



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 20, 2021 – 02:11 PM JST

PDB ID : 7DMW  
Title : Crystal structure of CcpC regulatory domain in complex with citrate from *Bacillus amyloliquefaciens*  
Authors : Chen, J.; Wang, L.; Shang, F.; Liu, W.; Chen, Y.; Lan, J.; Bu, T.; Bai, X.; Xu, Y.  
Deposited on : 2020-12-08  
Resolution : 2.29 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

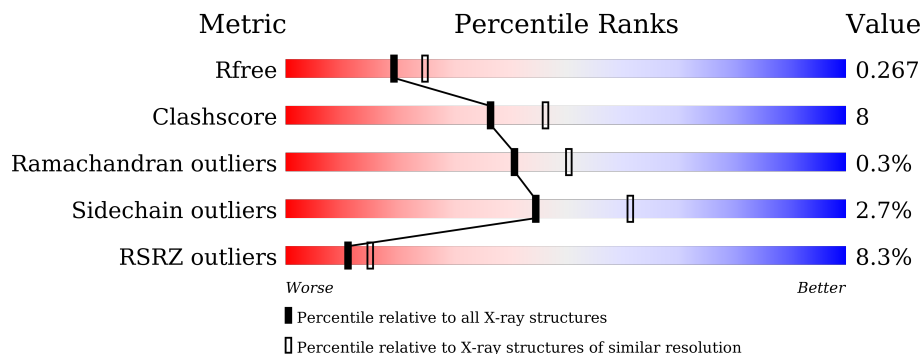
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.29 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	293	 3% 58% 10% 32%
1	B	293	 % 61% 6% 32%
1	C	293	 4% 53% 15% 32%
1	D	293	 9% 46% 19% 33%
1	E	293	 11% 46% 14% 38%

## 2 Entry composition [i](#)

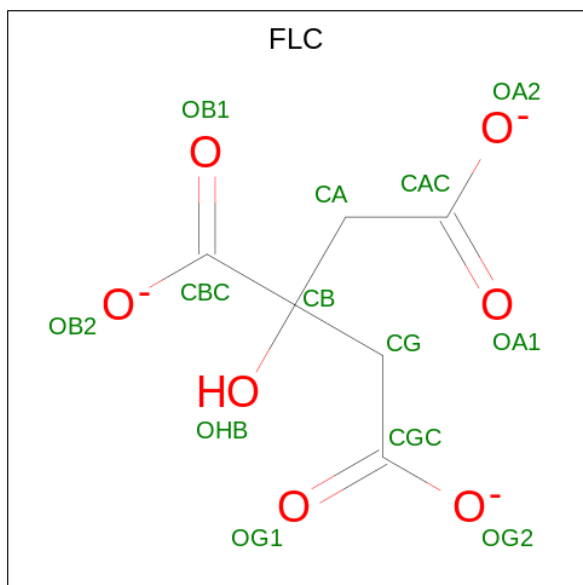
There are 3 unique types of molecules in this entry. The entry contains 8194 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CcpC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	200	Total 1637	C 1059	N 272	O 299	S 7	0	0	0
1	B	199	Total 1627	C 1053	N 269	O 298	S 7	0	0	0
1	C	200	Total 1637	C 1059	N 272	O 299	S 7	0	0	0
1	D	195	Total 1597	C 1034	N 263	O 293	S 7	0	0	0
1	E	182	Total 1478	C 956	N 241	O 274	S 7	0	0	0

- Molecule 2 is CITRATE ANION (three-letter code: FLC) (formula: C<sub>6</sub>H<sub>5</sub>O<sub>7</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	Total 13	C 6	O 7	0	0

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

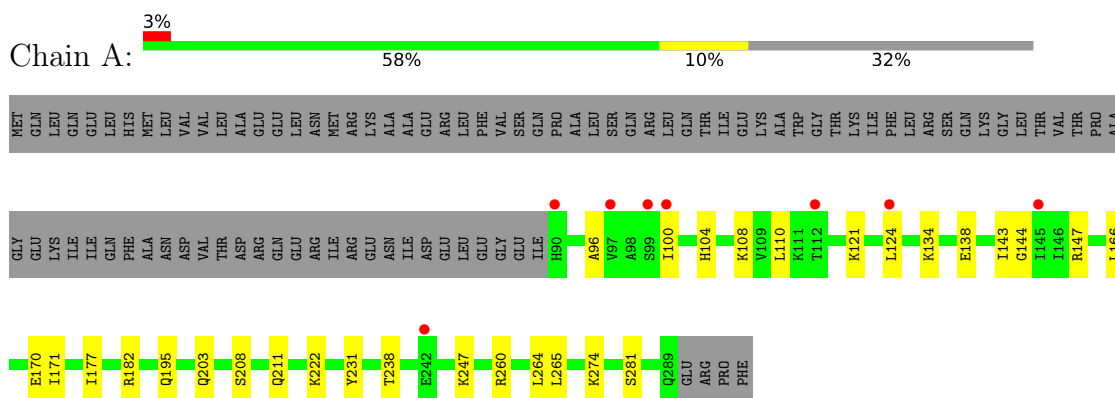
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	51	Total	O	0	0
			51	51		
3	B	54	Total	O	0	0
			54	54		
3	C	22	Total	O	0	0
			22	22		
3	D	17	Total	O	0	0
			17	17		
3	E	9	Total	O	0	0
			9	9		

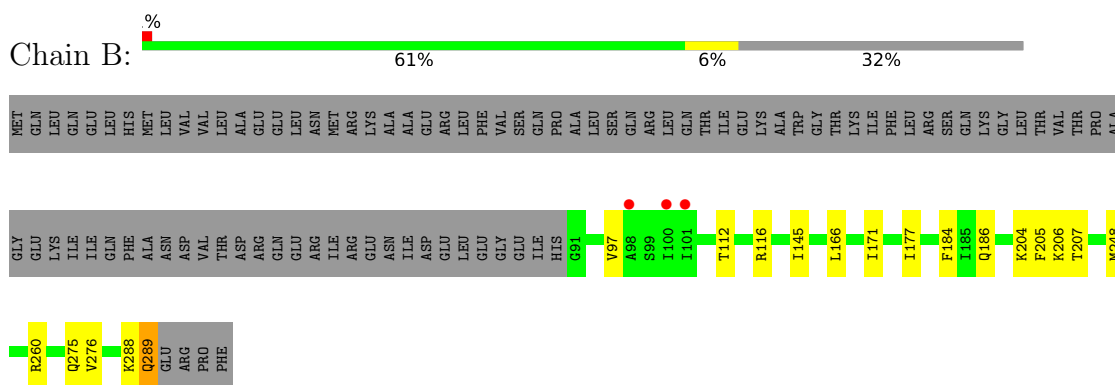
### 3 Residue-property plots [i](#)

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.

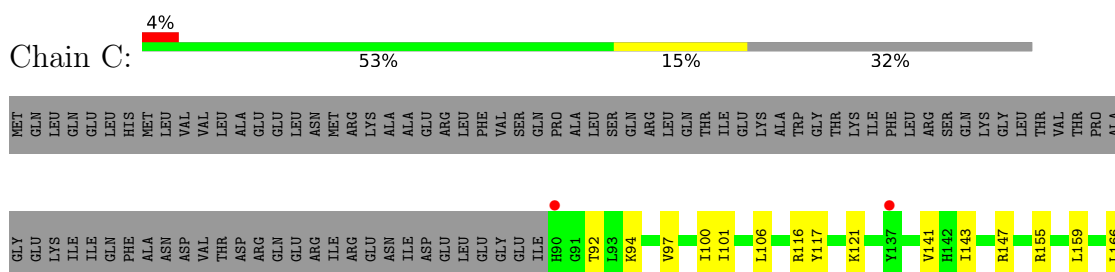
- Molecule 1: CcpC

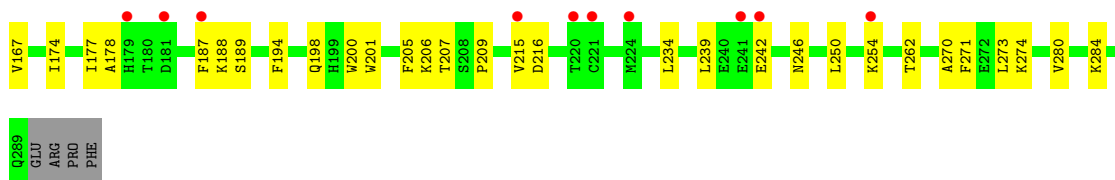


- Molecule 1: CcpC

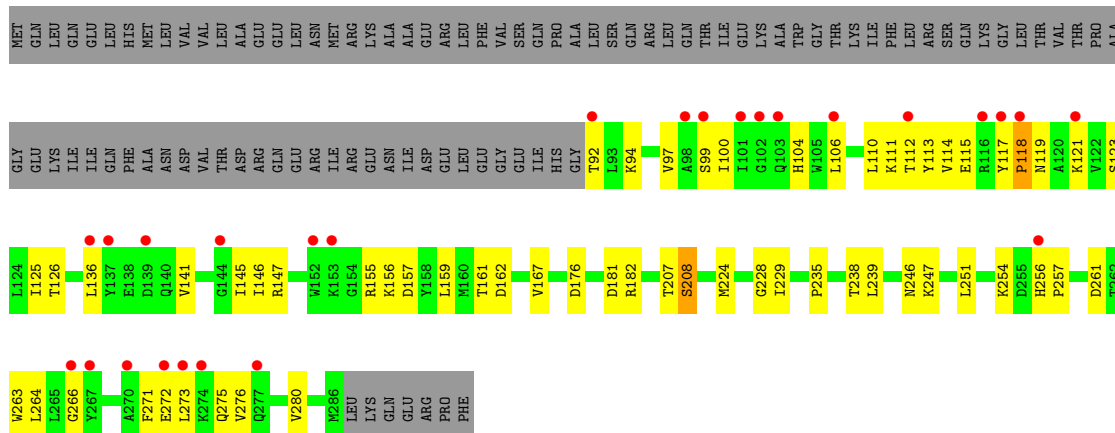


- Molecule 1: CcpC

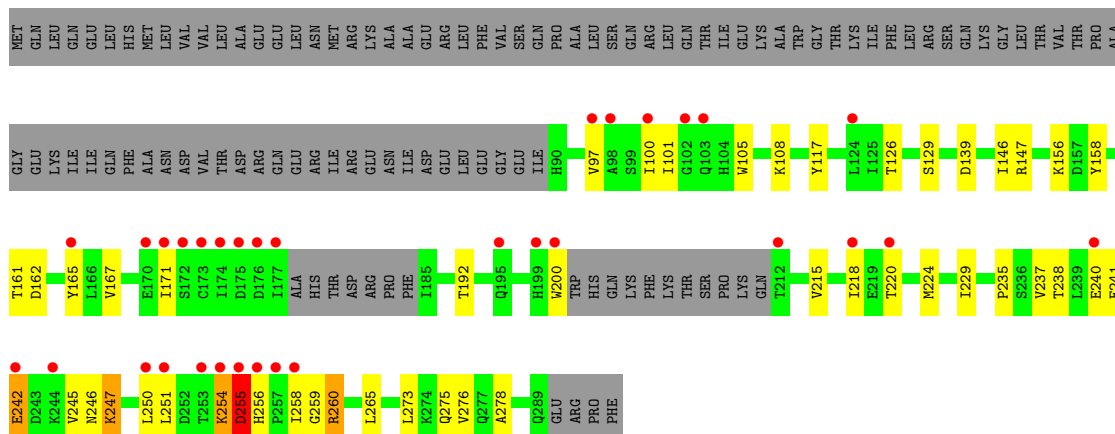




● Molecule 1: CcpC



● Molecule 1: CcpC



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.96Å 90.90Å 105.53Å 90.00° 106.18° 90.00°	Depositor
Resolution (Å)	29.71 – 2.29 39.34 – 2.29	Depositor EDS
% Data completeness (in resolution range)	96.5 (29.71-2.29) 96.5 (39.34-2.29)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.76 (at 2.29Å)	Xtrriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, $R_{free}$	0.207 , 0.267 0.207 , 0.267	Depositor DCC
$R_{free}$ test set	2000 reflections (3.59%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.6	Xtrriage
Anisotropy	0.438	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 52.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8194	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: FLC

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	0.44	0/1680	0.55	0/2278
1	B	0.45	0/1669	0.59	0/2263
1	C	0.43	0/1680	0.58	0/2278
1	D	0.40	0/1639	0.58	0/2224
1	E	0.37	0/1511	0.52	0/2046
All	All	0.42	0/8179	0.57	0/11089

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	272	GLU	Peptide

### 5.2 Too-close contacts [i](#)

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	1637	0	1638	18	1
1	B	1627	0	1631	12	0
1	C	1637	0	1638	27	1
1	D	1597	0	1596	35	0
1	E	1478	0	1484	38	0
2	A	13	0	5	0	0
2	B	13	0	5	0	0
2	C	13	0	5	1	0
2	D	13	0	5	1	0
2	E	13	0	5	1	0
3	A	51	0	0	3	0
3	B	54	0	0	1	0
3	C	22	0	0	2	0
3	D	17	0	0	0	0
3	E	9	0	0	0	0
All	All	8194	0	8012	127	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 8.

All (127) 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:C:92:THR:HG22	1:C:121:LYS:HB2	1.48	0.94
1:E:245:VAL:HG23	1:E:247:LYS:HZ2	1.35	0.92
1:E:192:THR:HG23	1:E:260:ARG:HH22	1.37	0.89
1:A:166:LEU:O	3:A:401:HOH:O	1.93	0.84
1:E:245:VAL:O	1:E:247:LYS:NZ	2.10	0.83
1:D:92:THR:HA	1:D:121:LYS:HB2	1.62	0.81
1:D:147:ARG:NH2	1:D:162:ASP:OD1	2.14	0.81
1:E:245:VAL:CG2	1:E:247:LYS:HZ2	1.95	0.80
1:A:247:LYS:HA	3:A:401:HOH:O	1.85	0.74
1:C:209:PRO:O	3:C:401:HOH:O	2.11	0.68
1:E:254:LYS:O	1:E:256:HIS:N	2.29	0.66
1:C:216:ASP:OD2	3:C:402:HOH:O	2.13	0.66
1:E:224:MET:HG2	1:E:229:ILE:HD12	1.79	0.65
1:E:240:GLU:OE1	1:E:241:GLU:HG3	1.98	0.63
1:E:192:THR:HG23	1:E:260:ARG:NH2	2.11	0.63
1:D:112:THR:HA	1:D:115:GLU:HG2	1.81	0.61
1:D:224:MET:HB3	1:D:229:ILE:HD12	1.82	0.61
1:B:204:LYS:NZ	3:B:404:HOH:O	2.33	0.60
1:E:158:TYR:OH	1:E:161:THR:OG1	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:LYS:HD2	1:E:265:LEU:HD21	1.84	0.59
1:D:159:LEU:HD13	1:D:264:LEU:HB2	1.85	0.58
1:D:113:TYR:O	1:D:117:TYR:HB2	2.04	0.57
1:E:147:ARG:NH1	1:E:162:ASP:OD2	2.33	0.57
1:C:174:ILE:O	1:C:177:ILE:HG12	2.06	0.56
1:D:182:ARG:NH2	1:D:228:GLY:O	2.38	0.55
1:E:245:VAL:CG2	1:E:247:LYS:NZ	2.69	0.55
1:C:167:VAL:HA	1:C:246:ASN:O	2.07	0.55
1:D:157:ASP:HB2	1:D:264:LEU:HB3	1.89	0.54
1:D:159:LEU:CD1	1:D:264:LEU:HB2	2.38	0.54
1:D:136:LEU:HD11	1:D:266:GLY:HA2	1.88	0.54
1:C:270:ALA:HA	1:C:273:LEU:HD12	1.90	0.53
1:D:100:ILE:O	1:D:104:HIS:HB2	2.07	0.53
1:D:92:THR:N	1:D:275:GLN:HE21	2.07	0.53
1:E:171:ILE:HD12	1:E:171:ILE:H	1.74	0.52
1:C:159:LEU:HB2	1:C:262:THR:O	2.10	0.52
1:D:235:PRO:HG2	1:D:238:THR:HG23	1.92	0.52
1:C:177:ILE:HD12	1:C:201:TRP:CZ3	2.44	0.52
1:E:129:SER:HB3	1:E:146:ILE:HG23	1.91	0.52
1:B:184:PHE:CZ	1:B:186:GLN:HB3	2.45	0.52
1:D:111:LYS:HA	1:D:114:VAL:HG22	1.92	0.52
1:A:177:ILE:HD11	1:A:231:TYR:CG	2.45	0.51
1:A:177:ILE:HD11	1:A:231:TYR:CD2	2.45	0.51
1:D:167:VAL:HA	1:D:246:ASN:O	2.09	0.51
1:D:97:VAL:HG21	1:D:106:LEU:HD22	1.94	0.50
1:D:273:LEU:HB3	1:D:275:GLN:OE1	2.10	0.50
1:B:171:ILE:HD13	1:B:177:ILE:HD13	1.94	0.50
1:D:156:LYS:HE3	1:D:263:TRP:CZ3	2.47	0.50
1:E:235:PRO:O	1:E:238:THR:HG22	2.12	0.50
1:E:245:VAL:C	1:E:247:LYS:NZ	2.65	0.50
1:E:156:LYS:HG3	1:E:265:LEU:CD2	2.42	0.49
1:E:167:VAL:HA	1:E:246:ASN:O	2.12	0.49
1:A:104:HIS:CD2	1:A:238:THR:HG22	2.48	0.49
1:A:124:LEU:HB3	1:C:215:VAL:HG12	1.95	0.48
1:C:101:ILE:HD11	1:C:147:ARG:HH11	1.78	0.48
1:C:234:LEU:HD12	1:C:239:LEU:HD21	1.94	0.48
1:B:112:THR:HG22	1:B:116:ARG:CD	2.44	0.48
1:E:215:VAL:HG11	1:E:220:THR:HB	1.94	0.48
1:E:251:LEU:HD23	1:E:255:ASP:O	2.14	0.48
1:D:106:LEU:HG	1:D:110:LEU:HG	1.95	0.47
1:E:273:LEU:HD23	1:E:275:GLN:HE22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:101:ILE:HG23	1:E:105:TRP:HB3	1.97	0.47
1:E:97:VAL:O	1:E:126:THR:HA	2.15	0.47
1:E:156:LYS:HG3	1:E:265:LEU:HD23	1.98	0.46
1:A:134:LYS:NZ	1:A:138:GLU:OE2	2.32	0.46
1:B:166:LEU:HD22	1:B:248:MET:HE2	1.98	0.46
1:D:145:ILE:O	1:D:146:ILE:HD13	2.16	0.46
1:B:97:VAL:HG13	1:B:145:ILE:HB	1.97	0.46
1:B:112:THR:HG22	1:B:116:ARG:HD3	1.96	0.46
1:D:155:ARG:HB3	1:D:271:PHE:CE2	2.51	0.46
1:A:171:ILE:HD13	1:A:177:ILE:HD12	1.97	0.45
1:C:116:ARG:NH2	1:C:117:TYR:OH	2.49	0.45
1:E:165:TYR:HA	1:E:250:LEU:HD23	1.98	0.45
1:A:222:LYS:NZ	1:A:238:THR:O	2.37	0.45
1:C:201:TRP:HE1	1:C:207:THR:HG23	1.81	0.45
1:E:100:ILE:HG23	2:E:301:FLC:OA2	2.16	0.45
1:D:125:ILE:O	1:D:125:ILE:HG13	2.16	0.45
1:E:241:GLU:OE2	1:E:242:GLU:N	2.50	0.45
1:C:200:TRP:CZ2	1:C:250:LEU:HG	2.52	0.45
1:D:207:THR:OG1	1:D:208:SER:N	2.49	0.45
1:D:161:THR:OG1	1:D:261:ASP:OD1	2.33	0.45
1:D:254:LYS:HE3	1:D:254:LYS:HB2	1.59	0.45
1:E:258:ILE:HD12	1:E:259:GLY:H	1.82	0.45
1:E:245:VAL:C	1:E:247:LYS:HZ2	2.19	0.45
1:B:205:PHE:C	1:B:207:THR:H	2.21	0.44
1:C:201:TRP:CD1	1:C:209:PRO:HD3	2.53	0.44
1:C:242:GLU:H	1:C:242:GLU:CD	2.21	0.43
1:C:155:ARG:HB3	1:C:271:PHE:CE2	2.53	0.43
1:E:275:GLN:HG2	1:E:276:VAL:N	2.33	0.43
1:C:143:ILE:HD13	1:C:143:ILE:HA	1.84	0.43
1:A:264:LEU:C	1:A:265:LEU:HD12	2.39	0.43
1:C:94:LYS:O	1:C:141:VAL:HB	2.19	0.43
1:D:94:LYS:O	1:D:141:VAL:HB	2.19	0.43
1:C:239:LEU:HD23	1:C:239:LEU:HA	1.85	0.43
1:D:118:PRO:HB2	1:D:119:ASN:H	1.63	0.43
1:B:288:LYS:O	1:B:289:GLN:HG3	2.18	0.42
1:D:100:ILE:HD11	1:D:147:ARG:NE	2.34	0.42
1:D:254:LYS:HB2	1:D:256:HIS:CE1	2.54	0.42
1:D:276:VAL:O	1:D:280:VAL:HG23	2.19	0.42
1:A:195:GLN:HG3	3:A:413:HOH:O	2.20	0.42
1:E:156:LYS:CD	1:E:265:LEU:HD21	2.48	0.42
1:A:96:ALA:O	1:A:144:GLY:HA2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:GLN:NE2	1:D:176:ASP:OD1	2.51	0.41
1:E:156:LYS:CG	1:E:265:LEU:CD2	2.98	0.41
1:A:121:LYS:HE3	1:A:121:LYS:HB2	1.83	0.41
1:E:117:TYR:CE2	1:E:278:ALA:HB1	2.55	0.41
1:E:235:PRO:HB2	1:E:237:VAL:HG12	2.02	0.41
1:A:143:ILE:HA	1:A:143:ILE:HD13	1.80	0.41
1:A:171:ILE:HD11	1:A:182:ARG:HD3	2.02	0.41
1:D:97:VAL:O	1:D:126:THR:HA	2.20	0.41
1:D:251:LEU:HD23	1:D:257:PRO:HA	2.03	0.41
1:E:100:ILE:HG21	1:E:218:ILE:HD12	2.02	0.41
1:A:100:ILE:HD11	1:A:147:ARG:CZ	2.50	0.41
1:C:194:PHE:O	1:C:198:GLN:HG2	2.20	0.41
1:E:241:GLU:CD	1:E:242:GLU:H	2.24	0.41
1:C:178:ALA:HB2	1:C:205:PHE:CD1	2.56	0.41
1:A:110:LEU:HD23	1:A:110:LEU:HA	1.86	0.41
1:B:204:LYS:O	1:B:204:LYS:HG3	2.21	0.41
1:C:254:LYS:HD2	1:C:254:LYS:HA	1.83	0.41
1:C:187:PHE:CZ	1:C:189:SER:HB3	2.56	0.41
1:C:100:ILE:HG12	2:C:301:FLC:OA1	2.21	0.40
1:C:280:VAL:HG13	1:C:284:LYS:NZ	2.35	0.40
1:E:100:ILE:HD11	1:E:147:ARG:NE	2.36	0.40
1:B:275:GLN:HG2	1:B:276:VAL:N	2.37	0.40
1:C:97:VAL:HG21	1:C:106:LEU:HD22	2.03	0.40
1:D:99:SER:HB2	2:D:301:FLC:OA1	2.22	0.40
1:B:166:LEU:HD22	1:B:248:MET:CE	2.52	0.40
1:D:114:VAL:HG21	1:E:229:ILE:HG23	2.04	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:170:GLU:OE1	1:C:188:LYS:NZ[4_455]	2.18	0.02

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	198/293 (68%)	191 (96%)	7 (4%)	0	100	100
1	B	197/293 (67%)	191 (97%)	6 (3%)	0	100	100
1	C	198/293 (68%)	190 (96%)	8 (4%)	0	100	100
1	D	193/293 (66%)	184 (95%)	8 (4%)	1 (0%)	29	35
1	E	176/293 (60%)	163 (93%)	11 (6%)	2 (1%)	14	15
All	All	962/1465 (66%)	919 (96%)	40 (4%)	3 (0%)	41	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	118	PRO
1	E	242	GLU
1	E	255	ASP

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

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	182/264 (69%)	176 (97%)	6 (3%)	38	53
1	B	181/264 (69%)	178 (98%)	3 (2%)	60	76
1	C	182/264 (69%)	179 (98%)	3 (2%)	62	78
1	D	178/264 (67%)	173 (97%)	5 (3%)	43	60
1	E	165/264 (62%)	158 (96%)	7 (4%)	30	42
All	All	888/1320 (67%)	864 (97%)	24 (3%)	44	61

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	LYS
1	A	208	SER

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Mol	Chain	Res	Type
1	A	211	GLN
1	A	260	ARG
1	A	274	LYS
1	A	281	SER
1	B	206	LYS
1	B	260	ARG
1	B	289	GLN
1	C	166	LEU
1	C	206	LYS
1	C	274	LYS
1	D	123	SER
1	D	181	ASP
1	D	208	SER
1	D	239	LEU
1	D	247	LYS
1	E	108	LYS
1	E	139	ASP
1	E	200	TRP
1	E	247	LYS
1	E	254	LYS
1	E	255	ASP
1	E	260	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	119	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FLC	B	301	-	3,12,12	1.23	1 (33%)	3,17,17	1.55	1 (33%)
2	FLC	E	301	-	3,12,12	1.23	0	3,17,17	2.13	1 (33%)
2	FLC	D	301	-	3,12,12	1.18	0	3,17,17	1.54	1 (33%)
2	FLC	C	301	-	3,12,12	0.74	0	3,17,17	2.33	1 (33%)
2	FLC	A	300	-	3,12,12	1.46	1 (33%)	3,17,17	2.56	1 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FLC	B	301	-	-	0/6/16/16	-
2	FLC	E	301	-	-	0/6/16/16	-
2	FLC	D	301	-	-	0/6/16/16	-
2	FLC	C	301	-	-	0/6/16/16	-
2	FLC	A	300	-	-	0/6/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	FLC	OHB-CB	-2.25	1.39	1.43
2	B	301	FLC	OHB-CB	-2.02	1.39	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	FLC	CB-CA-CAC	-3.95	108.65	114.98
2	C	301	FLC	CB-CA-CAC	-3.80	108.90	114.98
2	E	301	FLC	CB-CG-CGC	-3.50	109.38	114.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	FLC	CB-CA-CAC	-2.44	111.08	114.98
2	D	301	FLC	CB-CG-CGC	-2.18	111.49	114.98

There are no chirality outliers.

There are no torsion outliers.

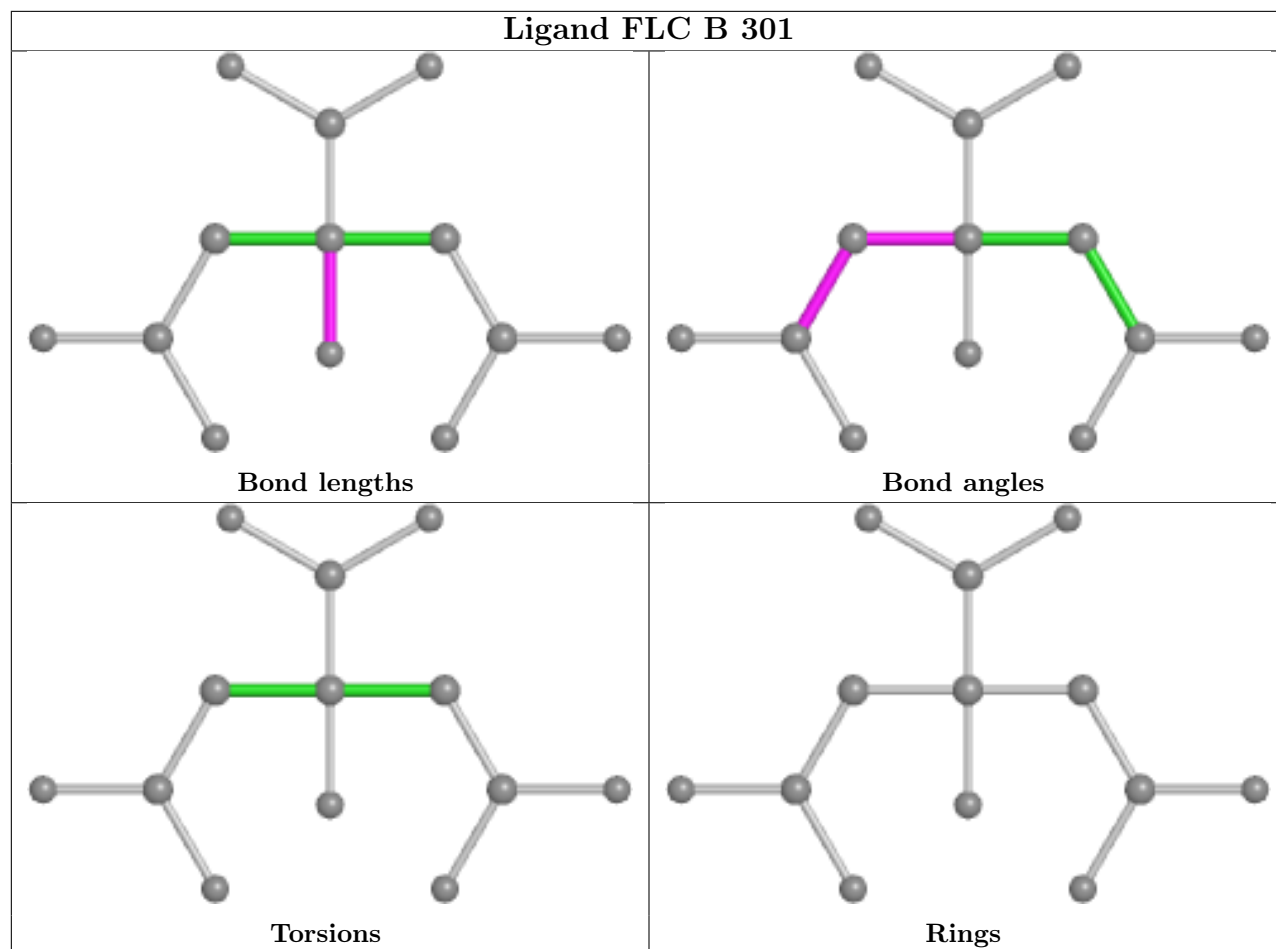
There are no ring outliers.

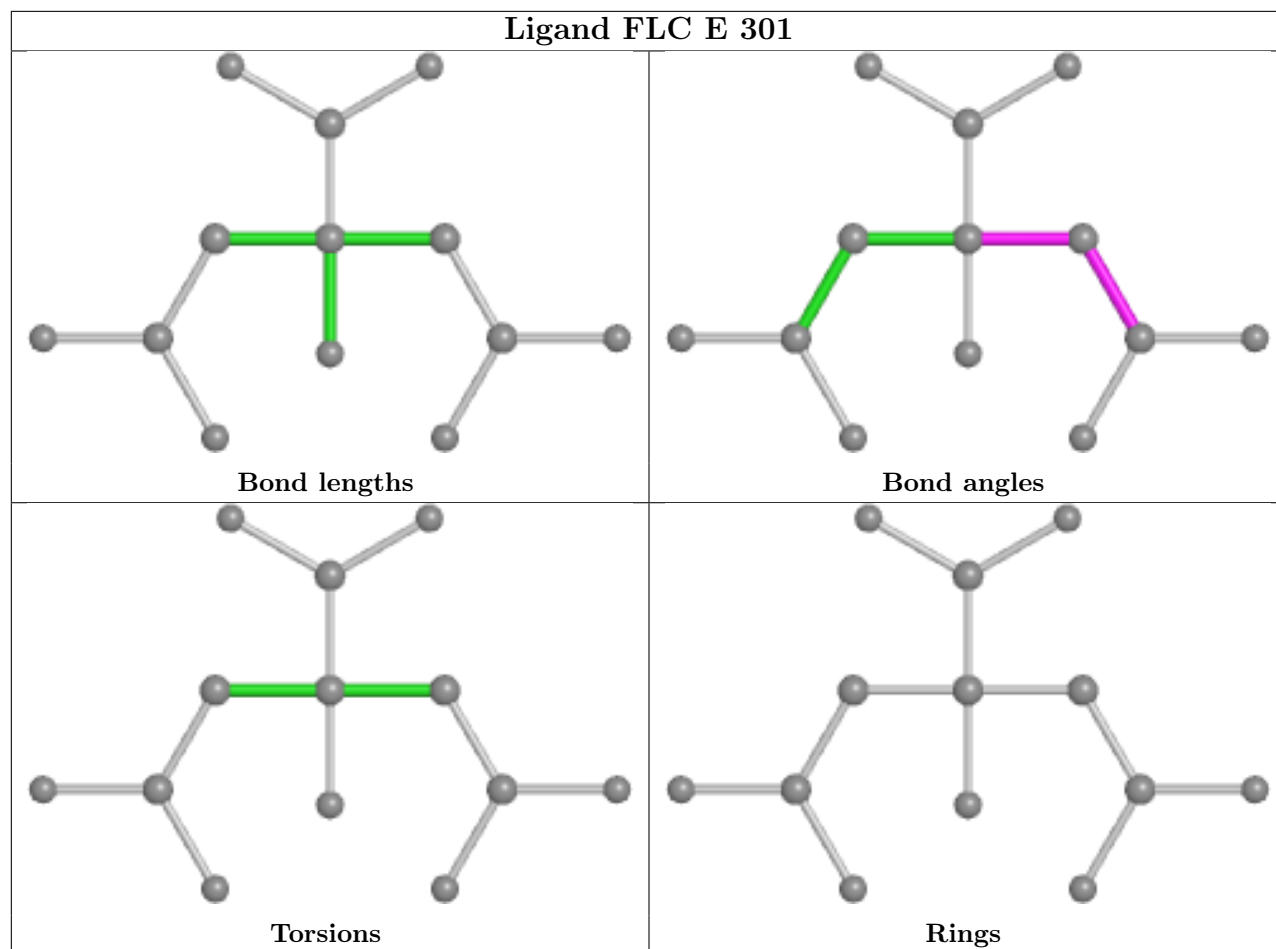
3 monomers are involved in 3 short contacts:

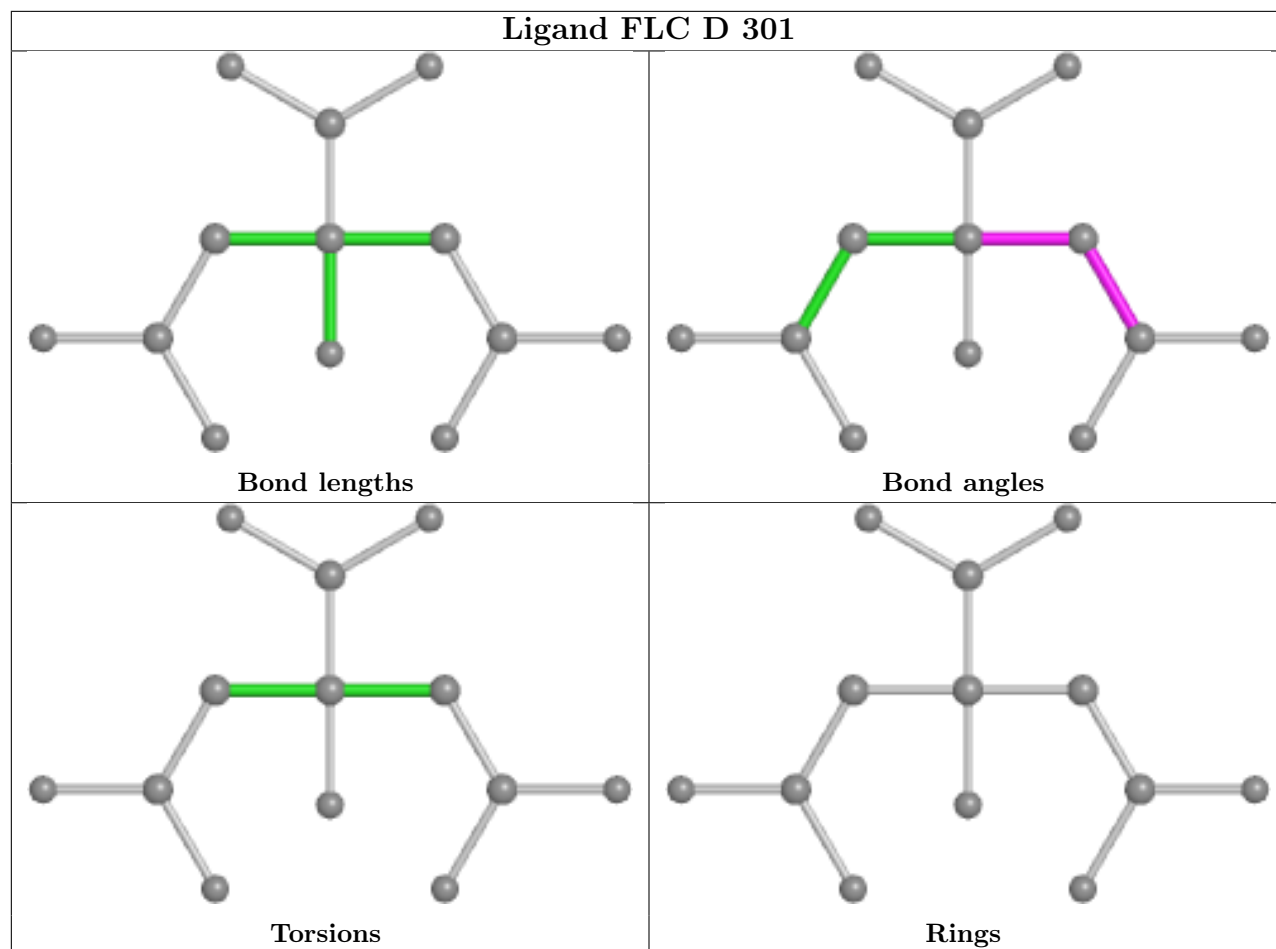
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	FLC	1	0
2	D	301	FLC	1	0
2	C	301	FLC	1	0

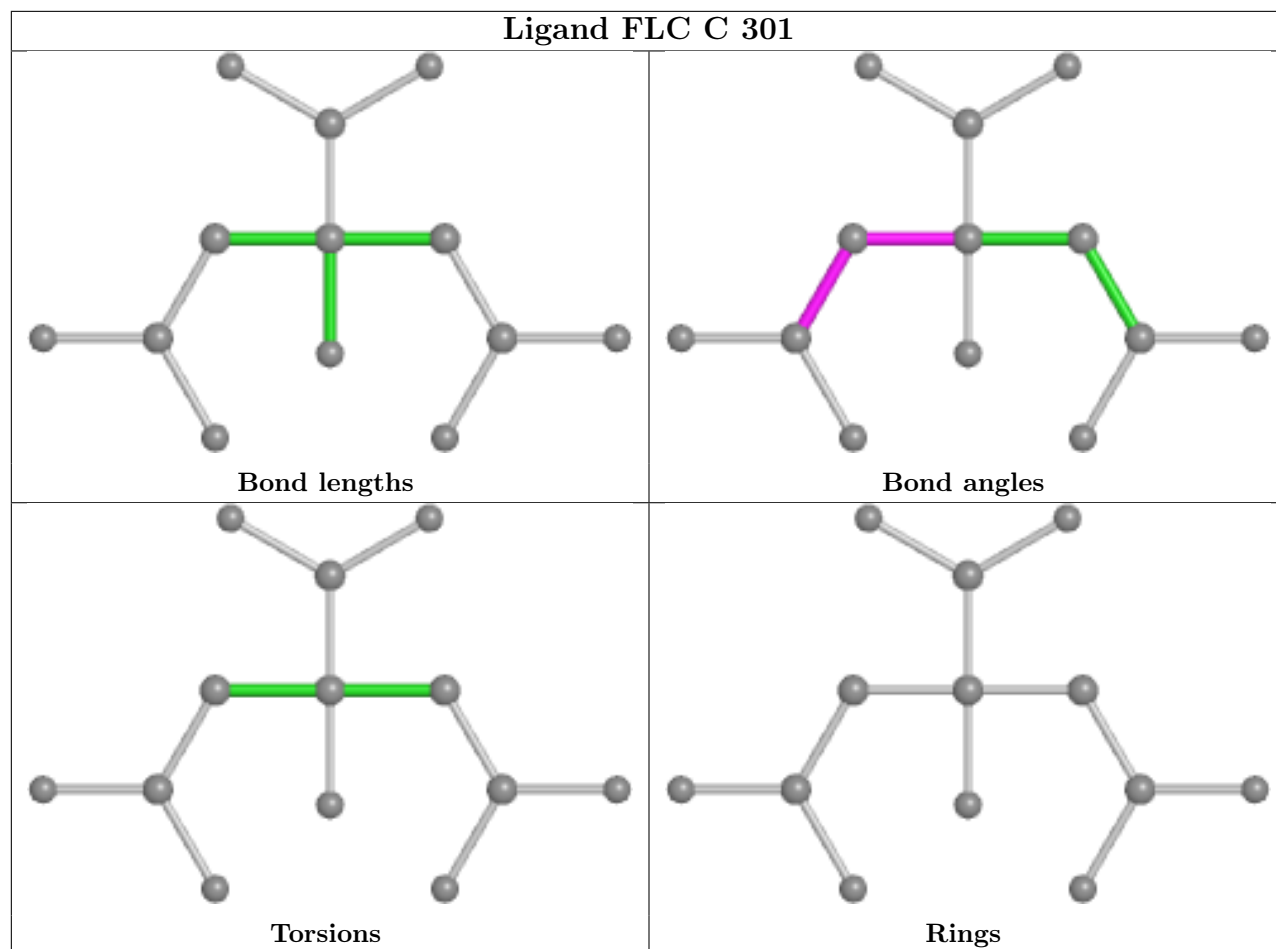
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

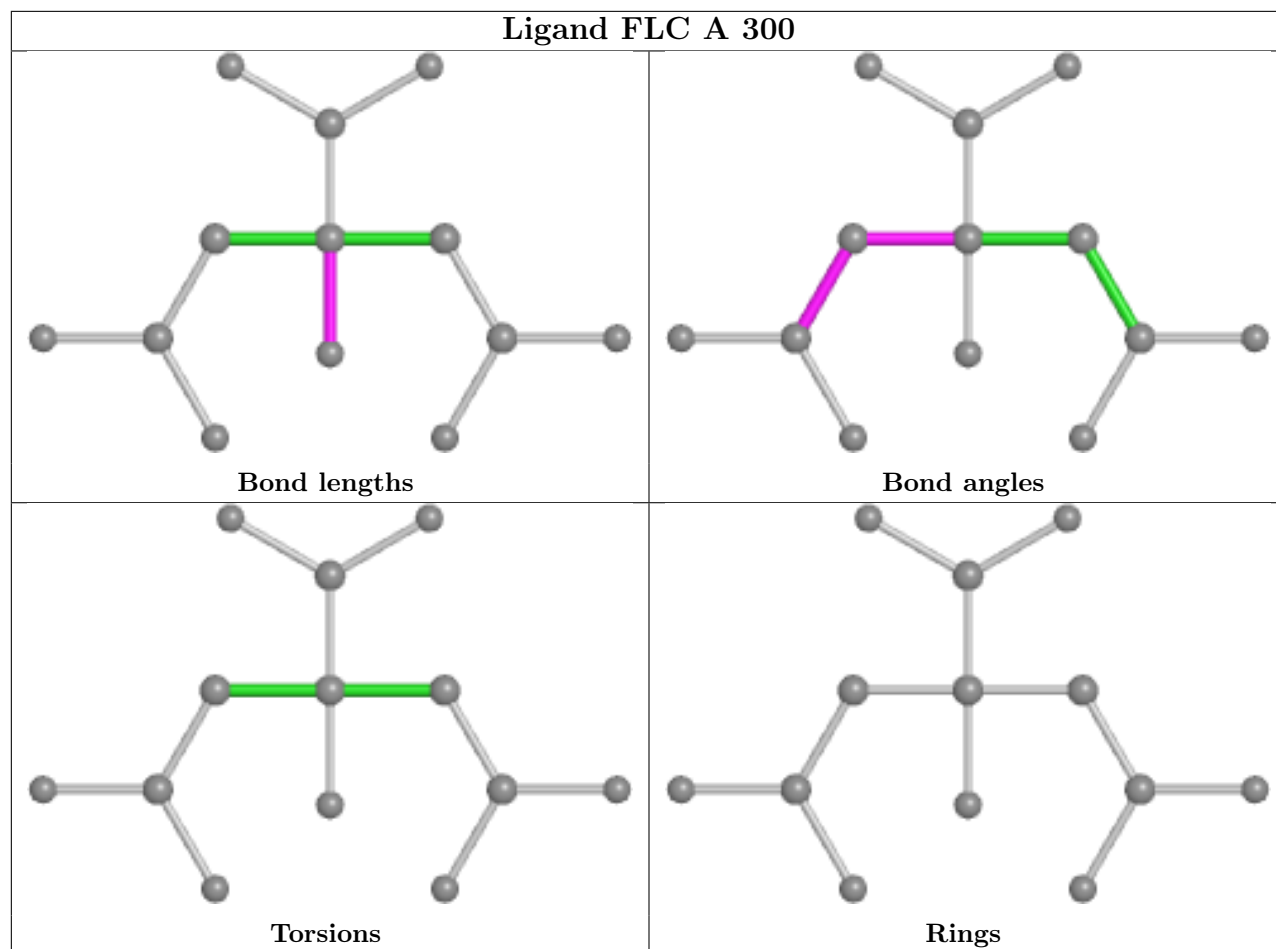












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	200/293 (68%)	0.24	8 (4%) 38 45	36, 51, 70, 89	0
1	B	199/293 (67%)	0.17	3 (1%) 73 79	36, 50, 70, 85	0
1	C	200/293 (68%)	0.30	12 (6%) 21 28	43, 57, 82, 100	0
1	D	195/293 (66%)	0.78	26 (13%) 3 4	46, 67, 103, 110	0
1	E	182/293 (62%)	0.93	32 (17%) 1 1	48, 70, 110, 124	0
All	All	976/1465 (66%)	0.48	81 (8%) 11 15	36, 57, 101, 124	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	250	LEU	5.5
1	E	177	ILE	5.5
1	D	273	LEU	5.0
1	E	251	LEU	4.7
1	E	174	ILE	4.6
1	E	199	HIS	4.5
1	D	92	THR	4.5
1	E	173	CYS	4.4
1	E	258	ILE	4.1
1	D	112	THR	4.0
1	E	175	ASP	3.9
1	E	200	TRP	3.8
1	E	253	THR	3.7
1	D	267	TYR	3.7
1	E	195	GLN	3.6
1	C	181	ASP	3.6
1	D	152	TRP	3.6
1	E	255	ASP	3.5
1	C	137	TYR	3.5
1	D	118	PRO	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	254	LYS	3.3
1	D	266	GLY	3.3
1	C	224	MET	3.3
1	C	220	THR	3.3
1	E	176	ASP	3.2
1	D	137	TYR	3.2
1	D	103	GLN	3.2
1	D	144	GLY	3.0
1	E	170	GLU	3.0
1	D	102	GLY	3.0
1	C	179	HIS	3.0
1	C	215	VAL	3.0
1	D	272	GLU	2.9
1	D	99	SER	2.8
1	E	212	THR	2.7
1	D	101	ILE	2.7
1	E	172	SER	2.7
1	E	240	GLU	2.6
1	D	116	ARG	2.6
1	A	112	THR	2.5
1	D	153	LYS	2.5
1	D	274	LYS	2.5
1	D	277	GLN	2.5
1	E	100	ILE	2.5
1	E	165	TYR	2.5
1	D	139	ASP	2.5
1	D	117	TYR	2.5
1	E	242	GLU	2.5
1	A	100	ILE	2.5
1	C	221	CYS	2.4
1	A	145	ILE	2.3
1	B	100	ILE	2.3
1	D	98	ALA	2.3
1	D	136	LEU	2.3
1	E	256	HIS	2.3
1	D	106	LEU	2.3
1	D	121	LYS	2.3
1	E	244	LYS	2.3
1	A	97	VAL	2.3
1	D	270	ALA	2.3
1	E	103	GLN	2.2
1	D	256	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	218	ILE	2.2
1	E	220	THR	2.2
1	A	242	GLU	2.2
1	A	124	LEU	2.2
1	C	254	LYS	2.1
1	A	90	HIS	2.1
1	C	241	GLU	2.1
1	E	98	ALA	2.1
1	B	101	ILE	2.1
1	E	257	PRO	2.1
1	C	90	HIS	2.1
1	E	97	VAL	2.1
1	E	102	GLY	2.1
1	C	242	GLU	2.0
1	E	171	ILE	2.0
1	A	99	SER	2.0
1	B	98	ALA	2.0
1	C	187	PHE	2.0
1	E	124	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	FLC	E	301	13/13	0.93	0.13	64,69,75,77	0
2	FLC	C	301	13/13	0.94	0.16	44,48,53,53	0
2	FLC	B	301	13/13	0.94	0.16	44,47,50,52	0
2	FLC	D	301	13/13	0.96	0.15	61,63,67,68	0

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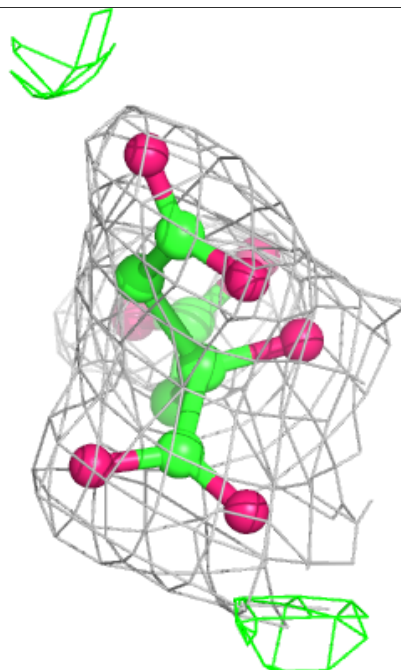
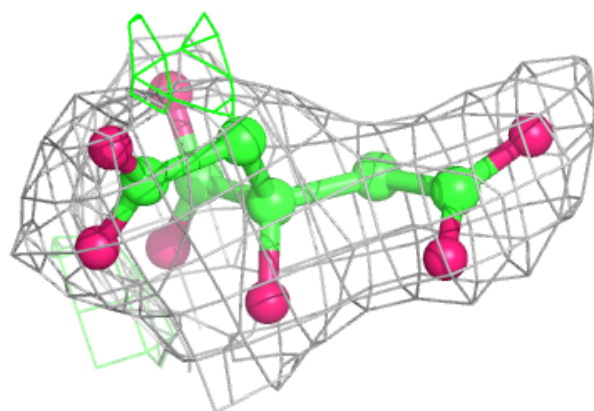
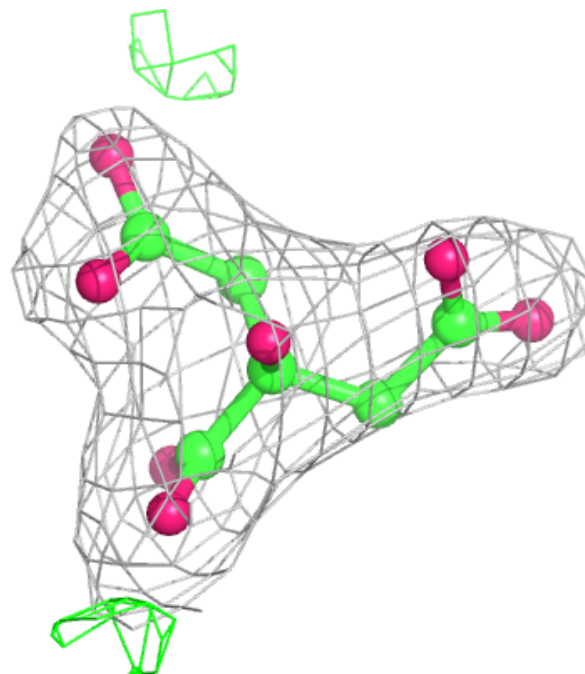
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FLC	A	300	13/13	0.96	0.16	39,42,49,50	0

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.

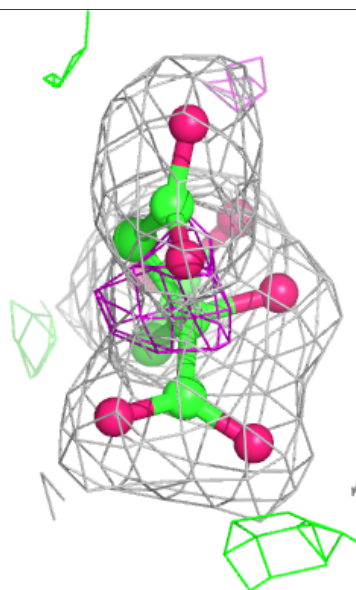
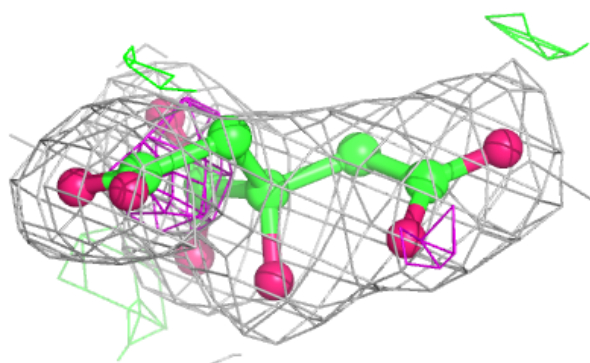
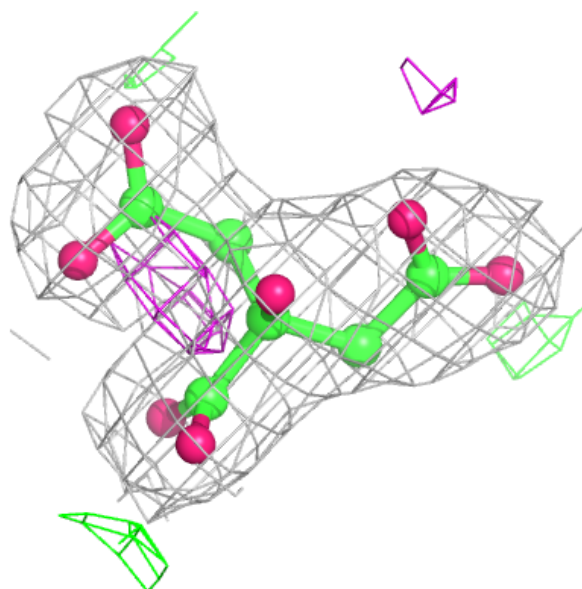
**Electron density around FLC E 301:**

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



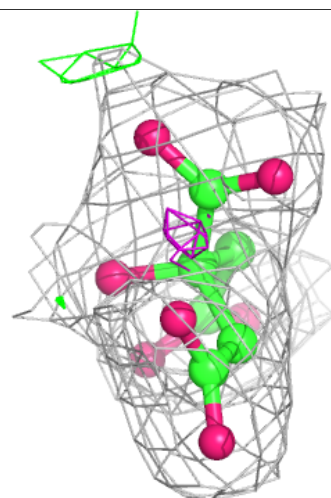
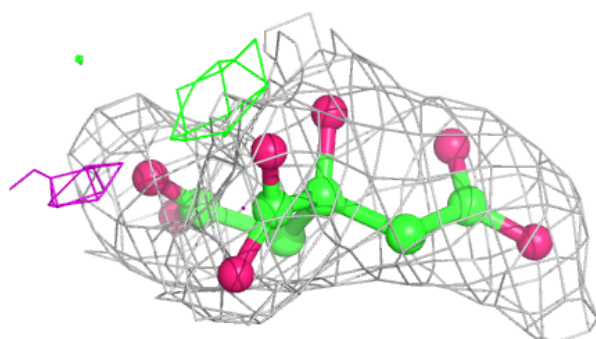
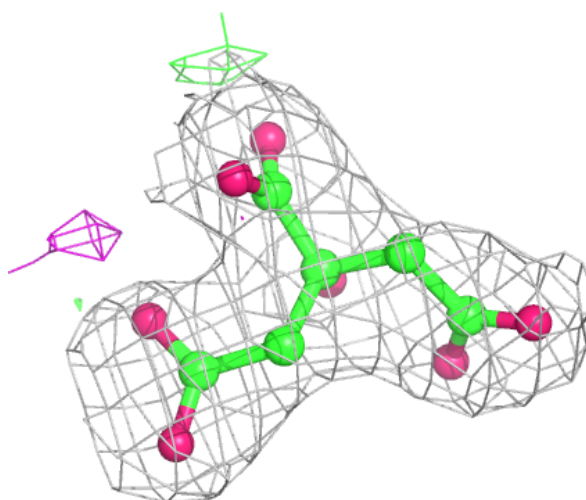
**Electron density around FLC C 301:**

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



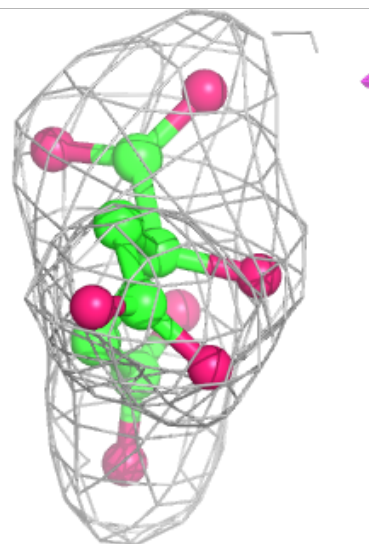
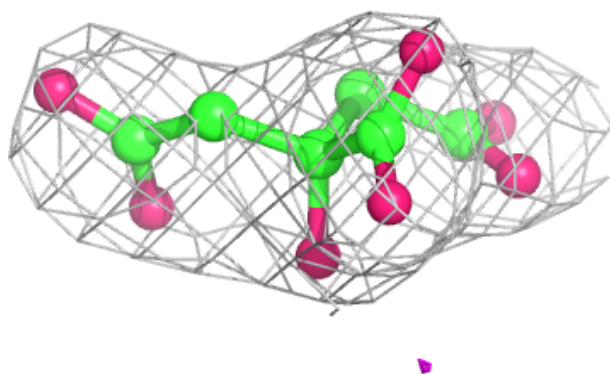
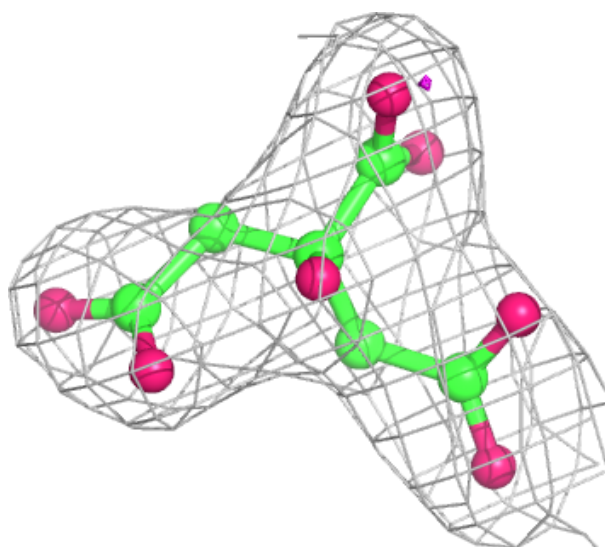
**Electron density around FLC B 301:**

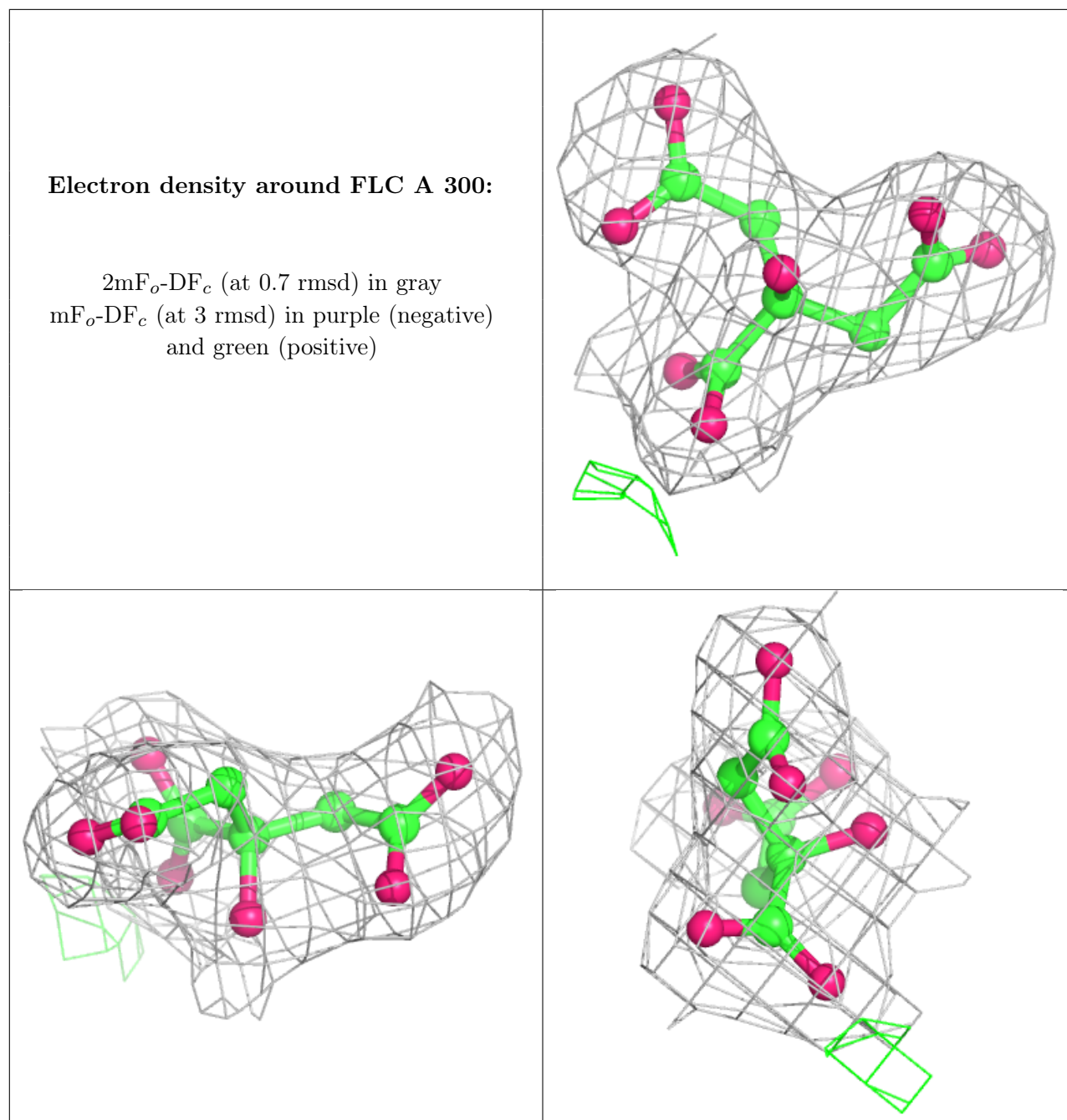
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FLC 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)





## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.