



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2022 – 12:05 PM JST

PDB ID : 7WL0  
Title : Crystal structure of human ALKBH5 in complex with N-oxalylglycine (NOG) and m6A-containing ssRNA  
Authors : Kaur, S.; McDonough, M.A.; Schofield, C.J.; Aik, W.S.  
Deposited on : 2022-01-12  
Resolution : 2.50 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.

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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 : 2.27  
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) : 2.27

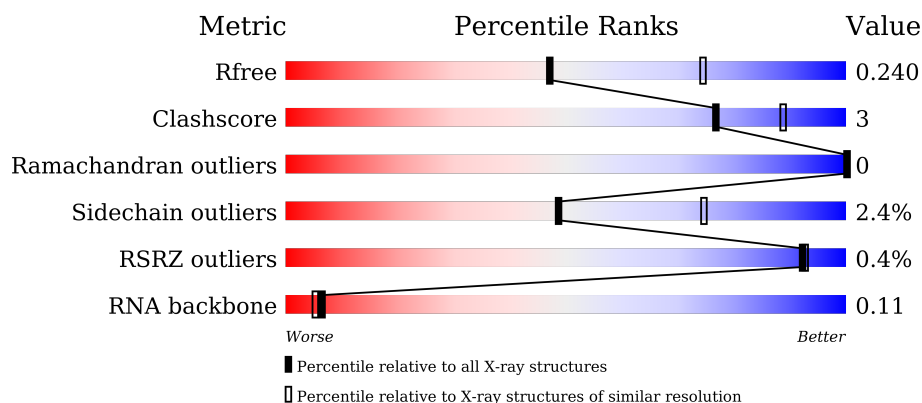
# 1 Overall quality at a glance

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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)
RNA backbone	3102	1008 (2.84-2.16)

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	220	
1	C	220	
1	E	220	
1	G	220	

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Mol	Chain	Length	Quality of chain
1	I	220	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>87%12%</div></div></div>
2	B	8	<div><div><div></div><div></div><div></div></div><div>62%38%</div></div>
2	D	8	<div><div><div></div><div></div><div></div></div><div>50%12%38%</div></div>
2	F	8	<div><div><div></div><div></div><div></div></div><div>88%12%</div></div>
2	H	8	<div><div><div></div><div></div><div></div></div><div>38%12%50%</div></div>
2	J	8	<div><div><div></div><div></div><div></div></div><div>25%25%50%</div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9362 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 RNA demethylase ALKBH5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1688	1071	303	308	6			
1	C	218	Total	C	N	O	S	0	0	0
			1737	1101	313	317	6			
1	E	216	Total	C	N	O	S	0	0	0
			1704	1081	308	309	6			
1	G	219	Total	C	N	O	S	0	0	0
			1709	1084	309	310	6			
1	I	218	Total	C	N	O	S	0	0	0
			1669	1064	297	302	6			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	SER	-	expression tag	UNP Q6P6C2
C	73	SER	-	expression tag	UNP Q6P6C2
E	73	SER	-	expression tag	UNP Q6P6C2
G	73	SER	-	expression tag	UNP Q6P6C2
I	73	SER	-	expression tag	UNP Q6P6C2

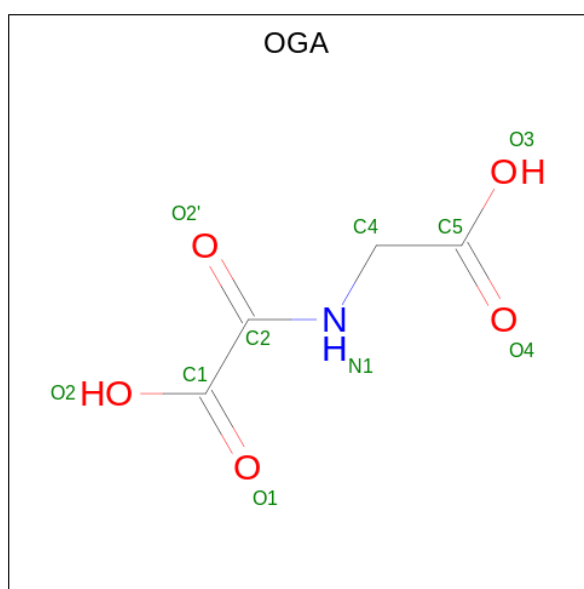
- Molecule 2 is a RNA chain called RNA (5'-R(\*UP\*GP\*GP\*(6MZ)P\*CP\*UP\*GP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	8	Total	C	N	O	P	0	0	0
			169	77	30	55	7			
2	D	5	Total	C	N	O	P	0	0	0
			106	49	20	33	4			
2	F	8	Total	C	N	O	P	0	0	0
			169	77	30	55	7			
2	H	4	Total	C	N	O	P	0	0	0
			89	40	18	27	4			
2	J	4	Total	C	N	O	P	0	0	0
			89	40	18	27	4			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

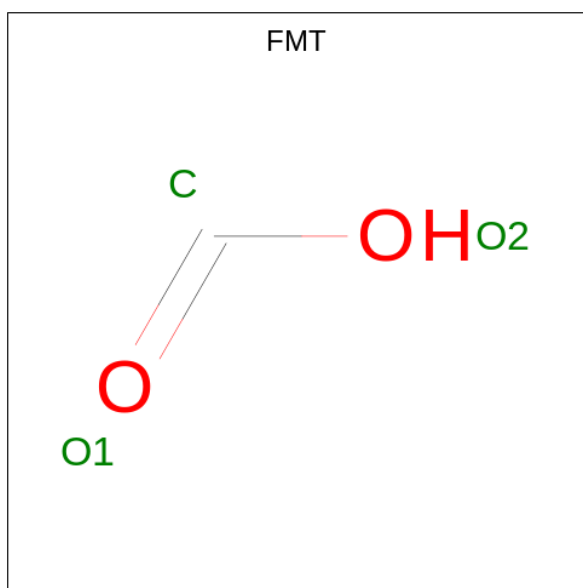
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		
3	E	1	Total	Mn	0	0
			1	1		
3	G	1	Total	Mn	0	0
			1	1		
3	I	1	Total	Mn	0	0
			1	1		

- Molecule 4 is N-OXALYLGLYCINE (three-letter code: OGA) (formula:  $C_4H_5NO_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			10	4	1	5		
4	C	1	Total	C	N	O	0	0
			10	4	1	5		
4	E	1	Total	C	N	O	0	0
			10	4	1	5		
4	G	1	Total	C	N	O	0	0
			10	4	1	5		
4	I	1	Total	C	N	O	0	0
			10	4	1	5		

- Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula:  $\text{CH}_2\text{O}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			3	1	2		


- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	44	Total	O	0	0
			44	44		
6	B	6	Total	O	0	0
			6	6		
6	C	39	Total	O	0	0
			39	39		
6	D	4	Total	O	0	0
			4	4		
6	E	30	Total	O	0	0
			30	30		
6	F	4	Total	O	0	0
			4	4		
6	G	29	Total	O	0	0
			29	29		
6	H	2	Total	O	0	0
			2	2		
6	I	16	Total	O	0	0
			16	16		
6	J	1	Total	O	0	0
			1	1		

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


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

- Molecule 1: RNA demethylase ALKBH5

Chain A: 




- Molecule 1: RNA demethylase ALKBH5

Chain C: 




- Molecule 1: RNA demethylase ALKBH5

Chain E: 




- Molecule 1: RNA demethylase ALKBH5

Chain G: 



- Molecule 1: RNA demethylase ALKBH5

Chain I: 



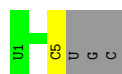
- Molecule 2: RNA (5'-R(\*UP\*GP\*GP\*(6MZ)P\*CP\*UP\*GP\*C)-3')

Chain B:  62% 38%




- Molecule 2: RNA (5'-R(\*UP\*GP\*GP\*(6MZ)P\*CP\*UP\*GP\*C)-3')

Chain D:  50% 12% 38%




- Molecule 2: RNA (5'-R(\*UP\*GP\*GP\*(6MZ)P\*CP\*UP\*GP\*C)-3')

Chain F:  88% 12%



- Molecule 2: RNA (5'-R(\*UP\*GP\*GP\*(6MZ)P\*CP\*UP\*GP\*C)-3')

Chain H:  38% 12% 50%



- Molecule 2: RNA (5'-R(\*UP\*GP\*GP\*(6MZ)P\*CP\*UP\*GP\*C)-3')

Chain J:  25% 25% 50%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.77Å 132.37Å 77.96Å 90.00° 100.99° 90.00°	Depositor
Resolution (Å)	58.67 – 2.50 66.25 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (58.67-2.50) 99.9 (66.25-2.50)	Depositor EDS
$R_{merge}$	0.49	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.196 , 0.240 0.196 , 0.240	Depositor DCC
$R_{free}$ test set	2067 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.4	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 30.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9362	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.89% 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: FMT, 6MZ, MN, OGA

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	0.27	0/1726	0.41	0/2339
1	C	0.25	0/1775	0.41	0/2401
1	E	0.25	0/1742	0.41	0/2359
1	G	0.27	0/1747	0.41	0/2369
1	I	0.25	0/1707	0.40	0/2321
2	B	0.18	0/161	0.72	0/247
2	D	0.14	0/91	0.63	0/138
2	F	0.14	0/161	0.70	0/247
2	H	0.13	0/72	0.72	0/108
2	J	0.11	0/72	0.64	0/108
All	All	0.25	0/9254	0.43	0/12637

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

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	1688	0	1664	9	0
1	C	1737	0	1728	9	0
1	E	1704	0	1684	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1709	0	1672	13	0
1	I	1669	0	1617	13	0
2	B	169	0	90	1	0
2	D	106	0	58	0	0
2	F	169	0	90	0	0
2	H	89	0	47	0	0
2	J	89	0	47	1	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
4	A	10	0	3	1	0
4	C	10	0	3	1	0
4	E	10	0	3	0	0
4	G	10	0	3	2	0
4	I	10	0	3	0	0
5	C	3	0	1	0	0
6	A	44	0	0	0	0
6	B	6	0	0	0	0
6	C	39	0	0	0	0
6	D	4	0	0	0	0
6	E	30	0	0	0	0
6	F	4	0	0	0	0
6	G	29	0	0	0	0
6	H	2	0	0	0	0
6	I	16	0	0	0	0
6	J	1	0	0	0	0
All	All	9362	0	8713	54	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 3.

All (54) 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:E:90:ARG:HB2	1:E:255:VAL:HB	1.83	0.60
1:A:90:ARG:HB2	1:A:255:VAL:HB	1.83	0.60
1:C:279:VAL:HG11	4:C:302:OGA:O4	2.03	0.59
1:G:74:GLN:HE22	1:I:188:ASN:HB2	1.67	0.58
1:G:204:HIS:CE1	4:G:302:OGA:O2'	2.56	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:192:ILE:HG12	1:I:280:ILE:HG12	1.88	0.55
1:E:137:GLU:HB2	1:E:189:SER:HB2	1.89	0.55
1:G:177:VAL:HG11	1:G:184:GLU:HG2	1.87	0.54
1:G:74:GLN:HE22	1:I:188:ASN:CB	2.22	0.52
1:C:81:GLU:HG2	1:C:243:VAL:HG11	1.93	0.51
1:I:155:LEU:HB2	1:I:291:ARG:HG2	1.93	0.50
1:G:204:HIS:NE2	4:G:302:OGA:O2'	2.45	0.50
1:A:97:GLN:OE1	1:E:274:LYS:NZ	2.45	0.49
1:I:137:GLU:HB2	1:I:189:SER:HB2	1.94	0.49
1:E:93:ARG:HD2	1:E:252:SER:HB3	1.93	0.49
1:A:218:VAL:HG22	1:A:253:VAL:HG22	1.95	0.49
1:C:113:ARG:HG3	1:C:118:LEU:HB2	1.94	0.48
1:E:239:VAL:HG11	1:E:269:ARG:HG2	1.95	0.47
1:I:203:SER:HA	1:I:267:CYS:HB3	1.95	0.47
1:E:218:VAL:HG22	1:E:253:VAL:HG22	1.97	0.47
1:C:203:SER:HA	1:C:267:CYS:HB3	1.96	0.47
1:I:90:ARG:HB2	1:I:255:VAL:HB	1.97	0.47
1:A:207:PRO:HB3	1:A:209:HIS:CE1	2.51	0.46
1:G:120:ASN:ND2	1:G:160:ASP:O	2.48	0.46
1:C:239:VAL:HG11	1:C:269:ARG:HG2	1.97	0.46
1:A:266:HIS:CD2	4:A:302:OGA:O2'	2.68	0.46
1:C:173:ILE:HG12	1:C:282:LEU:HD22	1.98	0.46
1:G:205:VAL:HG23	1:G:265:THR:HG22	1.98	0.45
1:I:205:VAL:HG23	1:I:265:THR:HG22	1.98	0.45
1:A:186:PHE:HA	1:A:284:LYS:HE2	1.98	0.45
1:E:203:SER:HA	1:E:267:CYS:HB3	1.98	0.45
1:A:89:ILE:HD13	1:A:246:LEU:HD22	1.99	0.45
1:C:135:PHE:HB3	1:C:164:ILE:HA	1.98	0.45
1:E:135:PHE:HB3	1:E:164:ILE:HA	1.99	0.44
1:G:193:ASN:HB2	1:G:279:VAL:HG13	2.00	0.44
1:G:203:SER:HA	1:G:267:CYS:HB3	2.00	0.44
1:A:91:GLN:HA	1:A:253:VAL:O	2.18	0.44
1:I:239:VAL:HG11	1:I:269:ARG:HG2	1.99	0.44
1:A:155:LEU:HB2	1:A:291:ARG:HG2	2.00	0.44
2:B:7:G:OP1	2:B:7:G:N2	2.30	0.44
1:E:205:VAL:HG23	1:E:265:THR:HG22	2.00	0.43
1:C:193:ASN:HB2	1:C:279:VAL:HG12	2.02	0.42
1:E:193:ASN:HB2	1:E:279:VAL:HG12	2.00	0.42
1:G:239:VAL:HG11	1:G:269:ARG:HG2	2.00	0.42
1:E:233:GLN:HB2	1:E:238:ARG:HB2	2.01	0.42
1:E:91:GLN:HA	1:E:253:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:90:ARG:HB3	1:G:255:VAL:HB	2.02	0.41
1:G:125:ASP:HB3	1:G:132:LYS:HB2	2.02	0.41
1:G:137:GLU:HB2	1:G:189:SER:HB2	2.01	0.41
1:I:106:ARG:HB3	1:I:167:TRP:CE2	2.55	0.41
1:I:224:SER:OG	1:I:225:ALA:N	2.52	0.41
1:C:155:LEU:HB2	1:C:291:ARG:HG2	2.02	0.41
1:I:219:SER:OG	1:I:277:ARG:NH2	2.54	0.41
1:I:283:ARG:HH12	2:J:4:6MZ:H9C1	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	212/220 (96%)	208 (98%)	4 (2%)	0	100	100
1	C	216/220 (98%)	209 (97%)	7 (3%)	0	100	100
1	E	214/220 (97%)	209 (98%)	5 (2%)	0	100	100
1	G	217/220 (99%)	211 (97%)	6 (3%)	0	100	100
1	I	216/220 (98%)	211 (98%)	5 (2%)	0	100	100
All	All	1075/1100 (98%)	1048 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	181/194 (93%)	175 (97%)	6 (3%)	38	64
1	C	188/194 (97%)	184 (98%)	4 (2%)	53	78
1	E	182/194 (94%)	178 (98%)	4 (2%)	52	77
1	G	180/194 (93%)	176 (98%)	4 (2%)	52	77
1	I	173/194 (89%)	169 (98%)	4 (2%)	50	76
All	All	904/970 (93%)	882 (98%)	22 (2%)	49	74

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	LEU
1	A	170	GLN
1	A	182	ILE
1	A	233	GLN
1	A	238	ARG
1	A	282	LEU
1	C	76	LEU
1	C	92	MET
1	C	102	LYS
1	C	146	GLN
1	E	92	MET
1	E	112	SER
1	E	166	GLU
1	E	257	SER
1	G	74	GLN
1	G	162	ASP
1	G	182	ILE
1	G	248	VAL
1	I	77	GLN
1	I	92	MET
1	I	94	LEU
1	I	174	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	174	GLN
1	G	74	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	6/8 (75%)	2 (33%)	0
2	D	3/8 (37%)	1 (33%)	0
2	F	6/8 (75%)	1 (16%)	0
2	H	2/8 (25%)	1 (50%)	0
2	J	2/8 (25%)	1 (50%)	0
All	All	19/40 (47%)	6 (31%)	0

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	5	C
2	B	8	C
2	D	5	C
2	F	5	C
2	H	5	C
2	J	5	C

There are no RNA pucker outliers to report.

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

5 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	$\# Z  > 2$
2	6MZ	D	4	2	18,25,26	0.62	0	16,36,39	0.69	0
2	6MZ	J	4	2	18,25,26	0.61	0	16,36,39	0.68	0
2	6MZ	B	4	2	18,25,26	0.61	0	16,36,39	0.68	0
2	6MZ	F	4	2	18,25,26	0.63	0	16,36,39	0.79	0
2	6MZ	H	4	2	18,25,26	0.60	0	16,36,39	0.68	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
2	6MZ	D	4	2	-	0/5/27/28	0/3/3/3
2	6MZ	J	4	2	-	0/5/27/28	0/3/3/3
2	6MZ	B	4	2	-	1/5/27/28	0/3/3/3
2	6MZ	F	4	2	-	1/5/27/28	0/3/3/3
2	6MZ	H	4	2	-	0/5/27/28	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	4	6MZ	N1-C6-N6-C9
2	F	4	6MZ	N1-C6-N6-C9

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	4	6MZ	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	OGA	E	302	3	3,9,9	0.84	0	4,11,11	1.35	0
4	OGA	C	302	3	3,9,9	0.82	0	4,11,11	0.90	0
4	OGA	G	302	3	3,9,9	0.85	0	4,11,11	1.24	0
4	OGA	I	302	3	3,9,9	0.55	0	4,11,11	0.93	0
5	FMT	C	303	-	0,2,2	-	-	0,1,1	-	-
4	OGA	A	302	3	3,9,9	0.84	0	4,11,11	1.50	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OGA	E	302	3	-	0/3/9/9	-
4	OGA	C	302	3	-	1/3/9/9	-
4	OGA	G	302	3	-	0/3/9/9	-
4	OGA	I	302	3	-	0/3/9/9	-
4	OGA	A	302	3	-	1/3/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	302	OGA	C5-C4-N1-C2
4	C	302	OGA	C5-C4-N1-C2

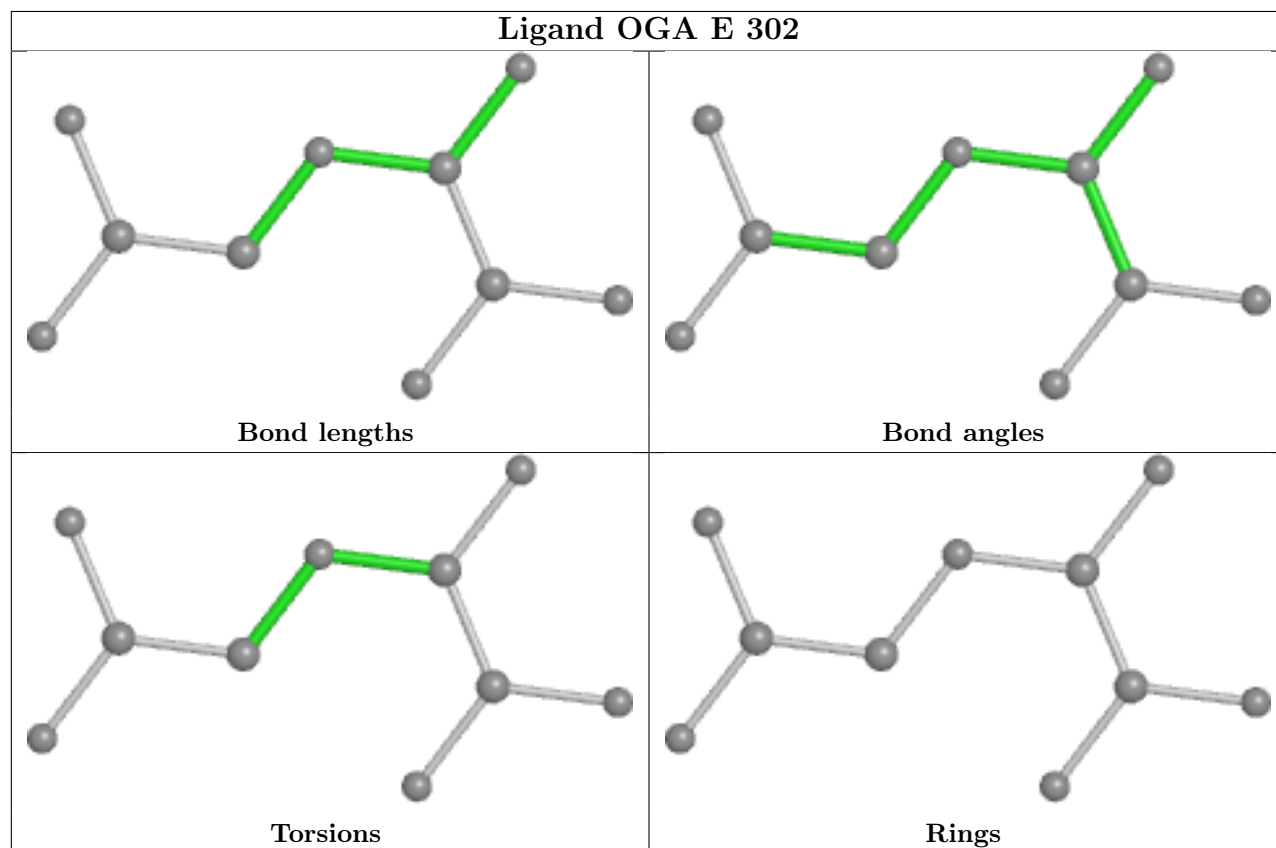
There are no ring outliers.

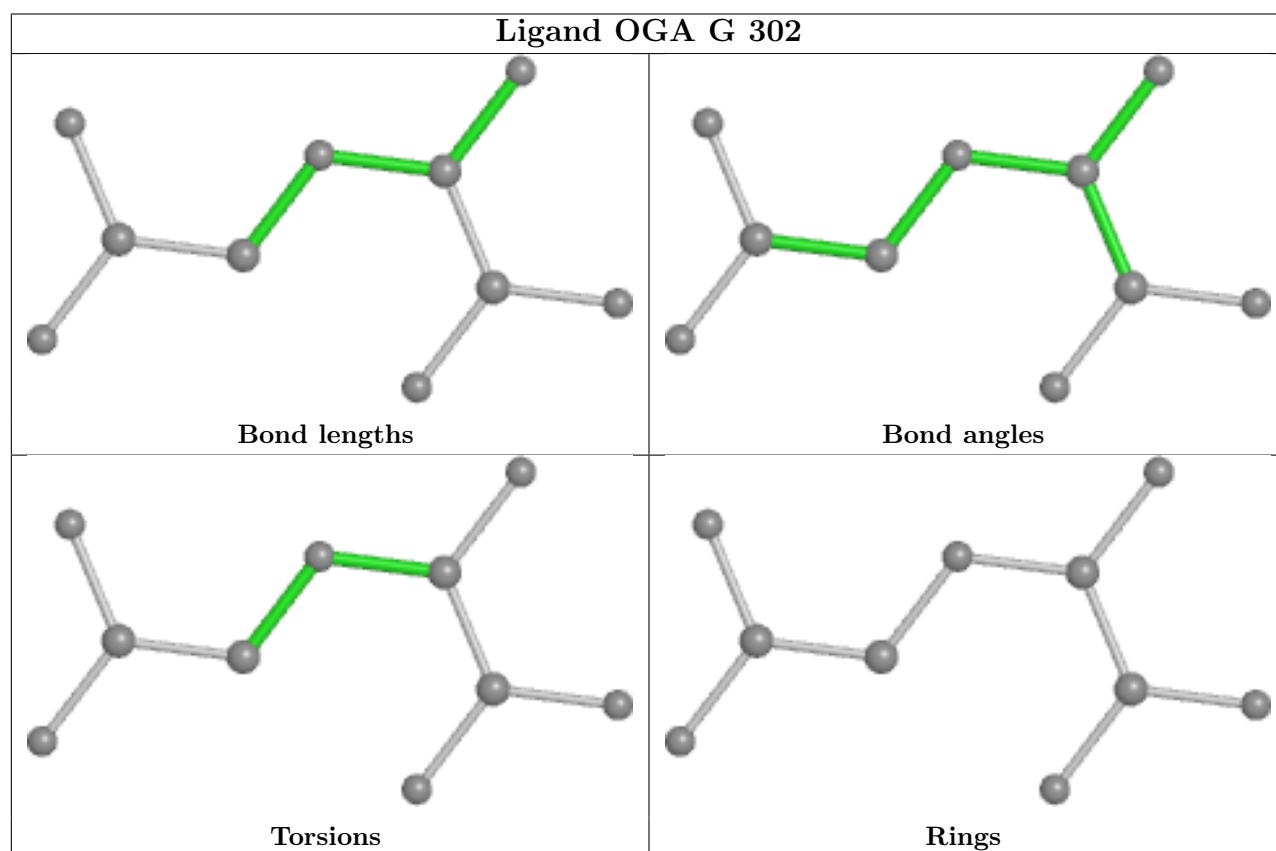
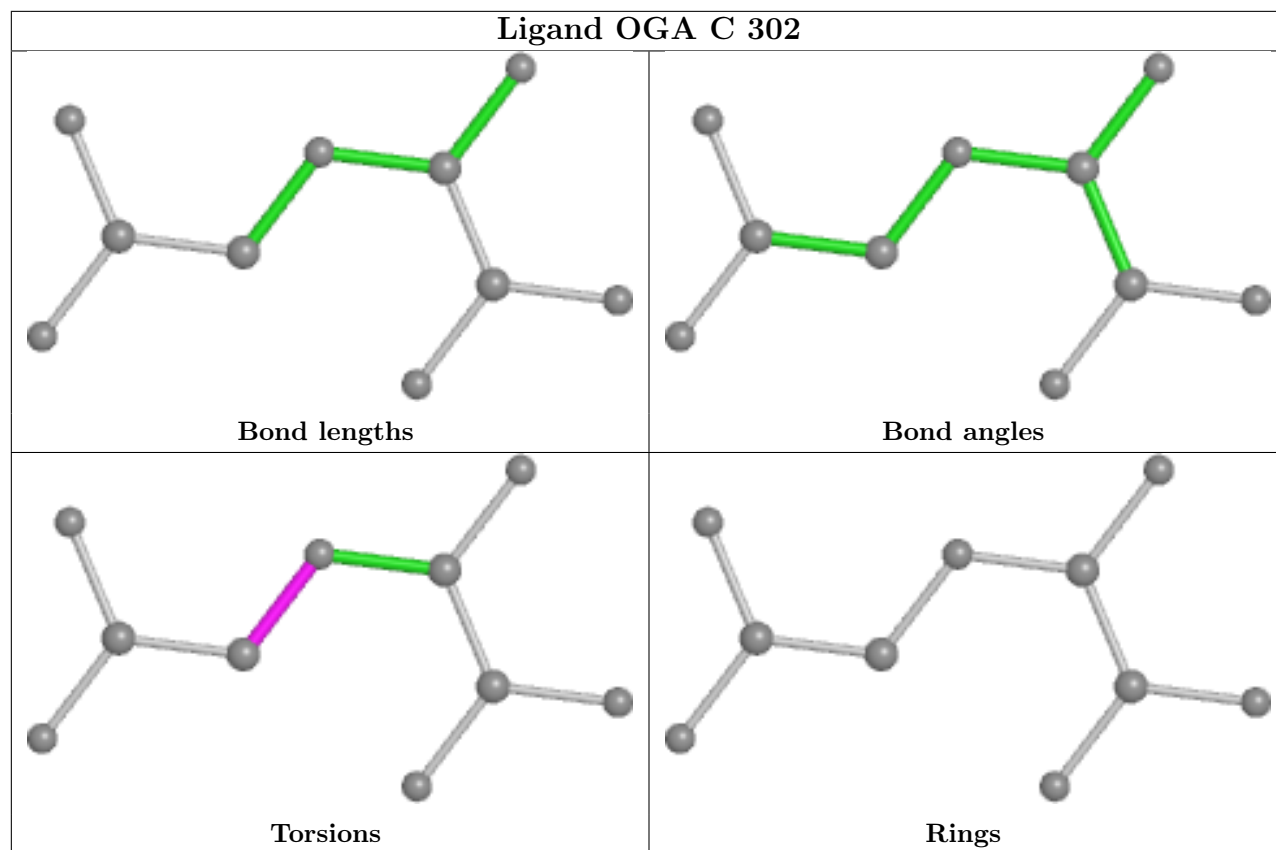
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	302	OGA	1	0
4	G	302	OGA	2	0
4	A	302	OGA	1	0

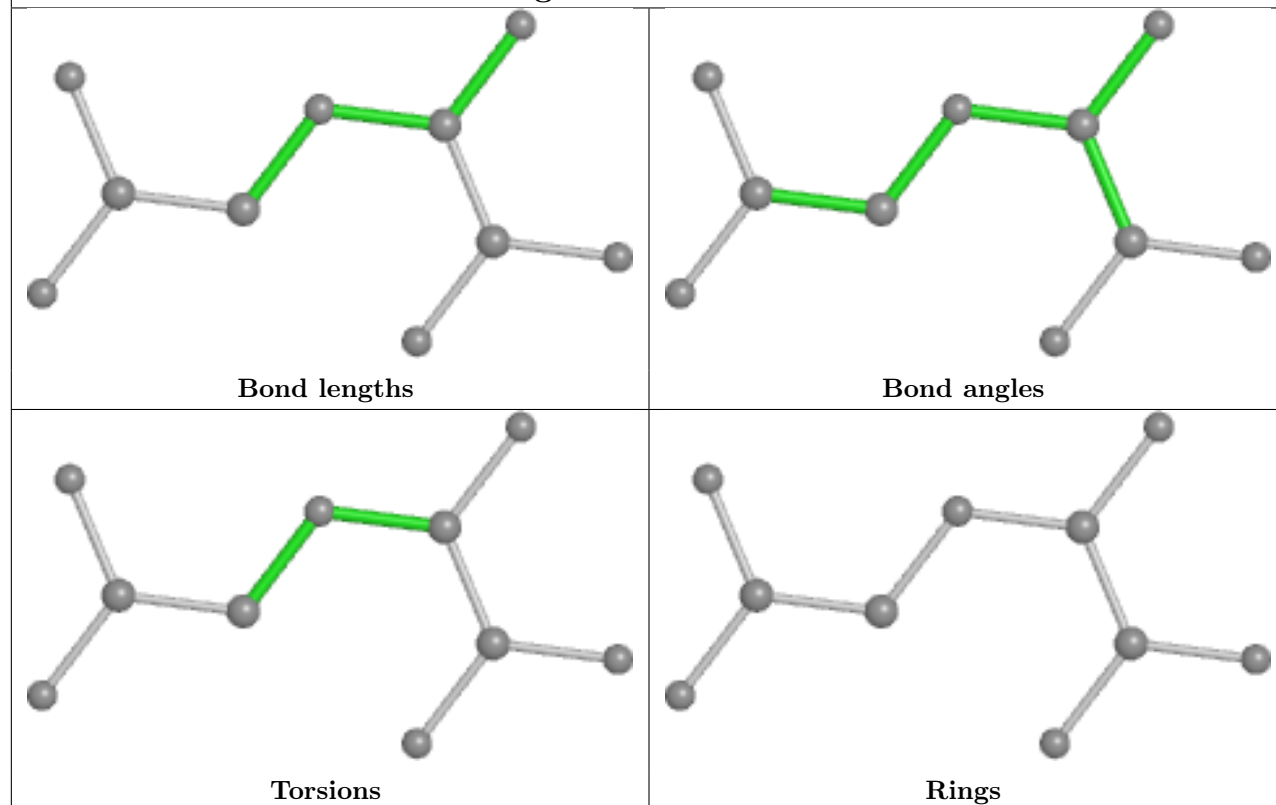
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

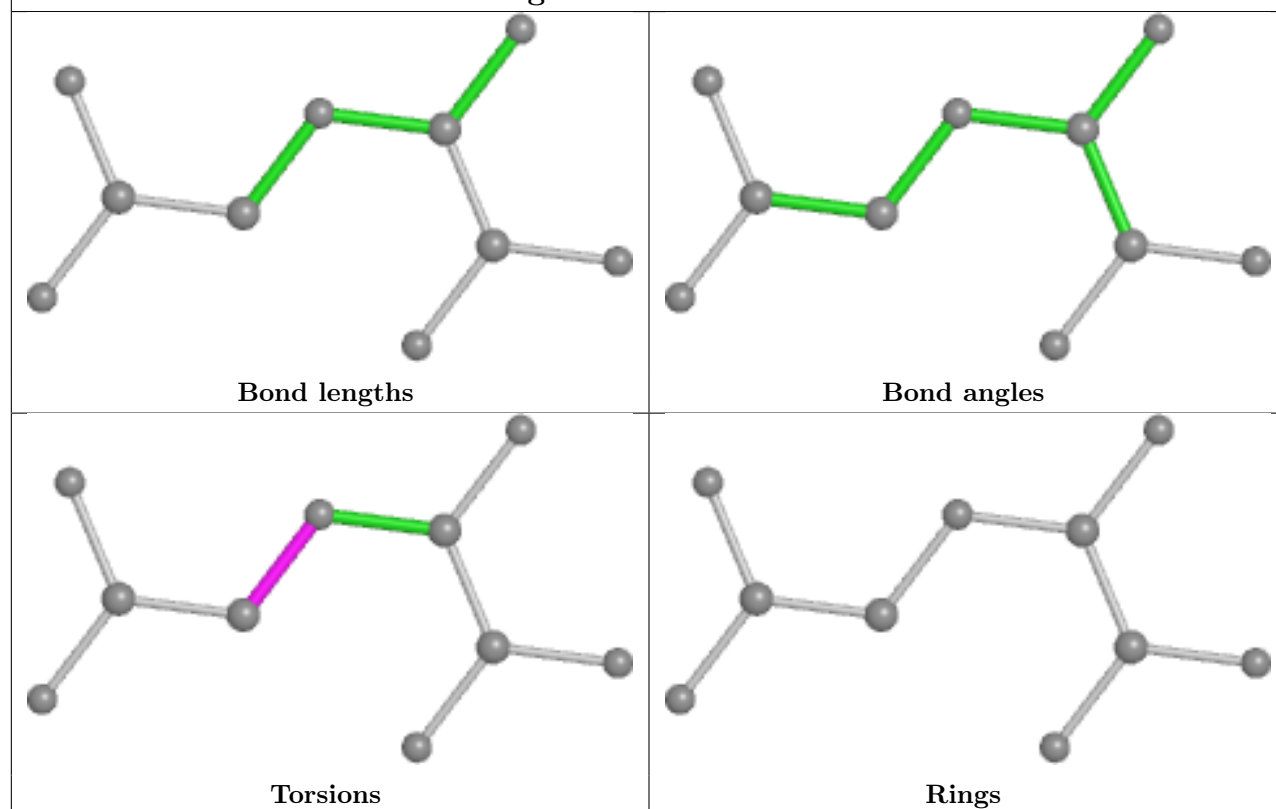




## Ligand OGA I 302



## Ligand OGA A 302



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [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	214/220 (97%)	-0.10	0 <a href="#">100</a> <a href="#">100</a>	32, 41, 57, 63	0
1	C	218/220 (99%)	-0.13	1 (0%) <a href="#">91</a> <a href="#">91</a>	34, 40, 57, 84	0
1	E	216/220 (98%)	-0.05	0 <a href="#">100</a> <a href="#">100</a>	35, 45, 62, 99	0
1	G	219/220 (99%)	-0.12	0 <a href="#">100</a> <a href="#">100</a>	34, 46, 63, 82	0
1	I	218/220 (99%)	0.02	3 (1%) <a href="#">75</a> <a href="#">77</a>	40, 61, 81, 100	0
2	B	7/8 (87%)	-0.05	0 <a href="#">100</a> <a href="#">100</a>	42, 58, 94, 131	0
2	D	4/8 (50%)	0.03	0 <a href="#">100</a> <a href="#">100</a>	45, 47, 60, 102	0
2	F	7/8 (87%)	0.08	0 <a href="#">100</a> <a href="#">100</a>	50, 61, 102, 133	0
2	H	3/8 (37%)	-0.71	0 <a href="#">100</a> <a href="#">100</a>	54, 54, 60, 64	0
2	J	3/8 (37%)	-0.39	0 <a href="#">100</a> <a href="#">100</a>	62, 62, 76, 77	0
All	All	1109/1140 (97%)	-0.08	4 (0%) <a href="#">92</a> <a href="#">93</a>	32, 45, 72, 133	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	292	LEU	3.5
1	C	148	ARG	2.5
1	I	160	ASP	2.4
1	I	171	LEU	2.2

### 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( $\text{\AA}^2$ )	Q<0.9
2	6MZ	D	4	23/24	0.97	0.13	34,37,41,41	0
2	6MZ	H	4	23/24	0.97	0.14	43,45,50,54	0
2	6MZ	J	4	23/24	0.97	0.15	48,51,54,58	0
2	6MZ	B	4	23/24	0.98	0.13	33,37,38,39	0
2	6MZ	F	4	23/24	0.98	0.13	39,41,45,46	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

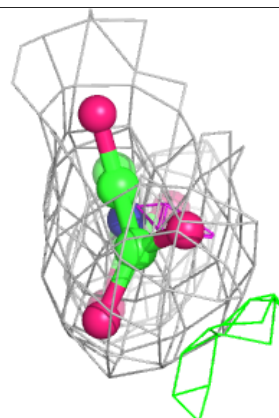
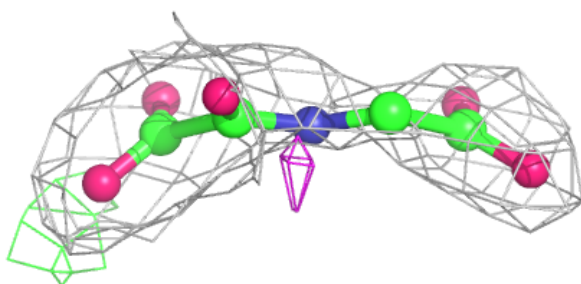
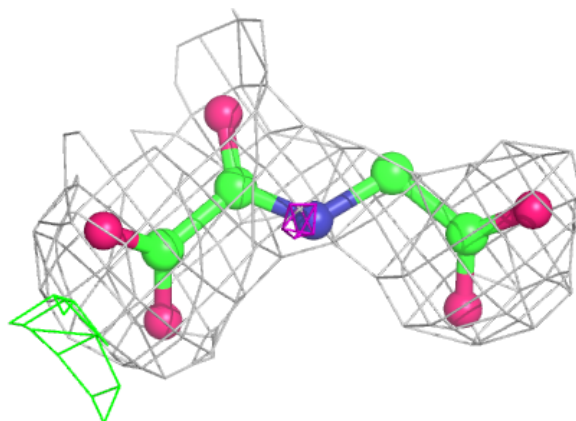
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
5	FMT	C	303	3/3	0.91	0.18	38,38,39,44	0
4	OGA	I	302	10/10	0.92	0.20	46,52,54,57	0
4	OGA	G	302	10/10	0.93	0.19	48,51,56,57	0
4	OGA	A	302	10/10	0.95	0.17	36,42,47,47	0
3	MN	A	301	1/1	0.95	0.23	54,54,54,54	0
4	OGA	E	302	10/10	0.96	0.17	42,45,46,51	0
4	OGA	C	302	10/10	0.96	0.17	44,47,56,57	0
3	MN	C	301	1/1	0.98	0.14	44,44,44,44	0
3	MN	E	301	1/1	0.98	0.11	43,43,43,43	0
3	MN	G	301	1/1	0.99	0.12	41,41,41,41	0
3	MN	I	301	1/1	0.99	0.11	36,36,36,36	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around OGA I 302:**

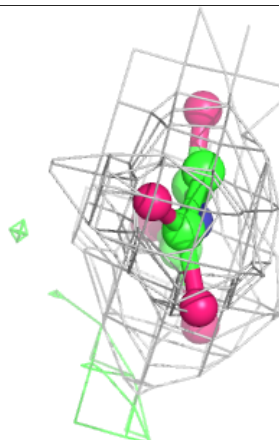
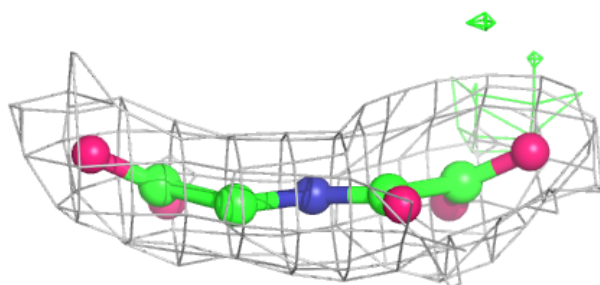
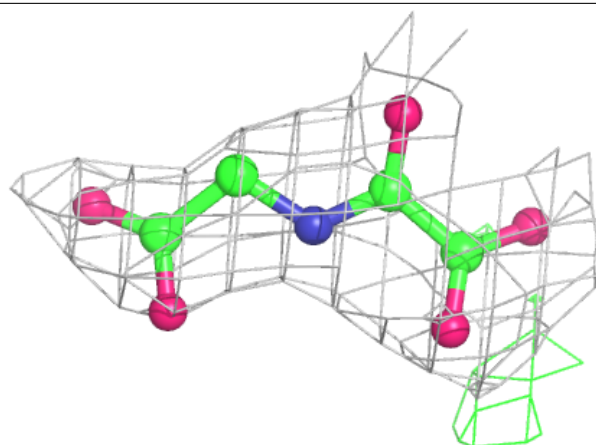
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



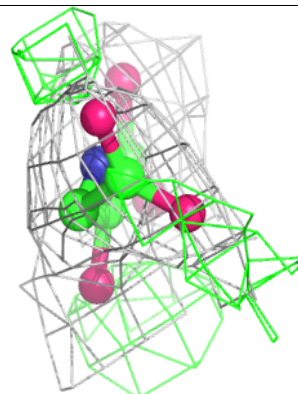
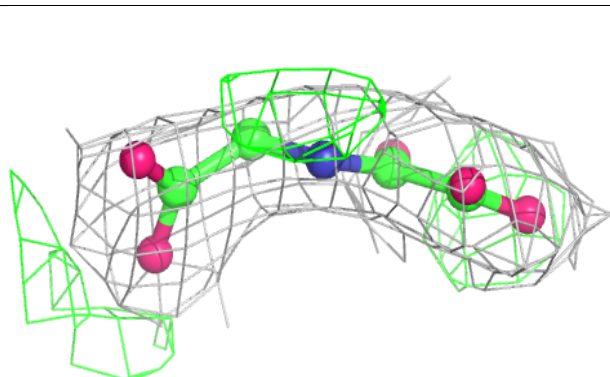
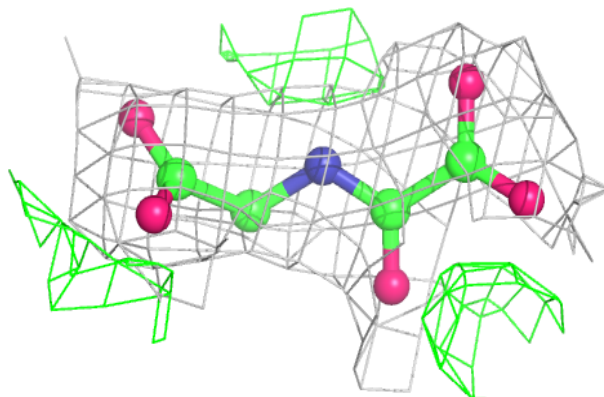


**Electron density around OGA G 302:**

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

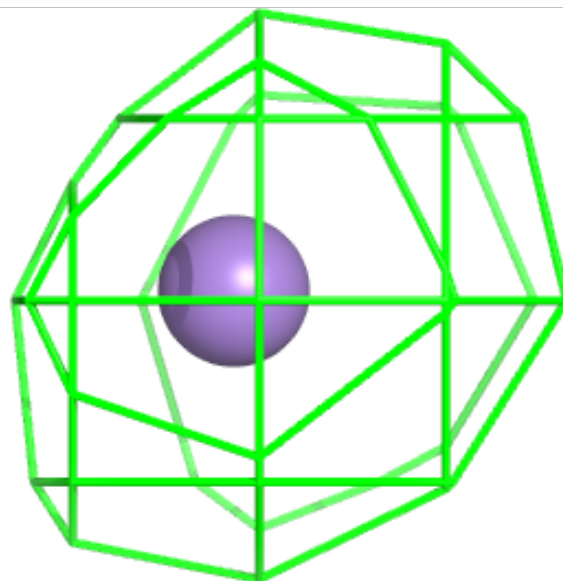
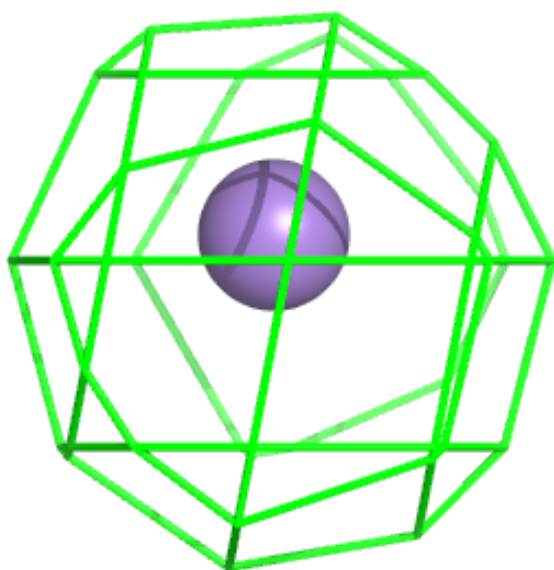
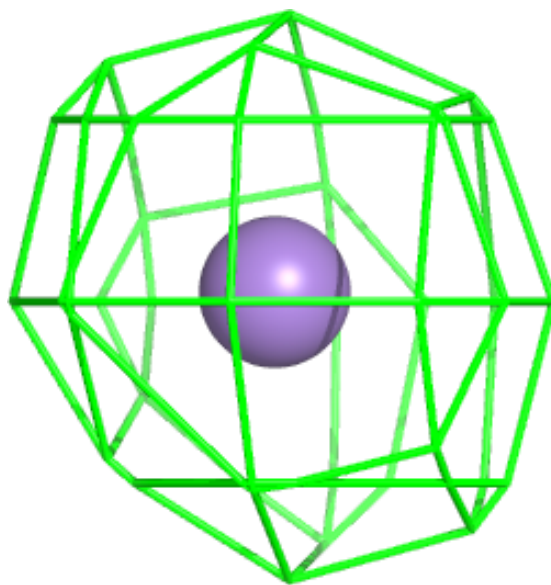
**Electron density around OGA A 302:**

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



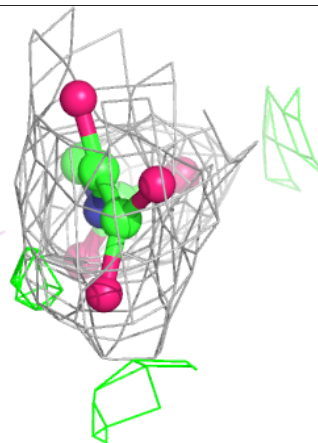
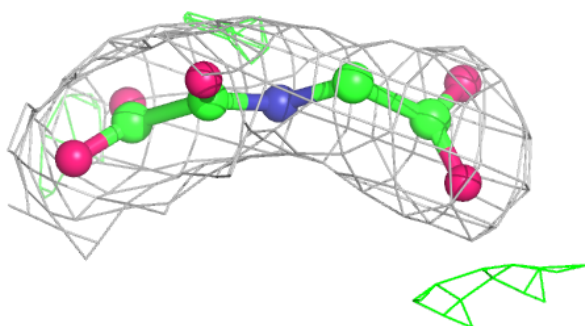
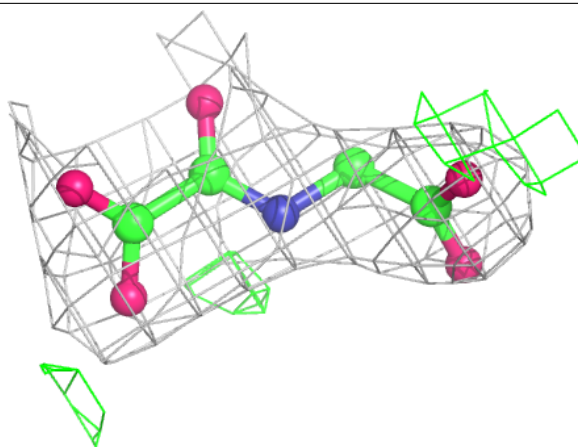
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and green (positive)



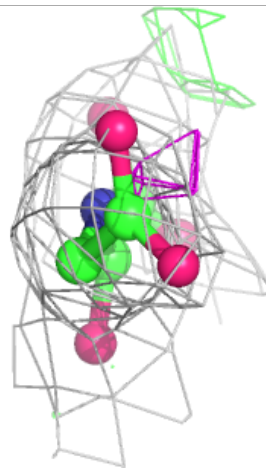
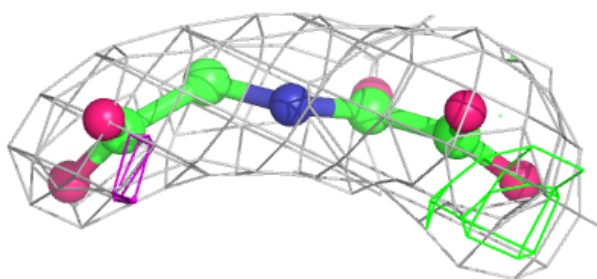
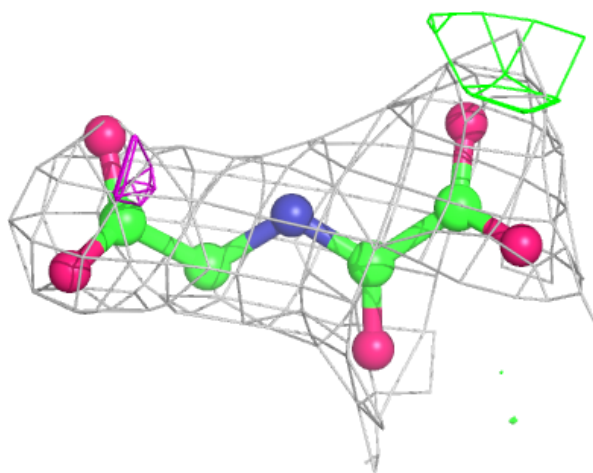
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and green (positive)



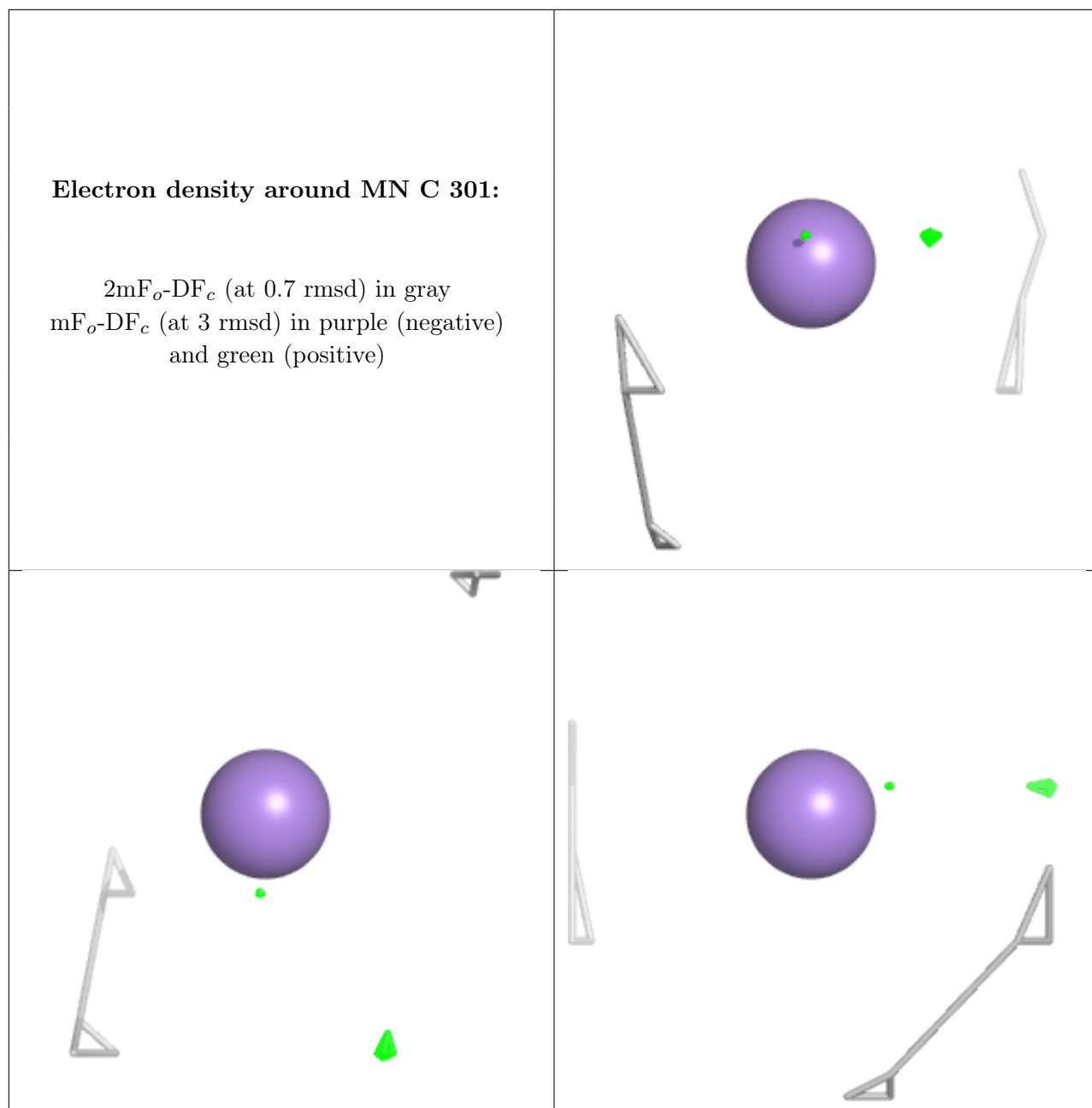
**Electron density around OGA C 302:**

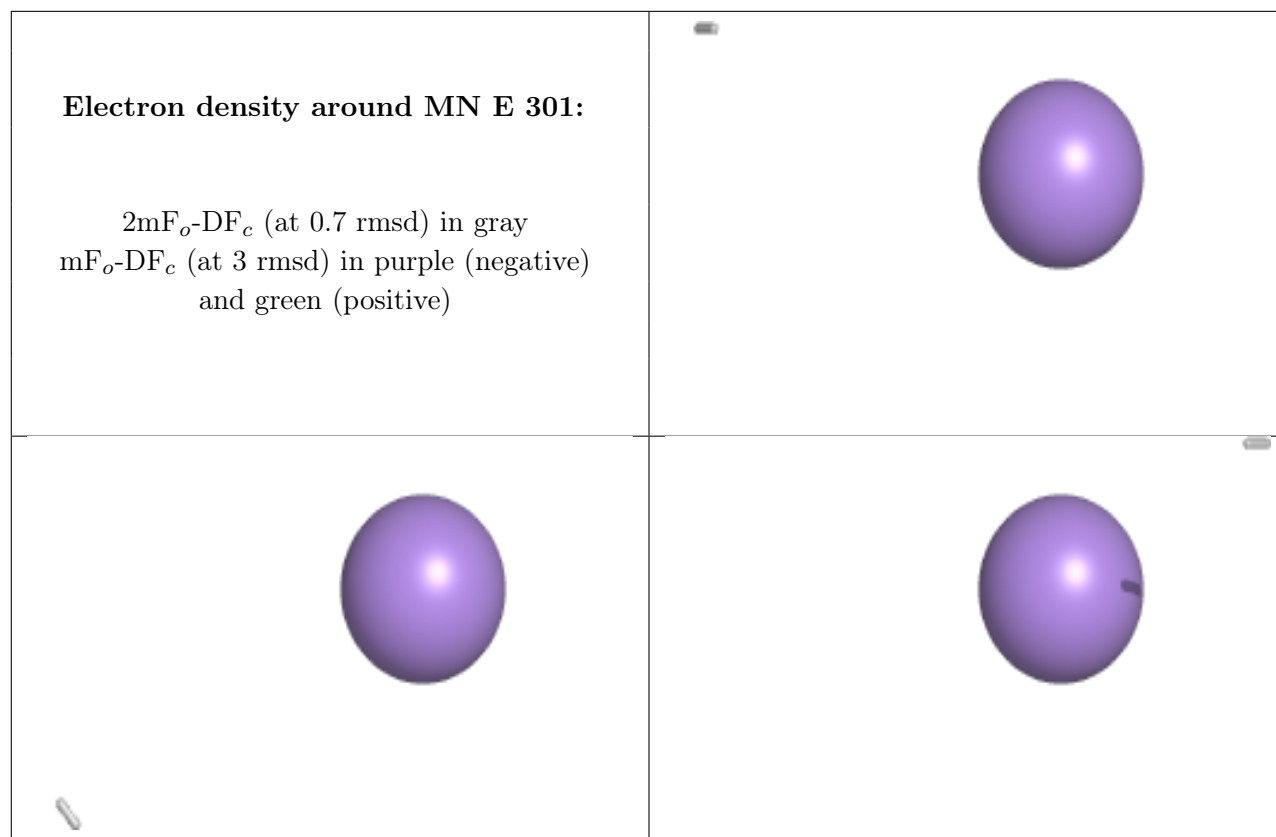
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

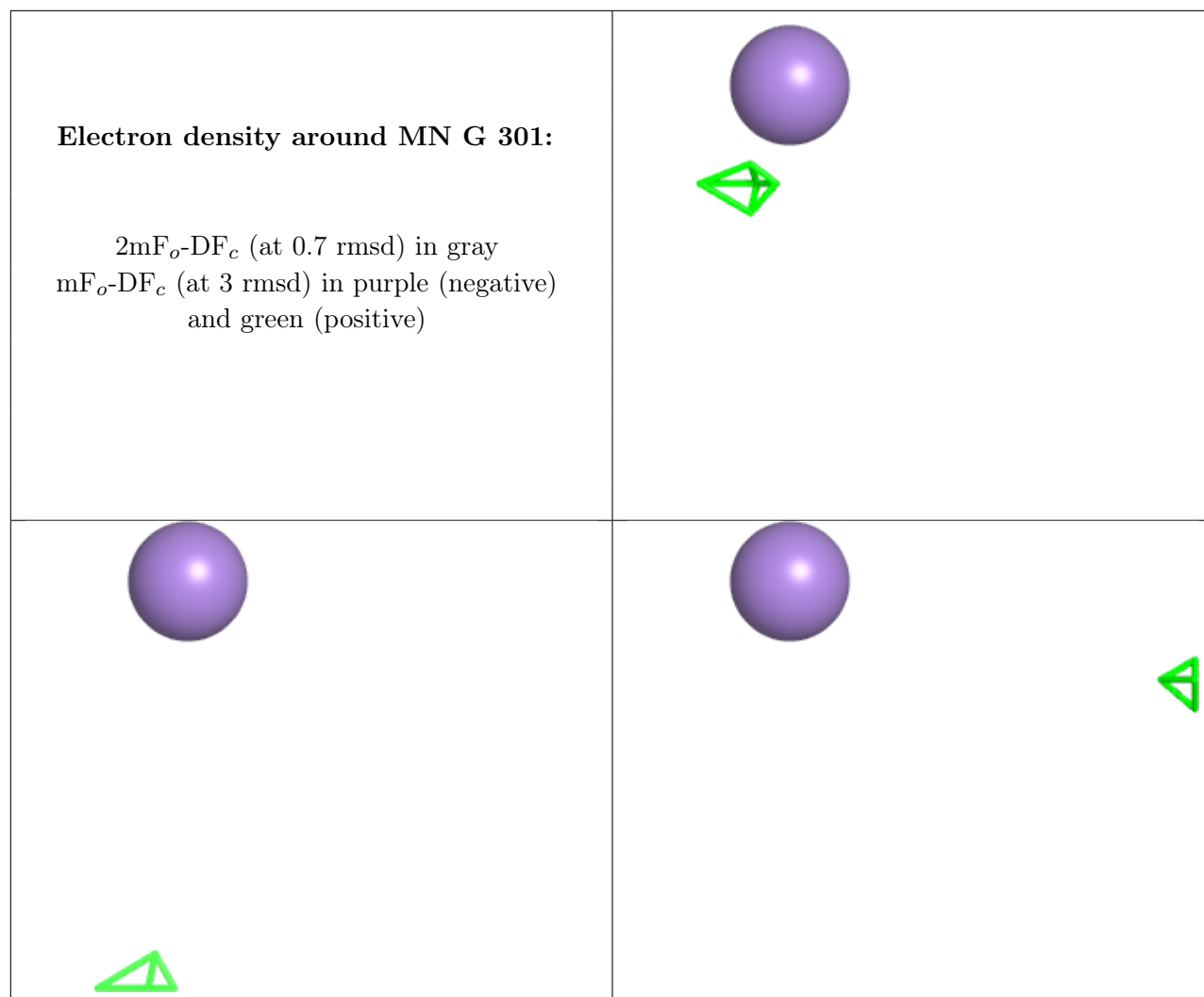


**Electron density around MN C 301:**

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

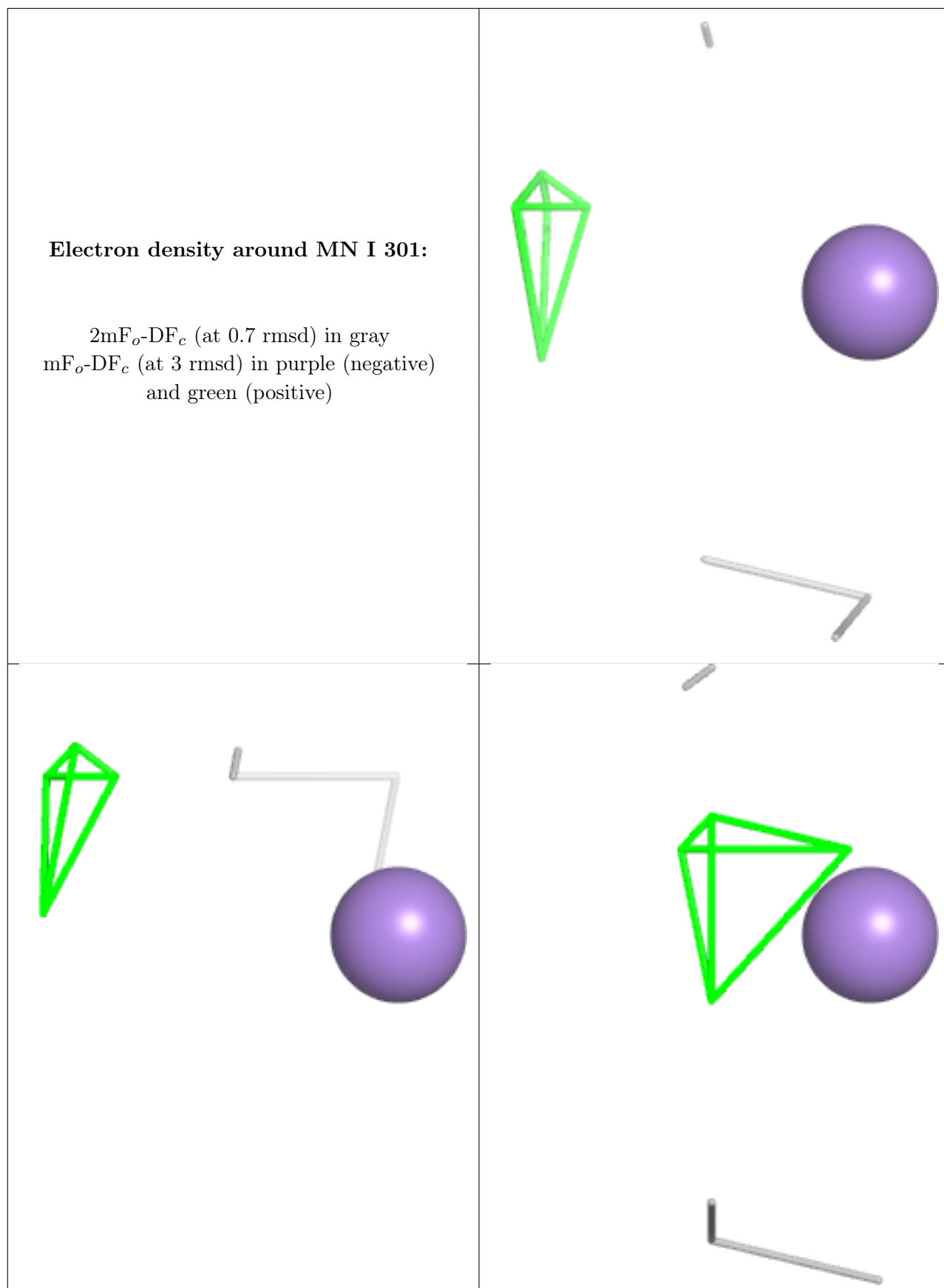






**Electron density around MN I 301:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.