



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 12:46 PM EDT

PDB ID : 7UJ5  
Title : Crystal structure of glutamate racemase from *Helicobacter pylori* in complex with D-glutamate  
Authors : Cooling, G.T.; Spies, M.A.  
Deposited on : 2022-03-30  
Resolution : 1.75 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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

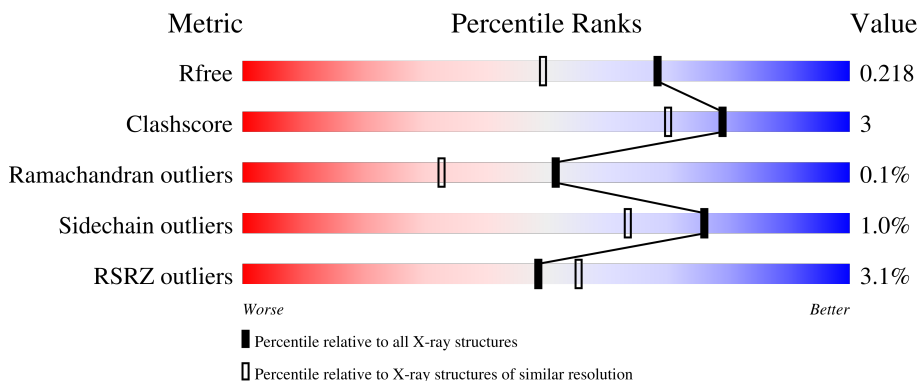
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	257	 2% (red), 91% (green), 8% (yellow)
1	B	257	 3% (red), 91% (green), 8% (yellow)
1	C	257	 4% (red), 96% (green), . (yellow)
1	D	257	 3% (red), 93% (green), 6% (yellow)

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 16807 atoms, of which 7900 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 Glutamate racemase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	256	3909	1285	1950	307	359	8	1	2	0
1	B	256	3934	1289	1964	313	360	8	0	2	0
1	C	256	3930	1291	1960	314	357	8	0	1	0
1	D	256	3939	1291	1967	311	362	8	0	2	0

There are 24 discrepancies between the modelled and reference sequences:

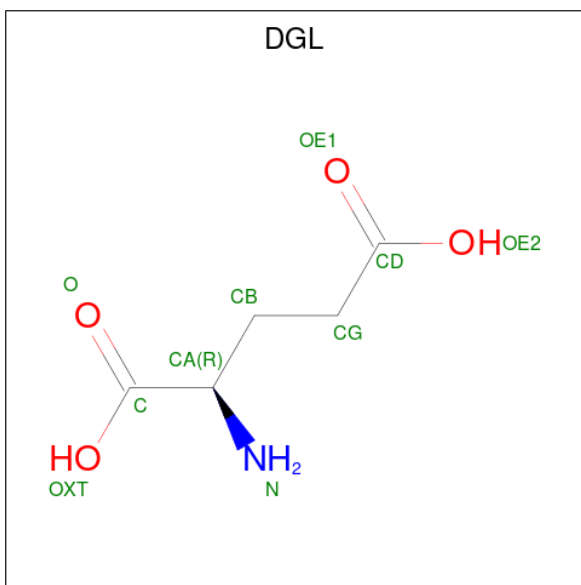
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP K2K6A3
A	0	HIS	-	expression tag	UNP K2K6A3
A	24	ILE	LEU	conflict	UNP K2K6A3
A	27	LYS	GLU	conflict	UNP K2K6A3
A	62	LYS	GLN	conflict	UNP K2K6A3
A	84	HIS	TYR	conflict	UNP K2K6A3
B	-1	SER	-	expression tag	UNP K2K6A3
B	0	HIS	-	expression tag	UNP K2K6A3
B	24	ILE	LEU	conflict	UNP K2K6A3
B	27	LYS	GLU	conflict	UNP K2K6A3
B	62	LYS	GLN	conflict	UNP K2K6A3
B	84	HIS	TYR	conflict	UNP K2K6A3
C	-1	SER	-	expression tag	UNP K2K6A3
C	0	HIS	-	expression tag	UNP K2K6A3
C	24	ILE	LEU	conflict	UNP K2K6A3
C	27	LYS	GLU	conflict	UNP K2K6A3
C	62	LYS	GLN	conflict	UNP K2K6A3
C	84	HIS	TYR	conflict	UNP K2K6A3
D	-1	SER	-	expression tag	UNP K2K6A3
D	0	HIS	-	expression tag	UNP K2K6A3
D	24	ILE	LEU	conflict	UNP K2K6A3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	27	LYS	GLU	conflict	UNP K2K6A3
D	62	LYS	GLN	conflict	UNP K2K6A3
D	84	HIS	TYR	conflict	UNP K2K6A3

- Molecule 2 is D-GLUTAMIC ACID (three-letter code: DGL) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
2	A	1	Total	C	H	N	O	0	0
			17	5	7	1	4		
2	B	1	Total	C	H	N	O	0	0
			17	5	7	1	4		
2	C	1	Total	C	H	N	O	0	0
			17	5	7	1	4		
2	D	1	Total	C	H	N	O	0	0
			17	5	7	1	4		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			13	3	7	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	C	1	Total	C	H	O	0	0
			14	3	8	3		
3	D	1	Total	C	H	O	0	0
			14	3	8	3		

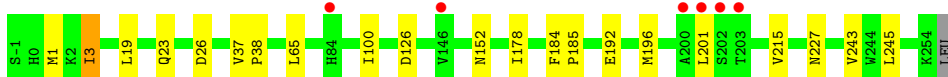
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	228	Total	O	0	0
			228	228		
4	B	253	Total	O	0	0
			253	253		
4	C	243	Total	O	0	0
			243	243		
4	D	248	Total	O	0	0
			248	248		

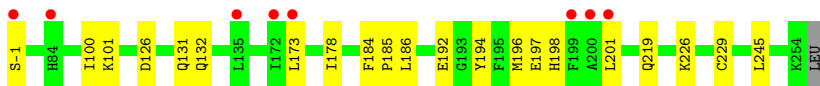
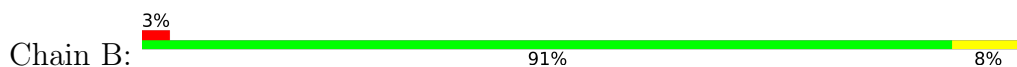
### 3 Residue-property plots [i](#)

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.

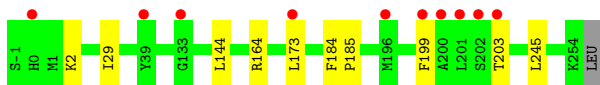
- Molecule 1: Glutamate racemase



- Molecule 1: Glutamate racemase



- Molecule 1: Glutamate racemase



- Molecule 1: Glutamate racemase



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.04Å 86.33Å 107.66Å 90.00° 91.62° 90.00°	Depositor
Resolution (Å)	40.06 – 1.75 40.06 – 1.75	Depositor EDS
% Data completeness (in resolution range)	97.3 (40.06-1.75) 97.3 (40.06-1.75)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 1.75Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.179 , 0.220 0.177 , 0.218	Depositor DCC
$R_{free}$ test set	5544 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.2	Xtrriage
Anisotropy	0.341	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 43.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16807	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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: DGL, GOL

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	0.54	0/2016	0.65	0/2747
1	B	0.55	0/2036	0.67	0/2773
1	C	0.55	0/2025	0.65	0/2753
1	D	0.56	0/2038	0.68	0/2776
All	All	0.55	0/8115	0.66	0/11049

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	1959	1950	1940	14	0
1	B	1970	1964	1946	14	0
1	C	1970	1960	1963	9	0
1	D	1972	1967	1949	10	0
2	A	10	7	7	0	0
2	B	10	7	7	0	0
2	C	10	7	7	0	0
2	D	10	7	7	0	0
3	A	6	7	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	8	8	1	0
3	C	6	8	8	0	0
3	D	6	8	8	1	0
4	A	228	0	0	2	0
4	B	253	0	0	0	0
4	C	243	0	0	0	0
4	D	248	0	0	2	0
All	All	8907	7900	7858	45	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 3.

All (45) 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:B:173:LEU:HD11	1:B:201:LEU:HD21	1.79	0.63
1:A:100:ILE:CD1	1:A:178:ILE:HD11	2.32	0.60
1:D:190:LYS:NZ	4:D:401:HOH:O	2.34	0.60
1:C:2:LYS:CE	1:C:29:ILE:HD11	2.32	0.59
1:A:100:ILE:HD11	1:A:178:ILE:HD11	1.83	0.59
1:C:173:LEU:HB2	1:C:199:PHE:CD2	2.41	0.55
1:D:194:TYR:CZ	3:D:302:GOL:H32	2.41	0.55
1:B:186:LEU:HD23	3:B:302:GOL:H31	1.89	0.55
1:A:3[A]:ILE:HD13	1:A:65:LEU:HD22	1.89	0.54
1:A:100:ILE:HD11	1:A:178:ILE:CD1	2.37	0.54
1:C:2:LYS:HE2	1:C:29:ILE:HD11	1.90	0.54
1:D:229:CYS:HB3	4:D:582:HOH:O	2.08	0.53
1:A:23:GLN:HB2	1:A:227:ASN:HA	1.91	0.52
1:B:100:ILE:HD11	1:B:178:ILE:HD11	1.95	0.49
1:A:196:MET:HA	1:A:201:LEU:HB2	1.95	0.48
1:C:2:LYS:HE3	1:C:29:ILE:HD11	1.96	0.48
1:B:219:GLN:OE1	1:B:226:LYS:HE3	2.14	0.47
1:A:192:GLU:O	1:A:196:MET:HG3	2.14	0.47
1:B:100:ILE:CD1	1:B:178:ILE:HD11	2.44	0.47
1:A:19:LEU:HD23	1:A:215:VAL:HG22	1.96	0.47
1:B:131:GLN:OE1	1:B:132:GLN:NE2	2.48	0.47
1:A:152:ASN:OD1	3:A:302:GOL:H2	2.16	0.45
1:D:184:PHE:N	1:D:185:PRO:CD	2.80	0.45
1:A:243:VAL:HG23	4:A:540:HOH:O	2.16	0.45
1:C:203:THR:O	1:C:203:THR:HG23	2.16	0.45
1:B:101:LYS:HE2	1:B:132:GLN:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:ILE:CD1	1:D:178:ILE:HD11	2.48	0.43
1:D:59:LYS:HB2	1:D:60:PRO:HD3	2.00	0.43
1:A:3[A]:ILE:HD13	1:A:65:LEU:HB3	2.01	0.43
1:D:13:PHE:CZ	1:D:249:ALA:HB2	2.54	0.43
1:C:144:LEU:HD22	1:D:148:LEU:HD12	2.00	0.42
1:C:2:LYS:HE2	1:C:29:ILE:CD1	2.47	0.42
1:B:194:TYR:CE2	1:B:198:HIS:CD2	3.08	0.42
1:C:184:PHE:N	1:C:185:PRO:CD	2.83	0.42
1:B:-1:SER:HA	1:B:229:CYS:SG	2.60	0.41
1:C:164:ARG:HH21	1:D:157:GLU:CD	2.23	0.41
1:A:37:VAL:CG2	1:A:38:PRO:HA	2.49	0.41
1:B:184:PHE:N	1:B:185:PRO:CD	2.83	0.41
1:A:184:PHE:N	1:A:185:PRO:CD	2.84	0.41
1:A:1:MET:HB2	4:A:424:HOH:O	2.20	0.41
1:B:192:GLU:O	1:B:196:MET:HG3	2.21	0.41
1:B:197:GLU:OE1	1:B:198:HIS:CE1	2.74	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	256/257 (100%)	249 (97%)	7 (3%)	0	100	100
1	B	256/257 (100%)	248 (97%)	8 (3%)	0	100	100
1	C	255/257 (99%)	246 (96%)	9 (4%)	0	100	100
1	D	256/257 (100%)	247 (96%)	8 (3%)	1 (0%)	34	17
All	All	1023/1028 (100%)	990 (97%)	32 (3%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	0	HIS

### 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	208/223 (93%)	203 (98%)	5 (2%)	49	26
1	B	211/223 (95%)	209 (99%)	2 (1%)	78	67
1	C	209/223 (94%)	208 (100%)	1 (0%)	88	83
1	D	212/223 (95%)	211 (100%)	1 (0%)	88	83
All	All	840/892 (94%)	831 (99%)	9 (1%)	76	60

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3[A]	ILE
1	A	3[B]	ILE
1	A	26	ASP
1	A	126	ASP
1	A	245	LEU
1	B	126	ASP
1	B	245	LEU
1	C	245	LEU
1	D	202	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	227	ASN
1	D	219	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 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	DGL	C	301	-	8,9,9	1.02	0	10,11,11	0.94	0
3	GOL	C	302	-	5,5,5	1.37	1 (20%)	5,5,5	1.04	0
2	DGL	A	301	-	8,9,9	1.04	0	10,11,11	1.08	0
3	GOL	A	302	-	5,5,5	1.34	1 (20%)	5,5,5	1.26	0
3	GOL	D	302	-	5,5,5	0.69	0	5,5,5	1.01	0
3	GOL	B	302	-	5,5,5	1.16	0	5,5,5	0.93	0
2	DGL	B	301	-	8,9,9	1.12	0	10,11,11	1.16	1 (10%)
2	DGL	D	301	-	8,9,9	1.01	1 (12%)	10,11,11	0.98	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	DGL	C	301	-	-	2/9/9/9	-
3	GOL	C	302	-	-	4/4/4/4	-
2	DGL	A	301	-	-	2/9/9/9	-
3	GOL	A	302	-	-	4/4/4/4	-
3	GOL	D	302	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	302	-	-	4/4/4/4	-
2	DGL	B	301	-	-	3/9/9/9	-
2	DGL	D	301	-	-	2/9/9/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	GOL	C3-C2	2.27	1.61	1.51
3	C	302	GOL	C3-C2	2.19	1.60	1.51
2	D	301	DGL	OXT-C	-2.08	1.23	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	DGL	OXT-C-CA	2.22	120.96	113.38

There are no chirality outliers.

All (21) torsion outliers are listed below:

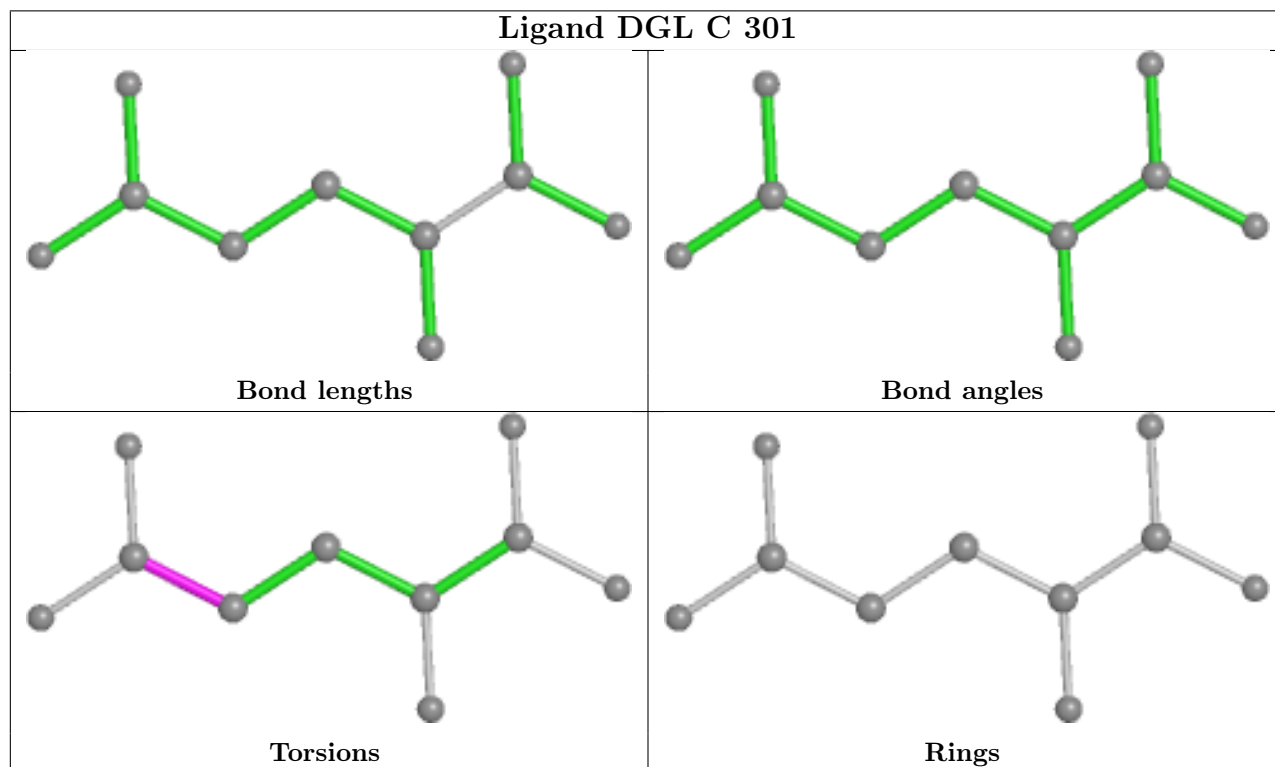
Mol	Chain	Res	Type	Atoms
3	A	302	GOL	O1-C1-C2-O2
3	A	302	GOL	O1-C1-C2-C3
3	A	302	GOL	C1-C2-C3-O3
3	B	302	GOL	C1-C2-C3-O3
3	C	302	GOL	O1-C1-C2-O2
3	C	302	GOL	O1-C1-C2-C3
3	C	302	GOL	C1-C2-C3-O3
3	A	302	GOL	O2-C2-C3-O3
3	C	302	GOL	O2-C2-C3-O3
3	B	302	GOL	O1-C1-C2-O2
3	B	302	GOL	O2-C2-C3-O3
2	C	301	DGL	OE1-CD-CG-CB
2	A	301	DGL	OE2-CD-CG-CB
2	C	301	DGL	OE2-CD-CG-CB
2	D	301	DGL	OE2-CD-CG-CB
2	D	301	DGL	OE1-CD-CG-CB
2	B	301	DGL	OE2-CD-CG-CB
2	B	301	DGL	OE1-CD-CG-CB
2	A	301	DGL	OE1-CD-CG-CB
2	B	301	DGL	CA-CB-CG-CD
3	B	302	GOL	O1-C1-C2-C3

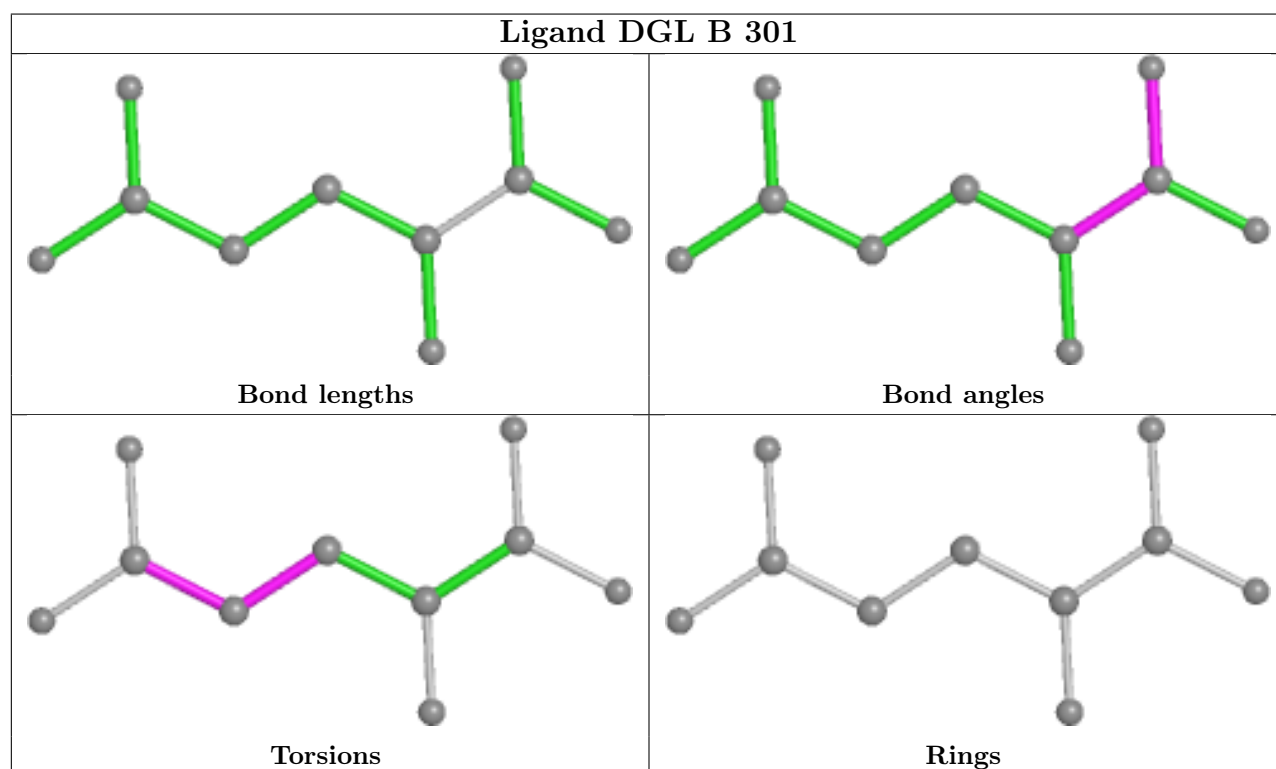
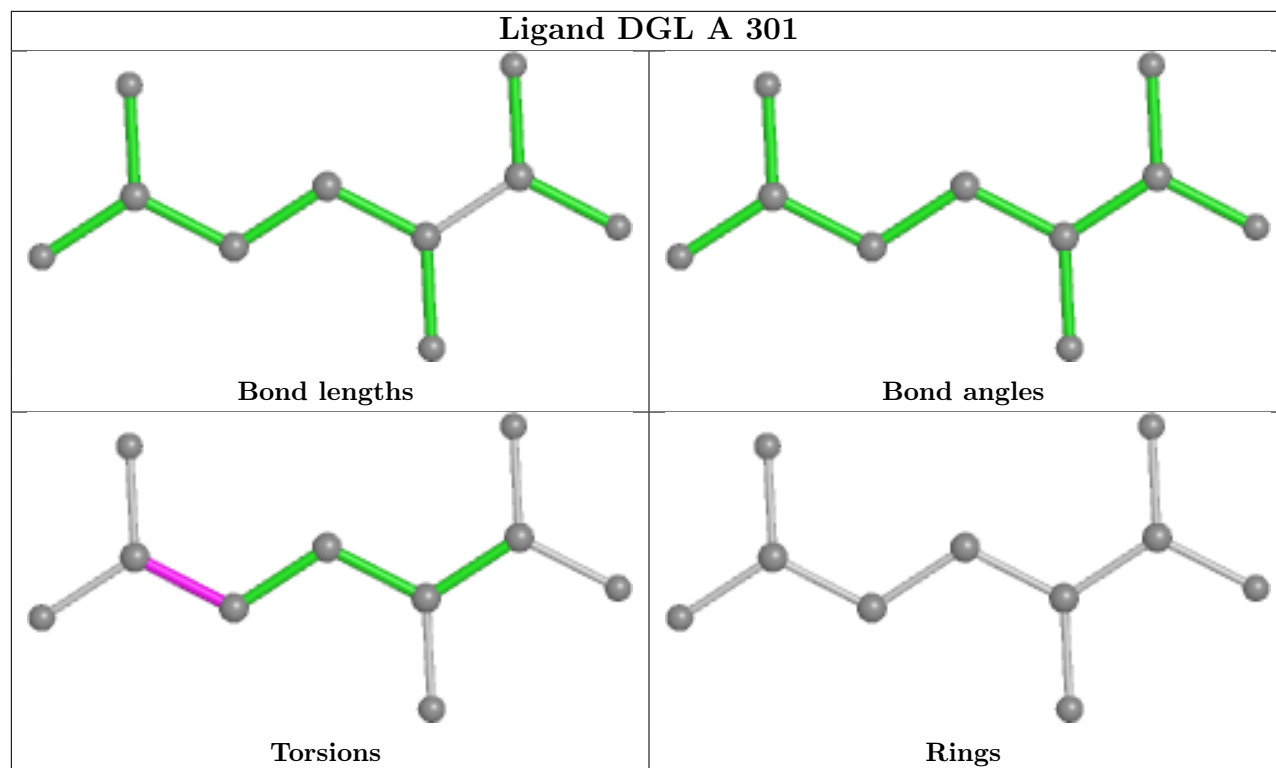
There are no ring outliers.

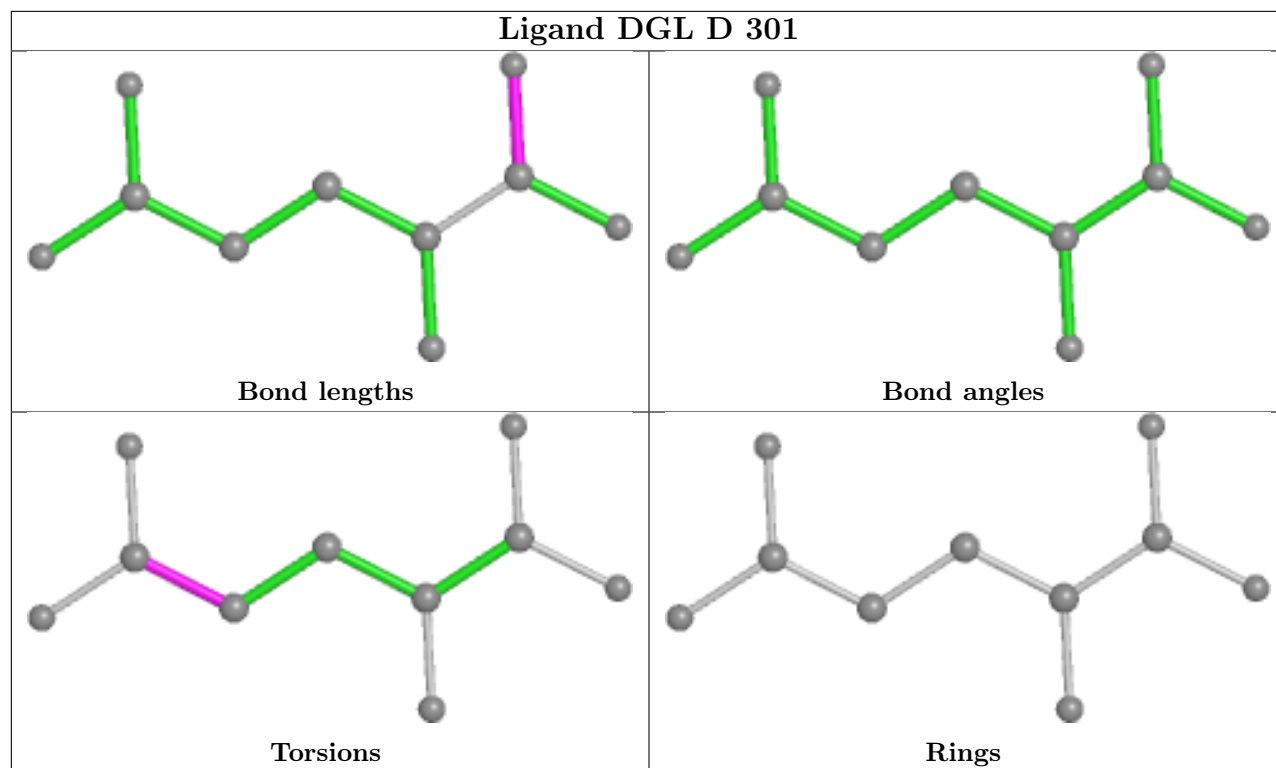
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	GOL	1	0
3	D	302	GOL	1	0
3	B	302	GOL	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	256/257 (99%)	0.14	6 (2%) 60 67	14, 25, 43, 52	0
1	B	256/257 (99%)	0.08	8 (3%) 49 55	14, 23, 43, 56	0
1	C	256/257 (99%)	0.19	10 (3%) 39 45	12, 22, 46, 59	0
1	D	256/257 (99%)	0.09	8 (3%) 49 55	13, 23, 43, 56	0
All	All	1024/1028 (99%)	0.13	32 (3%) 49 55	12, 23, 44, 59	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	200	ALA	6.9
1	C	201	LEU	5.8
1	C	199	PHE	5.4
1	B	199[A]	PHE	4.4
1	C	173	LEU	4.4
1	C	203	THR	4.3
1	A	200	ALA	4.2
1	A	84	HIS	4.1
1	D	-1	SER	4.0
1	D	84	HIS	3.9
1	B	-1	SER	3.8
1	B	172	ILE	3.7
1	C	202	SER	3.7
1	D	173	LEU	3.6
1	A	201	LEU	3.6
1	D	135	LEU	3.4
1	B	200	ALA	3.3
1	B	201	LEU	3.0
1	A	203	THR	2.9
1	C	0	HIS	2.8
1	A	202	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	133	GLY	2.6
1	D	0	HIS	2.6
1	D	199[A]	PHE	2.2
1	B	135	LEU	2.2
1	A	146	VAL	2.1
1	C	196	MET	2.1
1	C	39	TYR	2.0
1	C	133	GLY	2.0
1	B	173	LEU	2.0
1	B	84	HIS	2.0
1	D	85	SER	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](#)

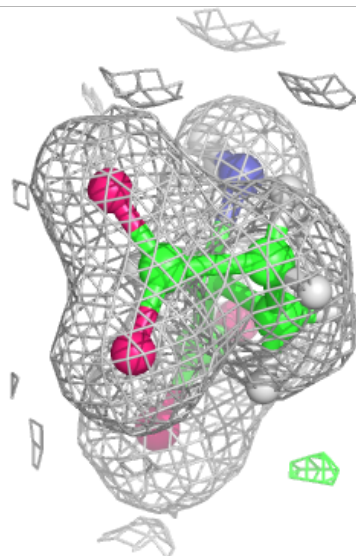
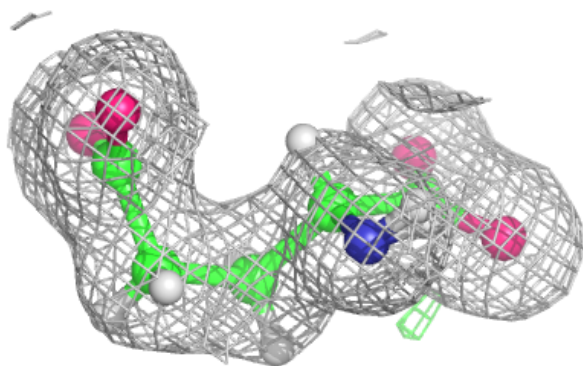
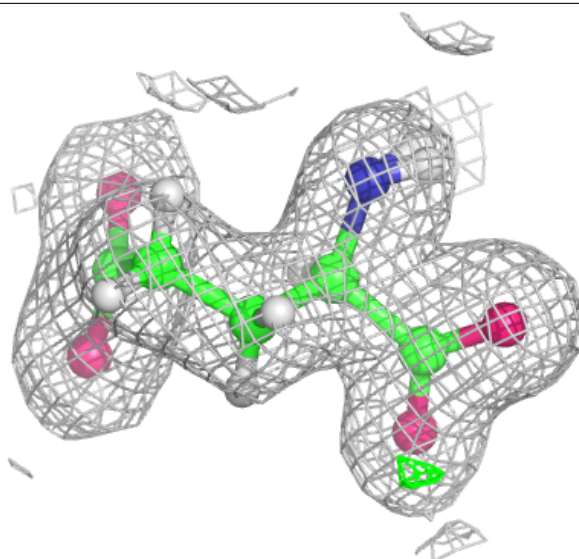
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	GOL	C	302	6/6	0.89	0.20	21,37,55,55	0
3	GOL	B	302	6/6	0.90	0.24	26,43,53,54	0
3	GOL	D	302	6/6	0.90	0.23	41,49,57,69	0
3	GOL	A	302	6/6	0.91	0.12	25,37,45,54	0
2	DGL	A	301	10/10	0.98	0.14	12,16,19,19	0
2	DGL	D	301	10/10	0.98	0.10	11,13,19,19	0
2	DGL	C	301	10/10	0.99	0.15	12,14,18,18	0
2	DGL	B	301	10/10	0.99	0.13	13,15,17,19	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.

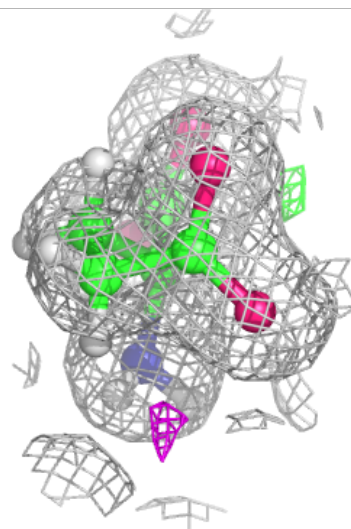
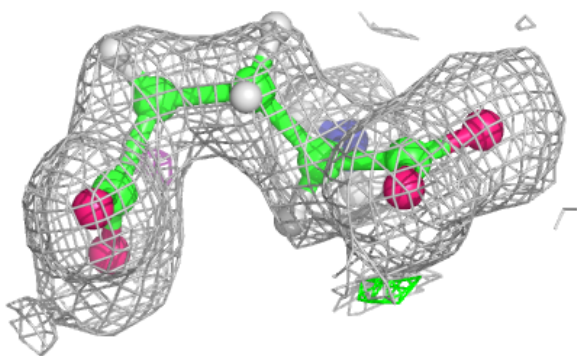
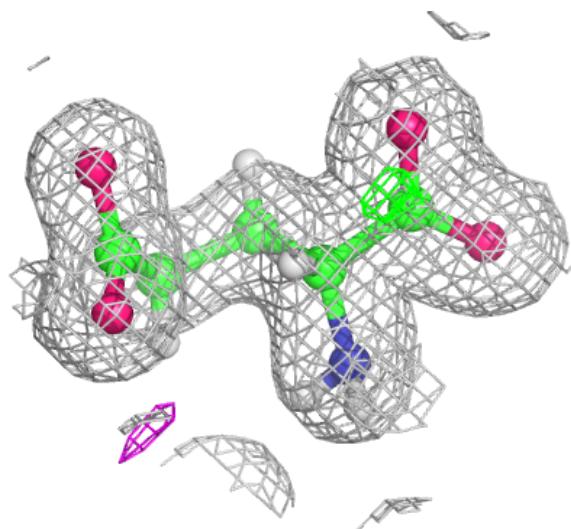
**Electron density around DGL A 301:**

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



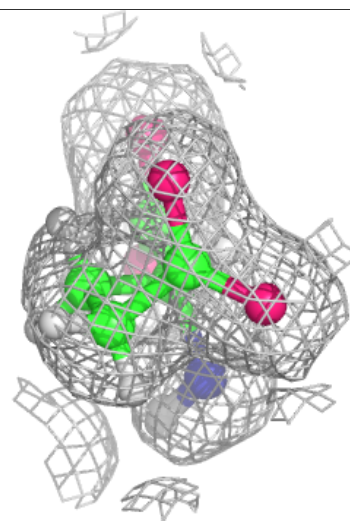
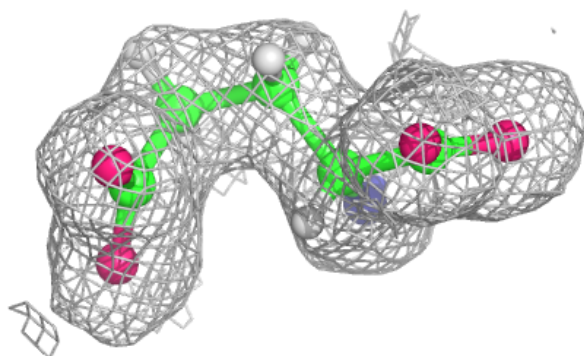
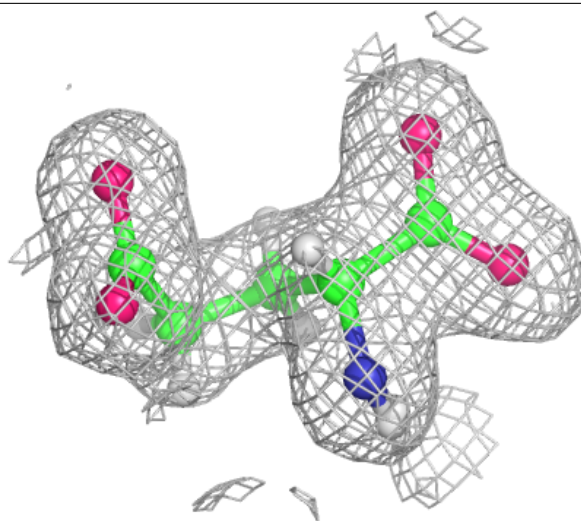
**Electron density around DGL D 301:**

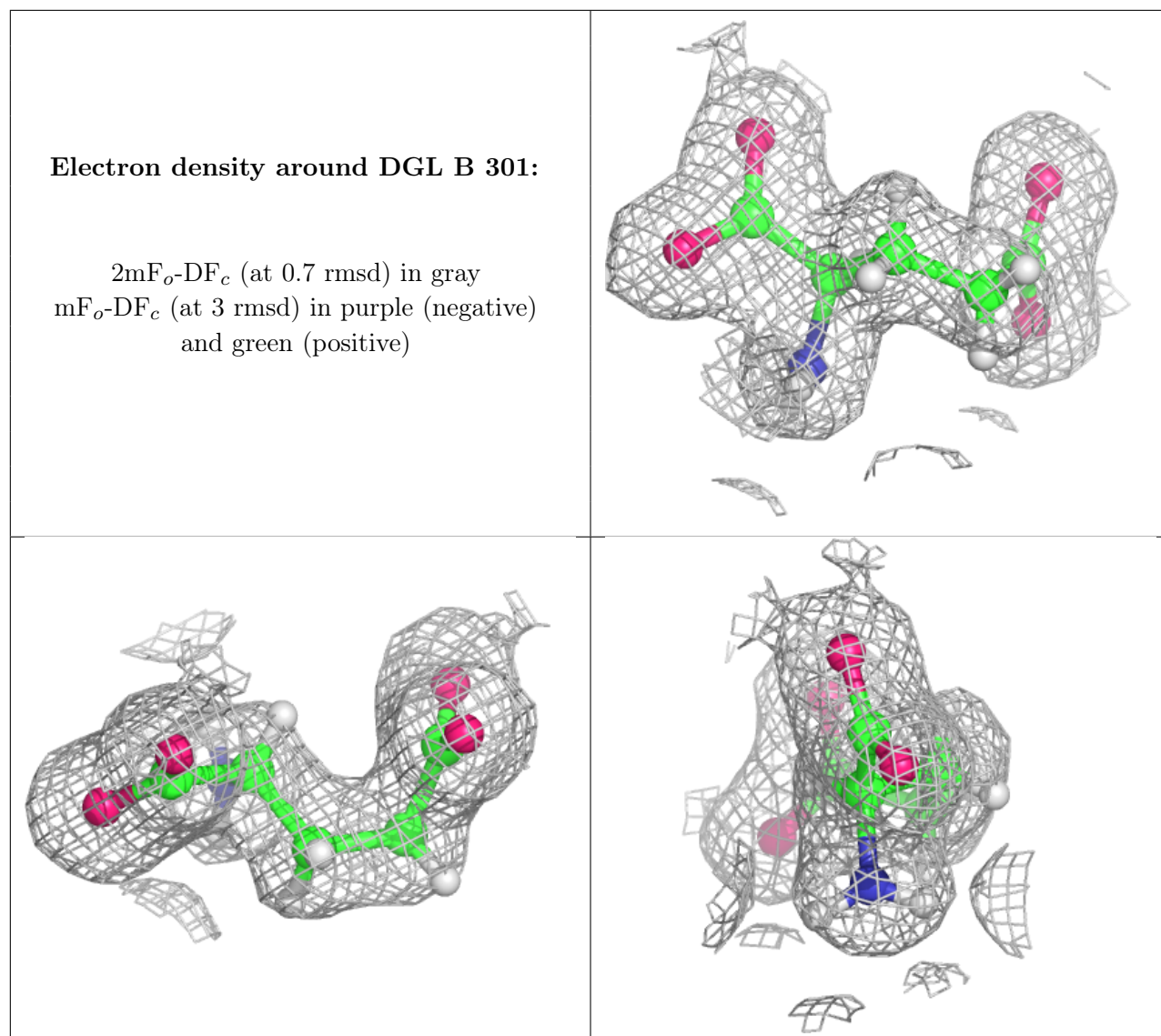
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around DGL 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.