



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2025 – 11:31 am BST

PDB ID : 9HHY / pdb\_00009hhY  
Title : Crystal Structure of the Coxiella burnetii 2-methylisocitrate lyase Bound to Inhibitor Isocitric Acid  
Authors : Stuart, W.; Isupov, M.; Harmer, N.J.  
Deposited on : 2024-11-22  
Resolution : 2.33 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 : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.4, CSD as541be (2020)  
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) : 2.45.1

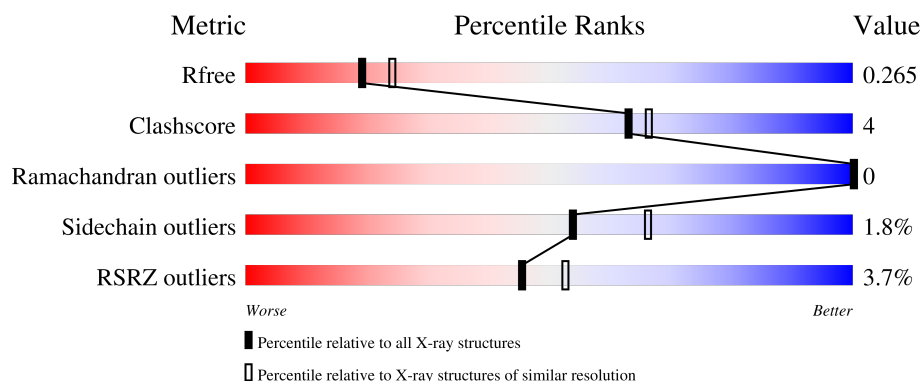
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.33 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	2747 (2.36-2.32)
Clashscore	180529	2936 (2.36-2.32)
Ramachandran outliers	177936	2912 (2.36-2.32)
Sidechain outliers	177891	2912 (2.36-2.32)
RSRZ outliers	164620	2747 (2.36-2.32)

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	312	<div> <div>6%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>7%</div> </div> </div>
1	B	312	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>8%</div> <div>8%</div> </div> </div>
1	C	312	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>7%</div> <div>8%</div> </div> </div>
1	D	312	<div> <div></div> <div> <div></div> <div>85%</div> <div>8%</div> <div>6%</div> </div> </div>
1	E	312	<div> <div>14%</div> <div> <div></div> <div>82%</div> <div>9%</div> <div>8%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	312	
1	G	312	
1	H	312	
1	I	312	
1	J	312	
1	K	312	
1	L	312	

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
3	EDO	D	308	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 27733 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 2-methylisocitrate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2242	1422	389	418	13			
1	B	287	Total	C	N	O	S	0	0	0
			2199	1392	381	413	13			
1	C	288	Total	C	N	O	S	0	0	0
			2210	1398	385	414	13			
1	D	292	Total	C	N	O	S	0	0	0
			2250	1428	390	419	13			
1	E	286	Total	C	N	O	S	0	0	0
			2190	1386	379	412	13			
1	F	287	Total	C	N	O	S	0	0	0
			2201	1393	383	412	13			
1	G	286	Total	C	N	O	S	0	0	0
			2190	1387	379	411	13			
1	H	287	Total	C	N	O	S	0	0	0
			2201	1393	383	412	13			
1	I	289	Total	C	N	O	S	0	0	0
			2222	1410	383	416	13			
1	J	288	Total	C	N	O	S	0	0	0
			2210	1398	385	414	13			
1	K	288	Total	C	N	O	S	0	0	0
			2210	1398	385	414	13			
1	L	287	Total	C	N	O	S	0	0	0
			2201	1393	383	412	13			

There are 264 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP Q83DG5
A	-20	HIS	-	expression tag	UNP Q83DG5
A	-19	HIS	-	expression tag	UNP Q83DG5
A	-18	HIS	-	expression tag	UNP Q83DG5
A	-17	HIS	-	expression tag	UNP Q83DG5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	HIS	-	expression tag	UNP Q83DG5
A	-15	HIS	-	expression tag	UNP Q83DG5
A	-14	SER	-	expression tag	UNP Q83DG5
A	-13	SER	-	expression tag	UNP Q83DG5
A	-12	GLY	-	expression tag	UNP Q83DG5
A	-11	VAL	-	expression tag	UNP Q83DG5
A	-10	ASP	-	expression tag	UNP Q83DG5
A	-9	LEU	-	expression tag	UNP Q83DG5
A	-8	GLY	-	expression tag	UNP Q83DG5
A	-7	THR	-	expression tag	UNP Q83DG5
A	-6	GLU	-	expression tag	UNP Q83DG5
A	-5	ASN	-	expression tag	UNP Q83DG5
A	-4	LEU	-	expression tag	UNP Q83DG5
A	-3	TYR	-	expression tag	UNP Q83DG5
A	-2	PHE	-	expression tag	UNP Q83DG5
A	-1	GLN	-	expression tag	UNP Q83DG5
A	0	SER	-	expression tag	UNP Q83DG5
B	-21	MET	-	initiating methionine	UNP Q83DG5
B	-20	HIS	-	expression tag	UNP Q83DG5
B	-19	HIS	-	expression tag	UNP Q83DG5
B	-18	HIS	-	expression tag	UNP Q83DG5
B	-17	HIS	-	expression tag	UNP Q83DG5
B	-16	HIS	-	expression tag	UNP Q83DG5
B	-15	HIS	-	expression tag	UNP Q83DG5
B	-14	SER	-	expression tag	UNP Q83DG5
B	-13	SER	-	expression tag	UNP Q83DG5
B	-12	GLY	-	expression tag	UNP Q83DG5
B	-11	VAL	-	expression tag	UNP Q83DG5
B	-10	ASP	-	expression tag	UNP Q83DG5
B	-9	LEU	-	expression tag	UNP Q83DG5
B	-8	GLY	-	expression tag	UNP Q83DG5
B	-7	THR	-	expression tag	UNP Q83DG5
B	-6	GLU	-	expression tag	UNP Q83DG5
B	-5	ASN	-	expression tag	UNP Q83DG5
B	-4	LEU	-	expression tag	UNP Q83DG5
B	-3	TYR	-	expression tag	UNP Q83DG5
B	-2	PHE	-	expression tag	UNP Q83DG5
B	-1	GLN	-	expression tag	UNP Q83DG5
B	0	SER	-	expression tag	UNP Q83DG5
C	-21	MET	-	initiating methionine	UNP Q83DG5
C	-20	HIS	-	expression tag	UNP Q83DG5
C	-19	HIS	-	expression tag	UNP Q83DG5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	HIS	-	expression tag	UNP Q83DG5
C	-17	HIS	-	expression tag	UNP Q83DG5
C	-16	HIS	-	expression tag	UNP Q83DG5
C	-15	HIS	-	expression tag	UNP Q83DG5
C	-14	SER	-	expression tag	UNP Q83DG5
C	-13	SER	-	expression tag	UNP Q83DG5
C	-12	GLY	-	expression tag	UNP Q83DG5
C	-11	VAL	-	expression tag	UNP Q83DG5
C	-10	ASP	-	expression tag	UNP Q83DG5
C	-9	LEU	-	expression tag	UNP Q83DG5
C	-8	GLY	-	expression tag	UNP Q83DG5
C	-7	THR	-	expression tag	UNP Q83DG5
C	-6	GLU	-	expression tag	UNP Q83DG5
C	-5	ASN	-	expression tag	UNP Q83DG5
C	-4	LEU	-	expression tag	UNP Q83DG5
C	-3	TYR	-	expression tag	UNP Q83DG5
C	-2	PHE	-	expression tag	UNP Q83DG5
C	-1	GLN	-	expression tag	UNP Q83DG5
C	0	SER	-	expression tag	UNP Q83DG5
D	-21	MET	-	initiating methionine	UNP Q83DG5
D	-20	HIS	-	expression tag	UNP Q83DG5
D	-19	HIS	-	expression tag	UNP Q83DG5
D	-18	HIS	-	expression tag	UNP Q83DG5
D	-17	HIS	-	expression tag	UNP Q83DG5
D	-16	HIS	-	expression tag	UNP Q83DG5
D	-15	HIS	-	expression tag	UNP Q83DG5
D	-14	SER	-	expression tag	UNP Q83DG5
D	-13	SER	-	expression tag	UNP Q83DG5
D	-12	GLY	-	expression tag	UNP Q83DG5
D	-11	VAL	-	expression tag	UNP Q83DG5
D	-10	ASP	-	expression tag	UNP Q83DG5
D	-9	LEU	-	expression tag	UNP Q83DG5
D	-8	GLY	-	expression tag	UNP Q83DG5
D	-7	THR	-	expression tag	UNP Q83DG5
D	-6	GLU	-	expression tag	UNP Q83DG5
D	-5	ASN	-	expression tag	UNP Q83DG5
D	-4	LEU	-	expression tag	UNP Q83DG5
D	-3	TYR	-	expression tag	UNP Q83DG5
D	-2	PHE	-	expression tag	UNP Q83DG5
D	-1	GLN	-	expression tag	UNP Q83DG5
D	0	SER	-	expression tag	UNP Q83DG5
E	-21	MET	-	initiating methionine	UNP Q83DG5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-20	HIS	-	expression tag	UNP Q83DG5
E	-19	HIS	-	expression tag	UNP Q83DG5
E	-18	HIS	-	expression tag	UNP Q83DG5
E	-17	HIS	-	expression tag	UNP Q83DG5
E	-16	HIS	-	expression tag	UNP Q83DG5
E	-15	HIS	-	expression tag	UNP Q83DG5
E	-14	SER	-	expression tag	UNP Q83DG5
E	-13	SER	-	expression tag	UNP Q83DG5
E	-12	GLY	-	expression tag	UNP Q83DG5
E	-11	VAL	-	expression tag	UNP Q83DG5
E	-10	ASP	-	expression tag	UNP Q83DG5
E	-9	LEU	-	expression tag	UNP Q83DG5
E	-8	GLY	-	expression tag	UNP Q83DG5
E	-7	THR	-	expression tag	UNP Q83DG5
E	-6	GLU	-	expression tag	UNP Q83DG5
E	-5	ASN	-	expression tag	UNP Q83DG5
E	-4	LEU	-	expression tag	UNP Q83DG5
E	-3	TYR	-	expression tag	UNP Q83DG5
E	-2	PHE	-	expression tag	UNP Q83DG5
E	-1	GLN	-	expression tag	UNP Q83DG5
E	0	SER	-	expression tag	UNP Q83DG5
F	-21	MET	-	initiating methionine	UNP Q83DG5
F	-20	HIS	-	expression tag	UNP Q83DG5
F	-19	HIS	-	expression tag	UNP Q83DG5
F	-18	HIS	-	expression tag	UNP Q83DG5
F	-17	HIS	-	expression tag	UNP Q83DG5
F	-16	HIS	-	expression tag	UNP Q83DG5
F	-15	HIS	-	expression tag	UNP Q83DG5
F	-14	SER	-	expression tag	UNP Q83DG5
F	-13	SER	-	expression tag	UNP Q83DG5
F	-12	GLY	-	expression tag	UNP Q83DG5
F	-11	VAL	-	expression tag	UNP Q83DG5
F	-10	ASP	-	expression tag	UNP Q83DG5
F	-9	LEU	-	expression tag	UNP Q83DG5
F	-8	GLY	-	expression tag	UNP Q83DG5
F	-7	THR	-	expression tag	UNP Q83DG5
F	-6	GLU	-	expression tag	UNP Q83DG5
F	-5	ASN	-	expression tag	UNP Q83DG5
F	-4	LEU	-	expression tag	UNP Q83DG5
F	-3	TYR	-	expression tag	UNP Q83DG5
F	-2	PHE	-	expression tag	UNP Q83DG5
F	-1	GLN	-	expression tag	UNP Q83DG5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	SER	-	expression tag	UNP Q83DG5
G	-21	MET	-	initiating methionine	UNP Q83DG5
G	-20	HIS	-	expression tag	UNP Q83DG5
G	-19	HIS	-	expression tag	UNP Q83DG5
G	-18	HIS	-	expression tag	UNP Q83DG5
G	-17	HIS	-	expression tag	UNP Q83DG5
G	-16	HIS	-	expression tag	UNP Q83DG5
G	-15	HIS	-	expression tag	UNP Q83DG5
G	-14	SER	-	expression tag	UNP Q83DG5
G	-13	SER	-	expression tag	UNP Q83DG5
G	-12	GLY	-	expression tag	UNP Q83DG5
G	-11	VAL	-	expression tag	UNP Q83DG5
G	-10	ASP	-	expression tag	UNP Q83DG5
G	-9	LEU	-	expression tag	UNP Q83DG5
G	-8	GLY	-	expression tag	UNP Q83DG5
G	-7	THR	-	expression tag	UNP Q83DG5
G	-6	GLU	-	expression tag	UNP Q83DG5
G	-5	ASN	-	expression tag	UNP Q83DG5
G	-4	LEU	-	expression tag	UNP Q83DG5
G	-3	TYR	-	expression tag	UNP Q83DG5
G	-2	PHE	-	expression tag	UNP Q83DG5
G	-1	GLN	-	expression tag	UNP Q83DG5
G	0	SER	-	expression tag	UNP Q83DG5
H	-21	MET	-	initiating methionine	UNP Q83DG5
H	-20	HIS	-	expression tag	UNP Q83DG5
H	-19	HIS	-	expression tag	UNP Q83DG5
H	-18	HIS	-	expression tag	UNP Q83DG5
H	-17	HIS	-	expression tag	UNP Q83DG5
H	-16	HIS	-	expression tag	UNP Q83DG5
H	-15	HIS	-	expression tag	UNP Q83DG5
H	-14	SER	-	expression tag	UNP Q83DG5
H	-13	SER	-	expression tag	UNP Q83DG5
H	-12	GLY	-	expression tag	UNP Q83DG5
H	-11	VAL	-	expression tag	UNP Q83DG5
H	-10	ASP	-	expression tag	UNP Q83DG5
H	-9	LEU	-	expression tag	UNP Q83DG5
H	-8	GLY	-	expression tag	UNP Q83DG5
H	-7	THR	-	expression tag	UNP Q83DG5
H	-6	GLU	-	expression tag	UNP Q83DG5
H	-5	ASN	-	expression tag	UNP Q83DG5
H	-4	LEU	-	expression tag	UNP Q83DG5
H	-3	TYR	-	expression tag	UNP Q83DG5

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-2	PHE	-	expression tag	UNP Q83DG5
H	-1	GLN	-	expression tag	UNP Q83DG5
H	0	SER	-	expression tag	UNP Q83DG5
I	-21	MET	-	initiating methionine	UNP Q83DG5
I	-20	HIS	-	expression tag	UNP Q83DG5
I	-19	HIS	-	expression tag	UNP Q83DG5
I	-18	HIS	-	expression tag	UNP Q83DG5
I	-17	HIS	-	expression tag	UNP Q83DG5
I	-16	HIS	-	expression tag	UNP Q83DG5
I	-15	HIS	-	expression tag	UNP Q83DG5
I	-14	SER	-	expression tag	UNP Q83DG5
I	-13	SER	-	expression tag	UNP Q83DG5
I	-12	GLY	-	expression tag	UNP Q83DG5
I	-11	VAL	-	expression tag	UNP Q83DG5
I	-10	ASP	-	expression tag	UNP Q83DG5
I	-9	LEU	-	expression tag	UNP Q83DG5
I	-8	GLY	-	expression tag	UNP Q83DG5
I	-7	THR	-	expression tag	UNP Q83DG5
I	-6	GLU	-	expression tag	UNP Q83DG5
I	-5	ASN	-	expression tag	UNP Q83DG5
I	-4	LEU	-	expression tag	UNP Q83DG5
I	-3	TYR	-	expression tag	UNP Q83DG5
I	-2	PHE	-	expression tag	UNP Q83DG5
I	-1	GLN	-	expression tag	UNP Q83DG5
I	0	SER	-	expression tag	UNP Q83DG5
J	-21	MET	-	initiating methionine	UNP Q83DG5
J	-20	HIS	-	expression tag	UNP Q83DG5
J	-19	HIS	-	expression tag	UNP Q83DG5
J	-18	HIS	-	expression tag	UNP Q83DG5
J	-17	HIS	-	expression tag	UNP Q83DG5
J	-16	HIS	-	expression tag	UNP Q83DG5
J	-15	HIS	-	expression tag	UNP Q83DG5
J	-14	SER	-	expression tag	UNP Q83DG5
J	-13	SER	-	expression tag	UNP Q83DG5
J	-12	GLY	-	expression tag	UNP Q83DG5
J	-11	VAL	-	expression tag	UNP Q83DG5
J	-10	ASP	-	expression tag	UNP Q83DG5
J	-9	LEU	-	expression tag	UNP Q83DG5
J	-8	GLY	-	expression tag	UNP Q83DG5
J	-7	THR	-	expression tag	UNP Q83DG5
J	-6	GLU	-	expression tag	UNP Q83DG5
J	-5	ASN	-	expression tag	UNP Q83DG5

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-4	LEU	-	expression tag	UNP Q83DG5
J	-3	TYR	-	expression tag	UNP Q83DG5
J	-2	PHE	-	expression tag	UNP Q83DG5
J	-1	GLN	-	expression tag	UNP Q83DG5
J	0	SER	-	expression tag	UNP Q83DG5
K	-21	MET	-	initiating methionine	UNP Q83DG5
K	-20	HIS	-	expression tag	UNP Q83DG5
K	-19	HIS	-	expression tag	UNP Q83DG5
K	-18	HIS	-	expression tag	UNP Q83DG5
K	-17	HIS	-	expression tag	UNP Q83DG5
K	-16	HIS	-	expression tag	UNP Q83DG5
K	-15	HIS	-	expression tag	UNP Q83DG5
K	-14	SER	-	expression tag	UNP Q83DG5
K	-13	SER	-	expression tag	UNP Q83DG5
K	-12	GLY	-	expression tag	UNP Q83DG5
K	-11	VAL	-	expression tag	UNP Q83DG5
K	-10	ASP	-	expression tag	UNP Q83DG5
K	-9	LEU	-	expression tag	UNP Q83DG5
K	-8	GLY	-	expression tag	UNP Q83DG5
K	-7	THR	-	expression tag	UNP Q83DG5
K	-6	GLU	-	expression tag	UNP Q83DG5
K	-5	ASN	-	expression tag	UNP Q83DG5
K	-4	LEU	-	expression tag	UNP Q83DG5
K	-3	TYR	-	expression tag	UNP Q83DG5
K	-2	PHE	-	expression tag	UNP Q83DG5
K	-1	GLN	-	expression tag	UNP Q83DG5
K	0	SER	-	expression tag	UNP Q83DG5
L	-21	MET	-	initiating methionine	UNP Q83DG5
L	-20	HIS	-	expression tag	UNP Q83DG5
L	-19	HIS	-	expression tag	UNP Q83DG5
L	-18	HIS	-	expression tag	UNP Q83DG5
L	-17	HIS	-	expression tag	UNP Q83DG5
L	-16	HIS	-	expression tag	UNP Q83DG5
L	-15	HIS	-	expression tag	UNP Q83DG5
L	-14	SER	-	expression tag	UNP Q83DG5
L	-13	SER	-	expression tag	UNP Q83DG5
L	-12	GLY	-	expression tag	UNP Q83DG5
L	-11	VAL	-	expression tag	UNP Q83DG5
L	-10	ASP	-	expression tag	UNP Q83DG5
L	-9	LEU	-	expression tag	UNP Q83DG5
L	-8	GLY	-	expression tag	UNP Q83DG5
L	-7	THR	-	expression tag	UNP Q83DG5

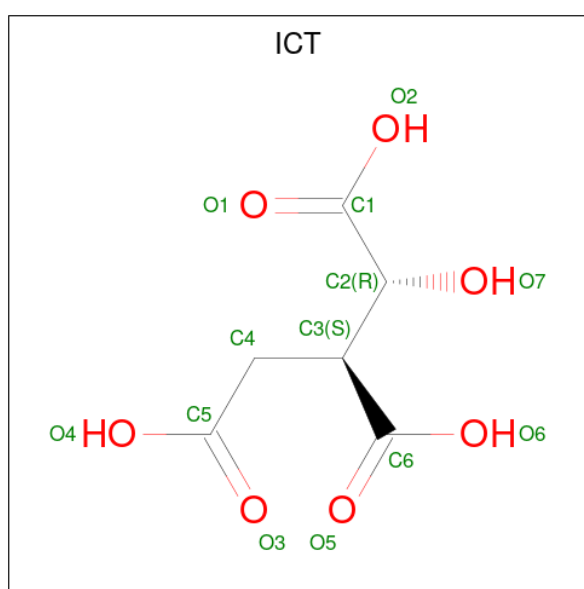
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Chain	Residue	Modelled	Actual	Comment	Reference
L	-6	GLU	-	expression tag	UNP Q83DG5
L	-5	ASN	-	expression tag	UNP Q83DG5
L	-4	LEU	-	expression tag	UNP Q83DG5
L	-3	TYR	-	expression tag	UNP Q83DG5
L	-2	PHE	-	expression tag	UNP Q83DG5
L	-1	GLN	-	expression tag	UNP Q83DG5
L	0	SER	-	expression tag	UNP Q83DG5

- Molecule 2 is ISOCITRIC ACID (CCD ID: ICT) (formula:  $C_6H_8O_7$ ) (labeled as "Ligand of Interest" by depositor).



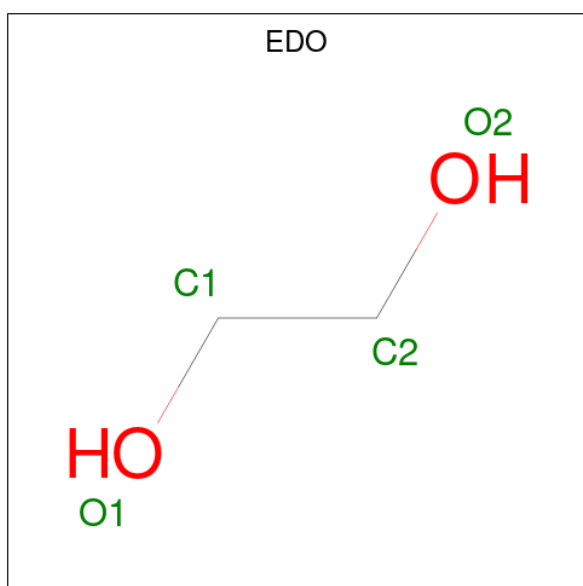
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 6 7	0	0
2	B	1	Total C O 13 6 7	0	0
2	C	1	Total C O 13 6 7	0	0
2	D	1	Total C O 13 6 7	0	0
2	E	1	Total C O 13 6 7	0	0
2	F	1	Total C O 13 6 7	0	0
2	G	1	Total C O 13 6 7	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	H	1	Total	C	O	0	0
			13	6	7		
2	I	1	Total	C	O	0	0
			13	6	7		
2	J	1	Total	C	O	0	0
			13	6	7		
2	K	1	Total	C	O	0	0
			13	6	7		
2	L	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	F	1	Total 4	C 2	O 2	0	0
3	F	1	Total 4	C 2	O 2	0	0
3	F	1	Total 4	C 2	O 2	0	0
3	G	1	Total 4	C 2	O 2	0	0
3	G	1	Total 4	C 2	O 2	0	0
3	G	1	Total 4	C 2	O 2	0	0
3	G	1	Total 4	C 2	O 2	0	0
3	G	1	Total 4	C 2	O 2	0	0
3	H	1	Total 4	C 2	O 2	0	0
3	H	1	Total 4	C 2	O 2	0	0
3	H	1	Total 4	C 2	O 2	0	0
3	H	1	Total 4	C 2	O 2	0	0
3	H	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	I	1	Total C O 4 2 2	0	0
3	J	1	Total C O 4 2 2	0	0
3	K	1	Total C O 4 2 2	0	0
3	L	1	Total C O 4 2 2	0	0
3	L	1	Total C O 4 2 2	0	0

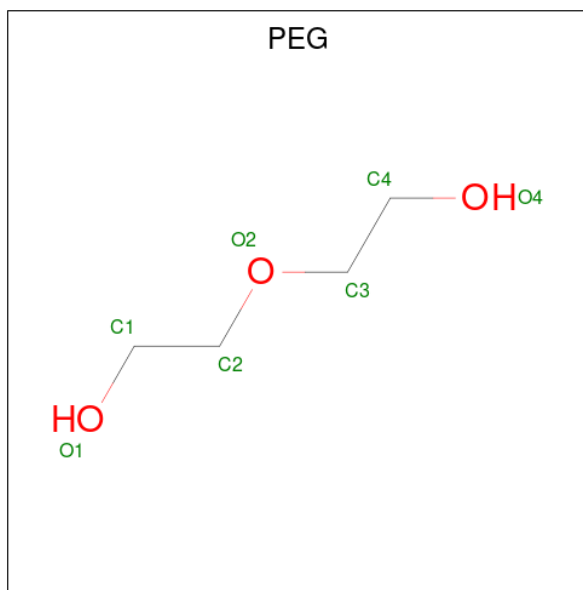
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0
4	G	1	Total Mg 1 1	0	0
4	H	1	Total Mg 1 1	0	0
4	I	1	Total Mg 1 1	0	0
4	J	1	Total Mg 1 1	0	0
4	K	1	Total Mg 1 1	0	0
4	L	1	Total Mg 1 1	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

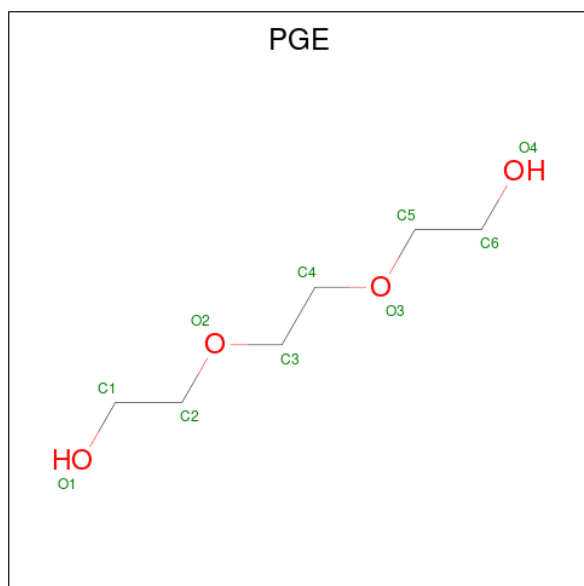
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0
5	B	1	Total Cl 1 1	0	0
5	C	1	Total Cl 1 1	0	0
5	D	1	Total Cl 1 1	0	0
5	E	1	Total Cl 1 1	0	0
5	F	1	Total Cl 1 1	0	0
5	G	1	Total Cl 1 1	0	0
5	H	1	Total Cl 1 1	0	0
5	I	1	Total Cl 1 1	0	0
5	J	1	Total Cl 1 1	0	0
5	K	1	Total Cl 1 1	0	0
5	L	2	Total Cl 2 2	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	J	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	97	Total	O	0	0
			97	97		
8	B	90	Total	O	0	0
			90	90		
8	C	90	Total	O	0	0
			90	90		
8	D	135	Total	O	0	0
			135	135		
8	E	24	Total	O	0	0
			24	24		
8	F	53	Total	O	0	0
			53	53		
8	G	73	Total	O	0	0
			73	73		
8	H	51	Total	O	0	0
			51	51		

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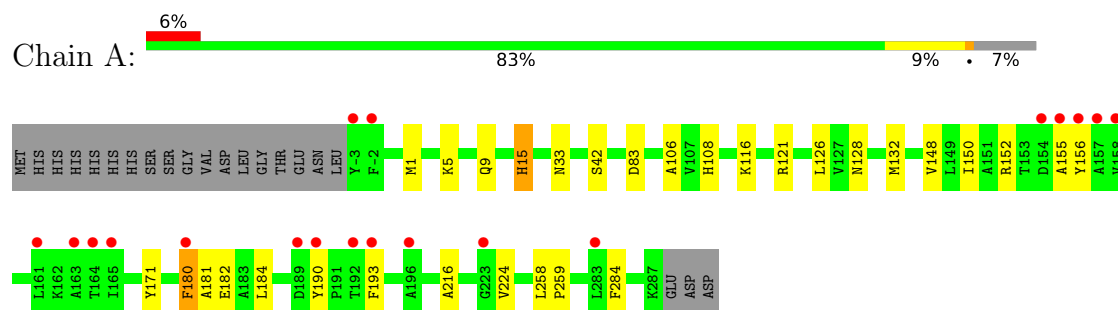
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	I	80	Total 80	O 80	0	0
8	J	86	Total 86	O 86	0	0
8	K	25	Total 25	O 25	0	0
8	L	77	Total 77	O 77	0	0

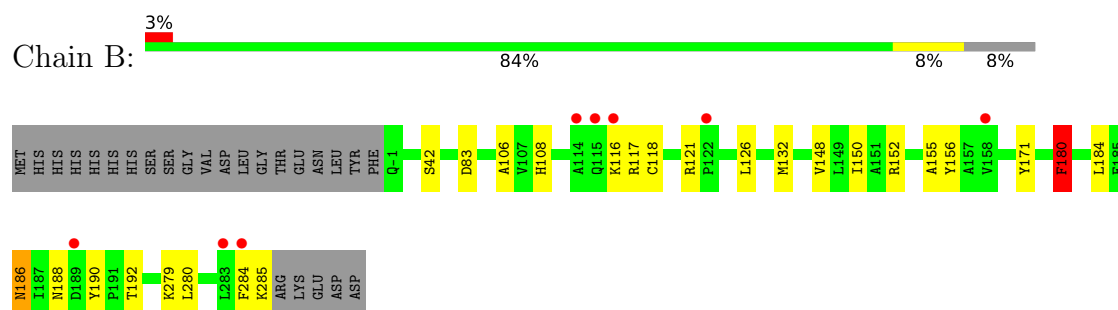
### 3 Residue-property plots

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.

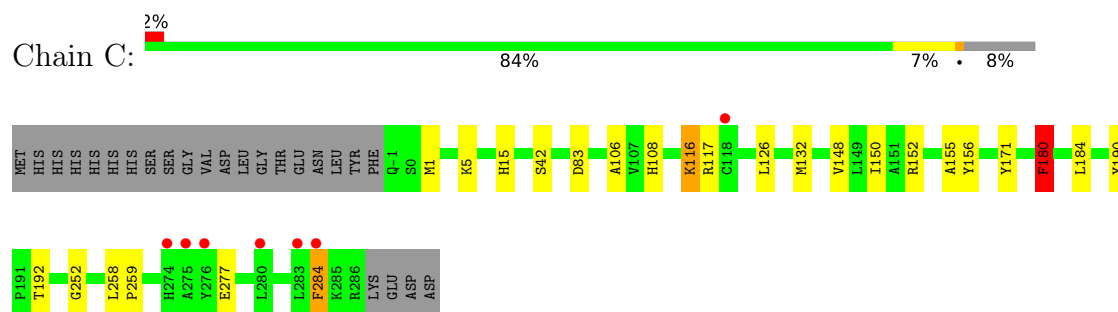
- Molecule 1: 2-methylisocitrate lyase



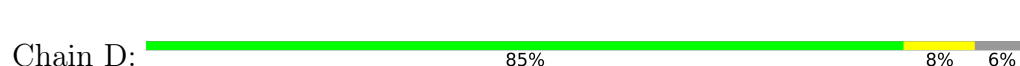
- Molecule 1: 2-methylisocitrate lyase

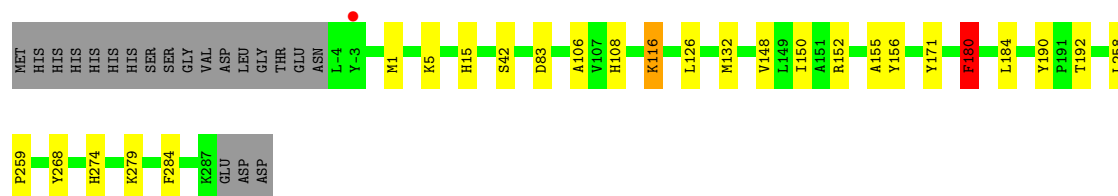


- Molecule 1: 2-methylisocitrate lyase

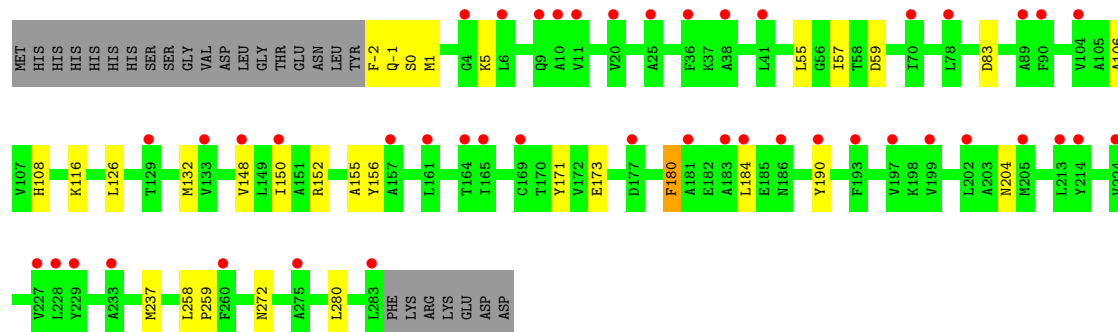
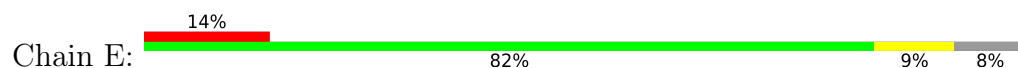


- Molecule 1: 2-methylisocitrate lyase

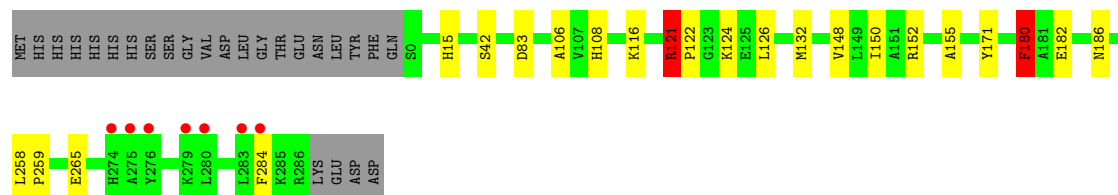
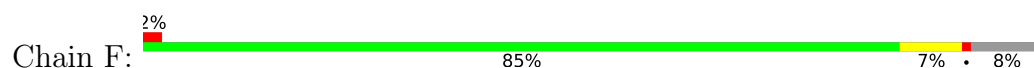




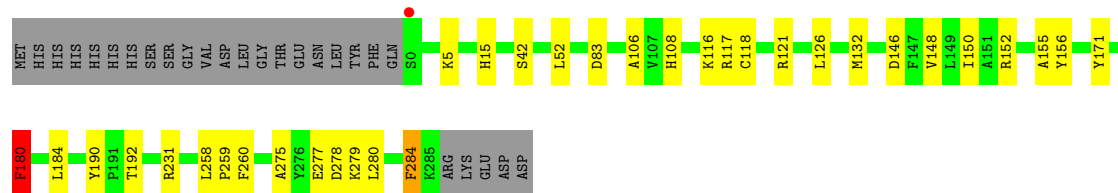
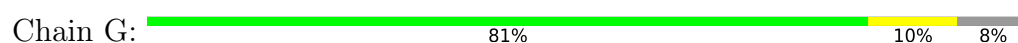
- Molecule 1: 2-methylisocitrate lyase



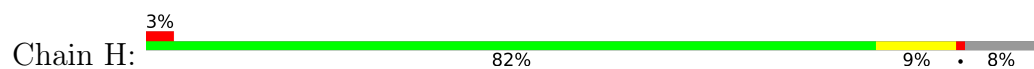
- Molecule 1: 2-methylisocitrate lyase

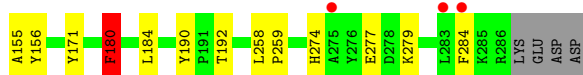


- Molecule 1: 2-methylisocitrate lyase

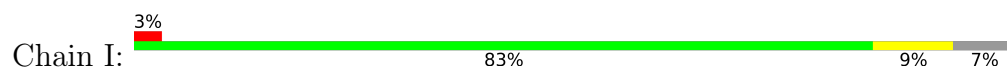


- Molecule 1: 2-methylisocitrate lyase

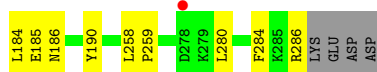
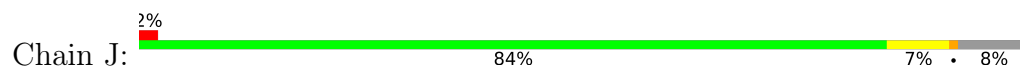




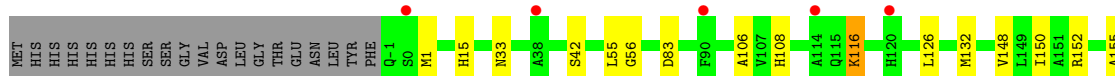
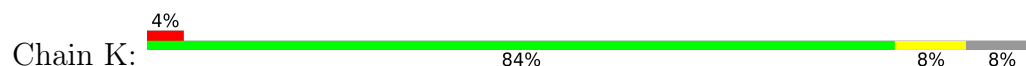
- Molecule 1: 2-methylisocitrate lyase



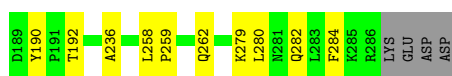
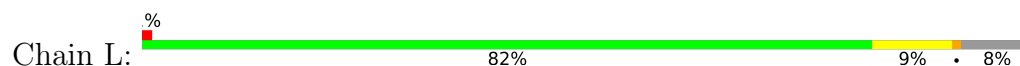
- Molecule 1: 2-methylisocitrate lyase



- Molecule 1: 2-methylisocitrate lyase



- Molecule 1: 2-methylisocitrate lyase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.78Å 115.55Å 195.24Å 90.00° 92.34° 90.00°	Depositor
Resolution (Å)	59.24 – 2.33 59.24 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.8 (59.24-2.33) 99.8 (59.24-2.33)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.04 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.214 , 0.265 0.214 , 0.265	Depositor DCC
$R_{free}$ test set	8849 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.9	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	27733	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.14% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ICT, PGE, EDO, PEG, CL

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	0.55	0/2282	1.01	2/3090 (0.1%)
1	B	0.55	0/2237	1.01	2/3031 (0.1%)
1	C	0.52	0/2248	0.99	3/3045 (0.1%)
1	D	0.54	0/2290	1.00	3/3101 (0.1%)
1	E	0.53	0/2228	1.01	2/3020 (0.1%)
1	F	0.51	0/2239	0.99	4/3033 (0.1%)
1	G	0.56	0/2228	1.04	3/3019 (0.1%)
1	H	0.52	0/2239	1.00	4/3033 (0.1%)
1	I	0.53	0/2262	1.03	5/3065 (0.2%)
1	J	0.53	0/2248	1.00	3/3045 (0.1%)
1	K	0.50	0/2248	0.98	3/3045 (0.1%)
1	L	0.57	0/2239	1.05	4/3033 (0.1%)
All	All	0.54	0/26988	1.01	38/36560 (0.1%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	121	ARG	CG-CD-NE	-7.11	96.36	112.00
1	L	118	CYS	CB-CA-C	6.25	120.59	110.96
1	E	-2	PHE	CA-CB-CG	6.11	119.91	113.80
1	G	15	HIS	CB-CA-C	5.87	120.00	111.02
1	A	15	HIS	CB-CA-C	5.83	119.95	111.02

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	2242	0	2256	18	0
1	B	2199	0	2212	17	0
1	C	2210	0	2225	17	0
1	D	2250	0	2267	26	0
1	E	2190	0	2199	21	0
1	F	2201	0	2217	17	0
1	G	2190	0	2204	23	0
1	H	2201	0	2217	19	0
1	I	2222	0	2230	21	0
1	J	2210	0	2225	22	0
1	K	2210	0	2225	16	0
1	L	2201	0	2217	20	0
2	A	13	0	5	1	0
2	B	13	0	5	0	0
2	C	13	0	5	0	0
2	D	13	0	5	0	0
2	E	13	0	5	1	0
2	F	13	0	5	1	0
2	G	13	0	5	0	0
2	H	13	0	5	0	0
2	I	13	0	5	0	0
2	J	13	0	5	1	0
2	K	13	0	5	0	0
2	L	13	0	5	0	0
3	A	8	0	12	0	0
3	B	16	0	24	0	0
3	C	4	0	6	0	0
3	D	28	0	42	6	0
3	F	12	0	18	0	0
3	G	20	0	30	1	0
3	H	20	0	30	0	0
3	I	4	0	6	0	0
3	J	4	0	6	0	0
3	K	4	0	6	0	0
3	L	8	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	2	0	0	0	0
6	E	7	0	10	0	0
7	J	10	0	14	0	0
8	A	97	0	0	5	0
8	B	90	0	0	3	0
8	C	90	0	0	0	0
8	D	135	0	0	0	0
8	E	24	0	0	1	0
8	F	53	0	0	2	0
8	G	73	0	0	5	0
8	H	51	0	0	1	0
8	I	80	0	0	5	0
8	J	86	0	0	2	0
8	K	25	0	0	3	0
8	L	77	0	0	1	0
All	All	27733	0	26970	211	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 4.

The worst 5 of 211 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:D:5:LYS:HD3	1:J:185:GLU:HB3	1.57	0.87
1:A:15:HIS:HB2	8:A:476:HOH:O	1.80	0.82
1:I:272:ASN:HB3	1:I:275:ALA:HB3	1.61	0.81
1:D:1:MET:HE2	1:D:5:LYS:HG2	1.62	0.81
1:E:57:ILE:HD11	1:H:90:PHE:HB2	1.63	0.79

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	289/312 (93%)	285 (99%)	4 (1%)	0	100	100
1	B	285/312 (91%)	281 (99%)	4 (1%)	0	100	100
1	C	286/312 (92%)	282 (99%)	4 (1%)	0	100	100
1	D	290/312 (93%)	286 (99%)	4 (1%)	0	100	100
1	E	284/312 (91%)	280 (99%)	4 (1%)	0	100	100
1	F	285/312 (91%)	281 (99%)	4 (1%)	0	100	100
1	G	284/312 (91%)	279 (98%)	5 (2%)	0	100	100
1	H	285/312 (91%)	281 (99%)	4 (1%)	0	100	100
1	I	287/312 (92%)	282 (98%)	5 (2%)	0	100	100
1	J	286/312 (92%)	282 (99%)	4 (1%)	0	100	100
1	K	286/312 (92%)	281 (98%)	5 (2%)	0	100	100
1	L	285/312 (91%)	279 (98%)	6 (2%)	0	100	100
All	All	3432/3744 (92%)	3379 (98%)	53 (2%)	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	231/250 (92%)	227 (98%)	4 (2%)	56	68
1	B	227/250 (91%)	223 (98%)	4 (2%)	54	66
1	C	228/250 (91%)	224 (98%)	4 (2%)	54	66
1	D	232/250 (93%)	227 (98%)	5 (2%)	47	58
1	E	226/250 (90%)	225 (100%)	1 (0%)	89	94
1	F	227/250 (91%)	223 (98%)	4 (2%)	54	66
1	G	226/250 (90%)	223 (99%)	3 (1%)	65	77
1	H	227/250 (91%)	221 (97%)	6 (3%)	41	51
1	I	229/250 (92%)	226 (99%)	3 (1%)	65	77
1	J	228/250 (91%)	224 (98%)	4 (2%)	54	66
1	K	228/250 (91%)	223 (98%)	5 (2%)	47	58
1	L	227/250 (91%)	221 (97%)	6 (3%)	41	51
All	All	2736/3000 (91%)	2687 (98%)	49 (2%)	54	66

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	180	PHE
1	J	116	LYS
1	H	192	THR
1	I	42	SER
1	J	286	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	115	GLN
1	L	282	GLN
1	J	75	HIS
1	L	103	GLN

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Mol	Chain	Res	Type
1	E	115	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 ⓘ

Of 71 ligands modelled in this entry, 25 are monoatomic - leaving 46 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	$\# Z  > 2$
3	EDO	A	302	-	3,3,3	0.14	0	2,2,2	0.73	0
3	EDO	B	302	-	3,3,3	0.12	0	2,2,2	0.28	0
3	EDO	H	302	-	3,3,3	0.18	0	2,2,2	0.19	0
2	ICT	K	301	4	12,12,12	1.02	0	13,16,16	1.16	1 (7%)
3	EDO	H	303	-	3,3,3	0.18	0	2,2,2	0.58	0
3	EDO	D	306	-	3,3,3	0.11	0	2,2,2	0.34	0
3	EDO	D	308	-	3,3,3	0.39	0	2,2,2	0.29	0
2	ICT	L	301	4	12,12,12	1.07	0	13,16,16	1.18	1 (7%)
3	EDO	B	303	-	3,3,3	0.28	0	2,2,2	0.38	0
2	ICT	E	301	4	12,12,12	1.10	0	13,16,16	1.20	2 (15%)
3	EDO	D	304	-	3,3,3	0.22	0	2,2,2	0.17	0
2	ICT	A	301	4	12,12,12	1.15	1 (8%)	13,16,16	1.19	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	F	302	-	3,3,3	0.07	0	2,2,2	0.24	0
3	EDO	D	307	-	3,3,3	0.22	0	2,2,2	0.10	0
3	EDO	I	302	-	3,3,3	0.15	0	2,2,2	0.35	0
3	EDO	D	301	-	3,3,3	0.25	0	2,2,2	0.20	0
3	EDO	G	302	-	3,3,3	0.20	0	2,2,2	0.20	0
2	ICT	C	301	4	12,12,12	1.04	0	13,16,16	1.39	2 (15%)
3	EDO	F	303	-	3,3,3	0.05	0	2,2,2	0.28	0
3	EDO	L	302	-	3,3,3	0.25	0	2,2,2	0.16	0
2	ICT	G	301	4	12,12,12	0.99	0	13,16,16	1.24	2 (15%)
3	EDO	G	306	-	3,3,3	0.30	0	2,2,2	0.74	0
3	EDO	H	306	-	3,3,3	0.19	0	2,2,2	0.24	0
3	EDO	D	305	-	3,3,3	0.13	0	2,2,2	0.41	0
3	EDO	L	303	-	3,3,3	0.06	0	2,2,2	0.08	0
3	EDO	G	304	-	3,3,3	0.09	0	2,2,2	0.15	0
3	EDO	D	303	-	3,3,3	0.29	0	2,2,2	0.42	0
2	ICT	F	301	4	12,12,12	1.09	0	13,16,16	1.10	1 (7%)
3	EDO	G	303	-	3,3,3	0.23	0	2,2,2	0.44	0
7	PGE	J	303	-	9,9,9	0.32	0	8,8,8	0.17	0
3	EDO	B	304	-	3,3,3	0.05	0	2,2,2	0.59	0
2	ICT	H	301	4	12,12,12	1.12	0	13,16,16	1.15	1 (7%)
3	EDO	A	303	-	3,3,3	0.27	0	2,2,2	0.73	0
2	ICT	D	302	4	12,12,12	1.03	0	13,16,16	1.15	1 (7%)
3	EDO	G	305	-	3,3,3	0.12	0	2,2,2	0.23	0
3	EDO	J	302	-	3,3,3	0.19	0	2,2,2	0.50	0
3	EDO	B	305	-	3,3,3	0.16	0	2,2,2	0.28	0
3	EDO	C	302	-	3,3,3	0.28	0	2,2,2	0.47	0
3	EDO	H	305	-	3,3,3	0.18	0	2,2,2	0.32	0
2	ICT	B	301	4	12,12,12	0.99	0	13,16,16	1.25	2 (15%)
3	EDO	H	304	-	3,3,3	0.12	0	2,2,2	0.67	0
2	ICT	I	301	4	12,12,12	1.05	0	13,16,16	1.33	1 (7%)
2	ICT	J	301	4	12,12,12	0.97	0	13,16,16	1.37	2 (15%)
3	EDO	F	304	-	3,3,3	0.09	0	2,2,2	0.17	0
3	EDO	K	302	-	3,3,3	0.17	0	2,2,2	0.24	0
6	PEG	E	302	-	6,6,6	0.24	0	5,5,5	0.12	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
3	EDO	A	302	-	-	1/1/1/1	-
3	EDO	B	302	-	-	0/1/1/1	-
3	EDO	H	302	-	-	1/1/1/1	-
2	ICT	K	301	4	-	8/16/16/16	-
3	EDO	H	303	-	-	1/1/1/1	-
3	EDO	D	306	-	-	1/1/1/1	-
3	EDO	D	308	-	-	1/1/1/1	-
2	ICT	L	301	4	-	10/16/16/16	-
3	EDO	B	303	-	-	1/1/1/1	-
2	ICT	E	301	4	-	6/16/16/16	-
3	EDO	D	304	-	-	0/1/1/1	-
2	ICT	A	301	4	-	9/16/16/16	-
3	EDO	F	302	-	-	1/1/1/1	-
3	EDO	D	307	-	-	1/1/1/1	-
3	EDO	I	302	-	-	0/1/1/1	-
3	EDO	D	301	-	-	0/1/1/1	-
3	EDO	G	302	-	-	1/1/1/1	-
2	ICT	C	301	4	-	10/16/16/16	-
3	EDO	F	303	-	-	1/1/1/1	-
3	EDO	L	302	-	-	1/1/1/1	-
2	ICT	G	301	4	-	10/16/16/16	-
3	EDO	G	306	-	-	1/1/1/1	-
3	EDO	H	306	-	-	1/1/1/1	-
3	EDO	D	305	-	-	0/1/1/1	-
3	EDO	L	303	-	-	0/1/1/1	-
3	EDO	G	304	-	-	1/1/1/1	-
3	EDO	D	303	-	-	0/1/1/1	-
2	ICT	F	301	4	-	10/16/16/16	-
3	EDO	G	303	-	-	1/1/1/1	-
7	PGE	J	303	-	-	6/7/7/7	-
3	EDO	B	304	-	-	0/1/1/1	-
2	ICT	H	301	4	-	10/16/16/16	-
3	EDO	A	303	-	-	1/1/1/1	-
2	ICT	D	302	4	-	7/16/16/16	-
3	EDO	G	305	-	-	1/1/1/1	-
3	EDO	J	302	-	-	1/1/1/1	-
3	EDO	B	305	-	-	0/1/1/1	-
3	EDO	C	302	-	-	1/1/1/1	-
3	EDO	H	305	-	-	1/1/1/1	-
2	ICT	B	301	4	-	10/16/16/16	-
3	EDO	H	304	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ICT	I	301	4	-	9/16/16/16	-
2	ICT	J	301	4	-	8/16/16/16	-
3	EDO	F	304	-	-	1/1/1/1	-
3	EDO	K	302	-	-	1/1/1/1	-
6	PEG	E	302	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	ICT	O4-C5	-2.14	1.23	1.30

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	301	ICT	O5-C6-C3	-2.61	116.41	122.95
2	C	301	ICT	O5-C6-C3	-2.32	117.14	122.95
2	A	301	ICT	O1-C1-C2	-2.27	115.66	121.63
2	G	301	ICT	O5-C6-C3	-2.25	117.30	122.95
2	D	302	ICT	O1-C1-C2	-2.19	115.88	121.63

There are no chirality outliers.

5 of 138 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	ICT	O7-C2-C3-C6
2	A	301	ICT	C2-C3-C4-C5
2	B	301	ICT	O7-C2-C3-C4
2	B	301	ICT	O7-C2-C3-C6
2	B	301	ICT	C2-C3-C4-C5

There are no ring outliers.

7 monomers are involved in 11 short contacts:

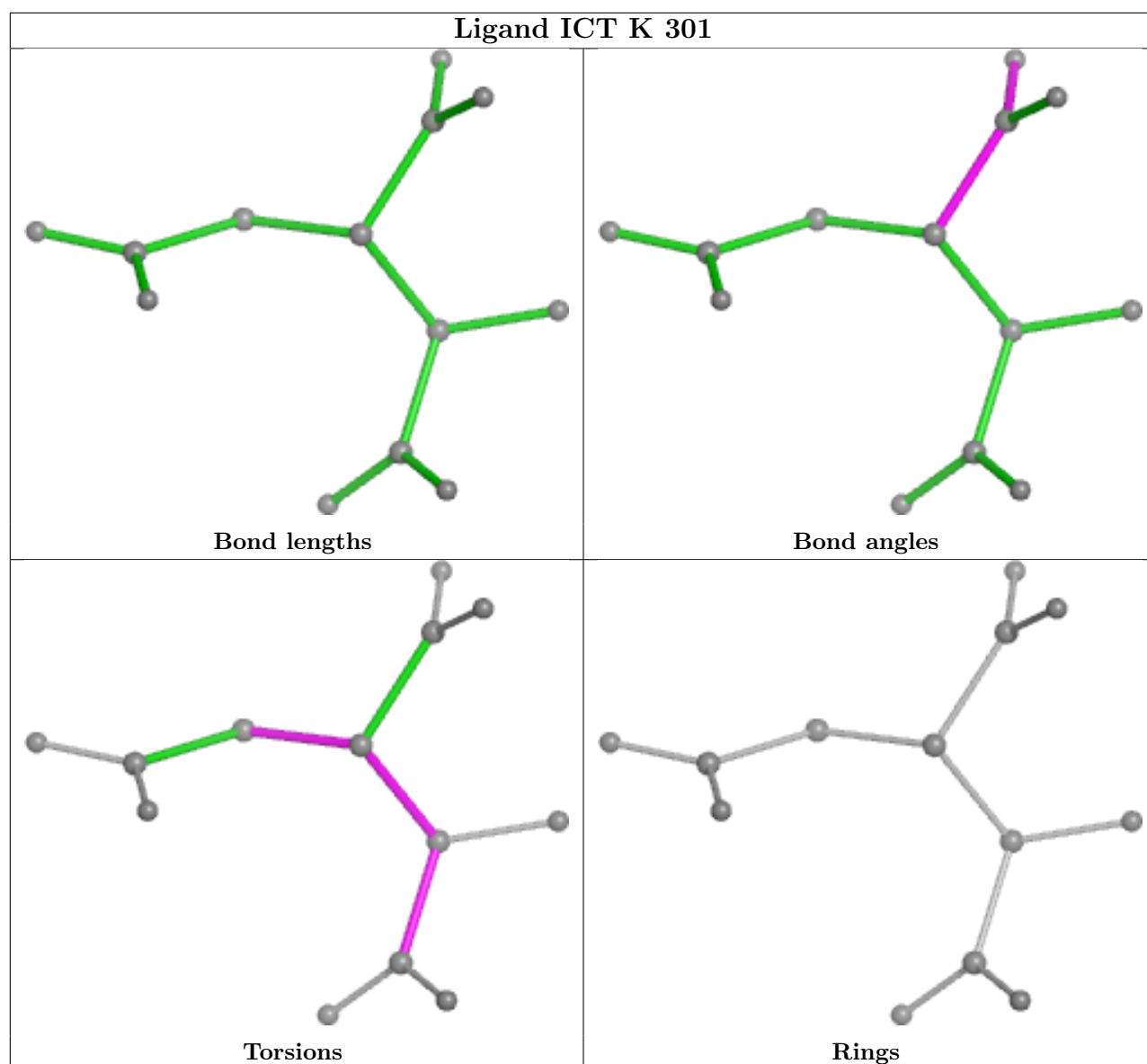
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	308	EDO	5	0
2	E	301	ICT	1	0
2	A	301	ICT	1	0
3	D	307	EDO	1	0
3	G	302	EDO	1	0
2	F	301	ICT	1	0

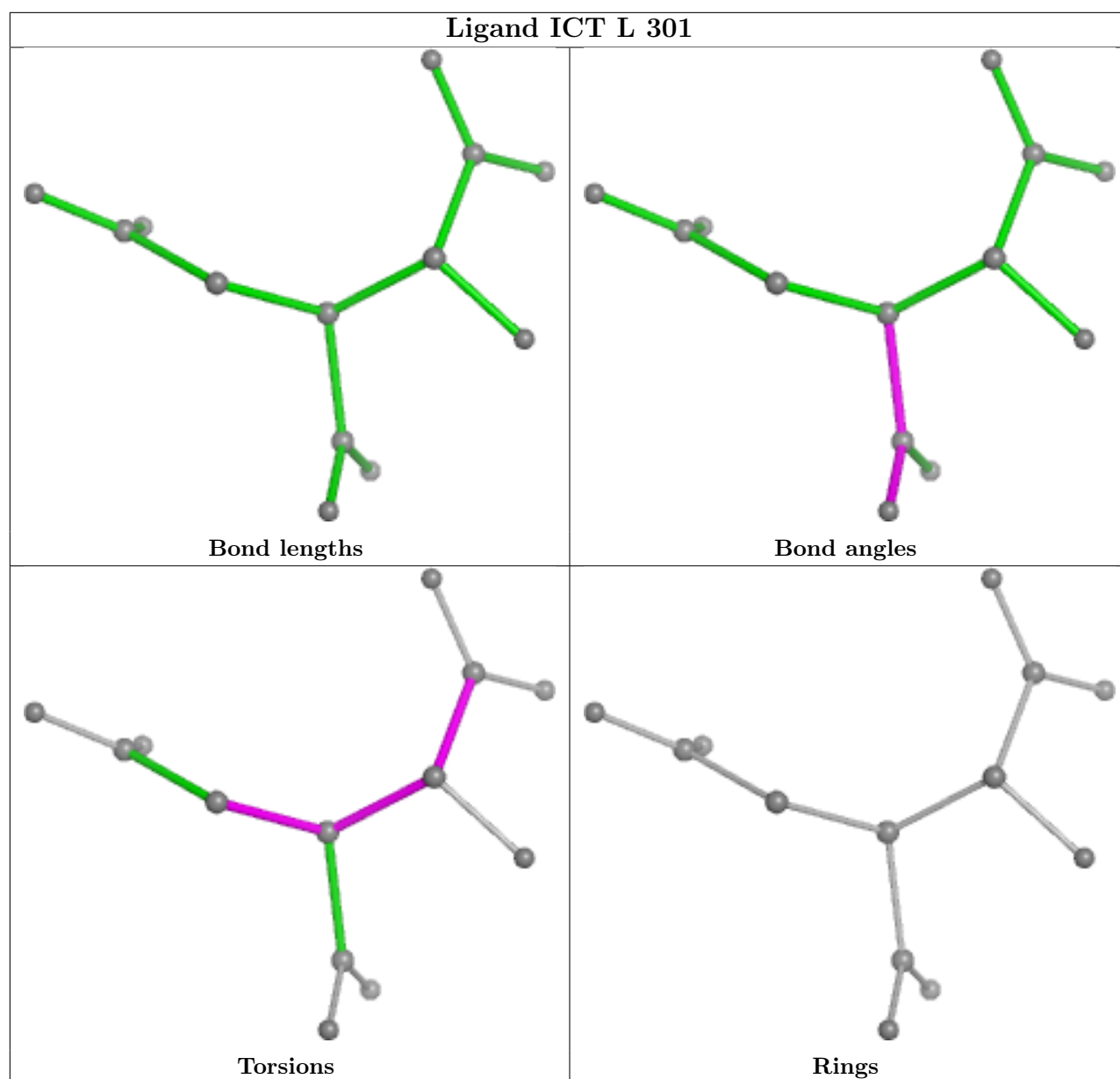
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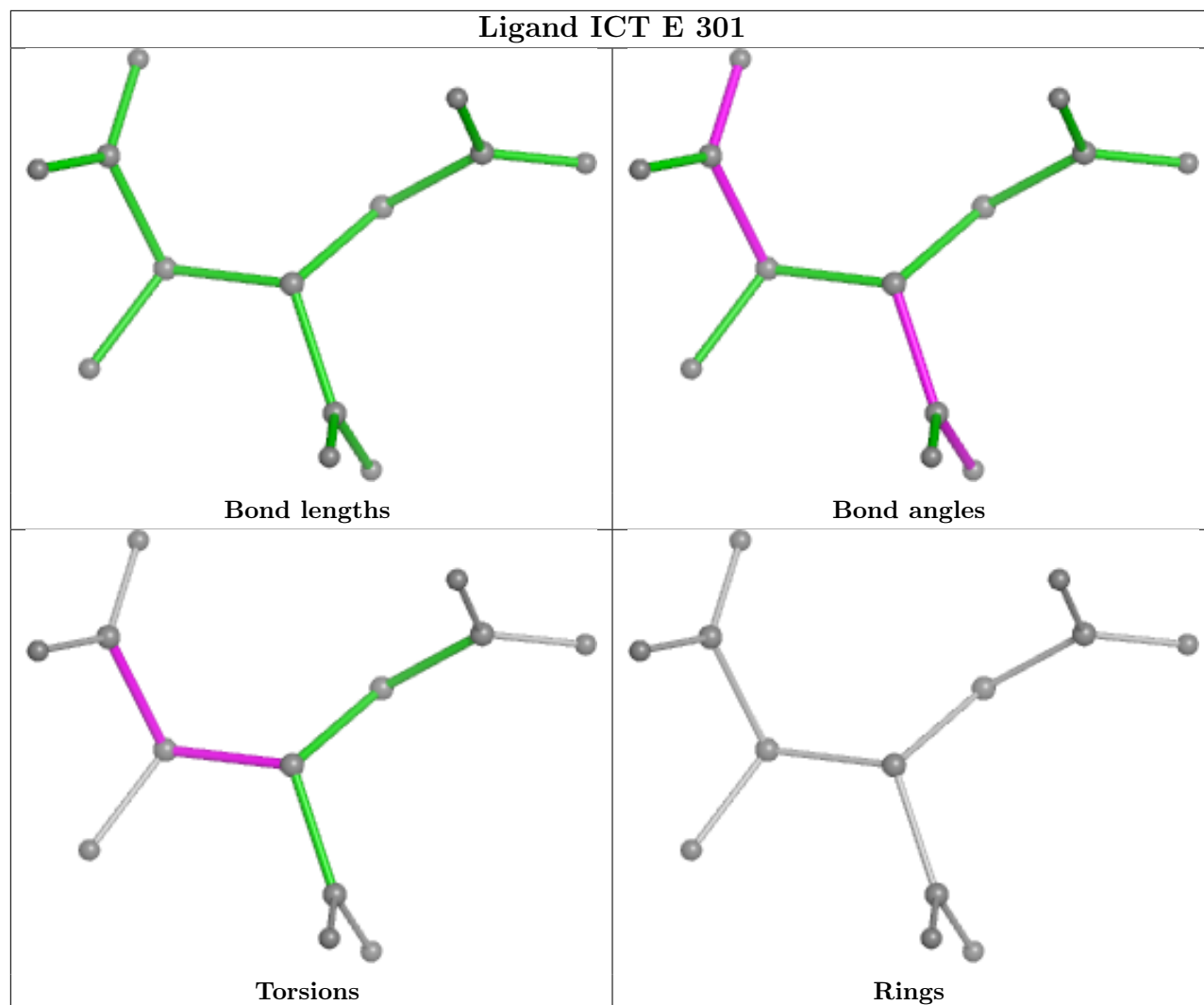
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	301	ICT	1	0

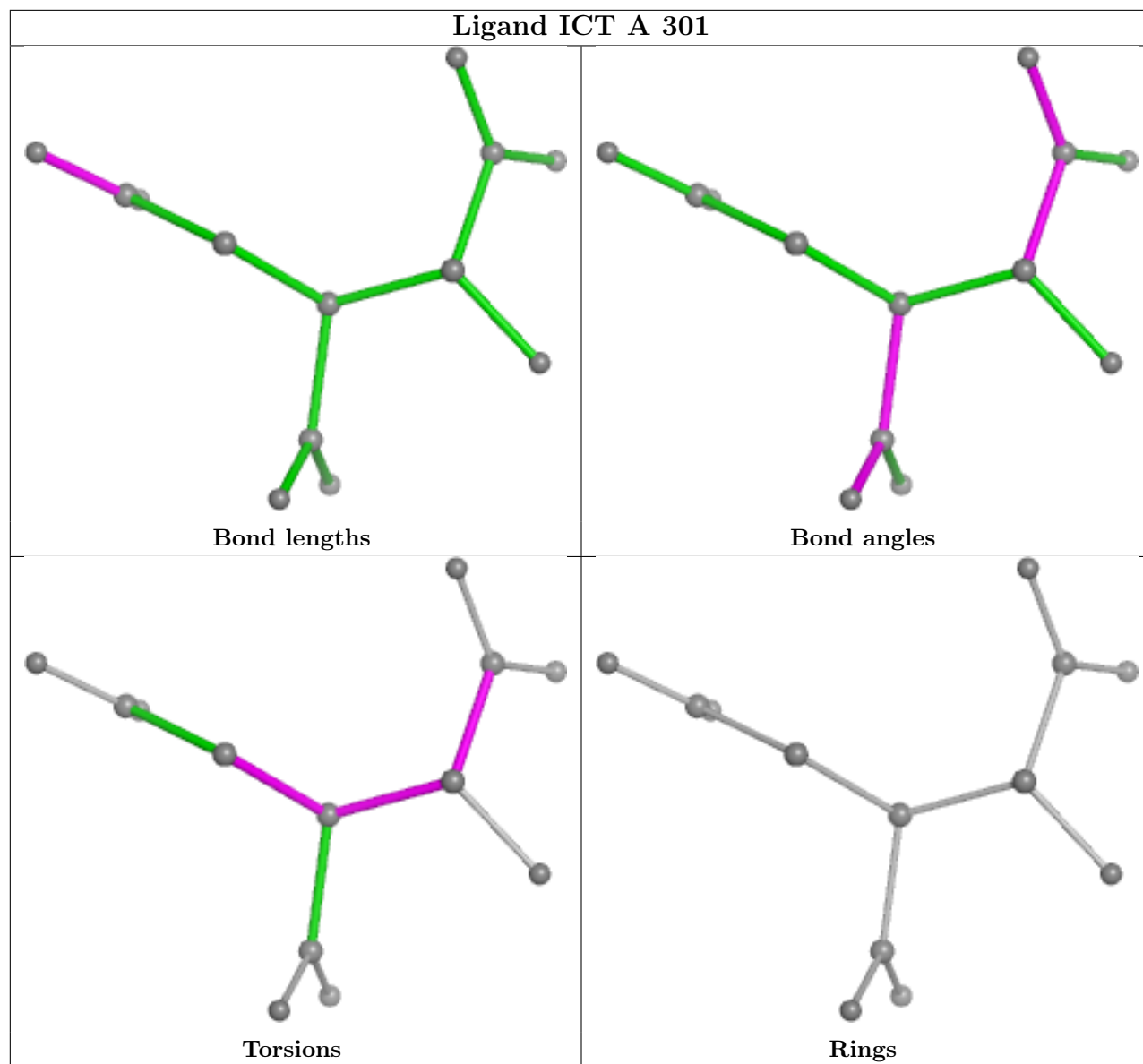
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

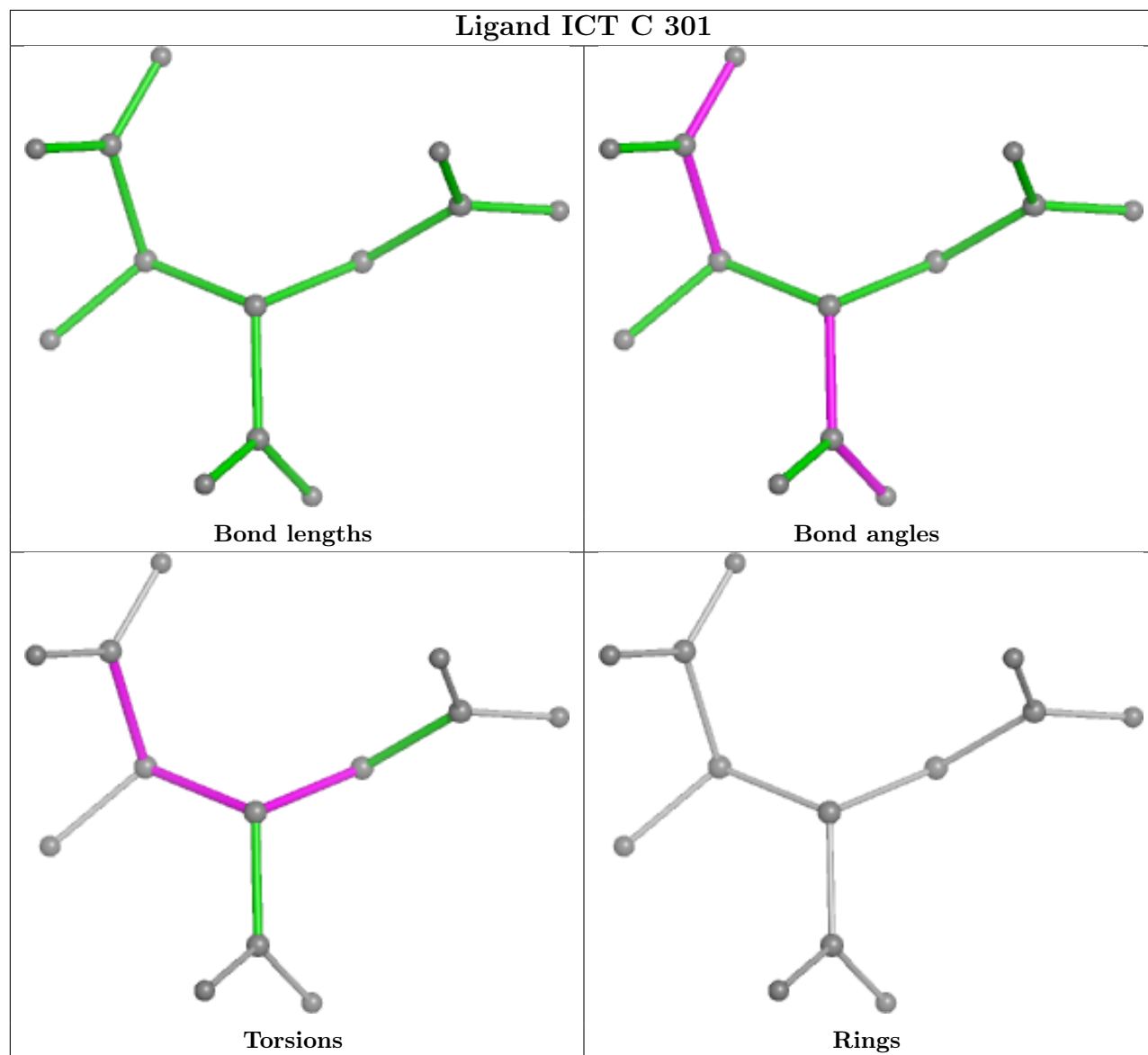




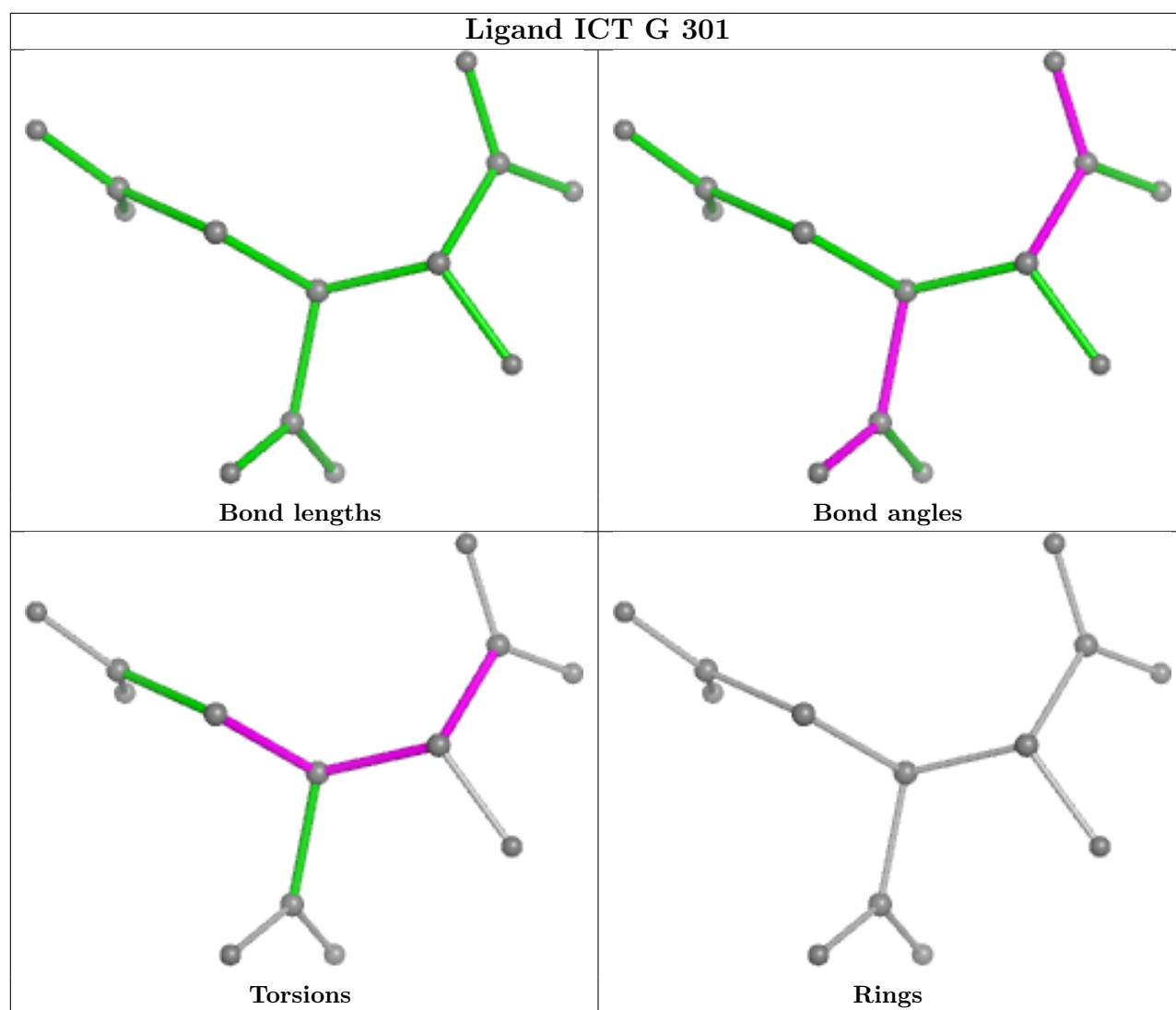
## Ligand ICT E 301

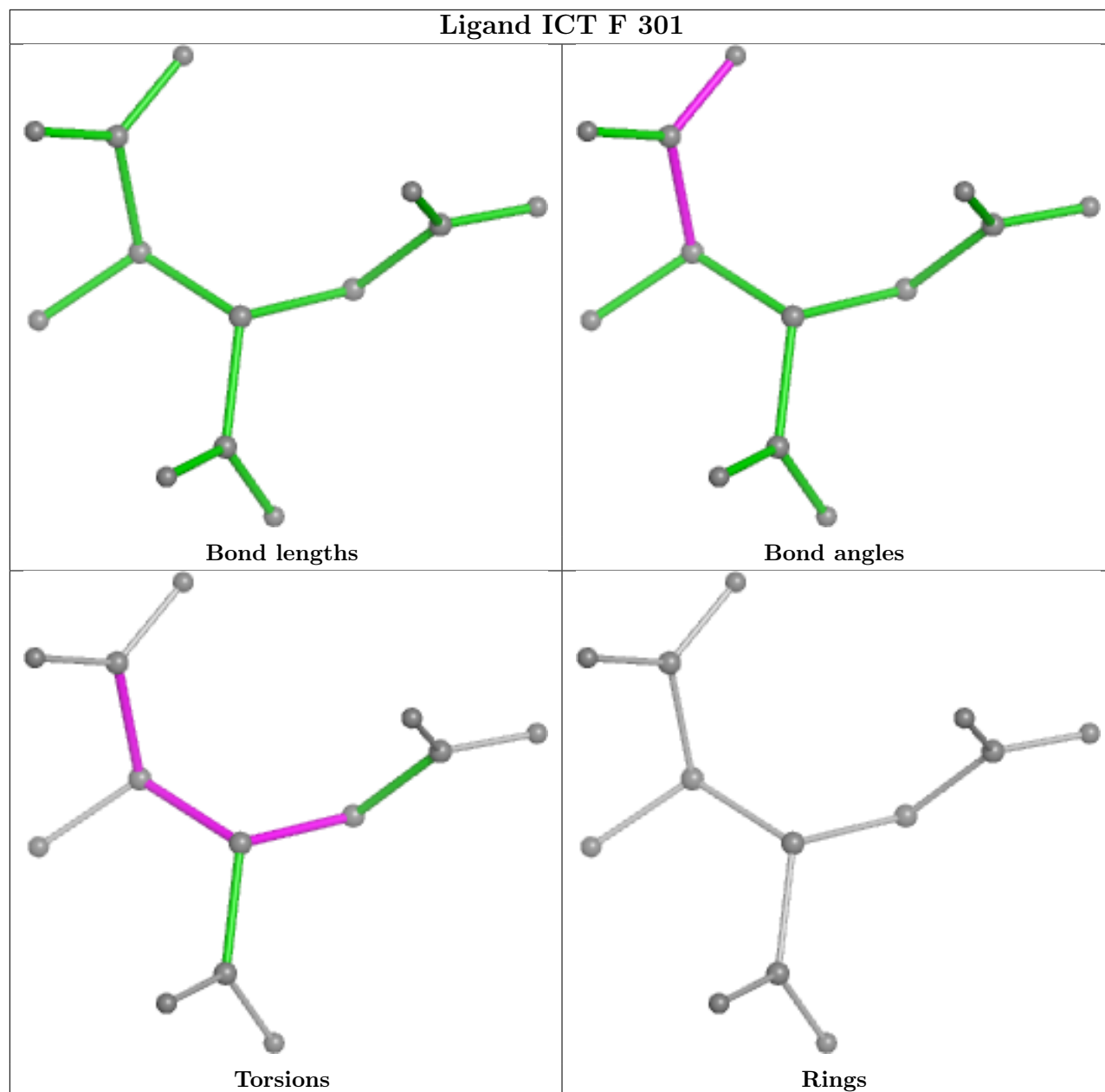


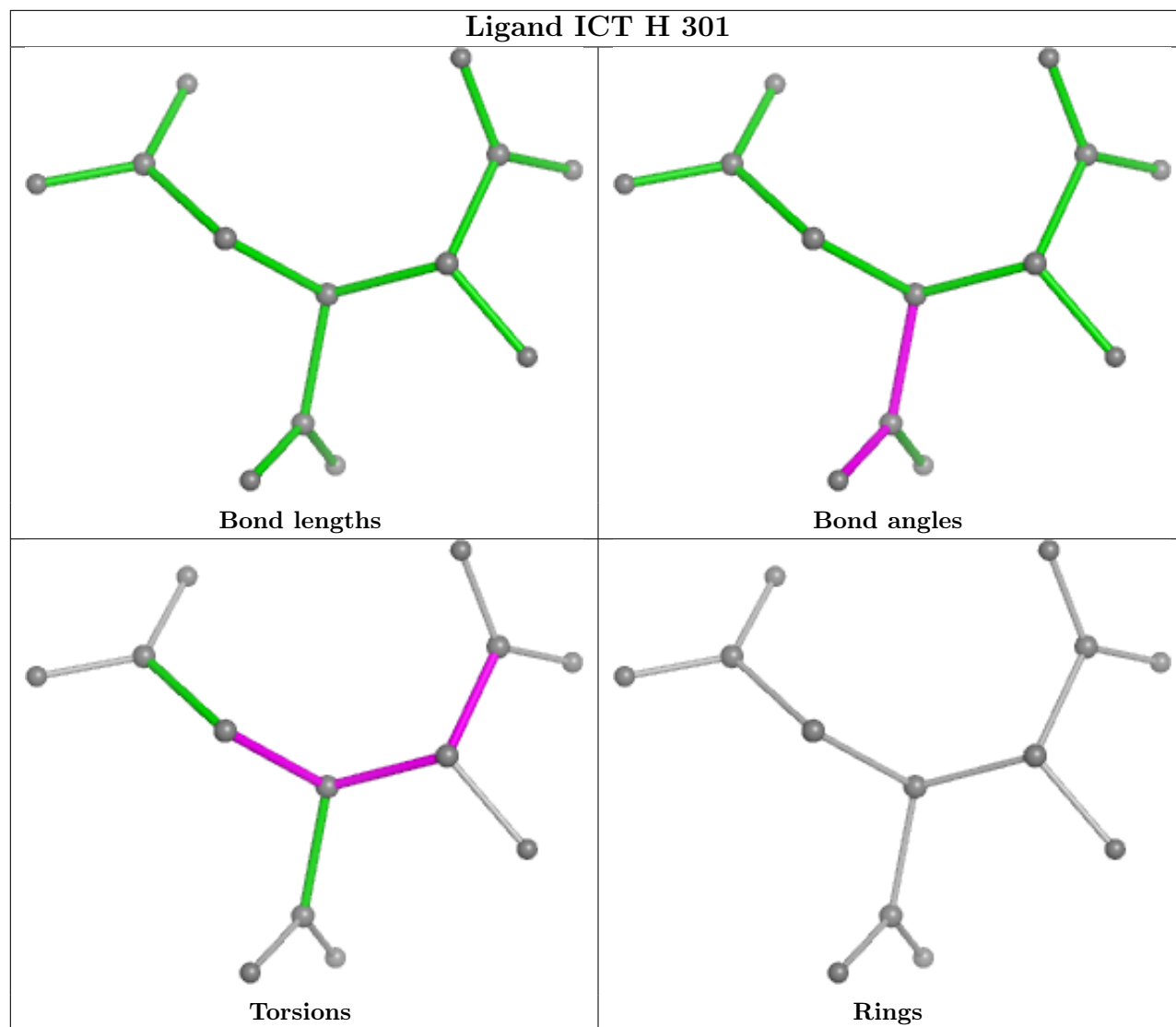




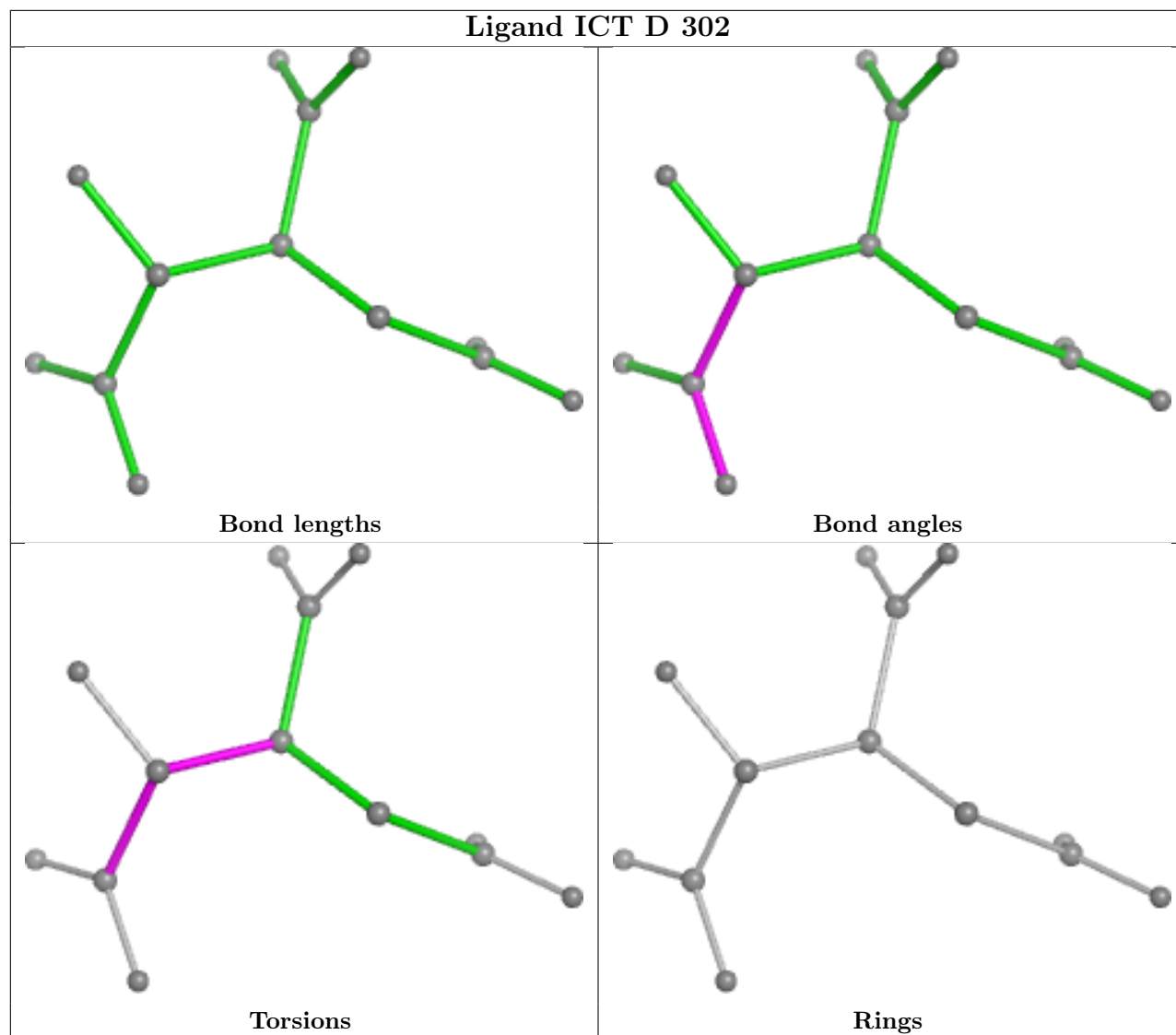




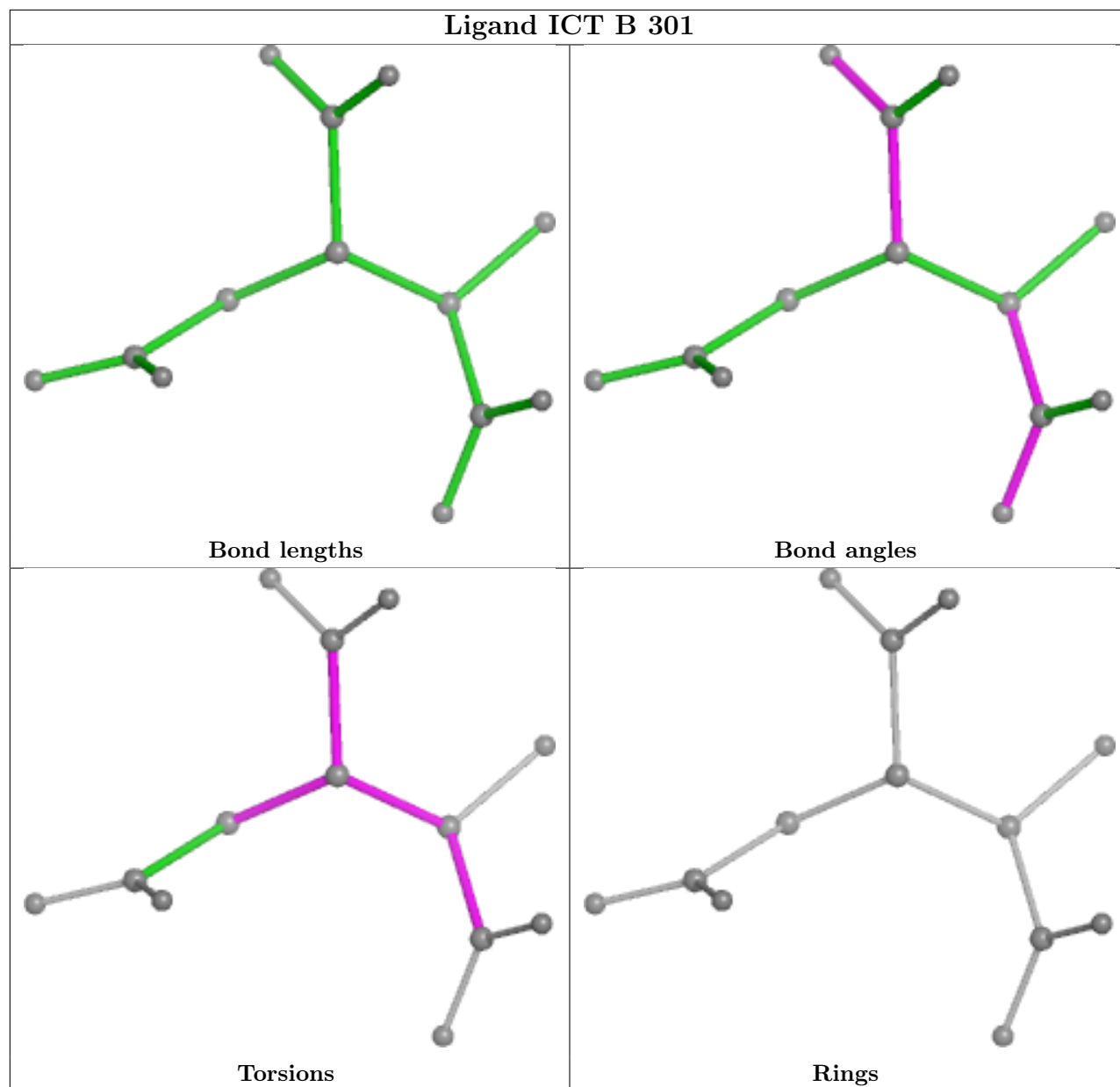


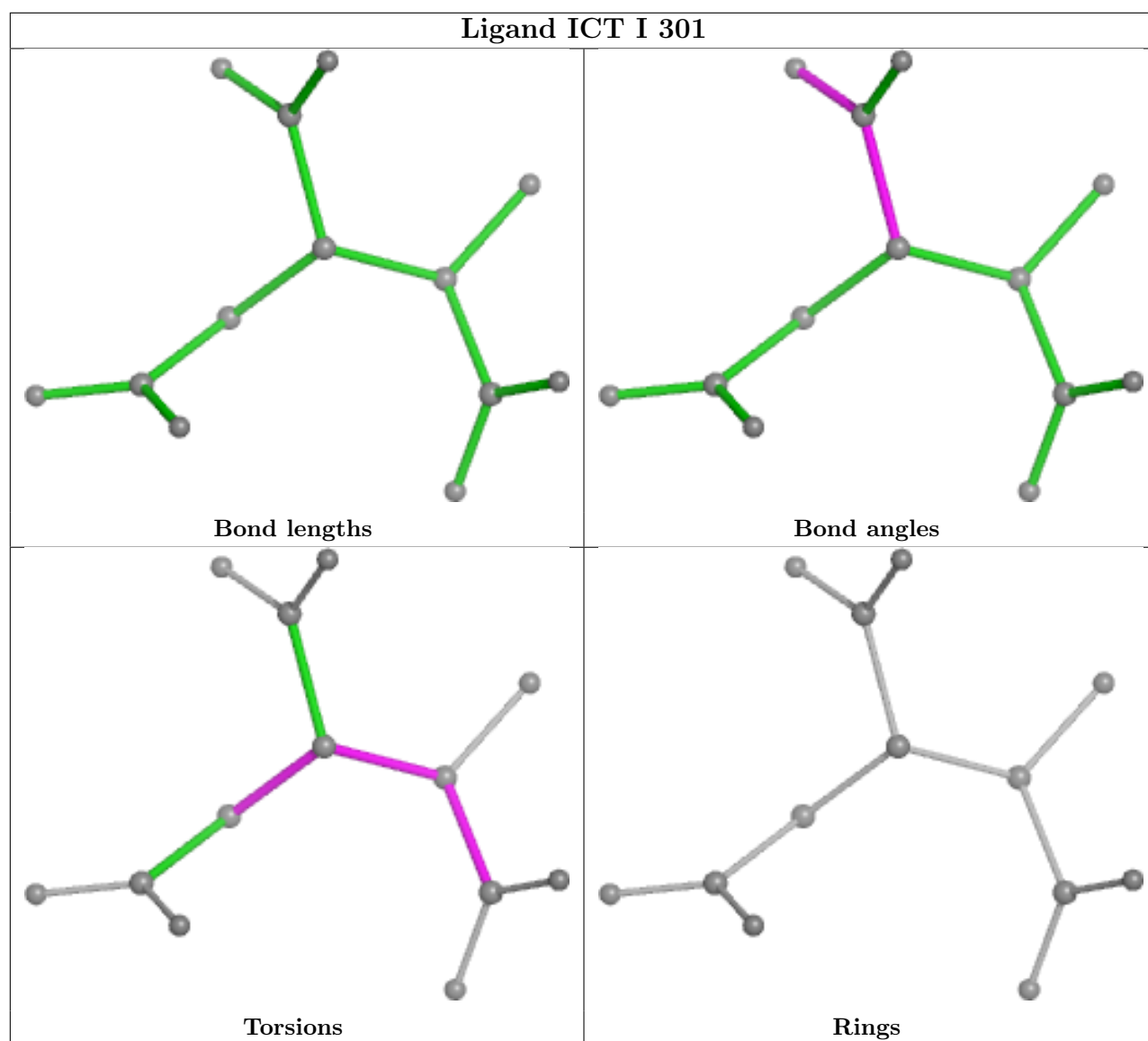


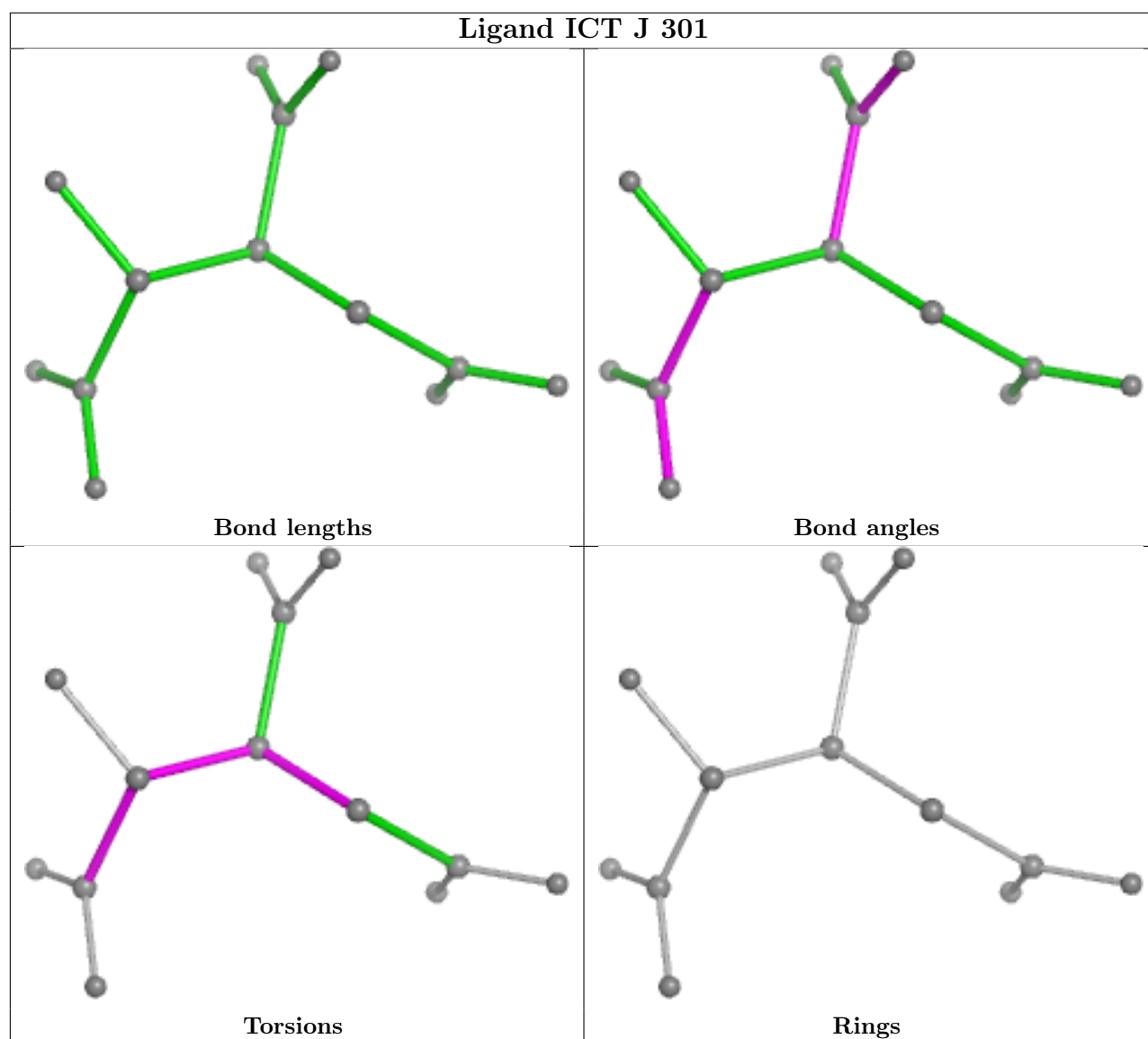
## Ligand ICT D 302



## Ligand ICT B 301







## 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	291/312 (93%)	0.11	19 (6%) 26 32	31, 55, 113, 149	0
1	B	287/312 (91%)	-0.18	8 (2%) 55 61	32, 50, 116, 150	0
1	C	288/312 (92%)	-0.04	7 (2%) 59 65	32, 57, 115, 208	0
1	D	292/312 (93%)	-0.52	1 (0%) 90 92	28, 44, 88, 154	0
1	E	286/312 (91%)	1.06	45 (15%) 6 8	49, 91, 133, 171	0
1	F	287/312 (91%)	-0.03	7 (2%) 59 65	37, 62, 113, 243	0
1	G	286/312 (91%)	-0.14	1 (0%) 90 92	38, 62, 103, 159	0
1	H	287/312 (91%)	-0.02	8 (2%) 55 61	41, 61, 112, 201	0
1	I	289/312 (92%)	-0.06	9 (3%) 51 58	34, 59, 107, 200	0
1	J	288/312 (92%)	-0.21	7 (2%) 59 65	36, 53, 110, 192	0
1	K	288/312 (92%)	0.53	14 (4%) 36 43	52, 86, 139, 176	0
1	L	287/312 (91%)	-0.18	3 (1%) 79 83	39, 55, 114, 188	0
All	All	3456/3744 (92%)	0.03	129 (3%) 45 53	28, 61, 123, 243	0

The worst 5 of 129 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	192	THR	5.3
1	I	284	PHE	4.3
1	A	157	ALA	4.1
1	B	283	LEU	3.9
1	F	283	LEU	3.7

### 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 ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

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
3	EDO	D	308	4/4	0.73	0.23	61,71,73,78	0
3	EDO	I	302	4/4	0.73	0.21	74,75,80,91	0
3	EDO	H	304	4/4	0.76	0.17	82,83,85,93	0
2	ICT	E	301	13/13	0.79	0.13	65,92,122,128	0
3	EDO	K	302	4/4	0.79	0.14	66,74,76,78	0
5	CL	L	305	1/1	0.79	0.09	96,96,96,96	0
3	EDO	D	304	4/4	0.80	0.18	65,69,76,81	0
3	EDO	G	304	4/4	0.80	0.13	73,77,79,80	0
3	EDO	D	307	4/4	0.81	0.13	60,67,75,96	0
3	EDO	H	302	4/4	0.81	0.12	61,64,86,87	0
3	EDO	H	306	4/4	0.82	0.16	76,78,83,87	0
3	EDO	D	305	4/4	0.83	0.10	54,68,69,89	0
6	PEG	E	302	7/7	0.83	0.13	81,90,102,110	0
3	EDO	F	304	4/4	0.84	0.14	59,64,67,81	0
2	ICT	J	301	13/13	0.84	0.13	69,94,118,119	0
3	EDO	A	302	4/4	0.84	0.12	62,64,68,74	0
2	ICT	H	301	13/13	0.85	0.13	64,93,118,124	0
5	CL	G	308	1/1	0.85	0.11	87,87,87,87	0
3	EDO	D	303	4/4	0.85	0.23	46,60,72,79	0
2	ICT	K	301	13/13	0.85	0.14	85,124,146,146	0
7	PGE	J	303	10/10	0.85	0.16	60,77,106,108	0
3	EDO	G	305	4/4	0.86	0.15	70,75,79,86	0
2	ICT	C	301	13/13	0.86	0.11	54,69,81,84	0
3	EDO	J	302	4/4	0.86	0.12	62,65,70,71	0
3	EDO	F	302	4/4	0.86	0.10	78,80,83,99	0
4	MG	J	304	1/1	0.87	0.10	111,111,111,111	0
2	ICT	L	301	13/13	0.89	0.10	67,101,125,136	0
3	EDO	G	302	4/4	0.89	0.12	58,68,71,80	0
3	EDO	B	303	4/4	0.89	0.09	58,66,70,71	0
3	EDO	H	305	4/4	0.89	0.13	64,64,83,83	0
3	EDO	L	302	4/4	0.89	0.10	58,70,71,71	0
4	MG	H	307	1/1	0.90	0.15	94,94,94,94	0

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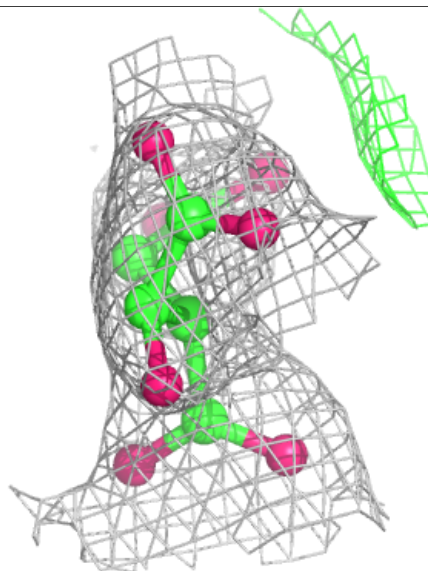
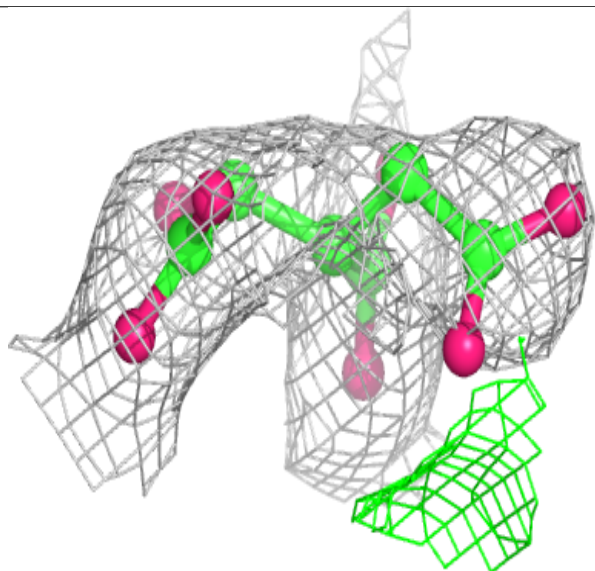
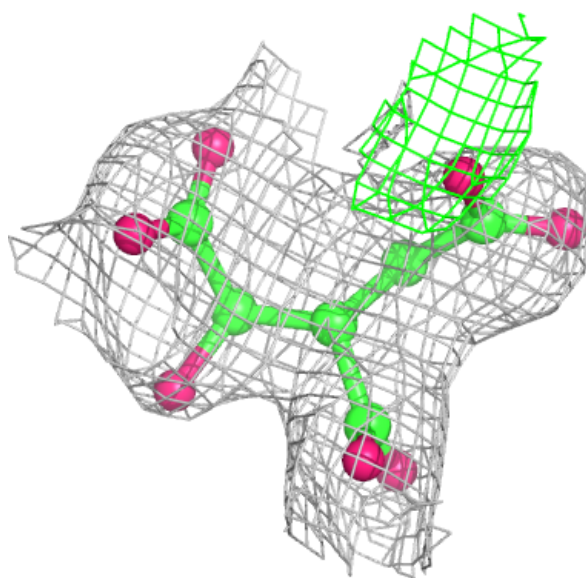
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CL	E	304	1/1	0.90	0.08	82,82,82,82	0
4	MG	B	306	1/1	0.91	0.08	85,85,85,85	0
3	EDO	A	303	4/4	0.91	0.10	51,60,61,66	0
3	EDO	G	303	4/4	0.91	0.11	58,74,76,78	0
4	MG	L	304	1/1	0.91	0.10	103,103,103,103	0
2	ICT	F	301	13/13	0.91	0.10	65,79,109,111	0
3	EDO	F	303	4/4	0.91	0.13	74,74,76,80	0
3	EDO	G	306	4/4	0.91	0.12	54,60,75,89	0
2	ICT	A	301	13/13	0.91	0.10	45,66,110,119	0
3	EDO	H	303	4/4	0.91	0.10	63,65,68,72	0
5	CL	C	304	1/1	0.92	0.10	80,80,80,80	0
3	EDO	B	304	4/4	0.92	0.08	45,53,54,66	0
3	EDO	C	302	4/4	0.92	0.09	64,64,66,67	0
4	MG	F	305	1/1	0.93	0.06	97,97,97,97	0
3	EDO	B	305	4/4	0.93	0.10	70,72,73,83	0
5	CL	H	308	1/1	0.93	0.07	72,72,72,72	0
5	CL	K	304	1/1	0.93	0.08	81,81,81,81	0
2	ICT	B	301	13/13	0.93	0.09	62,76,94,97	0
3	EDO	D	301	4/4	0.93	0.10	55,60,70,76	0
3	EDO	D	306	4/4	0.93	0.08	46,60,61,89	0
3	EDO	L	303	4/4	0.94	0.08	52,53,61,76	0
2	ICT	I	301	13/13	0.94	0.08	54,81,107,115	0
5	CL	D	310	1/1	0.95	0.10	57,57,57,57	0
2	ICT	D	302	13/13	0.95	0.07	48,65,81,86	0
2	ICT	G	301	13/13	0.95	0.07	58,80,111,116	0
4	MG	A	304	1/1	0.95	0.09	78,78,78,78	0
3	EDO	B	302	4/4	0.96	0.06	53,63,65,67	0
5	CL	F	306	1/1	0.96	0.07	71,71,71,71	0
4	MG	K	303	1/1	0.96	0.07	110,110,110,110	0
4	MG	G	307	1/1	0.96	0.12	80,80,80,80	0
5	CL	I	304	1/1	0.96	0.07	76,76,76,76	0
5	CL	A	305	1/1	0.96	0.09	73,73,73,73	0
5	CL	B	307	1/1	0.96	0.08	69,69,69,69	0
5	CL	L	306	1/1	0.96	0.07	73,73,73,73	0
4	MG	C	303	1/1	0.96	0.10	69,69,69,69	0
4	MG	I	303	1/1	0.96	0.06	76,76,76,76	0
5	CL	J	305	1/1	0.98	0.10	66,66,66,66	0
4	MG	E	303	1/1	0.98	0.09	77,77,77,77	0
4	MG	D	309	1/1	0.99	0.03	54,54,54,54	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.

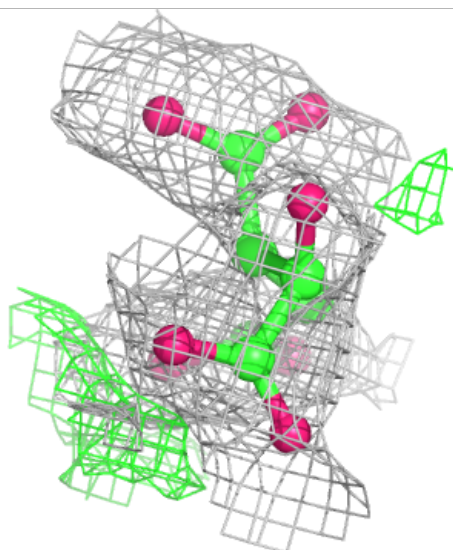
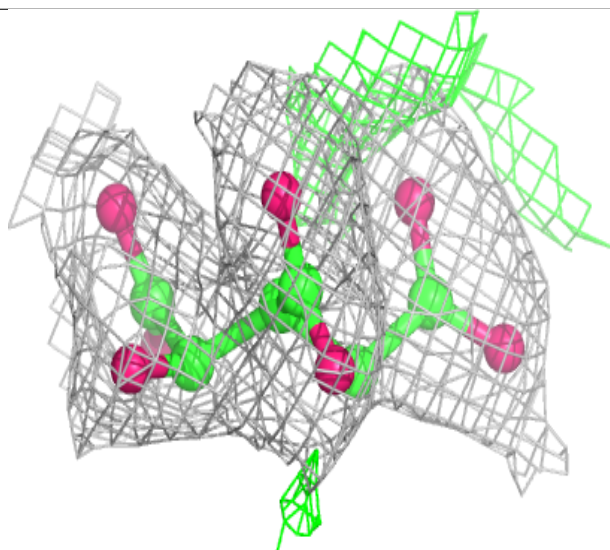
**Electron density around ICT E 301:**

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



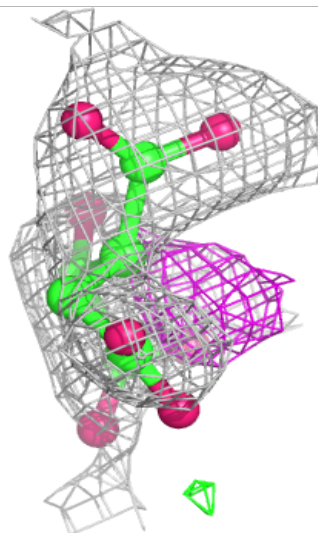
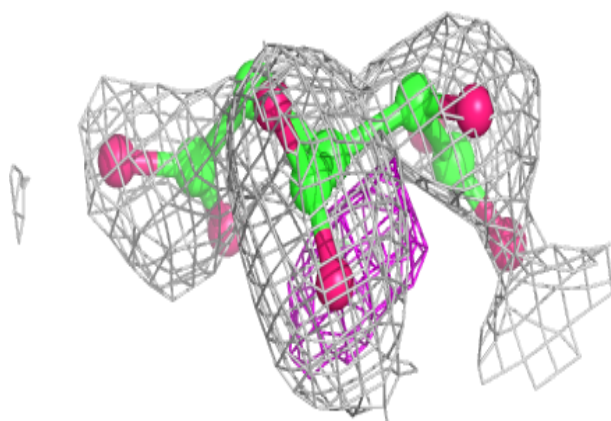
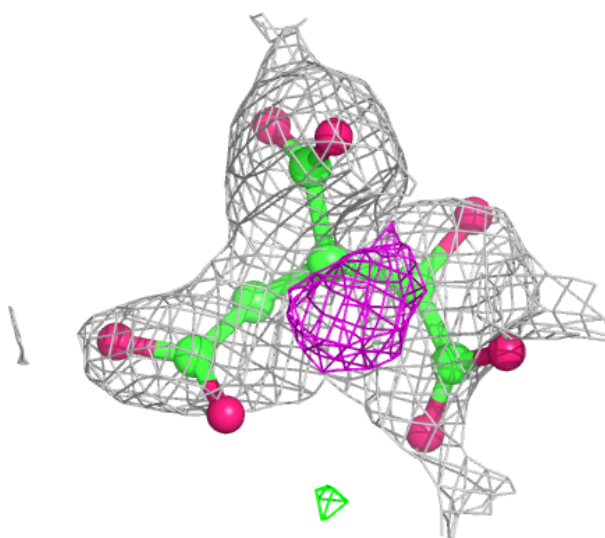
**Electron density around ICT J 301:**

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



**Electron density around ICT H 301:**

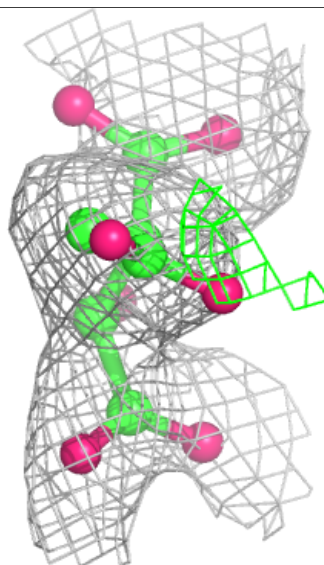
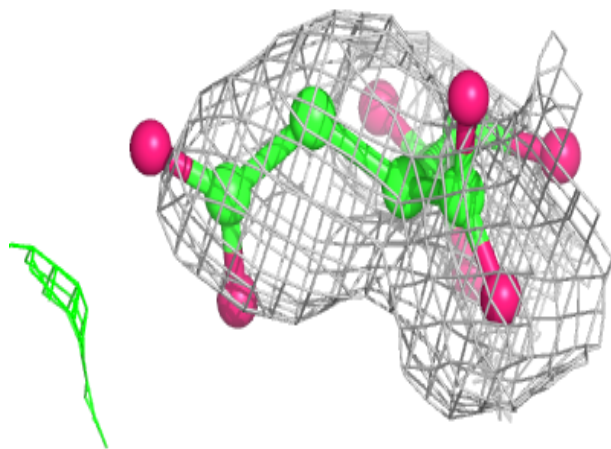
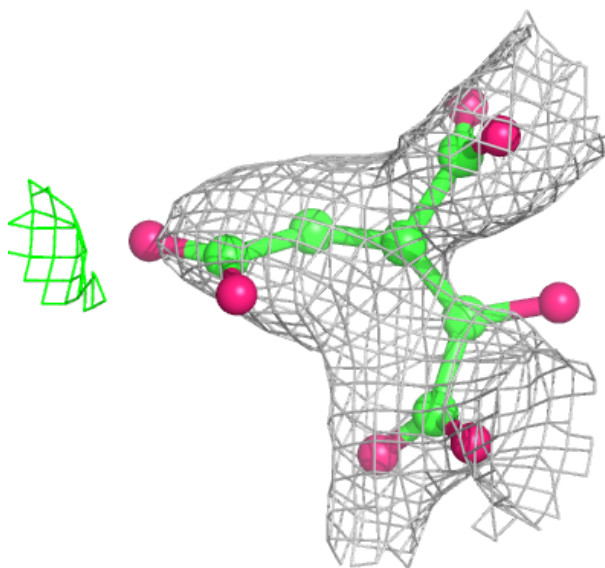
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





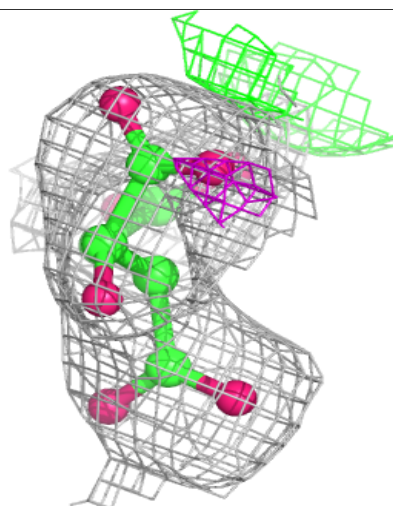
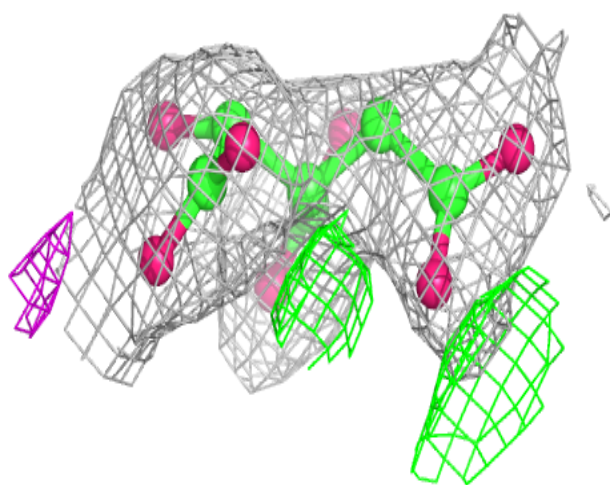
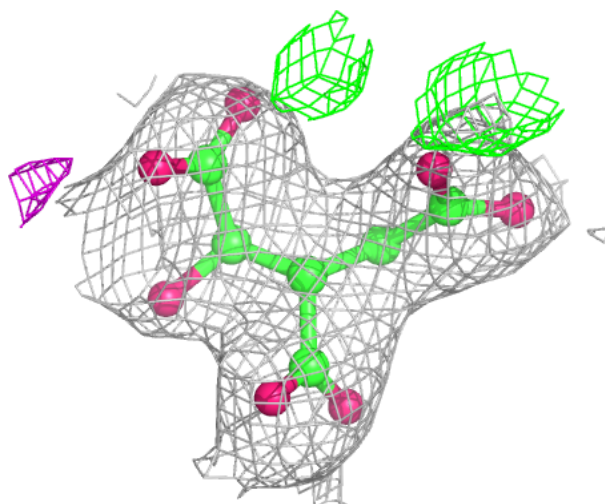
**Electron density around ICT K 301:**

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



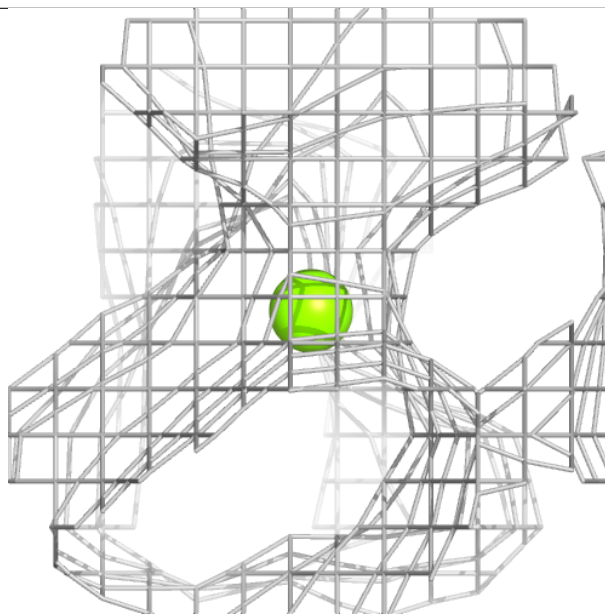
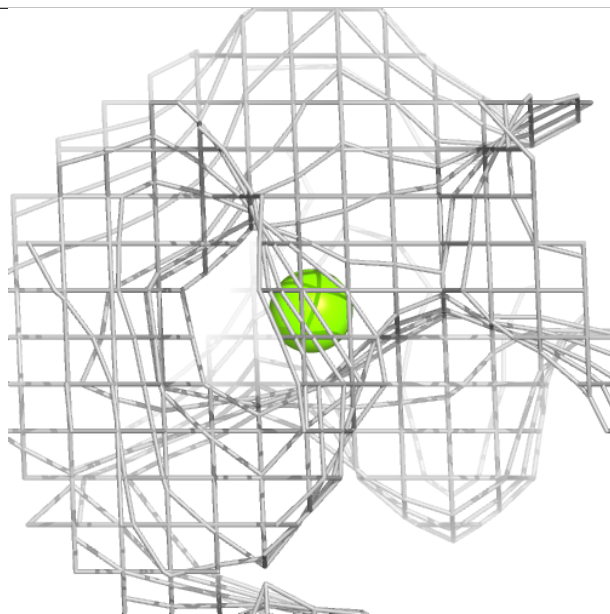
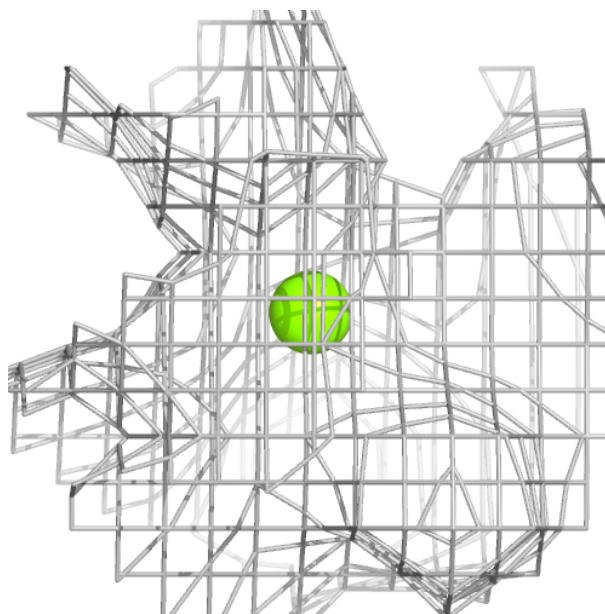
**Electron density around ICT C 301:**

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



**Electron density around MG J 304:**

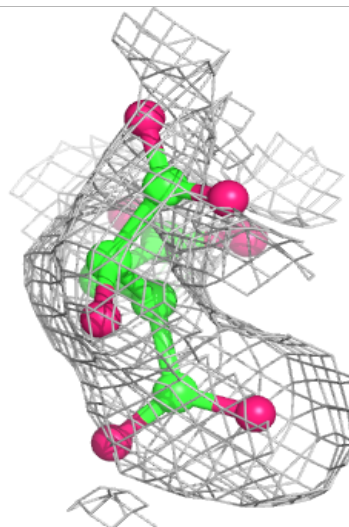
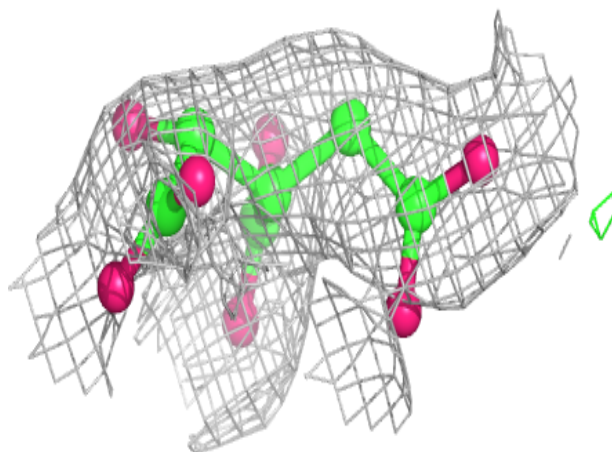
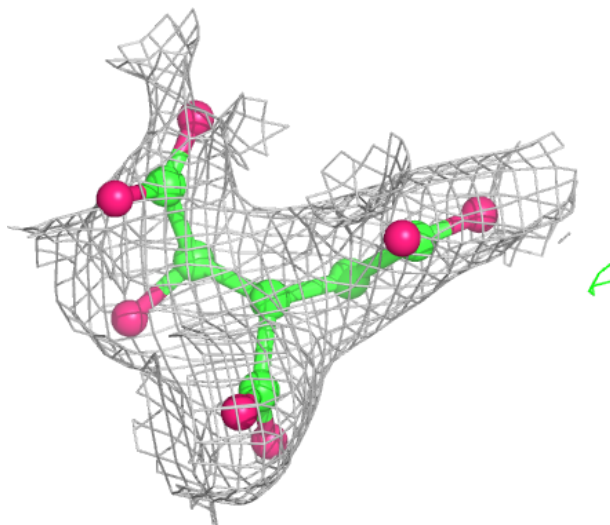
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





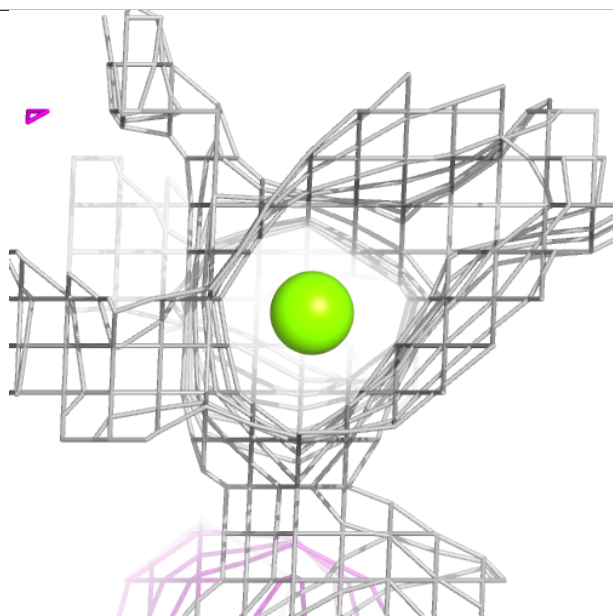
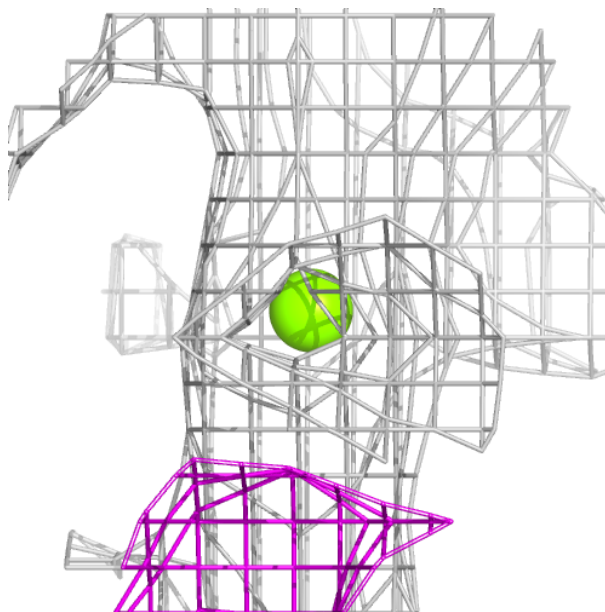
**Electron density around ICT L 301:**

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



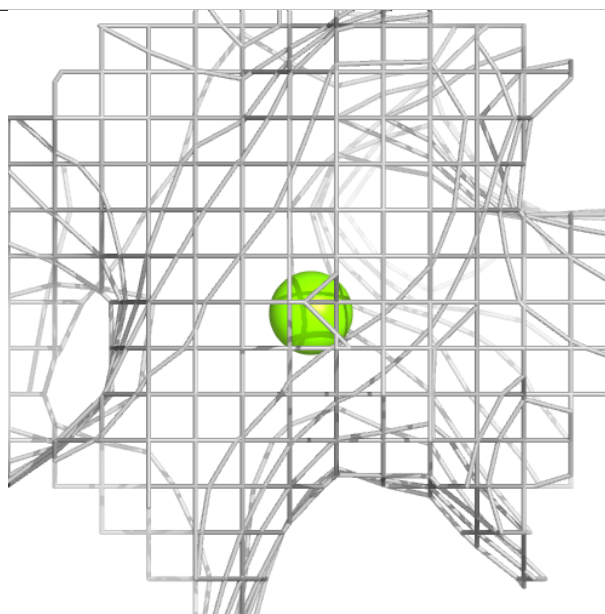
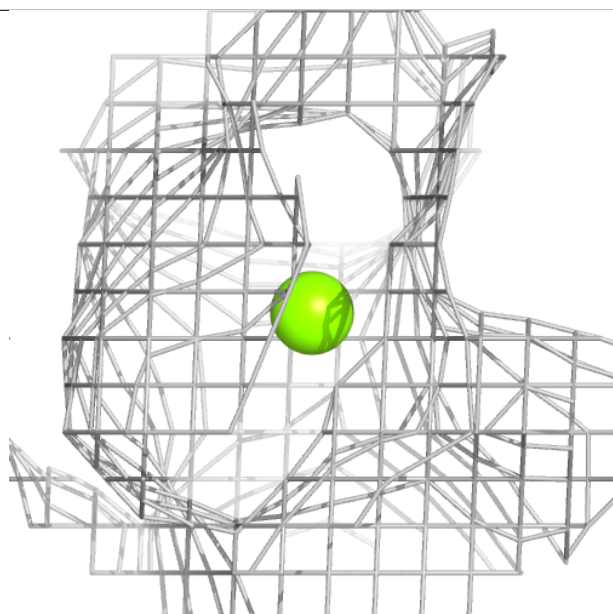
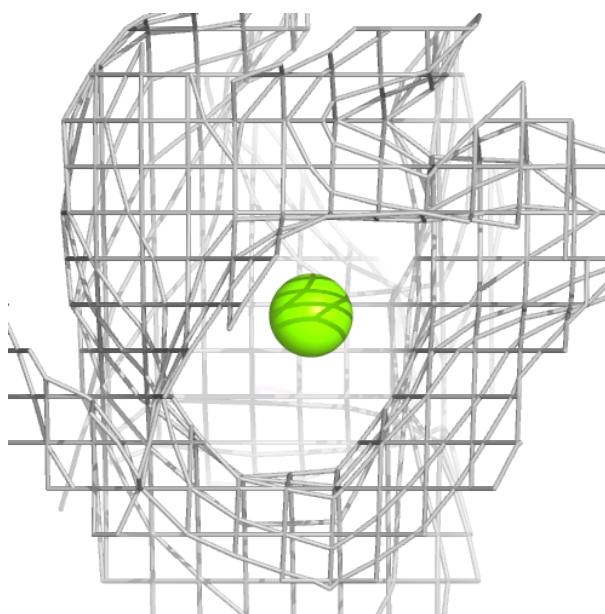
**Electron density around MG H 307:**

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



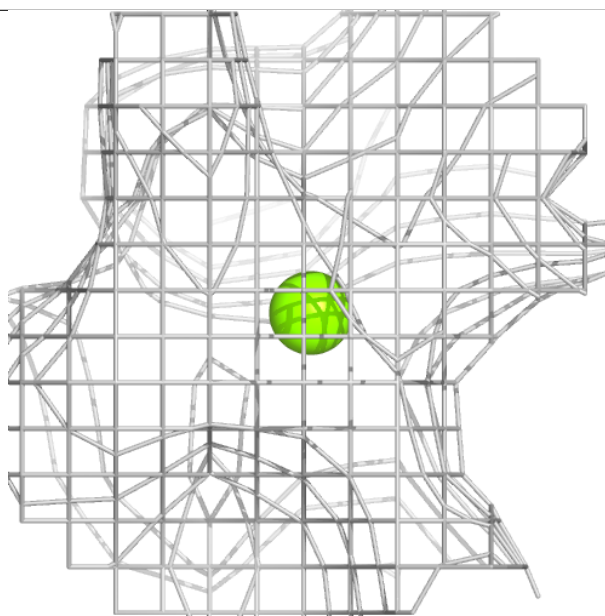
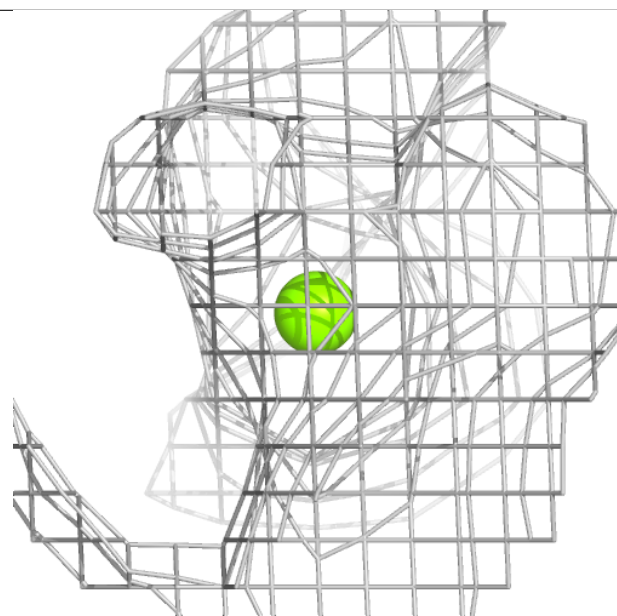
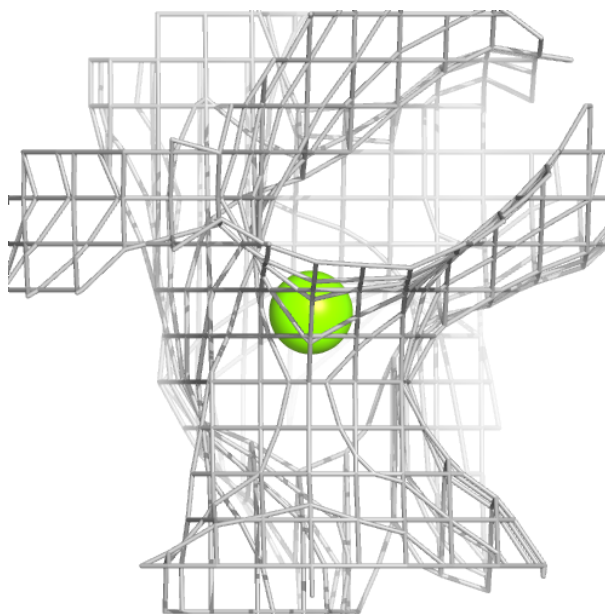
**Electron density around MG B 306:**

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



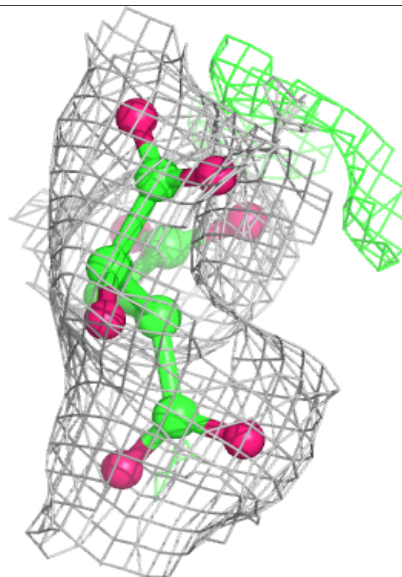
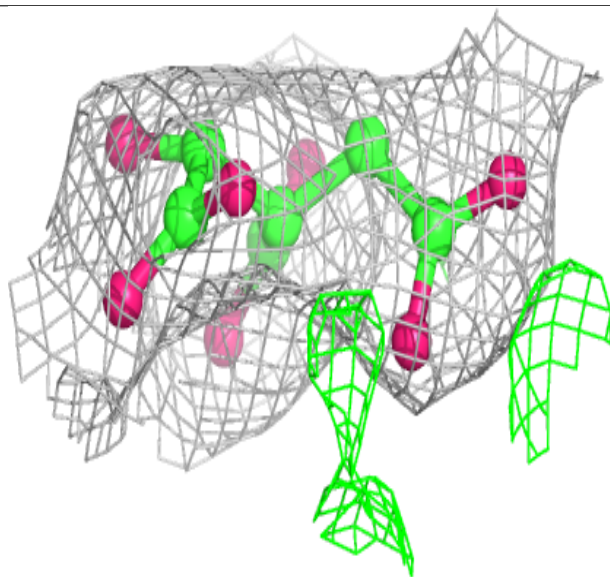
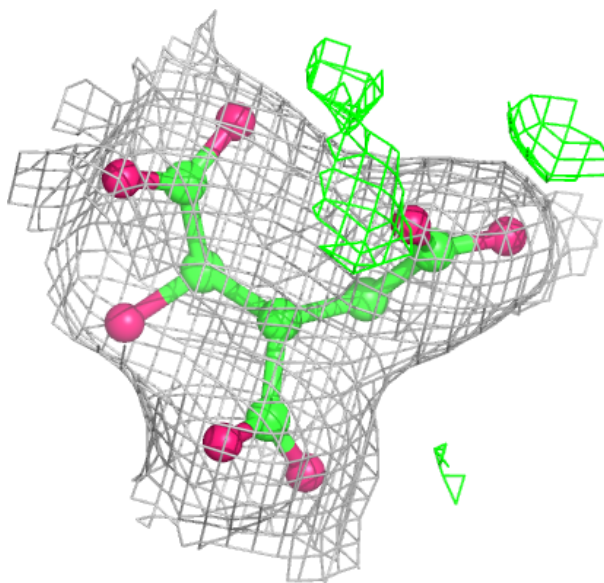
**Electron density around MG L 304:**

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



**Electron density around ICT F 301:**

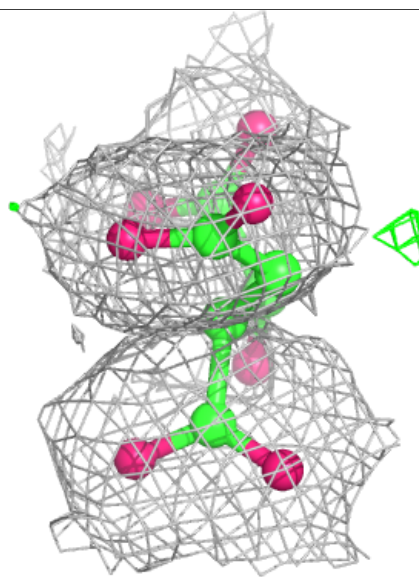
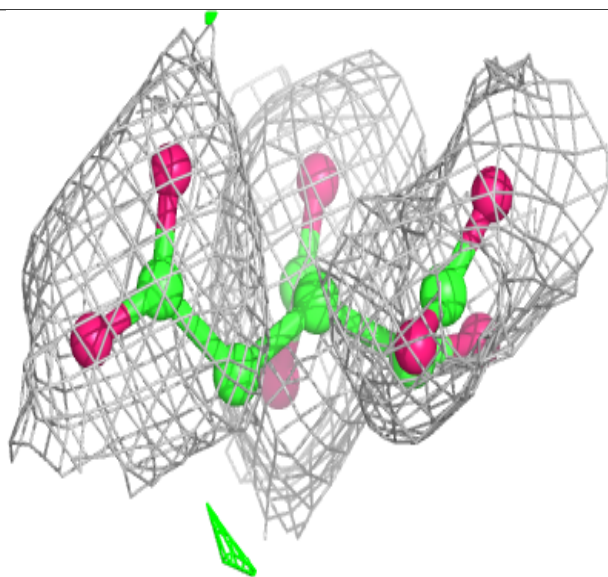
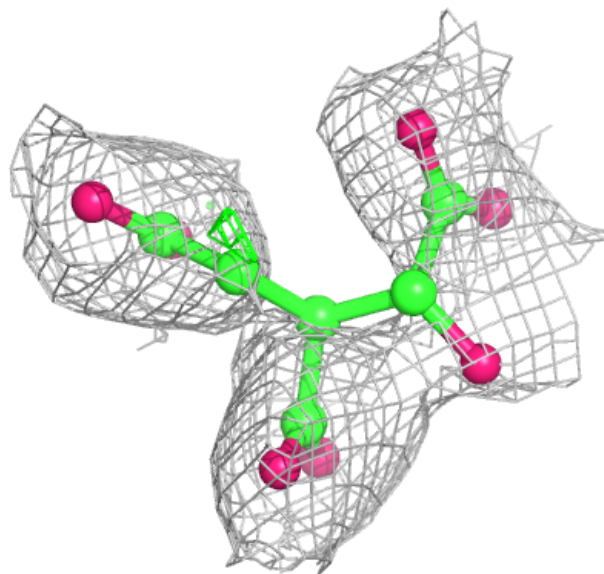
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





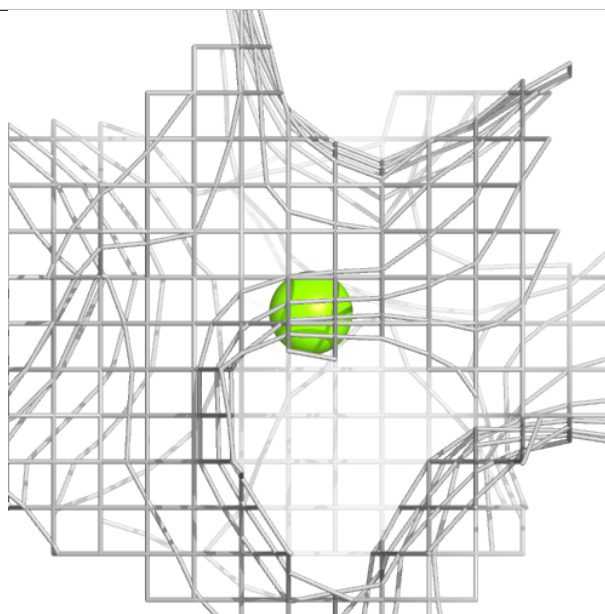
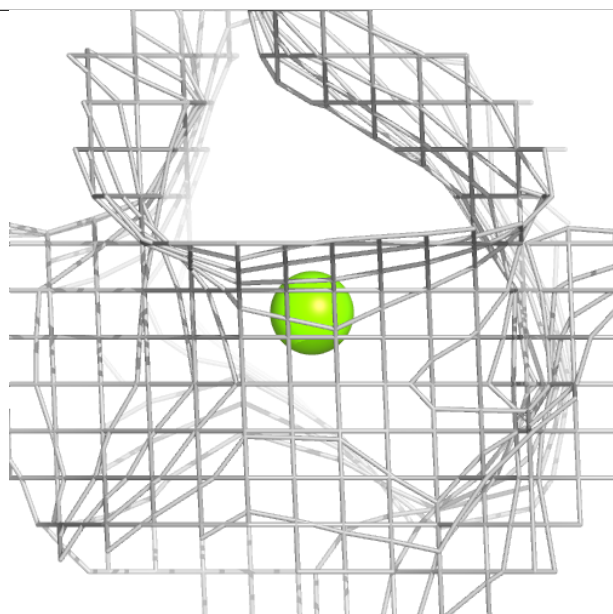
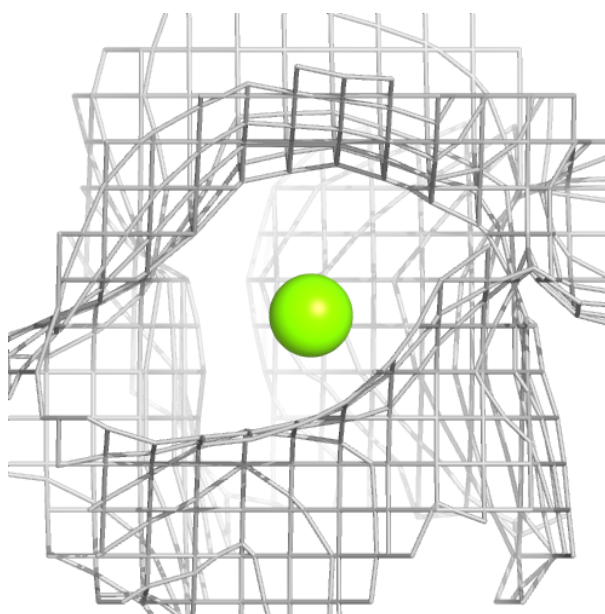
**Electron density around ICT A 301:**

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



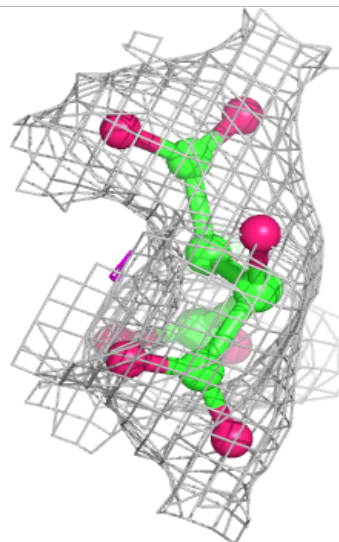
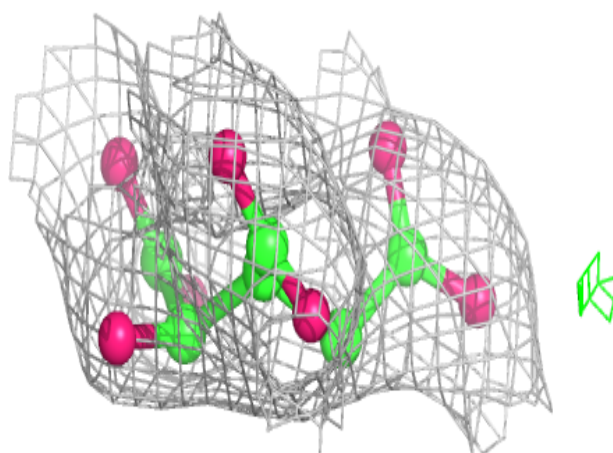
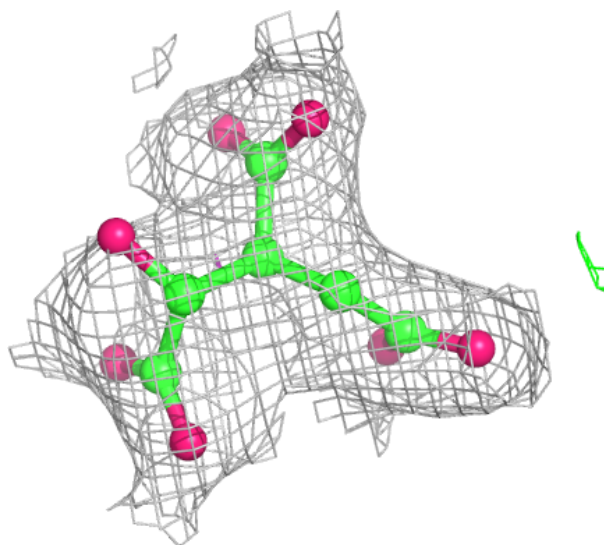
**Electron density around MG F 305:**

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



**Electron density around ICT B 301:**

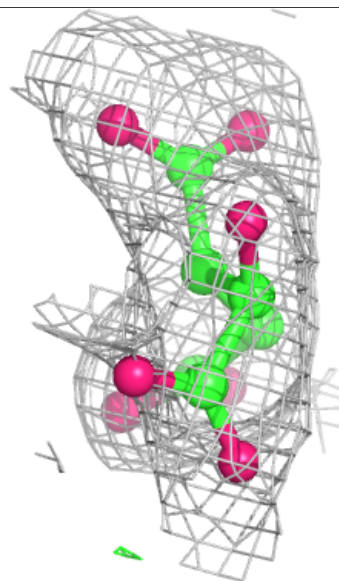
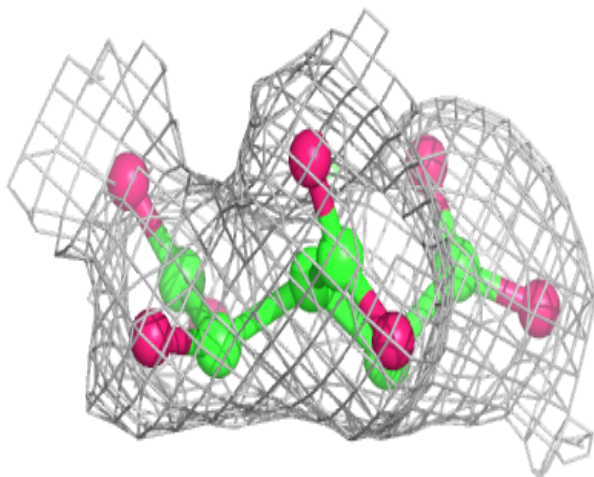
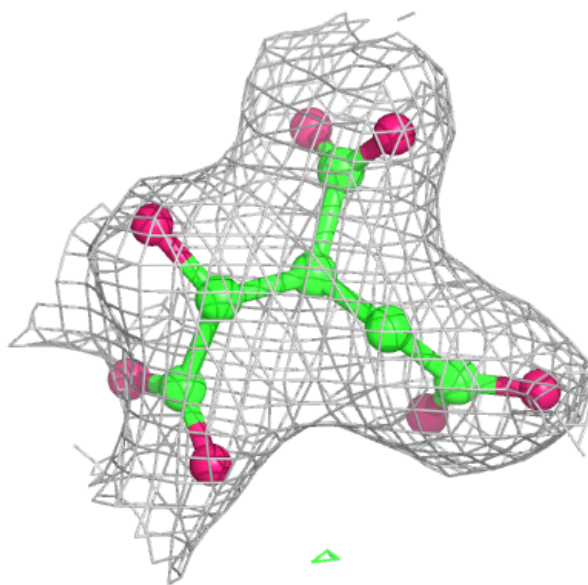
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





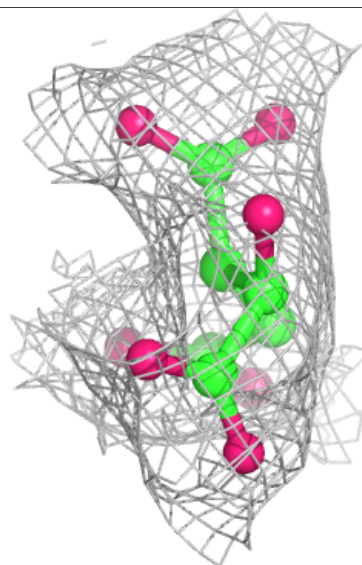
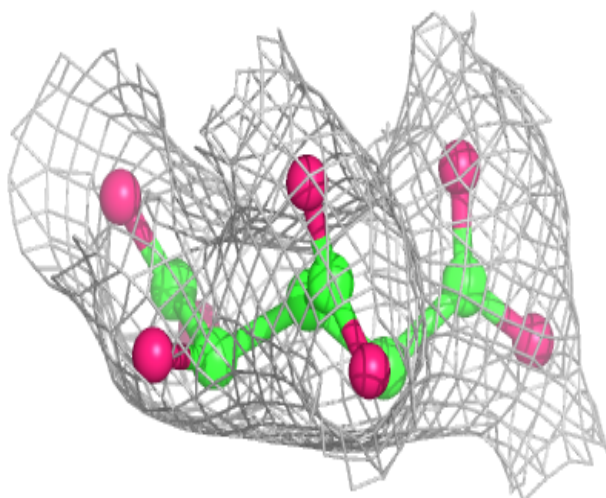
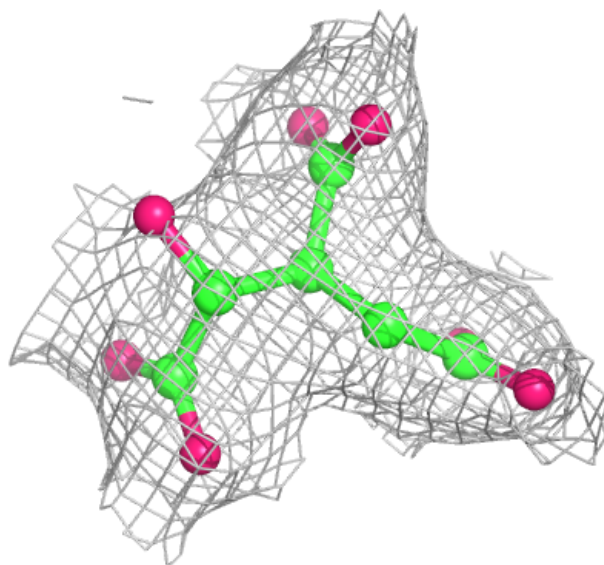
**Electron density around ICT I 301:**

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



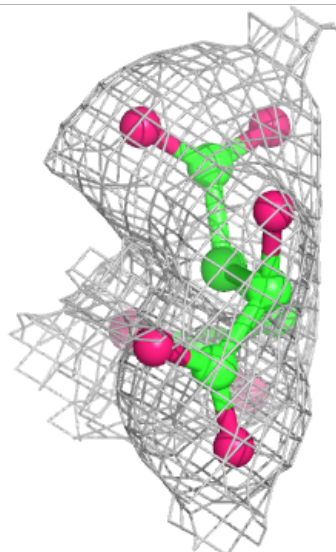
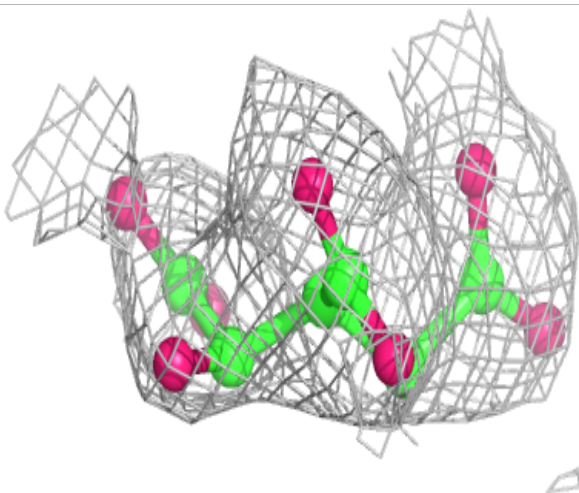
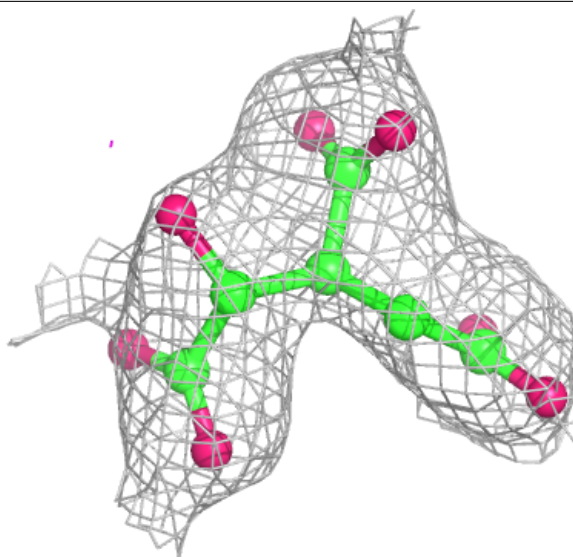
**Electron density around ICT D 302:**

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



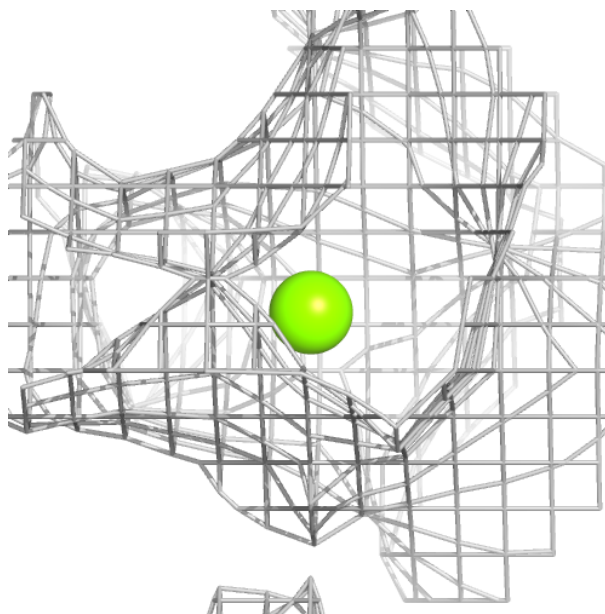
**Electron density around ICT G 301:**

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



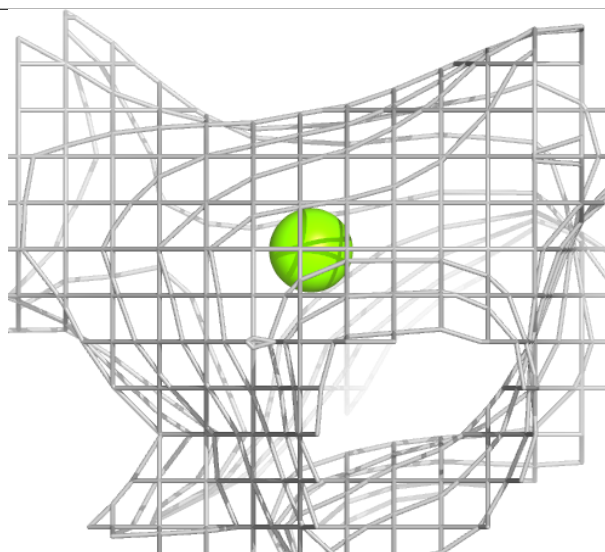
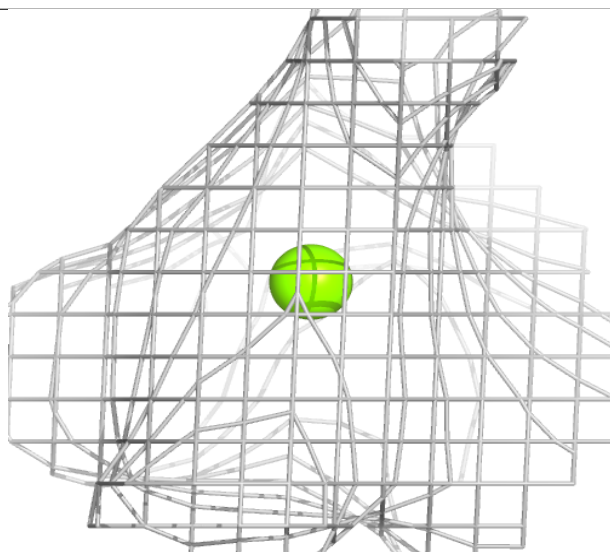
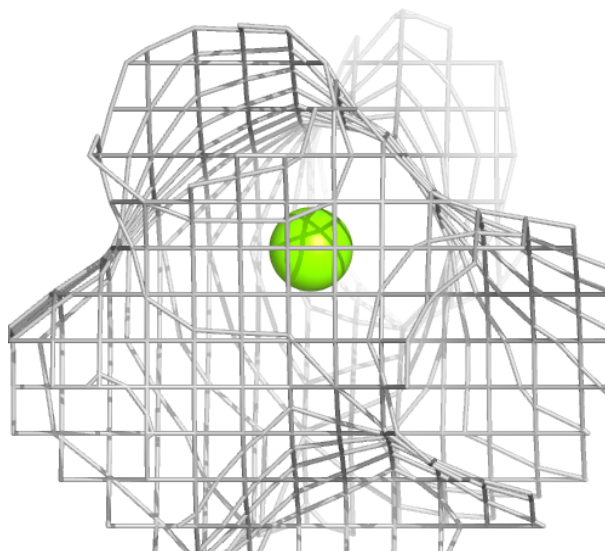
**Electron density around MG A 304:**

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



**Electron density around MG K 303:**

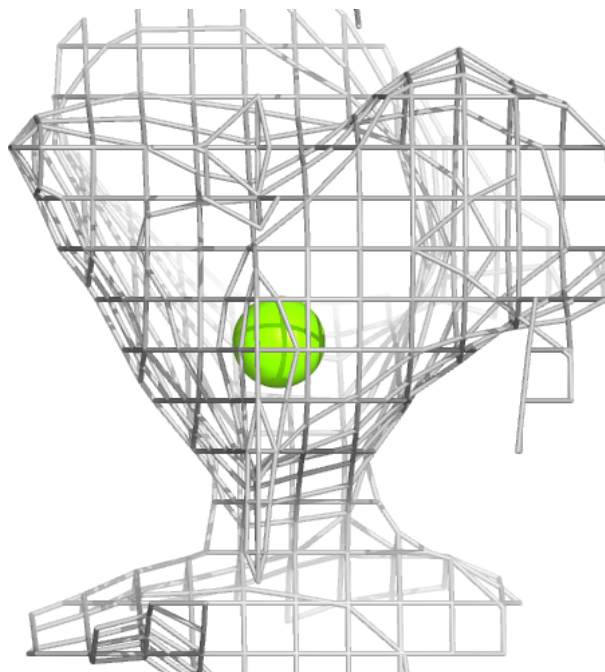
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





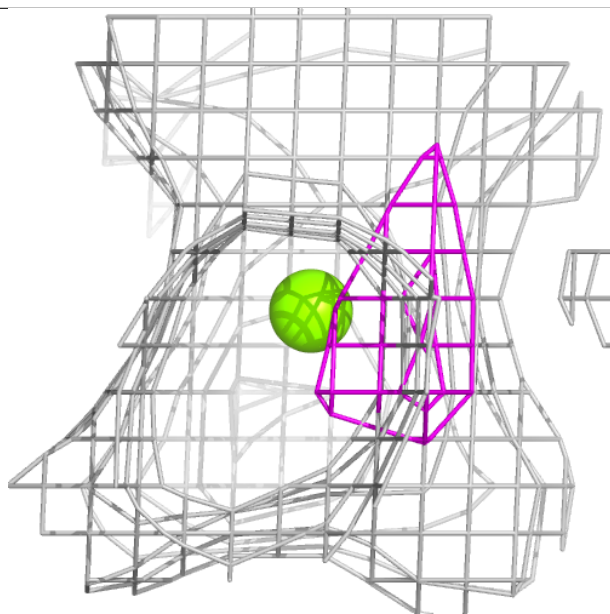
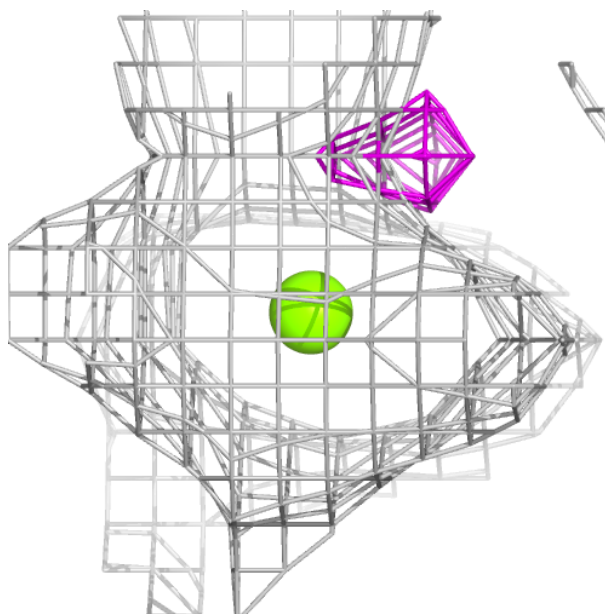
**Electron density around MG G 307:**

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



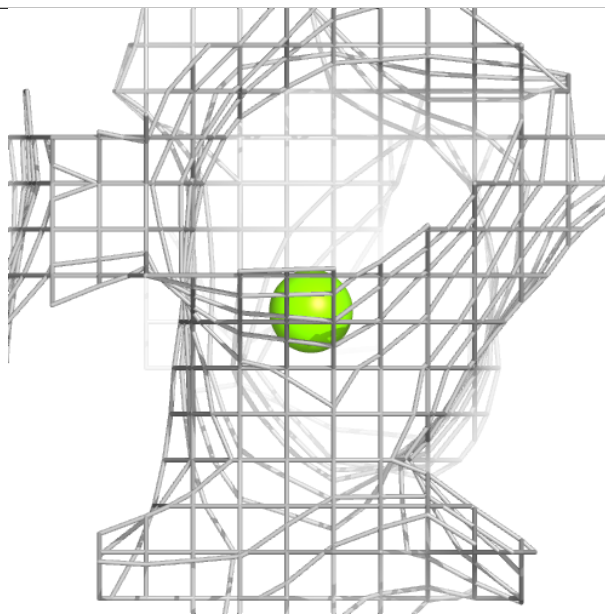
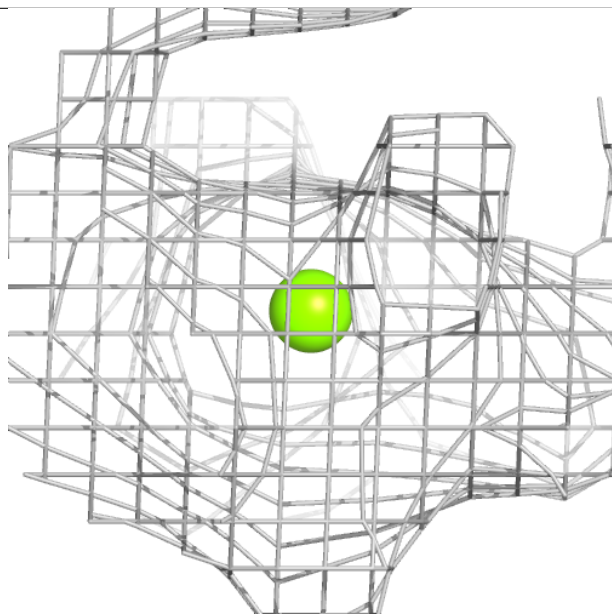
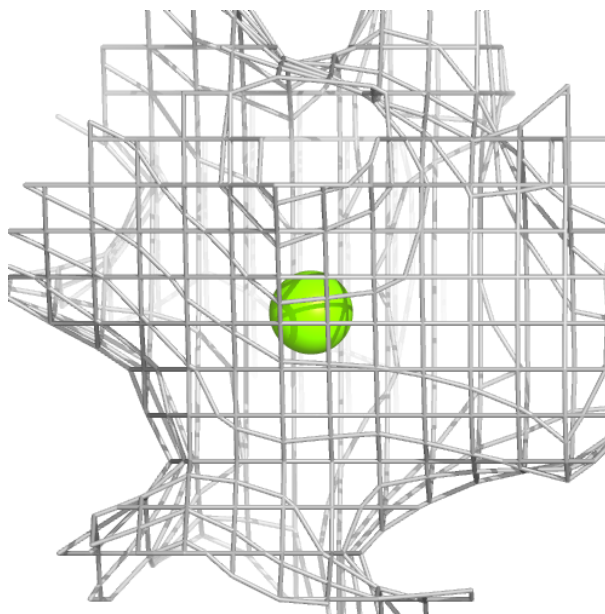
**Electron density around MG C 303:**

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



**Electron density around MG I 303:**

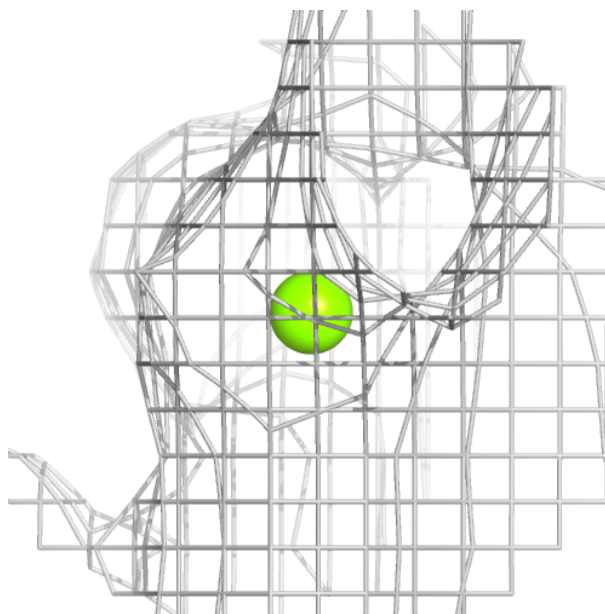
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





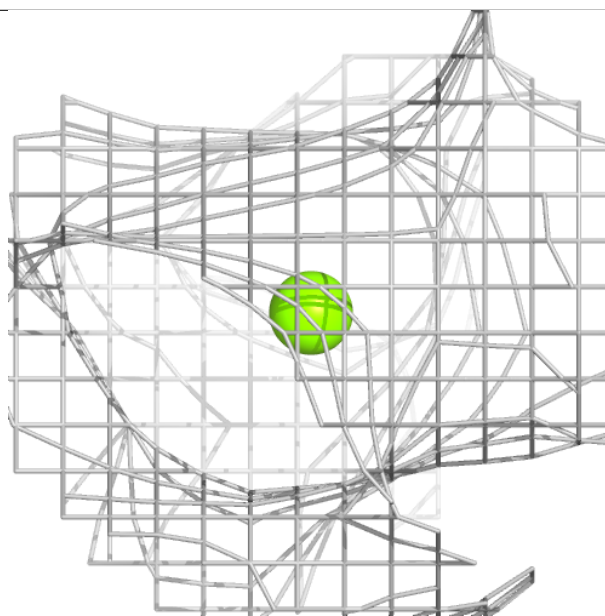
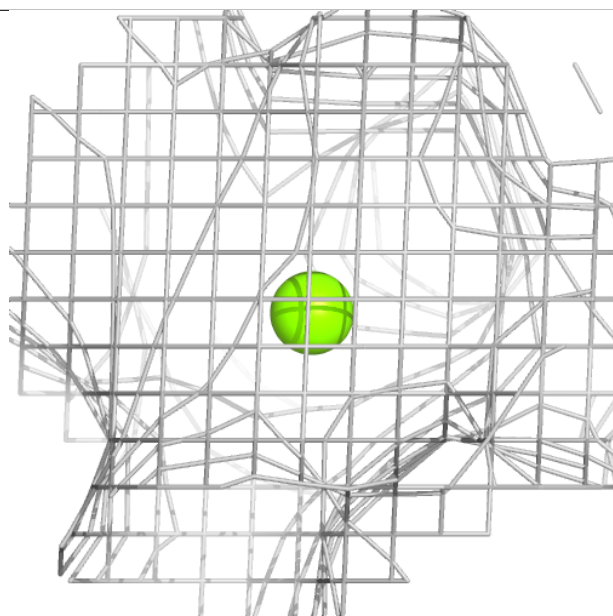
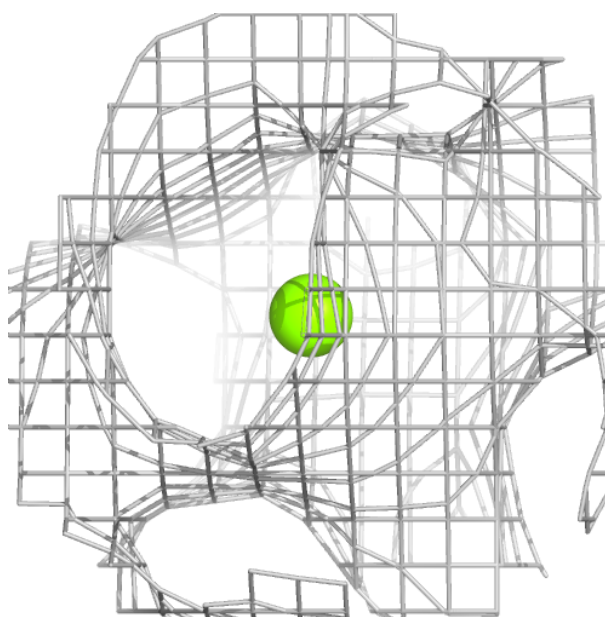
**Electron density around MG E 303:**

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



**Electron density around MG D 309:**

$2mF_o-DF_c$  (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.