



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 31, 2021 – 10:11 PM EDT

PDB ID : 3K3A  
Title : Crystal Structure of B/Perth Neuraminidase D197E mutant in complex with Oseltamivir  
Authors : Oakley, A.J.; McKimm-Breschkin, J.L.  
Deposited on : 2009-10-02  
Resolution : 2.59 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

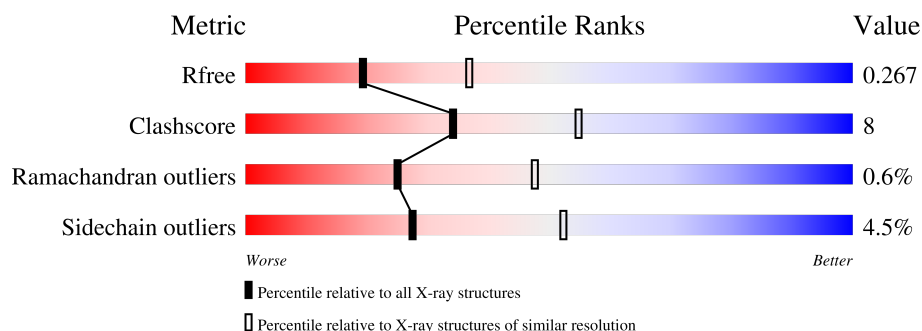
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 Å.

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












Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	397	79% 18% ..
1	B	397	79% 17% ..
1	C	397	81% 16% ..
1	D	397	76% 20% ..
1	E	397	77% 19% ..
1	F	397	80% 17% ..
1	G	397	79% 18% ..

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Mol	Chain	Length	Quality of chain
1	H	397	 81% 15% ..
1	I	397	 80% 17% ..
1	J	397	 78% 18% ..
1	K	397	 82% 15% ..
1	L	397	 77% 19% ..
1	M	397	 79% 18% ..
1	N	397	 79% 18% ..
1	O	397	 79% 18% ..
1	P	397	 82% 15% ..

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 49183 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.

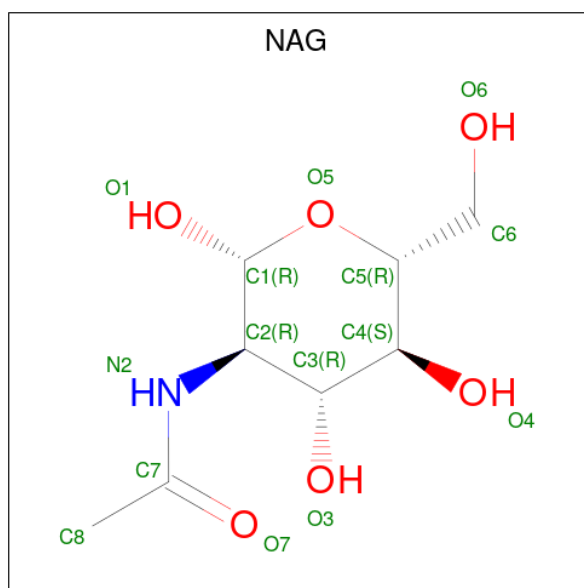
- Molecule 1 is a protein called Neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			2999	1882	519	569	29			
1	B	389	Total	C	N	O	S	0	0	0
			2999	1882	519	569	29			
1	C	389	Total	C	N	O	S	0	0	0
			2999	1882	519	569	29			
1	D	389	Total	C	N	O	S	0	0	0
			2999	1882	519	569	29			
1	E	389	Total	C	N	O	S	0	0	0
			2999	1882	519	569	29			
1	F	389	Total	C	N	O	S	0	0	0
			2999	1882	519	569	29			
1	G	389	Total	C	N	O	S	0	0	0
			2999	1882	519	569	29			
1	H	389	Total	C	N	O	S	0	0	0
			2999	1882	519	569	29			
1	I	389	Total	C	N	O	S	0	0	0
			2999	1882	519	569	29			
1	J	389	Total	C	N	O	S	0	0	0
			2999	1882	519	569	29			
1	K	389	Total	C	N	O	S	0	0	0
			2999	1882	519	569	29			
1	L	389	Total	C	N	O	S	0	0	0
			2999	1882	519	569	29			
1	M	389	Total	C	N	O	S	0	0	0
			2999	1882	519	569	29			
1	N	389	Total	C	N	O	S	0	0	0
			2999	1882	519	569	29			
1	O	389	Total	C	N	O	S	0	0	0
			2999	1882	519	569	29			
1	P	389	Total	C	N	O	S	0	0	0
			2999	1882	519	569	29			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	197	GLU	ASP	engineered mutation	UNP Q3S340
B	197	GLU	ASP	engineered mutation	UNP Q3S340
C	197	GLU	ASP	engineered mutation	UNP Q3S340
D	197	GLU	ASP	engineered mutation	UNP Q3S340
E	197	GLU	ASP	engineered mutation	UNP Q3S340
F	197	GLU	ASP	engineered mutation	UNP Q3S340
G	197	GLU	ASP	engineered mutation	UNP Q3S340
H	197	GLU	ASP	engineered mutation	UNP Q3S340
I	197	GLU	ASP	engineered mutation	UNP Q3S340
J	197	GLU	ASP	engineered mutation	UNP Q3S340
K	197	GLU	ASP	engineered mutation	UNP Q3S340
L	197	GLU	ASP	engineered mutation	UNP Q3S340
M	197	GLU	ASP	engineered mutation	UNP Q3S340
N	197	GLU	ASP	engineered mutation	UNP Q3S340
O	197	GLU	ASP	engineered mutation	UNP Q3S340
P	197	GLU	ASP	engineered mutation	UNP Q3S340

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		
2	G	1	Total	C	N	O	0	0
			14	8	1	5		
2	H	1	Total	C	N	O	0	0
			14	8	1	5		
2	I	1	Total	C	N	O	0	0
			14	8	1	5		
2	J	1	Total	C	N	O	0	0
			14	8	1	5		
2	K	1	Total	C	N	O	0	0
			14	8	1	5		
2	L	1	Total	C	N	O	0	0
			14	8	1	5		
2	M	1	Total	C	N	O	0	0
			14	8	1	5		
2	N	1	Total	C	N	O	0	0
			14	8	1	5		
2	O	1	Total	C	N	O	0	0
			14	8	1	5		
2	P	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

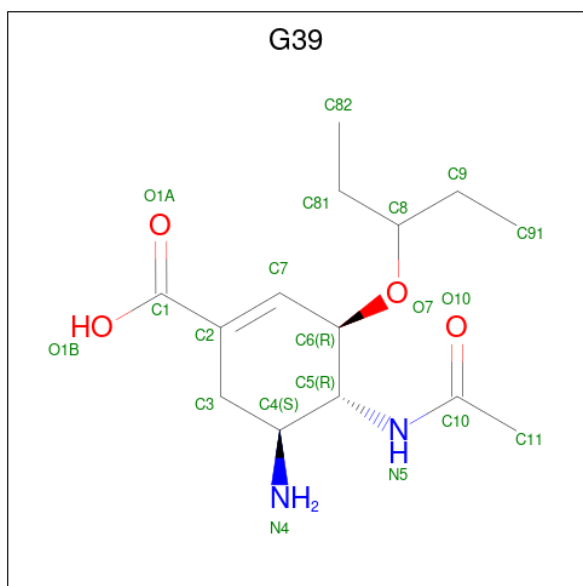
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	E	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	1	Total	Ca	0	0
			1	1		
3	G	1	Total	Ca	0	0
			1	1		
3	H	1	Total	Ca	0	0
			1	1		
3	I	1	Total	Ca	0	0
			1	1		
3	J	1	Total	Ca	0	0
			1	1		
3	K	1	Total	Ca	0	0
			1	1		
3	L	1	Total	Ca	0	0
			1	1		
3	M	1	Total	Ca	0	0
			1	1		
3	N	1	Total	Ca	0	0
			1	1		
3	O	1	Total	Ca	0	0
			1	1		
3	P	1	Total	Ca	0	0
			1	1		

- Molecule 4 is (3R,4R,5S)-4-(acetylamino)-5-amino-3-(pentan-3-yloxy)cyclohex-1-ene-1-carboxylic acid (three-letter code: G39) (formula: C<sub>14</sub>H<sub>24</sub>N<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 20	C 14	N 2	O 4	0	0
4	B	1	Total 20	C 14	N 2	O 4	0	0
4	C	1	Total 20	C 14	N 2	O 4	0	0
4	D	1	Total 20	C 14	N 2	O 4	0	0
4	E	1	Total 20	C 14	N 2	O 4	0	0
4	F	1	Total 20	C 14	N 2	O 4	0	0
4	G	1	Total 20	C 14	N 2	O 4	0	0
4	H	1	Total 20	C 14	N 2	O 4	0	0
4	I	1	Total 20	C 14	N 2	O 4	0	0
4	J	1	Total 20	C 14	N 2	O 4	0	0
4	K	1	Total 20	C 14	N 2	O 4	0	0
4	L	1	Total 20	C 14	N 2	O 4	0	0
4	M	1	Total 20	C 14	N 2	O 4	0	0
4	N	1	Total 20	C 14	N 2	O 4	0	0
4	O	1	Total 20	C 14	N 2	O 4	0	0
4	P	1	Total 20	C 14	N 2	O 4	0	0

- Molecule 5 is YTTRIUM (III) ION (three-letter code: YT3) (formula: Y).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Y 1	0	0
5	E	1	Total 1	Y 1	0	0
5	J	1	Total 1	Y 1	0	0
5	P	1	Total 1	Y 1	0	0

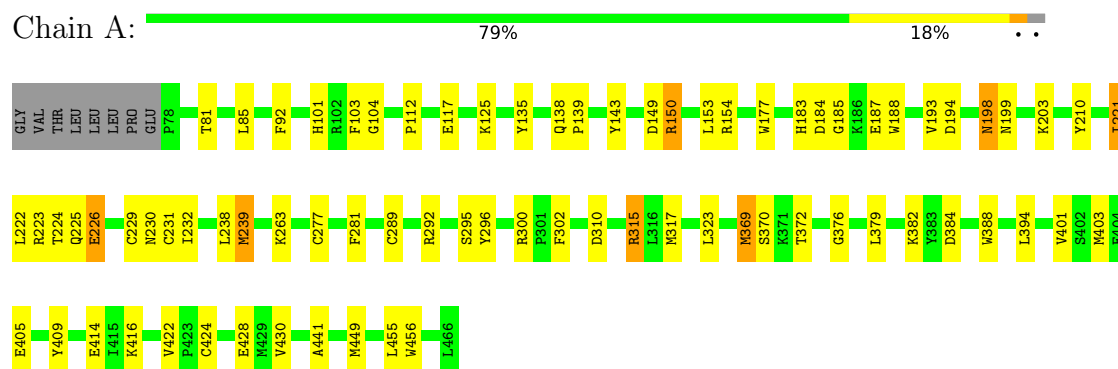
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	43	Total O 43 43	0	0
6	B	40	Total O 40 40	0	0
6	C	40	Total O 40 40	0	0
6	D	37	Total O 37 37	0	0
6	E	42	Total O 42 42	0	0
6	F	36	Total O 36 36	0	0
6	G	42	Total O 42 42	0	0
6	H	37	Total O 37 37	0	0
6	I	43	Total O 43 43	0	0
6	J	37	Total O 37 37	0	0
6	K	42	Total O 42 42	0	0
6	L	38	Total O 38 38	0	0
6	M	40	Total O 40 40	0	0
6	N	42	Total O 42 42	0	0
6	O	39	Total O 39 39	0	0
6	P	37	Total O 37 37	0	0

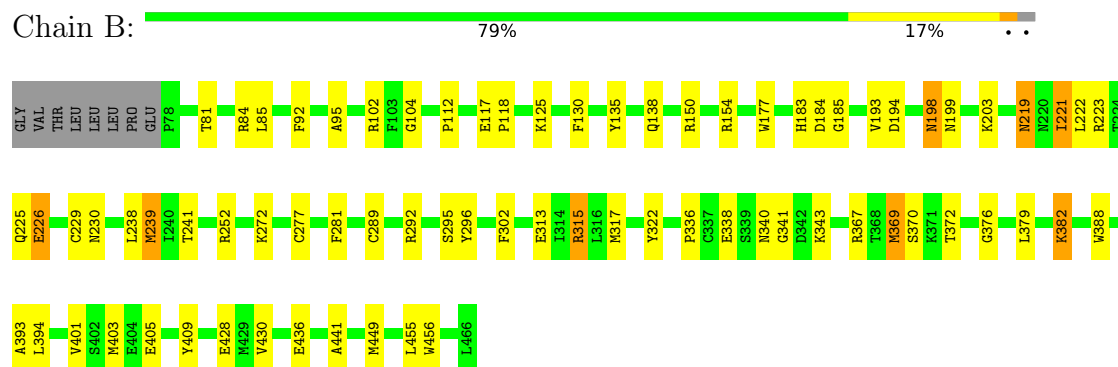
### 3 Residue-property plots [i](#)

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. 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. 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.

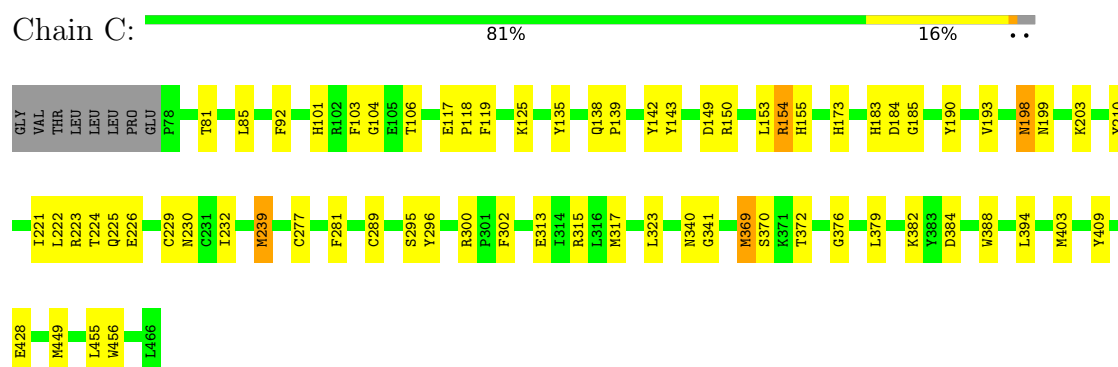
- Molecule 1: Neuraminidase



- Molecule 1: Neuraminidase

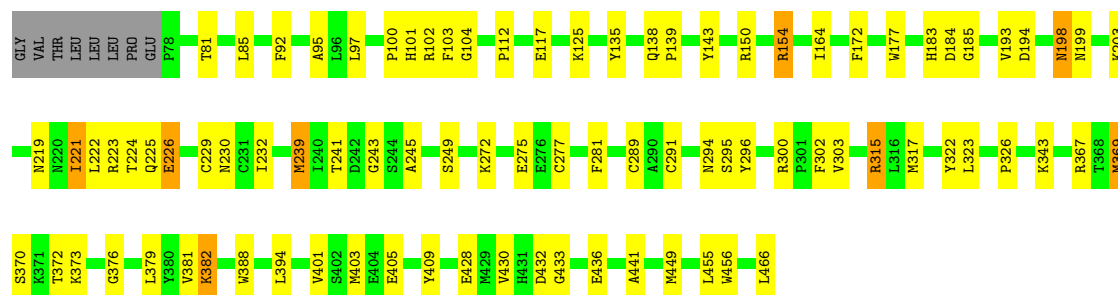


- Molecule 1: Neuraminidase




- Molecule 1: Neuraminidase

Chain D:  76% 20% ..




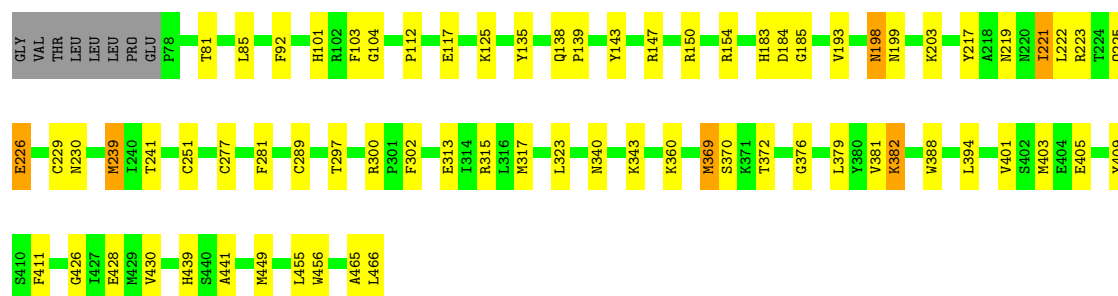
- Molecule 1: Neuraminidase

Chain E:  77% 19% ..




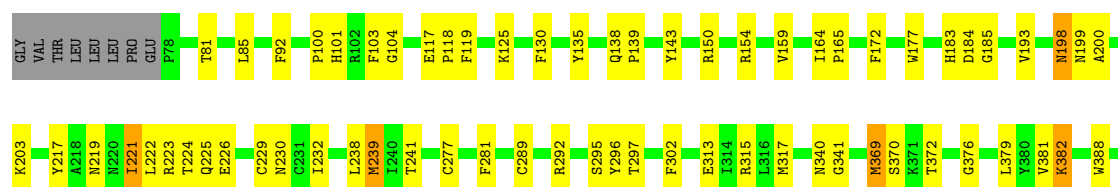
- Molecule 1: Neuraminidase

Chain F:  80% 17% ..



- Molecule 1: Neuraminidase

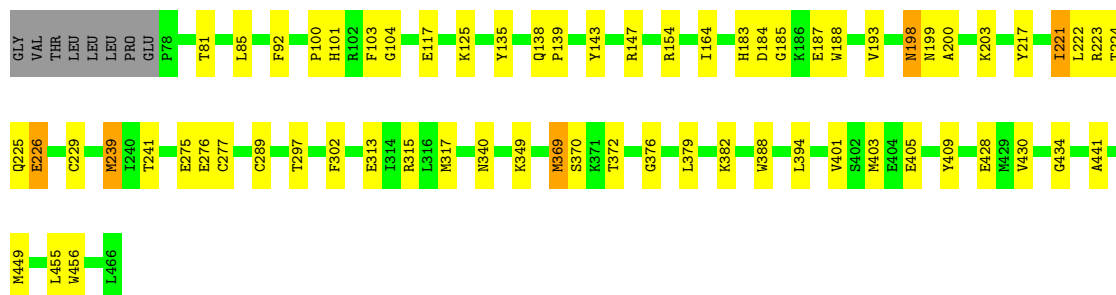
Chain G:  79% 18% ..





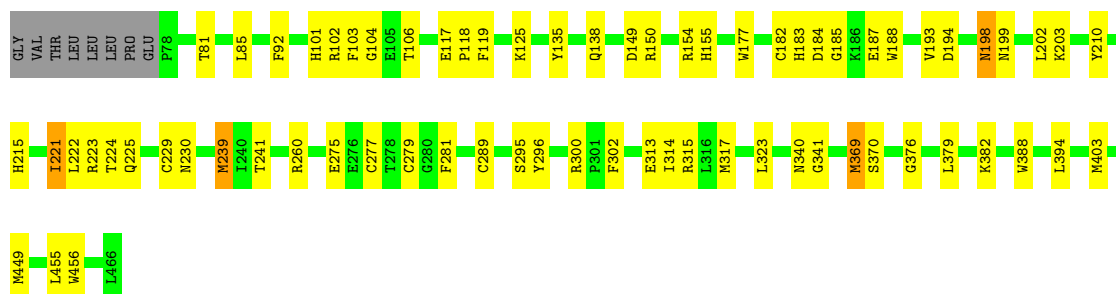
• Molecule 1: Neuraminidase

Chain H: 81% 15% ..



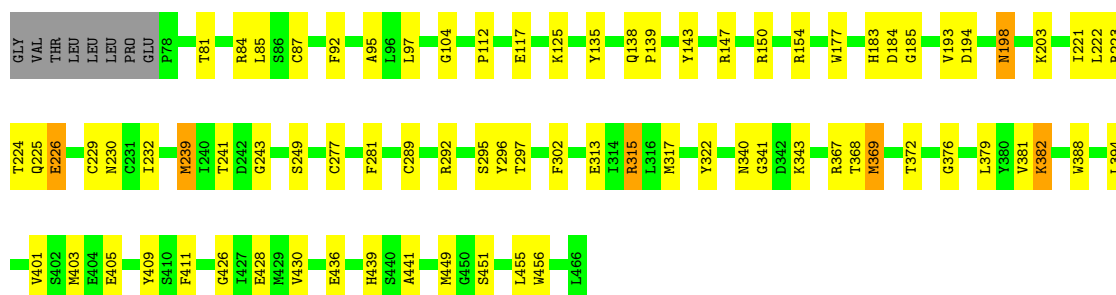
• Molecule 1: Neuraminidase

Chain I: 80% 17% ..



• Molecule 1: Neuraminidase

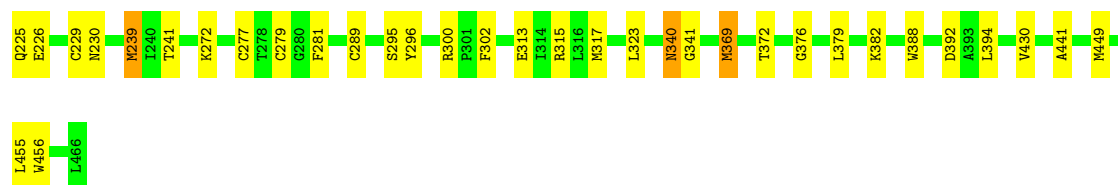
Chain J: 78% 18% ..



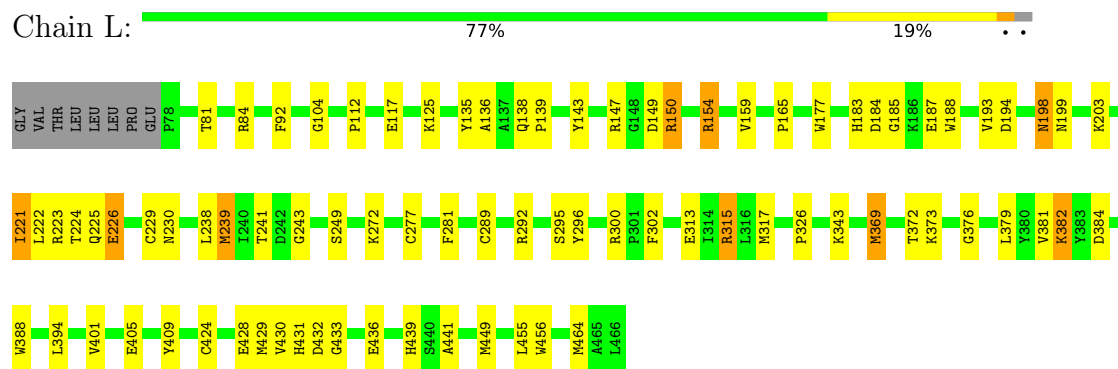
• Molecule 1: Neuraminidase

Chain K: 82% 15% ..

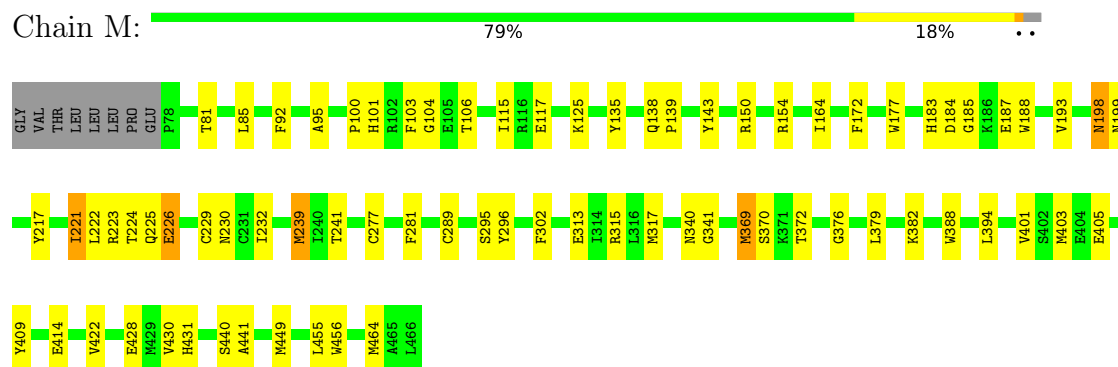




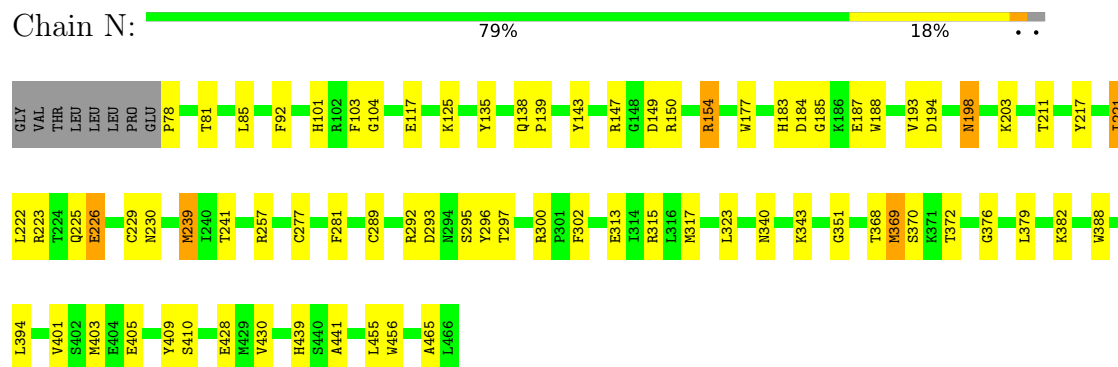
• Molecule 1: Neuraminidase



• Molecule 1: Neuraminidase

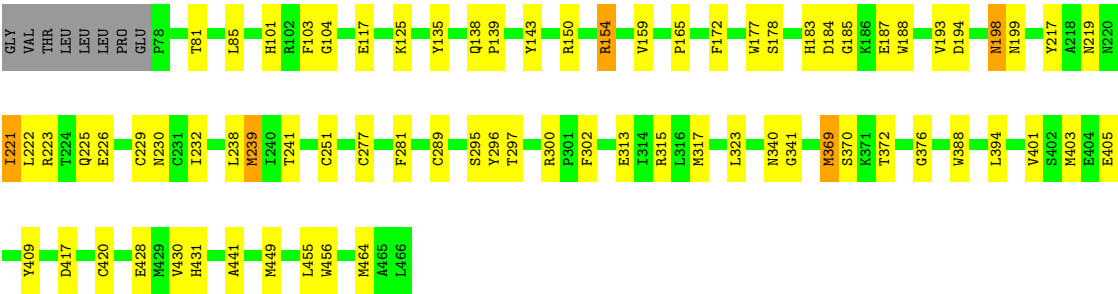


• Molecule 1: Neuraminidase

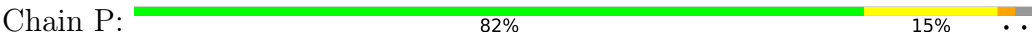


• Molecule 1: Neuraminidase





● Molecule 1: Neuraminidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.80Å 123.84Å 123.97Å 90.04° 90.17° 90.10°	Depositor
Resolution (Å)	49.69 – 2.59 49.65 – 2.25	Depositor EDS
% Data completeness (in resolution range)	96.3 (49.69-2.59) 90.8 (49.65-2.25)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.207 , 0.229 0.264 , 0.267	Depositor DCC
$R_{free}$ test set	14641 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.4	Xtriage
Anisotropy	0.803	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 100.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.377 for h,l,-k 0.377 for h,-l,k 0.419 for h,-k,-l 0.417 for -h,k,-l 0.428 for -h,-k,l 0.367 for -h,l,k 0.370 for -h,-l,-k	Xtriage
Reported twinning fraction	0.323 for H, K, L 0.224 for -H, K, -L 0.097 for H, -L, K 0.100 for -h,-k,l 0.256 for -H, L, K	Depositor
Outliers	0 of 289439 reflections	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	49183	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CA, G39, YT3

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	0.77	1/3072 (0.0%)	0.76	2/4150 (0.0%)
1	B	0.79	0/3072	0.78	4/4150 (0.1%)
1	C	0.78	0/3072	0.76	0/4150
1	D	0.77	0/3072	0.75	0/4150
1	E	0.83	2/3072 (0.1%)	0.76	0/4150
1	F	0.82	1/3072 (0.0%)	0.76	0/4150
1	G	0.81	0/3072	0.78	0/4150
1	H	0.82	0/3072	0.76	0/4150
1	I	0.79	2/3072 (0.1%)	0.76	1/4150 (0.0%)
1	J	0.76	0/3072	0.75	0/4150
1	K	0.78	2/3072 (0.1%)	0.76	0/4150
1	L	0.77	1/3072 (0.0%)	0.77	4/4150 (0.1%)
1	M	0.79	0/3072	0.77	0/4150
1	N	0.80	0/3072	0.75	1/4150 (0.0%)
1	O	0.81	1/3072 (0.0%)	0.76	0/4150
1	P	0.81	1/3072 (0.0%)	0.76	1/4150 (0.0%)
All	All	0.79	11/49152 (0.0%)	0.76	13/66400 (0.0%)

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	279	CYS	CB-SG	-7.67	1.69	1.82
1	E	289	CYS	CB-SG	-6.60	1.71	1.82
1	L	424	CYS	CB-SG	-6.08	1.72	1.82
1	K	182	CYS	CB-SG	-5.67	1.72	1.81
1	P	251	CYS	CB-SG	5.59	1.91	1.82

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	315	ARG	NE-CZ-NH2	-5.88	117.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	L	300	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	N	257	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	P	257	ARG	NE-CZ-NH2	-5.45	117.57	120.30

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	2999	0	2890	57	1
1	B	2999	0	2890	53	2
1	C	2999	0	2890	44	1
1	D	2999	0	2890	82	1
1	E	2999	0	2890	56	0
1	F	2999	0	2890	53	1
1	G	2999	0	2890	49	1
1	H	2999	0	2890	45	1
1	I	2999	0	2890	46	1
1	J	2999	0	2890	56	3
1	K	2999	0	2890	43	1
1	L	2999	0	2890	80	1
1	M	2999	0	2890	47	1
1	N	2999	0	2890	54	1
1	O	2999	0	2890	49	1
1	P	2999	0	2890	44	1
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
2	E	14	0	13	0	0
2	F	14	0	13	0	0
2	G	14	0	13	0	0
2	H	14	0	13	0	0
2	I	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	14	0	13	0	0
2	K	14	0	13	0	0
2	L	14	0	13	0	0
2	M	14	0	13	0	0
2	N	14	0	13	0	0
2	O	14	0	13	0	0
2	P	14	0	13	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
4	A	20	0	22	3	0
4	B	20	0	23	3	0
4	C	20	0	23	3	0
4	D	20	0	23	5	0
4	E	20	0	23	6	0
4	F	20	0	23	7	0
4	G	20	0	23	6	0
4	H	20	0	23	6	0
4	I	20	0	23	6	0
4	J	20	0	23	5	0
4	K	20	0	21	2	0
4	L	20	0	23	4	0
4	M	20	0	23	2	0
4	N	20	0	23	3	0
4	O	20	0	23	3	0
4	P	20	0	23	5	0
5	A	1	0	0	0	0
5	E	1	0	0	0	0
5	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	1	0	0	0	0
6	A	43	0	0	5	0
6	B	40	0	0	6	0
6	C	40	0	0	1	0
6	D	37	0	0	3	0
6	E	42	0	0	2	0
6	F	36	0	0	2	0
6	G	42	0	0	2	0
6	H	37	0	0	1	0
6	I	43	0	0	1	0
6	J	37	0	0	2	0
6	K	42	0	0	2	0
6	L	38	0	0	4	0
6	M	40	0	0	3	0
6	N	42	0	0	2	0
6	O	39	0	0	2	0
6	P	37	0	0	3	0
All	All	49183	0	46813	798	9

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 8.

The worst 5 of 798 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:N:81:THR:HG23	6:N:2047:HOH:O	1.31	1.30
1:F:81:THR:HG23	6:F:2047:HOH:O	1.30	1.28
1:P:81:THR:HG23	6:P:2047:HOH:O	1.39	1.22
1:O:81:THR:HG23	6:O:2047:HOH:O	1.39	1.20
1:H:81:THR:HG23	6:H:2047:HOH:O	1.38	1.18

The worst 5 of 9 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:343:LYS:NZ	1:J:436:GLU:O[1_554]	1.80	0.40
1:B:436:GLU:O	1:J:343:LYS:NZ[1_554]	1.86	0.34
1:C:315:ARG:NH2	1:H:217:TYR:O[1_556]	1.99	0.21
1:D:315:ARG:NH2	1:G:217:TYR:O[1_546]	2.04	0.16
1:I:315:ARG:NH2	1:N:217:TYR:O[1_446]	2.11	0.09

## 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	387/397 (98%)	359 (93%)	25 (6%)	3 (1%)	19	39
1	B	387/397 (98%)	360 (93%)	24 (6%)	3 (1%)	19	39
1	C	387/397 (98%)	358 (92%)	27 (7%)	2 (0%)	29	52
1	D	387/397 (98%)	361 (93%)	23 (6%)	3 (1%)	19	39
1	E	387/397 (98%)	359 (93%)	24 (6%)	4 (1%)	15	32
1	F	387/397 (98%)	361 (93%)	23 (6%)	3 (1%)	19	39
1	G	387/397 (98%)	363 (94%)	20 (5%)	4 (1%)	15	32
1	H	387/397 (98%)	359 (93%)	25 (6%)	3 (1%)	19	39
1	I	387/397 (98%)	361 (93%)	24 (6%)	2 (0%)	29	52
1	J	387/397 (98%)	357 (92%)	29 (8%)	1 (0%)	41	64
1	K	387/397 (98%)	361 (93%)	24 (6%)	2 (0%)	29	52
1	L	387/397 (98%)	359 (93%)	25 (6%)	3 (1%)	19	39
1	M	387/397 (98%)	362 (94%)	23 (6%)	2 (0%)	29	52
1	N	387/397 (98%)	359 (93%)	27 (7%)	1 (0%)	41	64
1	O	387/397 (98%)	361 (93%)	23 (6%)	3 (1%)	19	39
1	P	387/397 (98%)	363 (94%)	23 (6%)	1 (0%)	41	64
All	All	6192/6352 (98%)	5763 (93%)	389 (6%)	40 (1%)	25	47

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	199	ASN
1	B	199	ASN
1	B	219	ASN
1	D	199	ASN
1	E	219	ASN

### 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	320/329 (97%)	305 (95%)	15 (5%)	26	50
1	B	320/329 (97%)	306 (96%)	14 (4%)	28	53
1	C	320/329 (97%)	306 (96%)	14 (4%)	28	53
1	D	320/329 (97%)	305 (95%)	15 (5%)	26	50
1	E	320/329 (97%)	306 (96%)	14 (4%)	28	53
1	F	320/329 (97%)	306 (96%)	14 (4%)	28	53
1	G	320/329 (97%)	306 (96%)	14 (4%)	28	53
1	H	320/329 (97%)	306 (96%)	14 (4%)	28	53
1	I	320/329 (97%)	306 (96%)	14 (4%)	28	53
1	J	320/329 (97%)	304 (95%)	16 (5%)	24	47
1	K	320/329 (97%)	306 (96%)	14 (4%)	28	53
1	L	320/329 (97%)	305 (95%)	15 (5%)	26	50
1	M	320/329 (97%)	305 (95%)	15 (5%)	26	50
1	N	320/329 (97%)	305 (95%)	15 (5%)	26	50
1	O	320/329 (97%)	306 (96%)	14 (4%)	28	53
1	P	320/329 (97%)	307 (96%)	13 (4%)	30	56
All	All	5120/5264 (97%)	4890 (96%)	230 (4%)	27	52

5 of 230 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	106	THR
1	P	198	ASN
1	J	456	TRP
1	P	135	TYR
1	N	382	LYS

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

Mol	Chain	Res	Type
1	O	198	ASN
1	O	439	HIS
1	G	183	HIS
1	F	439	HIS
1	P	183	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 20 are monoatomic - leaving 32 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$
4	G39	E	1	-	17,20,20	1.78	4 (23%)	15,27,27	3.20	3 (20%)
4	G39	M	1	-	17,20,20	0.97	1 (5%)	15,27,27	1.68	2 (13%)
2	NAG	N	900	1	14,14,15	0.84	1 (7%)	17,19,21	1.72	2 (11%)
4	G39	B	1	-	17,20,20	1.46	3 (17%)	15,27,27	3.17	5 (33%)
4	G39	O	1	-	17,20,20	0.96	0	15,27,27	2.04	4 (26%)
4	G39	G	1	-	17,20,20	1.05	2 (11%)	15,27,27	2.61	5 (33%)
4	G39	C	1	-	17,20,20	1.21	3 (17%)	15,27,27	2.55	5 (33%)
4	G39	A	1	-	17,20,20	1.58	1 (5%)	15,27,27	2.66	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	G39	N	1	-	17,20,20	1.41	1 (5%)	15,27,27	2.13	6 (40%)
2	NAG	P	900	1	14,14,15	0.78	0	17,19,21	1.73	2 (11%)
2	NAG	L	900	1	14,14,15	0.53	0	17,19,21	1.45	3 (17%)
4	G39	F	1	-	17,20,20	1.04	1 (5%)	15,27,27	2.13	6 (40%)
2	NAG	C	900	1	14,14,15	0.56	0	17,19,21	1.28	3 (17%)
2	NAG	I	900	1	14,14,15	0.69	0	17,19,21	1.50	3 (17%)
2	NAG	A	900	1	14,14,15	0.62	0	17,19,21	1.65	3 (17%)
2	NAG	F	900	1	14,14,15	0.75	0	17,19,21	1.64	3 (17%)
2	NAG	D	900	1	14,14,15	0.47	0	17,19,21	1.47	2 (11%)
2	NAG	J	900	1	14,14,15	0.41	0	17,19,21	1.12	1 (5%)
2	NAG	H	900	1	14,14,15	0.63	0	17,19,21	1.68	2 (11%)
2	NAG	B	900	1	14,14,15	0.61	0	17,19,21	1.49	2 (11%)
2	NAG	K	900	1	14,14,15	0.62	0	17,19,21	1.34	2 (11%)
4	G39	I	1	-	17,20,20	1.09	0	15,27,27	2.18	4 (26%)
2	NAG	G	900	1	14,14,15	0.64	0	17,19,21	1.80	3 (17%)
4	G39	L	1	-	17,20,20	1.95	4 (23%)	15,27,27	3.04	6 (40%)
4	G39	P	1	-	17,20,20	1.12	1 (5%)	15,27,27	2.42	4 (26%)
2	NAG	E	900	1	14,14,15	0.52	0	17,19,21	1.83	3 (17%)
4	G39	D	1	-	17,20,20	1.40	1 (5%)	15,27,27	2.91	8 (53%)
2	NAG	M	900	1	14,14,15	0.52	0	17,19,21	1.75	2 (11%)
2	NAG	O	900	1	14,14,15	0.50	0	17,19,21	1.58	2 (11%)
4	G39	K	1	-	17,20,20	3.00	8 (47%)	15,27,27	3.30	5 (33%)
4	G39	H	1	-	17,20,20	1.33	4 (23%)	15,27,27	3.36	4 (26%)
4	G39	J	1	-	17,20,20	2.30	3 (17%)	15,27,27	2.30	5 (33%)

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	G39	E	1	-	-	2/12/32/32	0/1/1/1
4	G39	M	1	-	-	2/12/32/32	0/1/1/1
2	NAG	N	900	1	-	0/6/23/26	0/1/1/1
4	G39	B	1	-	-	2/12/32/32	0/1/1/1
4	G39	O	1	-	-	2/12/32/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	G39	G	1	-	-	3/12/32/32	0/1/1/1
4	G39	C	1	-	-	3/12/32/32	0/1/1/1
4	G39	A	1	-	-	0/12/32/32	0/1/1/1
4	G39	N	1	-	-	6/12/32/32	0/1/1/1
2	NAG	P	900	1	-	0/6/23/26	0/1/1/1
2	NAG	L	900	1	-	0/6/23/26	0/1/1/1
4	G39	F	1	-	-	2/12/32/32	0/1/1/1
2	NAG	C	900	1	-	0/6/23/26	0/1/1/1
2	NAG	I	900	1	-	0/6/23/26	0/1/1/1
2	NAG	A	900	1	-	0/6/23/26	0/1/1/1
2	NAG	F	900	1	-	0/6/23/26	0/1/1/1
2	NAG	D	900	1	-	0/6/23/26	0/1/1/1
2	NAG	J	900	1	-	0/6/23/26	0/1/1/1
2	NAG	H	900	1	-	0/6/23/26	0/1/1/1
2	NAG	B	900	1	-	0/6/23/26	0/1/1/1
2	NAG	K	900	1	-	0/6/23/26	0/1/1/1
4	G39	I	1	-	-	0/12/32/32	0/1/1/1
2	NAG	G	900	1	-	0/6/23/26	0/1/1/1
4	G39	L	1	-	-	1/12/32/32	0/1/1/1
4	G39	P	1	-	-	4/12/32/32	0/1/1/1
2	NAG	E	900	1	-	0/6/23/26	0/1/1/1
4	G39	D	1	-	-	4/12/32/32	0/1/1/1
2	NAG	M	900	1	-	0/6/23/26	0/1/1/1
2	NAG	O	900	1	-	0/6/23/26	0/1/1/1
4	G39	K	1	-	-	5/12/32/32	0/1/1/1
4	G39	H	1	-	-	0/12/32/32	0/1/1/1
4	G39	J	1	-	-	1/12/32/32	0/1/1/1

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	1	G39	C5-N5	-7.12	1.34	1.45
4	J	1	G39	C6-C7	7.05	1.60	1.50
4	N	1	G39	C4-C5	-5.25	1.46	1.52
4	A	1	G39	C6-C5	-5.21	1.46	1.53
4	E	1	G39	C4-C5	-5.04	1.46	1.52

The worst 5 of 114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	G39	C3-C2-C7	10.10	139.31	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1	G39	C3-C2-C7	9.30	137.77	119.87
4	K	1	G39	C5-N5-C10	7.77	142.07	123.18
4	B	1	G39	C4-C3-C2	7.57	118.72	109.75
4	G	1	G39	C3-C2-C7	6.79	132.94	119.87

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	1	G39	C9-C8-C81-C82
4	N	1	G39	O10-C10-N5-C5
4	N	1	G39	C7-C6-O7-C8
4	N	1	G39	C11-C10-N5-C5
4	P	1	G39	C11-C10-N5-C5

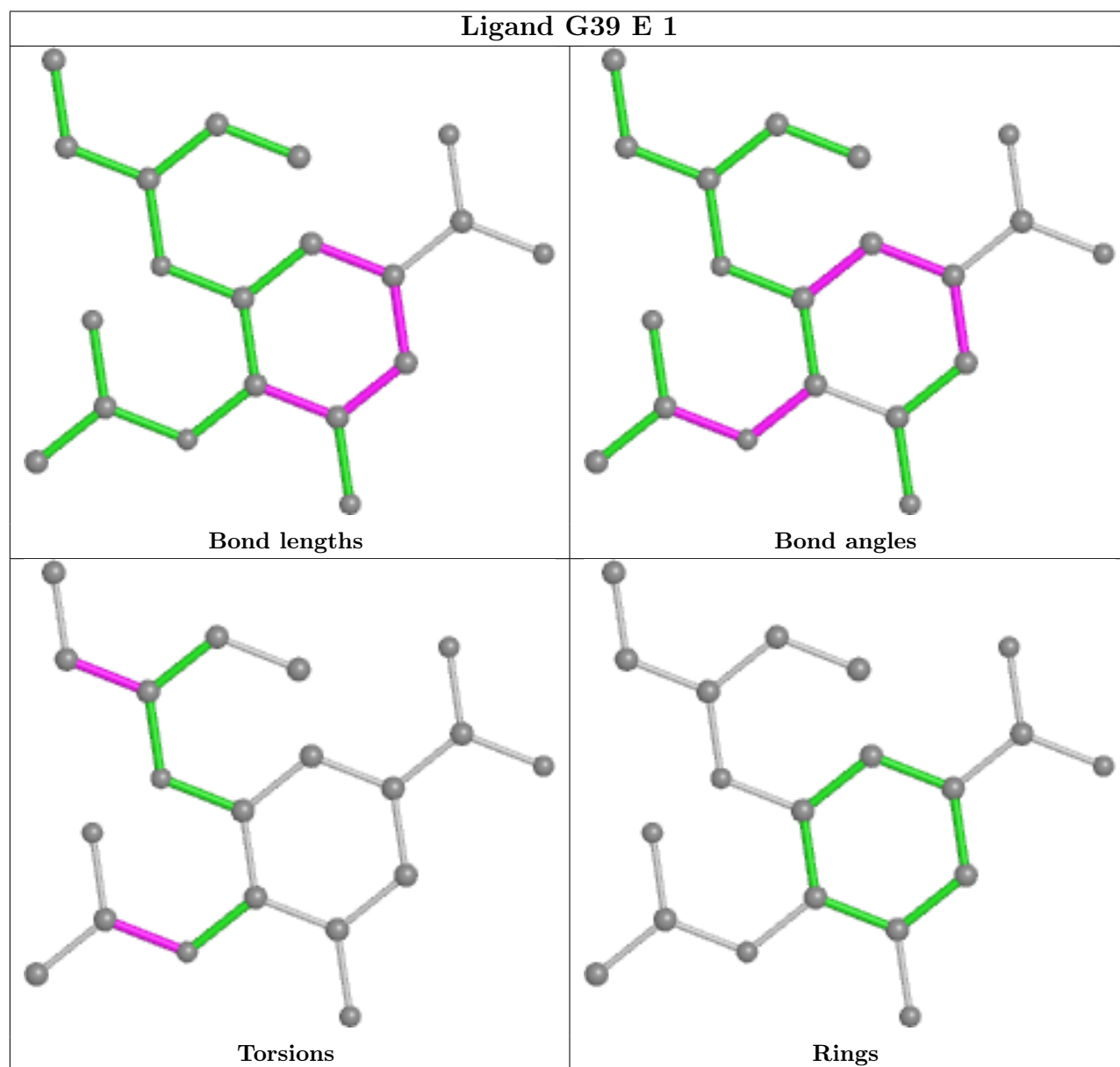
There are no ring outliers.

16 monomers are involved in 69 short contacts:

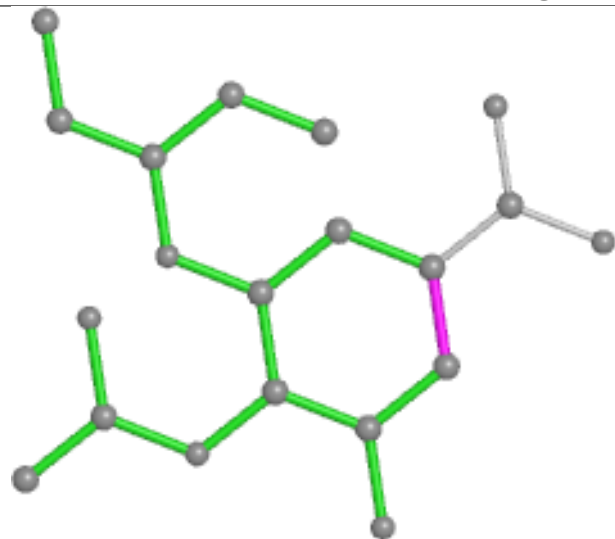
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	G39	6	0
4	M	1	G39	2	0
4	B	1	G39	3	0
4	O	1	G39	3	0
4	G	1	G39	6	0
4	C	1	G39	3	0
4	A	1	G39	3	0
4	N	1	G39	3	0
4	F	1	G39	7	0
4	I	1	G39	6	0
4	L	1	G39	4	0
4	P	1	G39	5	0
4	D	1	G39	5	0
4	K	1	G39	2	0
4	H	1	G39	6	0
4	J	1	G39	5	0

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

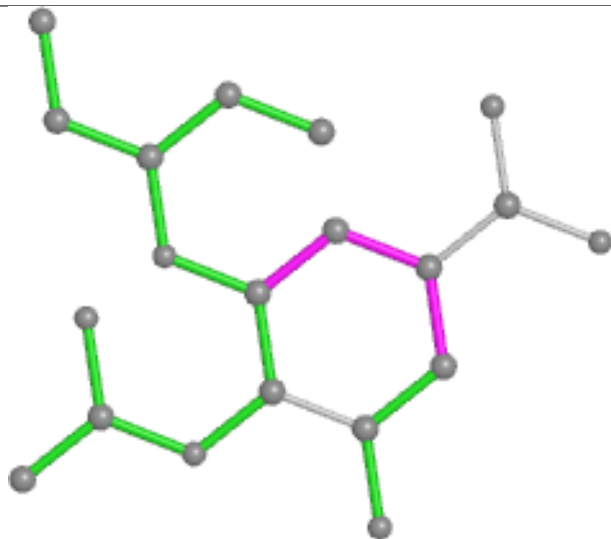
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified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



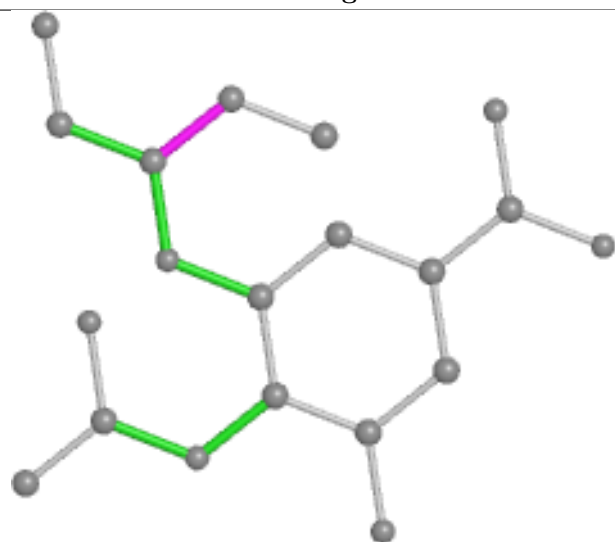
## Ligand G39 M 1



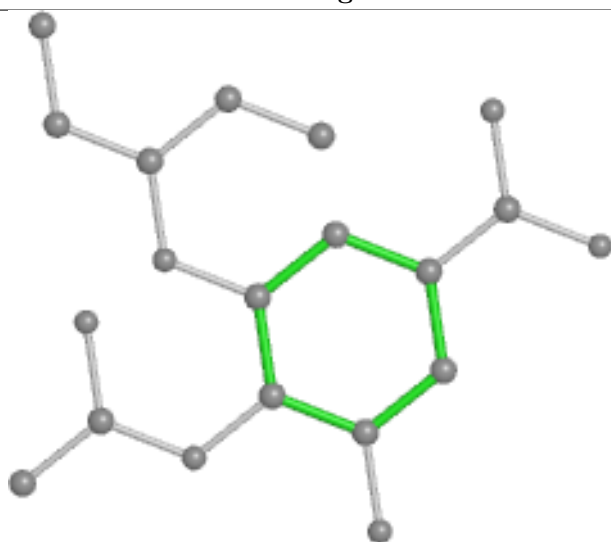
Bond lengths



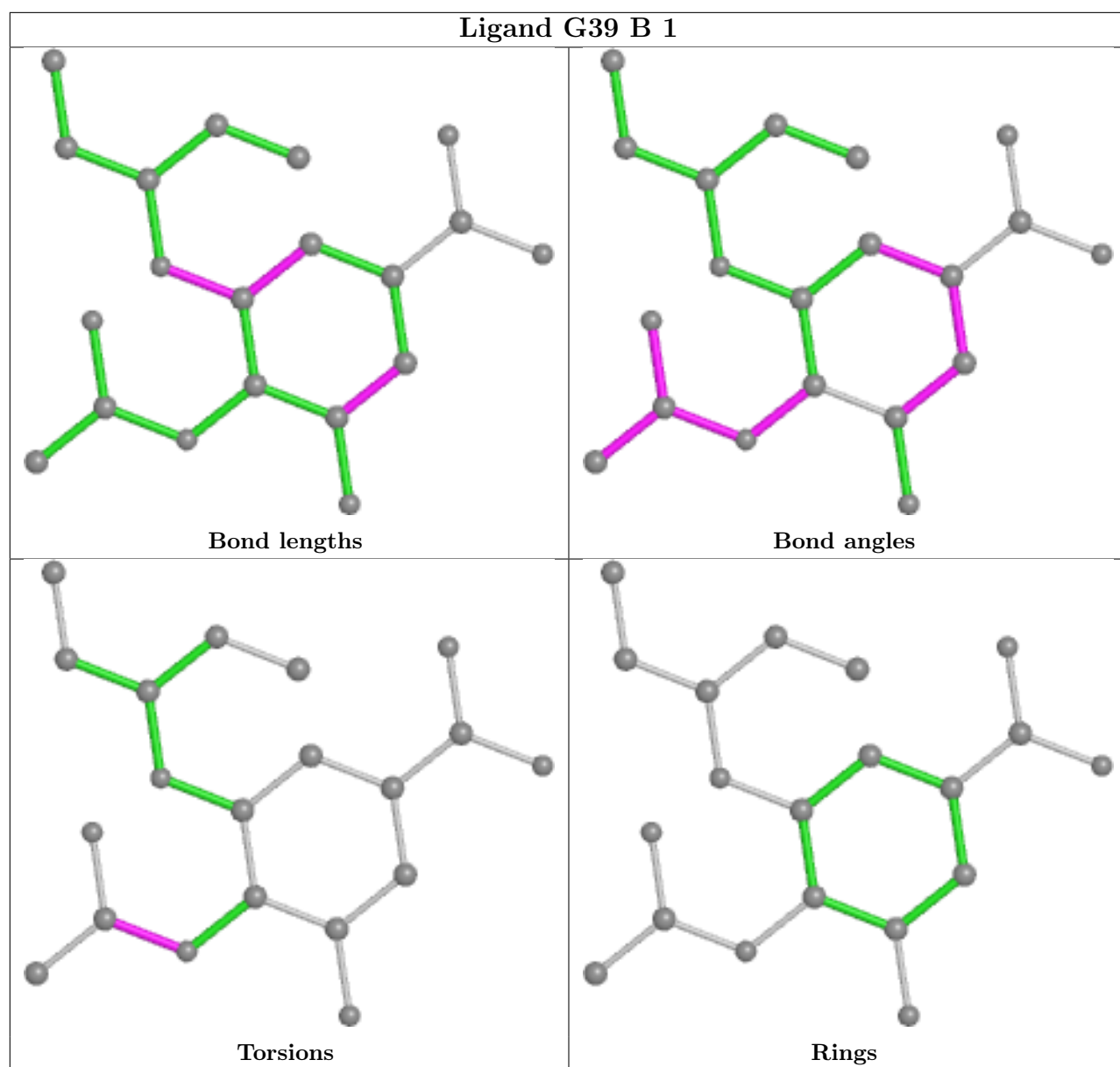
Bond angles

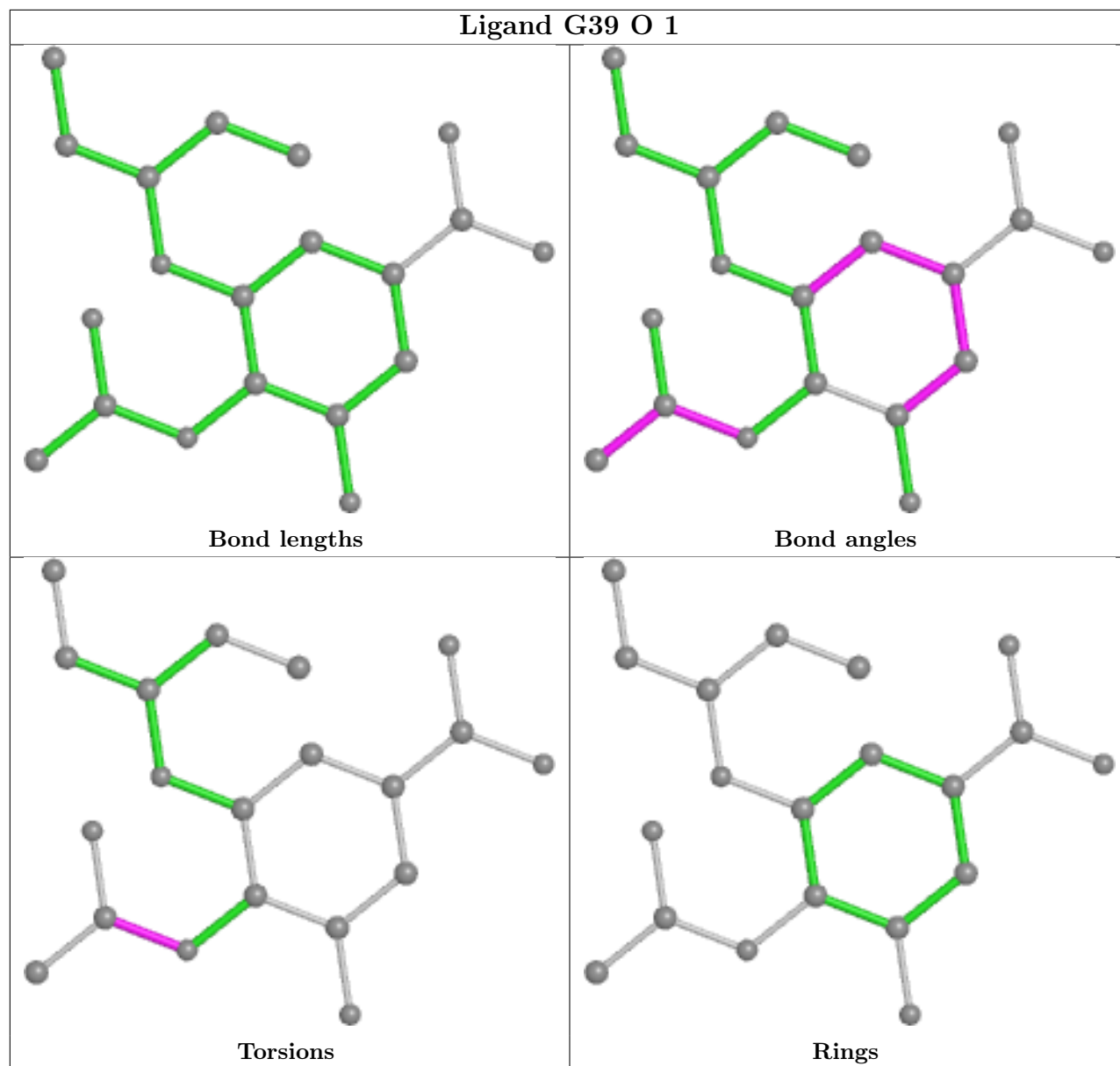


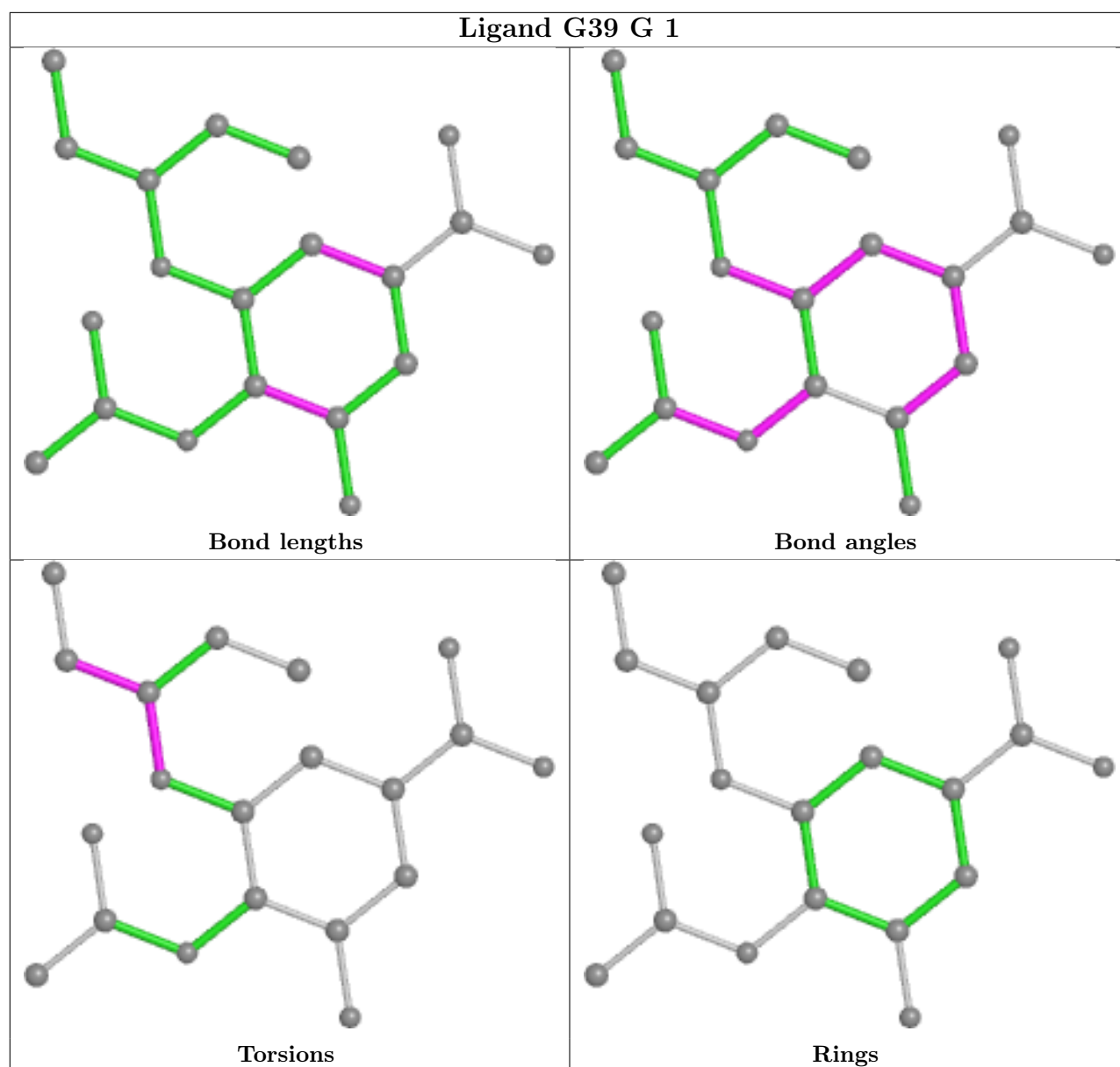
Torsions

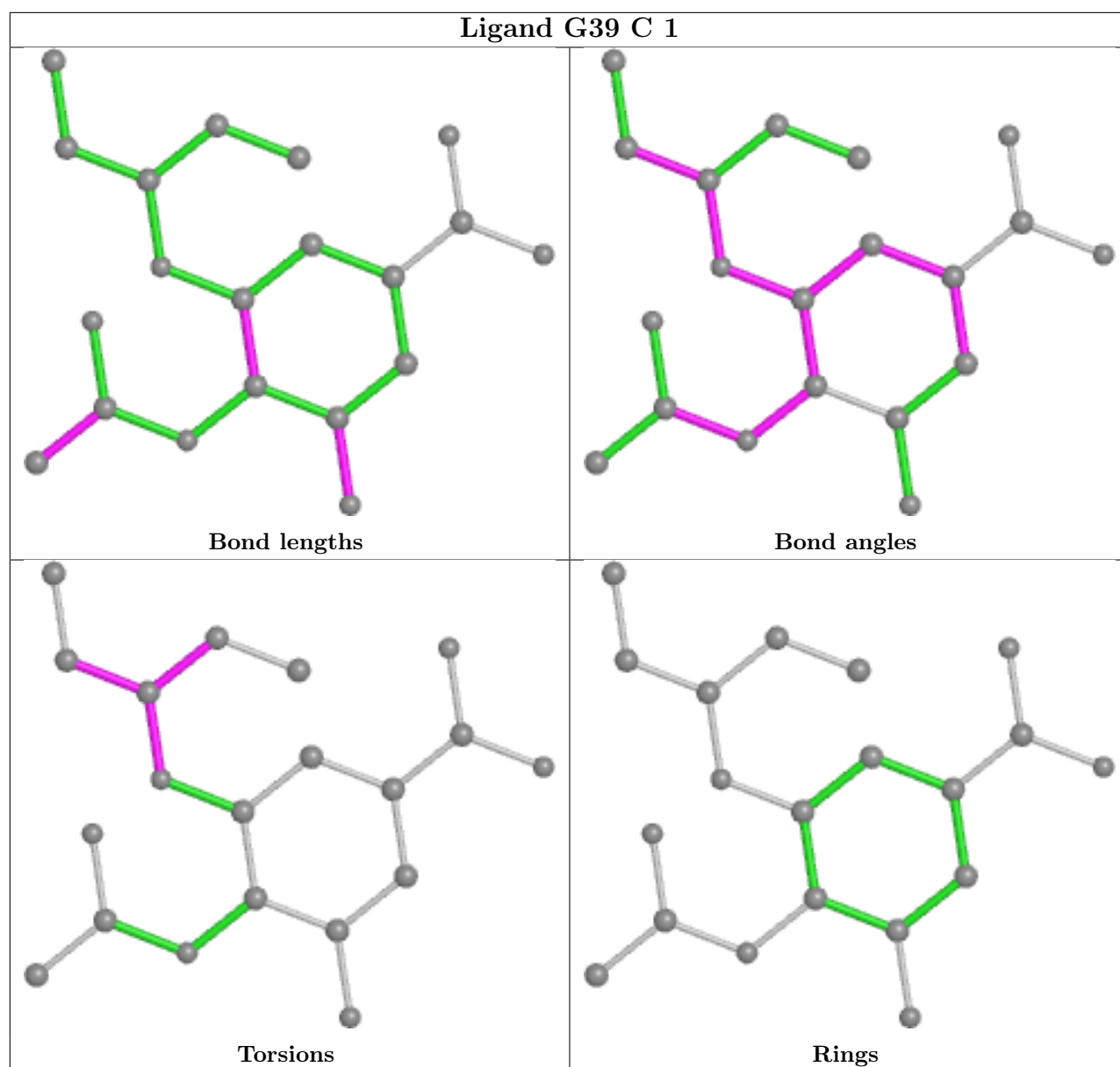


Rings

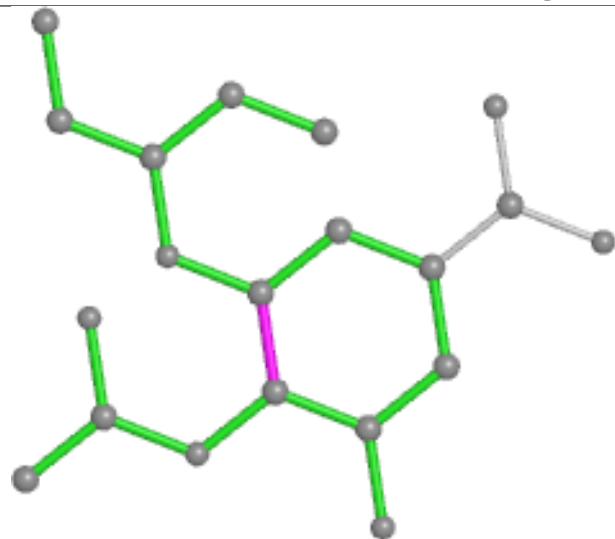




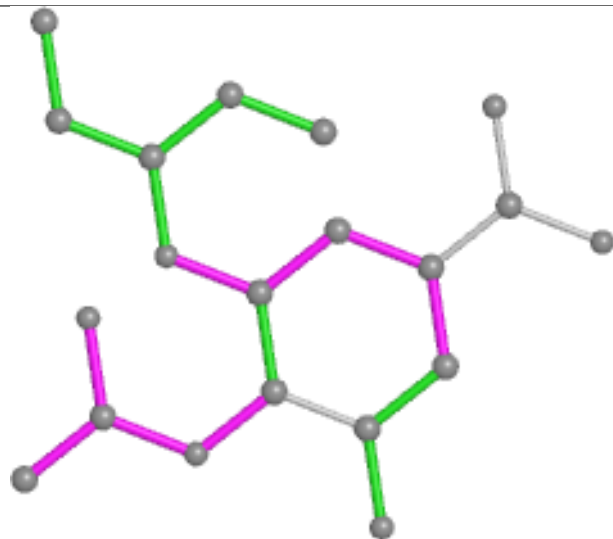




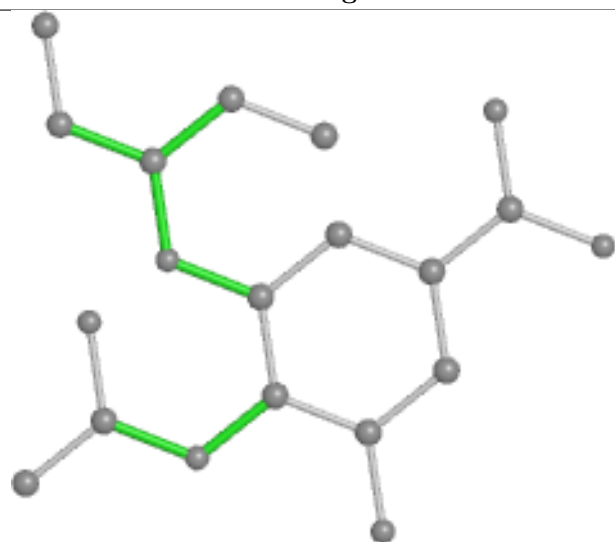
## Ligand G39 A 1



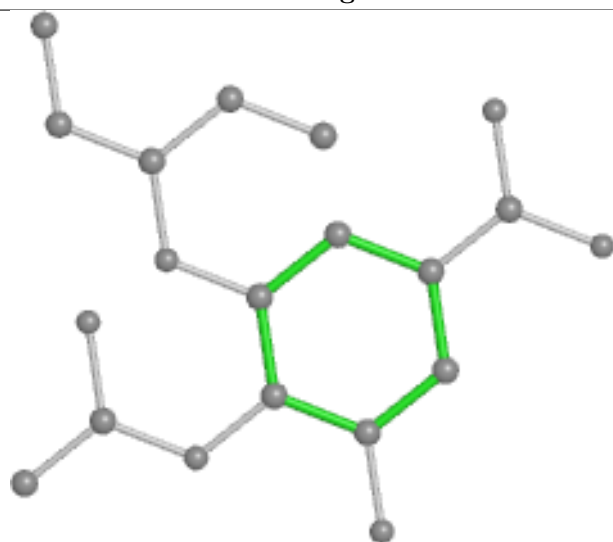
Bond lengths



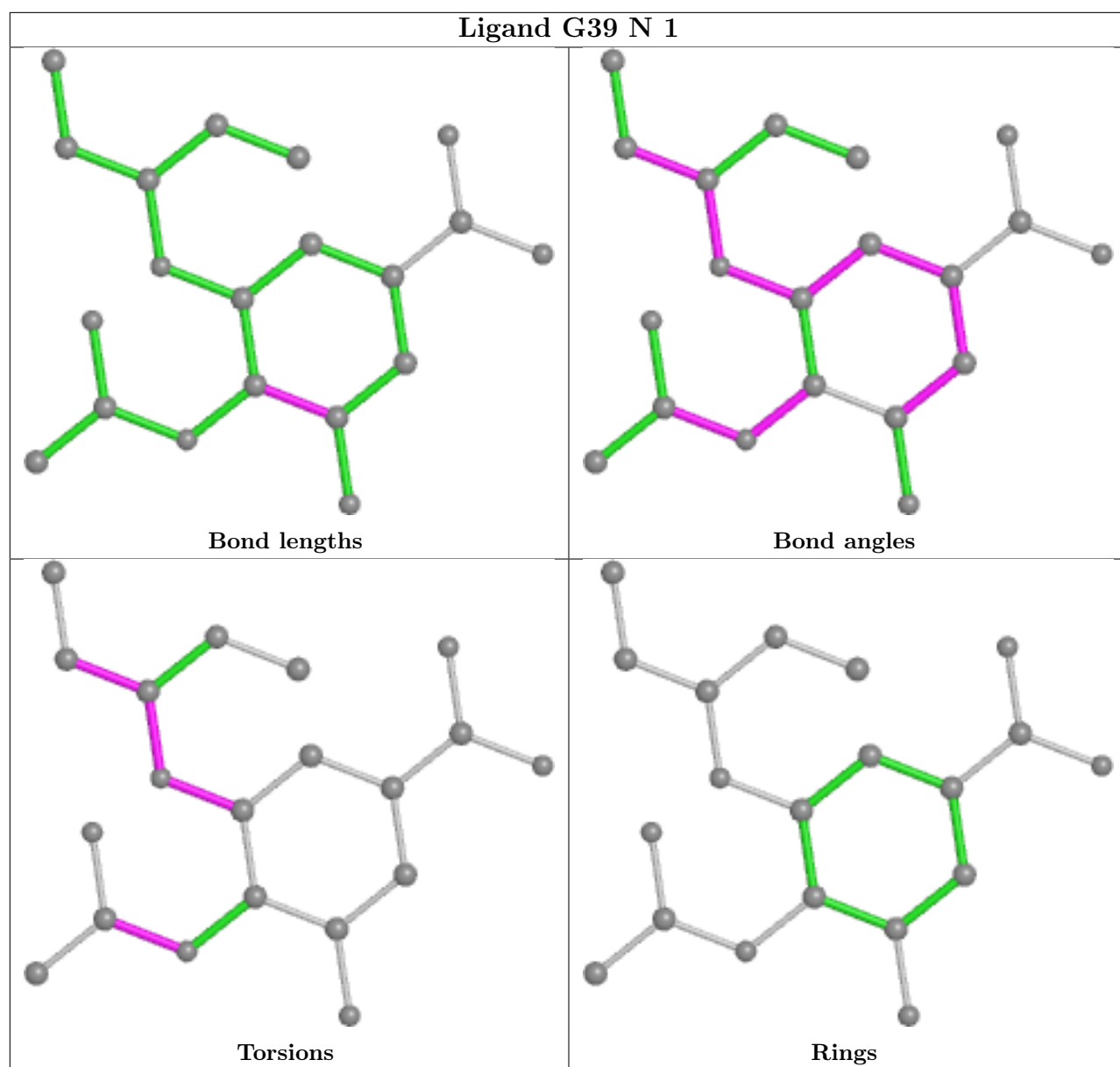
Bond angles

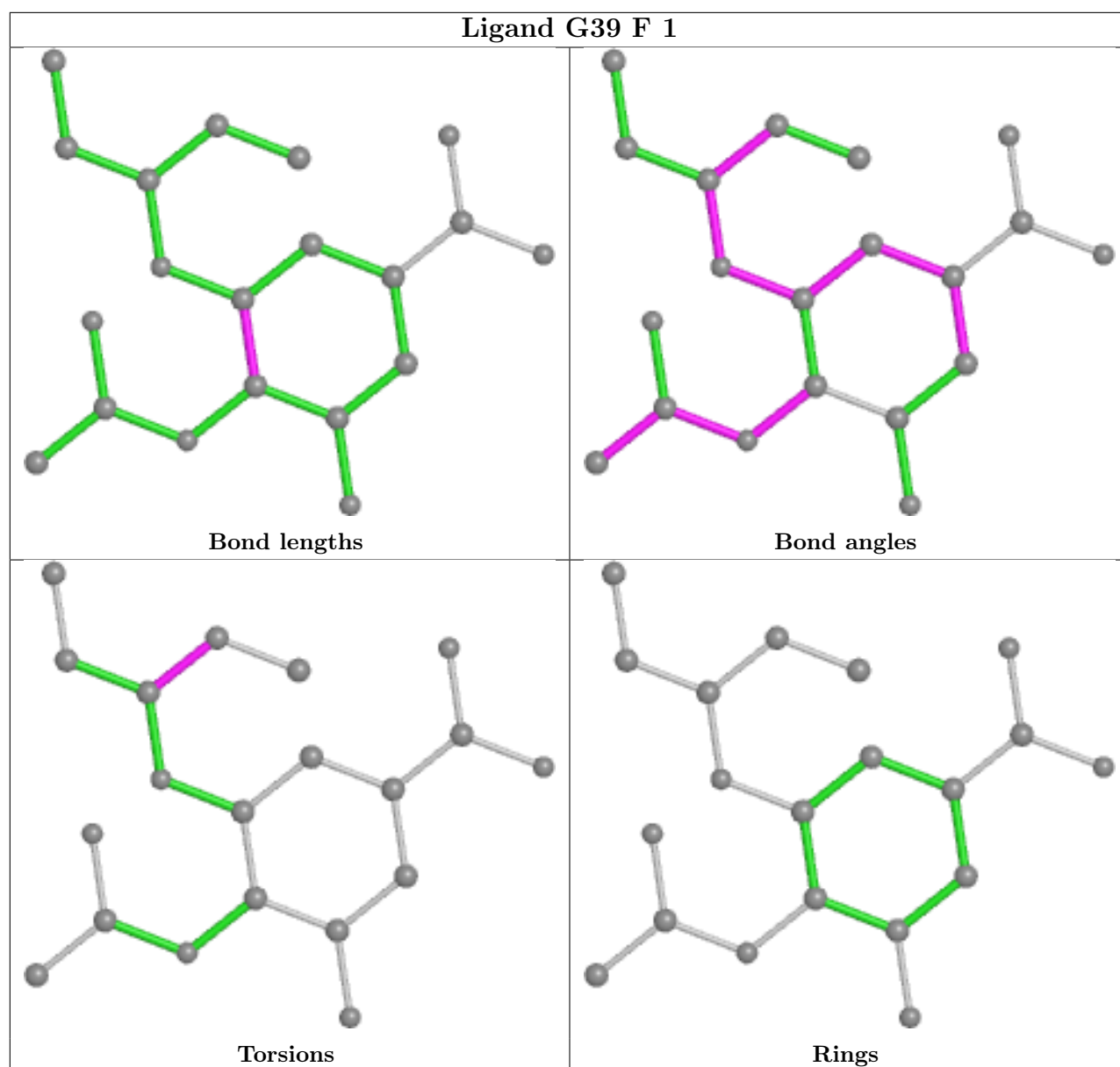


Torsions

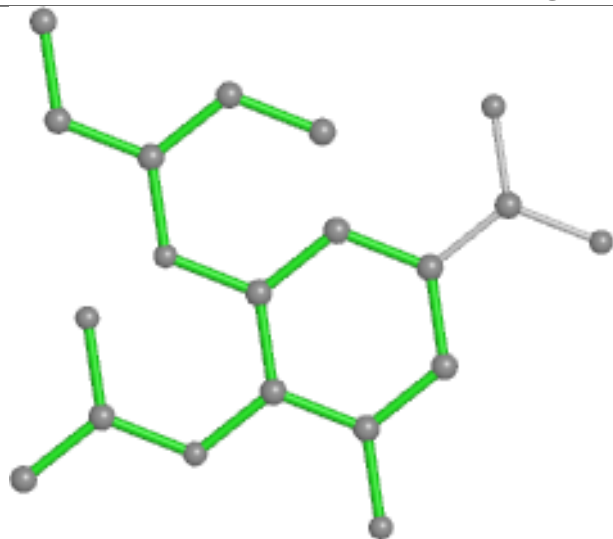


Rings

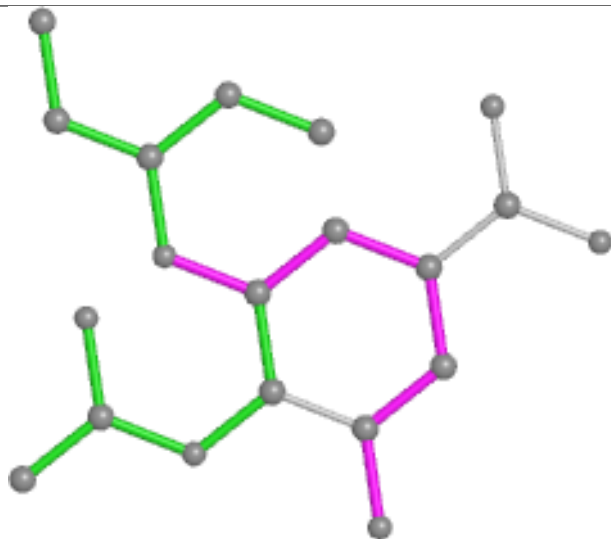




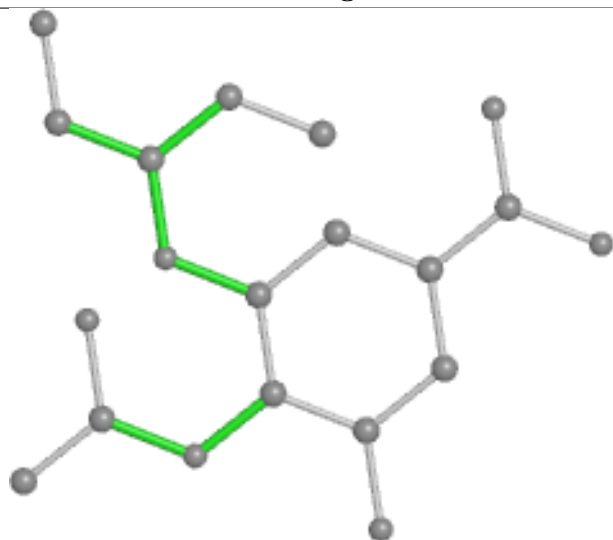
## Ligand G39 I 1



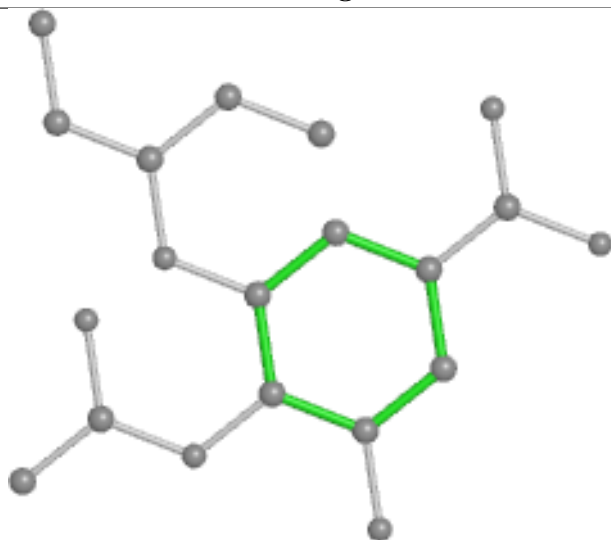
Bond lengths



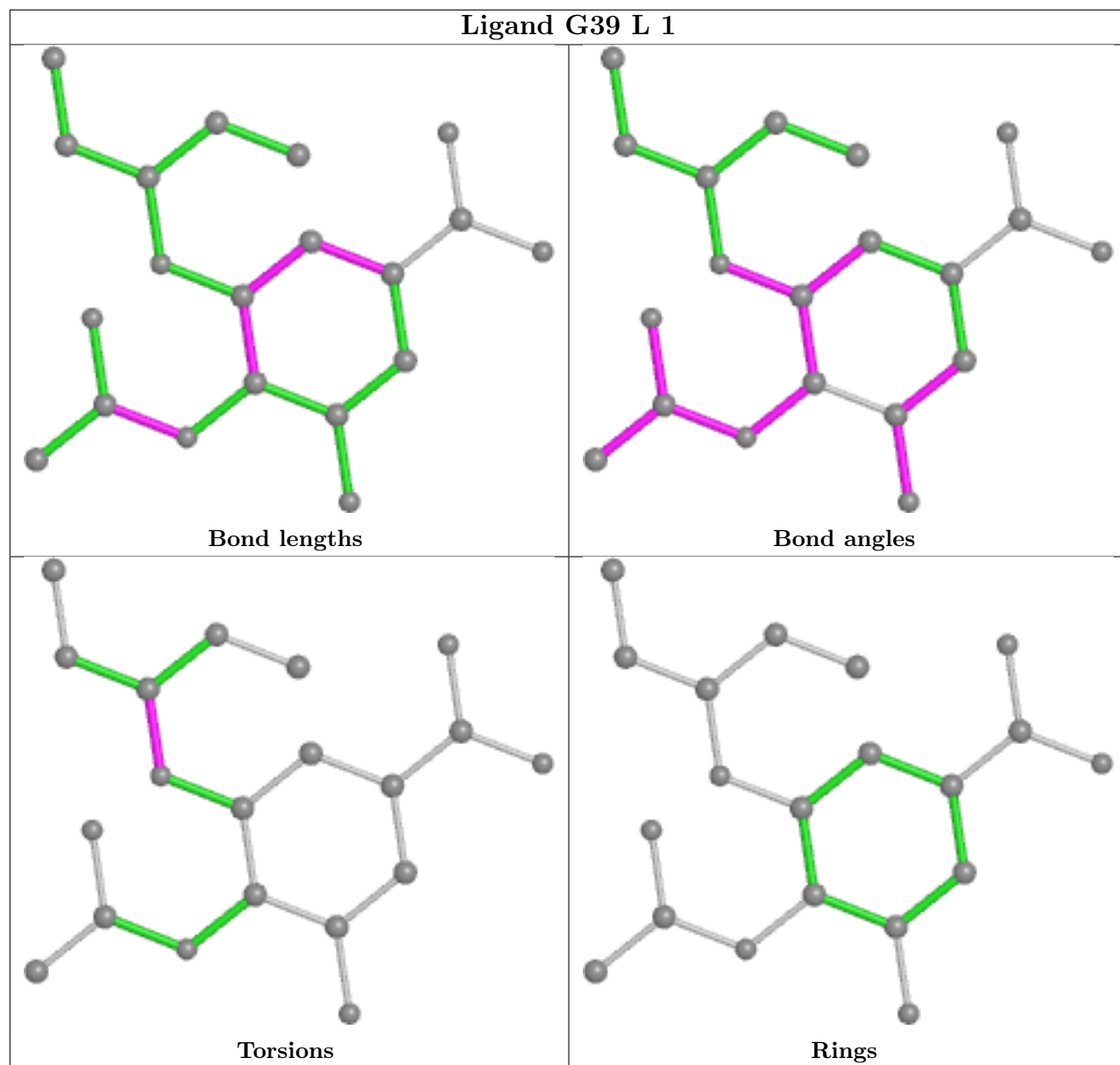
Bond angles

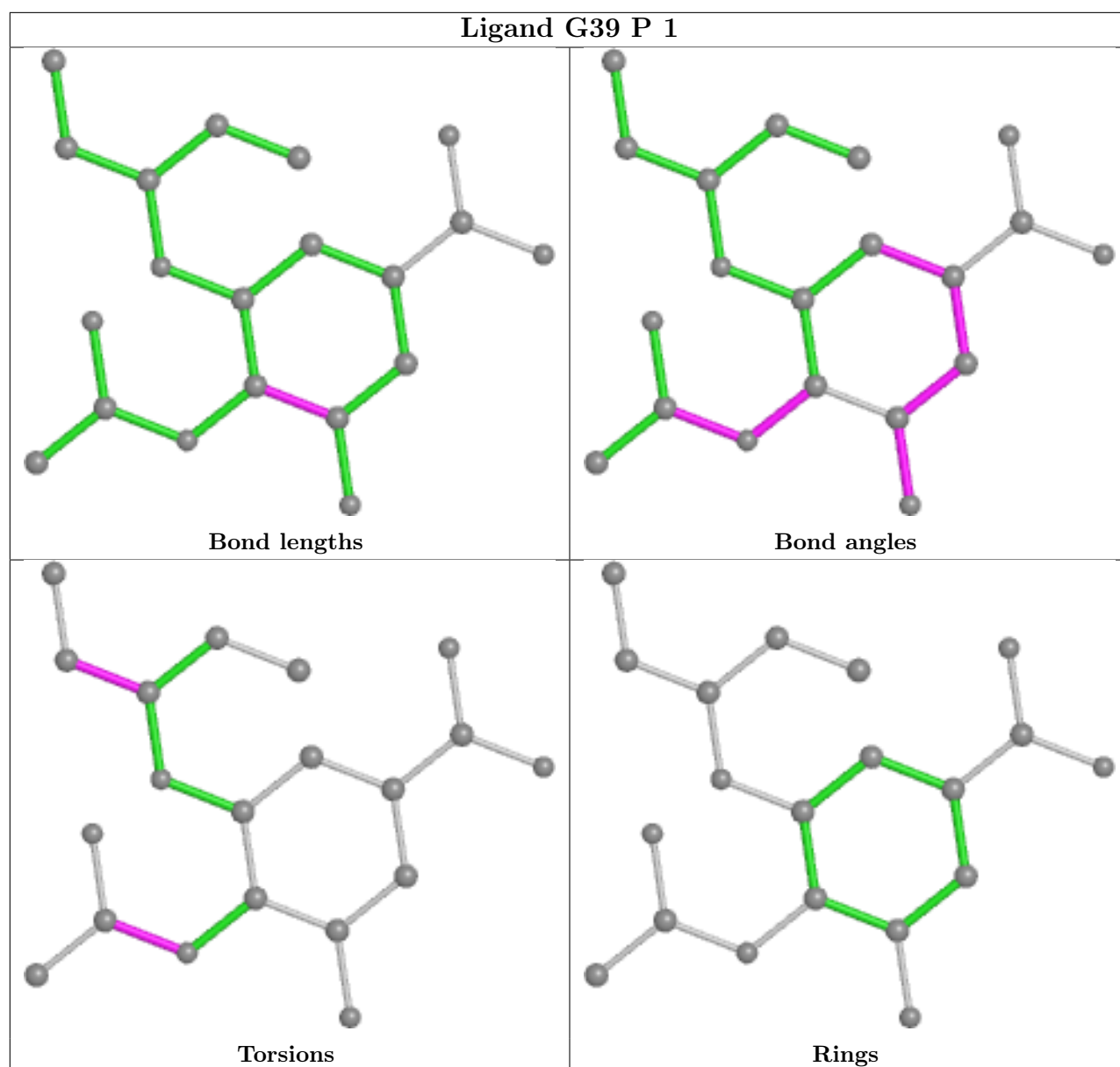


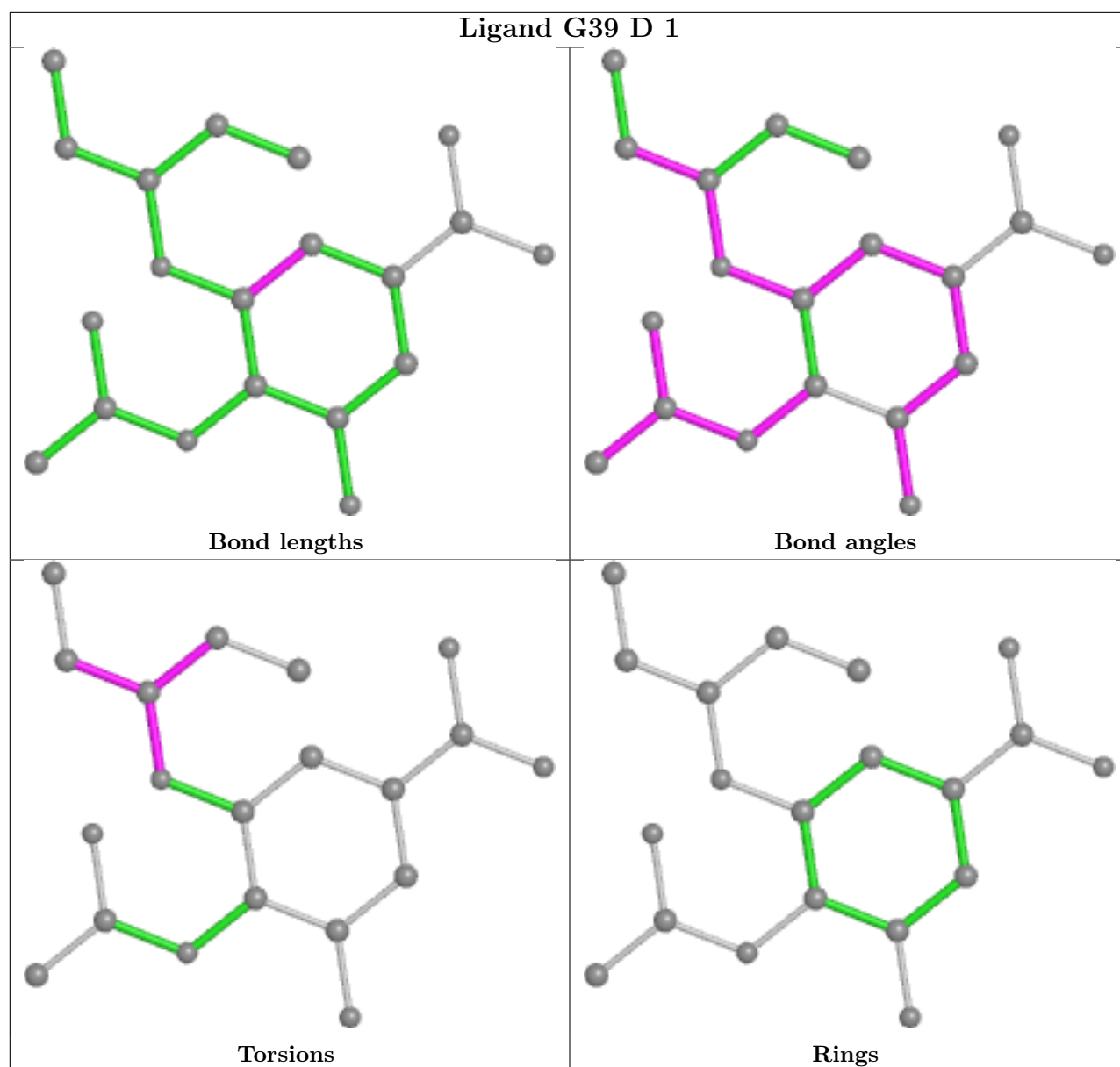
Torsions



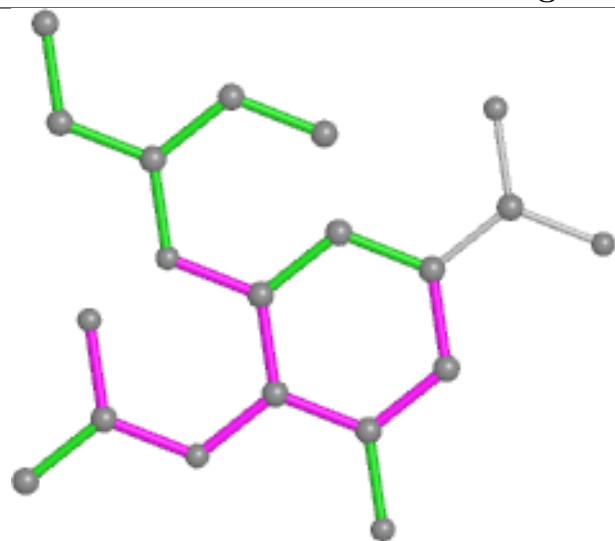
Rings



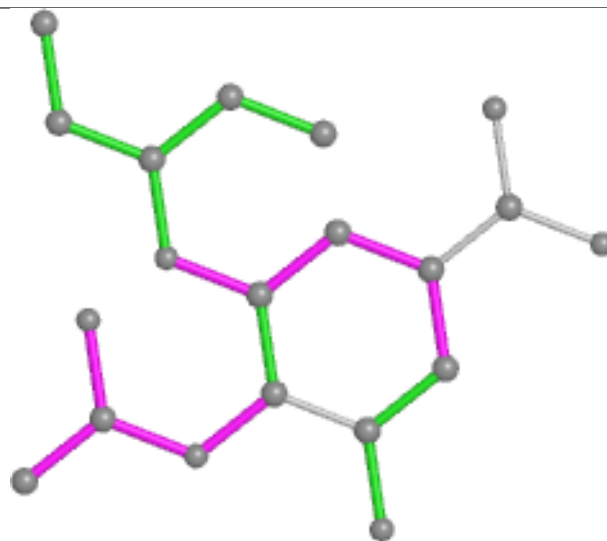




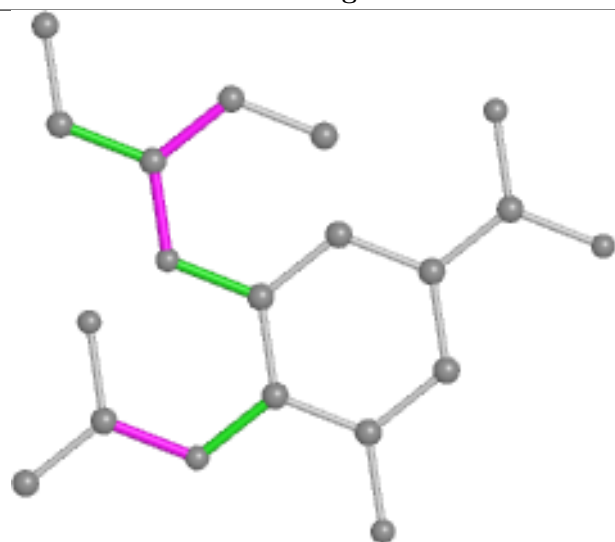
## Ligand G39 K 1



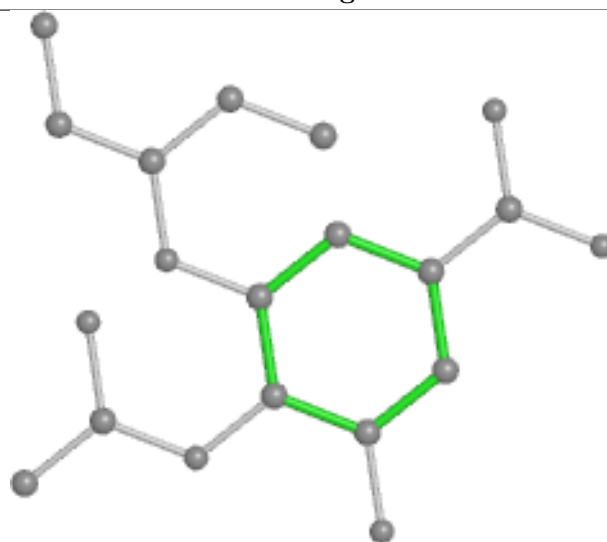
Bond lengths



Bond angles

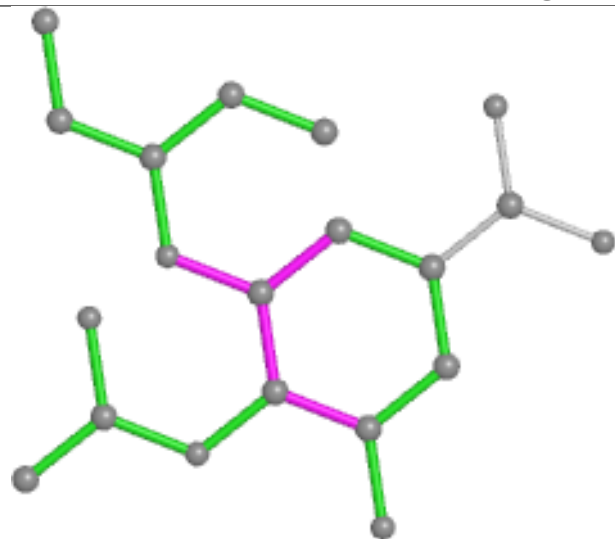


Torsions

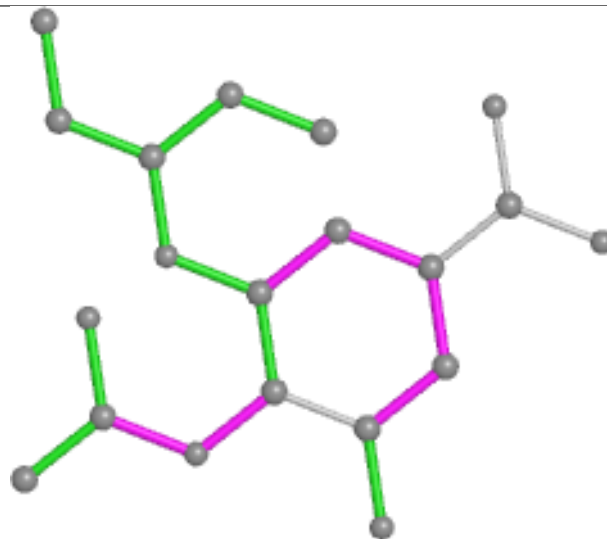


Rings

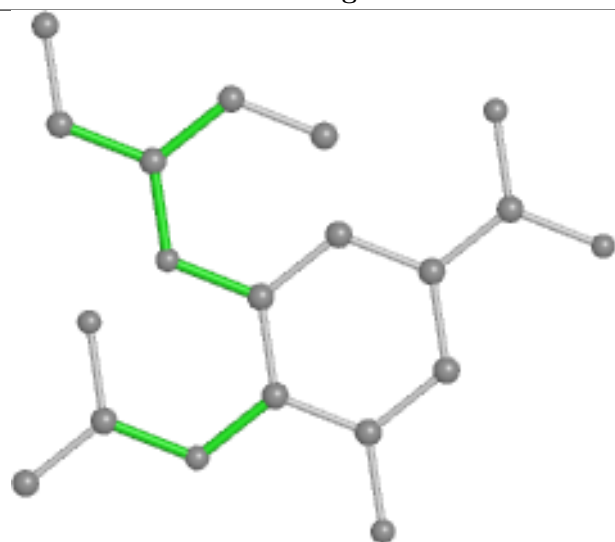
## Ligand G39 H 1



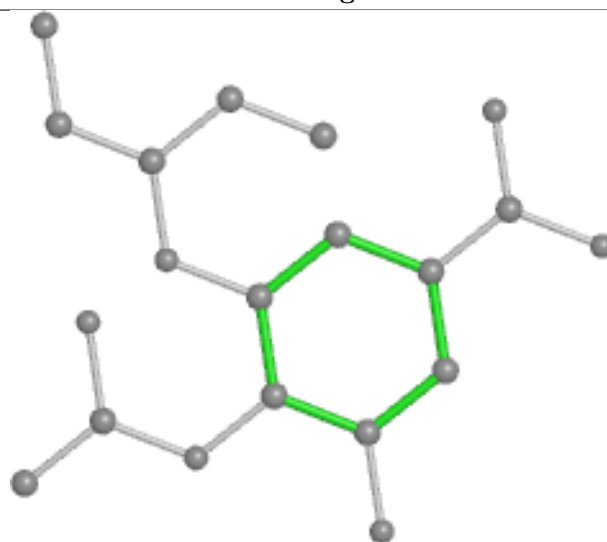
Bond lengths



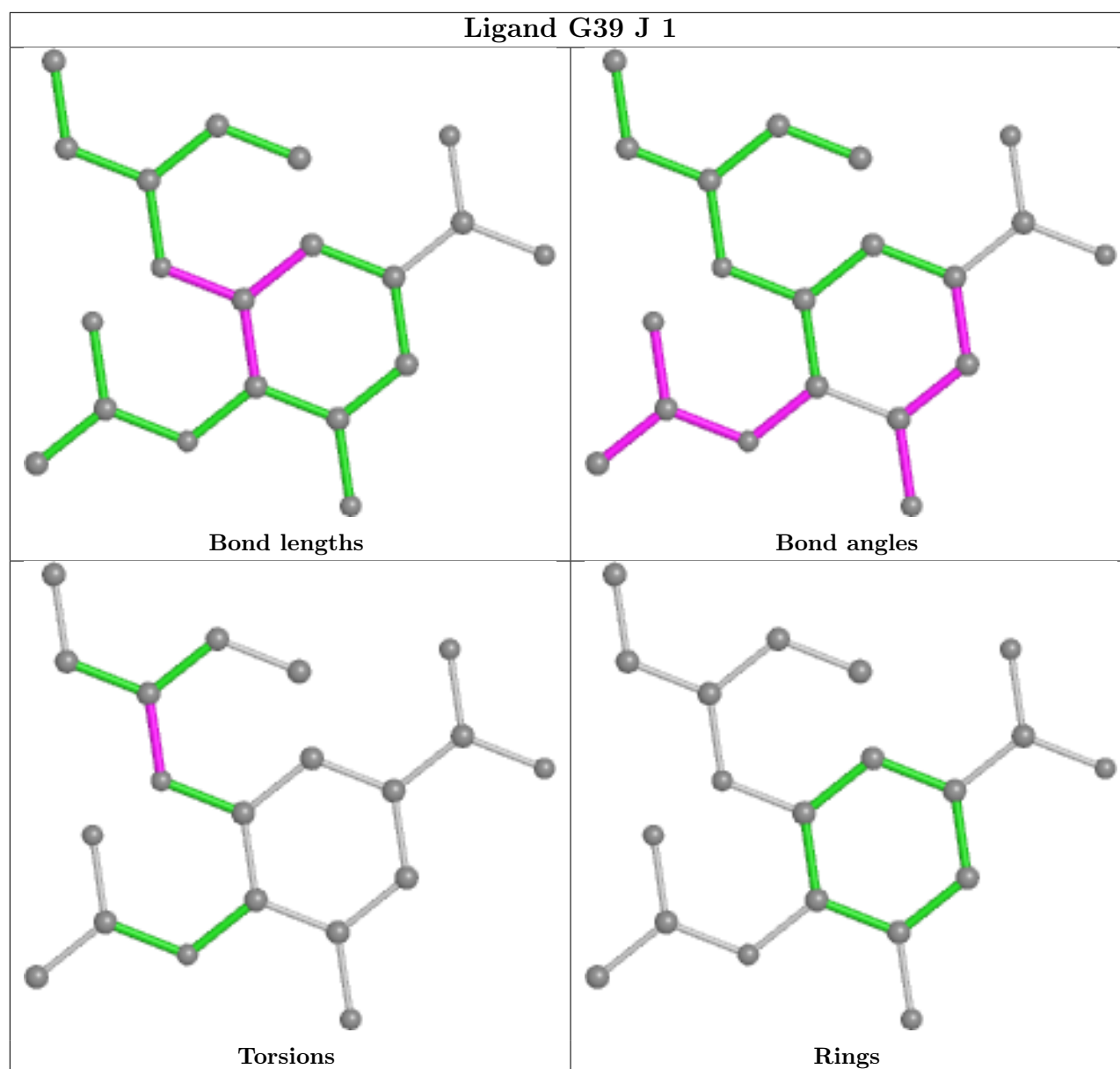
Bond angles



Torsions



Rings



## 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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

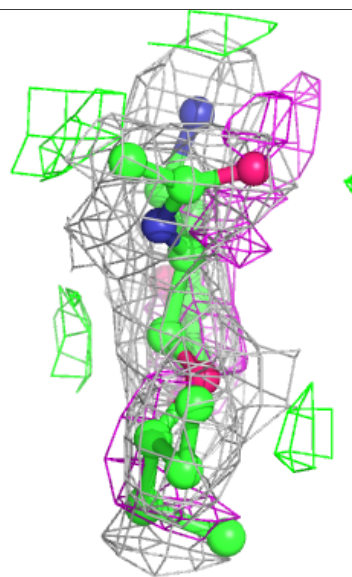
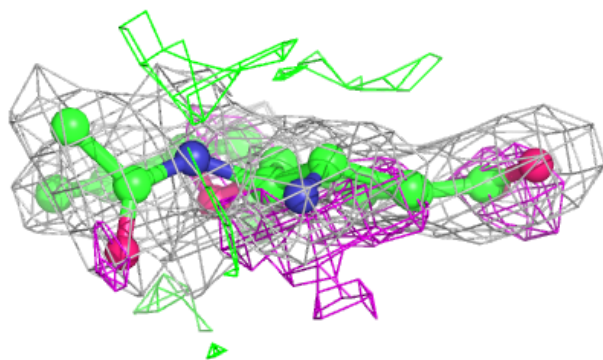
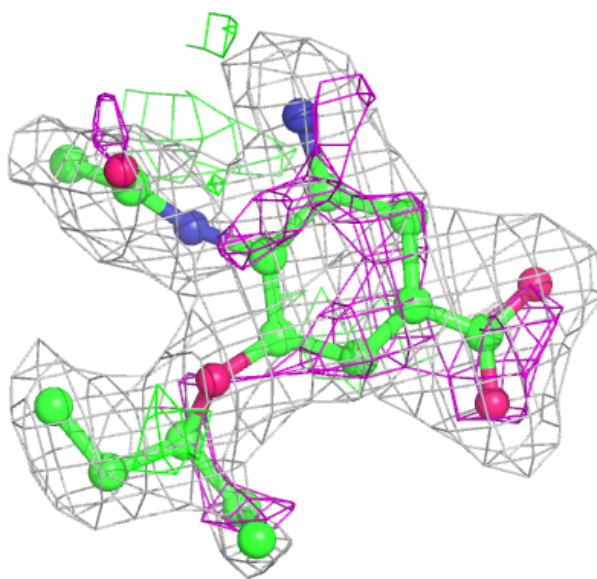
### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

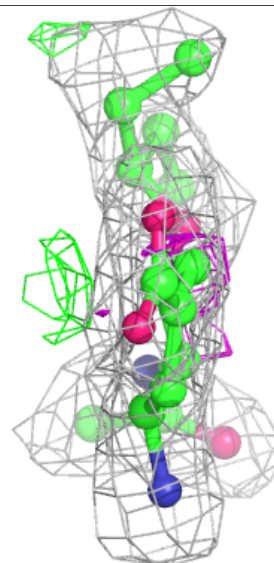
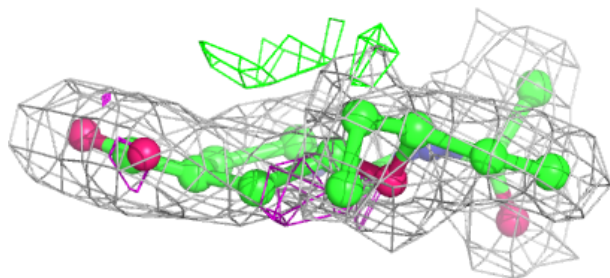
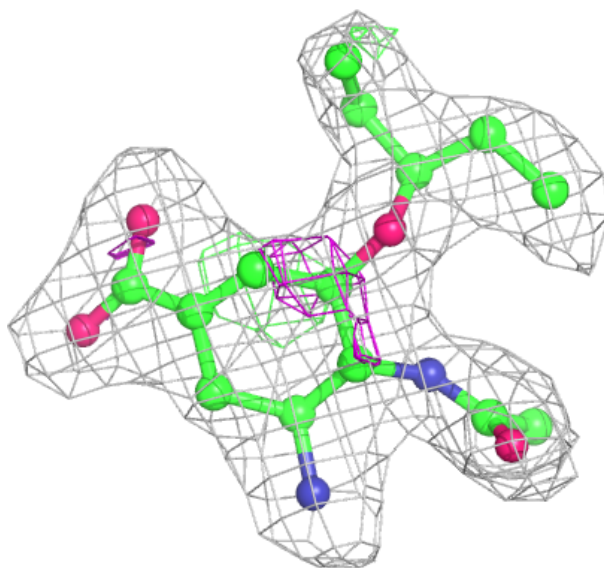
**Electron density around G39 A 1:**

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



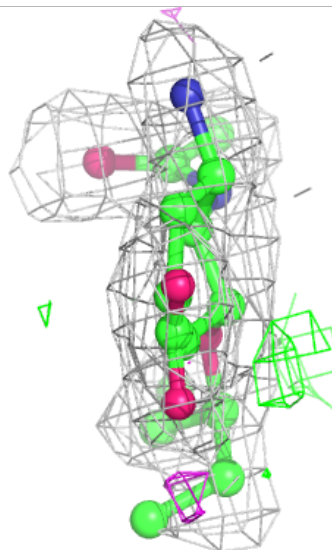
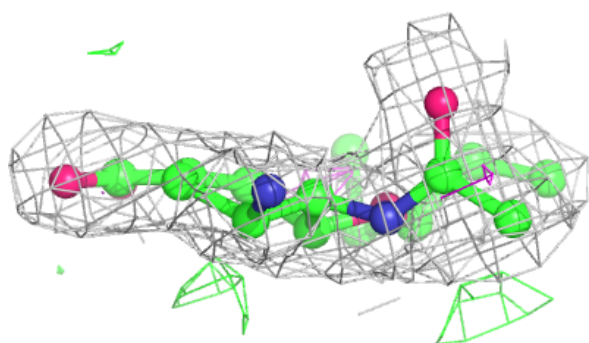
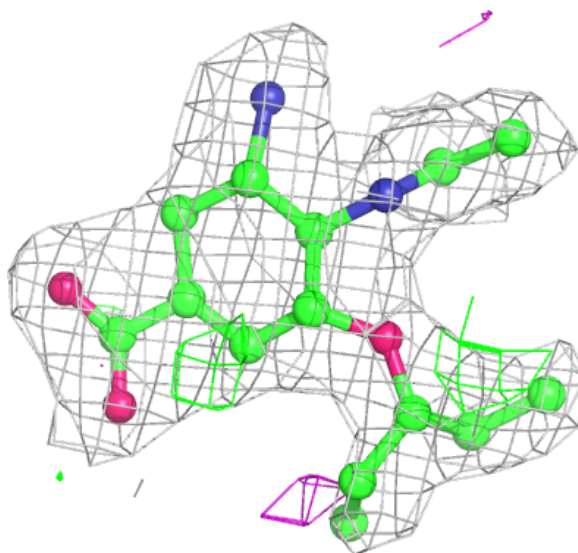
**Electron density around G39 B 1:**

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



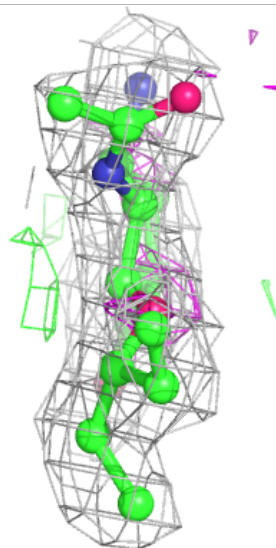
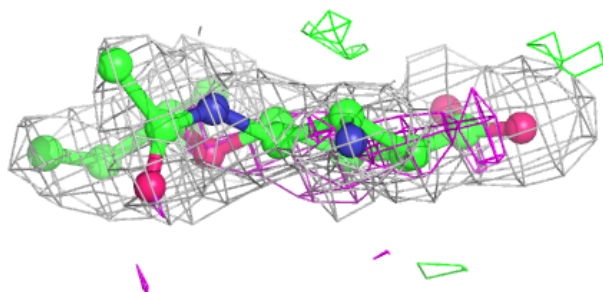
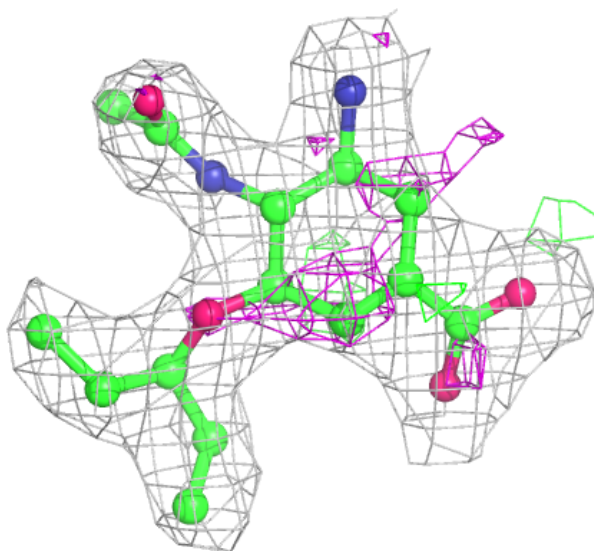
**Electron density around G39 C 1:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



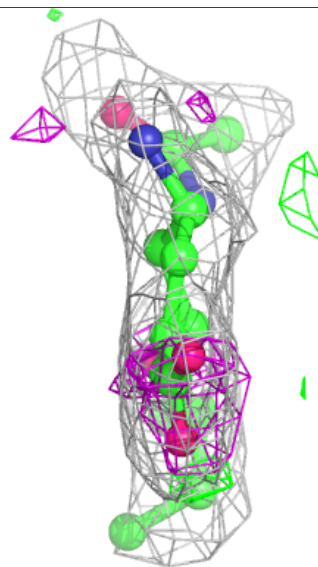
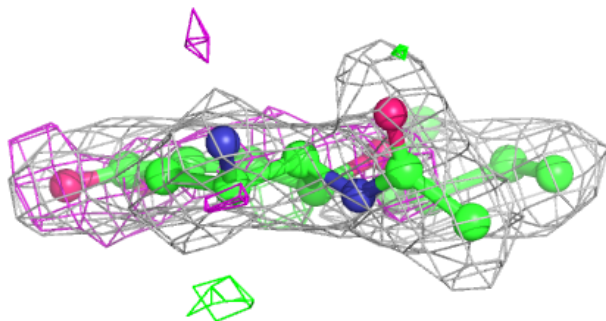
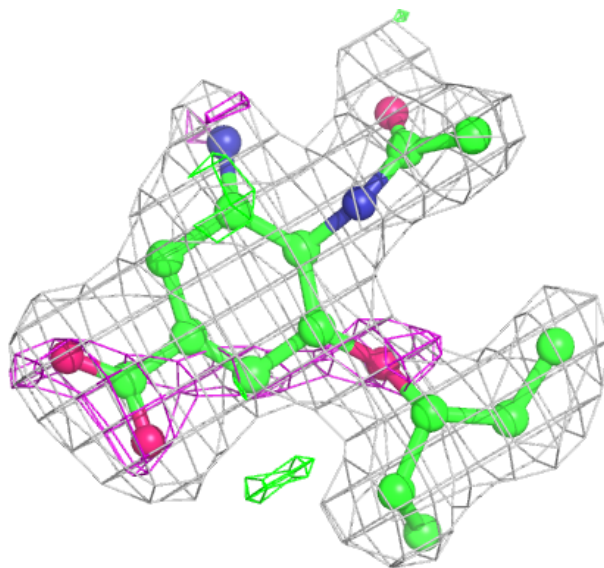
**Electron density around G39 D 1:**

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



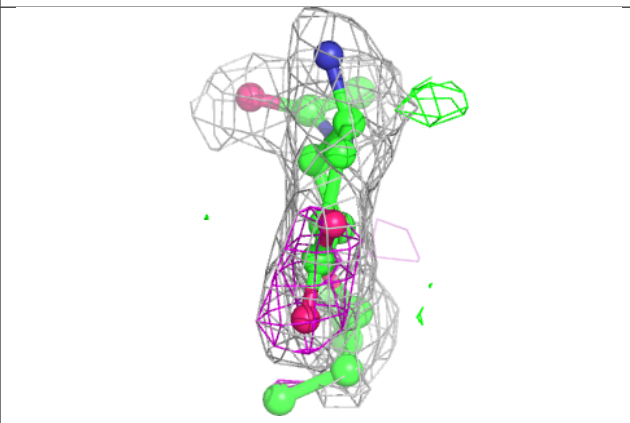
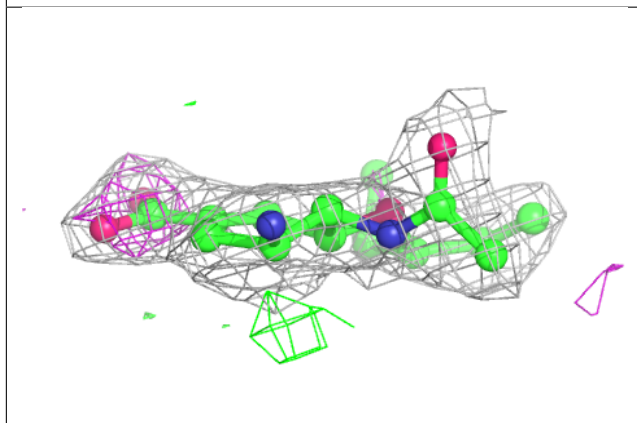
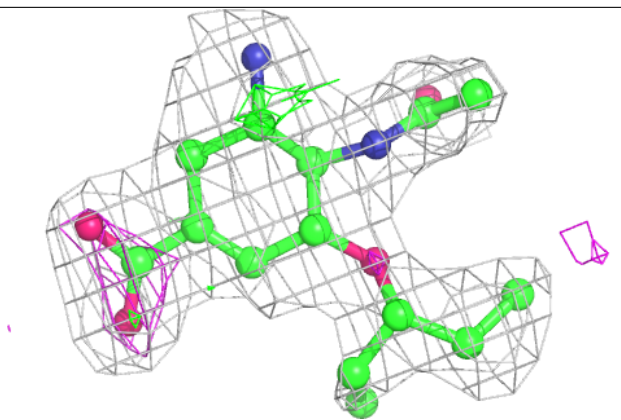
**Electron density around G39 E 1:**

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



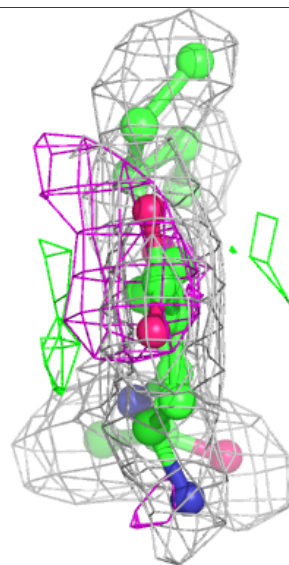
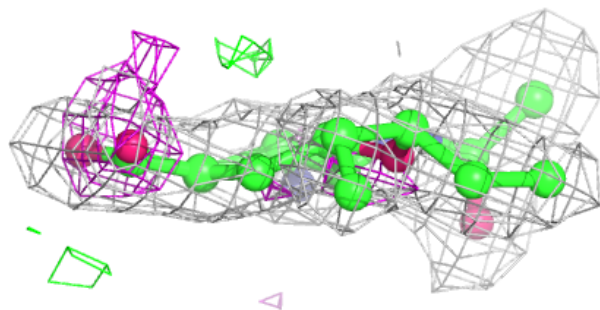
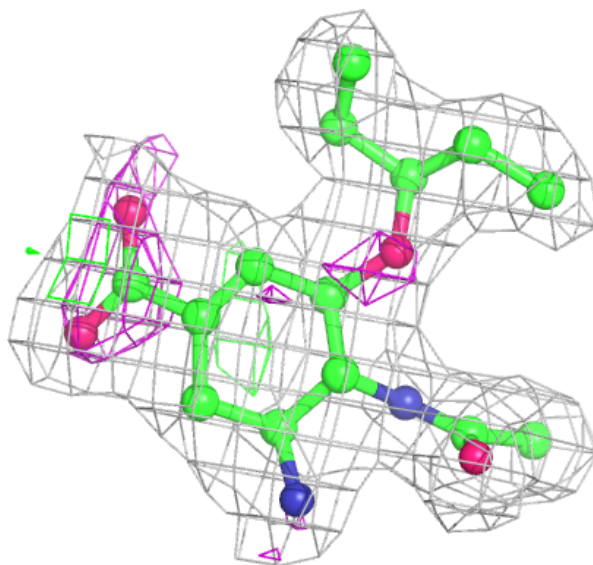
**Electron density around G39 F 1:**

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



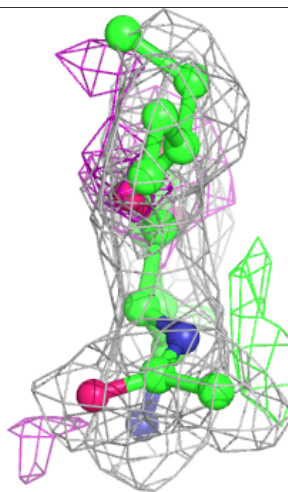
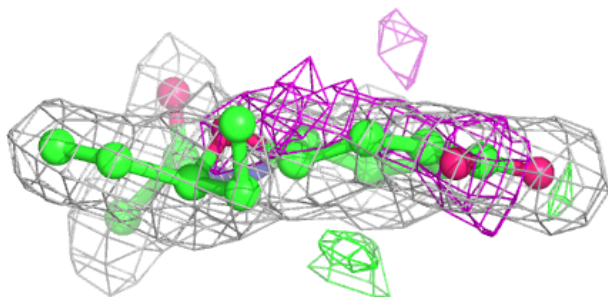
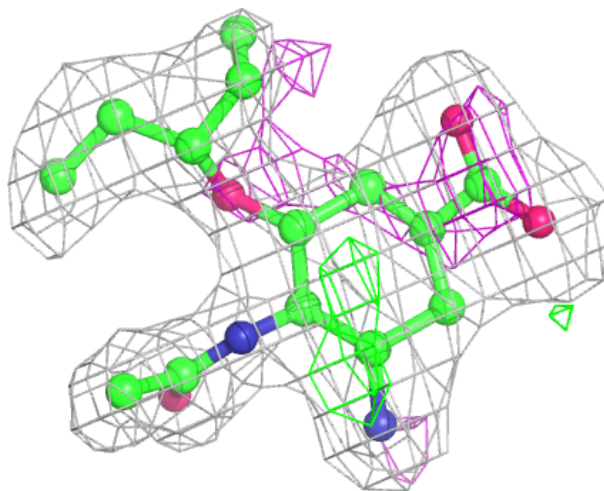
**Electron density around G39 G 1:**

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



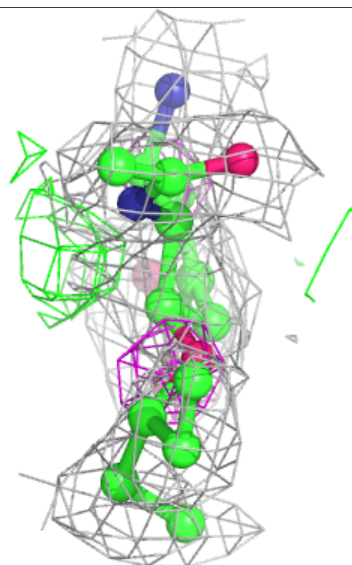
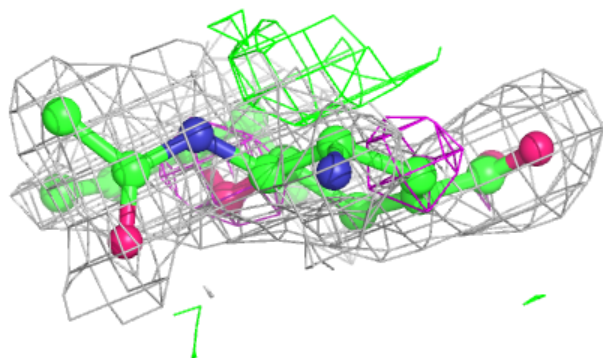
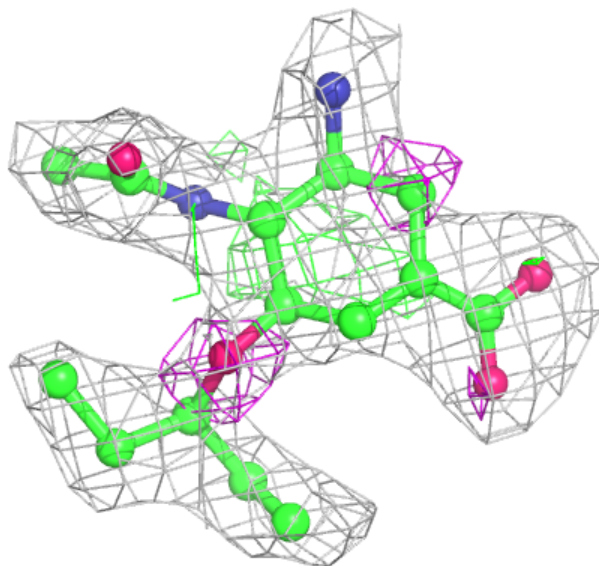
**Electron density around G39 H 1:**

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



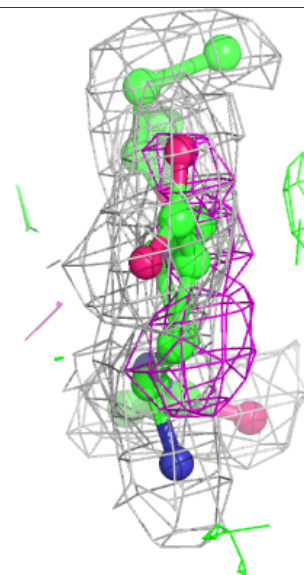
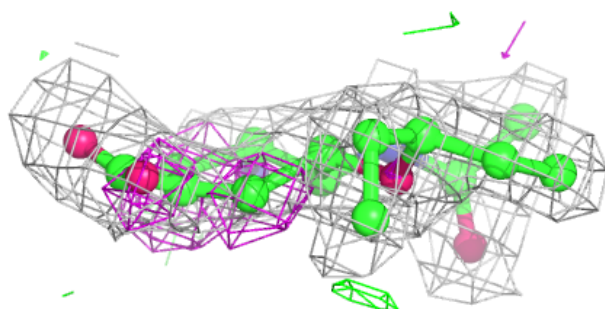
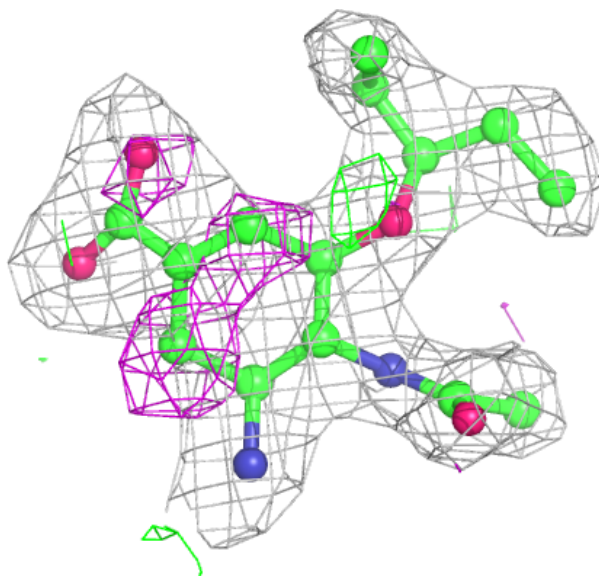
**Electron density around G39 I 1:**

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



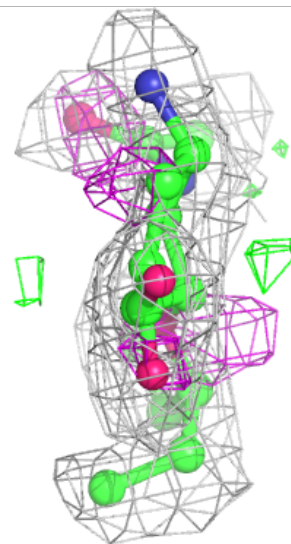
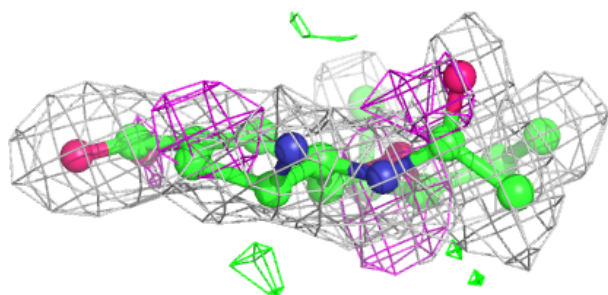
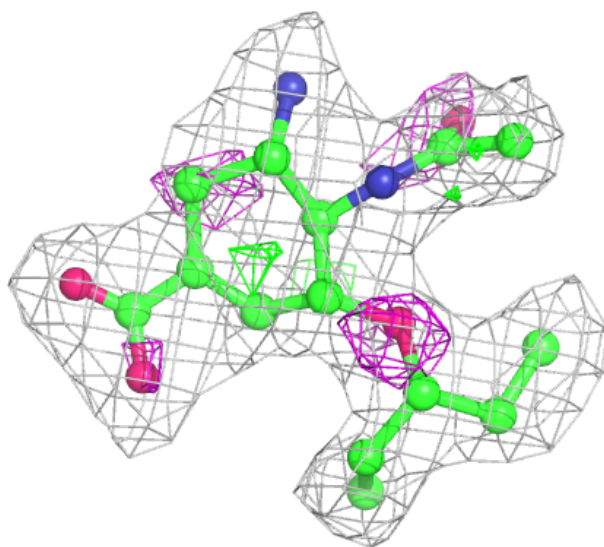
**Electron density around G39 J 1:**

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



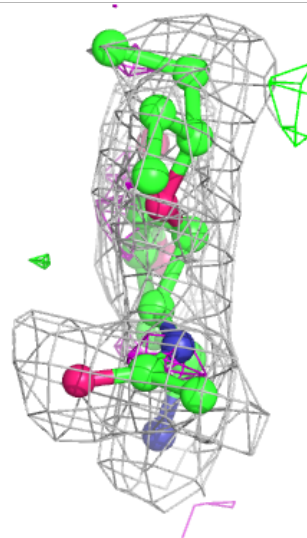
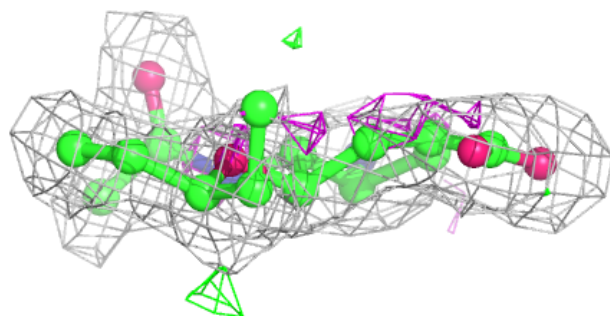
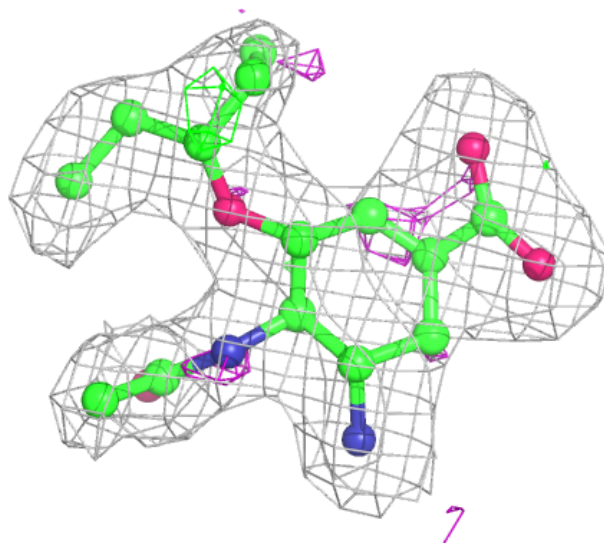
**Electron density around G39 K 1:**

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



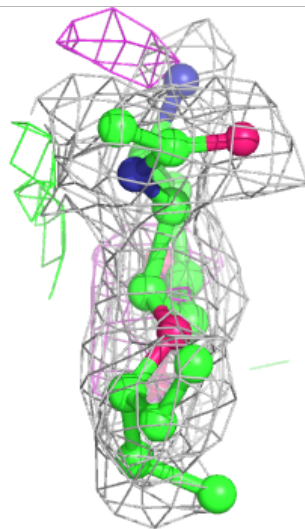
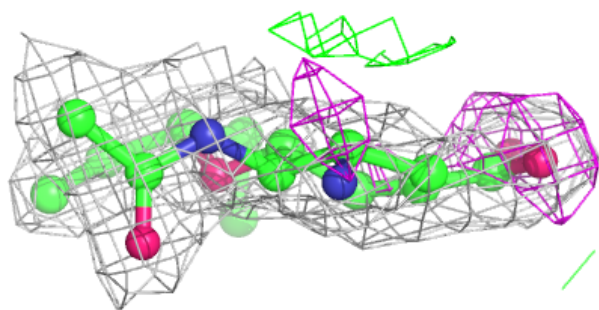
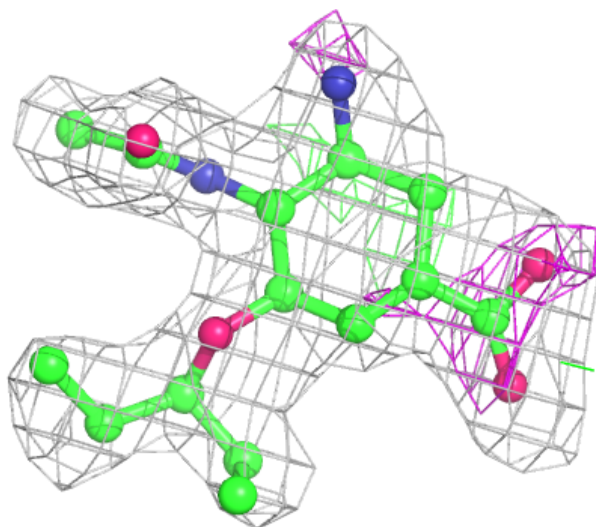
**Electron density around G39 L 1:**

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



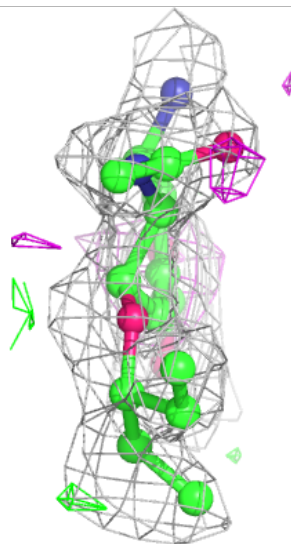
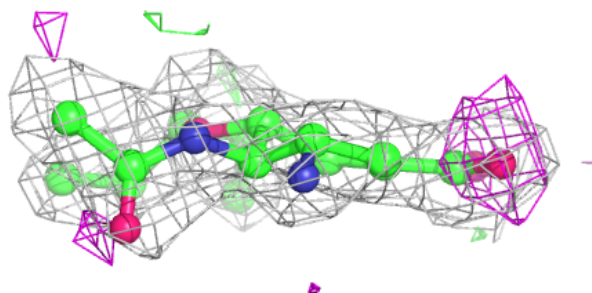
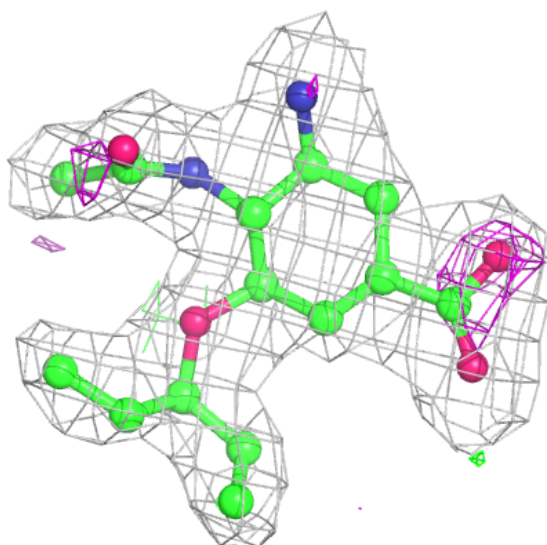
**Electron density around G39 M 1:**

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



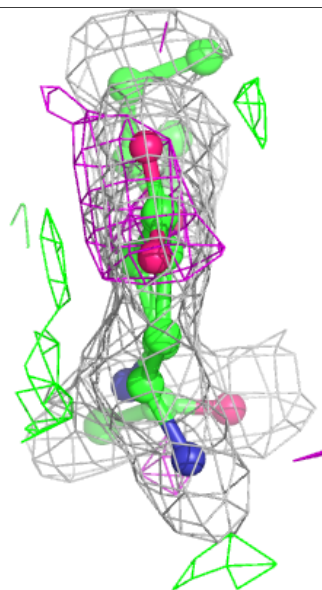
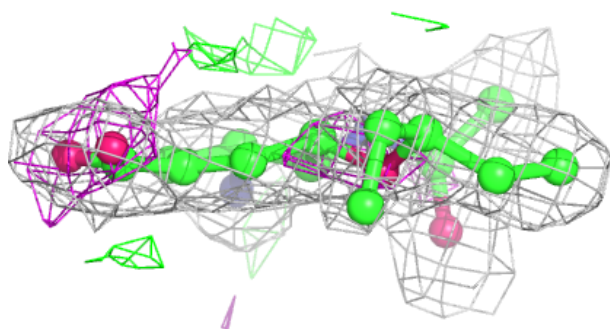
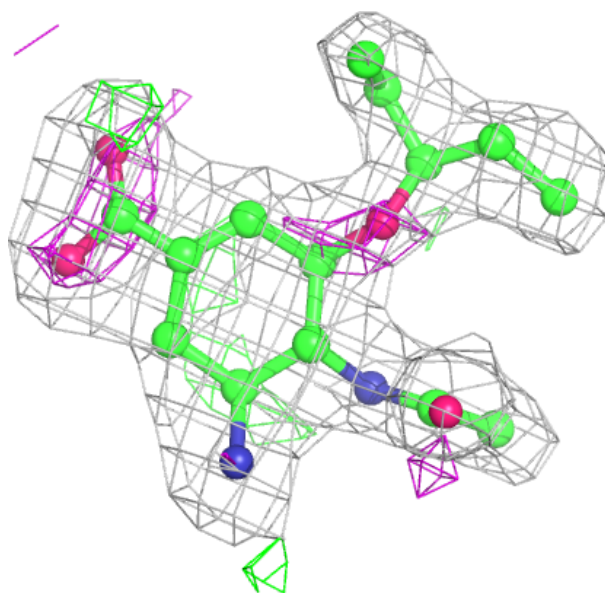
**Electron density around G39 N 1:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



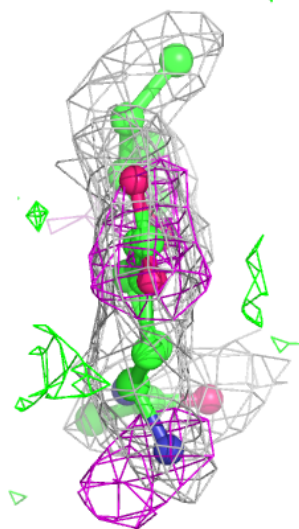
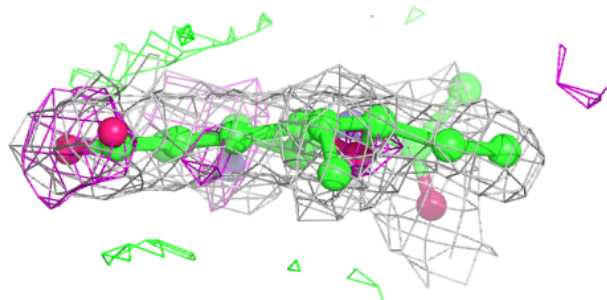
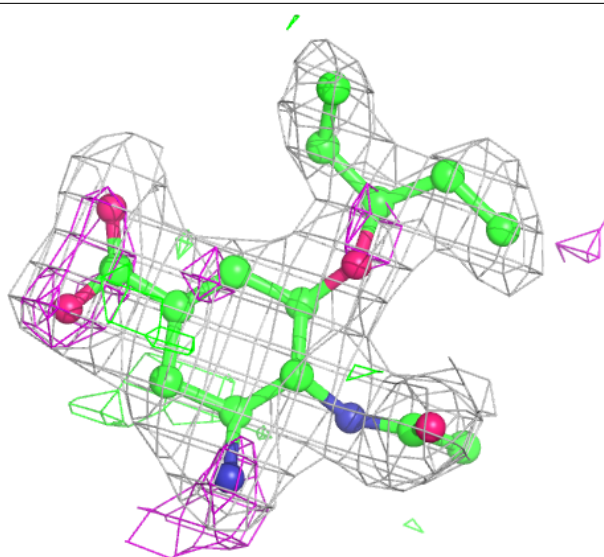
**Electron density around G39 O 1:**

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



**Electron density around G39 P 1:**

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



## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.