



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 18, 2025 – 01:11 pm BST

PDB ID : 9GHL / pdb\_00009ghl  
Title : Fe(II)-2-oxoglutarate-dependent pseudomonal iron uptake factor C in complex with malate  
Authors : Alshref, F.M.; Allen, M.D.; Sanguankiattichai, N.; Zaborskyte, G.; Schofield, C.J.  
Deposited on : 2024-08-15  
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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



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

MolProbity	:	4-5-2 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



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Mol	Chain	Length	Quality of chain
1	E	225	 85%15%
1	F	225	 79%21%

## 2 Entry composition [i](#)

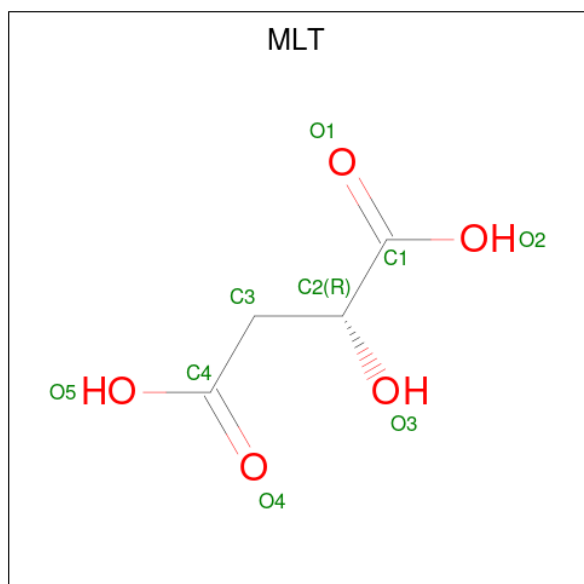
There are 5 unique types of molecules in this entry. The entry contains 11995 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PKHD-type hydroxylase PiuC.

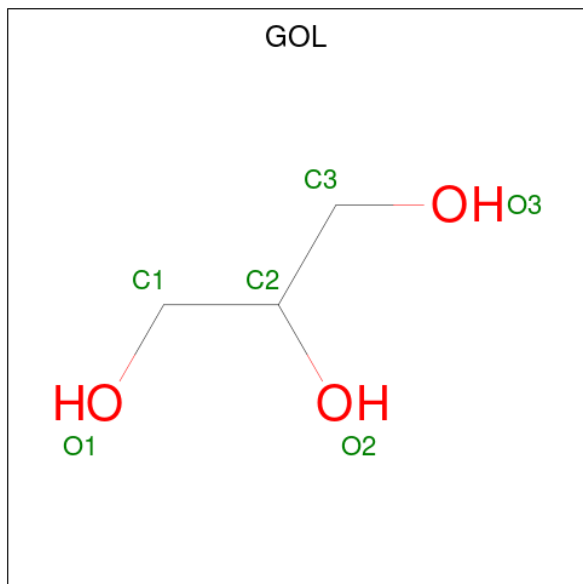
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	5	0
			1853	1177	333	339	4			
1	B	225	Total	C	N	O	S	0	6	0
			1861	1181	334	342	4			
1	C	225	Total	C	N	O	S	0	4	0
			1845	1171	332	338	4			
1	D	225	Total	C	N	O	S	0	3	0
			1836	1168	329	335	4			
1	E	225	Total	C	N	O	S	0	3	0
			1836	1168	329	335	4			
1	F	225	Total	C	N	O	S	0	3	0
			1836	1168	329	335	4			

- Molecule 2 is D-MALATE (CCD ID: MLT) (formula:  $C_4H_6O_5$ ) (labeled as "Ligand of Interest" by depositor).



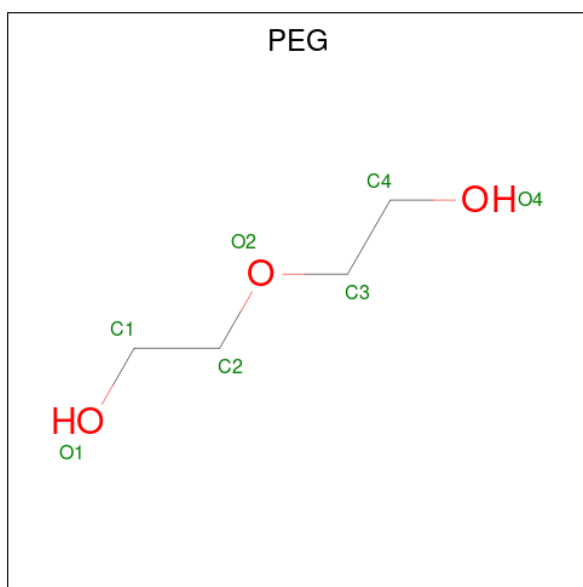
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	4	5		
2	B	1	Total	C	O	0	0
			9	4	5		
2	C	1	Total	C	O	0	0
			9	4	5		
2	D	1	Total	C	O	0	0
			9	4	5		
2	E	1	Total	C	O	0	0
			9	4	5		
2	F	1	Total	C	O	0	0
			9	4	5		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	E	1	Total	C	O	0	0
			7	4	3		
4	F	1	Total	C	O	0	0
			7	4	3		


- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	150	Total	O	0	0
			150	150		
5	B	161	Total	O	0	0
			161	161		
5	C	166	Total	O	0	0
			166	166		
5	D	115	Total	O	0	0
			115	115		
5	E	109	Total	O	0	0
			109	109		
5	F	113	Total	O	0	0
			113	113		

### 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: PKHD-type hydroxylase PiuC

Chain A:  85% 15%



- Molecule 1: PKHD-type hydroxylase PiuC

Chain B:  88% 12%




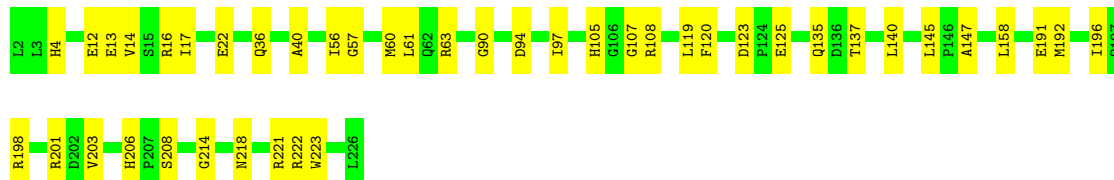
- Molecule 1: PKHD-type hydroxylase PiuC

Chain C:  87% 13%




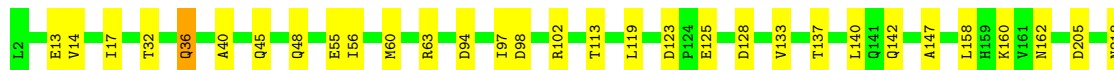
- Molecule 1: PKHD-type hydroxylase PiuC

Chain D:  81% 19%



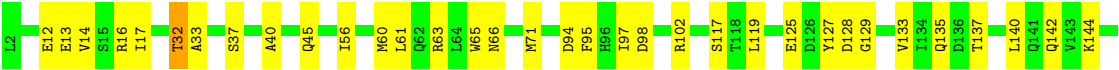
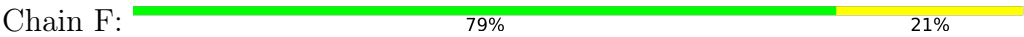
- Molecule 1: PKHD-type hydroxylase PiuC

Chain E:  85% 15%





● Molecule 1: PKHD-type hydroxylase PiuC



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.84Å 80.91Å 88.70Å 62.89° 62.90° 60.03°	Depositor
Resolution (Å)	59.58 – 2.00 59.58 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.3 (59.58-2.00) 96.1 (59.58-2.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.18 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.183 , 0.208 0.183 , 0.207	Depositor DCC
$R_{free}$ test set	1925 reflections (1.78%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.9	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 42.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.469 for -h+k,-h,-h+l 0.469 for -k,h-k,-k+l 0.039 for h,h-k,h-l 0.037 for -h+k,k,k-l 0.037 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	11995	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% 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: PEG, GOL, MLT

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	0.13	0/1902	0.33	0/2584
1	B	0.13	0/1910	0.34	0/2596
1	C	0.13	0/1894	0.34	0/2573
1	D	0.12	0/1885	0.34	0/2561
1	E	0.13	0/1885	0.33	0/2561
1	F	0.11	0/1885	0.30	0/2561
All	All	0.13	0/11361	0.33	0/15436

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	1853	0	1804	25	1
1	B	1861	0	1808	20	1
1	C	1845	0	1794	22	0
1	D	1836	0	1792	29	0
1	E	1836	0	1792	29	0
1	F	1836	0	1792	34	0
2	A	9	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	9	0	4	0	0
2	C	9	0	4	0	0
2	D	9	0	4	0	0
2	E	9	0	4	0	0
2	F	9	0	4	0	0
3	A	6	0	8	3	0
3	D	6	0	8	3	0
3	F	6	0	8	3	0
4	A	7	0	10	2	0
4	B	7	0	10	1	0
4	C	7	0	10	0	0
4	D	7	0	10	0	0
4	E	7	0	10	2	0
4	F	7	0	10	0	0
5	A	150	0	0	9	0
5	B	161	0	0	5	0
5	C	166	0	0	5	0
5	D	115	0	0	4	0
5	E	109	0	0	9	0
5	F	113	0	0	8	0
All	All	11995	0	10890	153	1

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 7.

All (153) 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:A:123:ASP:OD1	5:A:401:HOH:O	1.84	0.94
1:B:128:ASP:OD2	5:B:601:HOH:O	1.84	0.94
3:A:302:GOL:H11	1:E:223:TRP:HE1	1.32	0.93
1:B:142:GLN:NE2	5:B:602:HOH:O	2.01	0.92
1:F:98:ASP:OD2	5:F:401:HOH:O	1.88	0.91
1:C:223:TRP:HE1	3:F:302:GOL:H32	1.34	0.90
1:B:223:TRP:HE1	3:D:302:GOL:H32	1.38	0.89
1:C:109:GLU:OE1	5:C:401:HOH:O	1.90	0.88
1:C:123:ASP:OD1	5:C:402:HOH:O	1.94	0.86
1:F:33:ALA:N	5:F:402:HOH:O	2.07	0.85
1:D:198:ARG:HH11	1:D:201:ARG:HH22	1.29	0.81
1:E:205:ASP:OD2	5:E:401:HOH:O	2.00	0.80
1:E:102:ARG:NH1	5:E:407:HOH:O	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:HIS:HD2	1:C:208:SER:H	1.34	0.75
1:D:97:ILE:HG23	1:D:158:LEU:HD12	1.71	0.72
1:A:142:GLN:NE2	5:A:404:HOH:O	2.23	0.71
1:F:223:TRP:HE1	3:F:302:GOL:H11	1.54	0.71
1:E:55:GLU:OE2	5:E:402:HOH:O	2.08	0.71
1:F:33:ALA:O	5:F:402:HOH:O	2.09	0.70
1:B:182:GLU:OE1	5:B:603:HOH:O	2.10	0.69
1:F:128:ASP:OD2	5:F:403:HOH:O	2.10	0.68
1:E:123:ASP:OD2	5:E:403:HOH:O	2.10	0.68
1:A:206:HIS:ND1	1:A:207:PRO:HD2	2.09	0.68
1:C:128:ASP:OD2	5:C:403:HOH:O	2.12	0.67
1:A:128:ASP:OD2	5:A:402:HOH:O	2.13	0.67
1:E:128:ASP:OD2	5:E:404:HOH:O	2.12	0.66
1:D:223:TRP:HE1	3:D:302:GOL:H11	1.61	0.65
1:B:30:LYS:NZ	1:B:38:ALA:O	2.24	0.65
1:A:139:GLY:N	5:A:405:HOH:O	2.30	0.65
1:D:90:GLY:O	5:D:401:HOH:O	2.14	0.65
4:E:302:PEG:O4	5:E:405:HOH:O	2.15	0.64
1:D:123:ASP:OD1	5:D:402:HOH:O	2.15	0.63
1:B:102:ARG:NH2	5:B:604:HOH:O	2.16	0.62
1:A:223:TRP:HE1	3:A:302:GOL:H32	1.65	0.60
1:B:191:GLU:HG3	1:E:137:THR:HG23	1.81	0.60
1:C:191:GLU:HG3	1:D:137:THR:HG23	1.83	0.59
1:D:206:HIS:HD2	1:D:208:SER:H	1.50	0.59
1:E:36:GLN:OE1	5:E:406:HOH:O	2.17	0.58
1:E:17:ILE:HG23	1:E:56:ILE:HD13	1.85	0.58
1:F:14:VAL:HG11	1:F:147:ALA:HB1	1.86	0.58
1:E:123:ASP:HB3	1:E:125:GLU:OE1	2.03	0.58
1:E:14:VAL:HG11	1:E:147:ALA:HB1	1.86	0.57
1:B:206:HIS:ND1	1:B:207:PRO:HD2	2.19	0.57
1:D:214:GLY:HA2	1:E:97:ILE:HG12	1.85	0.57
1:F:66:ASN:OD1	5:F:404:HOH:O	2.17	0.57
1:F:13:GLU:O	1:F:17:ILE:HG13	2.04	0.57
1:F:98:ASP:OD1	5:F:405:HOH:O	2.17	0.57
1:A:136:ASP:HB2	5:A:405:HOH:O	2.04	0.57
3:A:302:GOL:H11	1:E:223:TRP:NE1	2.14	0.56
1:D:123:ASP:HB3	1:D:125:GLU:OE1	2.05	0.56
1:C:142:GLN:NE2	5:C:408:HOH:O	2.37	0.56
1:B:9:PHE:HE1	4:B:302:PEG:H12	1.71	0.56
1:F:17:ILE:HG23	1:F:56:ILE:HD13	1.88	0.55
1:A:198:ARG:NH1	1:A:202:ASP:OD2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:VAL:O	1:D:203:VAL:HG13	2.08	0.54
1:D:14:VAL:HG11	1:D:147:ALA:HB1	1.90	0.54
1:D:60:MET:HE3	1:D:119:LEU:HD12	1.89	0.54
1:D:17:ILE:HG23	1:D:56:ILE:HD13	1.89	0.53
1:A:97:ILE:HD12	1:A:98:ASP:H	1.74	0.53
1:E:48:GLN:HG2	5:E:446:HOH:O	2.09	0.53
1:F:133:VAL:HG22	1:F:142:GLN:HG2	1.90	0.53
1:F:125:GLU:H	1:F:125:GLU:CD	2.17	0.53
1:D:40:ALA:HB1	1:D:94:ASP:HB3	1.92	0.52
1:D:22:GLU:OE2	5:D:403:HOH:O	2.19	0.52
1:F:12:GLU:OE2	1:F:16:ARG:HG3	2.10	0.51
1:F:71:MET:HG3	5:F:491:HOH:O	2.09	0.51
1:F:135:GLN:HA	1:F:140:LEU:HD12	1.92	0.51
1:C:97:ILE:HD12	1:C:98:ASP:H	1.75	0.51
1:C:182:GLU:OE2	5:C:404:HOH:O	2.19	0.51
1:C:58:GLU:O	1:C:62:GLN:HG3	2.12	0.49
1:F:40:ALA:HB1	1:F:94:ASP:HB3	1.94	0.49
1:F:127:TYR:CE2	1:F:144:LYS:HE3	2.46	0.49
1:D:4:HIS:CD2	1:D:145:LEU:HD13	2.47	0.49
1:E:32:THR:OG1	1:E:45:GLN:NE2	2.46	0.49
1:B:223:TRP:NE1	3:D:302:GOL:H32	2.19	0.49
1:C:41:LYS:HD2	1:C:93:PHE:CE2	2.47	0.49
1:C:137:THR:HG23	1:D:191:GLU:HG2	1.94	0.49
1:C:133:VAL:HG22	1:C:142:GLN:HG2	1.96	0.48
1:A:194:GLN:OE1	5:A:403:HOH:O	2.20	0.48
1:A:203:VAL:HG22	1:A:206:HIS:HB2	1.96	0.48
1:F:97:ILE:HB	1:F:158:LEU:HD12	1.95	0.48
1:A:133:VAL:HG22	1:A:142:GLN:HG2	1.95	0.48
1:B:57:GLY:O	1:B:61[A]:LEU:HG	2.13	0.48
1:D:218:ASN:O	1:D:222:ARG:HG3	2.14	0.47
1:A:59:ALA:HB1	4:A:303:PEG:H11	1.95	0.47
1:A:127:TYR:CE2	1:A:144:LYS:HE3	2.50	0.47
1:B:97:ILE:HD12	1:B:98:ASP:H	1.78	0.47
1:C:125:GLU:H	1:C:125:GLU:CD	2.20	0.47
1:B:128:ASP:CG	1:B:166:ARG:HE	2.23	0.47
1:E:125:GLU:H	1:E:125:GLU:CD	2.23	0.47
1:E:40:ALA:HB1	1:E:94:ASP:HB3	1.97	0.46
1:F:60:MET:HE3	1:F:119:LEU:HD12	1.97	0.46
1:D:135:GLN:HA	1:D:140:LEU:HD23	1.96	0.46
1:E:218:ASN:O	1:E:222:ARG:HG3	2.15	0.46
1:E:133:VAL:HG22	1:E:142:GLN:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:MET:HE2	1:A:216:TYR:HB2	1.97	0.46
1:E:225:GLU:OE2	5:E:408:HOH:O	2.21	0.46
1:B:218:ASN:O	1:B:222:ARG:HG3	2.16	0.46
1:F:97:ILE:HD12	1:F:98:ASP:H	1.81	0.46
1:A:190:PHE:O	1:A:194:GLN:HG2	2.16	0.45
1:C:61:LEU:HD12	1:C:65[A]:TRP:CD1	2.51	0.45
1:E:97:ILE:HD12	1:E:98:ASP:H	1.81	0.45
1:E:13:GLU:CD	1:E:63:ARG:HH22	2.25	0.45
1:A:125:GLU:H	1:A:125:GLU:CD	2.25	0.45
1:D:221[B]:ARG:NH1	1:E:113:THR:OG1	2.49	0.45
1:E:60:MET:HE3	1:E:119:LEU:HD12	1.98	0.45
1:C:127:TYR:CE2	1:C:144:LYS:HE3	2.52	0.44
4:A:303:PEG:H42	5:A:532:HOH:O	2.17	0.44
1:C:206:HIS:CD2	1:C:207:PRO:HD2	2.53	0.44
1:F:32:THR:OG1	1:F:45:GLN:NE2	2.50	0.44
1:A:135:GLN:HB2	1:A:140:LEU:HD23	2.00	0.44
1:F:190:PHE:O	1:F:194:GLN:HG2	2.18	0.44
1:D:13:GLU:CD	1:D:63:ARG:HH22	2.25	0.44
5:D:425:HOH:O	1:F:210:ILE:HD11	2.17	0.44
1:A:214:GLY:HA2	1:B:97:ILE:HG21	2.00	0.43
1:B:133:VAL:HG22	1:B:142:GLN:HG2	2.00	0.43
1:F:218:ASN:O	1:F:222:ARG:HG3	2.19	0.43
1:A:57:GLY:O	1:A:61[A]:LEU:HG	2.18	0.43
1:A:191:GLU:HG3	1:F:137:THR:HG23	2.01	0.43
1:F:33:ALA:HB1	1:F:37:SER:OG	2.19	0.43
1:A:138:TYR:N	5:A:405:HOH:O	2.44	0.43
1:F:203:VAL:HG22	1:F:206:HIS:HB2	2.00	0.43
1:B:202:ASP:HB2	1:D:206:HIS:HE1	1.84	0.42
1:C:4:HIS:CE1	1:C:145:LEU:HD22	2.52	0.42
1:E:160:LYS:HE3	1:E:162:ASN:OD1	2.19	0.42
1:F:102:ARG:NH1	5:F:415:HOH:O	2.51	0.42
1:F:129:GLY:O	1:F:144:LYS:NZ	2.50	0.42
1:D:105:HIS:C	1:D:107:GLY:H	2.27	0.42
1:C:128:ASP:HB2	1:C:166:ARG:HB3	2.02	0.42
1:F:117:SER:HB3	1:F:150:LEU:HD11	2.00	0.42
1:B:127:TYR:CE2	1:B:144:LYS:HE3	2.55	0.42
1:D:198:ARG:HH11	1:D:201:ARG:NH2	2.07	0.42
1:C:29:GLY:C	1:C:41:LYS:HE2	2.45	0.42
1:E:56:ILE:HG12	4:E:302:PEG:H31	2.02	0.41
1:E:97:ILE:HB	1:E:158:LEU:HD12	2.01	0.41
1:D:12:GLU:OE1	1:D:16:ARG:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:TRP:NE1	3:F:302:GOL:H32	2.16	0.41
1:D:192:MET:O	1:D:196:ILE:HG13	2.21	0.41
1:F:95:PHE:HA	1:F:160:LYS:HB3	2.02	0.41
1:B:203:VAL:HG22	1:B:206:HIS:HB2	2.01	0.41
1:F:61[A]:LEU:O	1:F:65[A]:TRP:HD1	2.04	0.41
1:A:218:ASN:O	1:A:222:ARG:HG3	2.21	0.41
1:B:154:PRO:HD2	5:B:606:HOH:O	2.21	0.41
1:D:57:GLY:O	1:D:61[A]:LEU:HG	2.21	0.41
1:D:120:PHE:CD1	1:D:145:LEU:HB2	2.56	0.41
1:F:201:ARG:HG2	1:F:202:ASP:OD1	2.21	0.41
1:A:97:ILE:HD12	1:A:98:ASP:N	2.36	0.41
1:C:198:ARG:NH2	1:C:202:ASP:OD2	2.54	0.40
1:E:13:GLU:O	1:E:17:ILE:HG13	2.21	0.40
1:A:120:PHE:HE2	5:A:449:HOH:O	2.05	0.40
1:D:97:ILE:HG23	1:D:158:LEU:CD1	2.46	0.40
1:E:140:LEU:HD23	1:E:140:LEU:HA	1.83	0.40
1:F:13:GLU:CD	1:F:63:ARG:HH22	2.29	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LYS:NZ	1:B:125:GLU:OE2[1_655]	2.09	0.11

## 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	228/225 (101%)	224 (98%)	4 (2%)	0	100	100
1	B	229/225 (102%)	226 (99%)	2 (1%)	1 (0%)	30	27
1	C	227/225 (101%)	223 (98%)	3 (1%)	1 (0%)	30	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	226/225 (100%)	222 (98%)	2 (1%)	2 (1%)	14	10
1	E	226/225 (100%)	221 (98%)	4 (2%)	1 (0%)	30	27
1	F	226/225 (100%)	225 (100%)	1 (0%)	0	100	100
All	All	1362/1350 (101%)	1341 (98%)	16 (1%)	5 (0%)	30	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	36	GLN
1	E	36	GLN
1	B	36	GLN
1	D	36	GLN
1	D	108	ARG

### 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	197/192 (103%)	197 (100%)	0	100	100
1	B	198/192 (103%)	196 (99%)	2 (1%)	73	78
1	C	196/192 (102%)	196 (100%)	0	100	100
1	D	195/192 (102%)	195 (100%)	0	100	100
1	E	195/192 (102%)	195 (100%)	0	100	100
1	F	195/192 (102%)	194 (100%)	1 (0%)	86	90
All	All	1176/1152 (102%)	1173 (100%)	3 (0%)	92	94

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

Mol	Chain	Res	Type
1	B	221[A]	ARG
1	B	221[B]	ARG
1	F	32	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	HIS
1	A	62	GLN
1	A	135	GLN
1	A	194	GLN
1	B	42	HIS
1	B	62	GLN
1	B	66	ASN
1	C	42	HIS
1	C	62	GLN
1	C	66	ASN
1	C	206	HIS
1	D	42	HIS
1	D	206	HIS
1	E	197	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	F	302	-	5,5,5	1.07	0	5,5,5	0.94	0
3	GOL	D	302	-	5,5,5	1.14	0	5,5,5	0.94	0
2	MLT	A	301	-	8,8,8	1.07	0	10,10,10	1.59	1 (10%)
2	MLT	E	301	-	8,8,8	1.05	0	10,10,10	1.70	2 (20%)
2	MLT	D	301	-	8,8,8	1.05	0	10,10,10	1.67	2 (20%)
2	MLT	B	301	-	8,8,8	1.06	0	10,10,10	1.63	1 (10%)
3	GOL	A	302	-	5,5,5	1.17	0	5,5,5	0.85	0
2	MLT	F	301	-	8,8,8	1.04	0	10,10,10	1.69	2 (20%)
4	PEG	B	302	-	6,6,6	0.14	0	5,5,5	0.03	0
4	PEG	D	303	-	6,6,6	0.12	0	5,5,5	0.06	0
4	PEG	A	303	-	6,6,6	0.11	0	5,5,5	0.09	0
4	PEG	F	303	-	6,6,6	0.11	0	5,5,5	0.08	0
4	PEG	C	302	-	6,6,6	0.12	0	5,5,5	0.07	0
4	PEG	E	302	-	6,6,6	0.10	0	5,5,5	0.11	0
2	MLT	C	301	-	8,8,8	1.05	0	10,10,10	1.65	2 (20%)

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	GOL	F	302	-	-	2/4/4/4	-
3	GOL	D	302	-	-	2/4/4/4	-
2	MLT	A	301	-	-	4/8/8/8	-
2	MLT	E	301	-	-	4/8/8/8	-
2	MLT	D	301	-	-	4/8/8/8	-
2	MLT	B	301	-	-	4/8/8/8	-
3	GOL	A	302	-	-	2/4/4/4	-
2	MLT	F	301	-	-	5/8/8/8	-
4	PEG	B	302	-	-	2/4/4/4	-
4	PEG	D	303	-	-	3/4/4/4	-
4	PEG	A	303	-	-	2/4/4/4	-
4	PEG	F	303	-	-	2/4/4/4	-
4	PEG	C	302	-	-	0/4/4/4	-
4	PEG	E	302	-	-	2/4/4/4	-
2	MLT	C	301	-	-	5/8/8/8	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	MLT	O2-C1-C2	3.64	120.71	112.72
2	F	301	MLT	O2-C1-C2	3.61	120.65	112.72
2	D	301	MLT	O2-C1-C2	3.56	120.54	112.72
2	B	301	MLT	O2-C1-C2	3.50	120.42	112.72
2	C	301	MLT	O2-C1-C2	3.43	120.26	112.72
2	A	301	MLT	O2-C1-C2	3.38	120.15	112.72
2	F	301	MLT	O5-C4-C3	2.14	120.94	114.07
2	E	301	MLT	O5-C4-C3	2.10	120.79	114.07
2	C	301	MLT	O5-C4-C3	2.09	120.76	114.07
2	D	301	MLT	O5-C4-C3	2.09	120.75	114.07

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	GOL	O1-C1-C2-C3
4	A	303	PEG	O1-C1-C2-O2
4	D	303	PEG	O2-C3-C4-O4
3	A	302	GOL	O1-C1-C2-O2
4	E	302	PEG	O1-C1-C2-O2
4	B	302	PEG	O1-C1-C2-O2
4	B	302	PEG	O2-C3-C4-O4
4	D	303	PEG	O1-C1-C2-O2
2	E	301	MLT	O2-C1-C2-C3
3	F	302	GOL	O2-C2-C3-O3
4	F	303	PEG	C1-C2-O2-C3
4	E	302	PEG	C1-C2-O2-C3
3	D	302	GOL	O2-C2-C3-O3
3	D	302	GOL	C1-C2-C3-O3
2	A	301	MLT	C2-C3-C4-O5
4	A	303	PEG	C4-C3-O2-C2
2	D	301	MLT	C2-C3-C4-O5
2	E	301	MLT	C2-C3-C4-O5
2	C	301	MLT	O1-C1-C2-C3
2	C	301	MLT	O2-C1-C2-C3
2	E	301	MLT	O1-C1-C2-C3
2	F	301	MLT	O1-C1-C2-C3
2	A	301	MLT	C2-C3-C4-O4
2	D	301	MLT	C2-C3-C4-O4
2	E	301	MLT	C2-C3-C4-O4

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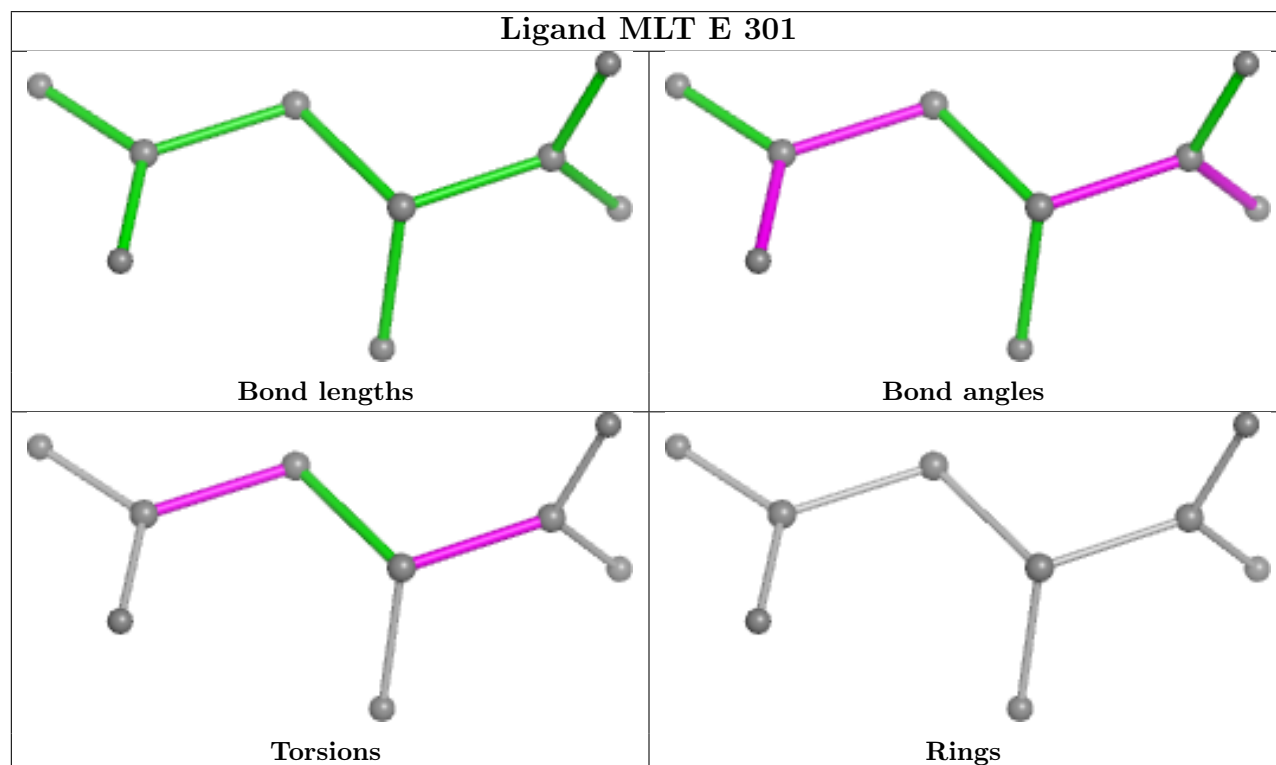
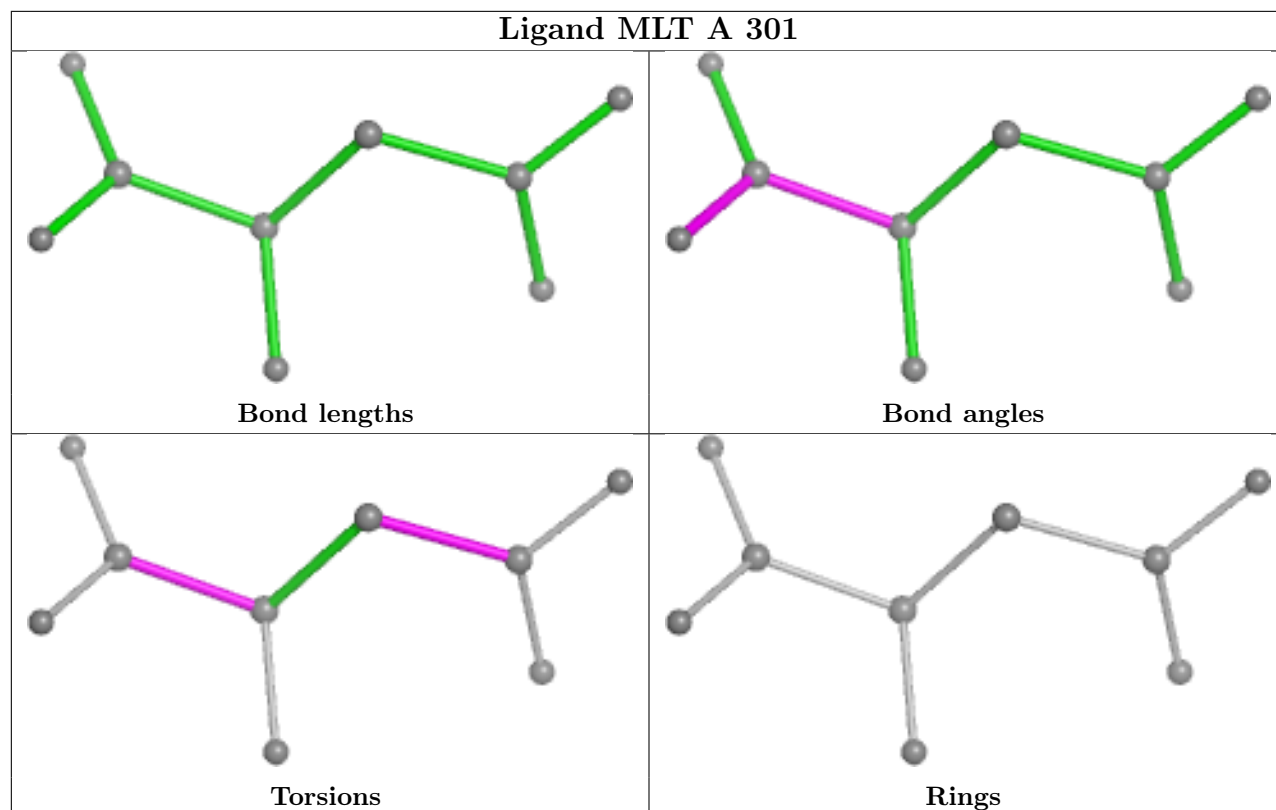
Mol	Chain	Res	Type	Atoms
2	F	301	MLT	C2-C3-C4-O4
2	F	301	MLT	C2-C3-C4-O5
4	F	303	PEG	O2-C3-C4-O4
4	D	303	PEG	C4-C3-O2-C2
2	A	301	MLT	O1-C1-C2-O3
2	A	301	MLT	O2-C1-C2-O3
2	B	301	MLT	O1-C1-C2-O3
2	B	301	MLT	O2-C1-C2-O3
2	C	301	MLT	O1-C1-C2-O3
2	C	301	MLT	O2-C1-C2-O3
2	D	301	MLT	O1-C1-C2-O3
2	D	301	MLT	O2-C1-C2-O3
2	F	301	MLT	O2-C1-C2-O3
2	C	301	MLT	C2-C3-C4-O5
3	F	302	GOL	C1-C2-C3-O3
2	B	301	MLT	O1-C1-C2-C3
2	B	301	MLT	O2-C1-C2-C3
2	F	301	MLT	O2-C1-C2-C3

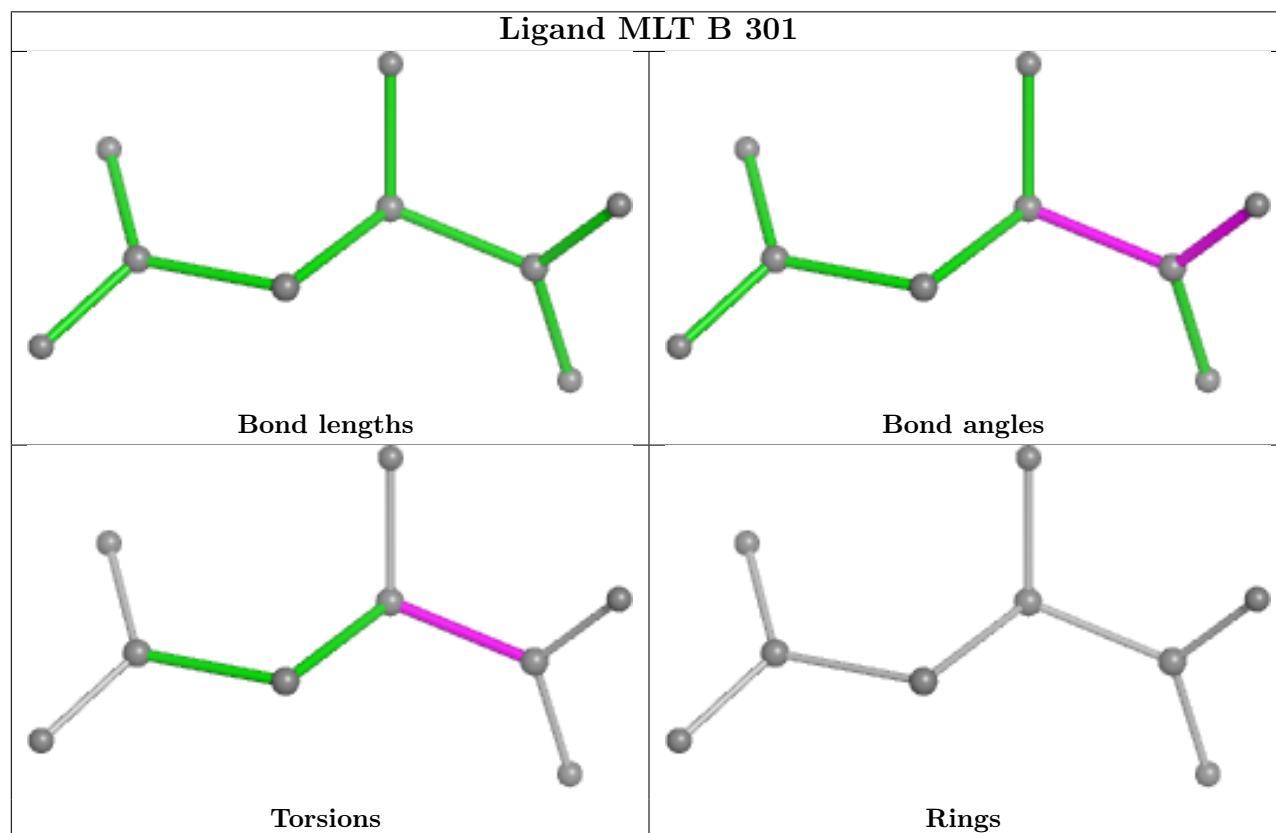
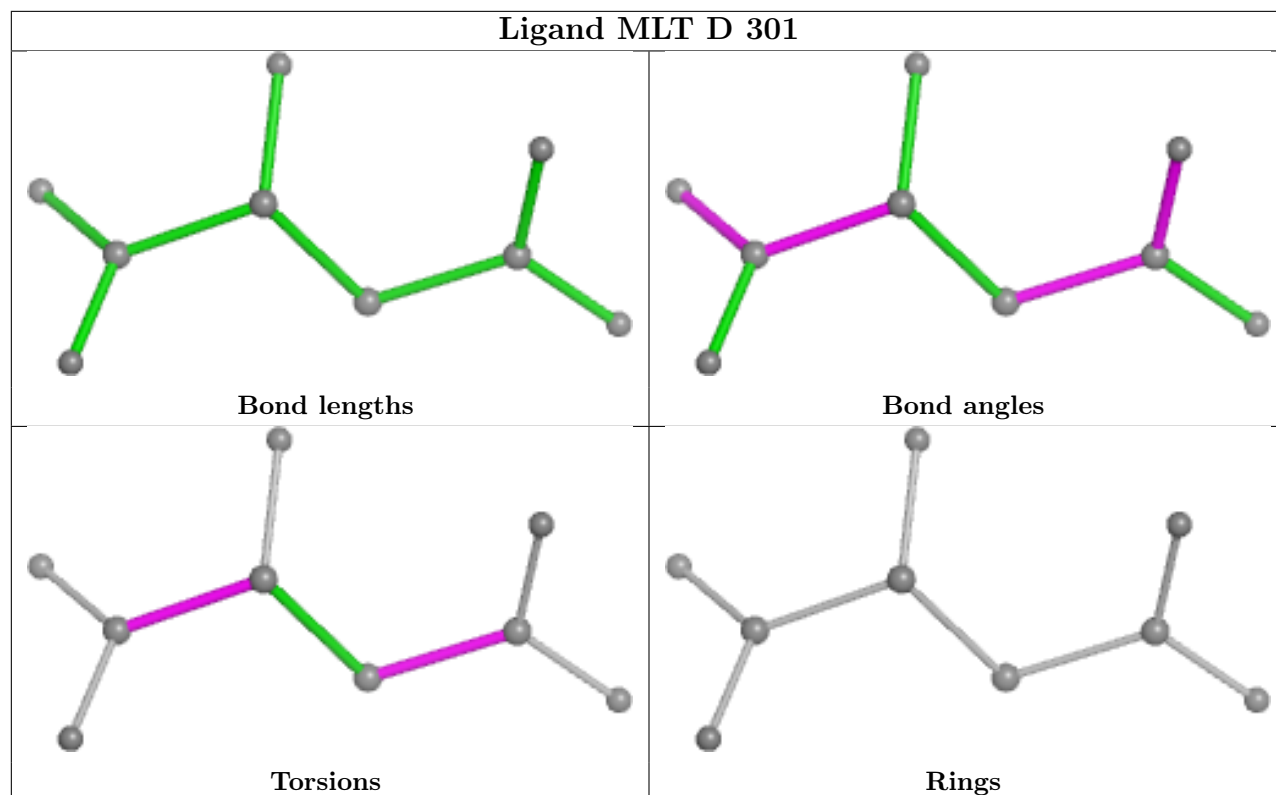
There are no ring outliers.

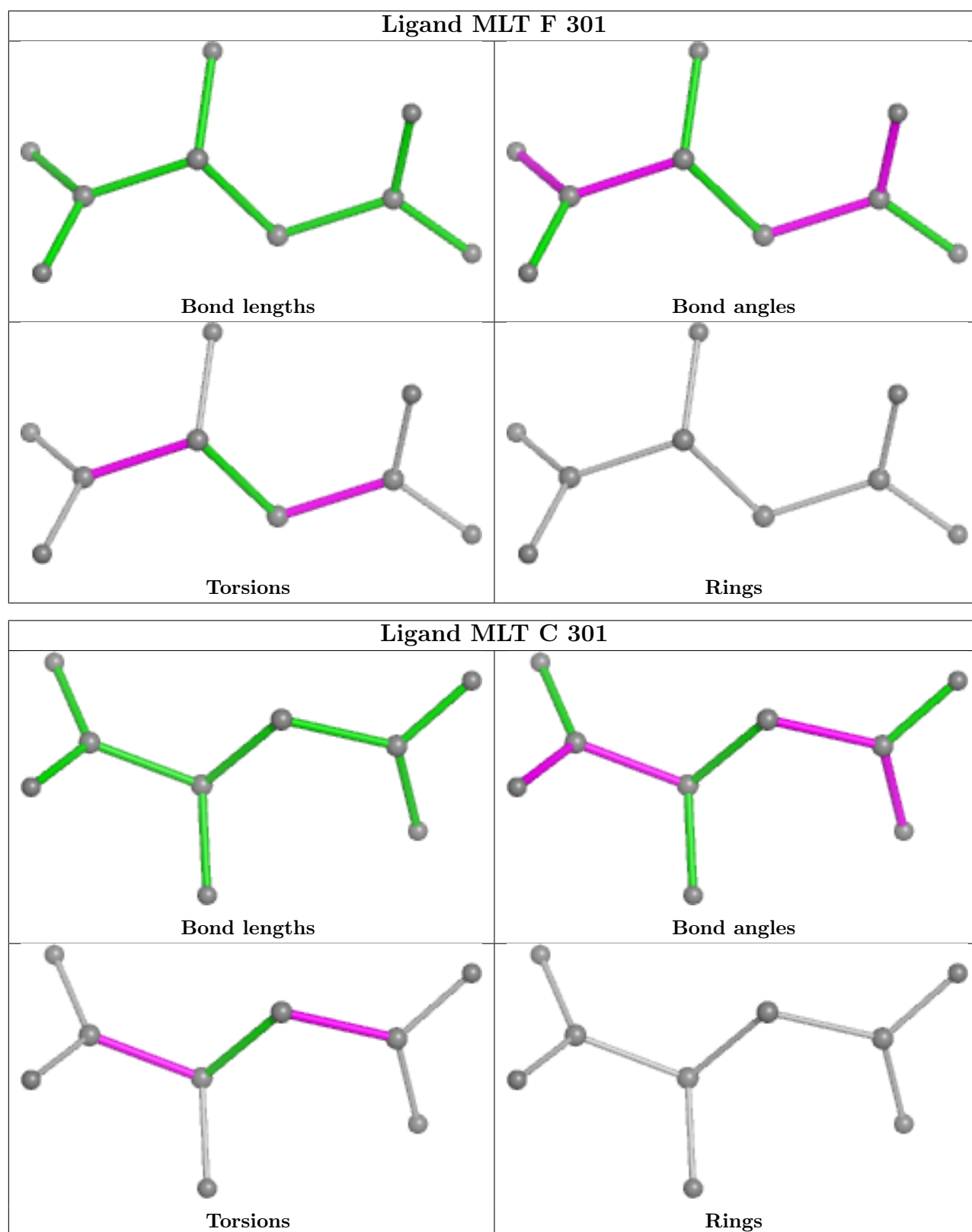
6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	302	GOL	3	0
3	D	302	GOL	3	0
3	A	302	GOL	3	0
4	B	302	PEG	1	0
4	A	303	PEG	2	0
4	E	302	PEG	2	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.







## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	225/225 (100%)	-1.41	0 100 100	13, 31, 74, 138	5 (2%)
1	B	225/225 (100%)	-1.42	0 100 100	13, 31, 72, 130	6 (2%)
1	C	225/225 (100%)	-1.41	0 100 100	13, 31, 72, 143	4 (1%)
1	D	225/225 (100%)	-1.34	0 100 100	14, 43, 77, 124	3 (1%)
1	E	225/225 (100%)	-1.35	0 100 100	14, 43, 75, 126	3 (1%)
1	F	225/225 (100%)	-1.34	0 100 100	14, 43, 75, 110	3 (1%)
All	All	1350/1350 (100%)	-1.38	0 100 100	13, 36, 75, 143	24 (1%)

There are no RSRZ outliers to report.

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.

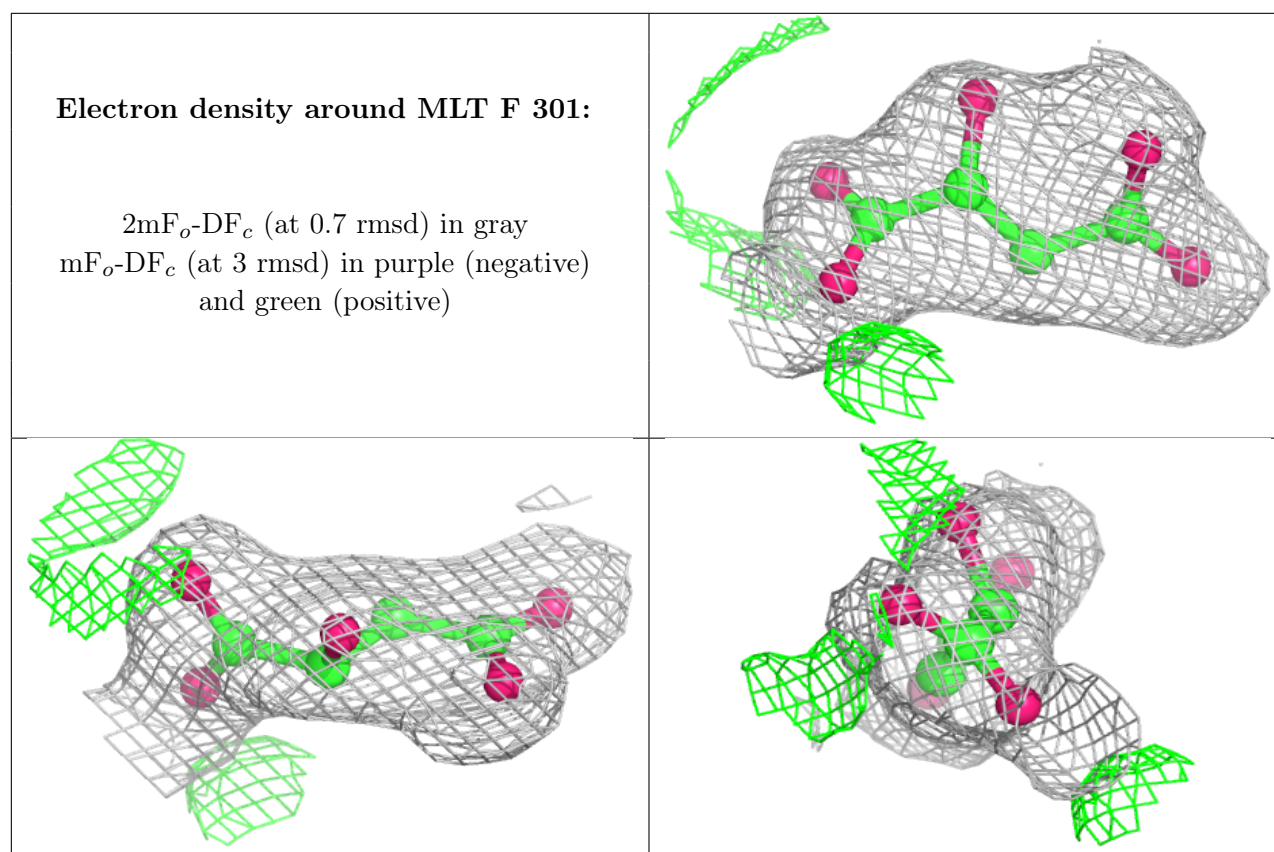
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MLT	F	301	9/9	0.98	0.05	41,44,54,55	0

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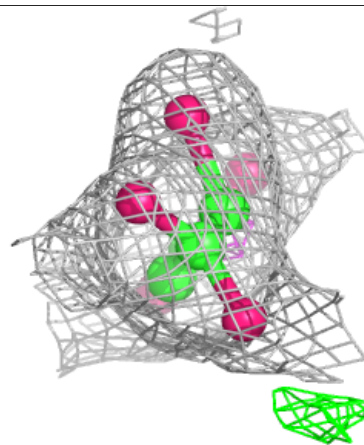
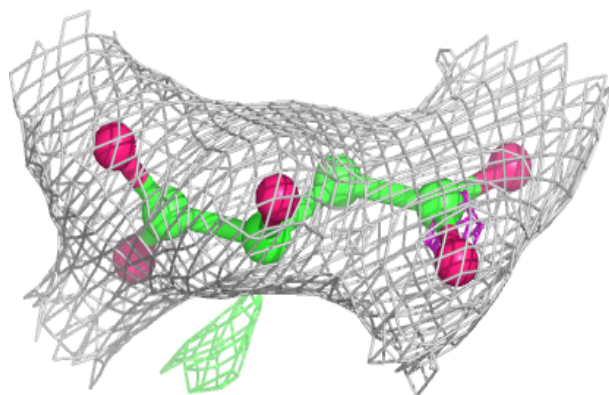
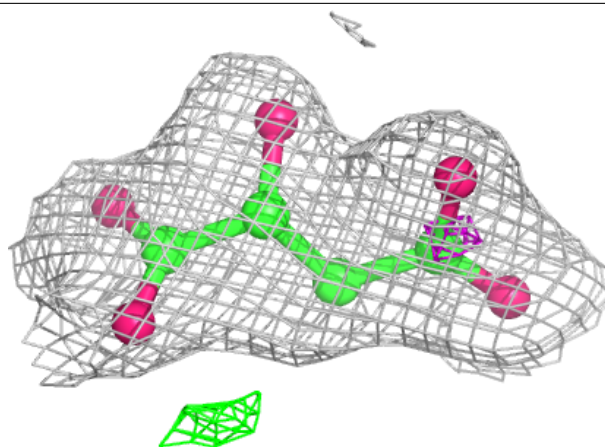
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PEG	B	302	7/7	0.98	0.07	41,50,51,56	0
4	PEG	C	302	7/7	0.98	0.05	44,47,53,55	0
2	MLT	D	301	9/9	0.99	0.05	39,42,57,57	0
2	MLT	E	301	9/9	0.99	0.04	38,41,56,57	0
2	MLT	A	301	9/9	0.99	0.03	30,35,45,46	0
3	GOL	A	302	6/6	0.99	0.04	27,38,48,53	0
3	GOL	D	302	6/6	0.99	0.04	35,42,44,50	0
3	GOL	F	302	6/6	0.99	0.03	32,39,43,51	0
4	PEG	A	303	7/7	0.99	0.04	43,48,52,56	0
2	MLT	B	301	9/9	0.99	0.05	26,32,43,43	0
2	MLT	C	301	9/9	0.99	0.04	27,33,44,46	0
4	PEG	D	303	7/7	0.99	0.05	40,53,61,62	0
4	PEG	E	302	7/7	0.99	0.04	41,46,57,63	0
4	PEG	F	303	7/7	0.99	0.05	47,53,57,61	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.



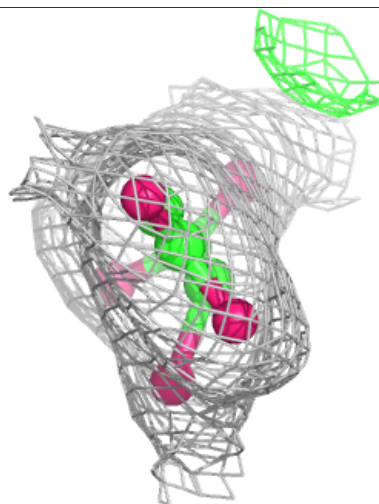
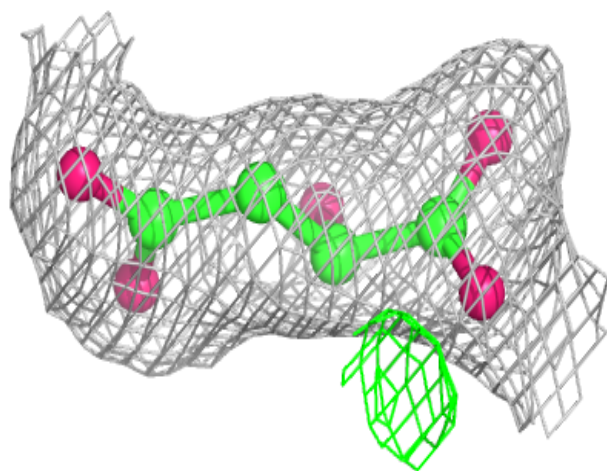
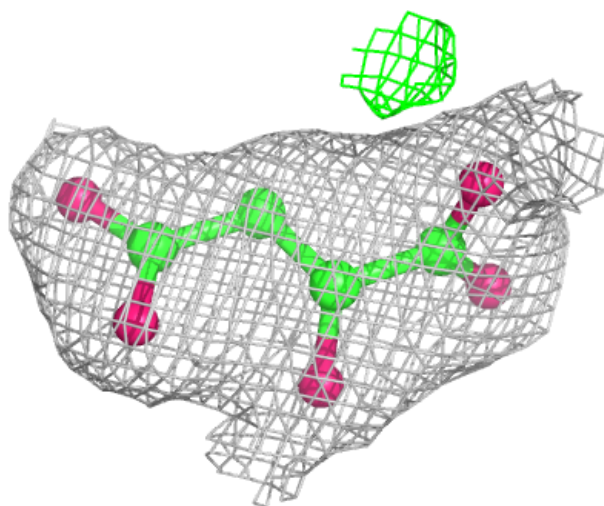
**Electron density around MLT D 301:**

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



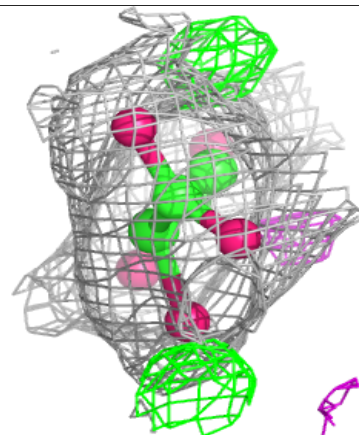
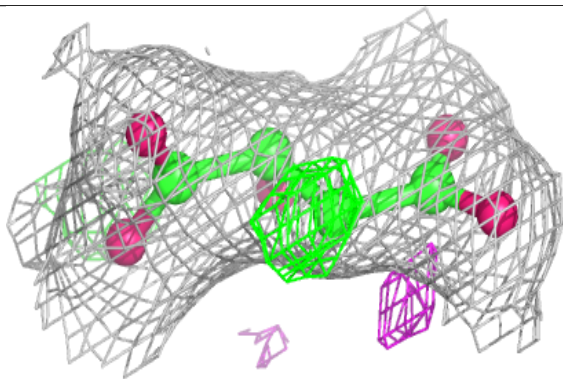
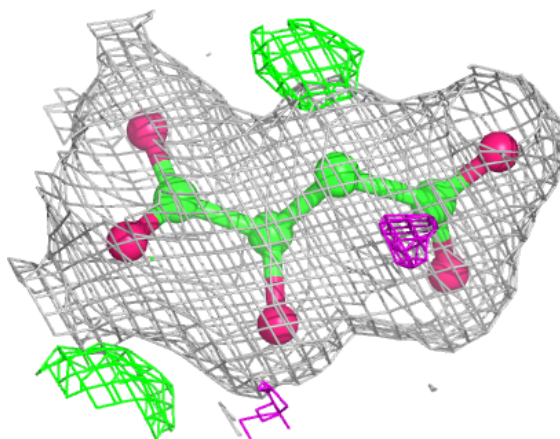
**Electron density around MLT E 301:**

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



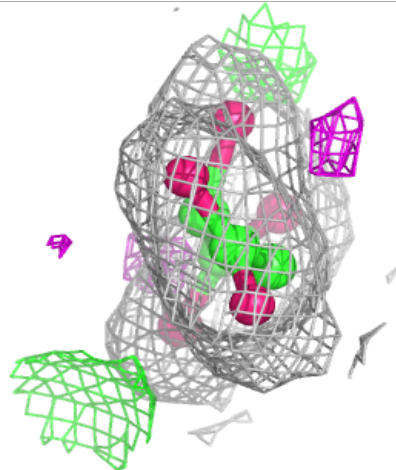
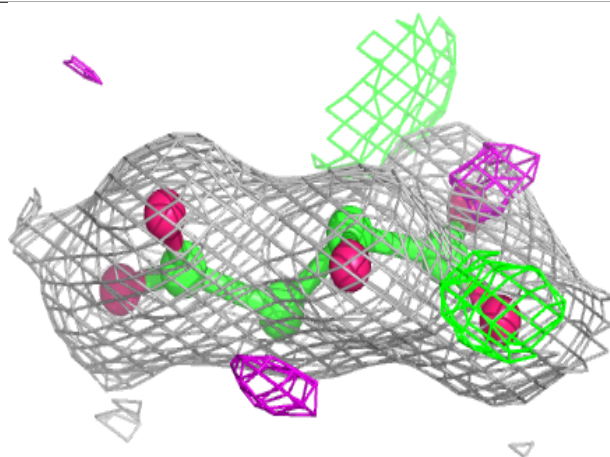
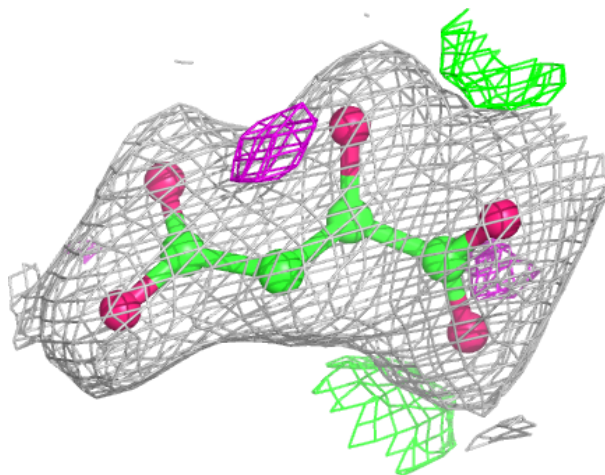
**Electron density around MLT A 301:**

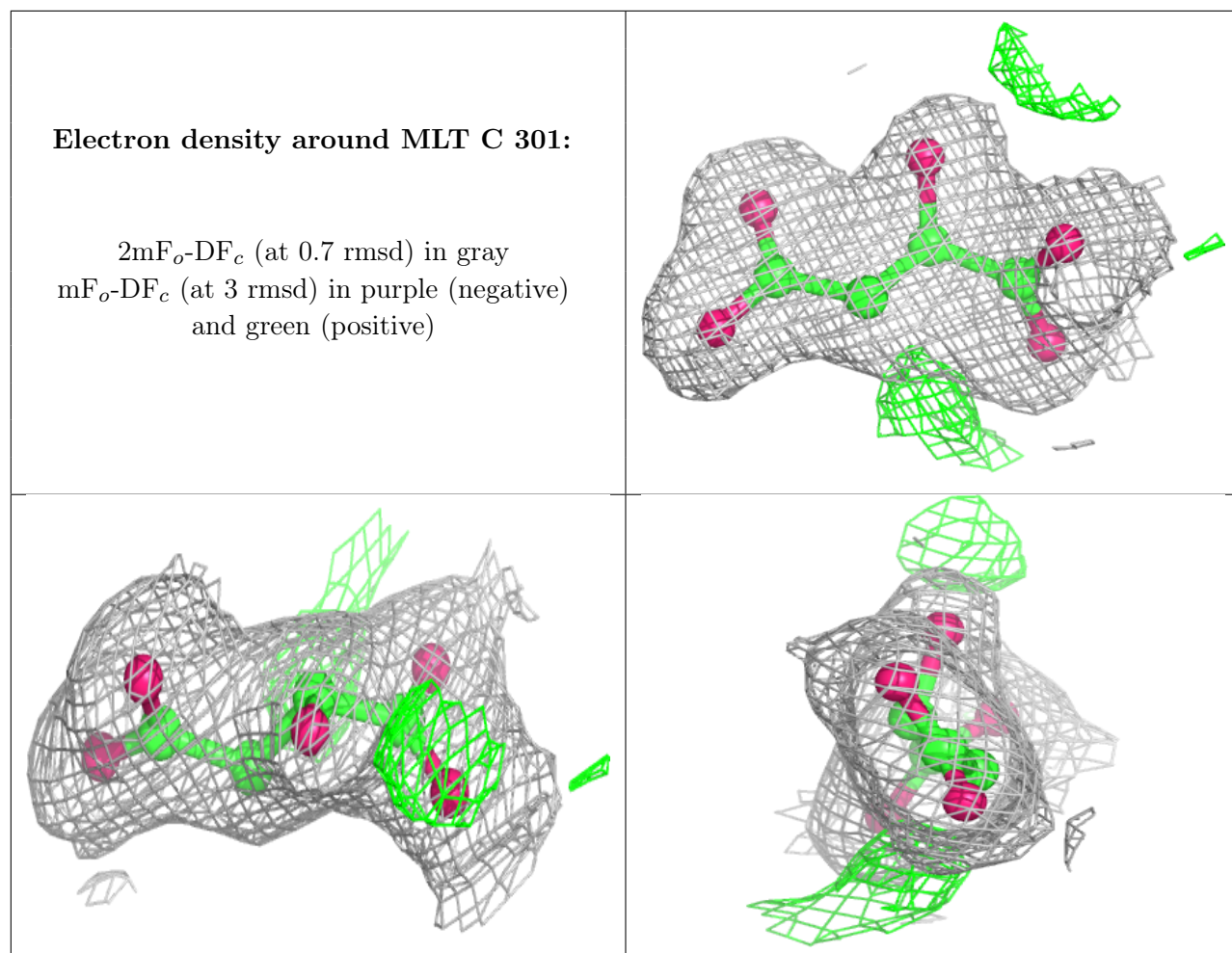
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around MLT 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)





## 6.5 Other polymers ⓘ

There are no such residues in this entry.