



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:44 PM UTC

PDB ID : 5ZZO / pdb_00005zzo
Title : Crystal structure of CcpE regulatory domain in complex with citrate from *Staphylococcus aureus*
Authors : Chen, J.; Wang, L.; Shang, F.; Xu, Y.
Deposited on : 2018-06-04
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

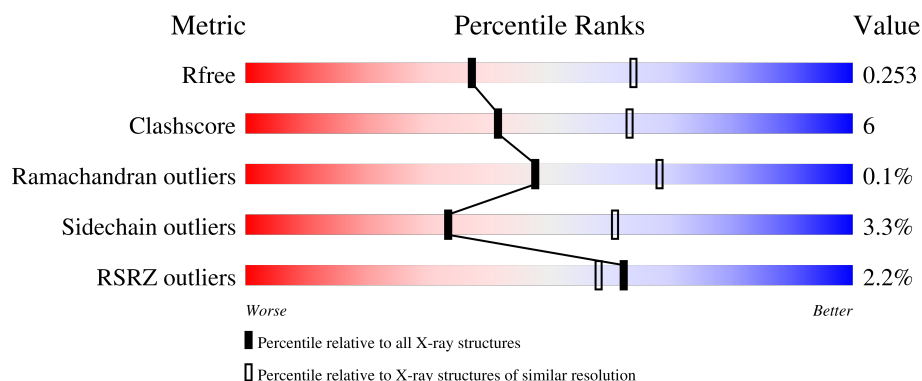
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 ≥ 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	201	2% 83% 12% ..
1	B	201	85% 10% ..
1	C	201	2% 86% 11% .
1	D	201	2% 82% 13% ..
1	E	201	2% 84% 12% ..

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Mol	Chain	Length	Quality of chain
1	F	201	5% 86% 12% ..

2 Entry composition [i](#)

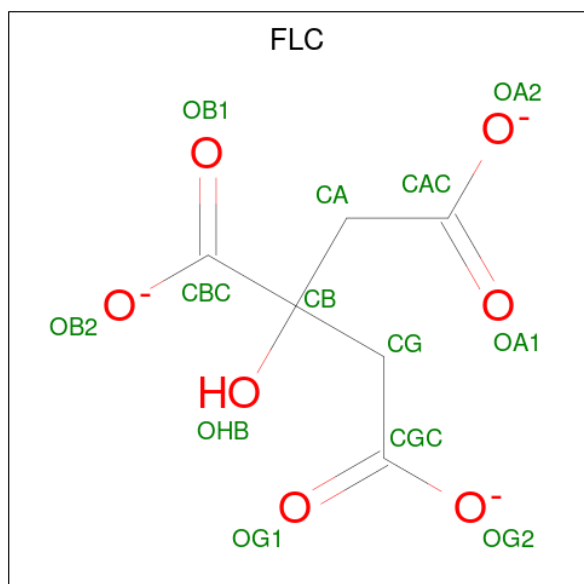
There are 3 unique types of molecules in this entry. The entry contains 19346 atoms, of which 9230 are hydrogens and 0 are deuteriums.

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 LysR family transcriptional regulator.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	194	Total	C	H	N	O	S	0	0	0
			3067	995	1516	247	299	10			
1	B	194	Total	C	H	N	O	S	0	0	0
			3064	994	1516	248	296	10			
1	C	196	Total	C	H	N	O	S	0	0	0
			3119	1007	1548	254	300	10			
1	D	196	Total	C	H	N	O	S	0	0	0
			3119	1007	1548	254	300	10			
1	E	195	Total	C	H	N	O	S	0	0	0
			3069	996	1517	248	298	10			
1	F	199	Total	C	H	N	O	S	0	0	0
			3149	1018	1555	258	308	10			

- Molecule 2 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			18	6	5	7		
2	B	1	Total	C	H	O	0	0
			18	6	5	7		
2	C	1	Total	C	H	O	0	0
			18	6	5	7		
2	D	1	Total	C	H	O	0	0
			18	6	5	7		
2	E	1	Total	C	H	O	0	0
			18	6	5	7		
2	F	1	Total	C	H	O	0	0
			18	6	5	7		

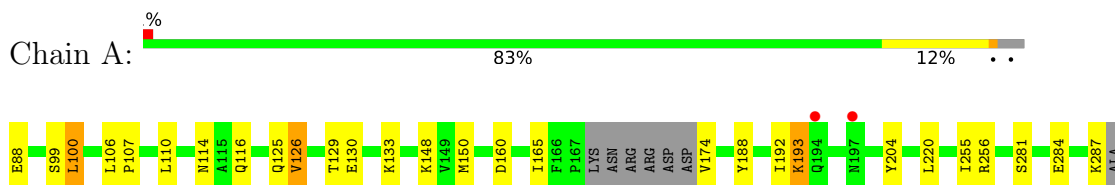
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	117	Total	O	0	0
			117	117		
3	B	108	Total	O	0	0
			108	108		
3	C	114	Total	O	0	0
			114	114		
3	D	101	Total	O	0	0
			101	101		
3	E	99	Total	O	0	0
			99	99		
3	F	112	Total	O	0	0
			112	112		

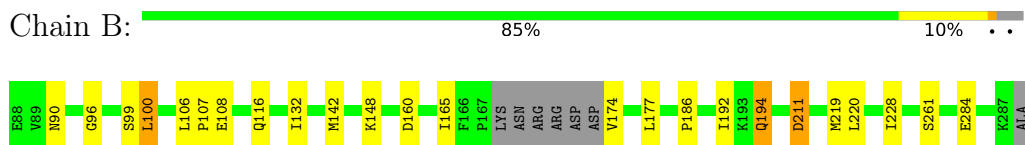
3 Residue-property plots

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.

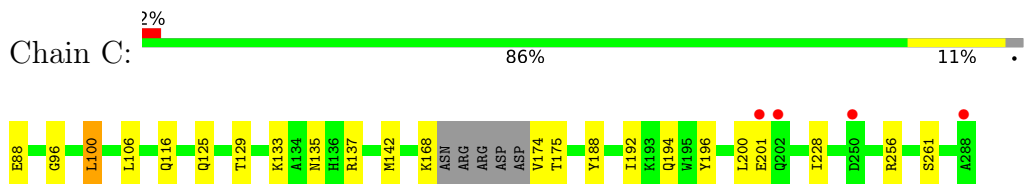
- Molecule 1: LysR family transcriptional regulator



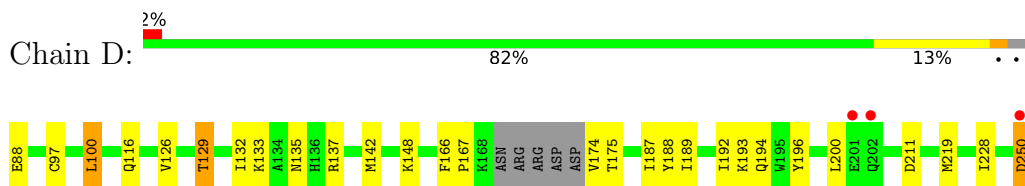
- Molecule 1: LysR family transcriptional regulator



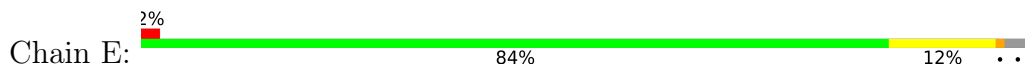
- Molecule 1: LysR family transcriptional regulator

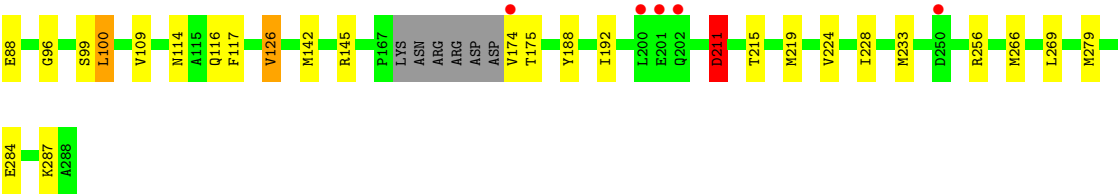


- Molecule 1: LysR family transcriptional regulator

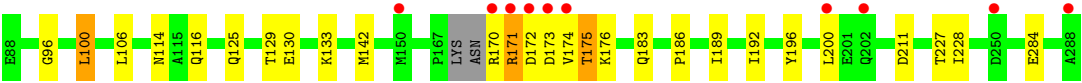
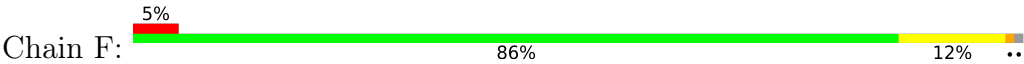


- Molecule 1: LysR family transcriptional regulator





• Molecule 1: LysR family transcriptional regulator



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	104.79Å 111.66Å 152.97Å 90.00° 95.14° 90.00°	Depositor
Resolution (Å)	31.89 – 2.50 31.89 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.2 (31.89-2.50) 93.5 (31.89-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.198 , 0.249 0.206 , 0.253	Depositor DCC
R_{free} test set	2000 reflections (1.64%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	19346	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 96.45 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.3624e-10. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.86	0/1584	0.91	0/2152
1	B	0.86	0/1581	0.96	1/2148 (0.0%)
1	C	0.85	0/1604	0.92	0/2177
1	D	0.87	0/1604	0.95	0/2177
1	E	0.88	0/1585	0.95	3/2154 (0.1%)
1	F	0.83	0/1627	0.94	1/2209 (0.0%)
All	All	0.86	0/9585	0.94	5/13017 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	211	ASP	CB-CA-C	-5.94	100.80	110.79
1	F	227	THR	N-CA-C	5.64	115.99	108.38
1	B	90	ASN	N-CA-C	5.38	122.26	110.80
1	E	117	PHE	CA-C-N	5.04	124.70	119.56
1	E	117	PHE	C-N-CA	5.04	124.70	119.56

There are no chirality outliers.

There are no planarity outliers.

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	1551	1516	1516	21	0
1	B	1548	1516	1516	17	0
1	C	1571	1548	1547	19	0
1	D	1571	1548	1547	18	1
1	E	1552	1517	1517	25	0
1	F	1594	1555	1555	21	0
2	A	13	5	5	0	0
2	B	13	5	5	0	0
2	C	13	5	5	1	0
2	D	13	5	5	1	0
2	E	13	5	5	1	0
2	F	13	5	5	0	0
3	A	117	0	0	7	1
3	B	108	0	0	8	1
3	C	114	0	0	11	0
3	D	101	0	0	5	0
3	E	99	0	0	11	1
3	F	112	0	0	13	1
All	All	10116	9230	9228	119	3

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 6.

All (119) 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:F:116:GLN:NE2	3:F:402:HOH:O	1.94	0.98
1:C:116:GLN:NE2	3:C:401:HOH:O	1.99	0.96
1:B:284:GLU:O	3:B:401:HOH:O	1.85	0.95
1:F:284:GLU:O	3:F:401:HOH:O	1.89	0.90
1:C:142:MET:SD	3:C:500:HOH:O	2.31	0.88
1:A:284:GLU:O	3:A:401:HOH:O	1.92	0.86
1:E:284:GLU:O	3:E:401:HOH:O	1.92	0.85
1:E:219:MET:SD	3:F:508:HOH:O	2.48	0.71
1:B:108:GLU:OE2	3:B:403:HOH:O	2.08	0.71
1:B:261:SER:OG	3:B:402:HOH:O	2.07	0.71
1:E:114:ASN:ND2	3:E:403:HOH:O	2.23	0.69
2:C:301:FLC:OA1	3:C:402:HOH:O	2.11	0.68
2:D:301:FLC:OA2	3:D:401:HOH:O	2.13	0.66
1:F:114:ASN:ND2	3:F:404:HOH:O	2.24	0.66
1:A:192:ILE:HD12	3:A:489:HOH:O	1.94	0.66
1:C:88:GLU:OE2	3:C:403:HOH:O	2.13	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:GLN:NE2	1:D:211:ASP:OD2	2.30	0.65
1:B:148:LYS:O	3:B:404:HOH:O	2.14	0.64
1:E:100:LEU:HD21	1:E:145:ARG:NE	2.16	0.60
1:E:100:LEU:HD22	3:E:496:HOH:O	2.00	0.60
1:E:192:ILE:HD12	3:E:485:HOH:O	2.01	0.60
1:C:88:GLU:N	3:C:412:HOH:O	2.35	0.60
1:A:160:ASP:OD1	3:A:403:HOH:O	2.17	0.60
1:E:211:ASP:OD1	1:F:125:GLN:NE2	2.37	0.58
1:C:201:GLU:N	1:C:201:GLU:OE1	2.37	0.58
1:A:114:ASN:ND2	3:A:406:HOH:O	2.25	0.57
1:D:88:GLU:N	3:D:411:HOH:O	2.38	0.57
1:E:88:GLU:N	3:E:411:HOH:O	2.38	0.56
1:B:219:MET:CE	3:C:492:HOH:O	2.54	0.55
1:B:211:ASP:OD1	1:C:125:GLN:NE2	2.40	0.54
1:F:192:ILE:HD12	3:F:493:HOH:O	2.07	0.54
1:E:224:VAL:HG11	3:F:508:HOH:O	2.08	0.54
1:B:160:ASP:CB	3:B:412:HOH:O	2.56	0.52
1:F:175:THR:HG23	3:F:500:HOH:O	2.09	0.52
1:A:129:THR:HG22	1:A:133:LYS:HE2	1.91	0.52
1:C:106:LEU:HD23	3:C:492:HOH:O	2.09	0.52
1:F:106:LEU:HD23	3:F:468:HOH:O	2.11	0.50
1:D:148:LYS:NZ	3:D:410:HOH:O	2.36	0.50
1:F:100:LEU:C	1:F:100:LEU:HD23	2.37	0.50
1:E:219:MET:CE	3:F:468:HOH:O	2.59	0.49
1:E:100:LEU:HD13	3:E:496:HOH:O	2.12	0.49
1:E:100:LEU:HD21	1:E:145:ARG:CD	2.43	0.49
1:B:194:GLN:HG3	3:B:489:HOH:O	2.13	0.49
1:E:114:ASN:ND2	3:E:413:HOH:O	2.46	0.49
1:E:188:TYR:CZ	1:E:256:ARG:HD3	2.47	0.49
1:C:188:TYR:CE2	1:C:256:ARG:CD	2.96	0.48
1:D:192:ILE:HG23	1:D:228:ILE:HD12	1.95	0.48
1:D:189:ILE:HG22	1:D:193:LYS:HE3	1.95	0.48
1:F:192:ILE:CD1	3:F:493:HOH:O	2.61	0.48
1:E:233:MET:CG	3:E:496:HOH:O	2.61	0.48
1:D:188:TYR:CE2	1:D:256:ARG:CD	2.97	0.47
1:C:116:GLN:OE1	3:C:405:HOH:O	2.20	0.47
1:D:187:ILE:HG12	3:D:418:HOH:O	2.15	0.47
1:B:186:PRO:HB2	1:E:266:MET:HE1	1.97	0.47
1:C:188:TYR:CE2	1:C:256:ARG:HD3	2.50	0.46
1:A:99:SER:HA	1:A:126:VAL:HG13	1.97	0.46
1:B:100:LEU:C	1:B:100:LEU:HD23	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:116:GLN:OE1	3:E:402:HOH:O	2.21	0.46
1:E:192:ILE:HG23	1:E:228:ILE:HD12	1.97	0.46
1:C:261:SER:OG	3:C:404:HOH:O	2.19	0.46
1:D:132:ILE:HG22	1:D:142:MET:SD	2.57	0.45
1:D:135:ASN:O	1:D:137:ARG:N	2.50	0.45
1:B:96:GLY:O	1:B:142:MET:HA	2.17	0.45
1:F:129:THR:HG22	1:F:133:LYS:HE2	1.98	0.45
1:B:192:ILE:HG23	1:B:228:ILE:HD12	1.99	0.44
1:D:100:LEU:C	1:D:100:LEU:HD12	2.42	0.44
1:F:96:GLY:O	1:F:142:MET:HA	2.17	0.44
1:A:110:LEU:HD12	1:D:219:MET:HE1	1.99	0.44
1:B:132:ILE:HG22	1:B:142:MET:HE3	1.99	0.44
1:A:129:THR:CG2	1:A:133:LYS:HE2	2.48	0.44
1:E:192:ILE:CD1	3:E:485:HOH:O	2.63	0.43
1:C:196:TYR:CD2	1:C:200:LEU:HD12	2.53	0.43
1:C:100:LEU:C	1:C:100:LEU:HD23	2.44	0.43
1:C:188:TYR:CZ	1:C:256:ARG:HD3	2.53	0.43
1:D:129:THR:HG22	1:D:133:LYS:HE2	2.00	0.43
1:D:196:TYR:CD2	1:D:200:LEU:HD12	2.52	0.43
1:A:287:LYS:O	3:A:404:HOH:O	2.21	0.43
1:C:192:ILE:HG23	1:C:228:ILE:HD12	2.00	0.43
1:F:116:GLN:OE1	3:F:403:HOH:O	2.21	0.43
2:E:301:FLC:CAC	3:E:443:HOH:O	2.66	0.43
1:F:174:VAL:HG23	3:F:500:HOH:O	2.18	0.43
1:C:129:THR:HG22	1:C:133:LYS:HE2	1.99	0.43
1:B:116:GLN:OE1	3:B:405:HOH:O	2.21	0.43
1:E:99:SER:HA	1:E:126:VAL:HG13	2.01	0.43
1:E:188:TYR:CE2	1:E:256:ARG:HD3	2.54	0.43
1:F:183:GLN:HB3	1:F:211:ASP:HA	2.00	0.43
1:A:193:LYS:HG2	1:A:204:TYR:CE1	2.54	0.43
1:A:130:GLU:OE1	1:A:130:GLU:N	2.46	0.42
1:F:189:ILE:CD1	3:F:455:HOH:O	2.67	0.42
1:F:192:ILE:HG23	1:F:228:ILE:HD12	2.01	0.42
1:B:165:ILE:HG21	1:B:220:LEU:HD21	2.01	0.42
1:B:160:ASP:CB	3:B:454:HOH:O	2.68	0.42
1:A:188:TYR:CZ	1:A:256:ARG:HD3	2.55	0.42
1:E:109:VAL:HG11	1:E:279:MET:HE1	2.02	0.41
1:C:135:ASN:O	1:C:137:ARG:N	2.54	0.41
1:C:116:GLN:HG3	3:C:415:HOH:O	2.20	0.41
1:A:106:LEU:N	1:A:107:PRO:CD	2.84	0.41
3:C:462:HOH:O	1:F:186:PRO:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:196:TYR:CD2	1:F:200:LEU:HD12	2.55	0.41
1:A:148:LYS:HE3	3:A:508:HOH:O	2.21	0.41
1:D:166:PHE:HB2	1:D:167:PRO:CD	2.51	0.41
1:A:116:GLN:OE1	3:A:405:HOH:O	2.22	0.41
1:E:215:THR:O	1:E:219:MET:HG2	2.20	0.41
1:A:100:LEU:HD12	1:A:100:LEU:C	2.46	0.41
1:A:193:LYS:HG2	1:A:204:TYR:CD1	2.56	0.41
1:D:250:ASP:HB3	1:D:251:ASN:H	1.77	0.41
1:F:170:ARG:HB3	1:F:173:ASP:HB3	2.02	0.41
1:A:160:ASP:O	1:A:255:ILE:HA	2.21	0.41
1:D:97:CYS:O	1:D:126:VAL:HA	2.21	0.40
1:E:96:GLY:O	1:E:142:MET:HA	2.21	0.40
1:F:170:ARG:O	1:F:171:ARG:HB2	2.21	0.40
1:A:165:ILE:HG21	1:A:220:LEU:HD21	2.03	0.40
1:C:96:GLY:O	1:C:142:MET:HA	2.21	0.40
1:D:188:TYR:CE2	1:D:256:ARG:HD3	2.56	0.40
1:E:266:MET:HE2	1:E:269:LEU:HD22	2.03	0.40
1:F:130:GLU:OE1	1:F:130:GLU:N	2.49	0.40
1:B:106:LEU:N	1:B:107:PRO:CD	2.85	0.40
1:A:188:TYR:CE2	1:A:256:ARG:CD	3.04	0.40
1:D:116:GLN:OE1	3:D:403:HOH:O	2.22	0.40

All (3) 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)
3:B:401:HOH:O	3:F:401:HOH:O[3_445]	1.80	0.40
3:A:401:HOH:O	3:E:401:HOH:O[3_545]	1.81	0.39
1:D:281:SER:OG	1:D:281:SER:OG[2_755]	2.14	0.06

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	190/201 (94%)	184 (97%)	6 (3%)	0	100	100
1	B	190/201 (94%)	182 (96%)	8 (4%)	0	100	100
1	C	192/201 (96%)	184 (96%)	8 (4%)	0	100	100
1	D	192/201 (96%)	186 (97%)	6 (3%)	0	100	100
1	E	191/201 (95%)	183 (96%)	8 (4%)	0	100	100
1	F	195/201 (97%)	188 (96%)	6 (3%)	1 (0%)	24	43
All	All	1150/1206 (95%)	1107 (96%)	42 (4%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	171	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	178/186 (96%)	171 (96%)	7 (4%)	28	55
1	B	177/186 (95%)	171 (97%)	6 (3%)	32	60
1	C	180/186 (97%)	175 (97%)	5 (3%)	38	66
1	D	180/186 (97%)	173 (96%)	7 (4%)	28	55
1	E	177/186 (95%)	171 (97%)	6 (3%)	32	60
1	F	182/186 (98%)	178 (98%)	4 (2%)	45	73
All	All	1074/1116 (96%)	1039 (97%)	35 (3%)	33	61

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	GLU
1	A	100	LEU
1	A	126	VAL
1	A	150	MET

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Mol	Chain	Res	Type
1	A	174	VAL
1	A	193	LYS
1	A	281	SER
1	B	99	SER
1	B	100	LEU
1	B	174	VAL
1	B	177	LEU
1	B	194	GLN
1	B	211	ASP
1	C	100	LEU
1	C	168	LYS
1	C	174	VAL
1	C	175	THR
1	C	194	GLN
1	D	100	LEU
1	D	129	THR
1	D	174	VAL
1	D	175	THR
1	D	194	GLN
1	D	250	ASP
1	D	281	SER
1	E	100	LEU
1	E	126	VAL
1	E	174	VAL
1	E	175	THR
1	E	211	ASP
1	E	287	LYS
1	F	100	LEU
1	F	172	ASP
1	F	175	THR
1	F	176	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	GLN
1	A	151	ASN
1	A	199	ASN
1	A	212	GLN
1	B	123	GLN
1	B	199	ASN
1	B	205	HIS

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Mol	Chain	Res	Type
1	B	212	GLN
1	C	190	ASN
1	C	191	GLN
1	C	199	ASN
1	C	212	GLN
1	D	194	GLN
1	D	199	ASN
1	D	205	HIS
1	D	212	GLN
1	E	135	ASN
1	E	147	ASN
1	E	199	ASN
1	E	212	GLN
1	F	116	GLN
1	F	125	GLN
1	F	147	ASN
1	F	199	ASN
1	F	212	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](#)

6 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	E	301	-	12,12,12	1.34	1 (8%)	17,17,17	1.50	2 (11%)
2	FLC	C	301	-	12,12,12	1.20	0	17,17,17	1.55	3 (17%)
2	FLC	A	301	-	12,12,12	1.15	0	17,17,17	1.61	2 (11%)
2	FLC	F	301	-	12,12,12	1.22	0	17,17,17	1.84	4 (23%)
2	FLC	B	301	-	12,12,12	1.12	0	17,17,17	1.63	3 (17%)
2	FLC	D	301	-	12,12,12	1.28	1 (8%)	17,17,17	1.73	4 (23%)

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	E	301	-	-	2/16/16/16	-
2	FLC	C	301	-	-	0/16/16/16	-
2	FLC	A	301	-	-	2/16/16/16	-
2	FLC	F	301	-	-	3/16/16/16	-
2	FLC	B	301	-	-	2/16/16/16	-
2	FLC	D	301	-	-	2/16/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	FLC	CB-CBC	2.35	1.55	1.53
2	E	301	FLC	OB1-CBC	2.02	1.28	1.22

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	FLC	OB2-CBC-CB	5.35	123.40	113.14
2	D	301	FLC	OB2-CBC-CB	4.60	121.97	113.14
2	A	301	FLC	OB2-CBC-CB	4.21	121.21	113.14
2	B	301	FLC	OB2-CBC-CB	3.67	120.18	113.14
2	E	301	FLC	OB2-CBC-CB	3.53	119.90	113.14
2	C	301	FLC	OB2-CBC-CB	3.48	119.81	113.14
2	D	301	FLC	OA2-CAC-CA	2.77	123.14	114.35
2	B	301	FLC	OG2-CGC-CG	2.55	122.43	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	FLC	OG2-CGC-OG1	-2.47	116.99	123.33
2	B	301	FLC	OG2-CGC-OG1	-2.41	117.13	123.33
2	D	301	FLC	OA2-CAC-OA1	-2.35	117.29	123.33
2	C	301	FLC	OB2-CBC-OB1	-2.33	116.39	123.86
2	F	301	FLC	OB2-CBC-OB1	-2.29	116.54	123.86
2	F	301	FLC	CG-CB-CBC	-2.12	105.34	110.03
2	C	301	FLC	OA2-CAC-OA1	-2.11	117.91	123.33
2	E	301	FLC	OA2-CAC-CA	2.10	121.01	114.35
2	D	301	FLC	OB2-CBC-OB1	-2.09	117.18	123.86
2	F	301	FLC	OHB-CB-CBC	2.04	111.85	108.96

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	301	FLC	CB-CA-CAC-OA1
2	E	301	FLC	CB-CA-CAC-OA2
2	A	301	FLC	CB-CA-CAC-OA1
2	A	301	FLC	CB-CA-CAC-OA2
2	D	301	FLC	CB-CG-CGC-OG1
2	D	301	FLC	CB-CG-CGC-OG2
2	B	301	FLC	CG-CB-CBC-OB1
2	B	301	FLC	CG-CB-CBC-OB2
2	F	301	FLC	CG-CB-CBC-OB2
2	F	301	FLC	CG-CB-CBC-OB1
2	F	301	FLC	CA-CB-CBC-OB2

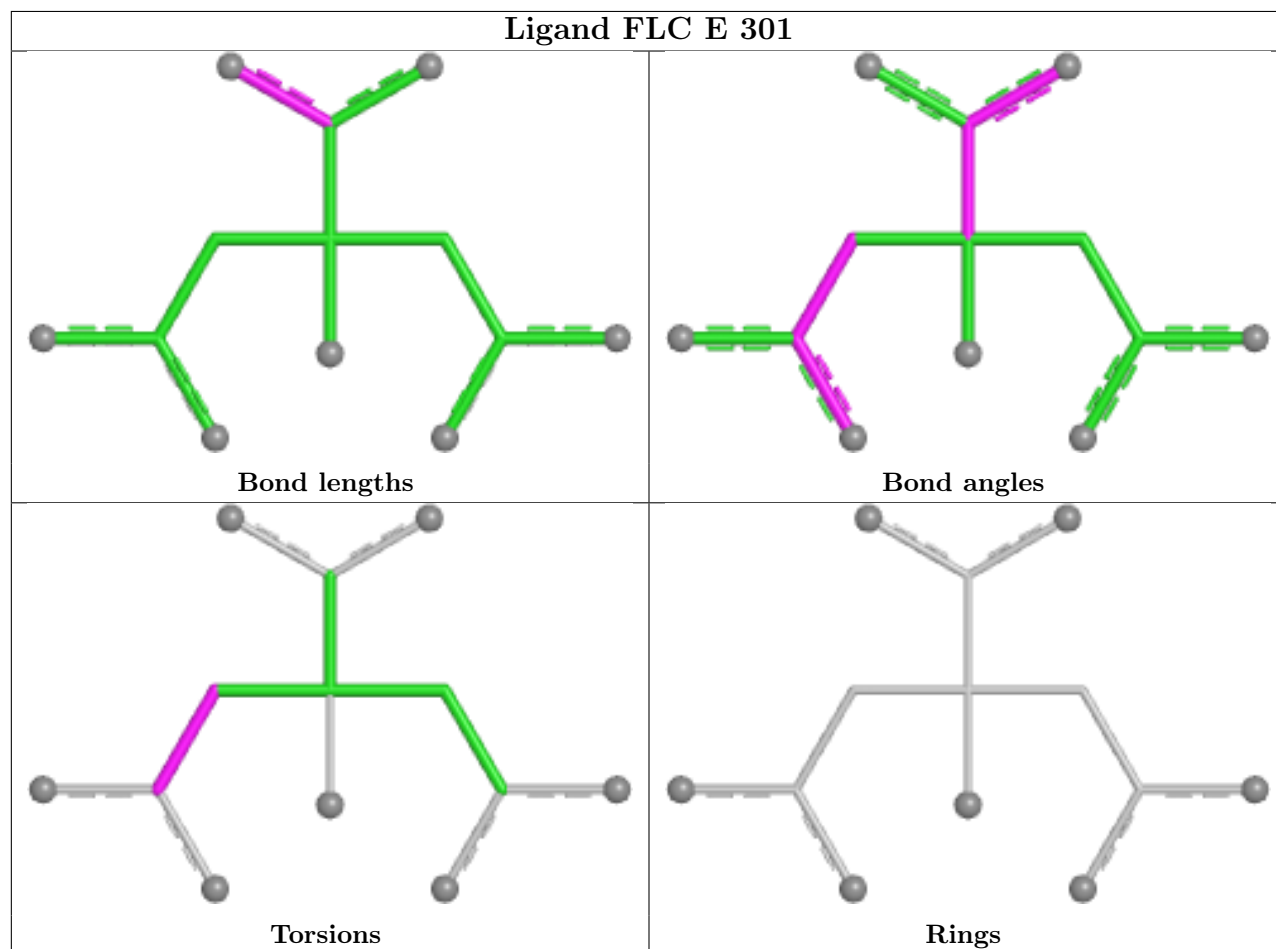
There are no ring outliers.

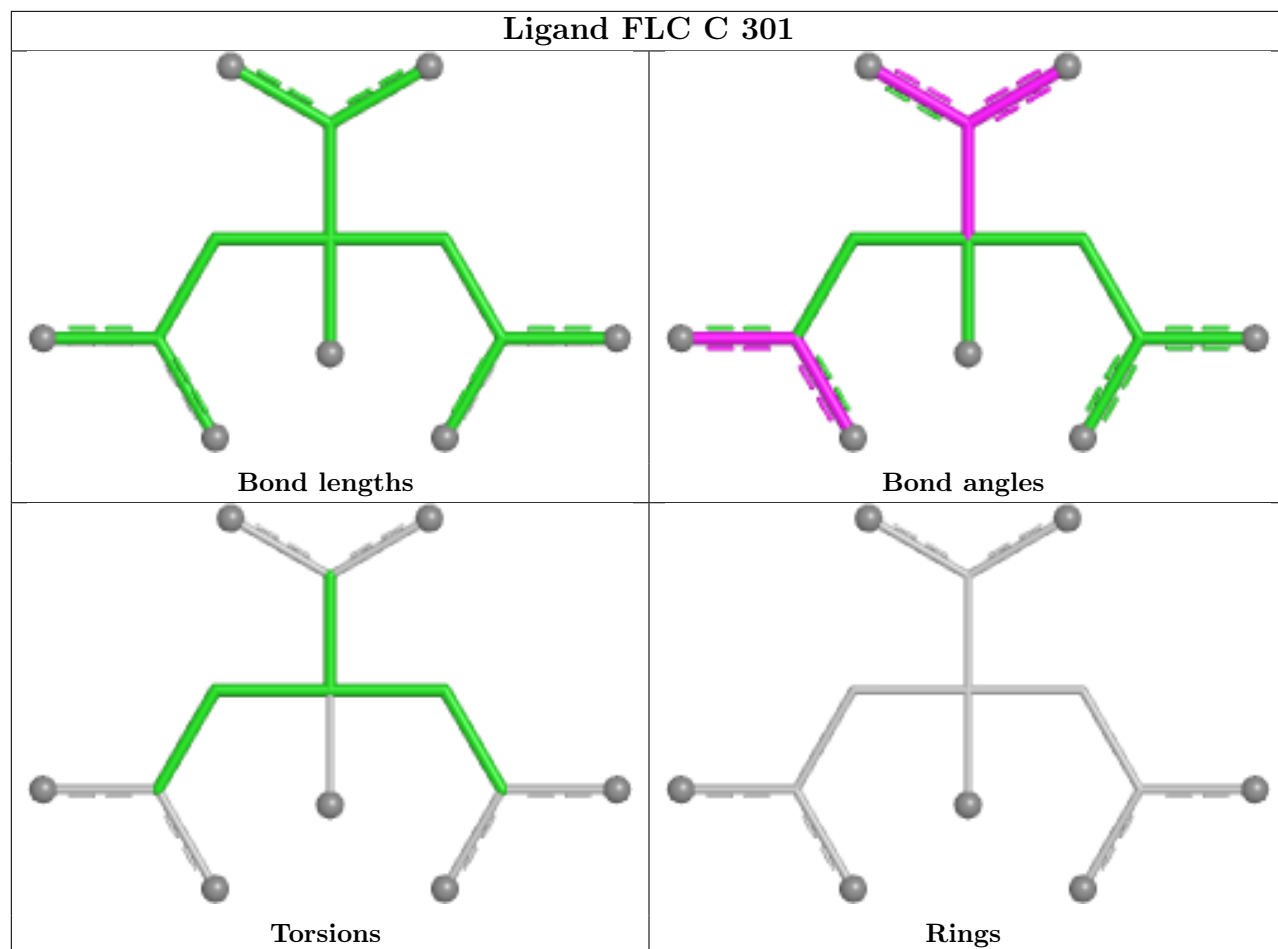
3 monomers are involved in 3 short contacts:

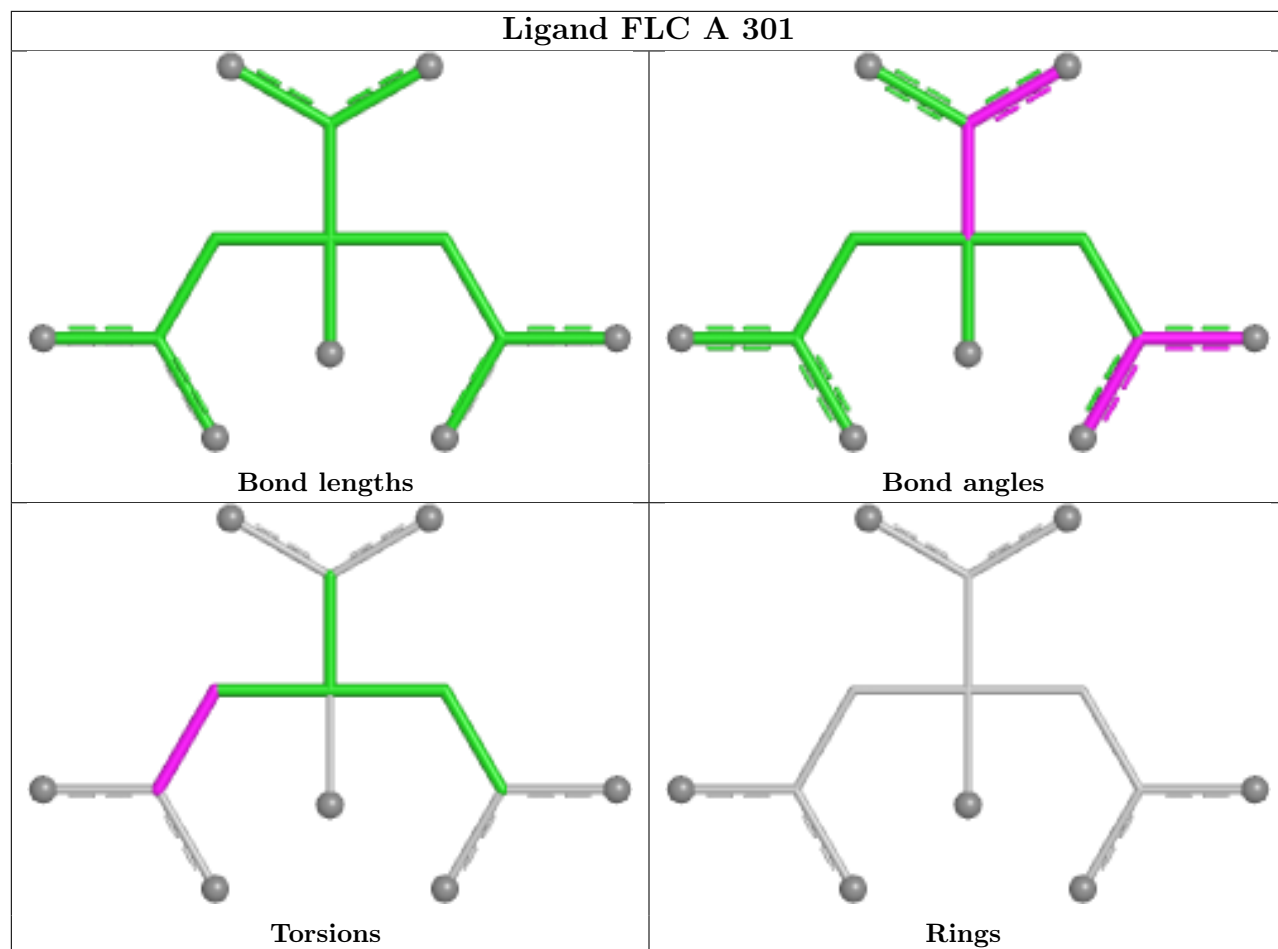
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	FLC	1	0
2	C	301	FLC	1	0
2	D	301	FLC	1	0

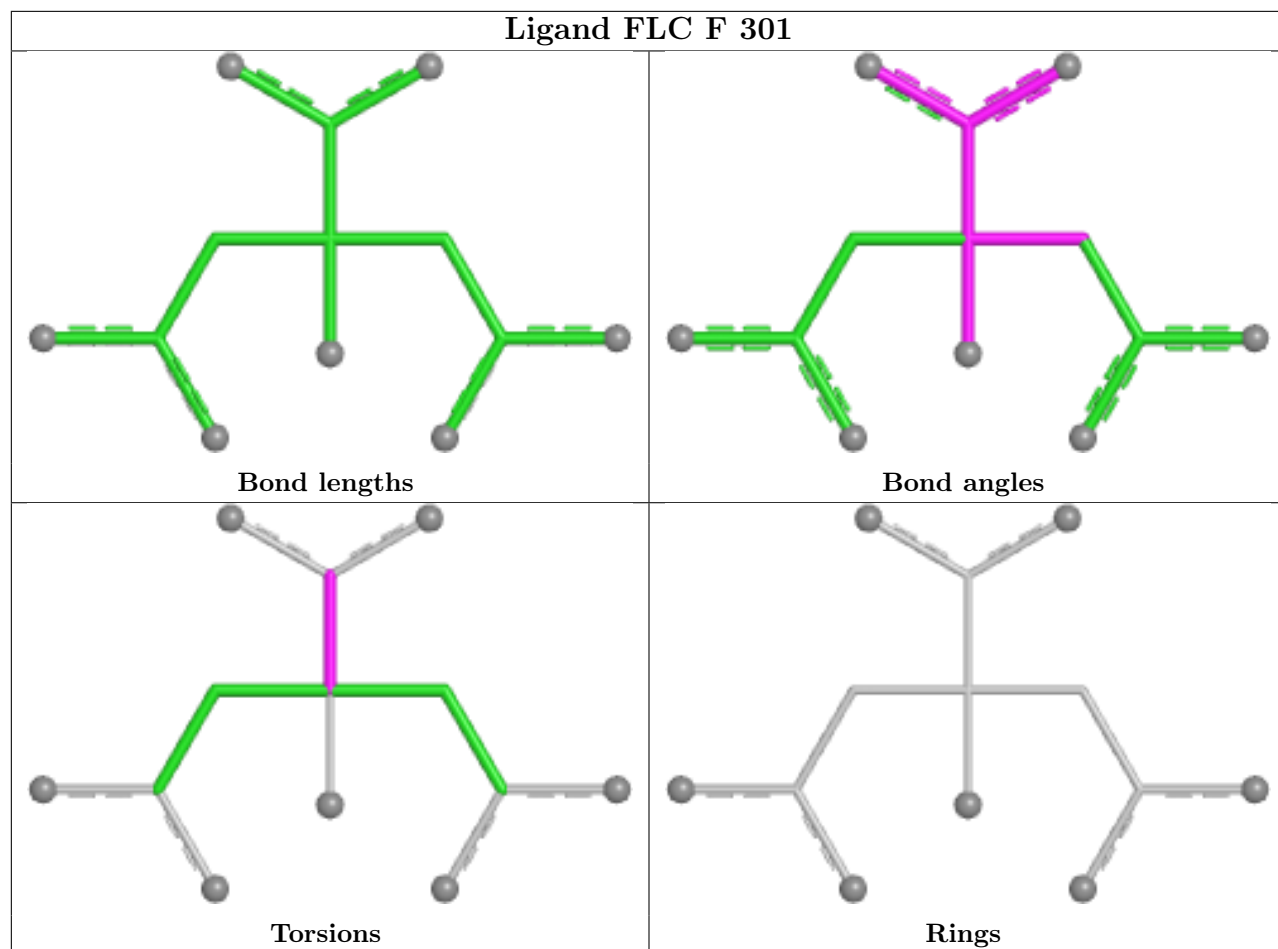
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

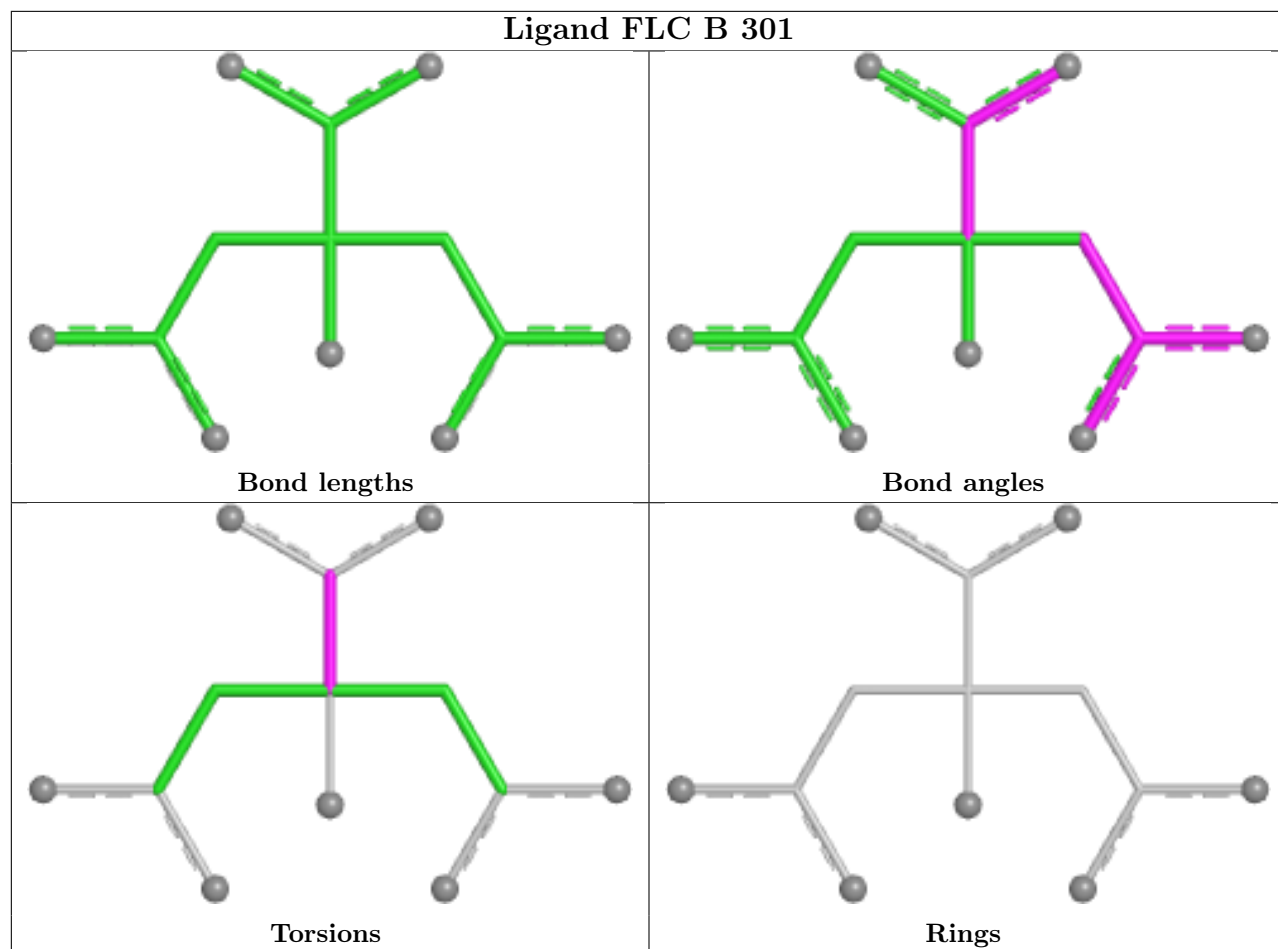
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

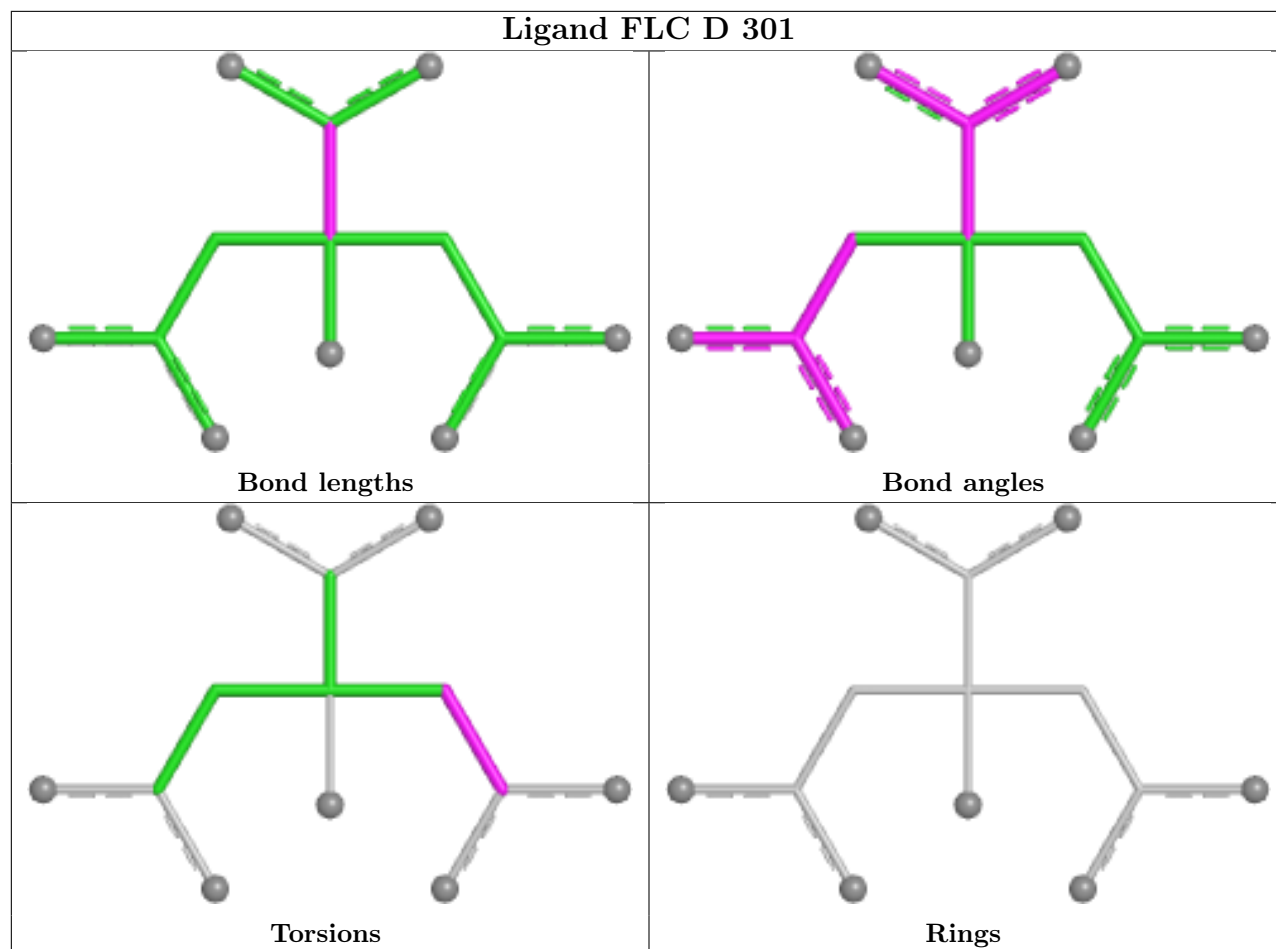












5.7 Other polymers [i](#)

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, 95th 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 ²)	Q<0.9
1	A	194/201 (96%)	-0.23	2 (1%) 79 76	22, 41, 74, 96	0
1	B	194/201 (96%)	-0.27	0 100 100	24, 40, 73, 88	0
1	C	196/201 (97%)	-0.25	4 (2%) 65 61	21, 41, 78, 162	0
1	D	196/201 (97%)	-0.25	5 (2%) 57 52	22, 40, 78, 158	1 (0%)
1	E	195/201 (97%)	-0.17	5 (2%) 57 52	22, 40, 81, 171	0
1	F	199/201 (99%)	-0.12	10 (5%) 34 30	22, 42, 85, 151	0
All	All	1174/1206 (97%)	-0.22	26 (2%) 62 58	21, 41, 78, 171	1 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	174	VAL	6.4
1	F	173	ASP	4.1
1	D	288	ALA	3.3
1	C	288	ALA	3.3
1	C	250	ASP	3.1
1	F	170	ARG	3.0
1	E	202	GLN	3.0
1	F	172	ASP	3.0
1	D	202	GLN	2.9
1	C	201	GLU	2.9
1	C	202	GLN	2.8
1	D	250	ASP	2.7
1	E	201	GLU	2.6
1	D	201	GLU	2.5
1	F	200	LEU	2.5
1	F	174	VAL	2.4
1	A	194	GLN	2.4
1	F	171	ARG	2.4
1	F	250	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	150	MET	2.2
1	E	200	LEU	2.2
1	E	250	ASP	2.2
1	A	197	ASN	2.1
1	F	202	GLN	2.1
1	D	251	ASN	2.1
1	F	288	ALA	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

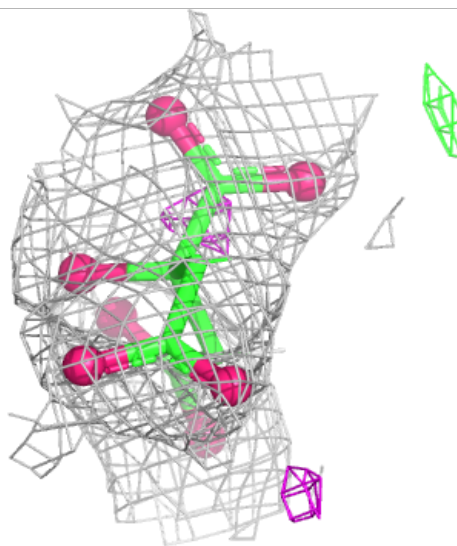
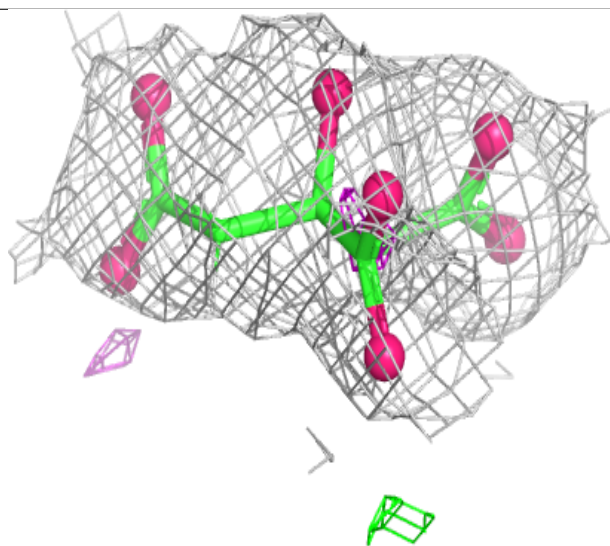
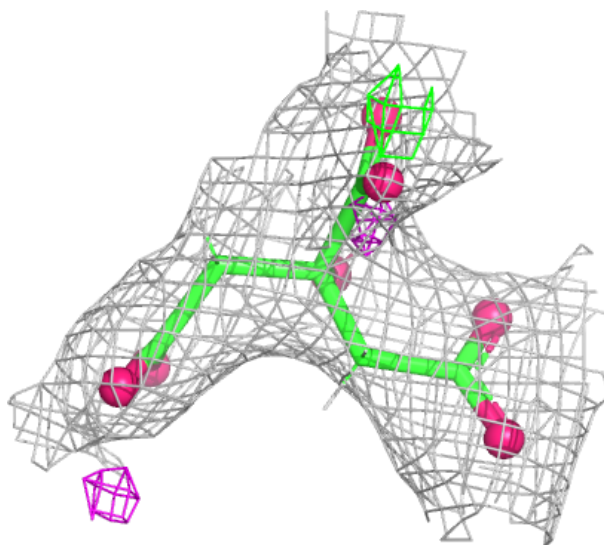
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FLC	E	301	13/13	0.94	0.08	35,43,53,54	0
2	FLC	F	301	13/13	0.94	0.09	29,52,63,68	0
2	FLC	D	301	13/13	0.95	0.08	28,47,57,57	0
2	FLC	A	301	13/13	0.95	0.08	37,49,60,64	0
2	FLC	B	301	13/13	0.95	0.08	39,46,54,56	0
2	FLC	C	301	13/13	0.96	0.08	30,51,66,66	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.

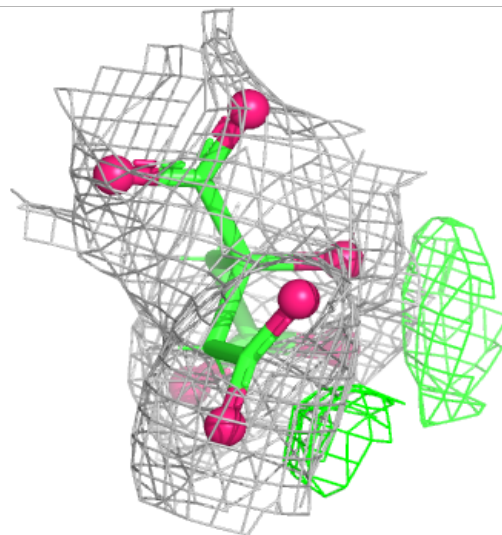
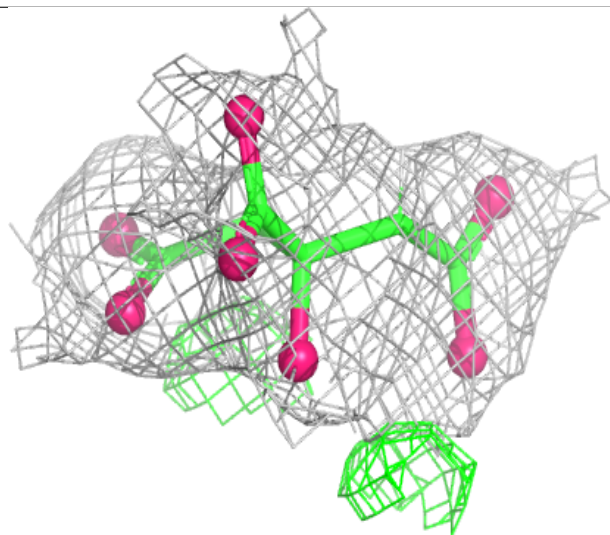
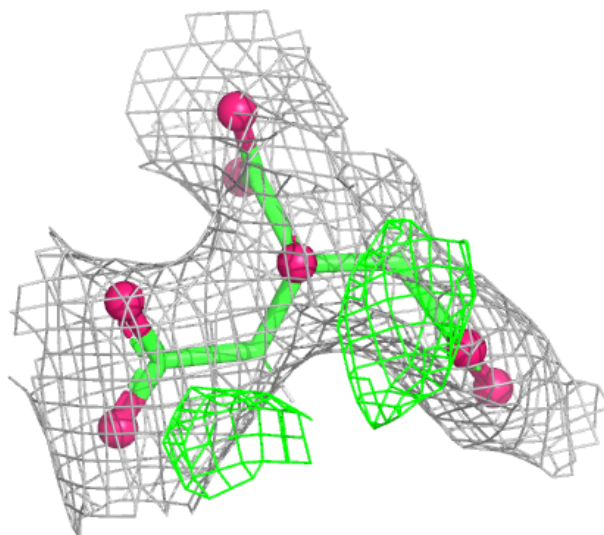
Electron density around FLC E 301:

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



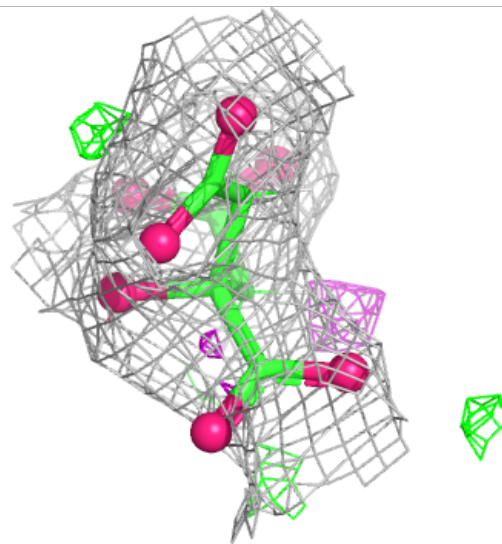
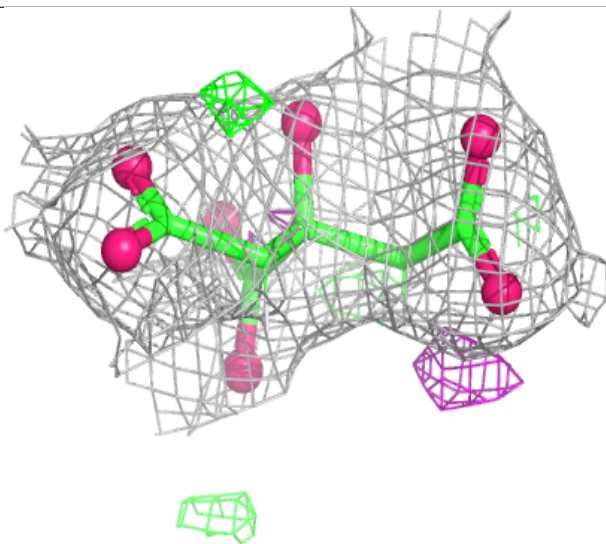
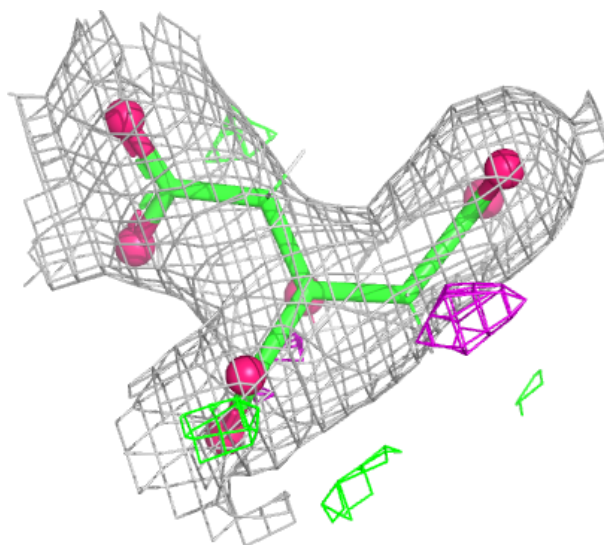
Electron density around FLC F 301:

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



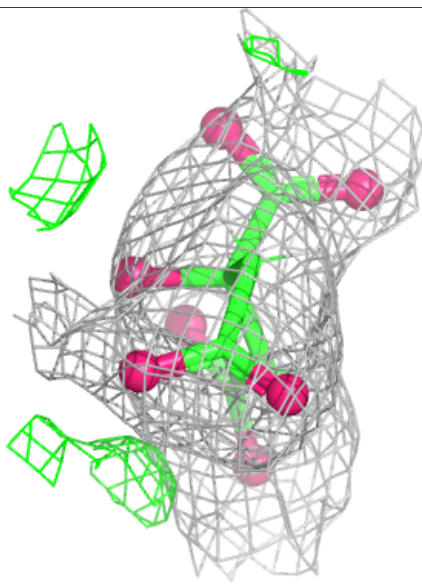
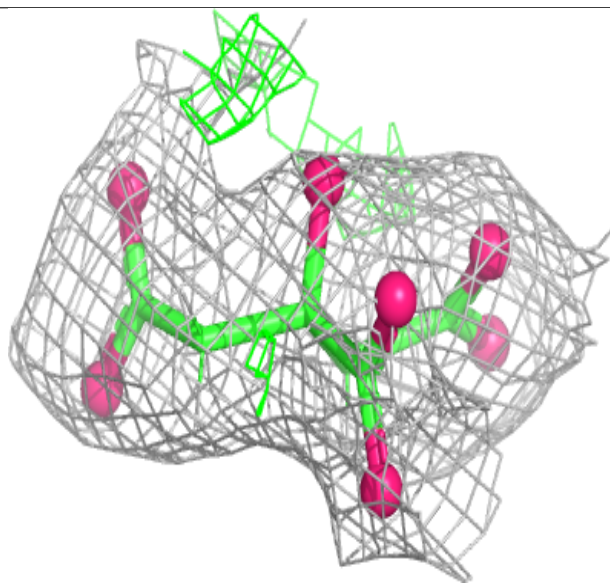
Electron density around FLC D 301:

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



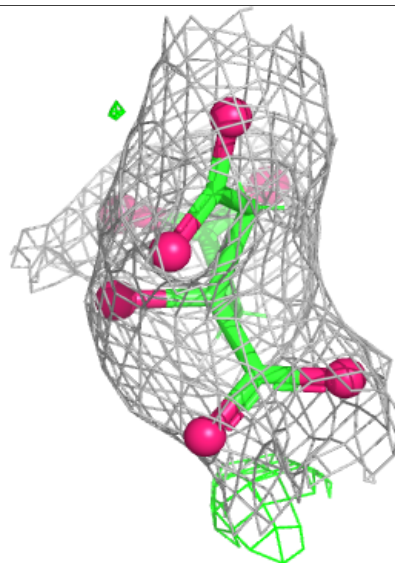
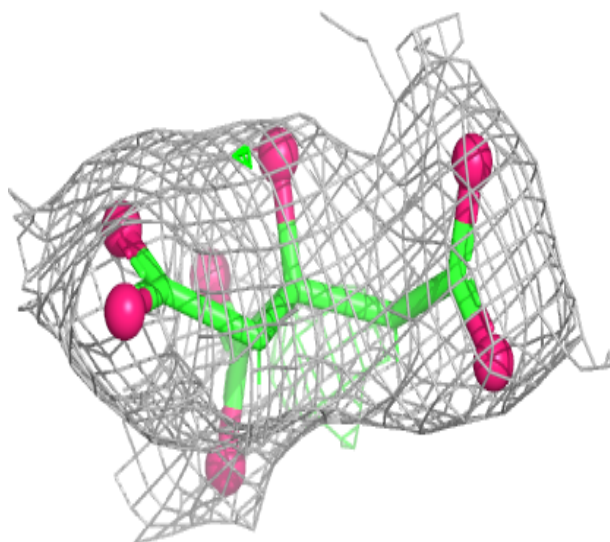
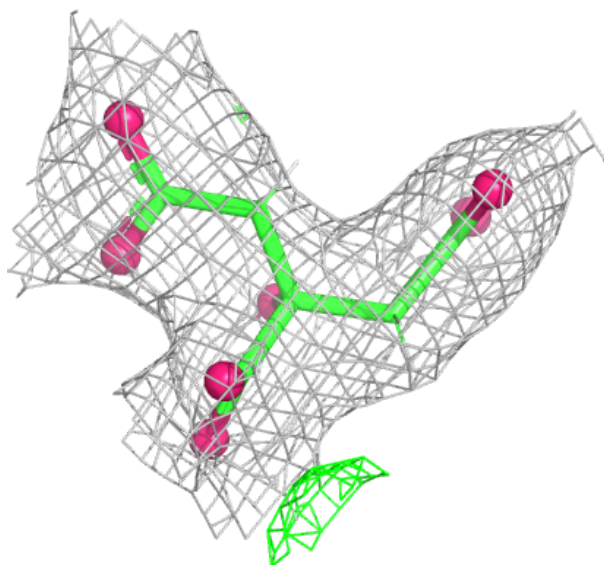
Electron density around FLC A 301:

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



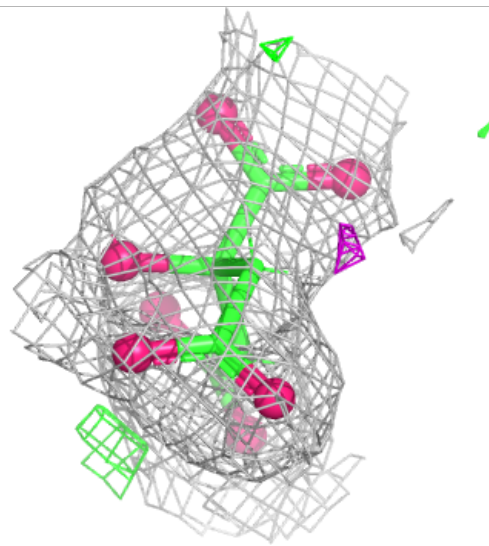
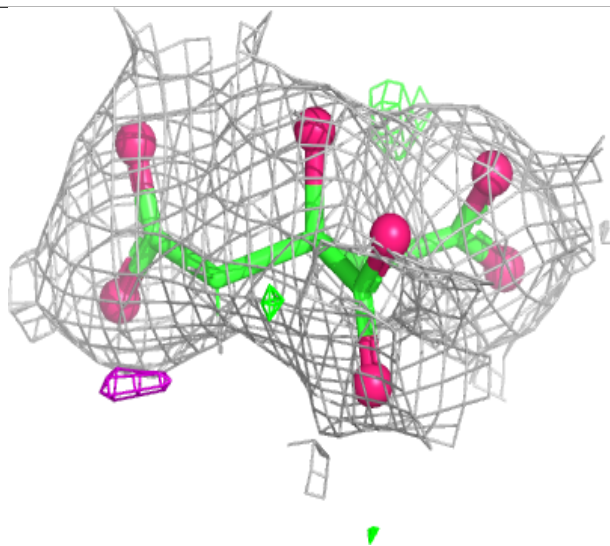
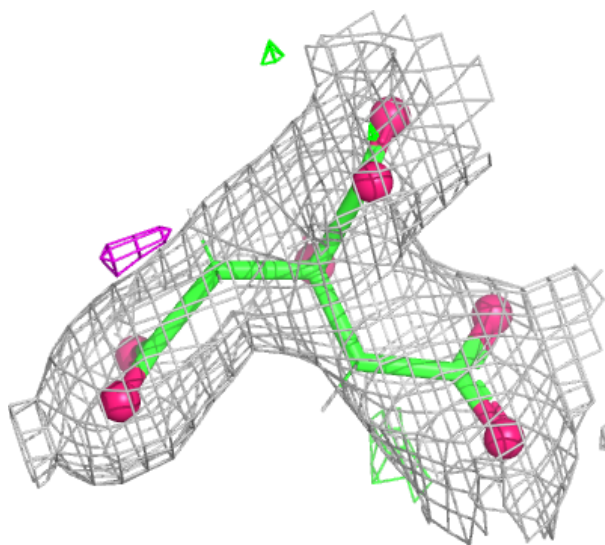
Electron density around FLC B 301:

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



Electron density around FLC 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)

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

There are no such residues in this entry.