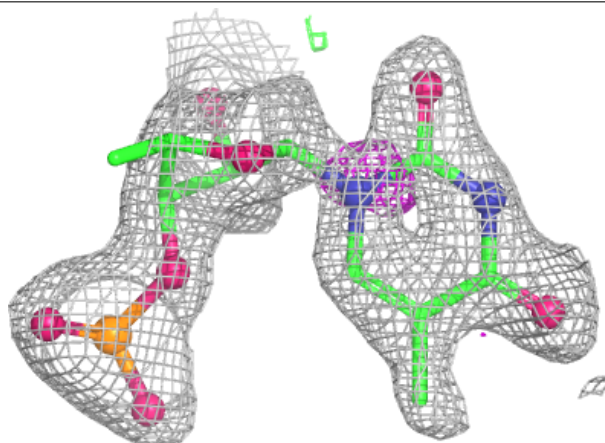


Electron density around 5GP B 102:

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and green (positive)

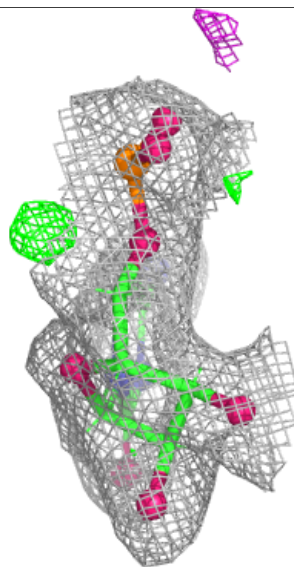
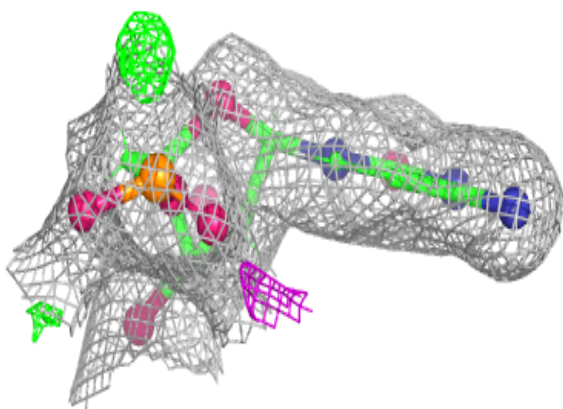
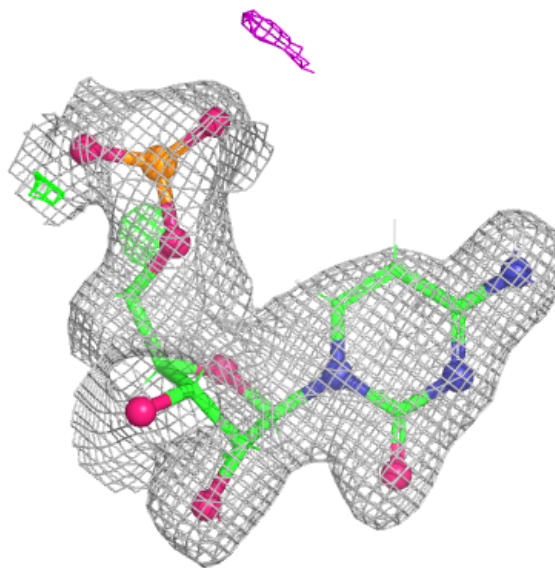
**Electron density around A1CY1 A 101:**

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and green (positive)



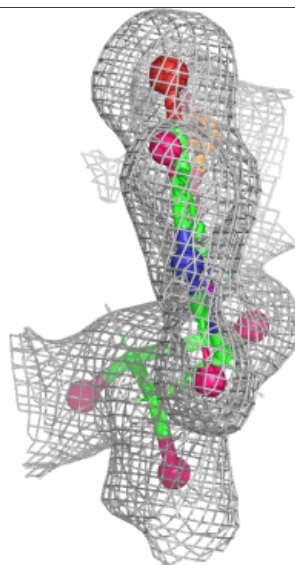
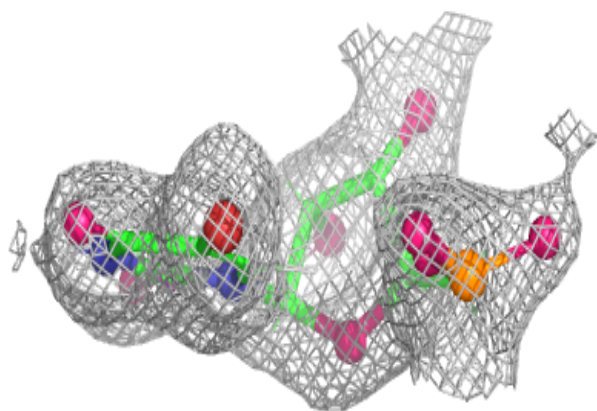
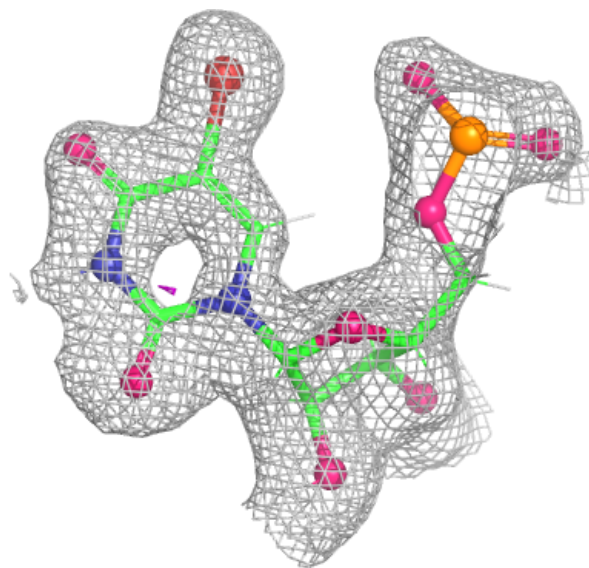
Electron density around C5P B 101:

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and green (positive)



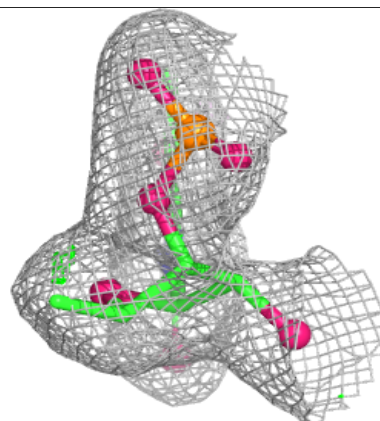
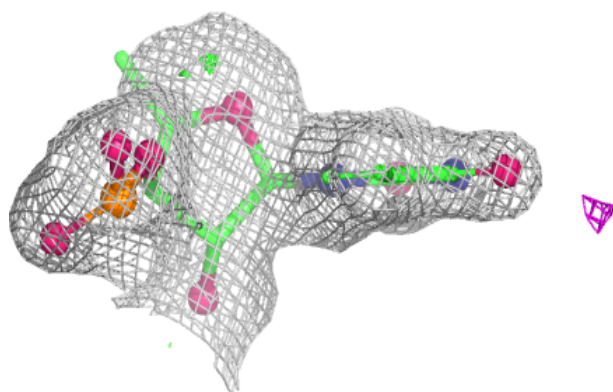
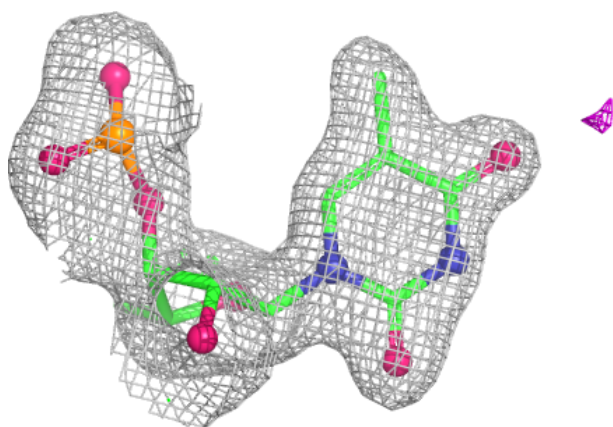
Electron density around 5BU F 101:

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and green (positive)



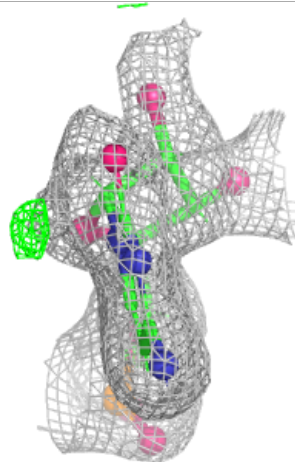
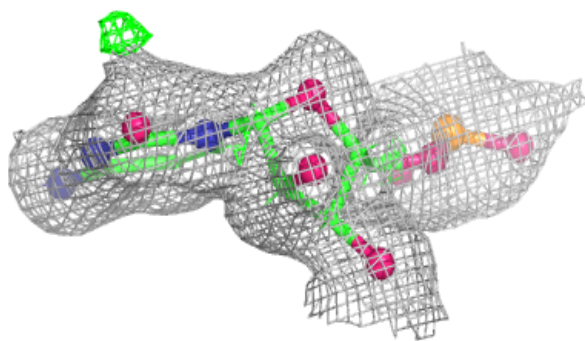
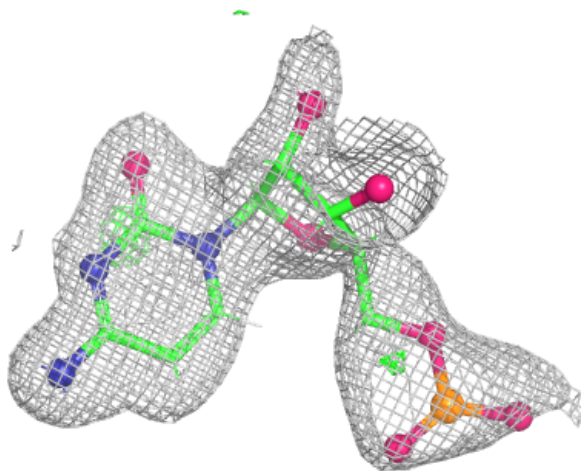
Electron density around A1CY1 B 105:

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and green (positive)



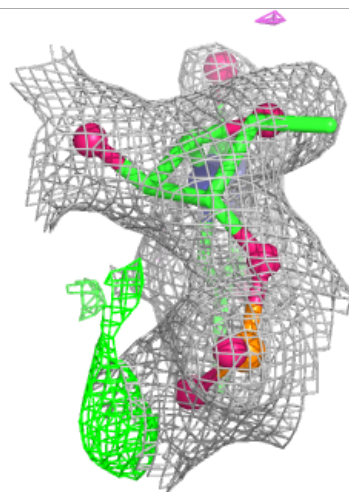
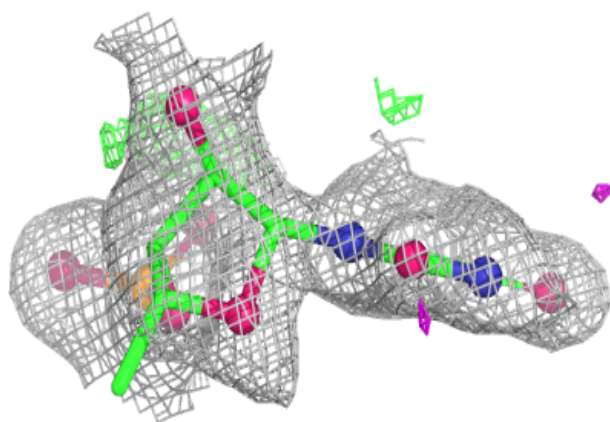
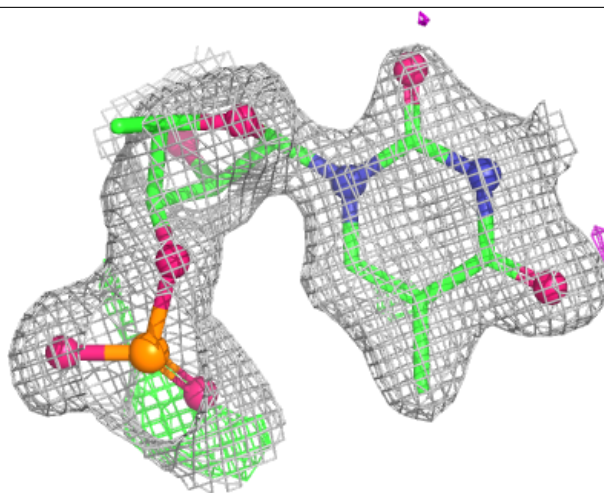
Electron density around C5P H 101:

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and green (positive)



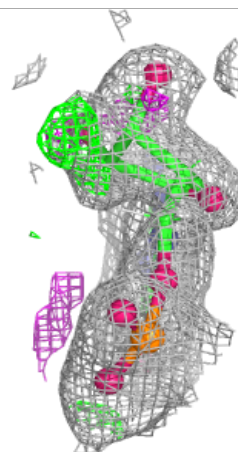
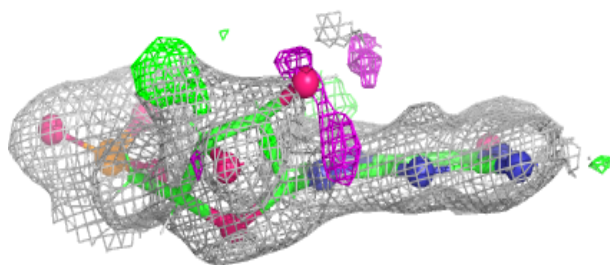
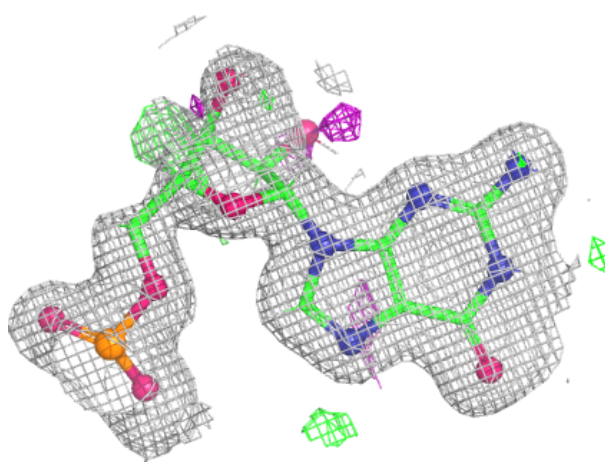
Electron density around A1CY1 F 106:

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and green (positive)



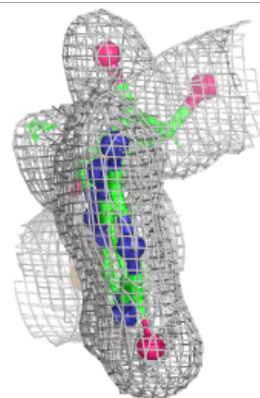
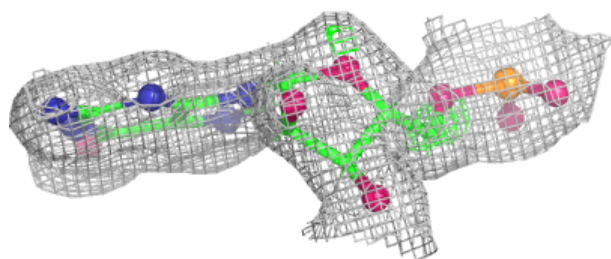
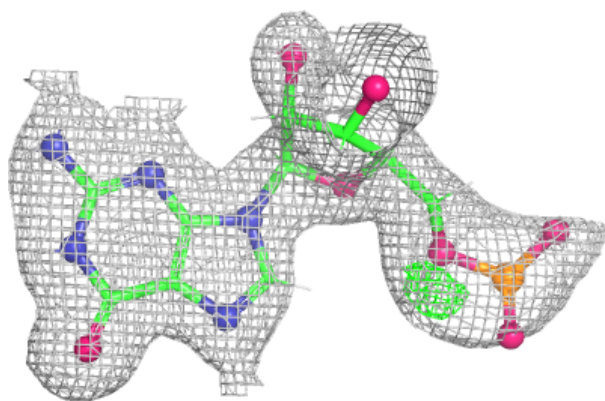
Electron density around 5GP H 104:

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and green (positive)



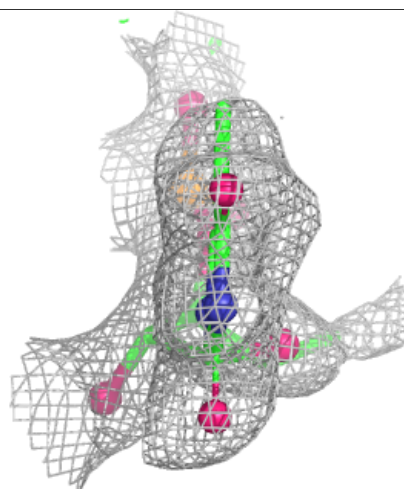
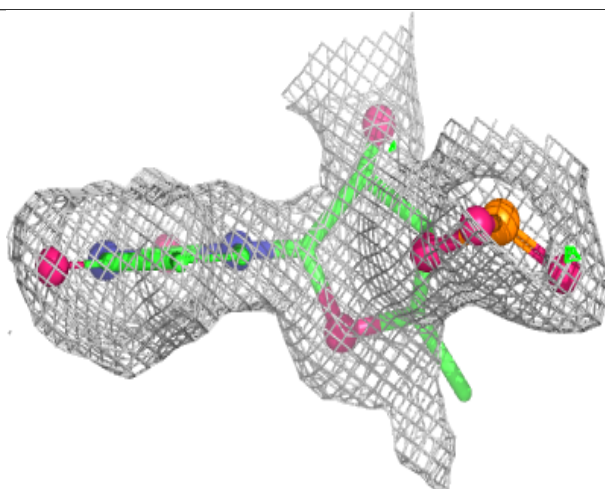
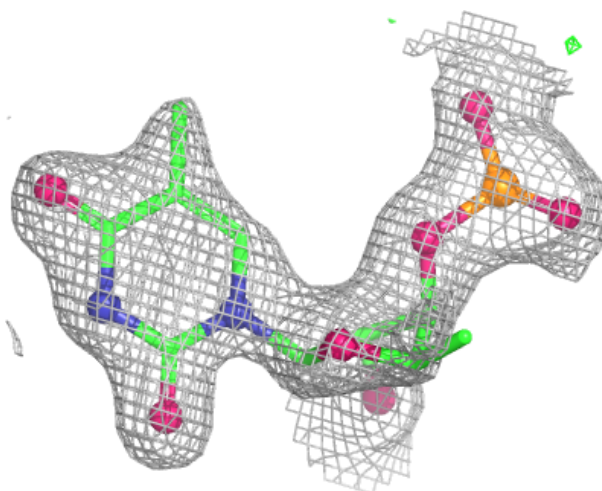
Electron density around 5GP G 105:

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and green (positive)



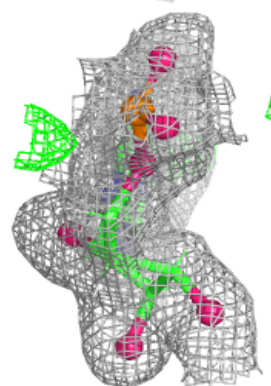
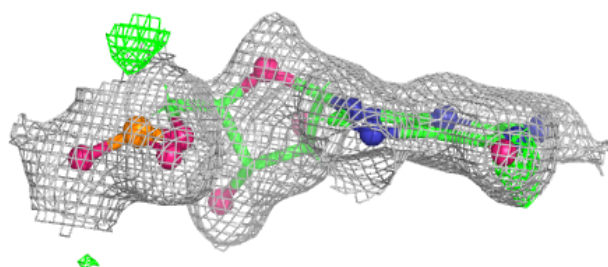
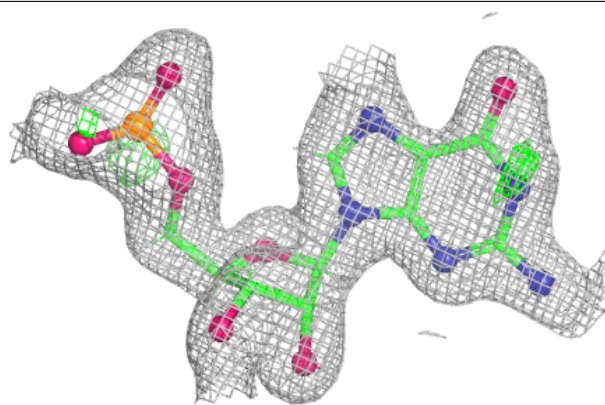
Electron density around A1CY1 G 101:

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and green (positive)



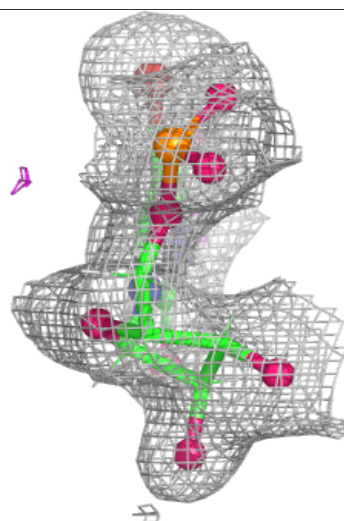
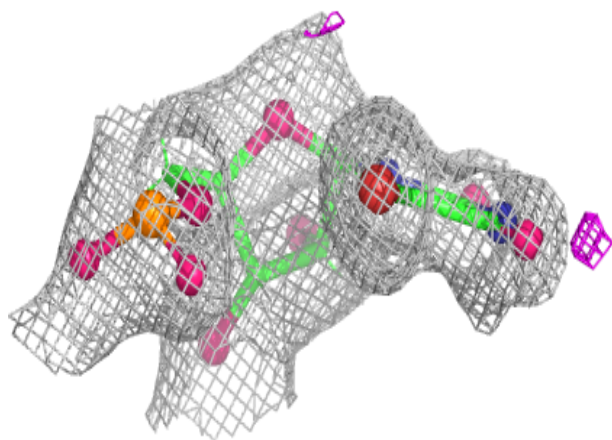
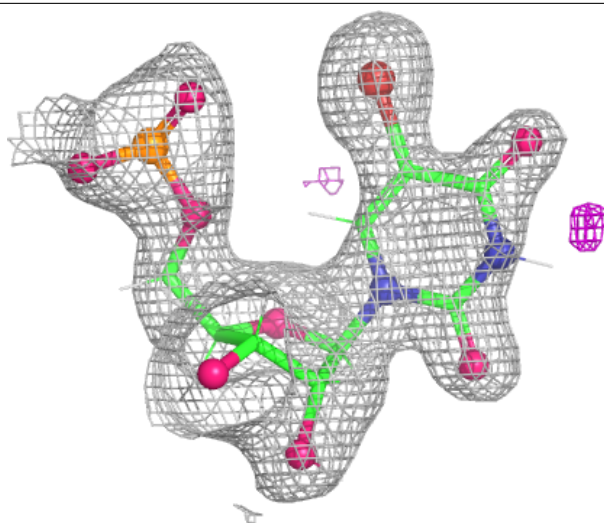
Electron density around 5GP F 105:

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and green (positive)



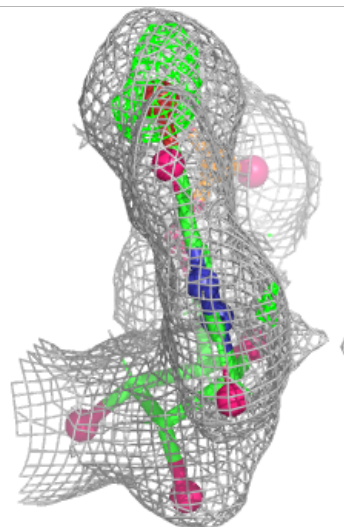
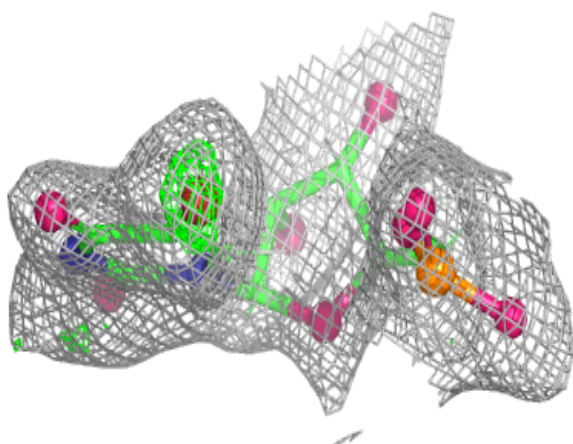
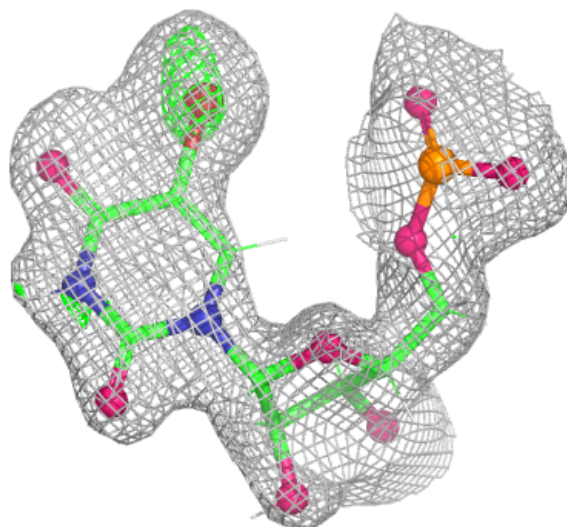
Electron density around 5BU D 101:

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



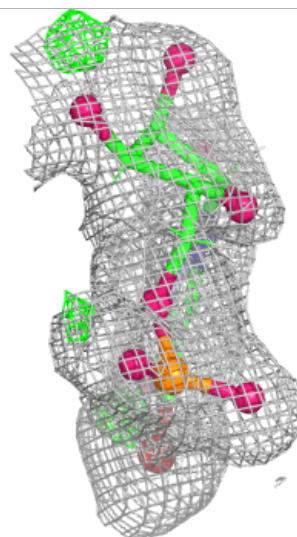
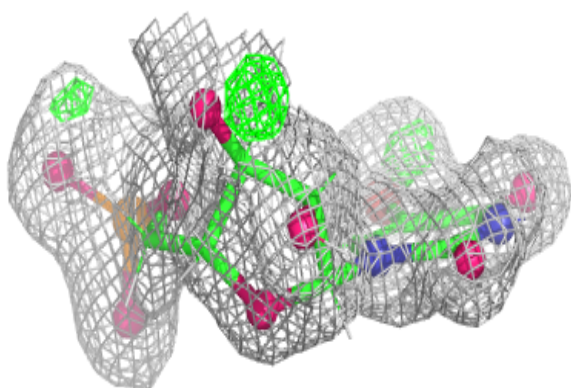
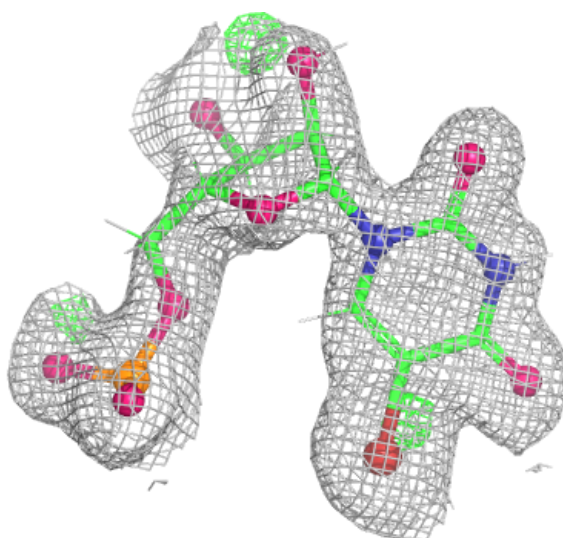
Electron density around 5BU A 103:

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



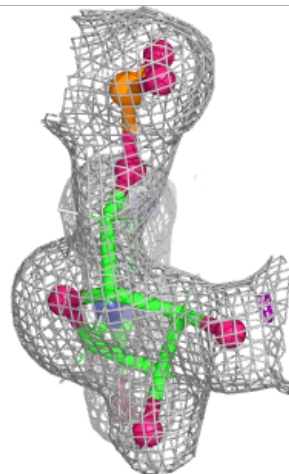
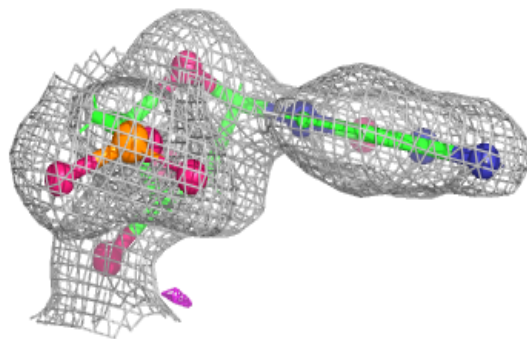
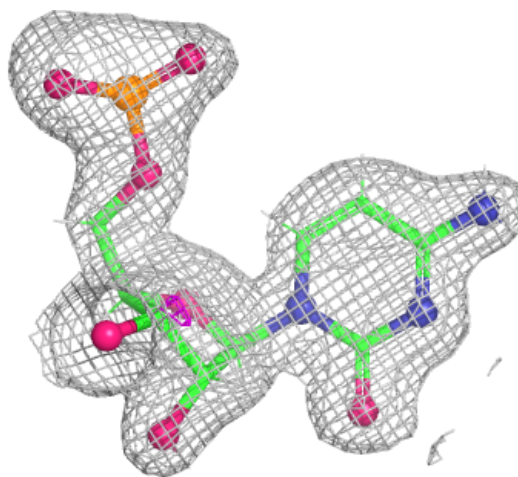
Electron density around 5BU A 102:

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



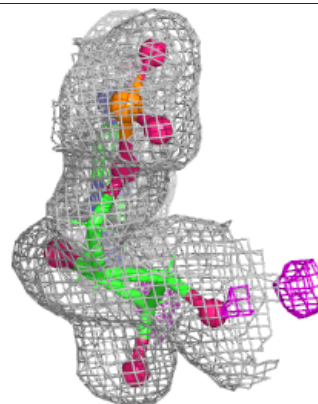
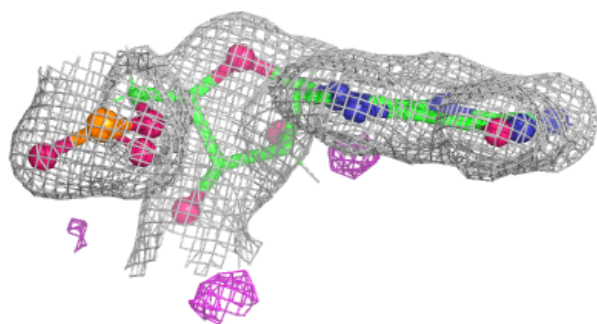
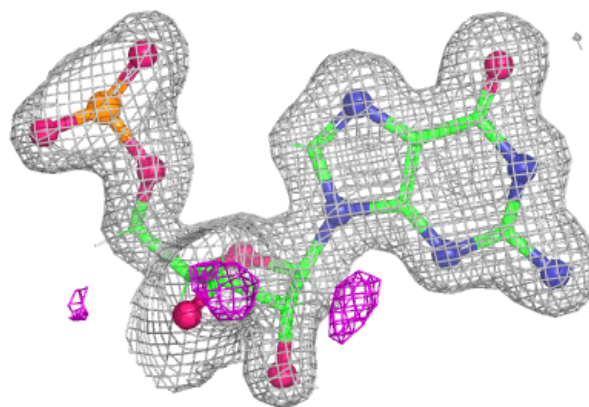
Electron density around C5P G 106:

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



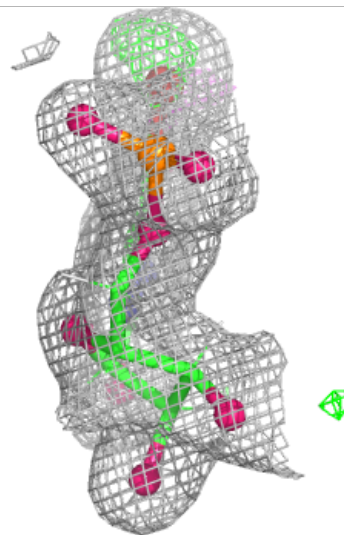
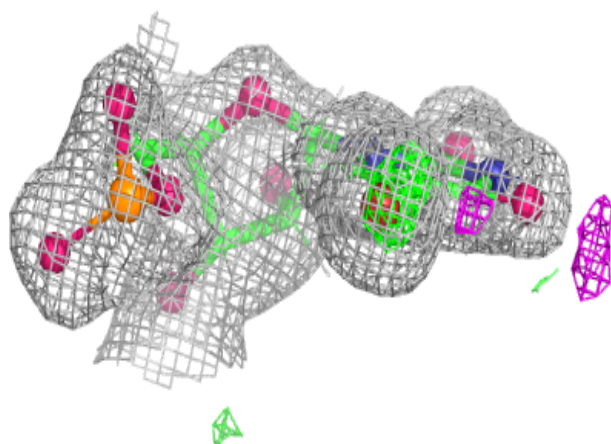
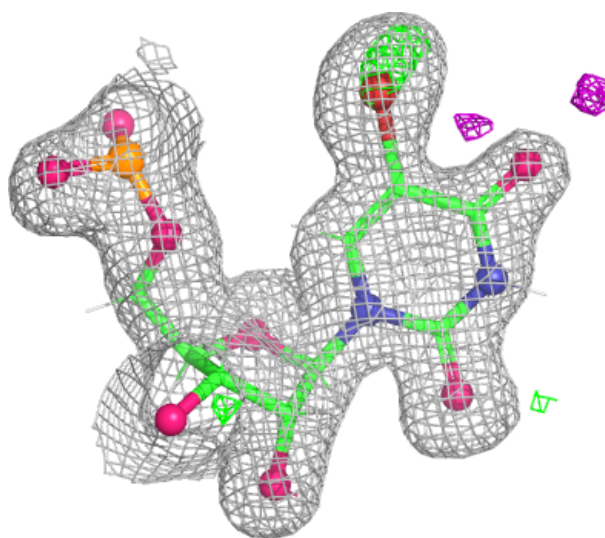
Electron density around 5GP A 105:

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



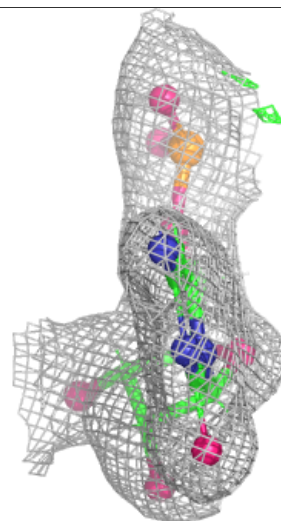
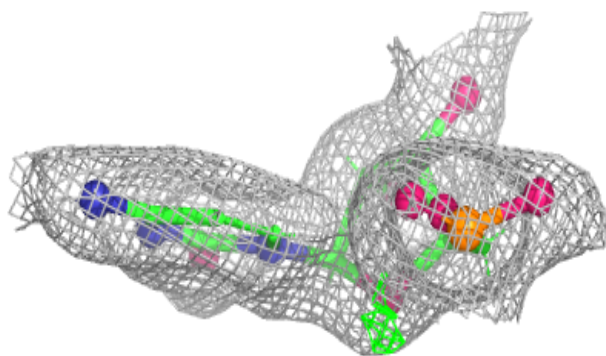
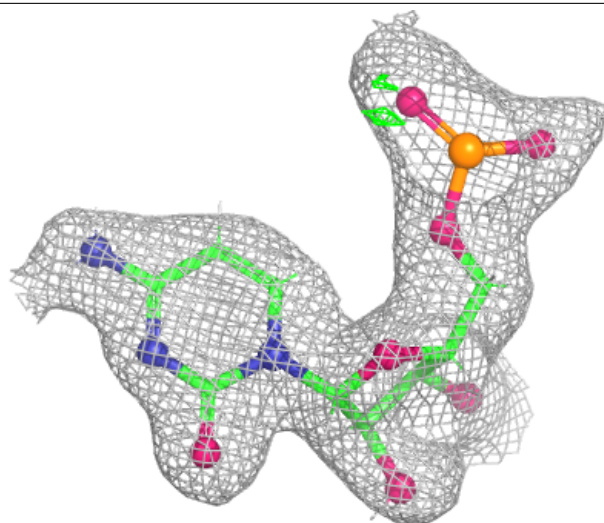
Electron density around 5BU G 102:

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



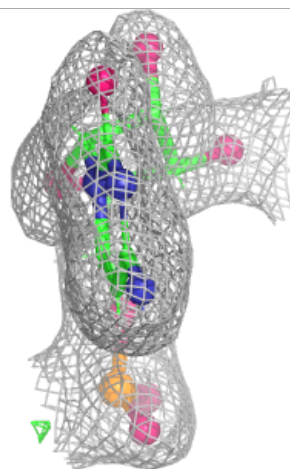
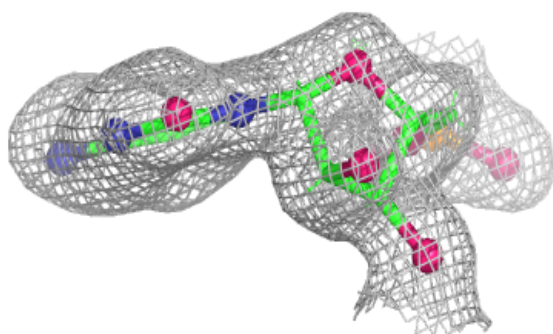
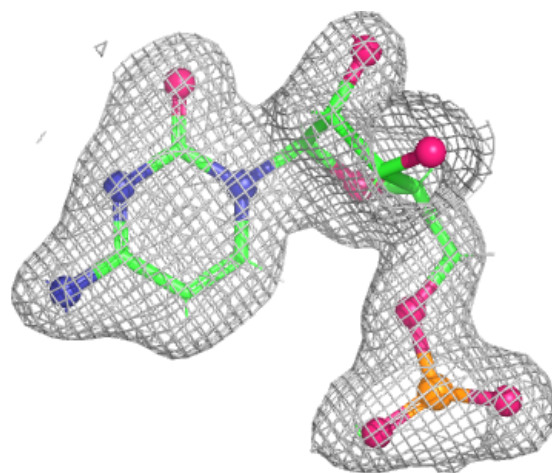
Electron density around C E 103:

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



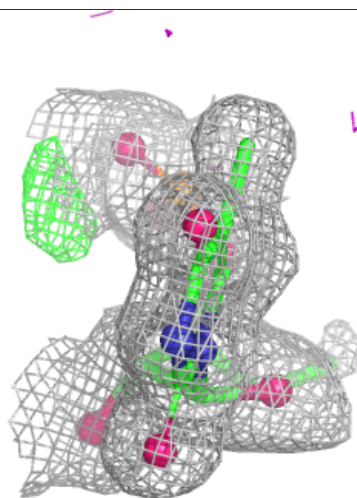
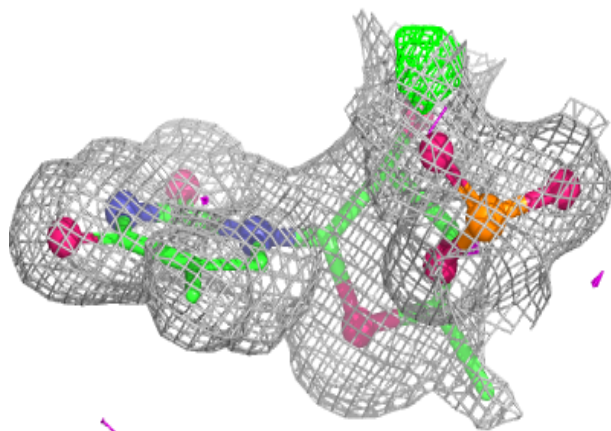
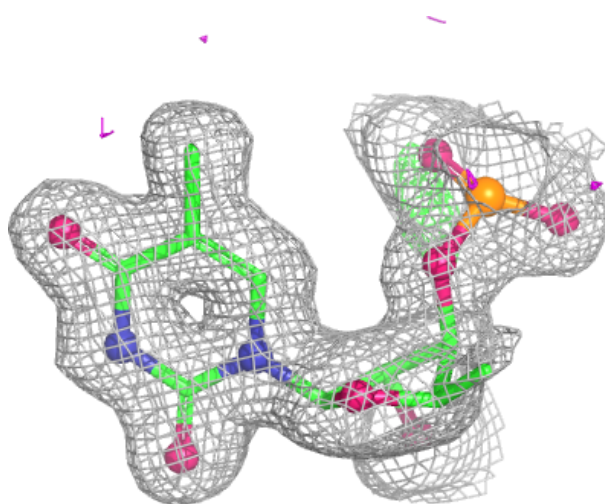
Electron density around C5P C 105:

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



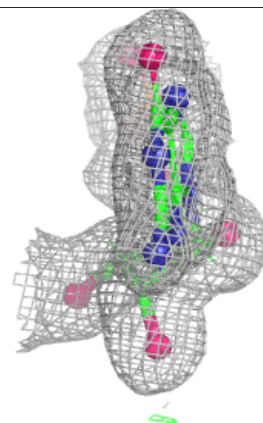
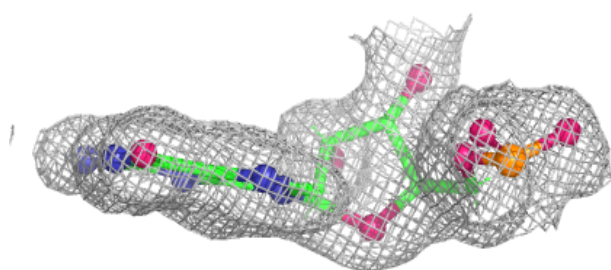
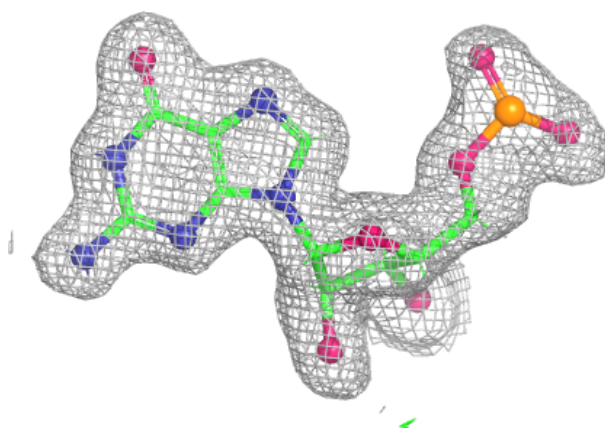
Electron density around A1CY1 H 105:

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

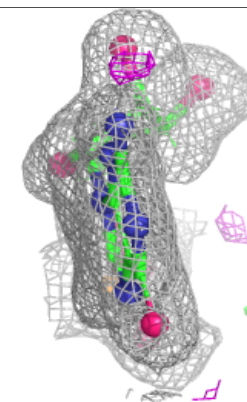
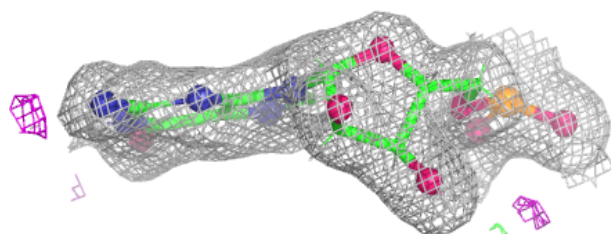
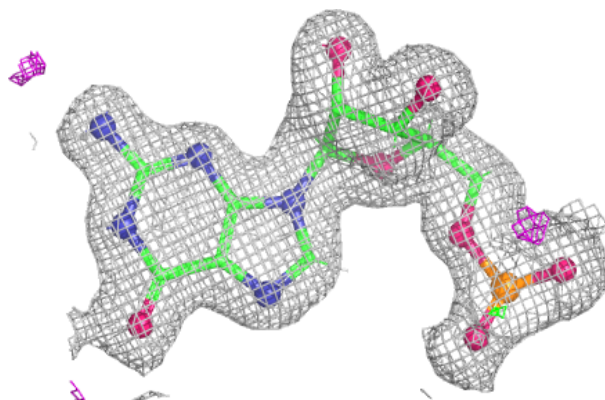


Electron density around 5GP E 104:

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

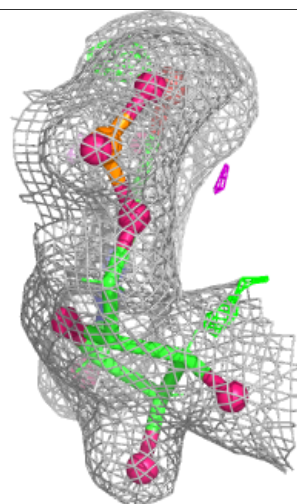
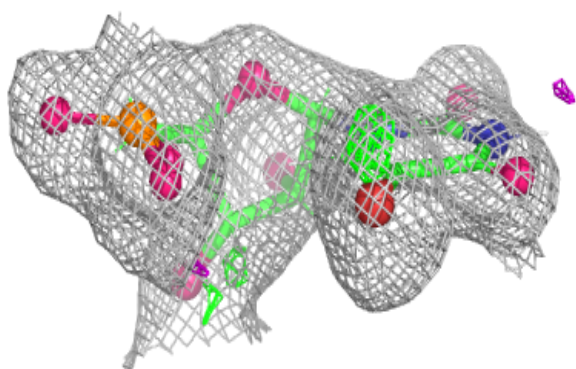
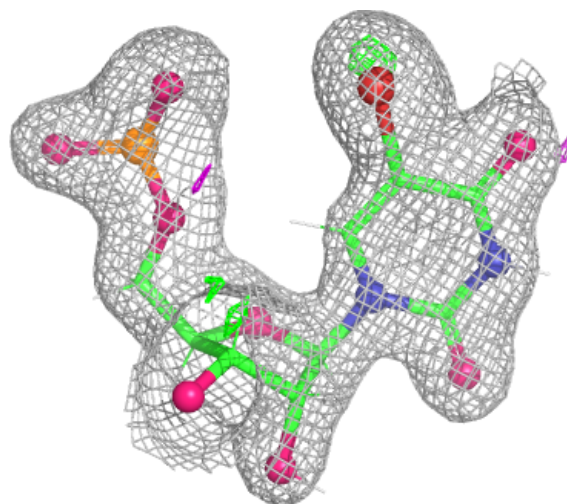
**Electron density around 5GP C 106:**

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



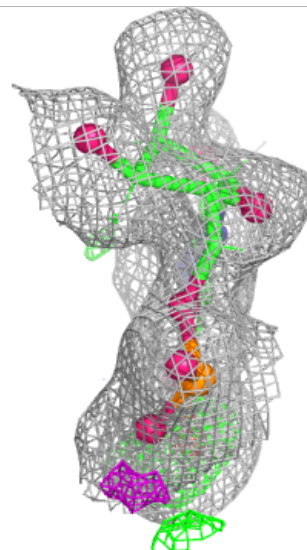
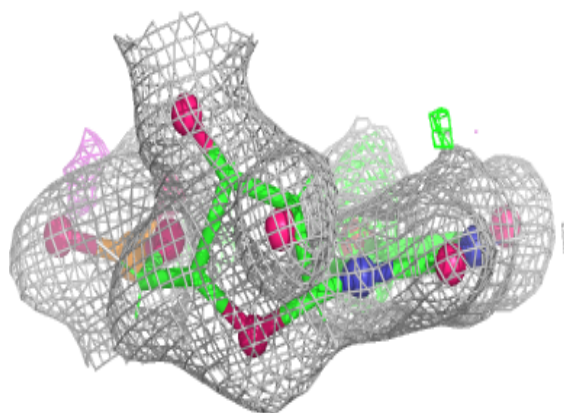
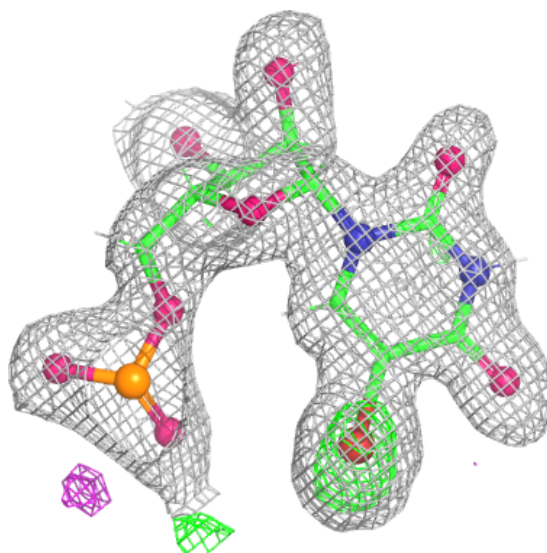
Electron density around 5BU E 102:

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



Electron density around 5BU G 103:

$2mF_o-DF_c$ (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.