



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 29, 2024 – 02:14 AM EDT

PDB ID : 2HU4  
Title : N1 neuraminidase in complex with oseltamivir 2  
Authors : Russell, R.J.; Haire, L.F.; Stevens, D.J.; Collins, P.J.; Lin, Y.P.; Blackburn, G.M.; Hay, A.J.; Gamblin, S.J.; Skehel, J.J.  
Deposited on : 2006-07-26  
Resolution : 2.50 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.

The types of validation reports are described at

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

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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 : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

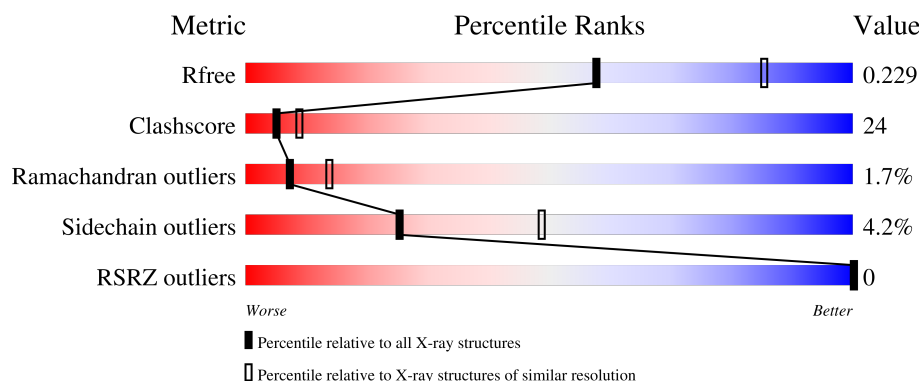
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	387	 63% 33% . .
1	B	387	 65% 30% . .
1	C	387	 63% 33% . .
1	D	387	 60% 35% 5% . .
1	E	387	 64% 32% . .

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Mol	Chain	Length	Quality of chain
1	F	387	 65% 31% . .
1	G	387	 63% 35% . .
1	H	387	 63% 34% . .

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23856 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.

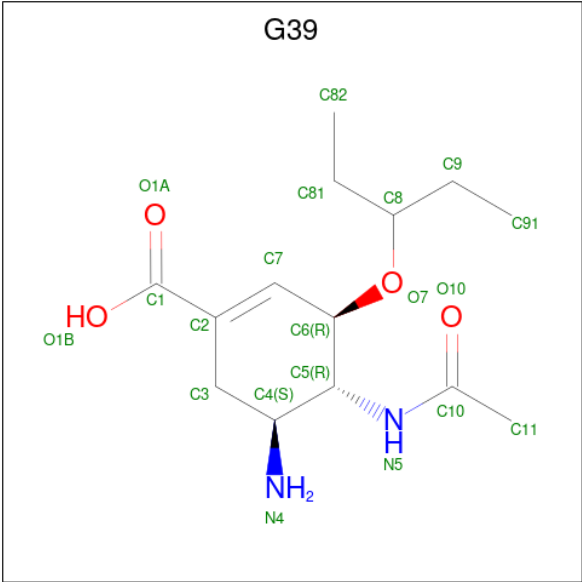
- Molecule 1 is a protein called Neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	0	0
			2962	1858	510	573	21			
1	B	385	Total	C	N	O	S	0	0	0
			2962	1858	510	573	21			
1	C	385	Total	C	N	O	S	0	0	0
			2962	1858	510	573	21			
1	D	385	Total	C	N	O	S	0	0	0
			2962	1858	510	573	21			
1	E	385	Total	C	N	O	S	0	0	0
			2962	1858	510	573	21			
1	F	385	Total	C	N	O	S	0	0	0
			2962	1858	510	573	21			
1	G	385	Total	C	N	O	S	0	0	0
			2962	1858	510	573	21			
1	H	385	Total	C	N	O	S	0	0	0
			2962	1858	510	573	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	252	TYR	HIS	engineered mutation	UNP Q6DPL2
B	252	TYR	HIS	engineered mutation	UNP Q6DPL2
C	252	TYR	HIS	engineered mutation	UNP Q6DPL2
D	252	TYR	HIS	engineered mutation	UNP Q6DPL2
E	252	TYR	HIS	engineered mutation	UNP Q6DPL2
F	252	TYR	HIS	engineered mutation	UNP Q6DPL2
G	252	TYR	HIS	engineered mutation	UNP Q6DPL2
H	252	TYR	HIS	engineered mutation	UNP Q6DPL2

- Molecule 2 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>).

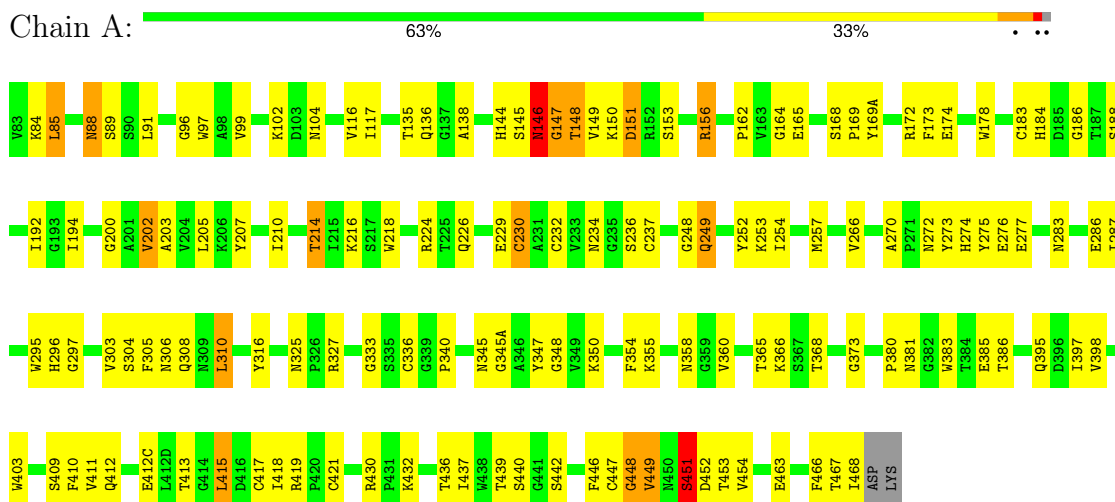


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			20	14	2	4		
2	B	1	Total	C	N	O	0	0
			20	14	2	4		
2	C	1	Total	C	N	O	0	0
			20	14	2	4		
2	D	1	Total	C	N	O	0	0
			20	14	2	4		
2	E	1	Total	C	N	O	0	0
			20	14	2	4		
2	F	1	Total	C	N	O	0	0
			20	14	2	4		
2	G	1	Total	C	N	O	0	0
			20	14	2	4		
2	H	1	Total	C	N	O	0	0
			20	14	2	4		

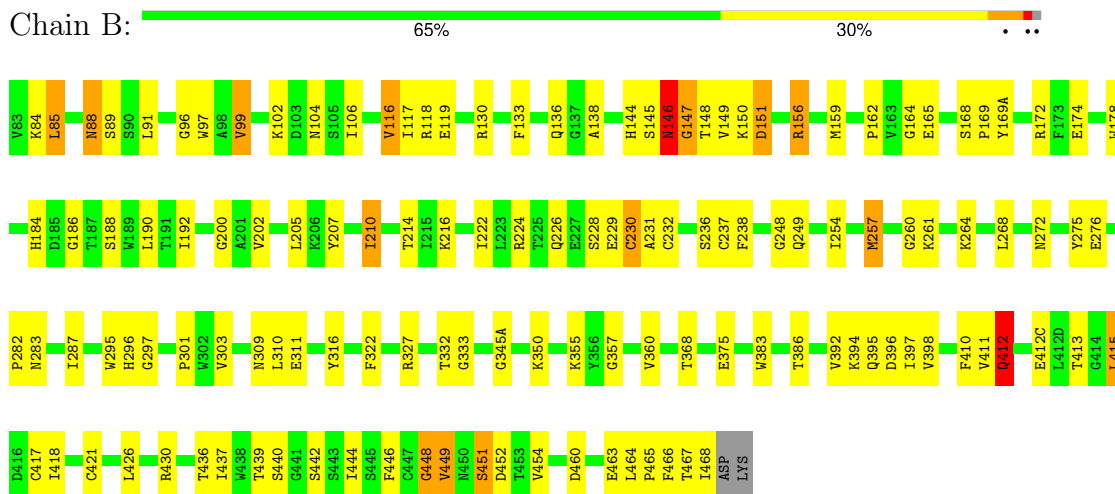
### 3 Residue-property plots

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: Neuraminidase

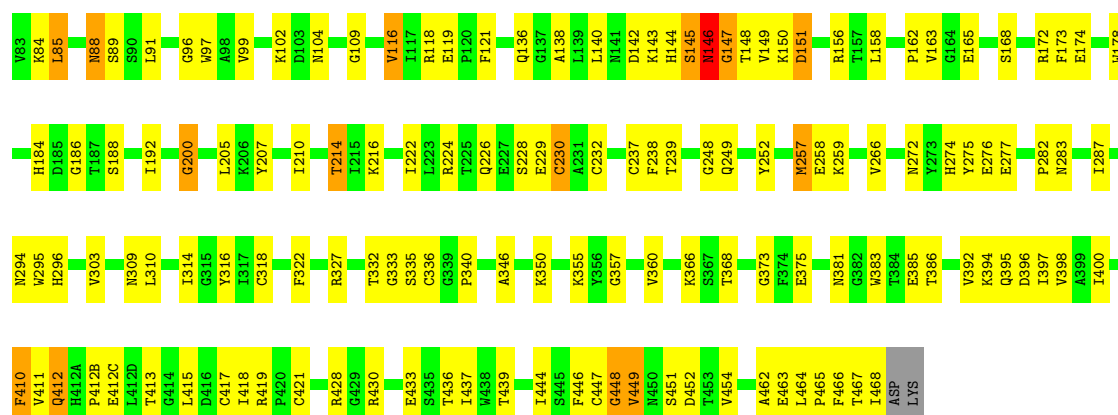


#### • Molecule 1: Neuraminidase



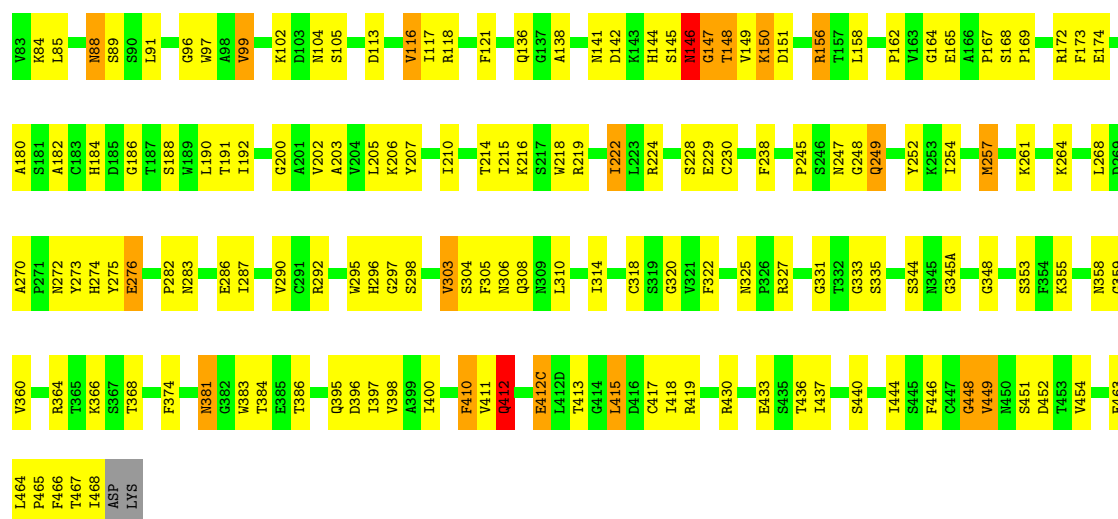
#### • Molecule 1: Neuraminidase





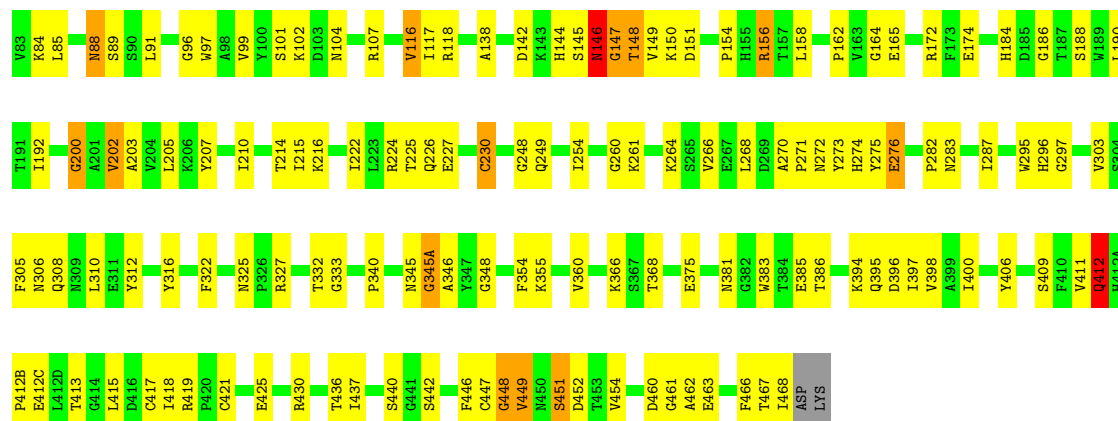
• Molecule 1: Neuraminidase

Chain D: 60% 35% 5% ..



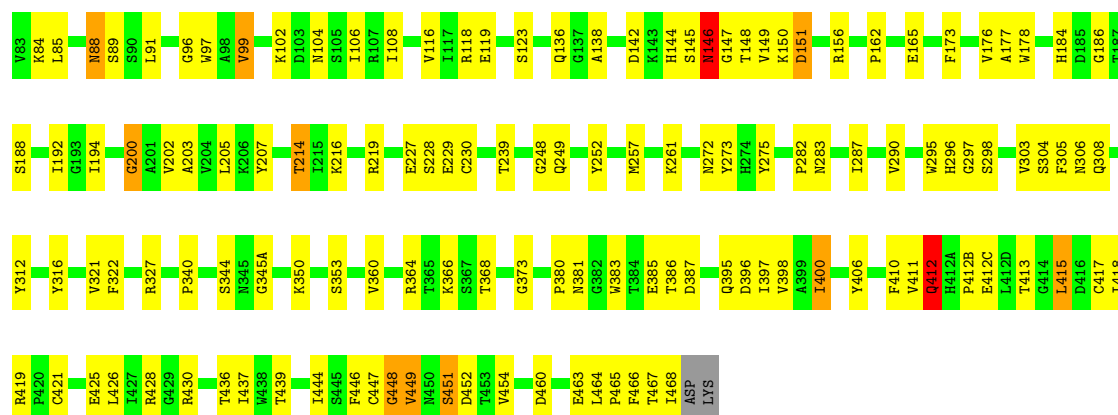
• Molecule 1: Neuraminidase

Chain E: 64% 32% ..



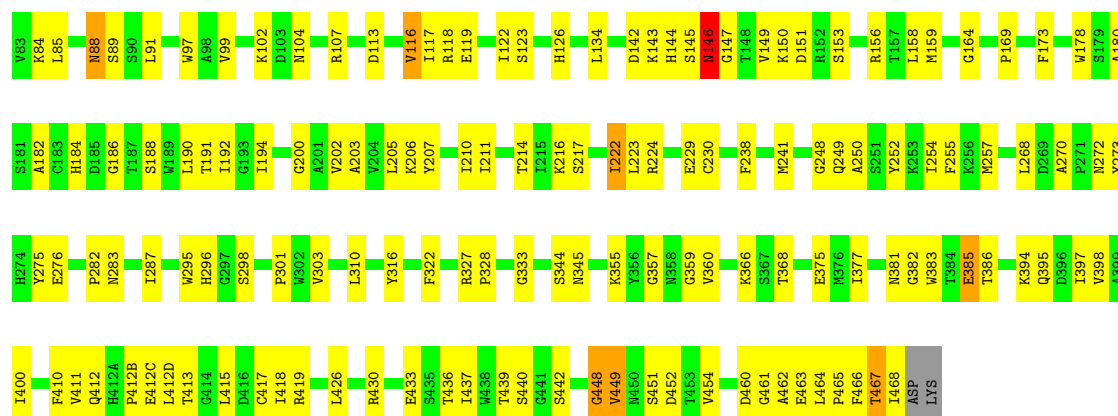
• Molecule 1: Neuraminidase

Chain F:  65% 31% ..



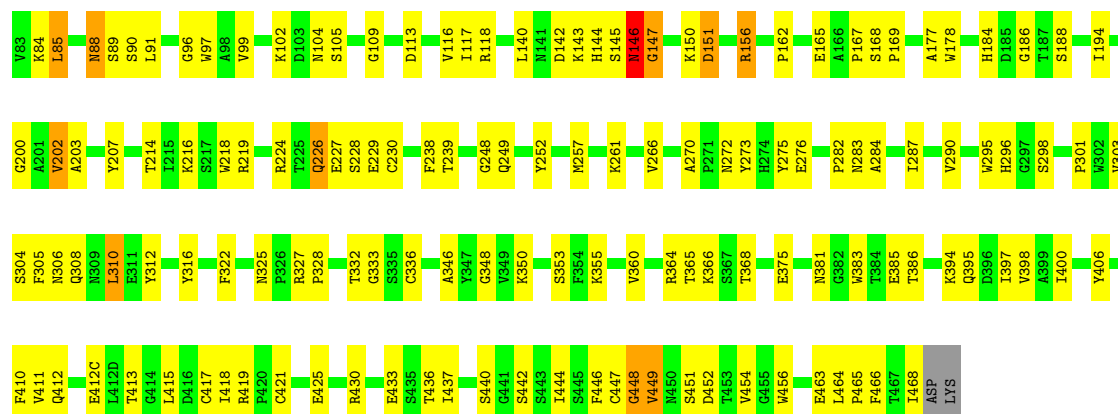
• Molecule 1: Neuraminidase

Chain G:  63% 35% ..



• Molecule 1: Neuraminidase

Chain H:  63% 34% ..





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	201.06Å 201.24Å 211.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 30.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.50) 93.0 (30.00-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.93 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.237 , 0.273 0.229 , 0.229	Depositor DCC
$R_{free}$ test set	6823 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.2	Xtriage
Anisotropy	0.602	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 0.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.079 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	23856	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.04% 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

### 5.1 Standard geometry

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

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	0.42	0/3045	0.72	0/4141
1	B	0.45	1/3045 (0.0%)	0.74	2/4141 (0.0%)
1	C	0.43	0/3045	0.74	1/4141 (0.0%)
1	D	0.47	2/3045 (0.1%)	0.77	3/4141 (0.1%)
1	E	0.47	1/3045 (0.0%)	0.72	1/4141 (0.0%)
1	F	0.48	1/3045 (0.0%)	0.73	1/4141 (0.0%)
1	G	0.42	0/3045	0.72	0/4141
1	H	0.42	0/3045	0.73	1/4141 (0.0%)
All	All	0.45	5/24360 (0.0%)	0.73	9/33128 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	412	GLN	C-N	-11.84	1.06	1.34
1	D	412	GLN	C-N	-10.38	1.10	1.34
1	E	412	GLN	C-N	-9.68	1.11	1.34
1	B	412	GLN	C-N	-9.25	1.12	1.34
1	D	410	PHE	C-N	-5.43	1.21	1.34

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	412	GLN	O-C-N	-9.63	107.29	122.70
1	D	412	GLN	CA-C-N	5.84	130.06	117.20
1	B	412	GLN	CB-CA-C	5.44	121.28	110.40
1	F	412	GLN	CB-CA-C	5.42	121.25	110.40
1	E	412	GLN	CB-CA-C	5.41	121.22	110.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	412	GLN	Mainchain
1	C	410	PHE	Mainchain
1	D	412	GLN	Mainchain
1	E	412	GLN	Mainchain
1	F	412	GLN	Mainchain

## 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	2962	0	2783	157	0
1	B	2962	0	2782	155	0
1	C	2962	0	2783	150	0
1	D	2962	0	2781	171	0
1	E	2962	0	2782	166	0
1	F	2962	0	2782	139	0
1	G	2962	0	2783	159	0
1	H	2962	0	2783	143	0
2	A	20	0	23	0	0
2	B	20	0	23	0	0
2	C	20	0	23	0	0
2	D	20	0	23	0	0
2	E	20	0	23	0	0
2	F	20	0	23	0	0
2	G	20	0	23	0	0
2	H	20	0	23	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	23856	0	22443	1126	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 24.

The worst 5 of 1126 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:G:327:ARG:O	1:G:368:THR:CG2	1.67	1.42
1:F:327:ARG:O	1:F:368:THR:CG2	1.73	1.37
1:H:327:ARG:O	1:H:368:THR:CG2	1.74	1.36
1:A:327:ARG:O	1:A:368:THR:CG2	1.71	1.35
1:B:327:ARG:O	1:B:368:THR:CG2	1.82	1.28

There are no symmetry-related clashes.

## 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	383/387 (99%)	350 (91%)	26 (7%)	7 (2%)	7	12
1	B	383/387 (99%)	347 (91%)	30 (8%)	6 (2%)	8	15
1	C	383/387 (99%)	348 (91%)	29 (8%)	6 (2%)	8	15
1	D	383/387 (99%)	347 (91%)	29 (8%)	7 (2%)	7	12
1	E	383/387 (99%)	338 (88%)	37 (10%)	8 (2%)	5	10
1	F	383/387 (99%)	344 (90%)	32 (8%)	7 (2%)	7	12
1	G	383/387 (99%)	348 (91%)	30 (8%)	5 (1%)	10	19
1	H	383/387 (99%)	345 (90%)	33 (9%)	5 (1%)	10	19
All	All	3064/3096 (99%)	2767 (90%)	246 (8%)	51 (2%)	7	14

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	B	146	ASN
1	C	146	ASN
1	C	448	GLY
1	D	146	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	329/331 (99%)	311 (94%)	18 (6%)	18	37
1	B	329/331 (99%)	316 (96%)	13 (4%)	27	51
1	C	329/331 (99%)	315 (96%)	14 (4%)	25	48
1	D	329/331 (99%)	312 (95%)	17 (5%)	19	39
1	E	329/331 (99%)	316 (96%)	13 (4%)	27	51
1	F	329/331 (99%)	318 (97%)	11 (3%)	33	59
1	G	329/331 (99%)	318 (97%)	11 (3%)	33	59
1	H	329/331 (99%)	315 (96%)	14 (4%)	25	48
All	All	2632/2648 (99%)	2521 (96%)	111 (4%)	25	49

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	296	HIS
1	H	442	SER
1	E	400	ILE
1	H	310	LEU
1	H	99	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	395	GLN
1	G	104	ASN
1	F	104	ASN
1	F	249	GLN
1	G	226	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

8 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$
2	G39	A	800	-	19,20,20	2.69	6 (31%)	20,27,27	2.10	6 (30%)
2	G39	G	806	-	19,20,20	2.70	6 (31%)	20,27,27	2.06	5 (25%)
2	G39	D	803	-	19,20,20	2.75	7 (36%)	20,27,27	2.11	7 (35%)
2	G39	E	804	-	19,20,20	2.67	8 (42%)	20,27,27	2.06	5 (25%)
2	G39	C	802	-	19,20,20	2.63	7 (36%)	20,27,27	2.09	6 (30%)
2	G39	H	807	-	19,20,20	2.81	7 (36%)	20,27,27	2.11	5 (25%)
2	G39	B	801	-	19,20,20	2.65	7 (36%)	20,27,27	2.11	5 (25%)
2	G39	F	805	-	19,20,20	2.66	7 (36%)	20,27,27	2.06	5 (25%)

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
2	G39	A	800	-	-	1/16/32/32	0/1/1/1
2	G39	G	806	-	-	4/16/32/32	0/1/1/1
2	G39	D	803	-	-	2/16/32/32	0/1/1/1
2	G39	E	804	-	-	2/16/32/32	0/1/1/1
2	G39	C	802	-	-	2/16/32/32	0/1/1/1
2	G39	H	807	-	-	1/16/32/32	0/1/1/1
2	G39	B	801	-	-	3/16/32/32	0/1/1/1
2	G39	F	805	-	-	2/16/32/32	0/1/1/1

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	807	G39	C3-C2	7.82	1.64	1.51
2	A	800	G39	C3-C2	7.68	1.64	1.51
2	D	803	G39	C3-C2	7.58	1.63	1.51
2	G	806	G39	C3-C2	7.49	1.63	1.51
2	B	801	G39	C3-C2	7.43	1.63	1.51

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	G39	C4-C3-C2	6.33	116.89	109.72
2	H	807	G39	C4-C3-C2	6.18	116.72	109.72
2	A	800	G39	C4-C3-C2	6.04	116.56	109.72
2	D	803	G39	C4-C3-C2	5.98	116.49	109.72
2	C	802	G39	C4-C3-C2	5.88	116.37	109.72

There are no chirality outliers.

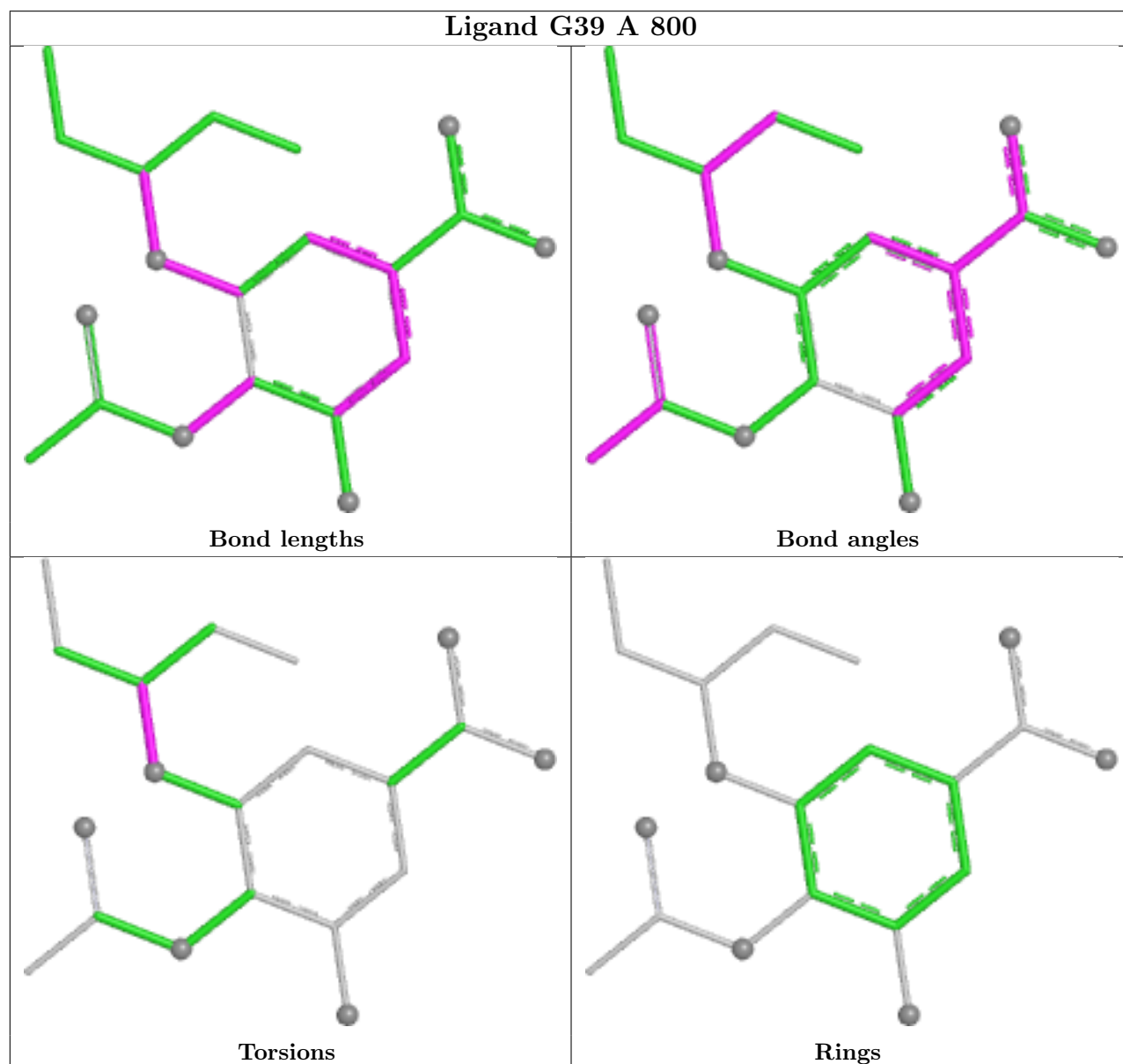
5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	G39	C9-C8-C81-C82
2	D	803	G39	C9-C8-C81-C82
2	F	805	G39	C9-C8-C81-C82
2	A	800	G39	C9-C8-O7-C6
2	B	801	G39	C9-C8-O7-C6

There are no ring outliers.

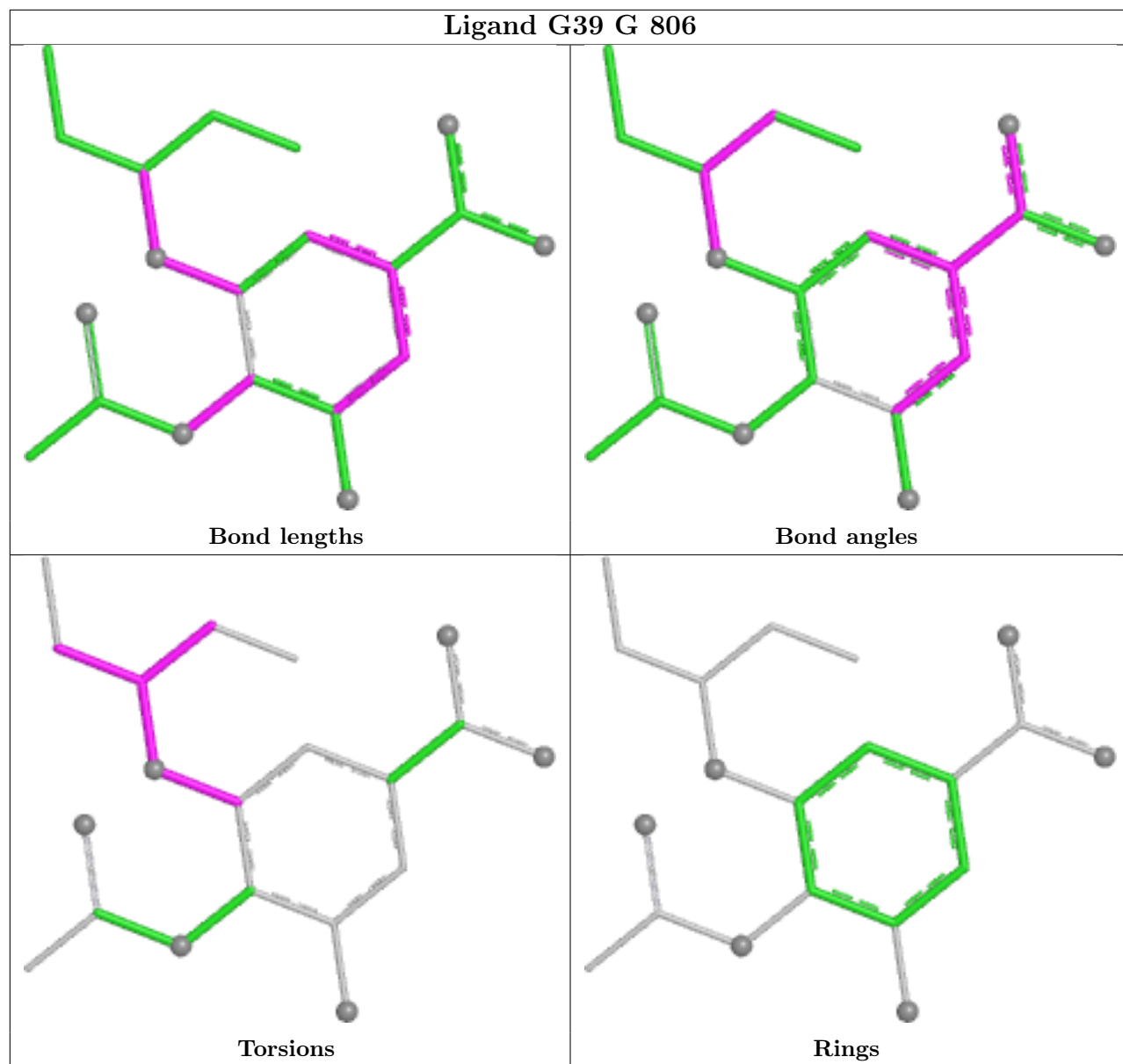
No monomer is involved in short contacts.

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.

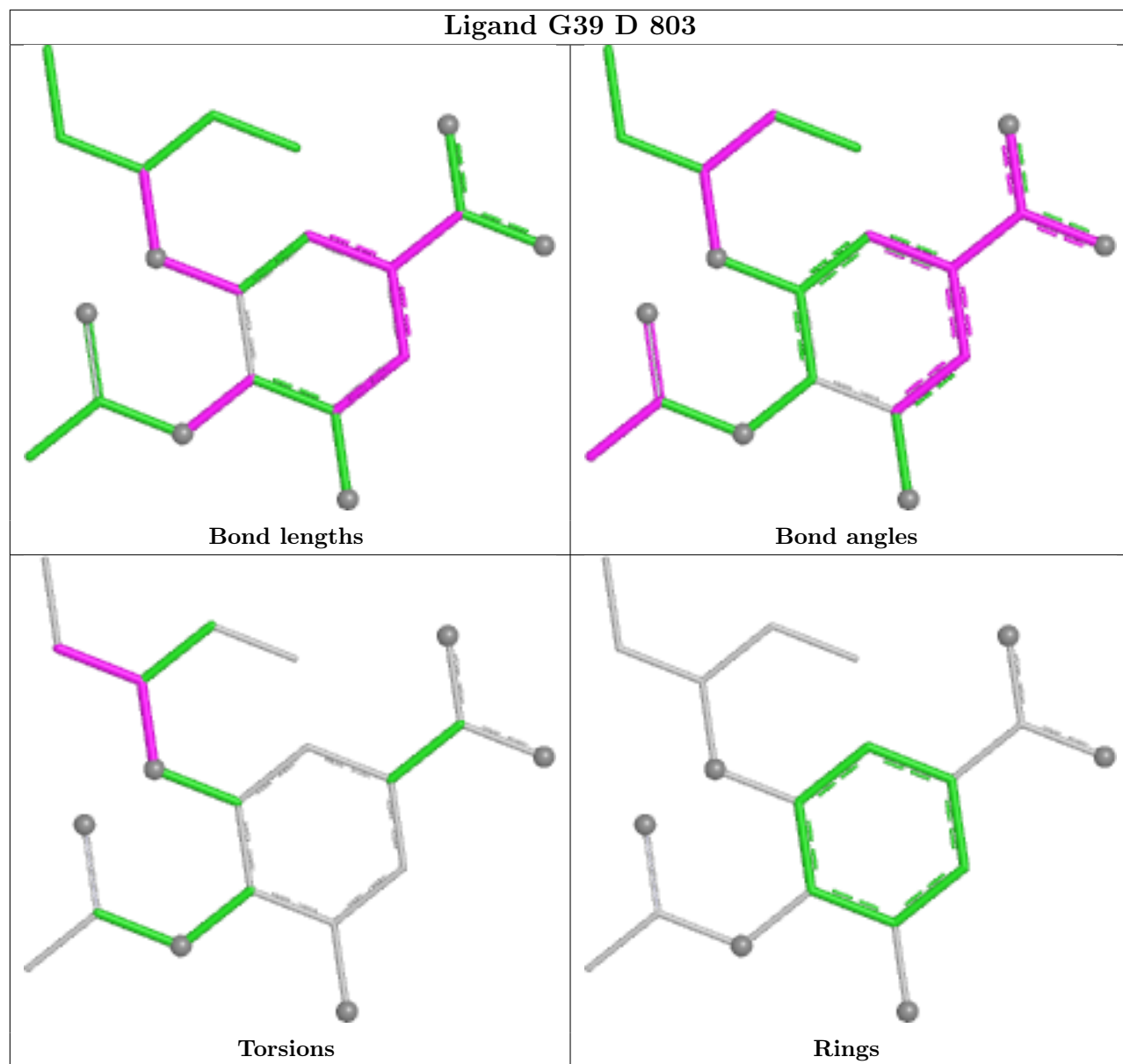




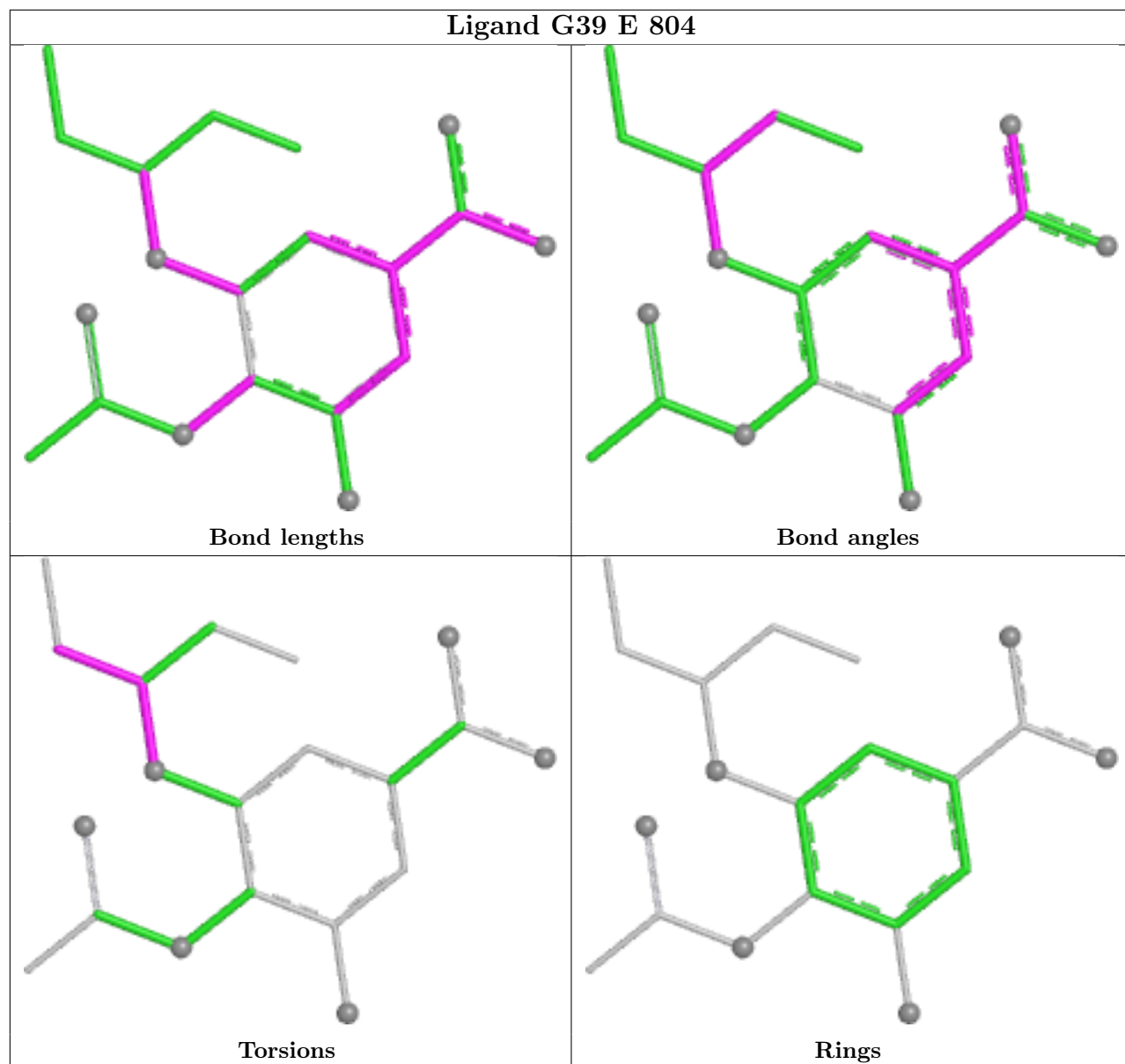
## Ligand G39 G 806



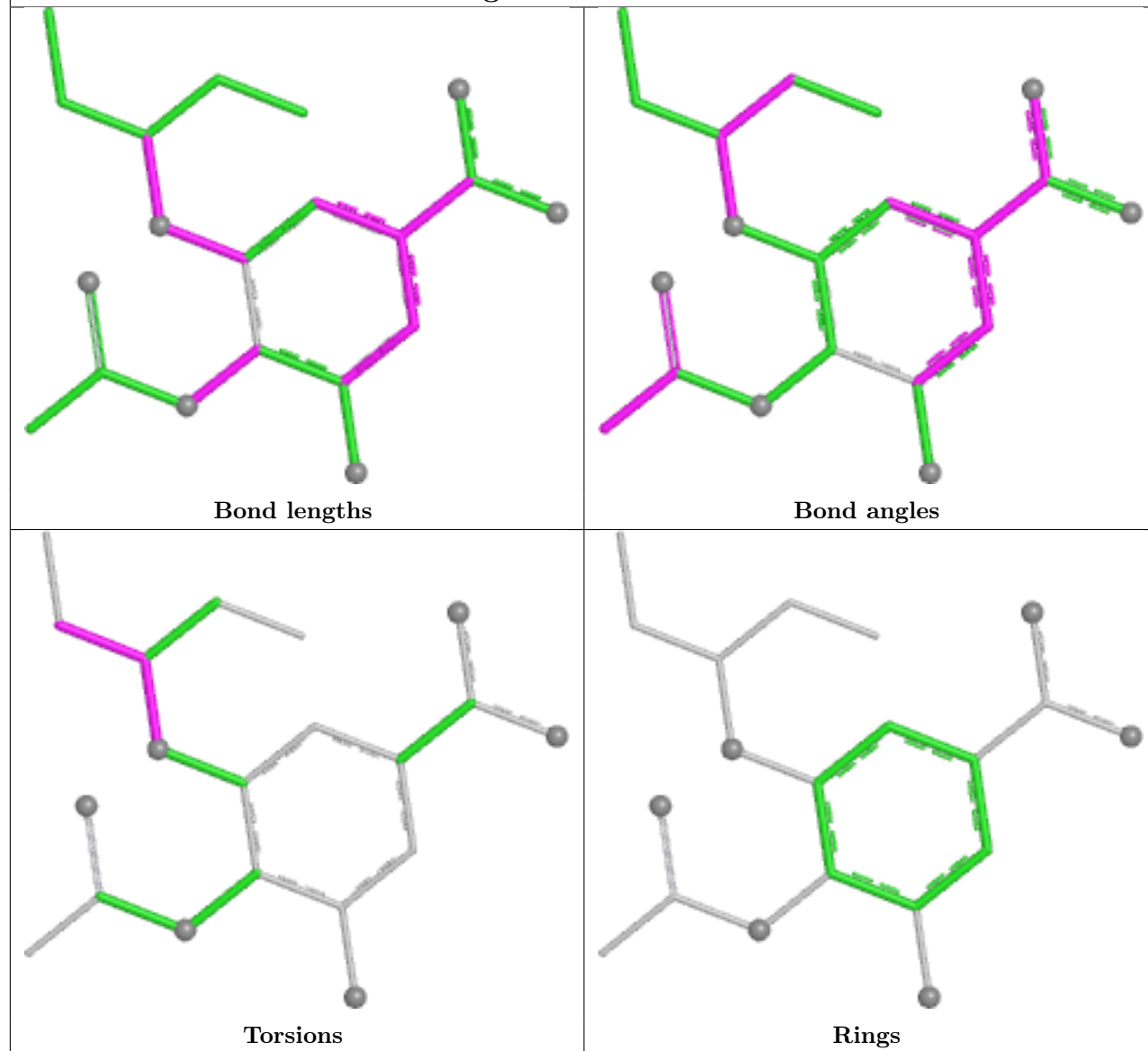
## Ligand G39 D 803



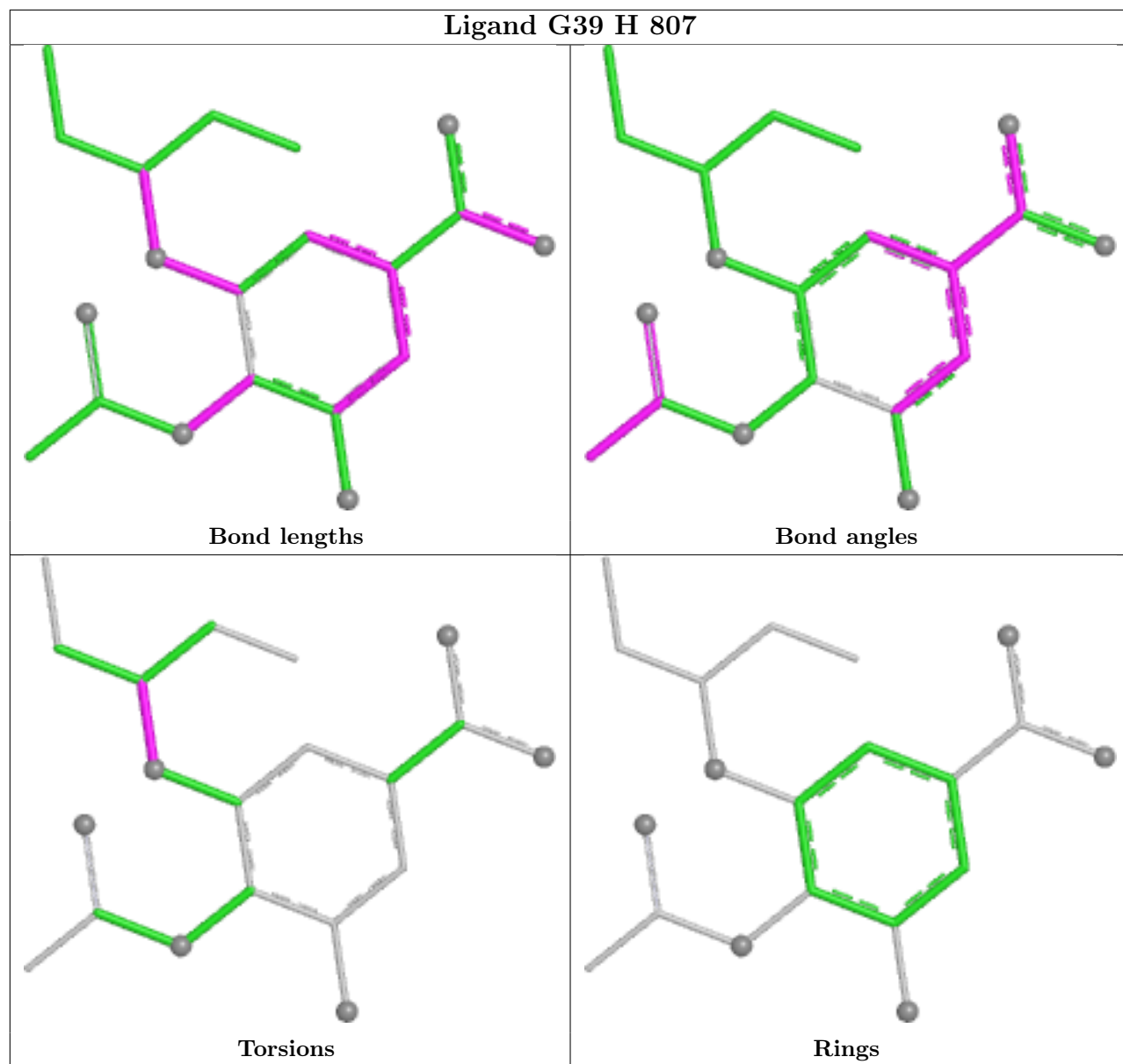
## Ligand G39 E 804



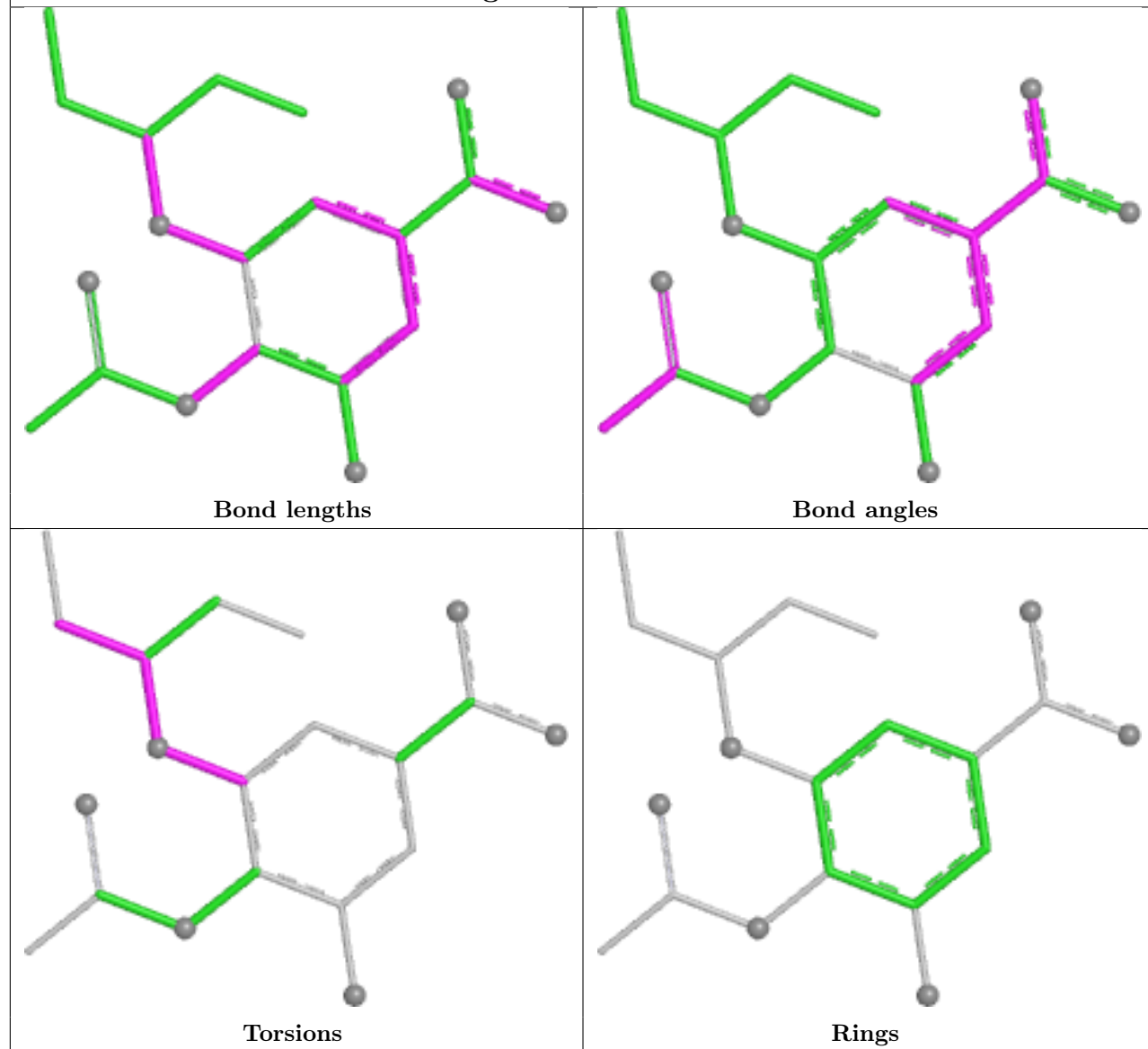
## Ligand G39 C 802

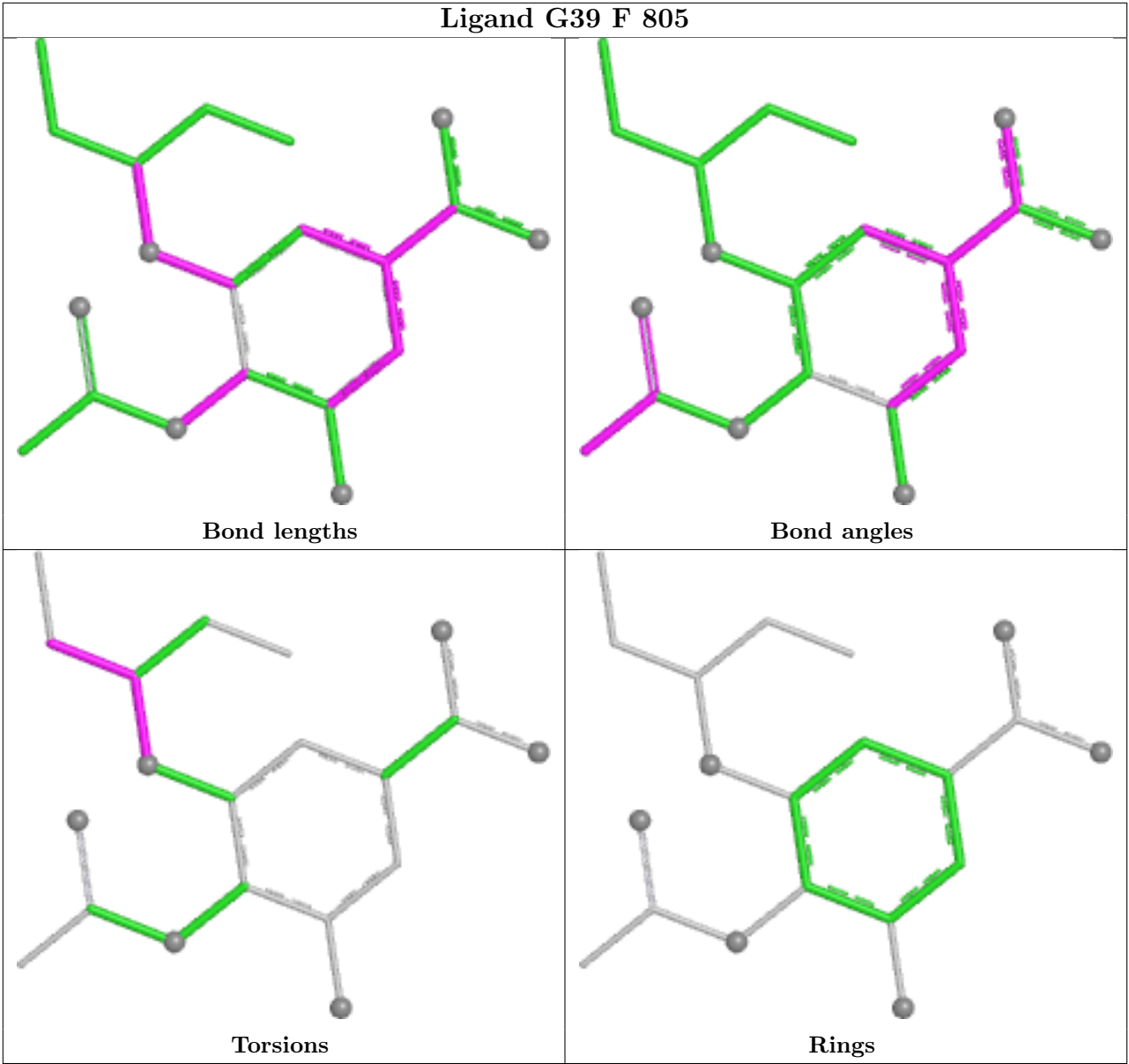


## Ligand G39 H 807



## Ligand G39 B 801





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	E	1
1	D	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Number of breaks
1	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	412:GLN	C	412(A):HIS	N	1.12
1	E	412:GLN	C	412(A):HIS	N	1.11
1	D	412:GLN	C	412(A):HIS	N	1.10
1	F	412:GLN	C	412(A):HIS	N	1.06



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	385/387 (99%)	-1.78	0 100 100	9, 18, 28, 40	0
1	B	385/387 (99%)	-1.79	0 100 100	8, 18, 28, 40	0
1	C	385/387 (99%)	-1.77	0 100 100	10, 18, 28, 41	0
1	D	385/387 (99%)	-1.79	0 100 100	10, 18, 29, 43	0
1	E	385/387 (99%)	-1.73	0 100 100	15, 24, 33, 43	0
1	F	385/387 (99%)	-1.73	0 100 100	12, 25, 35, 44	0
1	G	385/387 (99%)	-1.76	0 100 100	9, 21, 32, 43	0
1	H	385/387 (99%)	-1.74	0 100 100	14, 23, 34, 44	0
All	All	3080/3096 (99%)	-1.76	0 100 100	8, 21, 32, 44	0

There are no RSRZ outliers to report.

### 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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

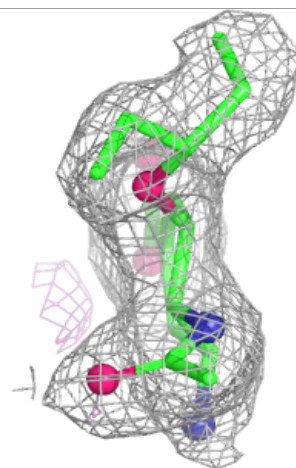
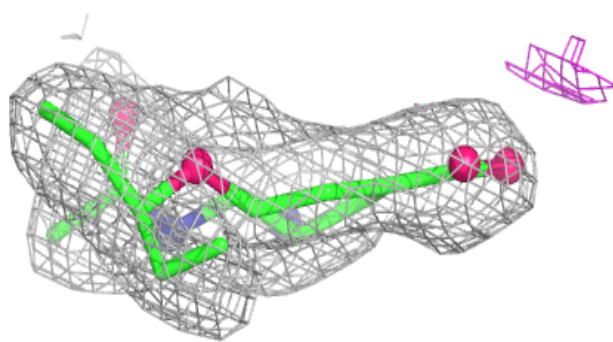
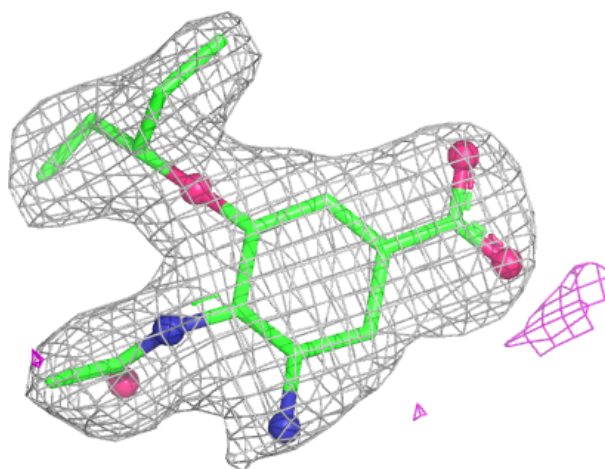
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	G39	C	802	20/20	0.99	0.03	24,26,28,31	0
2	G39	D	803	20/20	0.99	0.03	17,22,23,24	0
2	G39	E	804	20/20	0.99	0.03	21,24,26,26	0
2	G39	F	805	20/20	0.99	0.03	25,29,32,33	0
2	G39	G	806	20/20	0.99	0.02	18,21,23,23	0
2	G39	H	807	20/20	0.99	0.03	20,27,29,29	0
2	G39	A	800	20/20	1.00	0.02	20,24,26,26	0
2	G39	B	801	20/20	1.00	0.02	17,25,29,30	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.

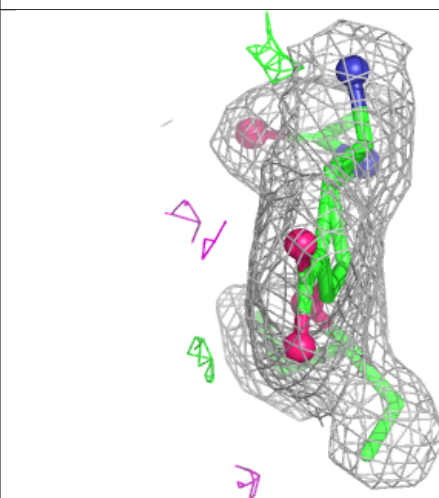
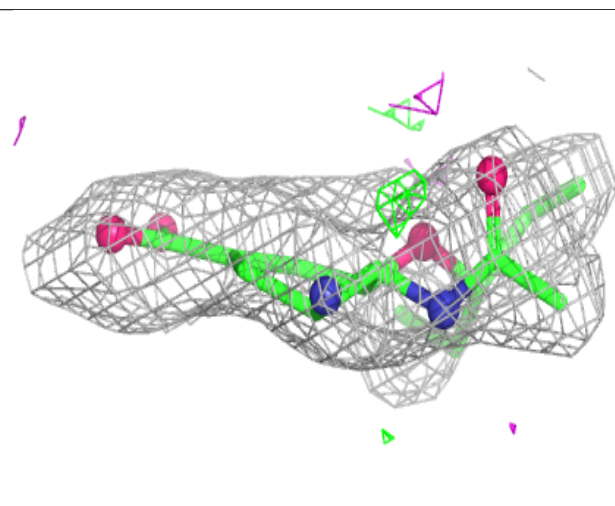
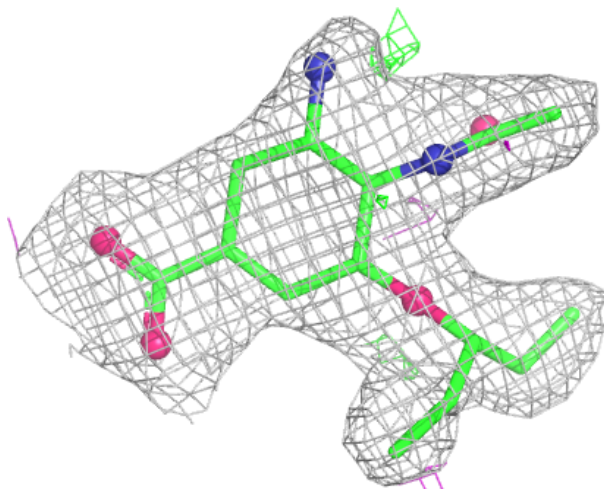
**Electron density around G39 C 802:**

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)



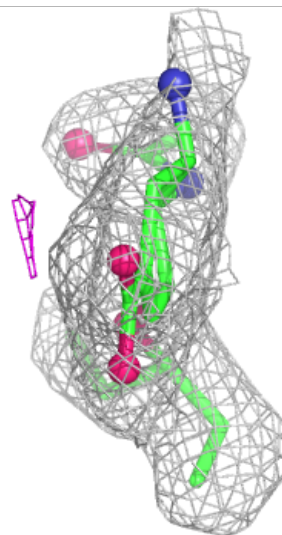
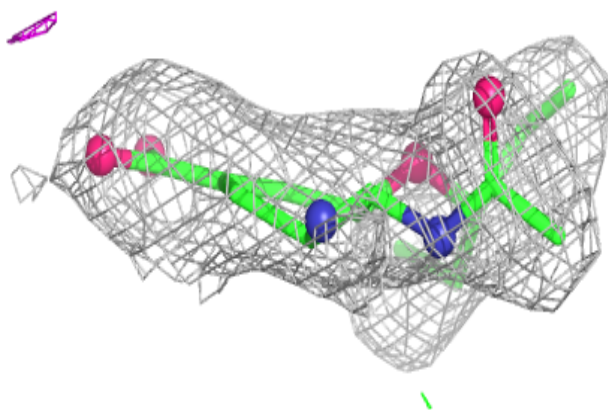
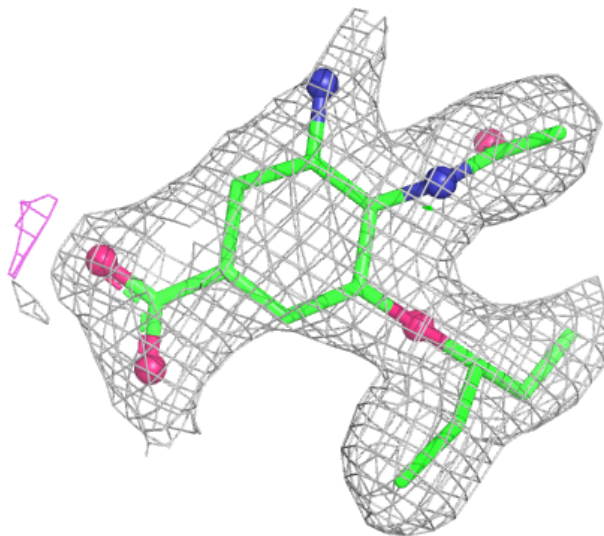
**Electron density around G39 D 803:**

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



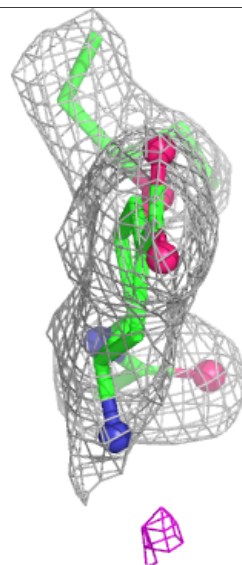
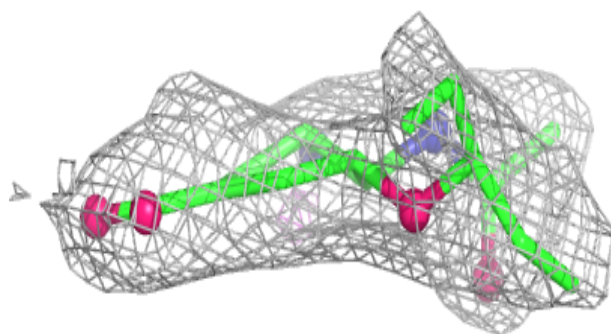
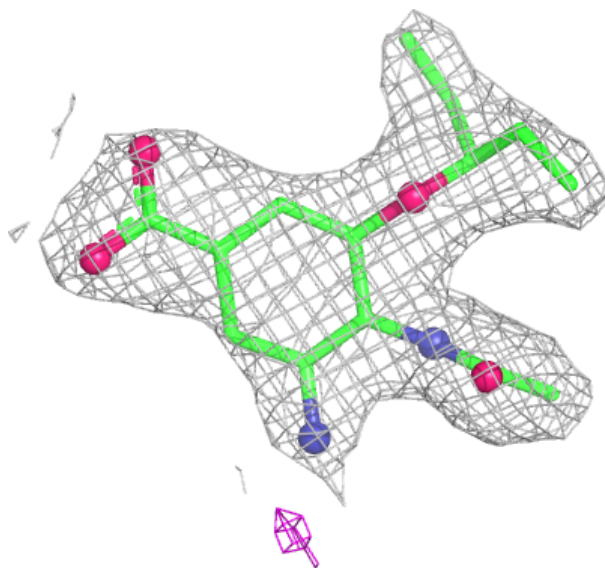
**Electron density around G39 E 804:**

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



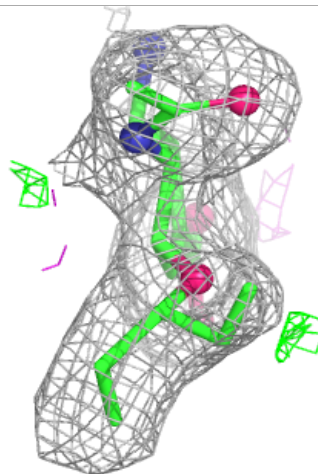
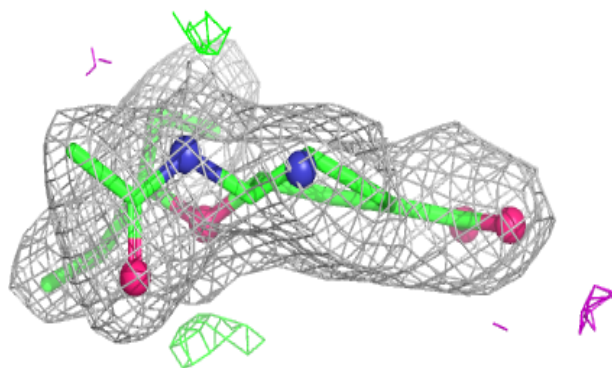
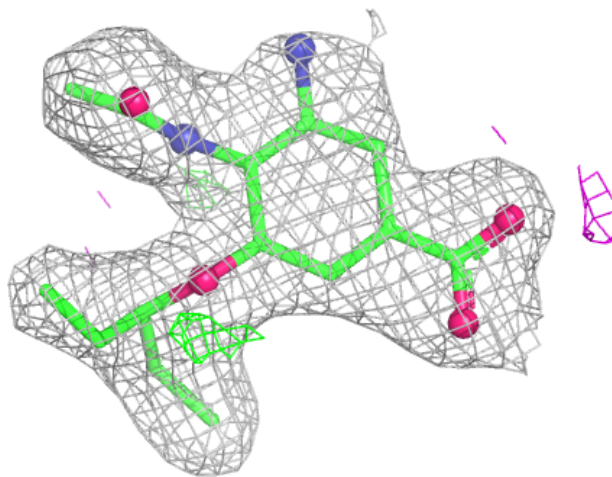
**Electron density around G39 F 805:**

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



**Electron density around G39 G 806:**

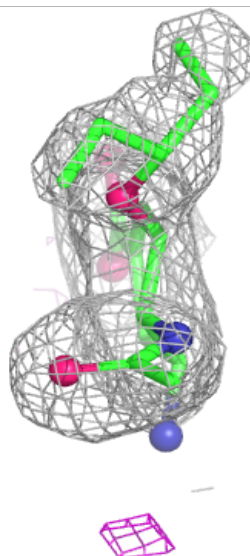
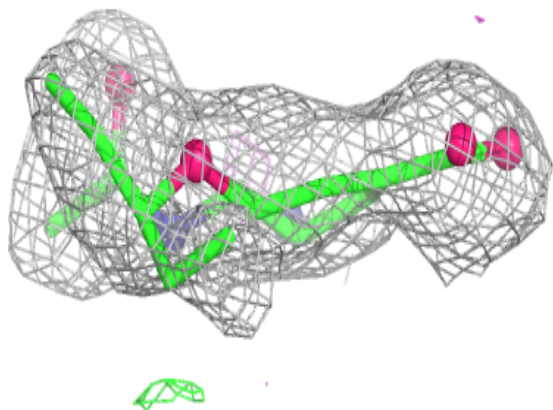
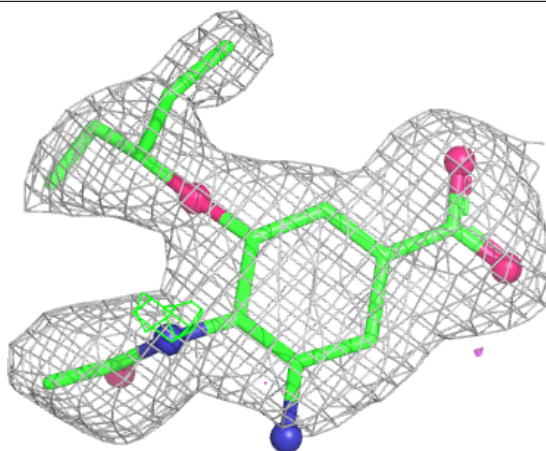
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





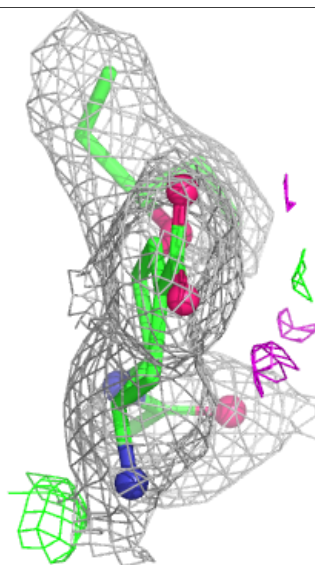
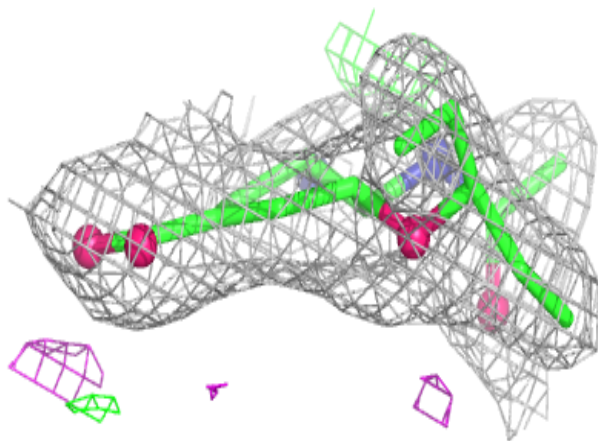
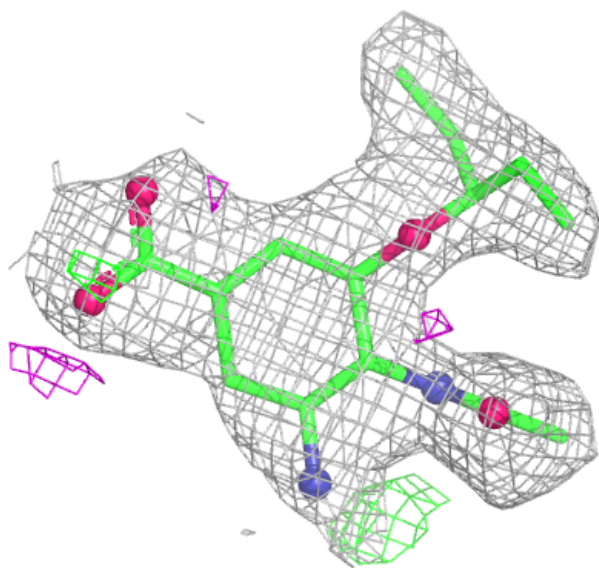
**Electron density around G39 H 807:**

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



**Electron density around G39 A 800:**

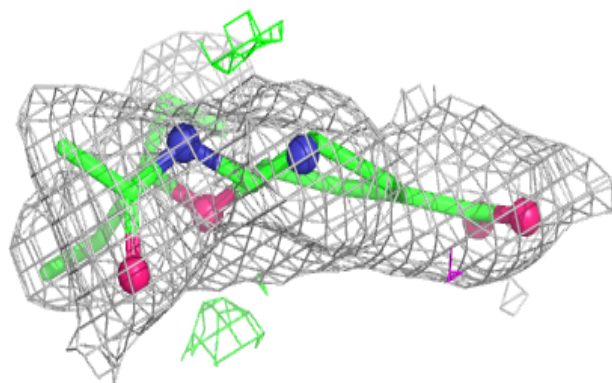
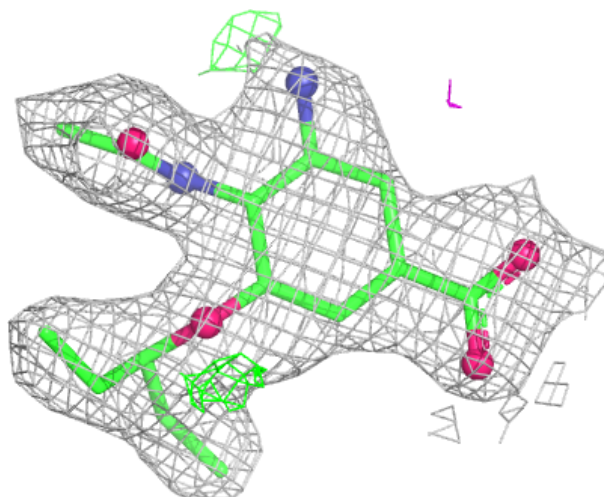
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around G39 B 801:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.