



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 22, 2025 – 02:11 PM EDT

PDB ID : 9DOY / pdb\_00009doy  
Title : Fibrillar assembly of an D-enantiopure, C-alpha methylated, macrocyclic beta-hairpin  
Authors : Samdin, T.D.; Lubkowski, J.; Anderson, C.F.; Schneider, J.P.  
Deposited on : 2024-09-20  
Resolution : 1.92 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](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)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

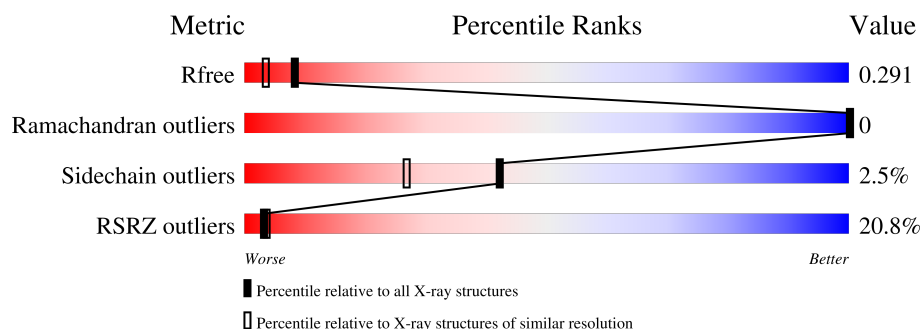
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.92 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	1028 (1.92-1.92)
Ramachandran outliers	177936	1087 (1.92-1.92)
Sidechain outliers	177891	1087 (1.92-1.92)
RSRZ outliers	164620	1028 (1.92-1.92)

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	13	
1	B	13	
1	C	13	
1	D	13	
1	E	13	
1	F	13	
1	a	13	

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Mol	Chain	Length	Quality of chain
1	b	13	
1	c	13	
1	d	13	
1	e	13	
1	f	13	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	I3C	a	102	-	X	-	-

## 2 Entry composition

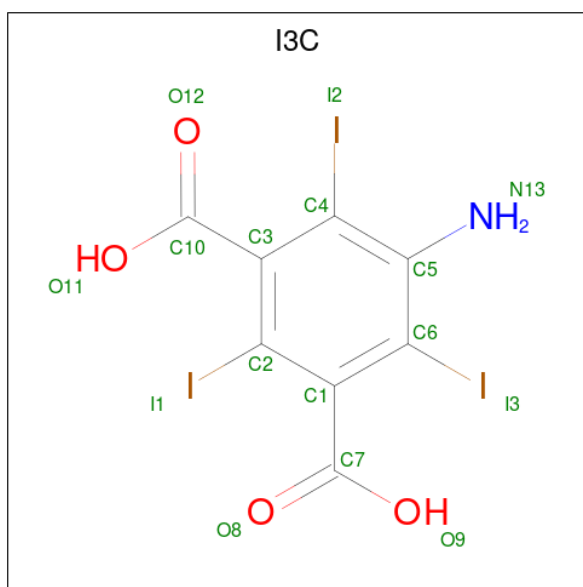
There are 3 unique types of molecules in this entry. The entry contains 1379 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-enantiopure, C-alpha methylated, macrocyclic beta-hairpin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	13	Total	C	N	O	0	0	0
			101	69	18	14			
1	a	13	Total	C	N	O	0	0	0
			101	69	18	14			
1	B	13	Total	C	N	O	0	1	0
			105	73	18	14			
1	b	13	Total	C	N	O	0	0	0
			101	69	18	14			
1	C	13	Total	C	N	O	0	0	0
			101	69	18	14			
1	c	13	Total	C	N	O	0	0	0
			101	69	18	14			
1	D	13	Total	C	N	O	0	1	0
			105	72	18	15			
1	d	13	Total	C	N	O	0	0	0
			101	69	18	14			
1	E	13	Total	C	N	O	0	1	0
			105	73	18	14			
1	e	13	Total	C	N	O	0	0	0
			101	69	18	14			
1	F	13	Total	C	N	O	0	0	0
			101	69	18	14			
1	f	13	Total	C	N	O	0	1	0
			105	73	18	14			

- Molecule 2 is 5-amino-2,4,6-triiodobenzene-1,3-dicarboxylic acid (CCD ID: I3C) (formula:  $C_8H_4I_3NO_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	a	1	Total 16	C 8	I 3	N 1	O 4	0	0
2	a	1	Total 16	C 8	I 3	N 1	O 4	0	0
2	C	1	Total 16	C 8	I 3	N 1	O 4	0	0
2	c	1	Total 16	C 8	I 3	N 1	O 4	0	0
2	D	1	Total 16	C 8	I 3	N 1	O 4	0	0
2	E	1	Total 16	C 8	I 3	N 1	O 4	0	0
2	f	1	Total 16	C 8	I 3	N 1	O 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	O	0	0
			3	3		
3	a	4	Total	O	0	0
			4	4		
3	B	4	Total	O	0	0
			4	4		
3	b	3	Total	O	0	0
			3	3		
3	C	3	Total	O	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	c	4	Total 4	O 4	0	0
3	D	3	Total 3	O 3	0	0
3	d	6	Total 6	O 6	0	0
3	E	2	Total 2	O 2	0	0
3	e	2	Total 2	O 2	0	0
3	F	4	Total 4	O 4	0	0
3	f	1	Total 1	O 1	0	0

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

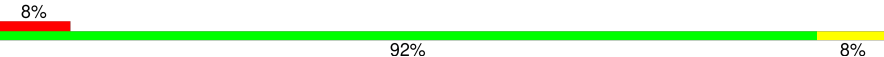
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

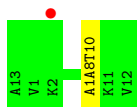
- Molecule 1: D-enantiopure, C-alpha methylated, macrocyclic beta-hairpin

Chain A: 




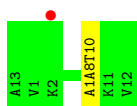
- Molecule 1: D-enantiopure, C-alpha methylated, macrocyclic beta-hairpin

Chain a: 




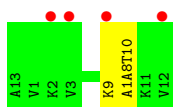
- Molecule 1: D-enantiopure, C-alpha methylated, macrocyclic beta-hairpin

Chain B: 




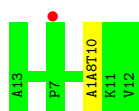
- Molecule 1: D-enantiopure, C-alpha methylated, macrocyclic beta-hairpin

Chain b: 

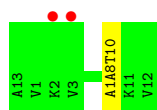
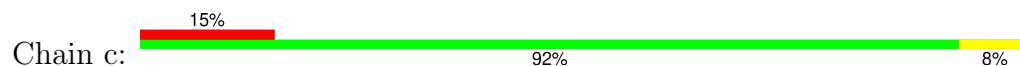


- Molecule 1: D-enantiopure, C-alpha methylated, macrocyclic beta-hairpin

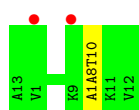
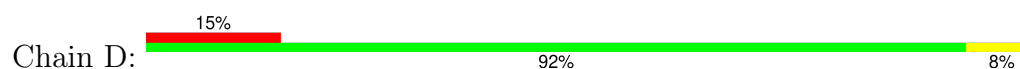
Chain C: 



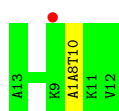
- Molecule 1: D-enantiopure, C-alpha methylated, macrocyclic beta-hairpin



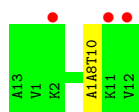
- Molecule 1: D-enantiopure, C-alpha methylated, macrocyclic beta-hairpin



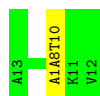
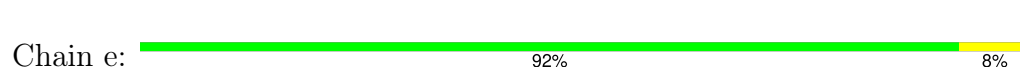
- Molecule 1: D-enantiopure, C-alpha methylated, macrocyclic beta-hairpin



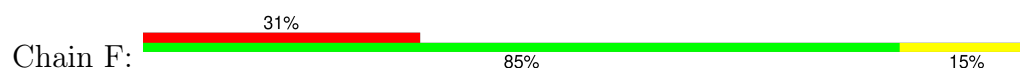
- Molecule 1: D-enantiopure, C-alpha methylated, macrocyclic beta-hairpin



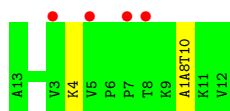
- Molecule 1: D-enantiopure, C-alpha methylated, macrocyclic beta-hairpin



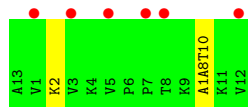
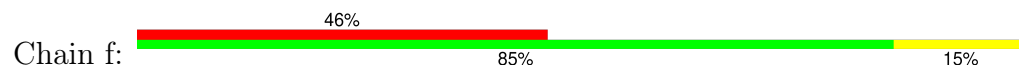
- Molecule 1: D-enantiopure, C-alpha methylated, macrocyclic beta-hairpin







- Molecule 1: D-enantiopure, C-alpha methylated, macrocyclic beta-hairpin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.48Å 57.48Å 113.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.43 – 1.92 40.43 – 1.92	Depositor EDS
% Data completeness (in resolution range)	94.0 (40.43-1.92) 94.1 (40.43-1.92)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	16.51 (at 1.92Å)	Xtrriage
Refinement program	REFMAC 5.8.0405	Depositor
R, $R_{free}$	0.246 , 0.296 0.247 , 0.291	Depositor DCC
$R_{free}$ test set	738 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.1	Xtrriage
Anisotropy	0.130	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 26.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	1379	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.96 % 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 1.4164e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: ORN, DPR, I3C, A1A8T

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	0.35	0/76	0.89	0/96
1	B	0.29	0/83	0.84	0/106
1	C	0.32	0/76	0.81	0/96
1	D	0.37	0/83	0.83	0/106
1	E	0.29	0/83	0.81	0/106
1	F	0.34	0/76	0.80	0/96
1	a	0.33	0/76	0.94	0/96
1	b	0.40	0/76	0.92	0/96
1	c	0.41	0/76	0.94	0/96
1	d	0.33	0/76	0.82	0/96
1	e	0.36	0/76	0.75	0/96
1	f	0.32	0/83	0.87	0/106
All	All	0.34	0/940	0.85	0/1192

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	9/13 (69%)	9 (100%)	0	0	100	100
1	B	10/13 (77%)	10 (100%)	0	0	100	100
1	C	9/13 (69%)	9 (100%)	0	0	100	100
1	D	10/13 (77%)	10 (100%)	0	0	100	100
1	E	10/13 (77%)	10 (100%)	0	0	100	100
1	F	9/13 (69%)	8 (89%)	1 (11%)	0	100	100
1	a	9/13 (69%)	9 (100%)	0	0	100	100
1	b	9/13 (69%)	9 (100%)	0	0	100	100
1	c	9/13 (69%)	9 (100%)	0	0	100	100
1	d	9/13 (69%)	9 (100%)	0	0	100	100
1	e	9/13 (69%)	9 (100%)	0	0	100	100
1	f	10/13 (77%)	10 (100%)	0	0	100	100
All	All	112/156 (72%)	111 (99%)	1 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	10/10 (100%)	10 (100%)	0	100	100
1	B	11/10 (110%)	11 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	10/10 (100%)	10 (100%)	0	100	100
1	D	11/10 (110%)	11 (100%)	0	100	100
1	E	11/10 (110%)	11 (100%)	0	100	100
1	F	10/10 (100%)	9 (90%)	1 (10%)	6	1
1	a	10/10 (100%)	10 (100%)	0	100	100
1	b	10/10 (100%)	9 (90%)	1 (10%)	6	1
1	c	10/10 (100%)	10 (100%)	0	100	100
1	d	10/10 (100%)	10 (100%)	0	100	100
1	e	10/10 (100%)	10 (100%)	0	100	100
1	f	11/10 (110%)	10 (91%)	1 (9%)	7	1
All	All	124/120 (103%)	121 (98%)	3 (2%)	42	28

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	b	9	LYS
1	F	4	LYS
1	f	2	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

36 non-standard protein/DNA/RNA residues 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
1	ORN	B	13	1	6,7,8	0.47	0	2,7,9	0.34	0
1	ORN	c	13	1	6,7,8	0.46	0	2,7,9	0.29	0
1	A1A8T	A	10	1	3,7,8	0.82	0	7,10,12	1.53	1 (14%)
1	ORN	E	13	1	6,7,8	0.43	0	2,7,9	0.24	0
1	A1A8T	D	10	1	3,7,8	0.71	0	7,10,12	1.51	2 (28%)
1	ORN	e	13	1	6,7,8	0.48	0	2,7,9	0.34	0
1	A1A8T	d	10	1	3,7,8	0.64	0	7,10,12	1.42	1 (14%)
1	A1A8T	f	10	1	3,7,8	0.45	0	7,10,12	1.18	1 (14%)
1	A1A8T	b	10	1	3,7,8	0.76	0	7,10,12	1.86	1 (14%)
1	ORN	f	13	1	6,7,8	0.40	0	2,7,9	0.12	0
1	A1A8T	B	10	1	3,7,8	0.63	0	7,10,12	2.45	3 (42%)
1	ORN	D	13	1	6,7,8	0.40	0	2,7,9	0.07	0
1	A1A8T	a	10	1	3,7,8	0.38	0	7,10,12	1.86	1 (14%)
1	A1A8T	C	10	1	3,7,8	0.63	0	7,10,12	1.25	1 (14%)
1	A1A8T	c	10	1	3,7,8	0.50	0	7,10,12	1.54	1 (14%)
1	ORN	A	13	1	6,7,8	0.44	0	2,7,9	0.19	0
1	A1A8T	E	10	1	3,7,8	0.73	0	7,10,12	1.39	1 (14%)
1	A1A8T	F	10	1	3,7,8	0.37	0	7,10,12	1.76	1 (14%)
1	ORN	d	13	1	6,7,8	0.43	0	2,7,9	0.14	0
1	ORN	b	13	1	6,7,8	0.36	0	2,7,9	0.21	0
1	ORN	F	13	1	6,7,8	0.39	0	2,7,9	0.15	0
1	A1A8T	e	10	1	3,7,8	0.66	0	7,10,12	1.60	1 (14%)
1	ORN	a	13	1	6,7,8	0.41	0	2,7,9	0.27	0
1	ORN	C	13	1	6,7,8	0.45	0	2,7,9	0.07	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
1	ORN	B	13	1	-	0/5/6/8	-
1	ORN	c	13	1	-	0/5/6/8	-
1	A1A8T	A	10	1	-	0/5/9/12	-
1	ORN	E	13	1	-	0/5/6/8	-
1	A1A8T	D	10	1	-	0/5/9/12	-
1	ORN	e	13	1	-	0/5/6/8	-
1	A1A8T	d	10	1	-	0/5/9/12	-
1	A1A8T	f	10	1	-	0/5/9/12	-
1	A1A8T	b	10	1	-	0/5/9/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	ORN	f	13	1	-	0/5/6/8	-
1	A1A8T	B	10	1	-	0/5/9/12	-
1	ORN	D	13	1	-	0/5/6/8	-
1	A1A8T	a	10	1	-	0/5/9/12	-
1	A1A8T	C	10	1	-	1/5/9/12	-
1	A1A8T	c	10	1	-	0/5/9/12	-
1	ORN	A	13	1	-	0/5/6/8	-
1	A1A8T	E	10	1	-	0/5/9/12	-
1	A1A8T	F	10	1	-	1/5/9/12	-
1	ORN	d	13	1	-	0/5/6/8	-
1	ORN	b	13	1	-	0/5/6/8	-
1	ORN	F	13	1	-	0/5/6/8	-
1	A1A8T	e	10	1	-	0/5/9/12	-
1	ORN	a	13	1	-	0/5/6/8	-
1	ORN	C	13	1	-	0/5/6/8	-

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	10	A1A8T	O-C-CA	-4.44	118.78	125.36
1	b	10	A1A8T	O-C-CA	-4.39	118.86	125.36
1	F	10	A1A8T	O-C-CA	-4.32	118.97	125.36
1	B	10	A1A8T	C1-CA-CB	4.29	119.86	112.12
1	B	10	A1A8T	O-C-CA	-3.80	119.73	125.36
1	e	10	A1A8T	O-C-CA	-3.79	119.75	125.36
1	c	10	A1A8T	O-C-CA	-3.75	119.80	125.36
1	E	10	A1A8T	O-C-CA	-3.50	120.17	125.36
1	A	10	A1A8T	O-C-CA	-3.37	120.37	125.36
1	C	10	A1A8T	O-C-CA	-3.16	120.68	125.36
1	D	10	A1A8T	O-C-CA	-3.01	120.90	125.36
1	f	10	A1A8T	O-C-CA	-2.93	121.03	125.36
1	d	10	A1A8T	O-C-CA	-2.74	121.30	125.36
1	B	10	A1A8T	C1-CA-C	-2.24	100.61	109.05
1	D	10	A1A8T	C1-CA-N	2.05	114.06	109.28

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	F	10	A1A8T	O-C-CA-C1

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Mol	Chain	Res	Type	Atoms
1	C	10	A1A8T	O-C-CA-C1

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

7 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	I3C	a	102	-	16,16,16	3.38	7 (43%)	24,24,24	6.59	17 (70%)
2	I3C	a	101	-	16,16,16	1.66	4 (25%)	24,24,24	3.54	8 (33%)
2	I3C	c	101	-	16,16,16	2.03	6 (37%)	24,24,24	4.20	13 (54%)
2	I3C	C	101	-	16,16,16	1.77	3 (18%)	24,24,24	3.24	10 (41%)
2	I3C	f	101	-	16,16,16	1.59	1 (6%)	24,24,24	3.57	11 (45%)
2	I3C	D	101	-	16,16,16	1.37	3 (18%)	24,24,24	3.59	8 (33%)
2	I3C	E	101	-	16,16,16	1.53	4 (25%)	24,24,24	4.48	13 (54%)

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	I3C	a	102	-	-	4/8/8/8	0/1/1/1
2	I3C	a	101	-	-	0/8/8/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	I3C	c	101	-	-	0/8/8/8	0/1/1/1
2	I3C	C	101	-	-	0/8/8/8	0/1/1/1
2	I3C	f	101	-	-	4/8/8/8	0/1/1/1
2	I3C	D	101	-	-	0/8/8/8	0/1/1/1
2	I3C	E	101	-	-	0/8/8/8	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	a	102	I3C	C6-I3	8.42	2.25	2.09
2	C	101	I3C	C6-I3	4.85	2.18	2.09
2	f	101	I3C	C6-I3	4.81	2.18	2.09
2	a	102	I3C	C1-C6	4.58	1.46	1.39
2	a	102	I3C	C1-C2	4.34	1.46	1.39
2	a	102	I3C	C5-C4	4.29	1.46	1.41
2	a	102	I3C	C4-I2	4.16	2.17	2.09
2	a	102	I3C	C5-C6	4.16	1.46	1.41
2	a	101	I3C	C4-I2	3.88	2.16	2.09
2	c	101	I3C	C2-I1	3.64	2.16	2.09
2	c	101	I3C	C4-I2	3.50	2.16	2.09
2	c	101	I3C	C6-I3	3.34	2.15	2.09
2	c	101	I3C	O9-C7	-3.30	1.20	1.30
2	a	102	I3C	C2-I1	3.27	2.15	2.09
2	E	101	I3C	C6-I3	3.00	2.15	2.09
2	D	101	I3C	C2-I1	2.70	2.14	2.09
2	c	101	I3C	O11-C10	-2.66	1.22	1.30
2	a	101	I3C	C5-C4	-2.57	1.37	1.41
2	E	101	I3C	C4-I2	2.51	2.14	2.09
2	C	101	I3C	C2-I1	2.35	2.14	2.09
2	E	101	I3C	C2-I1	2.33	2.14	2.09
2	D	101	I3C	C4-I2	2.27	2.14	2.09
2	D	101	I3C	O9-C7	-2.23	1.23	1.30
2	a	101	I3C	O9-C7	-2.13	1.24	1.30
2	E	101	I3C	O11-C10	-2.09	1.24	1.30
2	C	101	I3C	O9-C7	-2.08	1.24	1.30
2	c	101	I3C	O12-C10	2.04	1.28	1.22
2	a	101	I3C	C5-C6	2.01	1.43	1.41

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	a	102	I3C	C1-C6-C5	-17.00	109.35	122.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	a	102	I3C	C4-C5-C6	13.27	128.12	116.39
2	a	102	I3C	C5-C4-I2	11.89	129.48	118.47
2	E	101	I3C	C4-C5-N13	-11.00	112.70	121.76
2	f	101	I3C	C1-C6-C5	-10.53	114.26	122.27
2	c	101	I3C	C4-C5-C6	10.29	125.49	116.39
2	c	101	I3C	C3-C4-C5	-10.28	114.46	122.27
2	E	101	I3C	C1-C6-C5	-10.25	114.48	122.27
2	D	101	I3C	C4-C5-N13	-9.35	114.07	121.76
2	E	101	I3C	C4-C5-C6	9.34	124.65	116.39
2	a	101	I3C	C1-C6-C5	-9.17	115.30	122.27
2	a	101	I3C	C4-C5-N13	-8.56	114.71	121.76
2	a	102	I3C	C1-C2-I1	8.43	131.15	119.18
2	D	101	I3C	C4-C5-C6	8.22	123.66	116.39
2	a	101	I3C	C4-C5-C6	8.17	123.61	116.39
2	f	101	I3C	C4-C5-C6	8.07	123.53	116.39
2	D	101	I3C	C1-C6-C5	-8.04	116.16	122.27
2	a	102	I3C	C3-C4-C5	-7.92	116.25	122.27
2	C	101	I3C	C1-C6-C5	-7.68	116.43	122.27
2	a	102	I3C	C6-C5-N13	-7.54	115.55	121.76
2	c	101	I3C	C6-C5-N13	-7.51	115.58	121.76
2	a	102	I3C	C3-C2-I1	-7.44	108.60	119.18
2	c	101	I3C	C1-C6-C5	-7.25	116.76	122.27
2	E	101	I3C	C5-C6-I3	7.12	125.06	118.47
2	C	101	I3C	C6-C5-N13	-6.66	116.28	121.76
2	a	102	I3C	C4-C5-N13	-6.61	116.32	121.76
2	C	101	I3C	C4-C5-C6	6.31	121.97	116.39
2	a	102	I3C	C1-C6-I3	5.76	127.36	119.18
2	D	101	I3C	C3-C4-C5	-5.57	118.03	122.27
2	E	101	I3C	C3-C4-C5	-5.53	118.07	122.27
2	C	101	I3C	C1-C6-I3	5.50	126.99	119.18
2	D	101	I3C	C5-C6-I3	5.34	123.41	118.47
2	a	102	I3C	C5-C6-I3	5.21	123.29	118.47
2	f	101	I3C	C5-C6-I3	5.08	123.17	118.47
2	C	101	I3C	C2-C1-C7	-4.95	115.59	120.30
2	c	101	I3C	C5-C4-I2	4.88	122.98	118.47
2	E	101	I3C	C3-C4-I2	4.68	125.82	119.18
2	f	101	I3C	C6-C5-N13	-4.42	118.13	121.76
2	a	102	I3C	C2-C1-C7	-4.37	116.14	120.30
2	a	101	I3C	C3-C4-C5	-4.32	118.99	122.27
2	a	101	I3C	C5-C6-I3	4.24	122.39	118.47
2	f	101	I3C	C4-C5-N13	-4.19	118.31	121.76
2	c	101	I3C	C1-C6-I3	4.16	125.08	119.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	a	102	I3C	C2-C1-C6	4.04	124.27	119.01
2	f	101	I3C	C6-C1-C7	-3.87	116.62	120.30
2	a	101	I3C	C3-C4-I2	3.71	124.45	119.18
2	a	102	I3C	C2-C3-C10	-3.70	116.78	120.30
2	E	101	I3C	C2-C1-C7	-3.57	116.90	120.30
2	c	101	I3C	C4-C5-N13	-3.54	118.85	121.76
2	C	101	I3C	C5-C4-I2	3.49	121.70	118.47
2	a	102	I3C	C3-C4-I2	-3.46	114.26	119.18
2	C	101	I3C	C3-C4-C5	-3.32	119.75	122.27
2	C	101	I3C	C2-C1-C6	3.14	123.09	119.01
2	f	101	I3C	O11-C10-O12	-3.14	116.61	123.35
2	c	101	I3C	O9-C7-C1	3.02	123.17	114.67
2	f	101	I3C	C2-C1-C6	2.87	122.75	119.01
2	c	101	I3C	C2-C3-C4	2.72	122.55	119.01
2	E	101	I3C	O9-C7-C1	2.64	122.11	114.67
2	c	101	I3C	C4-C3-C10	-2.64	117.79	120.30
2	E	101	I3C	C5-C4-I2	-2.57	116.09	118.47
2	D	101	I3C	C2-C1-C7	-2.52	117.90	120.30
2	E	101	I3C	C2-C1-C6	2.50	122.26	119.01
2	E	101	I3C	C2-C3-C10	-2.44	117.98	120.30
2	f	101	I3C	O11-C10-C3	2.39	121.40	114.67
2	f	101	I3C	C1-C6-I3	2.39	122.57	119.18
2	c	101	I3C	C3-C4-I2	2.38	122.56	119.18
2	D	101	I3C	C3-C4-I2	2.37	122.55	119.18
2	a	102	I3C	O11-C10-C3	2.35	121.29	114.67
2	a	102	I3C	O9-C7-C1	2.29	121.11	114.67
2	a	101	I3C	C1-C6-I3	2.20	122.31	119.18
2	c	101	I3C	C1-C2-I1	2.20	122.30	119.18
2	c	101	I3C	O9-C7-O8	-2.19	118.64	123.35
2	E	101	I3C	C3-C2-I1	2.18	122.27	119.18
2	f	101	I3C	C3-C4-C5	-2.16	120.63	122.27
2	C	101	I3C	O9-C7-C1	2.15	120.72	114.67
2	a	102	I3C	C2-C3-C4	2.12	121.77	119.01
2	E	101	I3C	C4-C3-C10	2.09	122.29	120.30
2	a	101	I3C	C5-C4-I2	-2.06	116.56	118.47
2	C	101	I3C	C5-C6-I3	-2.05	116.57	118.47
2	D	101	I3C	O12-C10-C3	-2.03	116.32	121.18

There are no chirality outliers.

All (8) torsion outliers are listed below:

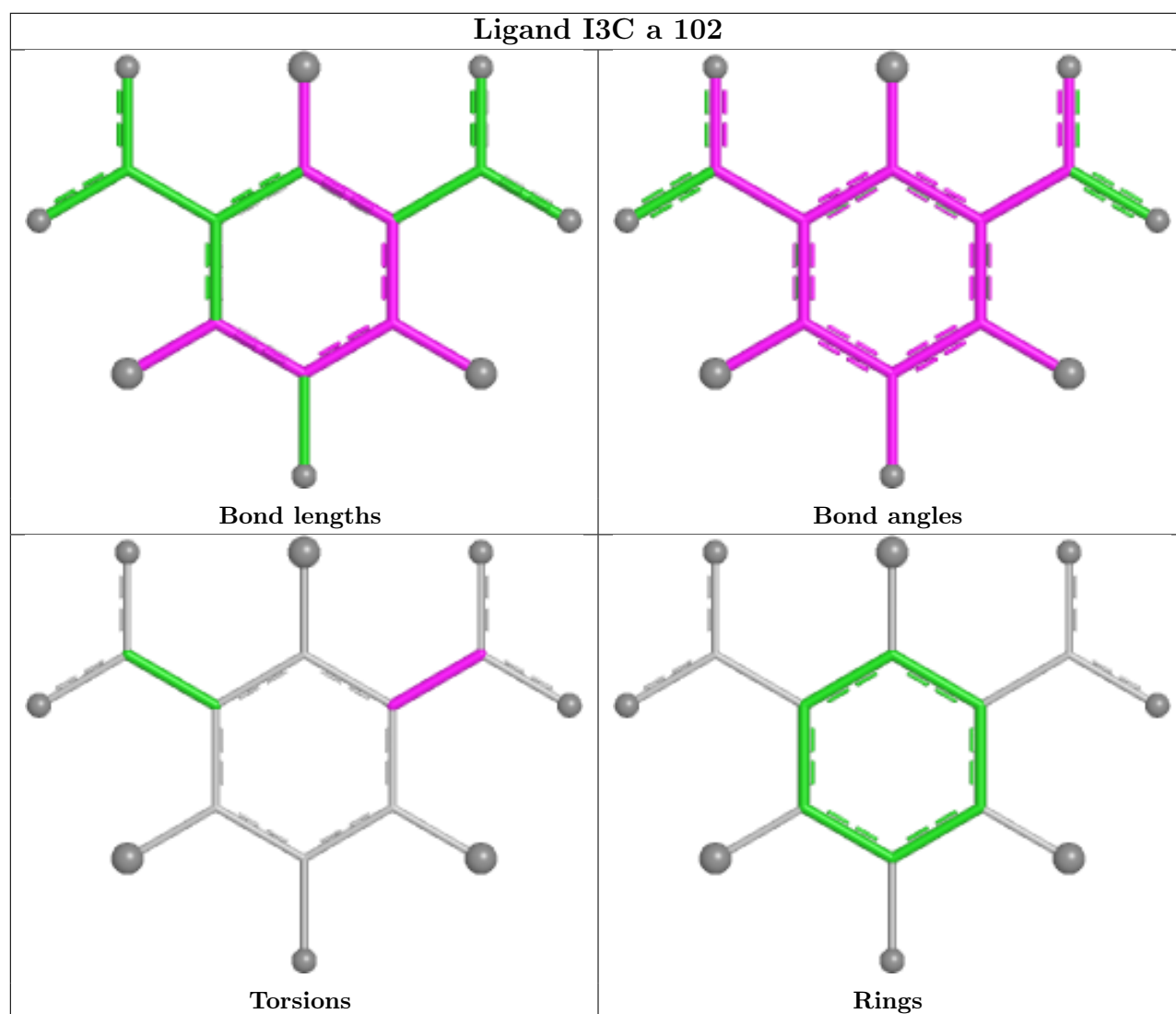
Mol	Chain	Res	Type	Atoms
2	f	101	I3C	O11-C10-C3-C4
2	f	101	I3C	O11-C10-C3-C2
2	f	101	I3C	O12-C10-C3-C4
2	f	101	I3C	O12-C10-C3-C2
2	a	102	I3C	C6-C1-C7-O8
2	a	102	I3C	C2-C1-C7-O9
2	a	102	I3C	C2-C1-C7-O8
2	a	102	I3C	C6-C1-C7-O9

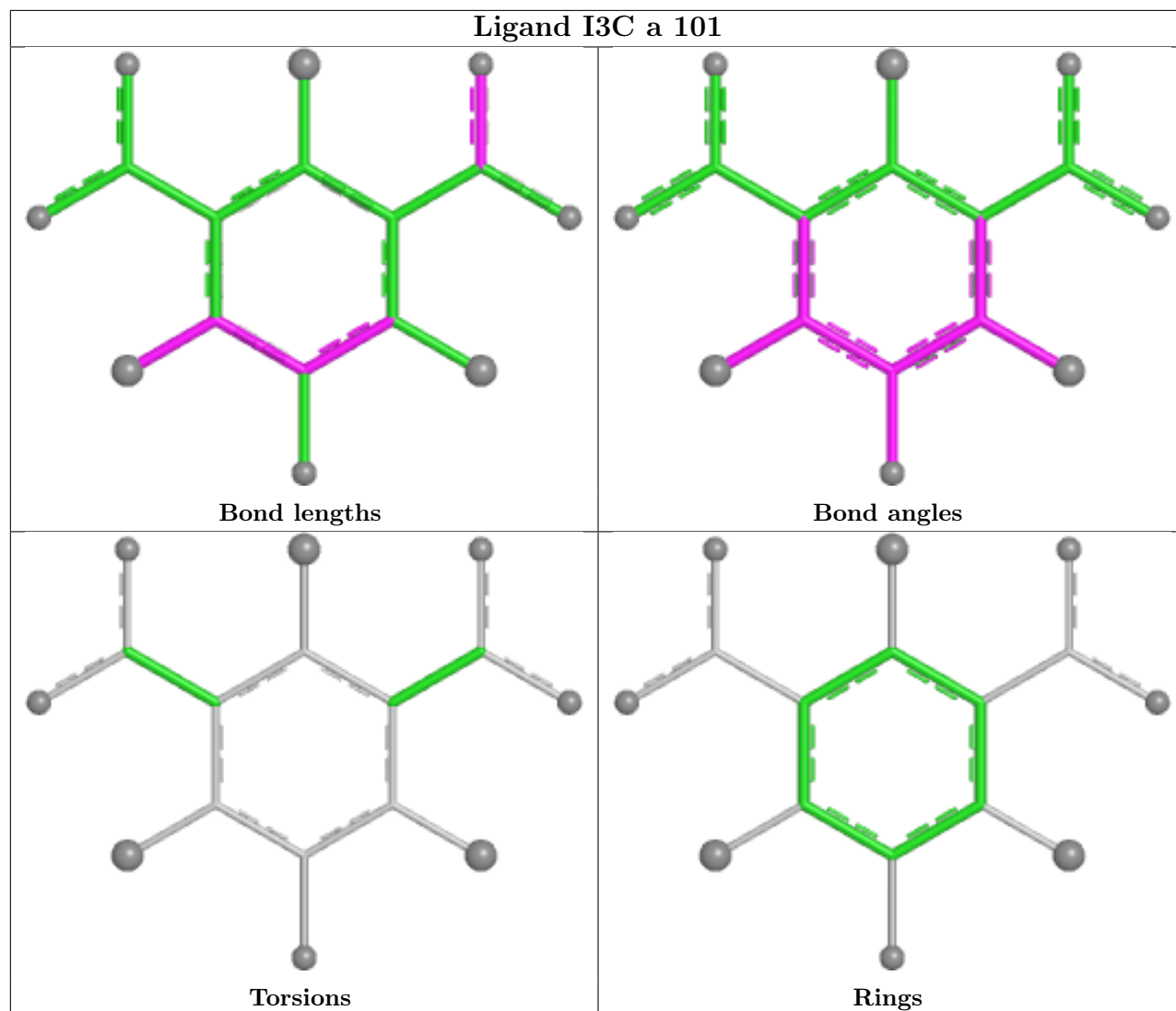
There are no ring outliers.

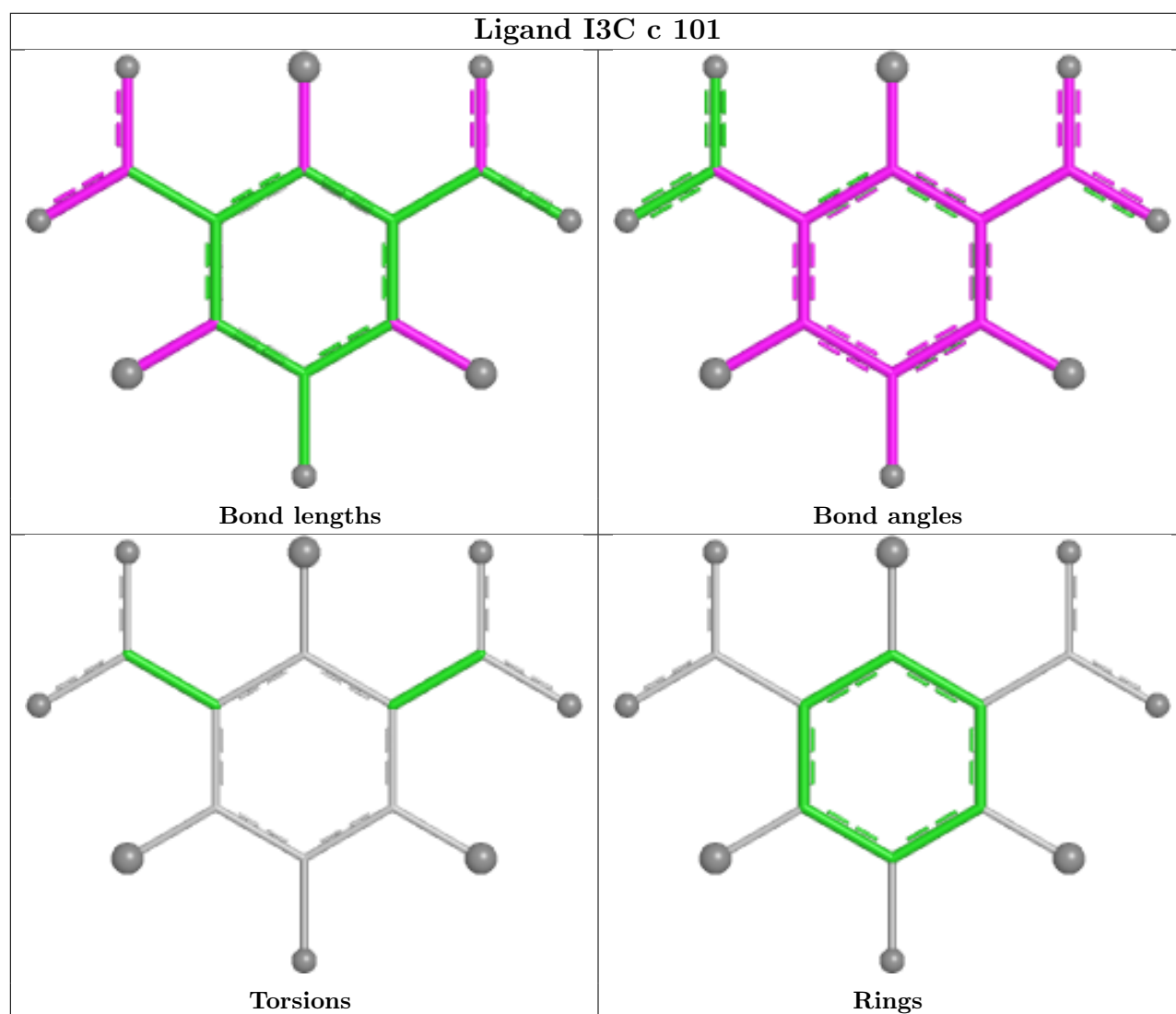
1 monomer is involved in 1 short contact:

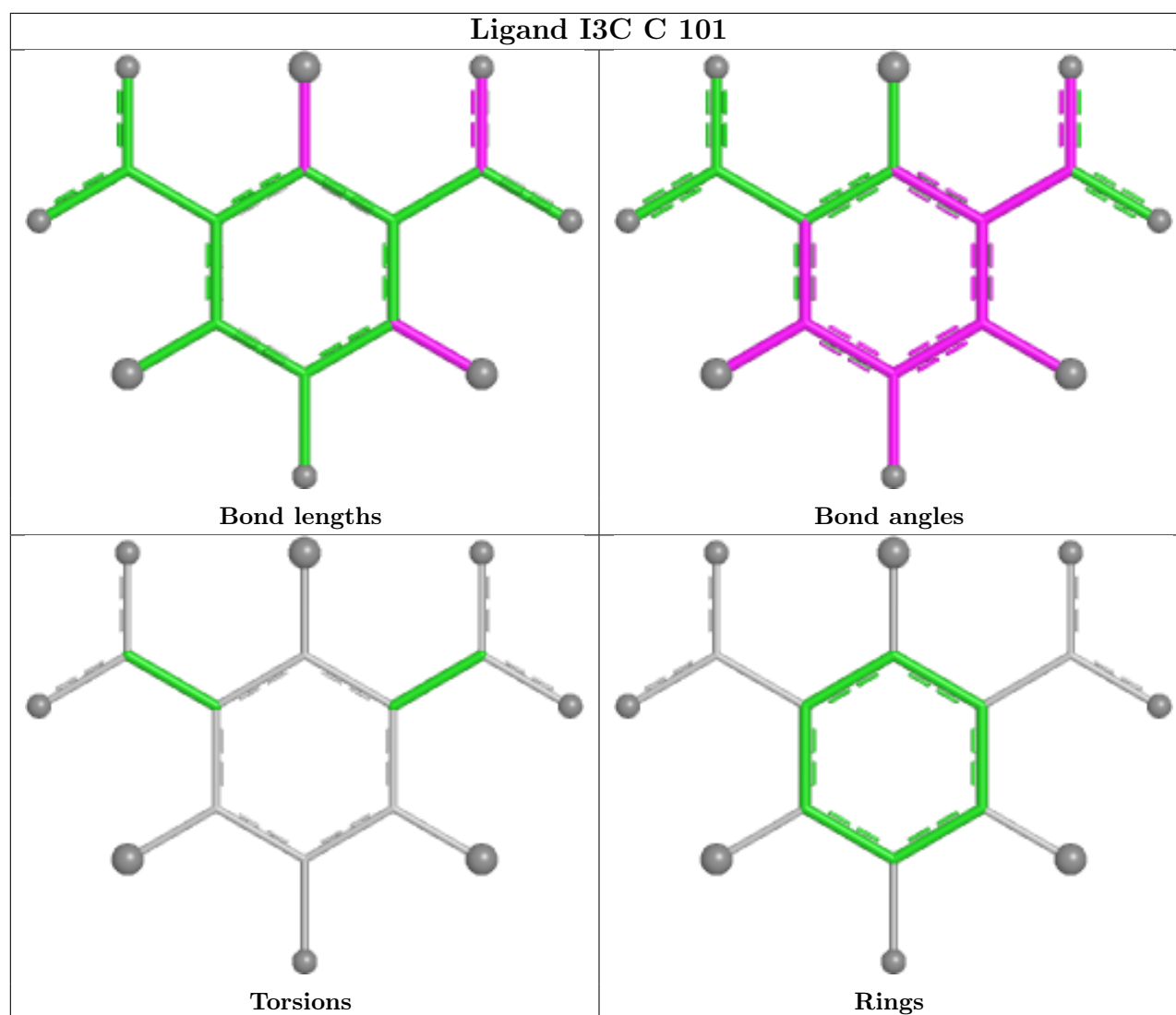
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	c	101	I3C	0	1

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

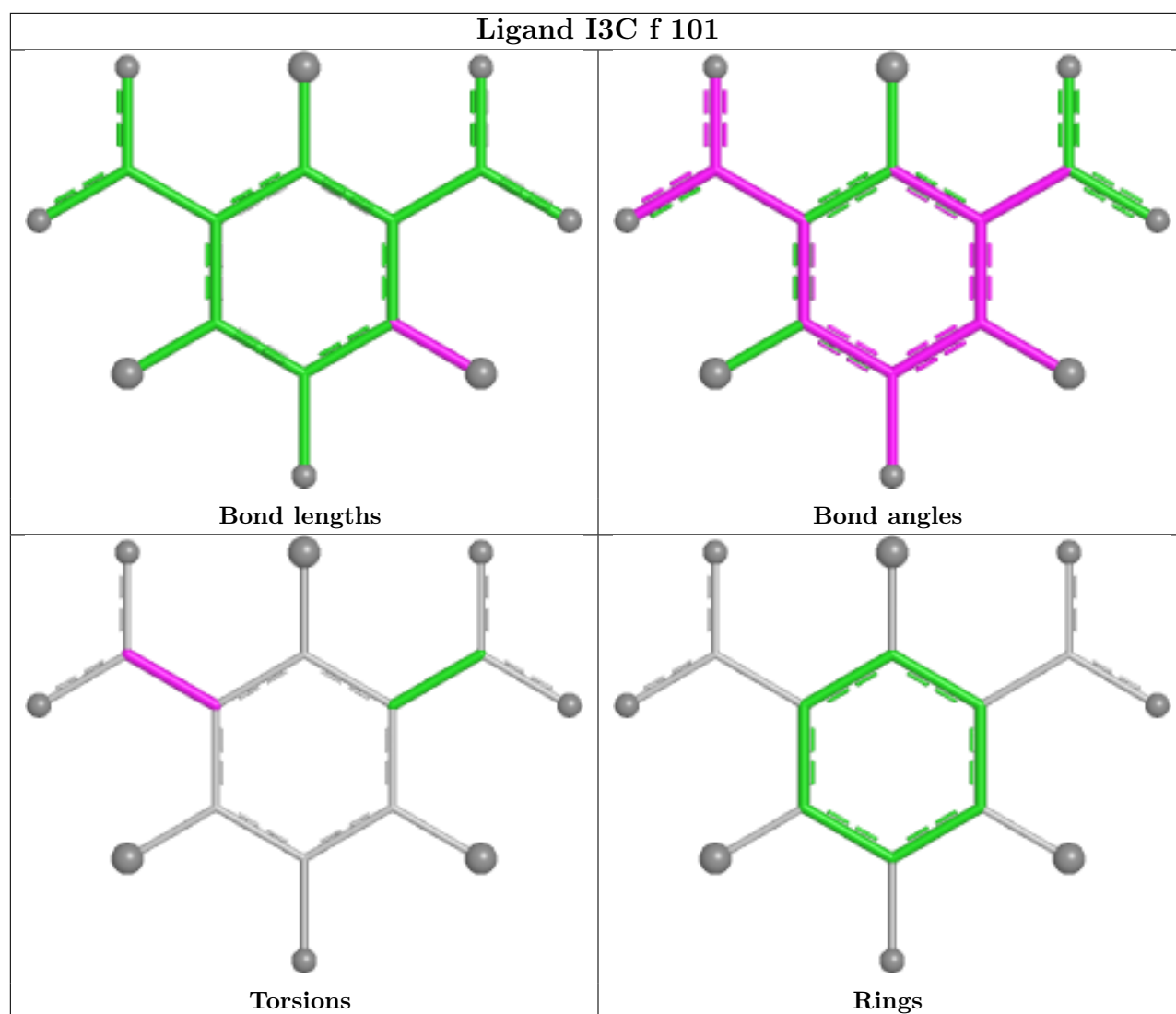


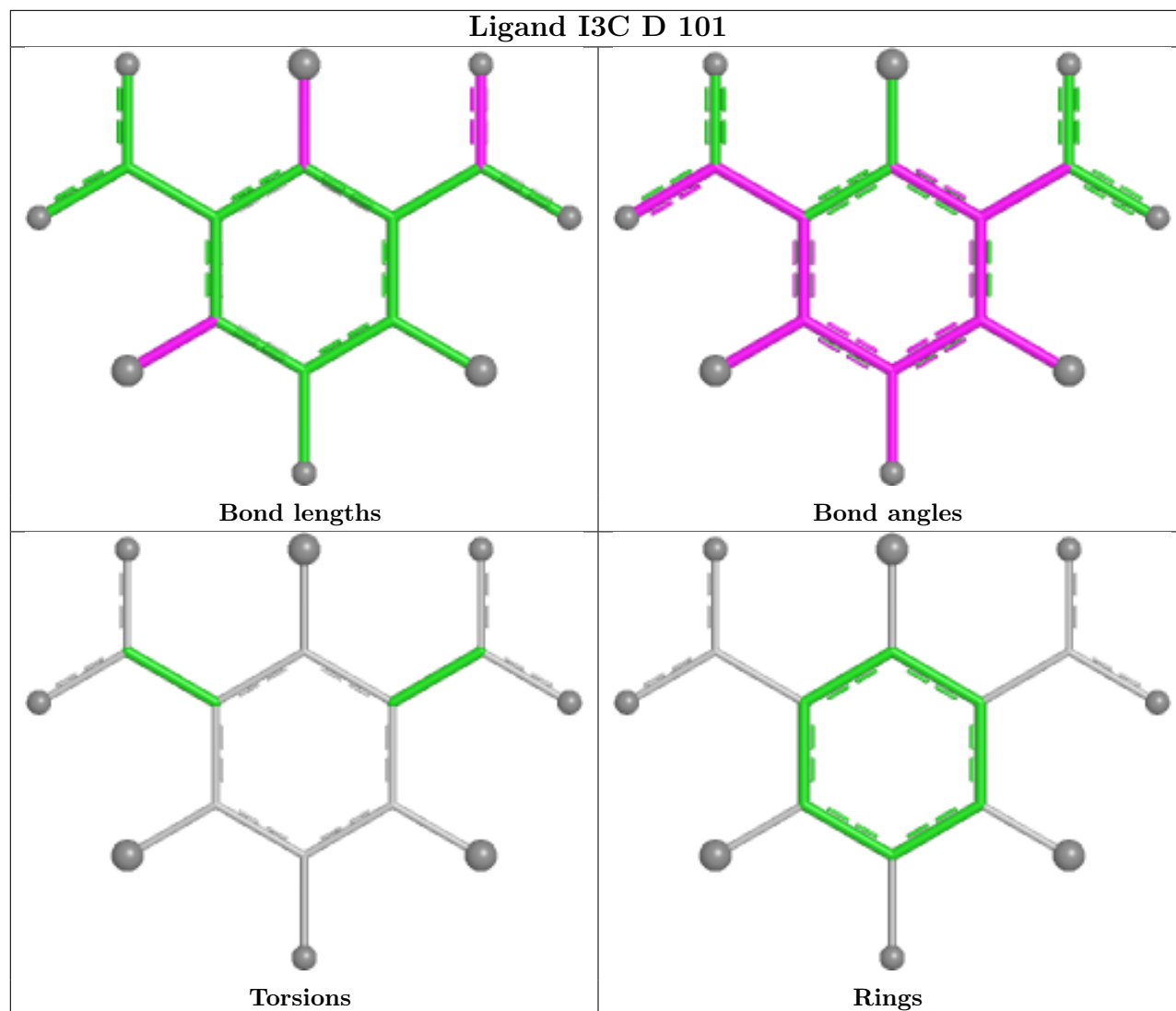


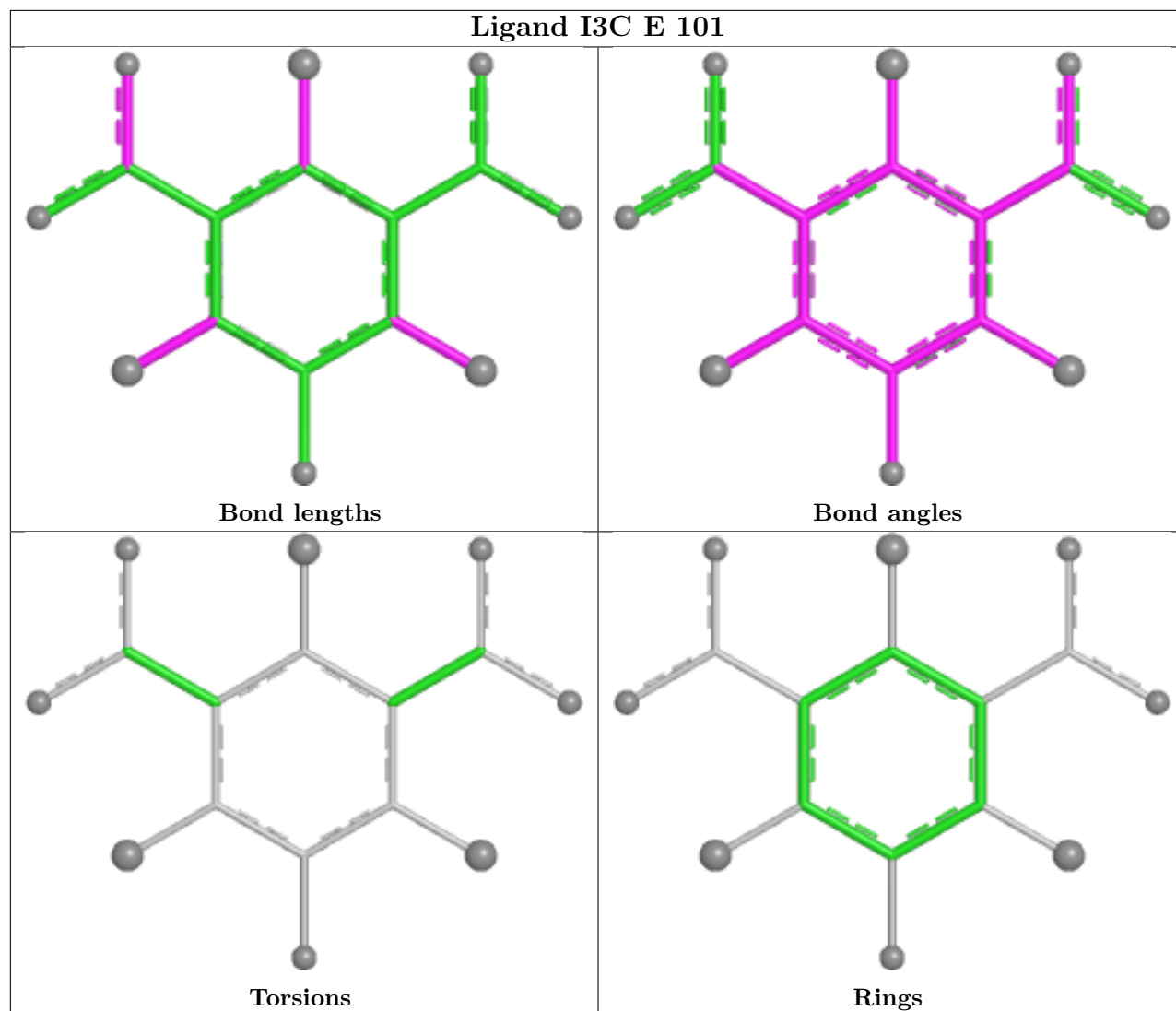












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	10/13 (76%)	0.75	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	20, 23, 25, 29	0
1	B	10/13 (76%)	0.86	1 (10%) <span style="border: 1px solid red; padding: 2px;">14</span> <span style="border: 1px solid red; padding: 2px;">18</span>	13, 23, 31, 31	1 (10%)
1	C	10/13 (76%)	1.33	1 (10%) <span style="border: 1px solid red; padding: 2px;">14</span> <span style="border: 1px solid red; padding: 2px;">18</span>	26, 29, 33, 36	0
1	D	10/13 (76%)	1.31	2 (20%) <span style="border: 1px solid red; padding: 2px;">3</span> <span style="border: 1px solid red; padding: 2px;">4</span>	15, 24, 27, 31	1 (10%)
1	E	10/13 (76%)	1.21	3 (30%) <span style="border: 1px solid red; padding: 2px;">1</span> <span style="border: 1px solid red; padding: 2px;">1</span>	14, 23, 28, 29	1 (10%)
1	F	10/13 (76%)	2.32	4 (40%) <span style="border: 1px solid red; padding: 2px;">1</span> <span style="border: 1px solid red; padding: 2px;">1</span>	21, 30, 39, 48	0
1	a	10/13 (76%)	0.65	1 (10%) <span style="border: 1px solid red; padding: 2px;">14</span> <span style="border: 1px solid red; padding: 2px;">18</span>	21, 25, 35, 36	0
1	b	10/13 (76%)	1.44	4 (40%) <span style="border: 1px solid red; padding: 2px;">1</span> <span style="border: 1px solid red; padding: 2px;">1</span>	21, 26, 38, 50	0
1	c	10/13 (76%)	1.19	2 (20%) <span style="border: 1px solid red; padding: 2px;">3</span> <span style="border: 1px solid red; padding: 2px;">4</span>	23, 27, 32, 33	0
1	d	10/13 (76%)	1.03	1 (10%) <span style="border: 1px solid red; padding: 2px;">14</span> <span style="border: 1px solid red; padding: 2px;">18</span>	22, 25, 31, 35	0
1	e	10/13 (76%)	0.94	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	20, 25, 30, 38	0
1	f	10/13 (76%)	2.47	6 (60%) <span style="border: 1px solid red; padding: 2px;">0</span> <span style="border: 1px solid red; padding: 2px;">0</span>	19, 34, 40, 48	1 (10%)
All	All	120/156 (76%)	1.29	25 (20%) <span style="border: 1px solid red; padding: 2px;">3</span> <span style="border: 1px solid red; padding: 2px;">4</span>	13, 26, 38, 50	4 (3%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	5	VAL	6.5
1	f	7	PRO	5.3
1	F	7	PRO	5.1
1	f	5	VAL	4.1
1	E	2	LYS	3.3
1	C	7	PRO	3.2
1	B	2	LYS	3.2
1	F	8	THR	3.1
1	D	9	LYS	3.1
1	f	1	VAL	3.1
1	f	8	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	b	9	LYS	2.8
1	a	2	LYS	2.6
1	d	9	LYS	2.4
1	b	2	LYS	2.3
1	c	2	LYS	2.3
1	c	3	VAL	2.2
1	f	12	VAL	2.2
1	b	3	VAL	2.2
1	b	12	VAL	2.2
1	f	3[A]	VAL	2.1
1	E	11	LYS	2.1
1	D	1	VAL	2.0
1	E	12	VAL	2.0
1	F	3	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
1	A1A8T	b	10	8/9	0.38	0.29	27,32,33,35	0
1	DPR	F	6	7/8	0.73	0.28	42,51,51,52	0
1	A1A8T	e	10	8/9	0.80	0.17	21,25,27,28	0
1	DPR	e	6	7/8	0.83	0.14	26,29,34,34	0
1	ORN	f	13	8/9	0.84	0.16	34,36,38,40	0
1	DPR	f	6	7/8	0.86	0.22	40,42,44,46	0
1	ORN	C	13	8/9	0.86	0.14	25,30,32,35	0
1	DPR	D	6	7/8	0.86	0.14	31,32,34,37	0
1	ORN	d	13	8/9	0.87	0.12	24,26,28,28	0
1	ORN	c	13	8/9	0.88	0.12	21,25,30,31	0
1	ORN	b	13	8/9	0.89	0.15	25,26,27,28	0
1	A1A8T	A	10	8/9	0.89	0.11	17,20,23,25	0
1	A1A8T	f	10	8/9	0.89	0.11	18,21,24,25	0
1	A1A8T	B	10	8/9	0.90	0.11	19,21,22,22	0
1	ORN	a	13	8/9	0.90	0.10	23,25,28,29	0
1	ORN	B	13	8/9	0.90	0.11	20,25,28,28	0
1	ORN	E	13	8/9	0.90	0.11	21,27,29,32	0
1	DPR	C	6	7/8	0.91	0.19	32,35,39,40	0
1	ORN	F	13	8/9	0.91	0.09	19,22,26,27	0

*Continued on next page...*

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	A1A8T	a	10	8/9	0.92	0.11	18,20,21,23	0
1	DPR	b	6	7/8	0.92	0.12	25,26,32,36	0
1	ORN	A	13	8/9	0.92	0.09	21,24,26,27	0
1	A1A8T	E	10	8/9	0.92	0.11	19,22,26,29	0
1	DPR	c	6	7/8	0.92	0.14	23,27,30,32	0
1	DPR	A	6	7/8	0.92	0.10	27,28,30,32	0
1	A1A8T	D	10	8/9	0.93	0.09	20,22,23,25	0
1	A1A8T	d	10	8/9	0.93	0.09	19,20,22,22	0
1	ORN	D	13	8/9	0.93	0.09	22,25,26,26	0
1	A1A8T	C	10	8/9	0.93	0.10	21,24,25,26	0
1	A1A8T	c	10	8/9	0.93	0.12	20,21,22,22	0
1	ORN	e	13	8/9	0.94	0.09	22,24,26,29	0
1	A1A8T	F	10	8/9	0.94	0.08	18,20,21,22	0
1	DPR	B	6	7/8	0.94	0.09	26,27,30,32	0
1	DPR	a	6	7/8	0.95	0.10	25,27,32,32	0
1	DPR	d	6	7/8	0.95	0.07	24,28,28,29	0
1	DPR	E	6	7/8	0.95	0.08	28,29,34,34	0

### 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.

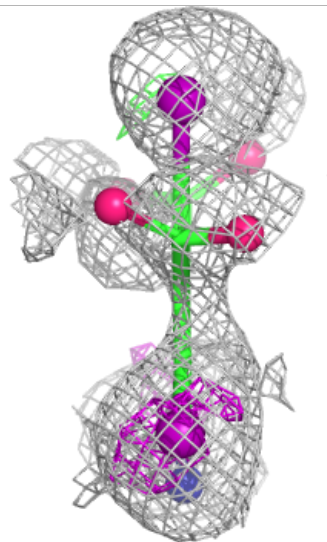
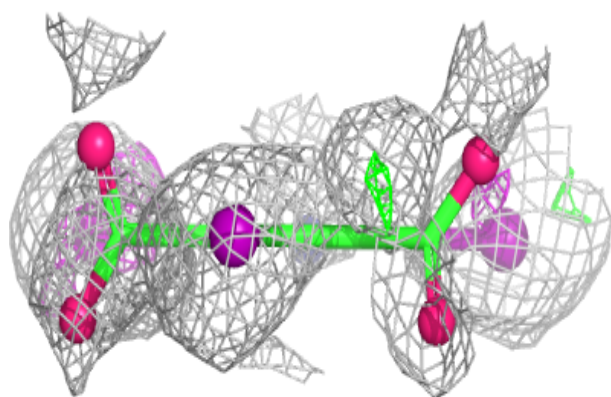
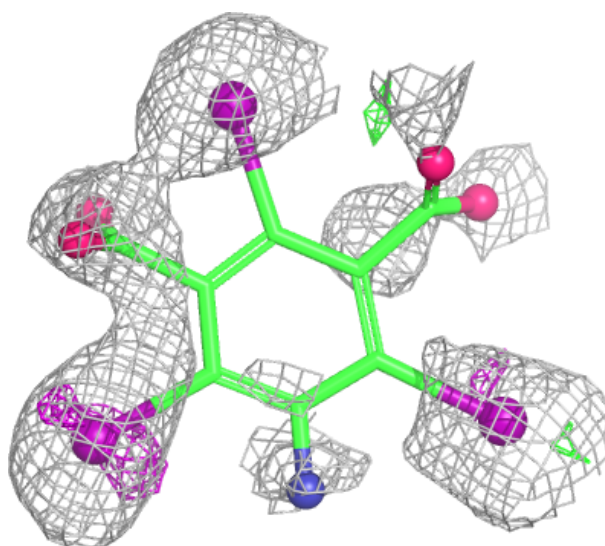
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	I3C	a	102	16/16	0.91	0.20	35,47,50,64	16
2	I3C	f	101	16/16	0.95	0.15	39,53,70,78	0
2	I3C	C	101	16/16	0.97	0.10	27,38,53,60	0
2	I3C	c	101	16/16	0.98	0.12	10,12,16,22	16
2	I3C	D	101	16/16	0.98	0.09	24,30,45,46	0
2	I3C	E	101	16/16	0.98	0.12	13,20,34,38	16
2	I3C	a	101	16/16	0.98	0.11	13,19,30,34	16

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.

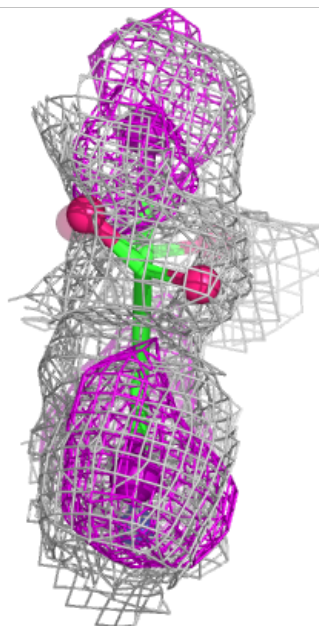
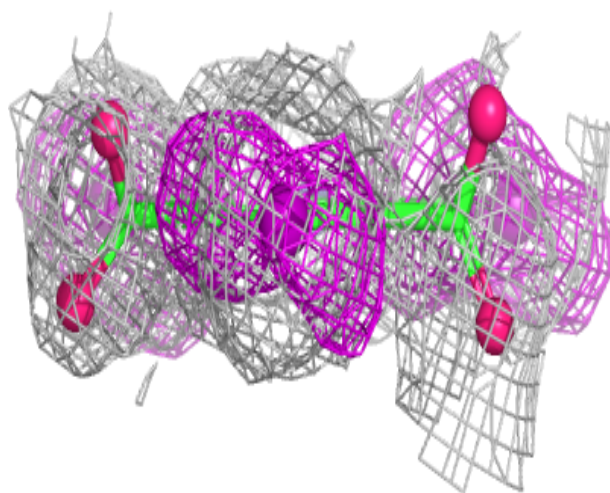
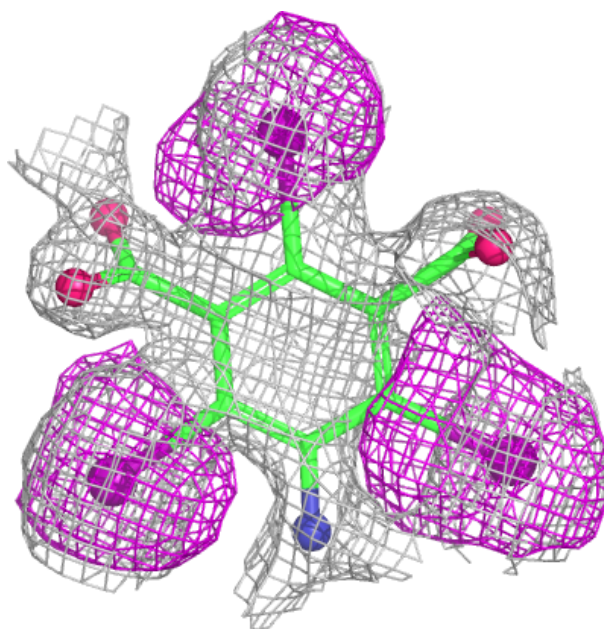
**Electron density around I3C a 102:**

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



**Electron density around I3C f 101:**

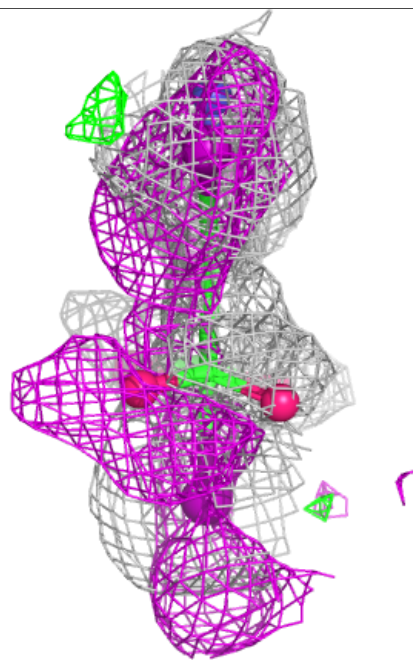
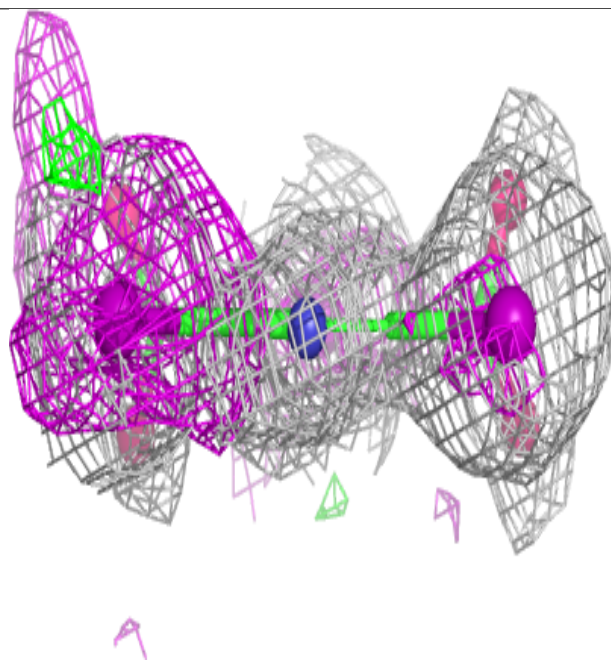
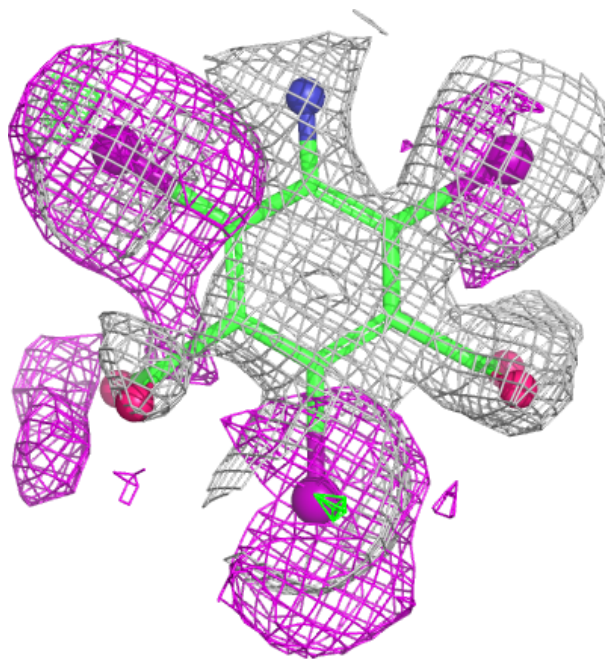
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





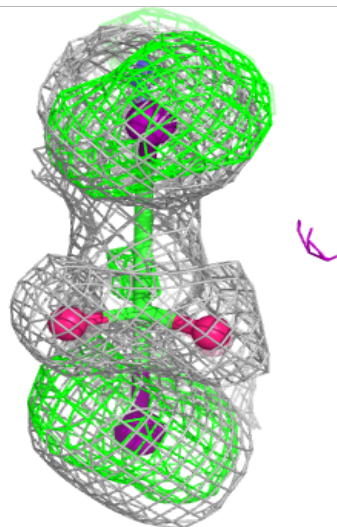
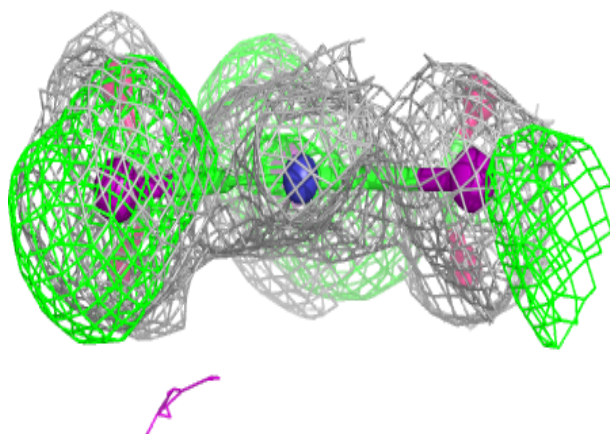
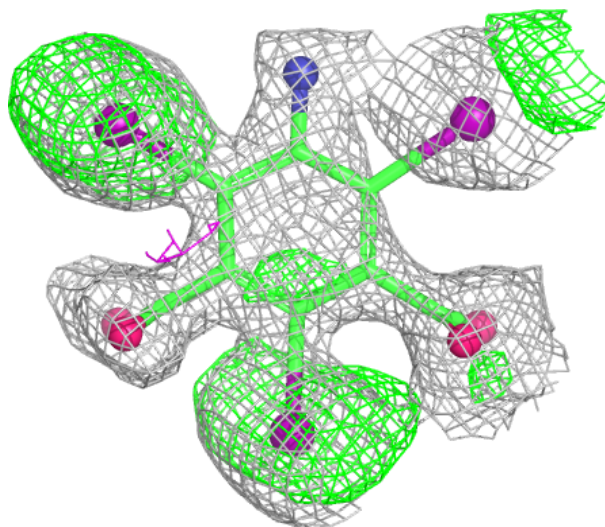
**Electron density around I3C C 101:**

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



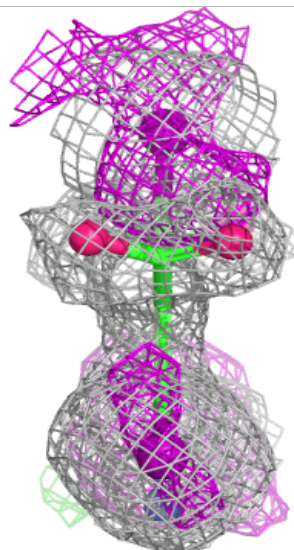
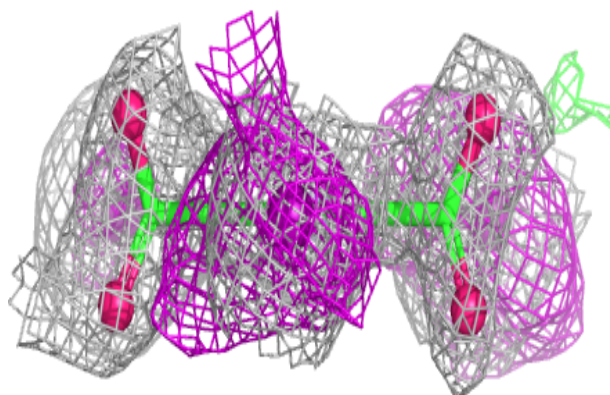
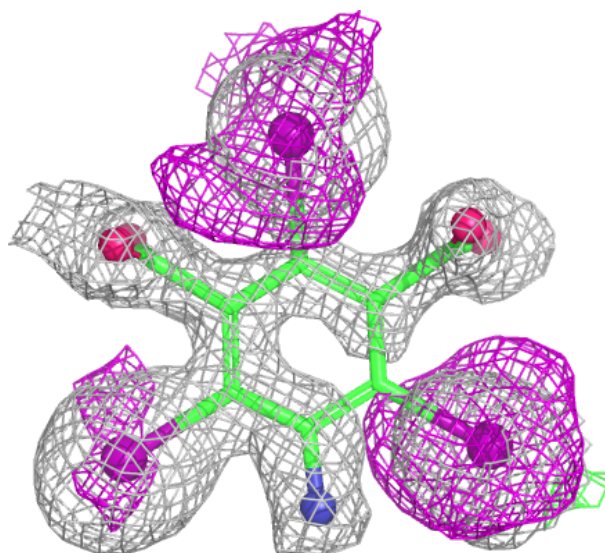
**Electron density around I3C c 101:**

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



**Electron density around I3C D 101:**

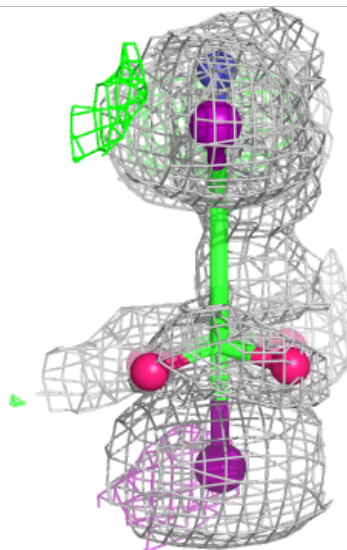
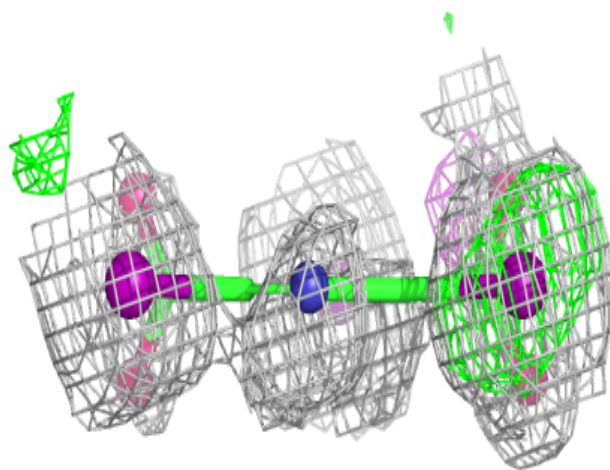
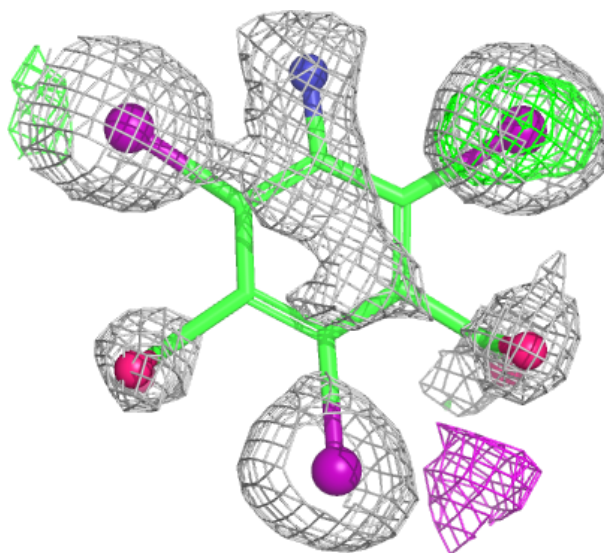
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





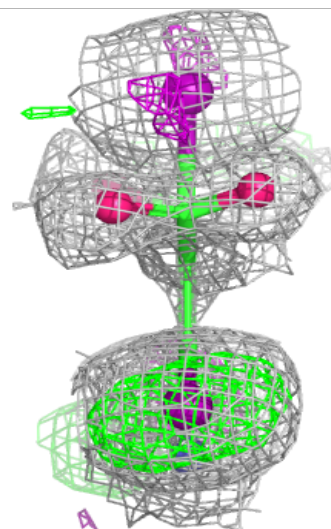
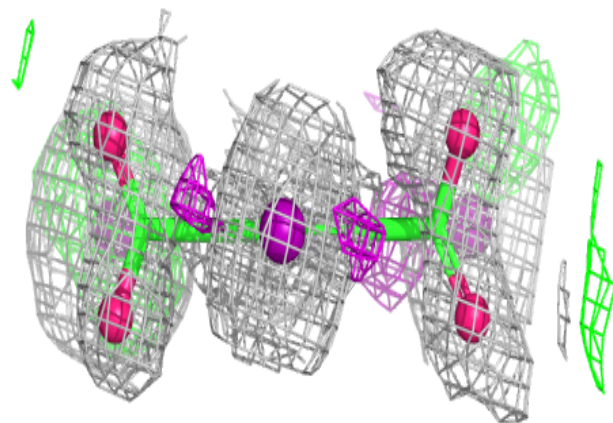
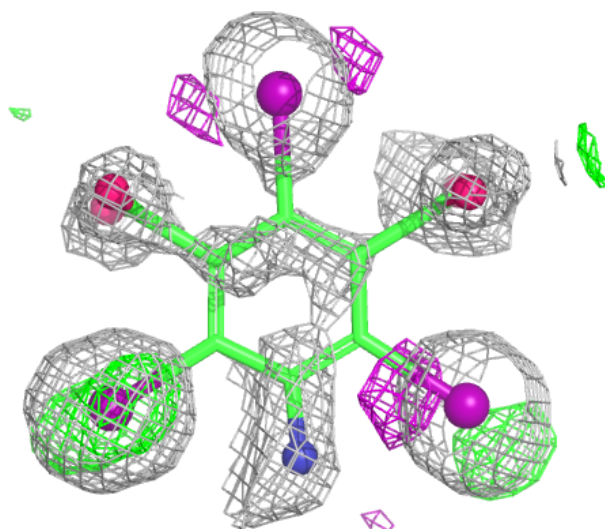
**Electron density around I3C E 101:**

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



**Electron density around I3C a 101:**

$2mF_o-DF_c$  (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.