



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 7, 2023 – 05:11 PM EST

PDB ID : 7FT3  
Title : SDCBP PanDDA analysis group deposition – The PDZ domains of SDCBP in complex with Z291279160  
Authors : Bradshaw, W.J.; Katis, V.L.; Bountra, C.; von Delft, F.; Brennan, P.E.  
Deposited on : 2023-01-24  
Resolution : 2.05 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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.32.1  
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) : 2.32.1

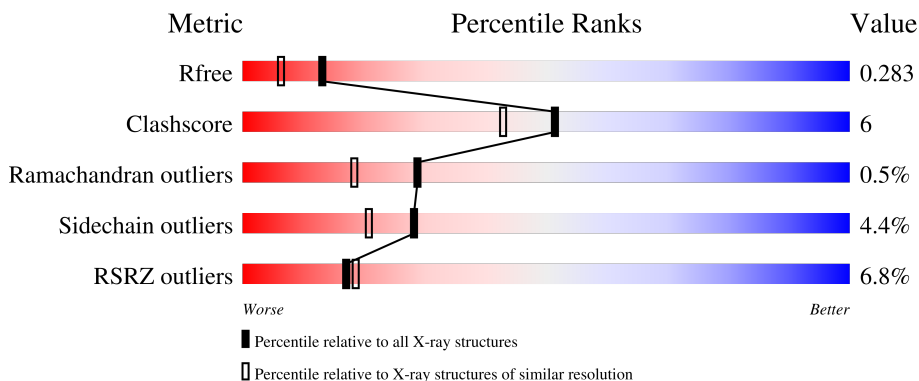
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	195	 5% 84% 12% ..
1	B	195	 5% 85% 13% ..
1	C	195	 11% 79% 18% ..
1	D	195	 6% 84% 12% ..

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6415 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 Syntenin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	191	1481	935	262	275	9	0	1	0
1	B	193	1495	943	264	279	9	0	1	0
1	C	193	1514	953	270	282	9	0	3	0
1	D	191	1489	939	263	278	9	0	2	0

There are 8 discrepancies between the modelled and reference sequences:

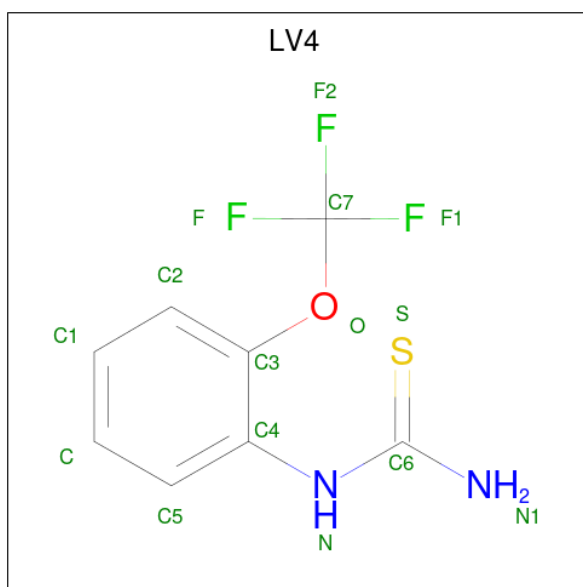
Chain	Residue	Modelled	Actual	Comment	Reference
A	104	SER	-	expression tag	UNP O00560
A	105	MET	-	expression tag	UNP O00560
B	104	SER	-	expression tag	UNP O00560
B	105	MET	-	expression tag	UNP O00560
C	104	SER	-	expression tag	UNP O00560
C	105	MET	-	expression tag	UNP O00560
D	104	SER	-	expression tag	UNP O00560
D	105	MET	-	expression tag	UNP O00560

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



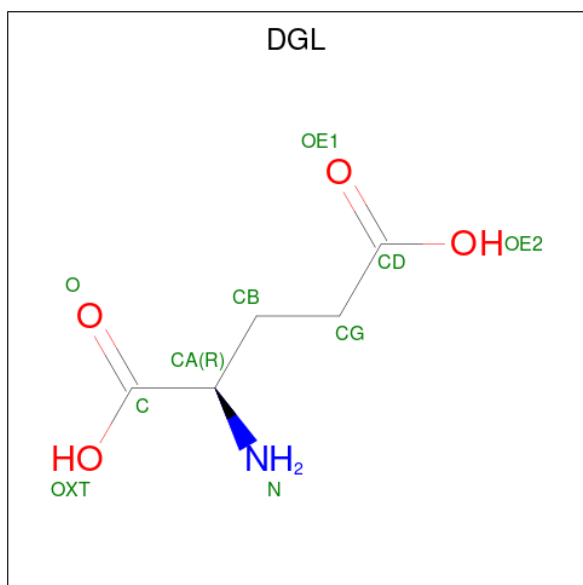
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

- Molecule 3 is 1-[2-(trifluoromethoxy)phenyl]thiourea (three-letter code: LV4) (formula:  $C_8H_7F_3N_2OS$ ) (labeled as "Ligand of Interest" by depositor).



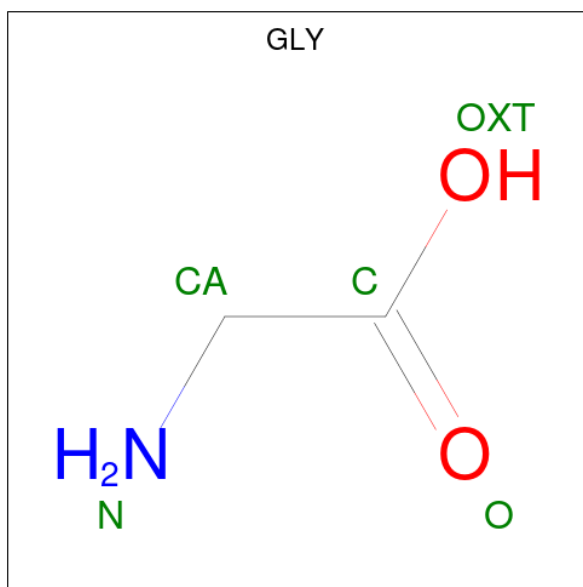
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf		
			Total	C	F	N	O			S	
3	B	1	Total	15	8	3	2	1	1	0	0
3	C	1	Total	15	8	3	2	1	1	0	0
3	C	1	Total	15	8	3	2	1	1	0	0
3	D	1	Total	15	8	3	2	1	1	0	0

- Molecule 4 is D-GLUTAMIC ACID (three-letter code: DGL) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	B	1	10	5	1	4	0	0
4	D	1	10	5	1	4	0	0

- Molecule 5 is GLYCINE (three-letter code: GLY) (formula: C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub>).



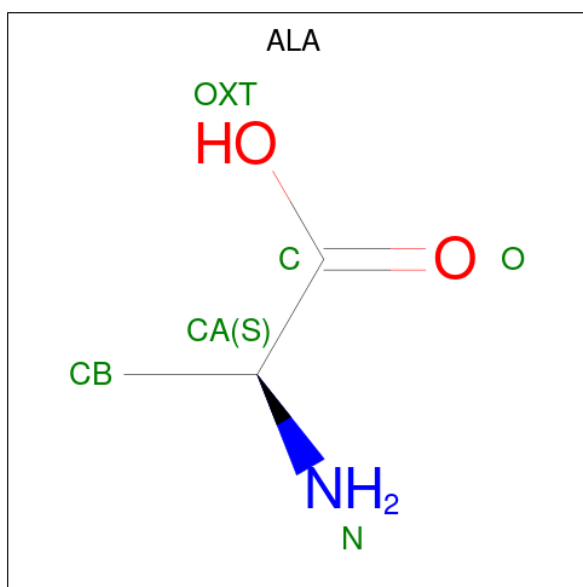
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	C	1	5	2	1	2	0	0
5	D	1	5	2	1	2	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is ALANINE (three-letter code: ALA) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	N	O	0	0
			6	3	1	2		

- Molecule 8 is water.

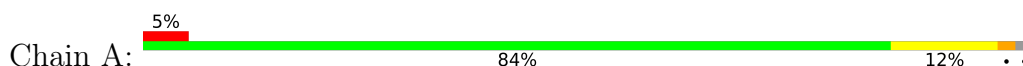
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	44	Total O 44 44	0	0
8	B	97	Total O 97 97	0	1
8	C	65	Total O 65 65	0	0
8	D	87	Total O 87 87	0	1



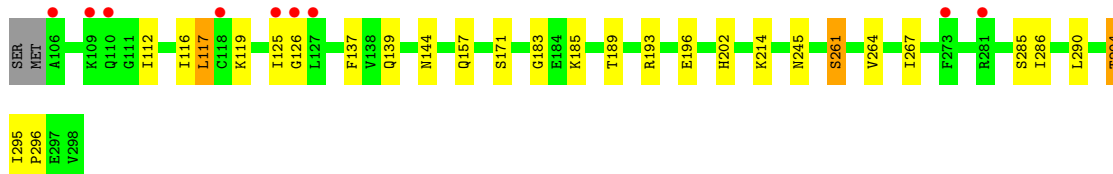
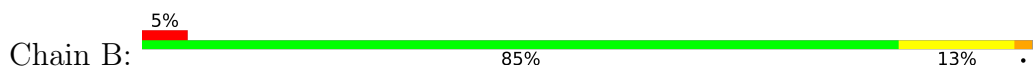
### 3 Residue-property plots [i](#)

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

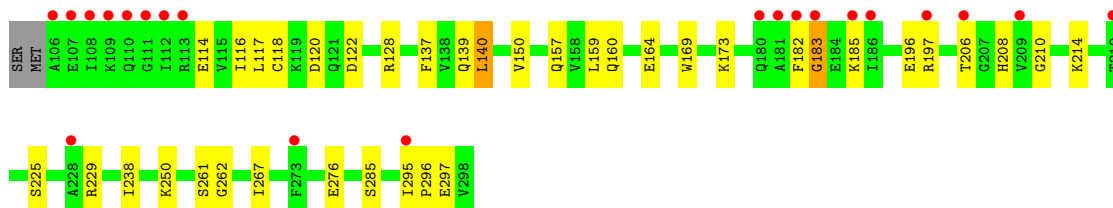
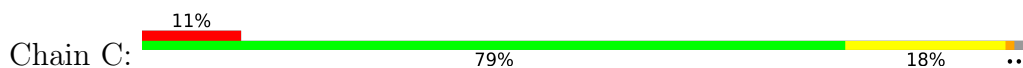
- Molecule 1: Syntenin-1



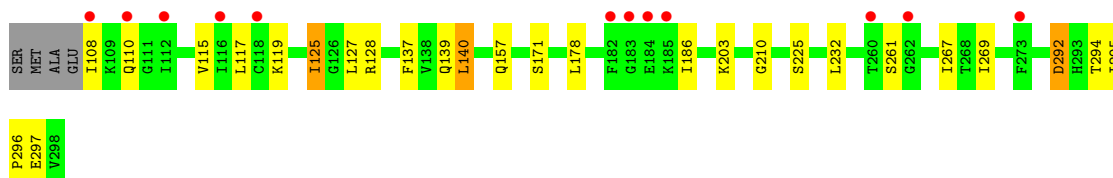
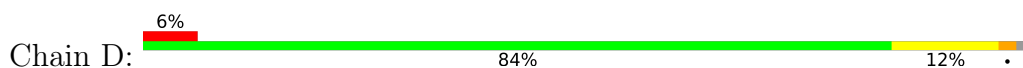
- Molecule 1: Syntenin-1



- Molecule 1: Syntenin-1



- Molecule 1: Syntenin-1



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.55Å 49.70Å 115.89Å 90.00° 95.04° 90.00°	Depositor
Resolution (Å)	115.45 – 2.05 115.45 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.6 (115.45-2.05) 99.6 (115.45-2.05)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 2.05Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.224 , 0.279 0.235 , 0.283	Depositor DCC
$R_{free}$ test set	2810 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.1	Xtrriage
Anisotropy	0.317	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6415	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.47 % 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 1.5416e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: SO4, DGL, EDO, LV4

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	0.77	0/1502	0.91	0/2019
1	B	0.88	1/1516 (0.1%)	1.02	0/2038
1	C	0.80	1/1535 (0.1%)	0.99	0/2063
1	D	0.90	1/1510 (0.1%)	1.03	0/2030
All	All	0.84	3/6063 (0.0%)	0.99	0/8150

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	A	0	1
1	B	0	1
1	D	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	292	ASP	CB-CG	6.83	1.66	1.51
1	C	276	GLU	CD-OE2	5.01	1.31	1.25
1	B	126	GLY	C-O	5.00	1.31	1.23

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	GLN	Peptide
1	B	214	LYS	Mainchain
1	D	127	LEU	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	1481	0	1530	17	0
1	B	1495	0	1541	17	0
1	C	1514	0	1558	20	0
1	D	1489	0	1533	15	0
2	A	4	0	6	0	0
2	B	8	0	12	0	0
2	C	12	0	18	0	0
2	D	8	0	12	0	0
3	B	15	0	0	0	0
3	C	30	0	0	0	0
3	D	15	0	0	0	0
4	B	10	0	7	1	0
4	D	10	0	7	0	0
5	C	5	0	2	0	0
5	D	5	0	2	0	0
6	D	15	0	0	0	0
7	D	6	0	4	0	0
8	A	44	0	0	0	0
8	B	97	0	0	1	0
8	C	65	0	0	1	0
8	D	87	0	0	0	0
All	All	6415	0	6232	69	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (69) 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:206:THR:HG1	1:C:208:HIS:HD1	1.03	0.91
1:C:137:PHE:CE2	1:C:157:GLN:HB2	2.26	0.70
1:C:229:ARG:NH2	8:C:402:HOH:O	2.28	0.67
1:C:296:PRO:HD2	1:C:297:GLU:OE1	1.95	0.66
1:A:108:ILE:HA	1:A:192:ASP:OD2	1.97	0.64
1:B:117:LEU:HD12	1:B:117:LEU:N	2.12	0.64
1:C:157:GLN:HG2	1:C:159:LEU:CD1	2.29	0.62
1:B:112:ILE:CG2	1:B:189:THR:HG22	2.28	0.62
1:C:196:GLU:O	1:C:197[B]:ARG:HD3	2.00	0.61
1:D:125:ILE:HD11	1:D:178:LEU:HD13	1.84	0.59
1:D:128:ARG:HB2	1:D:140:LEU:HB3	1.84	0.59
1:A:286:ILE:HG23	1:A:290:LEU:HD12	1.87	0.57
1:B:119:LYS:HB2	1:B:183:GLY:HA3	1.88	0.56
1:D:295:ILE:HB	1:D:296:PRO:HD2	1.91	0.53
1:C:128:ARG:HD3	1:C:140:LEU:HD22	1.89	0.53
1:C:128:ARG:CD	1:C:140:LEU:HD22	2.38	0.53
1:A:182:PHE:O	1:A:184:GLU:N	2.42	0.52
1:A:181:ALA:O	1:A:183:GLY:N	2.43	0.52
1:D:128:ARG:HH11	1:D:128:ARG:HG2	1.76	0.51
1:A:203:LYS:HA	1:A:208:HIS:O	2.11	0.51
1:C:261:SER:OG	1:C:262:GLY:N	2.42	0.51
1:D:119:LYS:CE	1:D:186:ILE:HD11	2.41	0.51
1:D:119:LYS:HE3	1:D:186:ILE:HD11	1.94	0.50
1:A:140:LEU:HD12	1:A:282:MET:SD	2.51	0.50
1:D:128:ARG:HG2	1:D:128:ARG:NH1	2.27	0.50
1:A:283:ALA:HB3	1:A:286:ILE:HD12	1.93	0.49
1:A:182:PHE:H	1:A:182:PHE:HD2	1.59	0.49
1:A:206:THR:OG1	1:A:208:HIS:ND1	2.40	0.48
1:B:171:SER:OG	4:B:304:DGL:OXT	2.31	0.47
1:D:203:LYS:NZ	1:D:261:SER:O	2.39	0.47
1:B:117:LEU:HD23	1:B:125:ILE:HG23	1.98	0.46
1:C:182:PHE:C	1:C:183:GLY:O	2.53	0.46
1:C:210:GLY:HA3	1:C:225:SER:CB	2.45	0.46
1:D:137:PHE:CE2	1:D:157:GLN:HB2	2.52	0.45
1:B:295:ILE:HA	1:B:296:PRO:HD3	1.87	0.44
1:C:120:ASP:OD1	1:C:122:ASP:N	2.51	0.44
1:D:267:ILE:HG13	1:D:269:ILE:HG23	1.99	0.44
1:B:193:ARG:HB3	1:B:196:GLU:HB2	2.00	0.44
1:A:153:ARG:HH11	1:A:153:ARG:HG3	1.82	0.44
1:D:210:GLY:HA3	1:D:225:SER:HB2	1.99	0.44
1:C:160:GLN:HA	1:C:164:GLU:O	2.18	0.44
1:B:112:ILE:CG2	1:B:189:THR:CG2	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ILE:HG23	1:B:185:LYS:HG2	2.00	0.43
1:C:297:GLU:O	1:C:297:GLU:HG2	2.18	0.43
1:B:125:ILE:HD12	1:B:125:ILE:N	2.34	0.43
1:B:202:HIS:CE1	1:B:264:VAL:HG22	2.53	0.43
1:A:112:ILE:HA	1:A:190:ILE:O	2.18	0.43
1:B:286:ILE:HG23	1:B:290:LEU:HD12	2.00	0.43
1:A:258:LEU:CD2	1:A:265:VAL:HG11	2.49	0.43
1:D:232:LEU:HD11	1:D:267:ILE:HD11	2.00	0.43
1:A:182:PHE:CD2	1:A:182:PHE:N	2.86	0.42
1:B:119:LYS:HB2	1:B:183:GLY:CA	2.49	0.42
1:B:261:SER:HB2	8:B:466:HOH:O	2.19	0.42
1:B:294:THR:HG22	1:B:295:ILE:N	2.34	0.42
1:C:128:ARG:HB2	1:C:140:LEU:HB3	2.01	0.42
1:A:140:LEU:HD11	1:A:286:ILE:HG22	2.02	0.42
1:B:245:ASN:OD1	1:B:245:ASN:C	2.58	0.42
1:C:295:ILE:HA	1:C:296:PRO:HD3	1.92	0.42
1:D:292:ASP:OD1	1:D:294:THR:HG23	2.20	0.42
1:D:210:GLY:HA3	1:D:225:SER:CB	2.51	0.41
1:B:137:PHE:CE2	1:B:157:GLN:HB2	2.55	0.41
1:A:161:ILE:HG13	1:A:166:CYS:SG	2.61	0.41
1:C:169:TRP:CE2	1:C:173:LYS:HE2	2.56	0.41
1:C:238:ILE:HG23	1:C:267:ILE:HG23	2.02	0.41
1:D:128:ARG:HH11	1:D:128:ARG:CG	2.34	0.41
1:A:235:GLU:OE1	1:A:235:GLU:HA	2.20	0.40
1:C:116:ILE:HG23	1:C:185:LYS:HG3	2.03	0.40
1:C:210:GLY:HA3	1:C:225:SER:HB2	2.04	0.40
1:A:286:ILE:HG23	1:A:290:LEU:CD1	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	190/195 (97%)	176 (93%)	11 (6%)	3 (2%)	9	2
1	B	192/195 (98%)	184 (96%)	8 (4%)	0	100	100
1	C	194/195 (100%)	182 (94%)	11 (6%)	1 (0%)	29	18
1	D	191/195 (98%)	185 (97%)	6 (3%)	0	100	100
All	All	767/780 (98%)	727 (95%)	36 (5%)	4 (0%)	29	18

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	PHE
1	A	183	GLY
1	C	183	GLY
1	A	193	ARG

### 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	166/168 (99%)	162 (98%)	4 (2%)	49	42
1	B	167/168 (99%)	160 (96%)	7 (4%)	30	22
1	C	169/168 (101%)	160 (95%)	9 (5%)	22	14
1	D	167/168 (99%)	158 (95%)	9 (5%)	22	13
All	All	669/672 (100%)	640 (96%)	29 (4%)	28	22

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	LEU
1	A	253	GLN
1	A	259	SER
1	A	295	ILE
1	B	117	LEU
1	B	139	GLN
1	B	144	ASN

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Mol	Chain	Res	Type
1	B	261	SER
1	B	267	ILE
1	B	285	SER
1	B	294	THR
1	C	114	GLU
1	C	117	LEU
1	C	118	CYS
1	C	139	GLN
1	C	140	LEU
1	C	150	VAL
1	C	214	LYS
1	C	250	LYS
1	C	285	SER
1	D	108	ILE
1	D	110	GLN
1	D	115	VAL
1	D	117	LEU
1	D	125	ILE
1	D	139	GLN
1	D	140	LEU
1	D	171	SER
1	D	297	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	A	180	GLN
1	A	237	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 [i](#)

20 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
6	SO4	D	306	-	4,4,4	0.38	0	6,6,6	0.14	0
5	GLY	D	309	-	4,4,4	1.07	0	3,4,4	1.33	0
7	ALA	D	307	-	5,5,5	1.13	1 (20%)	6,6,6	1.54	1 (16%)
3	LV4	D	301	-	15,15,15	2.91	3 (20%)	20,21,21	1.01	2 (10%)
4	DGL	B	304	-	8,9,9	1.04	1 (12%)	10,11,11	1.58	2 (20%)
5	GLY	C	306	-	4,4,4	1.05	0	3,4,4	1.16	0
2	EDO	C	305	-	3,3,3	0.27	0	2,2,2	0.54	0
2	EDO	A	301	-	3,3,3	0.20	0	2,2,2	0.03	0
3	LV4	C	302	-	15,15,15	2.56	4 (26%)	20,21,21	1.02	1 (5%)
2	EDO	B	302	-	3,3,3	0.31	0	2,2,2	0.28	0
2	EDO	B	303	-	3,3,3	0.53	0	2,2,2	0.55	0
2	EDO	C	304	-	3,3,3	0.10	0	2,2,2	0.27	0
2	EDO	D	303	-	3,3,3	0.13	0	2,2,2	0.34	0
2	EDO	C	303	-	3,3,3	0.11	0	2,2,2	0.10	0
6	SO4	D	304	-	4,4,4	0.37	0	6,6,6	0.06	0
3	LV4	C	301	-	15,15,15	3.03	3 (20%)	20,21,21	1.36	4 (20%)
6	SO4	D	305	-	4,4,4	0.38	0	6,6,6	0.05	0
4	DGL	D	308	-	8,9,9	0.99	0	10,11,11	1.09	0
3	LV4	B	301	-	15,15,15	4.43	4 (26%)	20,21,21	1.69	3 (15%)
2	EDO	D	302	-	3,3,3	0.06	0	2,2,2	0.13	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	303	-	-	0/1/1/1	-
2	EDO	C	305	-	-	1/1/1/1	-
2	EDO	A	301	-	-	0/1/1/1	-
3	LV4	C	302	-	-	0/9/9/9	0/1/1/1
5	GLY	D	309	-	-	0/2/2/2	-
3	LV4	C	301	-	-	0/9/9/9	0/1/1/1
4	DGL	D	308	-	-	4/9/9/9	-
7	ALA	D	307	-	-	0/4/4/4	-
2	EDO	C	304	-	-	1/1/1/1	-
3	LV4	B	301	-	-	1/9/9/9	0/1/1/1
3	LV4	D	301	-	-	0/9/9/9	0/1/1/1
2	EDO	D	303	-	-	0/1/1/1	-
2	EDO	C	303	-	-	1/1/1/1	-
4	DGL	B	304	-	-	0/9/9/9	-
2	EDO	B	302	-	-	1/1/1/1	-
5	GLY	C	306	-	-	2/2/2/2	-
2	EDO	D	302	-	-	1/1/1/1	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	LV4	C6-S	-13.43	1.50	1.69
3	B	301	LV4	C6-N1	6.92	1.45	1.32
3	C	301	LV4	C6-S	-6.87	1.59	1.69
3	C	301	LV4	C6-N1	6.80	1.45	1.32
3	B	301	LV4	C6-N	6.49	1.46	1.34
3	D	301	LV4	C6-N1	6.48	1.44	1.32
3	C	302	LV4	C6-N1	6.44	1.44	1.32
3	D	301	LV4	C6-S	-6.34	1.60	1.69
3	C	302	LV4	C6-N	6.15	1.45	1.34
3	C	301	LV4	C6-N	5.92	1.45	1.34
3	D	301	LV4	C6-N	5.83	1.44	1.34
3	B	301	LV4	C4-N	4.19	1.49	1.41
3	C	302	LV4	C6-S	-2.39	1.65	1.69
3	C	302	LV4	C4-N	2.32	1.46	1.41
7	D	307	ALA	OXT-C	-2.25	1.23	1.30
4	B	304	DGL	OXT-C	-2.04	1.23	1.30

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	LV4	S-C6-N1	-4.31	117.26	123.15
3	B	301	LV4	N1-C6-N	3.99	124.74	117.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	304	DGL	OXT-C-O	-3.42	116.33	124.09
7	D	307	ALA	OXT-C-O	-3.29	116.62	124.09
3	C	301	LV4	S-C6-N1	-3.28	118.67	123.15
3	C	301	LV4	N1-C6-N	2.44	121.90	117.43
3	D	301	LV4	N1-C6-N	2.41	121.84	117.43
3	C	302	LV4	S-C6-N1	-2.40	119.88	123.15
3	C	301	LV4	C3-C4-N	2.33	120.83	116.66
3	B	301	LV4	C4-N-C6	-2.31	118.70	126.45
4	B	304	DGL	OXT-C-CA	2.24	121.01	113.38
3	C	301	LV4	C4-N-C6	-2.05	119.54	126.45
3	D	301	LV4	S-C6-N	-2.03	116.70	121.07

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	306	GLY	O-C-CA-N
5	C	306	GLY	OXT-C-CA-N
2	C	305	EDO	O1-C1-C2-O2
2	D	302	EDO	O1-C1-C2-O2
3	B	301	LV4	C2-C3-O-C7
4	D	308	DGL	OXT-C-CA-CB
2	B	302	EDO	O1-C1-C2-O2
4	D	308	DGL	O-C-CA-CB
2	C	304	EDO	O1-C1-C2-O2
4	D	308	DGL	CA-CB-CG-CD
2	C	303	EDO	O1-C1-C2-O2
4	D	308	DGL	N-CA-CB-CG

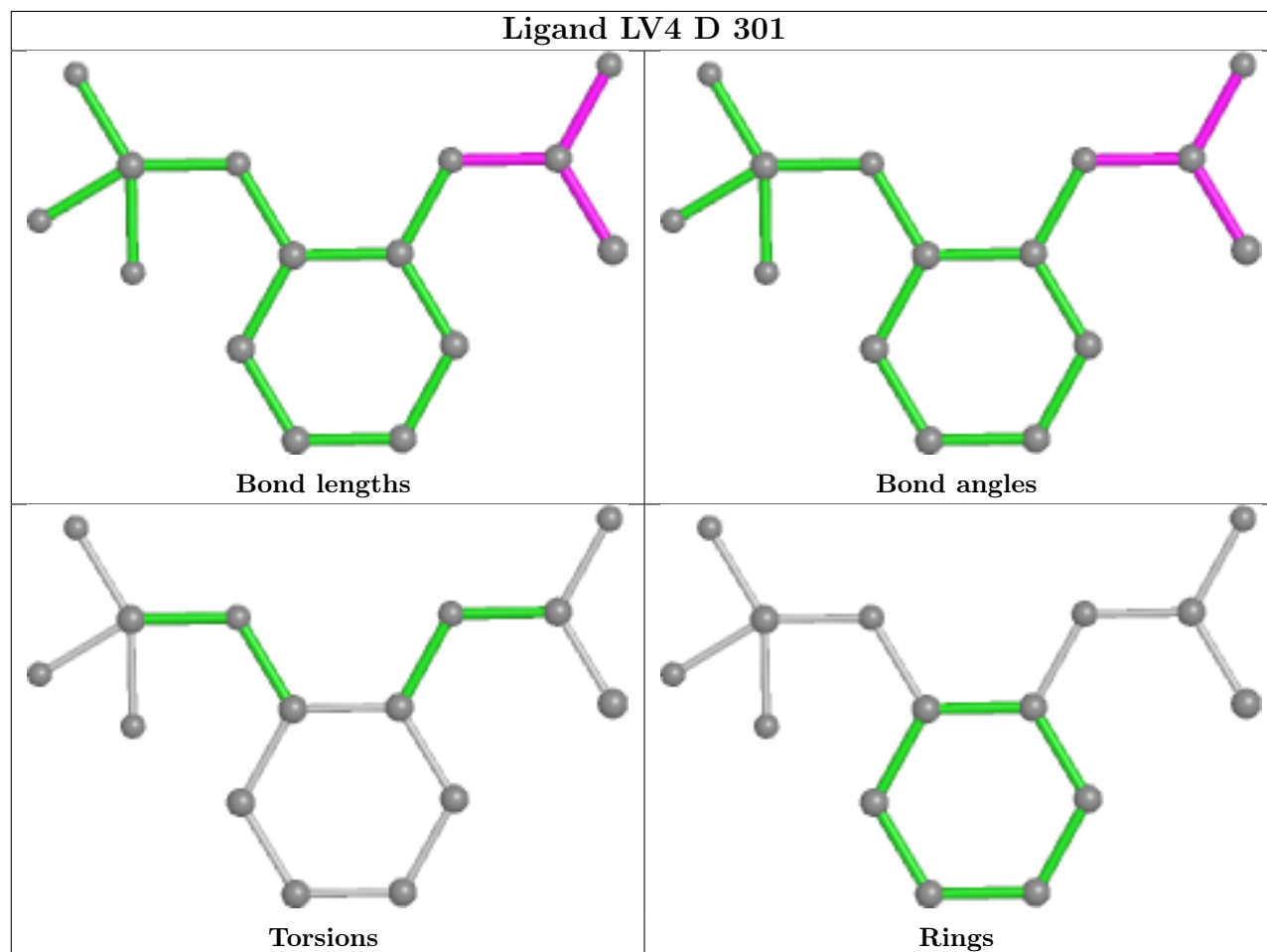
There are no ring outliers.

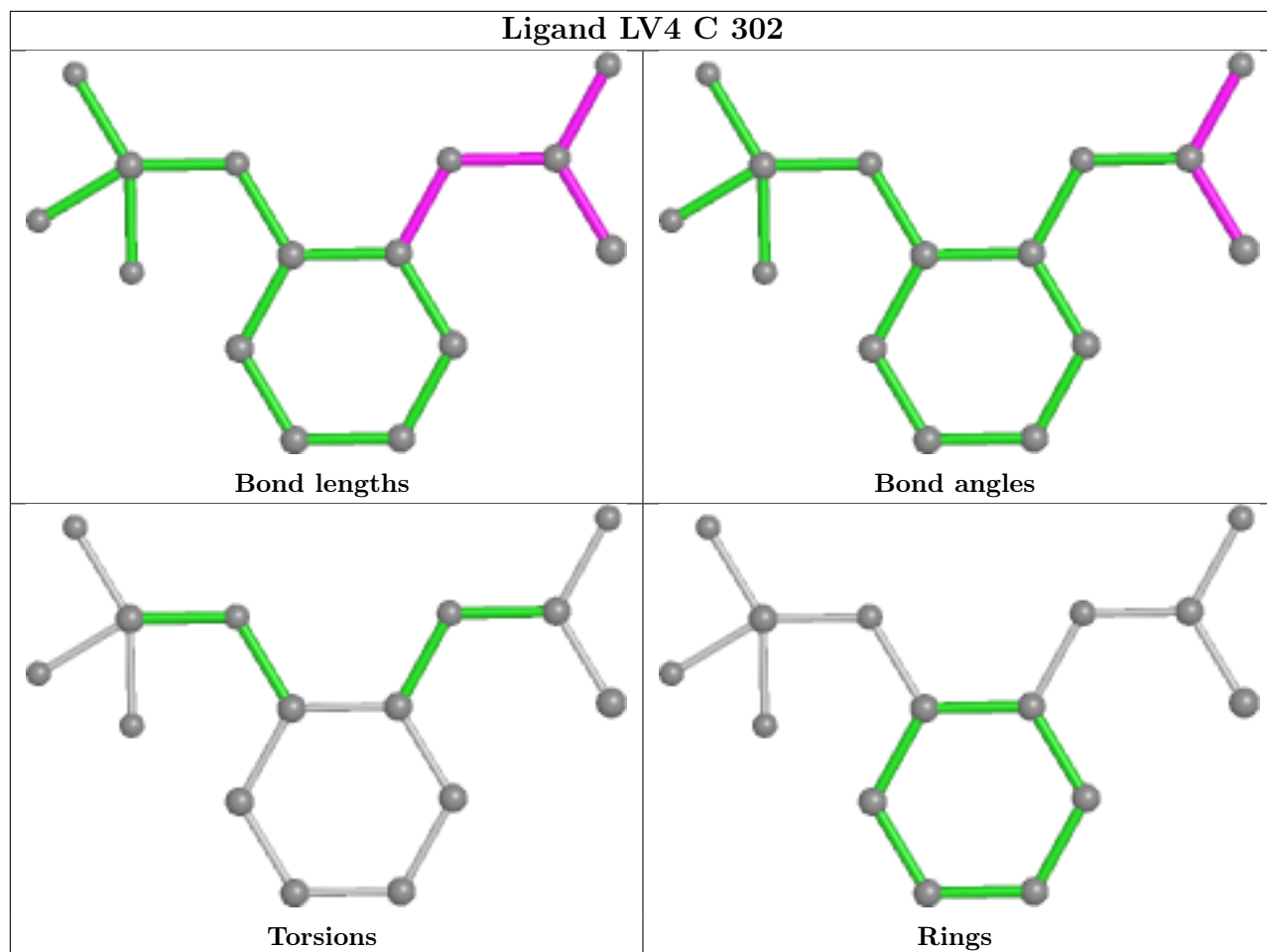
1 monomer is involved in 1 short contact:

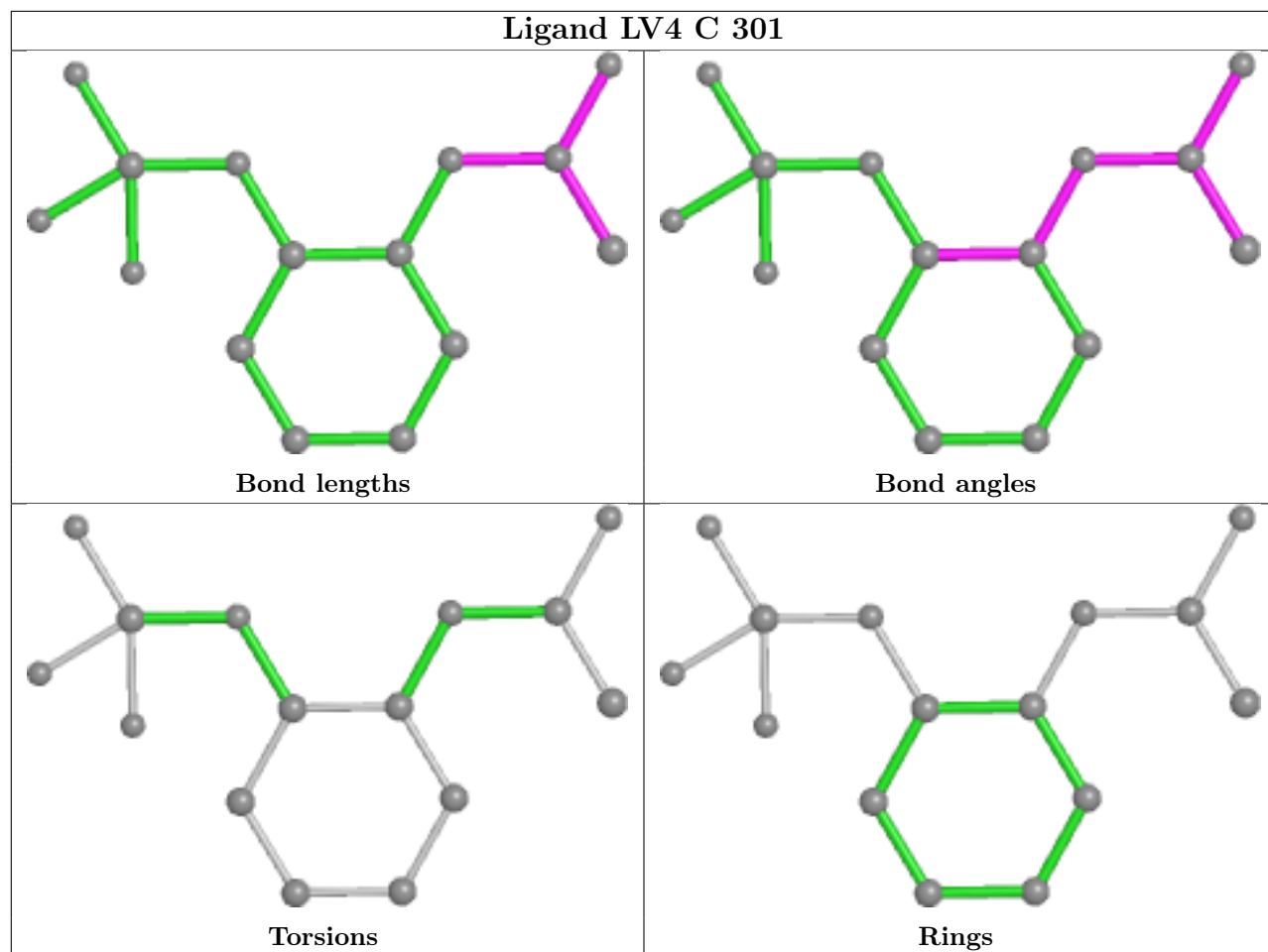
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	304	DGL	1	0

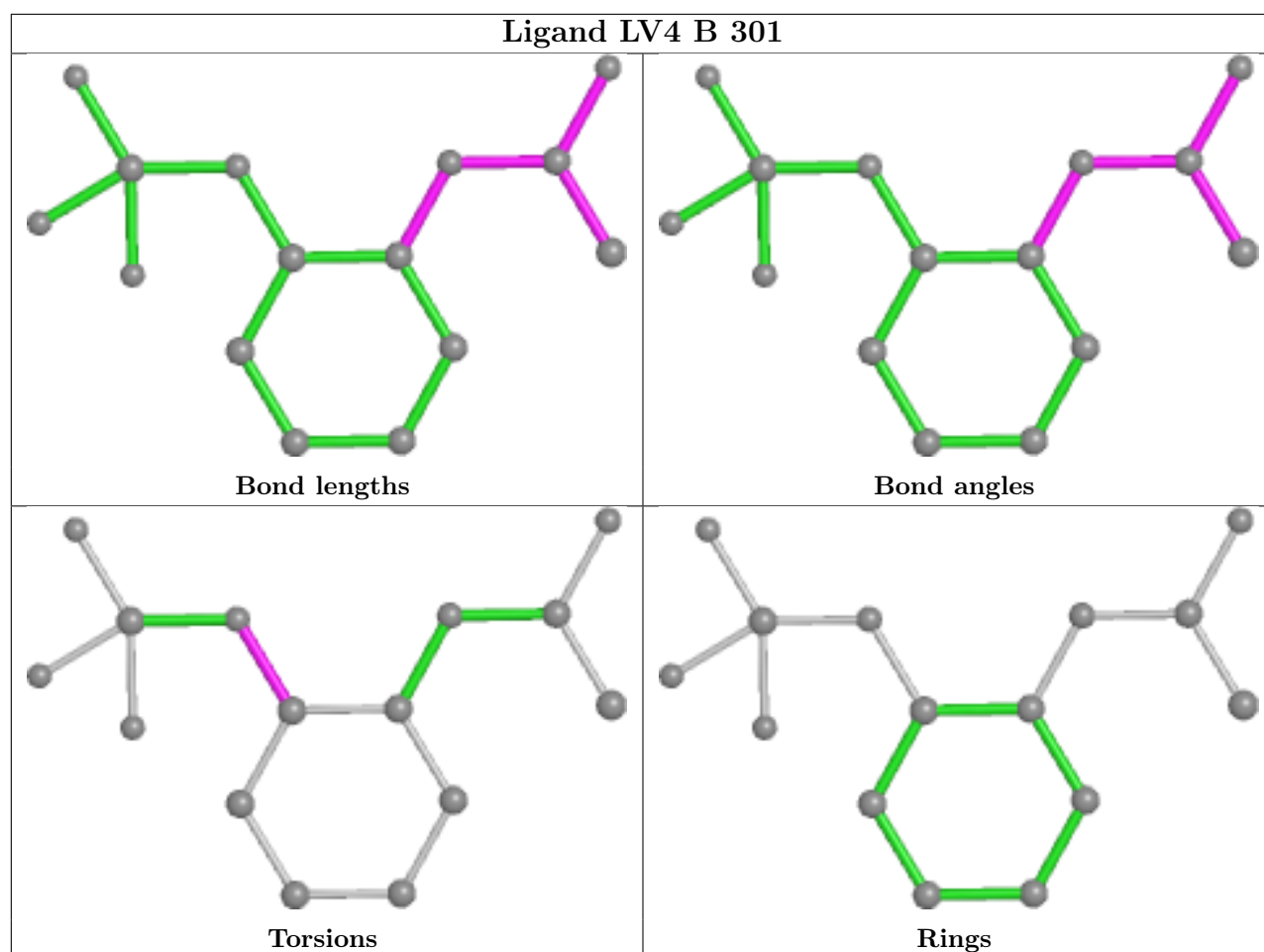
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 [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	191/195 (97%)	0.49	10 (5%) 27 29	35, 54, 86, 119	18 (9%)
1	B	193/195 (98%)	0.32	9 (4%) 31 33	31, 47, 65, 83	5 (2%)
1	C	193/195 (98%)	0.73	21 (10%) 5 5	34, 49, 77, 95	22 (11%)
1	D	191/195 (97%)	0.53	12 (6%) 20 21	31, 46, 67, 120	8 (4%)
All	All	768/780 (98%)	0.52	52 (6%) 17 18	31, 49, 79, 120	53 (6%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	184	GLU	10.0
1	C	112	ILE	9.5
1	C	106	ALA	9.1
1	C	108	ILE	8.2
1	C	111	GLY	7.9
1	C	110	GLN	6.8
1	C	109	LYS	6.0
1	D	182	PHE	6.0
1	D	183	GLY	5.8
1	A	110	GLN	5.7
1	C	180	GLN	5.2
1	B	106	ALA	5.2
1	C	113	ARG	4.7
1	C	181	ALA	4.5
1	A	109	LYS	4.4
1	C	107	GLU	4.2
1	A	182	PHE	4.1
1	B	273[A]	PHE	4.1
1	D	116	ILE	4.1
1	D	185	LYS	4.0
1	C	206	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	182	PHE	3.8
1	C	273[A]	PHE	3.6
1	B	127	LEU	3.4
1	C	295	ILE	3.4
1	D	273[A]	PHE	3.2
1	D	108	ILE	3.1
1	B	125	ILE	3.1
1	B	281	ARG	2.9
1	D	112	ILE	2.9
1	C	183	GLY	2.9
1	D	118	CYS	2.9
1	A	283	ALA	2.8
1	D	260	THR	2.7
1	D	262	GLY	2.7
1	A	282	MET	2.7
1	B	126	GLY	2.7
1	C	209	VAL	2.6
1	C	197[A]	ARG	2.6
1	A	281	ARG	2.6
1	D	110	GLN	2.6
1	C	185	LYS	2.5
1	A	108	ILE	2.4
1	A	273[A]	PHE	2.4
1	B	110	GLN	2.4
1	A	180	GLN	2.3
1	B	109	LYS	2.2
1	B	118	CYS	2.2
1	C	219	THR	2.2
1	C	228	ALA	2.1
1	C	186	ILE	2.0
1	A	264	VAL	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

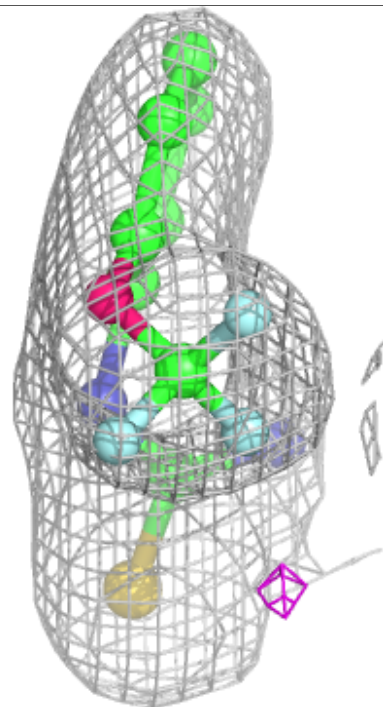
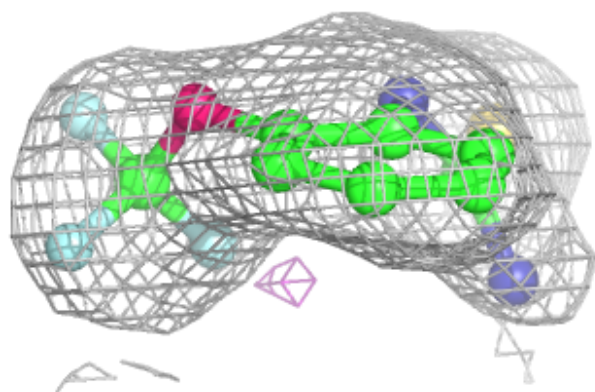
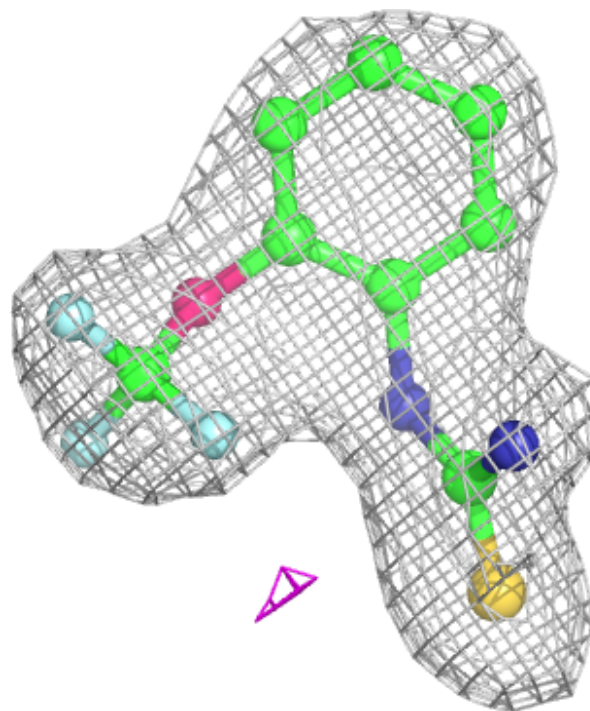
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
6	SO4	D	306	5/5	0.80	0.31	45,49,50,50	5
4	DGL	D	308	10/10	0.84	0.16	43,63,68,74	0
5	GLY	C	306	5/5	0.85	0.17	53,54,63,68	0
7	ALA	D	307	6/6	0.85	0.19	62,72,77,80	0
5	GLY	D	309	5/5	0.86	0.13	60,65,72,73	0
6	SO4	D	305	5/5	0.86	0.54	104,105,106,107	5
2	EDO	D	302	4/4	0.87	0.17	34,35,36,37	0
3	LV4	B	301	15/15	0.88	0.15	52,54,57,57	15
4	DGL	B	304	10/10	0.88	0.23	47,58,64,78	0
2	EDO	C	305	4/4	0.89	0.20	60,61,63,63	0
2	EDO	C	304	4/4	0.89	0.24	53,58,59,61	0
3	LV4	D	301	15/15	0.91	0.14	48,49,50,51	0
2	EDO	B	302	4/4	0.91	0.14	40,42,43,46	0
2	EDO	D	303	4/4	0.92	0.14	48,49,51,51	0
2	EDO	C	303	4/4	0.92	0.16	38,41,43,51	0
2	EDO	B	303	4/4	0.93	0.12	30,34,35,36	0
3	LV4	C	301	15/15	0.93	0.20	48,52,54,55	15
6	SO4	D	304	5/5	0.95	0.25	71,76,88,91	0
2	EDO	A	301	4/4	0.95	0.19	43,43,44,48	0
3	LV4	C	302	15/15	0.96	0.26	56,60,61,61	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.

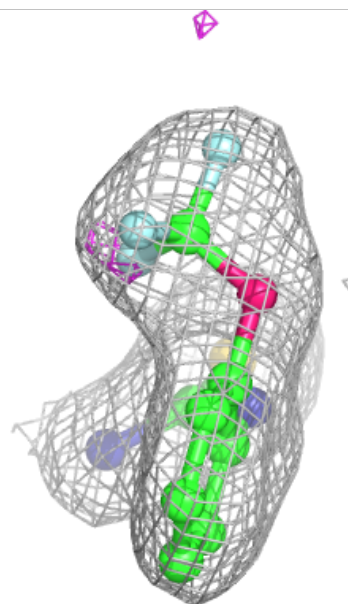
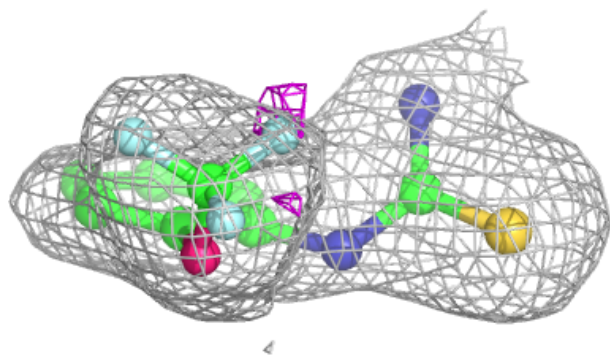
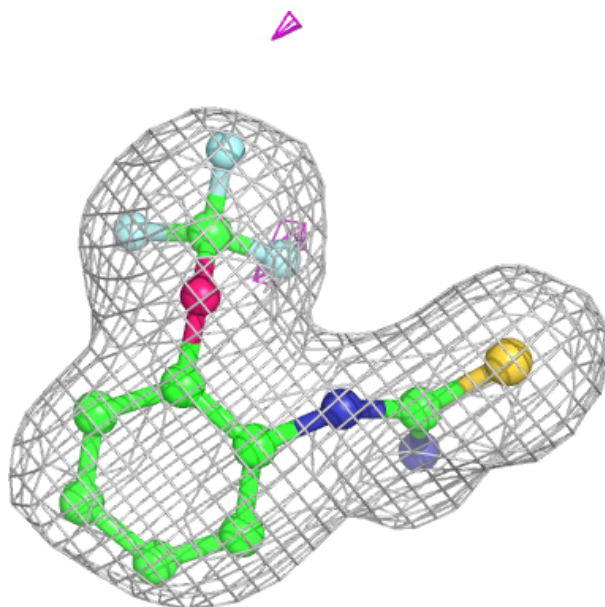
**Electron density around LV4 B 301:**

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



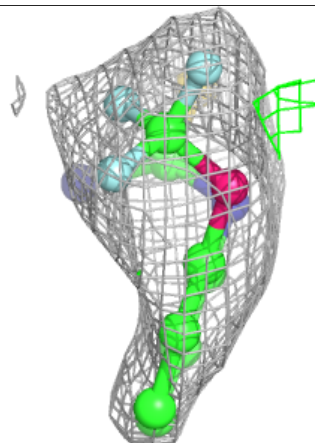
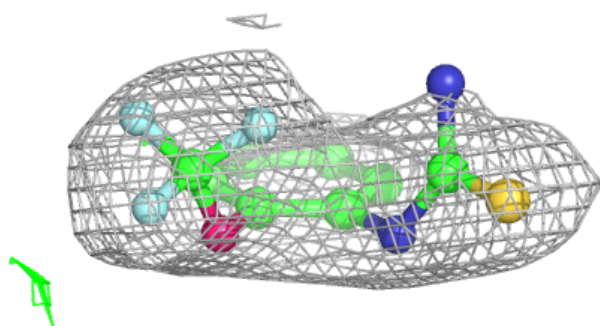
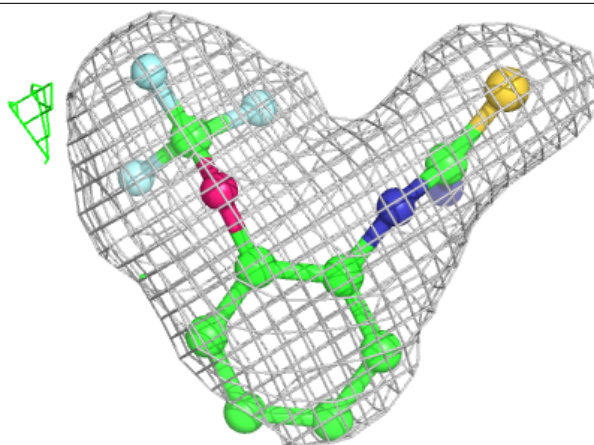
**Electron density around LV4 D 301:**

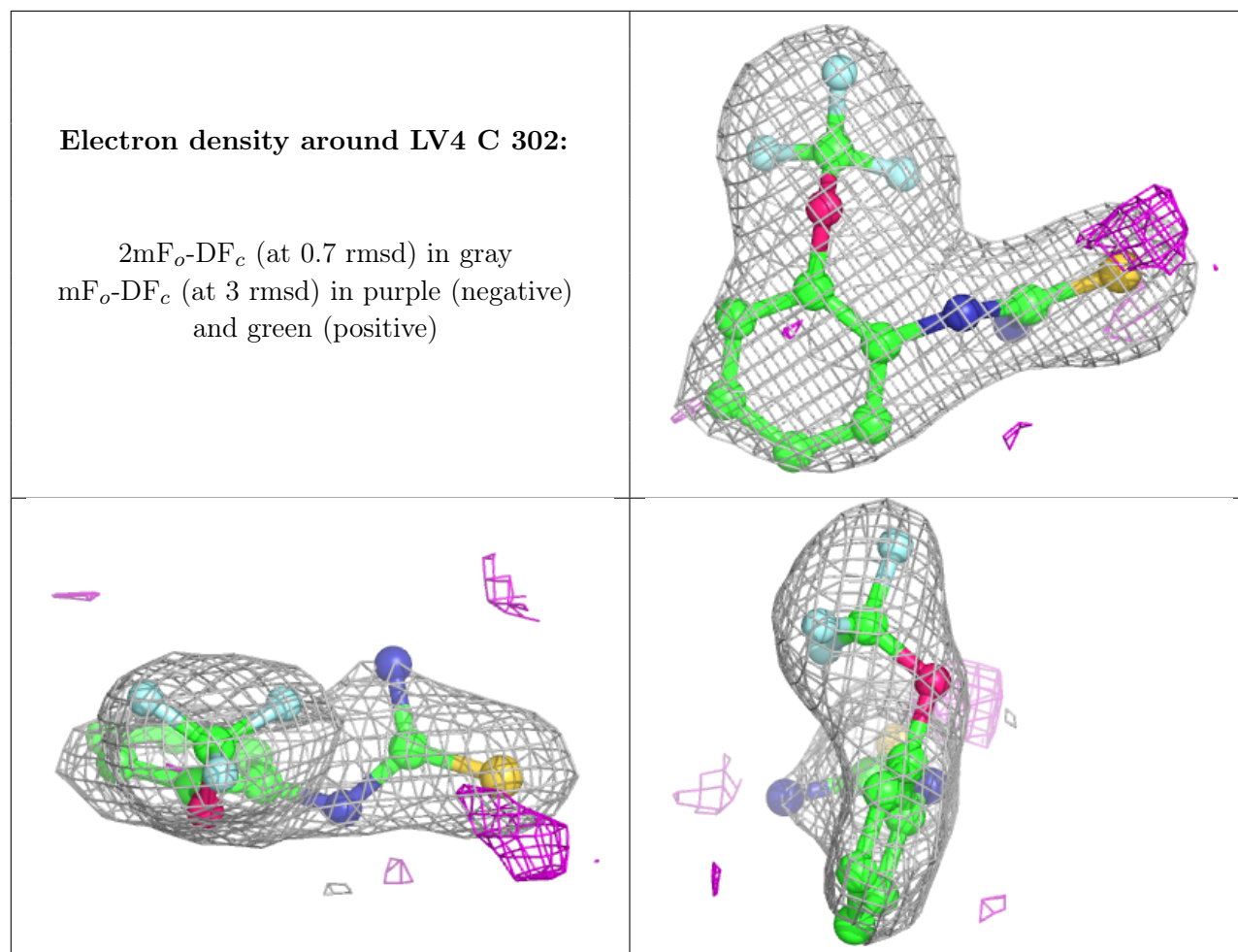
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around LV4 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.