



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2021 – 02:25 PM EDT

PDB ID : 7K2X  
Title : Crystal structure of CTX-M-14 E166A/K234R Beta-lactamase  
Authors : Lu, S.; Palzkill, T.; Sankaran, B.; Hu, L.; Soeung, V.; Prasad, B.V.V.  
Deposited on : 2020-09-09  
Resolution : 1.80 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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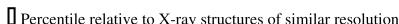
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.20  
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) : 2.20

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## X-RAY DIFFRACTION

A.


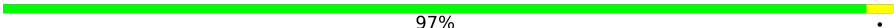
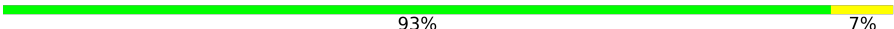


Similar resolution  
(#Entries, resolution range(Å))

Quality of chain

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Mol	Chain	Length	Quality of chain
1	F	260	 91% 8% .
1	G	260	 97% .
1	H	260	 93% 7%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17071 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 Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	1	0	0
			1938	1200	352	380	6			
1	B	260	Total	C	N	O	S	1	0	0
			1938	1200	352	380	6			
1	C	260	Total	C	N	O	S	1	0	0
			1938	1200	352	380	6			
1	D	260	Total	C	N	O	S	2	0	0
			1938	1200	352	380	6			
1	E	259	Total	C	N	O	S	1	0	0
			1934	1198	351	379	6			
1	F	260	Total	C	N	O	S	0	0	0
			1938	1200	352	380	6			
1	G	260	Total	C	N	O	S	1	0	0
			1938	1200	352	380	6			
1	H	260	Total	C	N	O	S	0	0	0
			1938	1200	352	380	6			

There are 16 discrepancies between the modelled and reference sequences:

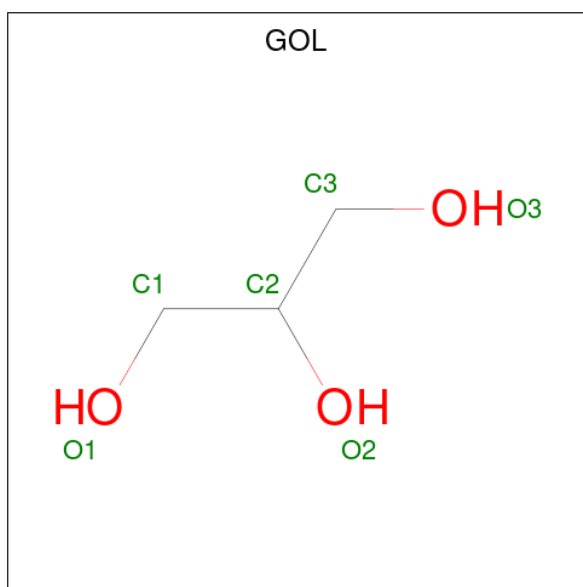
Chain	Residue	Modelled	Actual	Comment	Reference
A	166	ALA	GLU	engineered mutation	UNP A0A2H4FY00
A	240	ASP	GLY	conflict	UNP A0A2H4FY00
B	166	ALA	GLU	engineered mutation	UNP A0A2H4FY00
B	240	ASP	GLY	conflict	UNP A0A2H4FY00
C	166	ALA	GLU	engineered mutation	UNP A0A2H4FY00
C	240	ASP	GLY	conflict	UNP A0A2H4FY00
D	166	ALA	GLU	engineered mutation	UNP A0A2H4FY00
D	240	ASP	GLY	conflict	UNP A0A2H4FY00
E	166	ALA	GLU	engineered mutation	UNP A0A2H4FY00
E	240	ASP	GLY	conflict	UNP A0A2H4FY00
F	166	ALA	GLU	engineered mutation	UNP A0A2H4FY00
F	240	ASP	GLY	conflict	UNP A0A2H4FY00
G	166	ALA	GLU	engineered mutation	UNP A0A2H4FY00

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Chain	Residue	Modelled	Actual	Comment	Reference
G	240	ASP	GLY	conflict	UNP A0A2H4FY00
H	166	ALA	GLU	engineered mutation	UNP A0A2H4FY00
H	240	ASP	GLY	conflict	UNP A0A2H4FY00

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	E	1	Total C O 6 3 3	0	0
2	F	1	Total C O 6 3 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	187	Total O 187 187	0	0
3	B	204	Total O 204 204	0	0
3	C	181	Total O 181 181	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	180	Total 180	O 180	0	0
3	E	188	Total 188	O 188	0	0
3	F	197	Total 197	O 197	0	0
3	G	209	Total 209	O 209	0	0
3	H	201	Total 201	O 201	0	0

### 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: Beta-lactamase

Chain A:  95% 5%



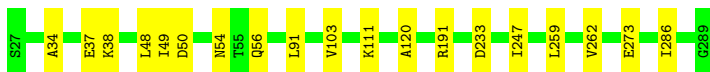
- Molecule 1: Beta-lactamase

Chain B:  94% 6%



- Molecule 1: Beta-lactamase

Chain C:  93% 7%



- Molecule 1: Beta-lactamase

Chain D:  94% 6%




- Molecule 1: Beta-lactamase

Chain E:  92% 8%



- Molecule 1: Beta-lactamase

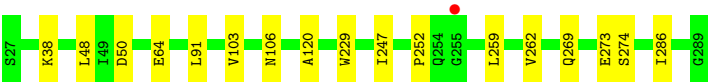
Chain F:  91% 8%



● Molecule 1: Beta-lactamase



● Molecule 1: Beta-lactamase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.37Å 83.37Å 232.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.23 – 1.80 45.23 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.23-1.80) 99.7 (45.23-1.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.16 (at 1.81Å)	Xtriage
Refinement program	PHENIX dev_3386	Depositor
R, $R_{free}$	0.181 , 0.224 0.181 , 0.224	Depositor DCC
$R_{free}$ test set	8348 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.3	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 43.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l 0.487 for h,-h-k,-l 0.032 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	17071	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	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 70.49 % 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 3.0943e-06. 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: 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	0.40	0/1967	0.58	1/2678 (0.0%)
1	B	0.38	0/1967	0.58	0/2678
1	C	0.39	0/1967	0.57	0/2678
1	D	0.39	0/1967	0.57	0/2678
1	E	0.40	0/1963	0.59	0/2673
1	F	0.40	0/1967	0.58	0/2678
1	G	0.39	0/1967	0.57	0/2678
1	H	0.40	0/1967	0.59	1/2678 (0.0%)
All	All	0.39	0/15732	0.58	2/21419 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	38	LYS	CD-CE-NZ	-5.44	99.19	111.70
1	A	98	LYS	CD-CE-NZ	-5.10	99.97	111.70

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	1938	0	1953	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1938	0	1953	9	0
1	C	1938	0	1953	10	0
1	D	1938	0	1953	9	0
1	E	1934	0	1950	15	0
1	F	1938	0	1953	17	0
1	G	1938	0	1953	2	0
1	H	1938	0	1953	8	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
2	E	6	0	8	0	0
2	F	6	0	8	0	0
3	A	187	0	0	2	1
3	B	204	0	0	1	1
3	C	181	0	0	1	1
3	D	180	0	0	0	1
3	E	188	0	0	3	0
3	F	197	0	0	4	4
3	G	209	0	0	0	3
3	H	201	0	0	0	3
All	All	17071	0	15653	75	7

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 2.

All (75) 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:35:ALA:HA	1:B:38:LYS:HE2	1.57	0.86
1:C:273:GLU:OE1	3:C:301:HOH:O	1.96	0.83
1:B:28:ALA:HA	1:B:31:GLN:HB2	1.63	0.81
1:F:89:GLN:NE2	3:F:401:HOH:O	2.07	0.73
1:C:54:ASN:OD1	1:C:191:ARG:NH1	2.21	0.70
1:E:204:ARG:HG2	1:E:204:ARG:HH11	1.58	0.67
1:C:34:ALA:O	1:C:38:LYS:HG2	1.95	0.66
1:E:54:ASN:OD1	1:E:191:ARG:NH2	2.27	0.61
1:B:35:ALA:HA	1:B:38:LYS:CE	2.30	0.61
1:D:50:ASP:HA	1:D:259:LEU:HD23	1.81	0.61
1:A:31:GLN:O	1:A:31:GLN:NE2	2.33	0.60
1:F:256:ARG:NH1	1:F:257:ALA:O	2.34	0.60
1:E:201:GLU:OE2	1:E:204:ARG:NH2	2.36	0.58
1:A:34:ALA:O	1:A:38:LYS:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:247:ILE:HG22	1:F:262:VAL:HG13	1.88	0.56
1:B:34:ALA:O	1:B:38:LYS:HG3	2.06	0.55
1:F:204:ARG:NH1	3:F:407:HOH:O	2.39	0.55
1:E:222:ARG:NH1	3:E:404:HOH:O	2.39	0.55
1:B:273:GLU:H	1:B:273:GLU:CD	2.10	0.55
1:F:201:GLU:OE2	1:F:204:ARG:NH2	2.41	0.54
1:D:48:LEU:HD22	1:D:286:ILE:HG23	1.90	0.54
1:D:34:ALA:O	1:D:38:LYS:HG2	2.09	0.52
1:C:50:ASP:HA	1:C:259:LEU:HD23	1.91	0.52
1:A:32:LYS:NZ	3:A:404:HOH:O	2.40	0.52
1:F:237:SER:HB2	3:F:502:HOH:O	2.09	0.51
1:F:37:GLU:OE1	1:F:38:LYS:NZ	2.37	0.51
1:H:50:ASP:HA	1:H:259:LEU:HD23	1.93	0.51
1:D:91:LEU:HB3	1:D:120:ALA:HB2	1.94	0.50
1:C:91:LEU:HB3	1:C:120:ALA:HB2	1.94	0.50
1:D:37:GLU:OE1	1:D:38:LYS:NZ	2.41	0.50
1:C:247:ILE:HG22	1:C:262:VAL:HG13	1.94	0.49
1:B:64:GLU:HG2	1:C:111:LYS:HD3	1.95	0.49
1:G:229:TRP:CE2	1:G:252:PRO:HB3	2.47	0.49
1:F:50:ASP:CG	1:F:256:ARG:HH22	2.16	0.49
1:E:208:VAL:HG12	1:E:212:LYS:HD2	1.94	0.49
1:F:256:ARG:HH11	1:F:256:ARG:HG3	1.77	0.48
1:A:73:LYS:HE3	1:A:135:MET:HB2	1.96	0.48
1:E:34:ALA:O	1:E:38:LYS:HG2	2.13	0.48
1:E:204:ARG:HG2	1:E:204:ARG:NH1	2.26	0.48
1:E:48:LEU:HD22	1:E:286:ILE:HG23	1.95	0.48
1:B:70:SER:OG	1:B:73:LYS:NZ	2.34	0.47
1:H:91:LEU:HB3	1:H:120:ALA:HB2	1.97	0.47
1:F:37:GLU:HB3	1:F:38:LYS:NZ	2.30	0.46
1:F:252:PRO:HB2	1:F:256:ARG:HG2	1.97	0.46
1:B:137:LYS:NZ	3:B:401:HOH:O	2.32	0.46
1:H:273:GLU:CD	1:H:274:SER:H	2.18	0.46
1:A:284:ARG:O	1:A:288:GLU:HG2	2.17	0.45
1:E:48:LEU:O	1:E:56:GLN:HA	2.16	0.45
1:C:48:LEU:HD22	1:C:286:ILE:HG23	1.98	0.45
1:H:269:GLN:OE1	1:H:269:GLN:N	2.48	0.45
1:F:50:ASP:OD2	1:F:256:ARG:NH2	2.50	0.45
1:F:88:LYS:NZ	3:F:408:HOH:O	2.45	0.45
1:F:48:LEU:HD22	1:F:286:ILE:HG23	1.98	0.44
1:E:252:PRO:HB2	1:E:256:ARG:HG2	1.99	0.44
1:B:229:TRP:CE2	1:B:252:PRO:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:91:LEU:HB3	1:F:120:ALA:HB2	2.00	0.44
1:E:91:LEU:HB3	1:E:120:ALA:HB2	1.99	0.44
1:E:256:ARG:NH1	1:E:257:ALA:O	2.51	0.44
1:D:256:ARG:HH11	1:D:256:ARG:HG3	1.83	0.43
1:E:111:LYS:HD3	1:H:64:GLU:HG2	2.00	0.43
1:F:68:MET:HG2	1:F:181:THR:HG22	2.01	0.43
1:D:247:ILE:HG22	1:D:262:VAL:HG13	2.01	0.43
1:C:37:GLU:HB3	1:C:38:LYS:NZ	2.34	0.43
1:H:48:LEU:HD22	1:H:286:ILE:HG23	2.00	0.42
1:H:247:ILE:HG22	1:H:262:VAL:HG22	2.01	0.42
1:D:273:GLU:OE1	1:D:273:GLU:HA	2.19	0.42
1:F:54:ASN:OD1	1:F:191:ARG:NH2	2.45	0.42
1:A:48:LEU:HD22	1:A:286:ILE:HG23	2.01	0.42
1:H:229:TRP:CE2	1:H:252:PRO:HB3	2.54	0.42
1:D:48:LEU:O	1:D:56:GLN:HA	2.19	0.41
1:E:87:GLN:OE1	3:E:401:HOH:O	2.22	0.41
1:C:49:ILE:HG12	1:C:56:GLN:HG2	2.01	0.41
1:G:68:MET:HG2	1:G:181:THR:HG22	2.02	0.41
1:E:204:ARG:NH1	3:E:411:HOH:O	2.54	0.41
1:A:237:SER:HB2	3:A:521:HOH:O	2.22	0.40

All (7) 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:403:HOH:O	3:F:566:HOH:O[2_554]	1.95	0.25
3:G:354:HOH:O	3:H:459:HOH:O[1_665]	2.10	0.10
3:F:500:HOH:O	3:H:337:HOH:O[1_665]	2.15	0.05
3:A:404:HOH:O	3:H:403:HOH:O[2_564]	2.16	0.04
3:F:562:HOH:O	3:G:487:HOH:O[1_655]	2.16	0.04
3:C:401:HOH:O	3:D:476:HOH:O[1_665]	2.19	0.01
3:F:533:HOH:O	3:G:478:HOH:O[1_655]	2.19	0.01

## 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	258/260 (99%)	253 (98%)	4 (2%)	1 (0%)	34	21
1	B	258/260 (99%)	254 (98%)	3 (1%)	1 (0%)	34	21
1	C	258/260 (99%)	253 (98%)	4 (2%)	1 (0%)	34	21
1	D	258/260 (99%)	253 (98%)	4 (2%)	1 (0%)	34	21
1	E	257/260 (99%)	253 (98%)	3 (1%)	1 (0%)	34	21
1	F	258/260 (99%)	254 (98%)	3 (1%)	1 (0%)	34	21
1	G	258/260 (99%)	254 (98%)	3 (1%)	1 (0%)	34	21
1	H	258/260 (99%)	253 (98%)	4 (2%)	1 (0%)	34	21
All	All	2063/2080 (99%)	2027 (98%)	28 (1%)	8 (0%)	34	21

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	VAL
1	B	103	VAL
1	C	103	VAL
1	D	103	VAL
1	G	103	VAL
1	H	103	VAL
1	E	103	VAL
1	F	103	VAL

### 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	202/202 (100%)	201 (100%)	1 (0%)	88	87
1	B	202/202 (100%)	200 (99%)	2 (1%)	76	71
1	C	202/202 (100%)	201 (100%)	1 (0%)	88	87
1	D	202/202 (100%)	202 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	202/202 (100%)	201 (100%)	1 (0%)	88	87
1	F	202/202 (100%)	198 (98%)	4 (2%)	55	44
1	G	202/202 (100%)	200 (99%)	2 (1%)	76	71
1	H	202/202 (100%)	201 (100%)	1 (0%)	88	87
All	All	1616/1616 (100%)	1604 (99%)	12 (1%)	84	81

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	B	106	ASN
1	B	256	ARG
1	C	233	ASP
1	E	233	ASP
1	F	106	ASN
1	F	191	ARG
1	F	233	ASP
1	F	256	ARG
1	G	106	ASN
1	G	233	ASP
1	H	106	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	192	GLN
1	C	89	GLN
1	C	92	ASN
1	D	271	ASN
1	E	31	GLN
1	E	87	GLN
1	F	192	GLN
1	G	92	ASN
1	G	254	GLN
1	H	89	GLN
1	H	192	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](#)

4 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	GOL	A	301	-	5,5,5	0.77	0	5,5,5	0.97	0
2	GOL	F	301	-	5,5,5	0.83	0	5,5,5	1.05	1 (20%)
2	GOL	B	301	-	5,5,5	0.62	0	5,5,5	1.00	0
2	GOL	E	301	-	5,5,5	0.78	0	5,5,5	0.99	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	GOL	A	301	-	-	0/4/4/4	-
2	GOL	F	301	-	-	0/4/4/4	-
2	GOL	B	301	-	-	0/4/4/4	-
2	GOL	E	301	-	-	0/4/4/4	-

There are no bond length outliers.



All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	GOL	C3-C2-C1	-2.03	103.83	111.70

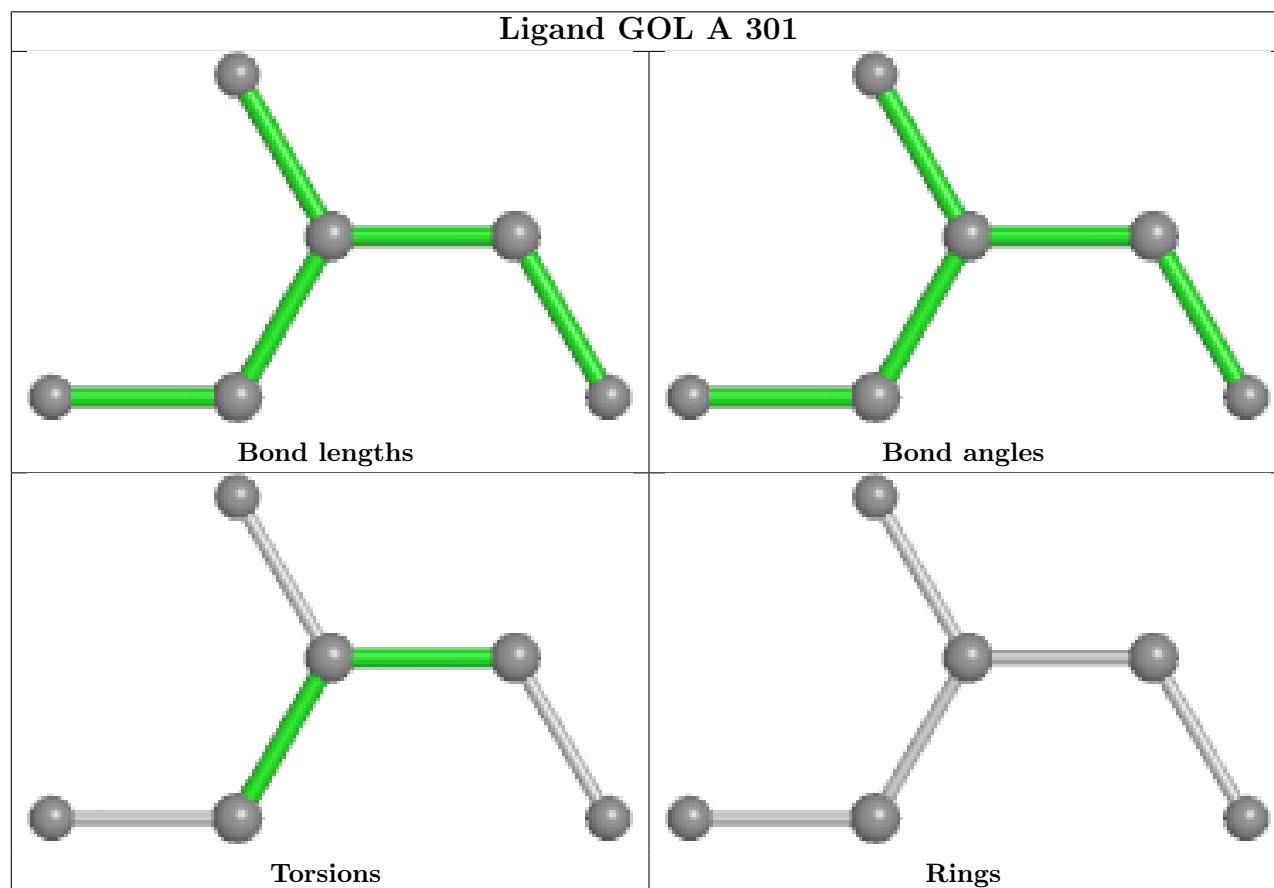
There are no chirality outliers.

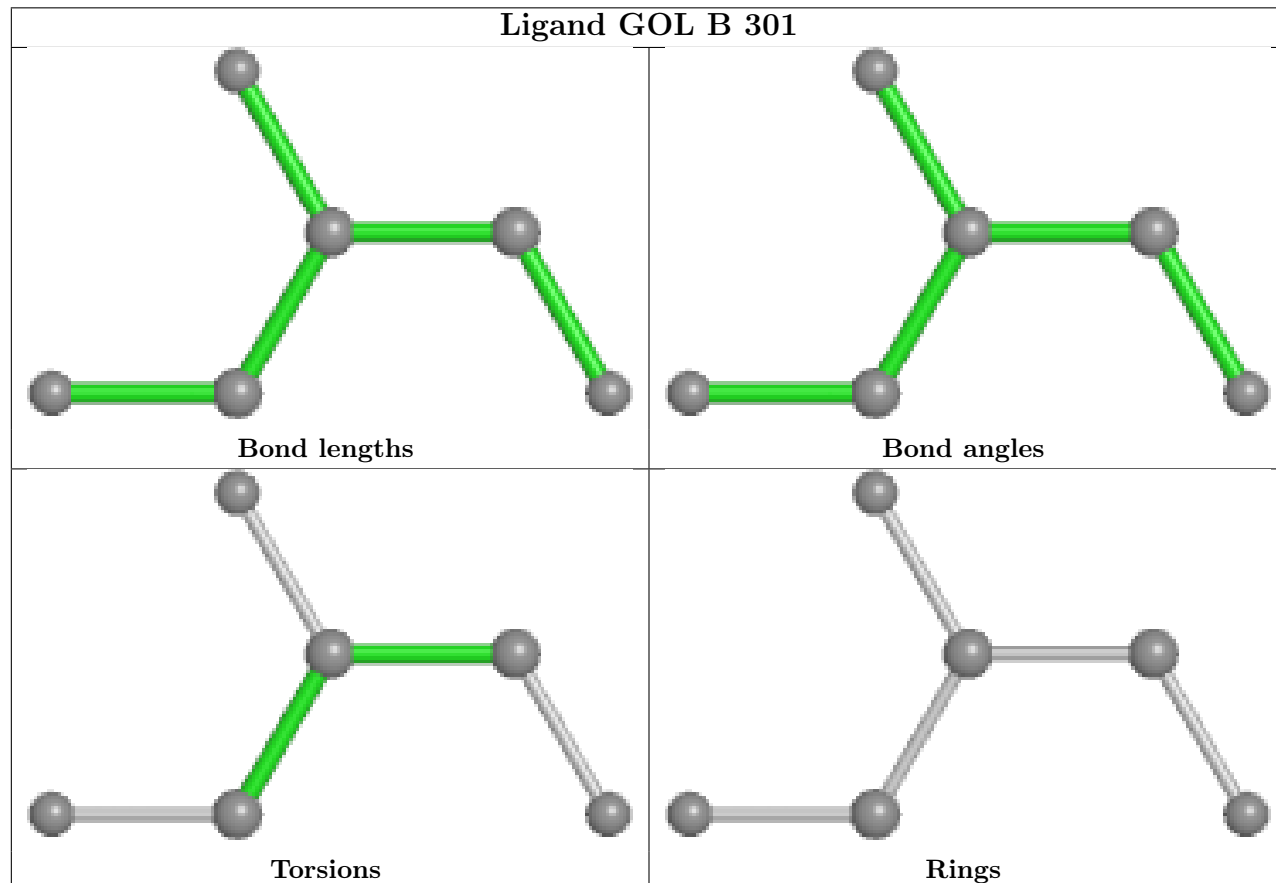
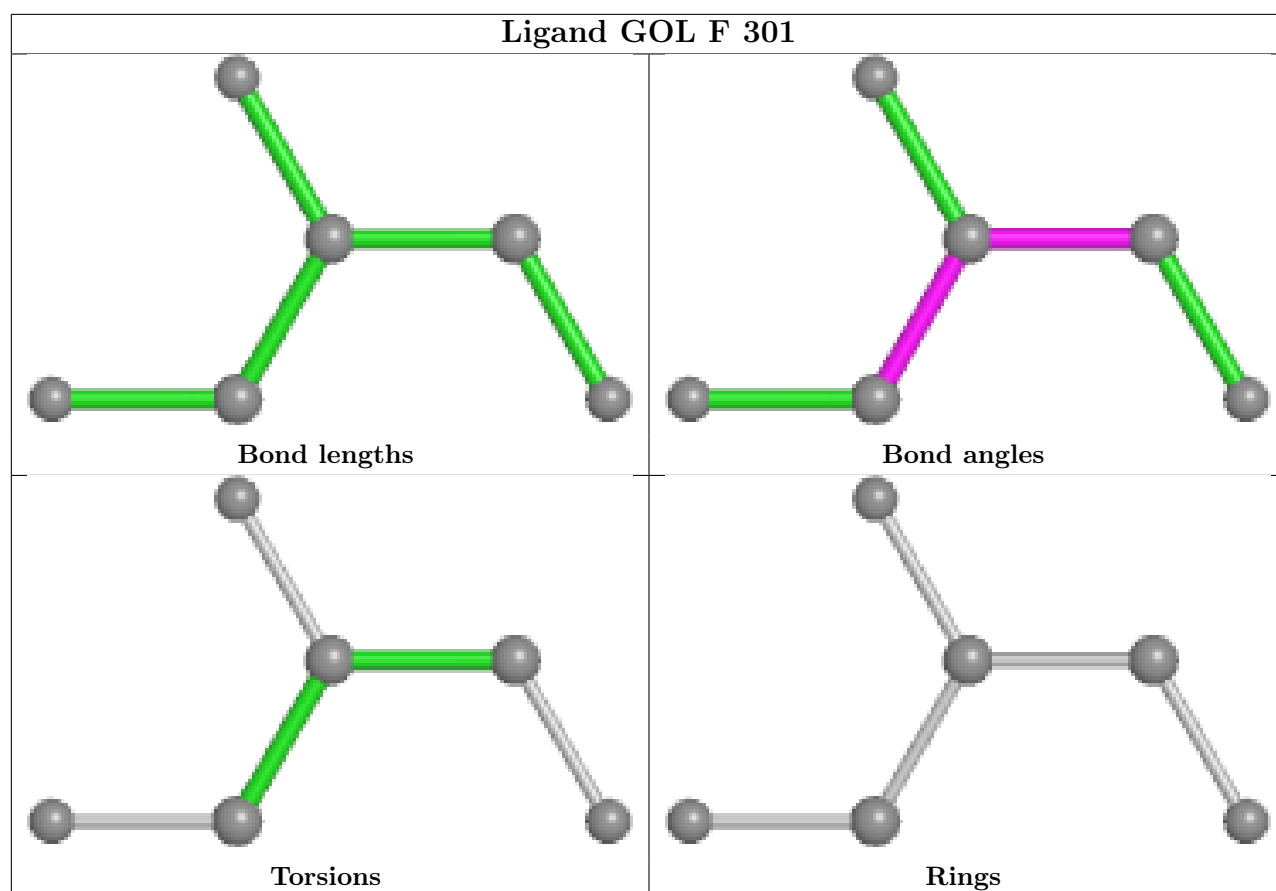
There are no torsion outliers.

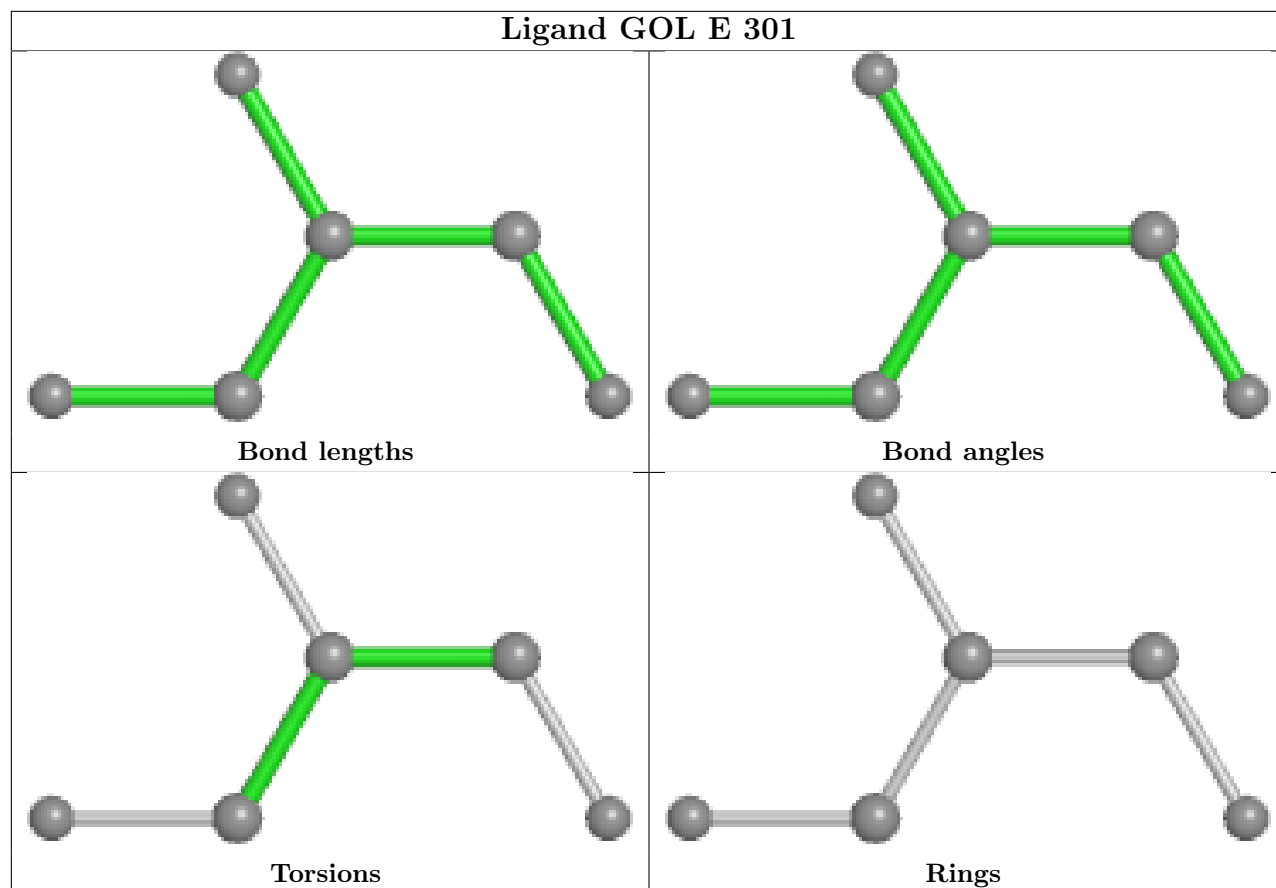
There are no ring outliers.

No monomer is involved in short contacts.

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	260/260 (100%)	-0.44	1 (0%) 92 90	13, 19, 36, 52	7 (2%)
1	B	260/260 (100%)	-0.50	0 100 100	12, 19, 35, 48	9 (3%)
1	C	260/260 (100%)	-0.48	0 100 100	12, 19, 33, 45	7 (2%)
1	D	260/260 (100%)	-0.46	1 (0%) 92 90	12, 19, 32, 43	6 (2%)
1	E	259/260 (99%)	-0.45	1 (0%) 92 90	12, 19, 33, 44	5 (1%)
1	F	260/260 (100%)	-0.47	0 100 100	12, 19, 33, 46	4 (1%)
1	G	260/260 (100%)	-0.49	1 (0%) 92 90	12, 19, 35, 46	6 (2%)
1	H	260/260 (100%)	-0.46	1 (0%) 92 90	12, 19, 36, 50	8 (3%)
All	All	2079/2080 (99%)	-0.47	5 (0%) 95 93	12, 19, 35, 52	52 (2%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	255	GLY	3.4
1	H	255	GLY	3.4
1	D	255	GLY	2.5
1	G	52	ALA	2.3
1	A	255	GLY	2.2

### 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](#)

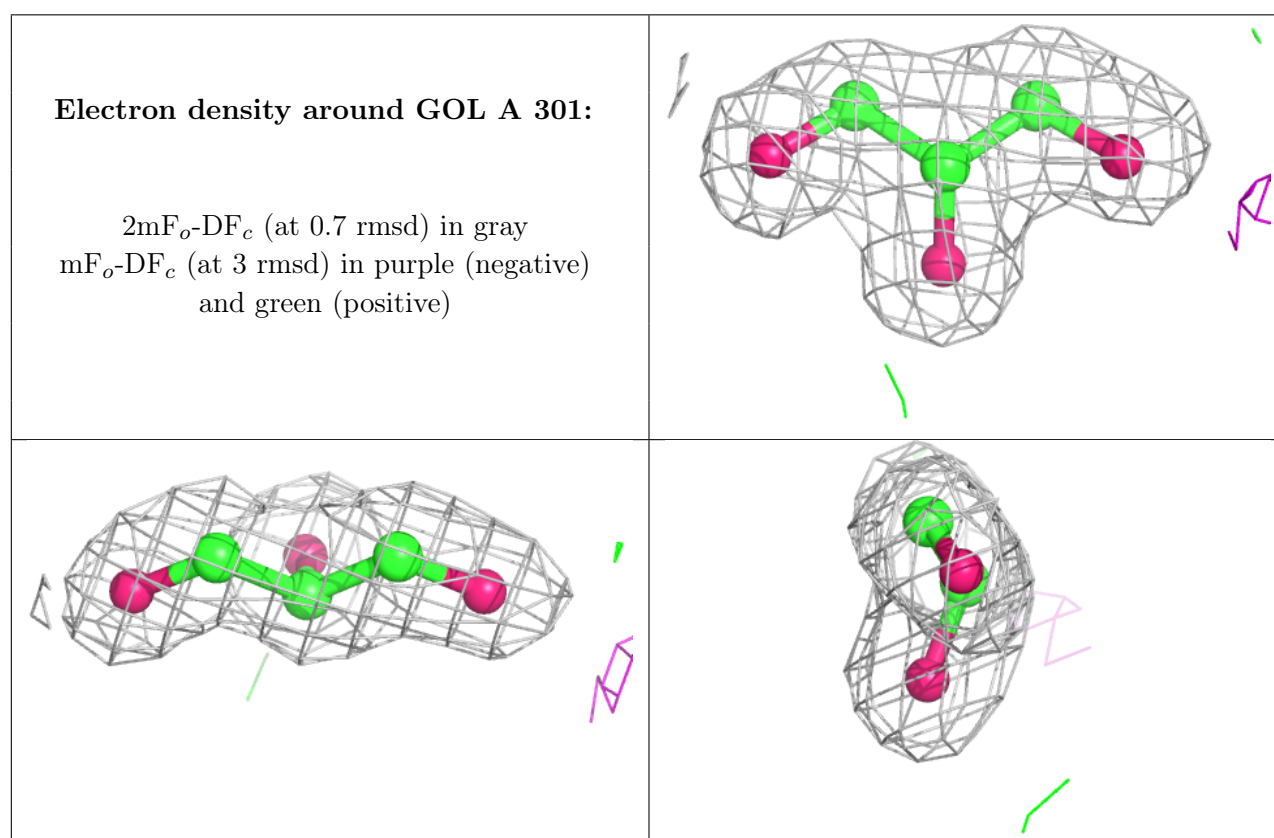
There are no monosaccharides in this entry.

## 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.

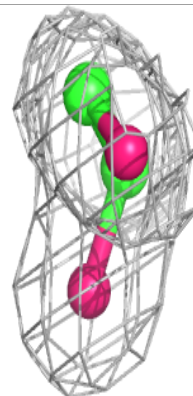
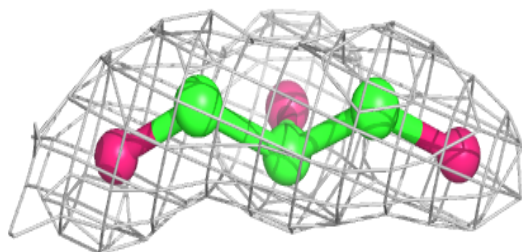
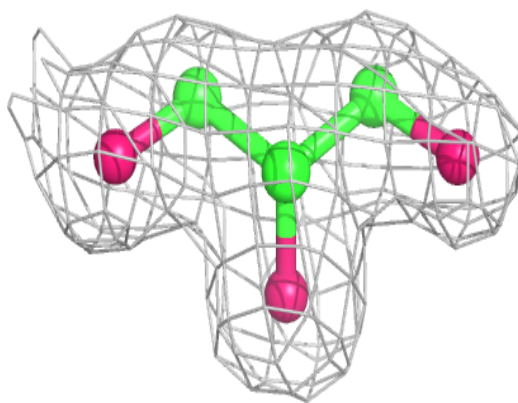
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	GOL	A	301	6/6	0.94	0.08	18,21,23,27	0
2	GOL	B	301	6/6	0.95	0.08	17,21,22,28	0
2	GOL	E	301	6/6	0.95	0.09	18,21,23,28	0
2	GOL	F	301	6/6	0.96	0.07	18,21,24,27	0

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.

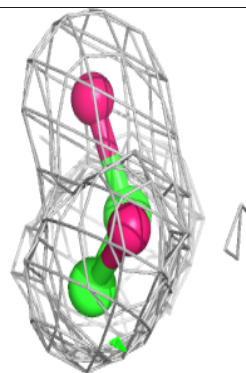
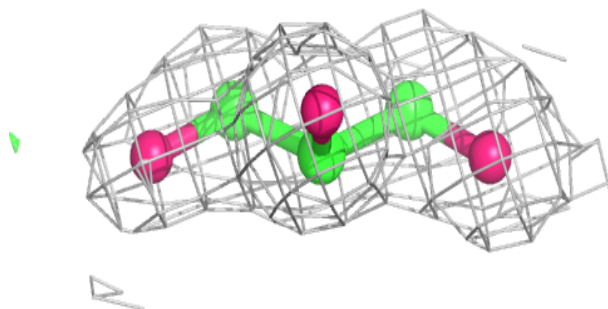
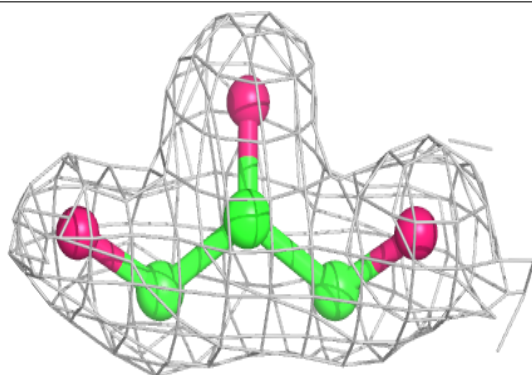


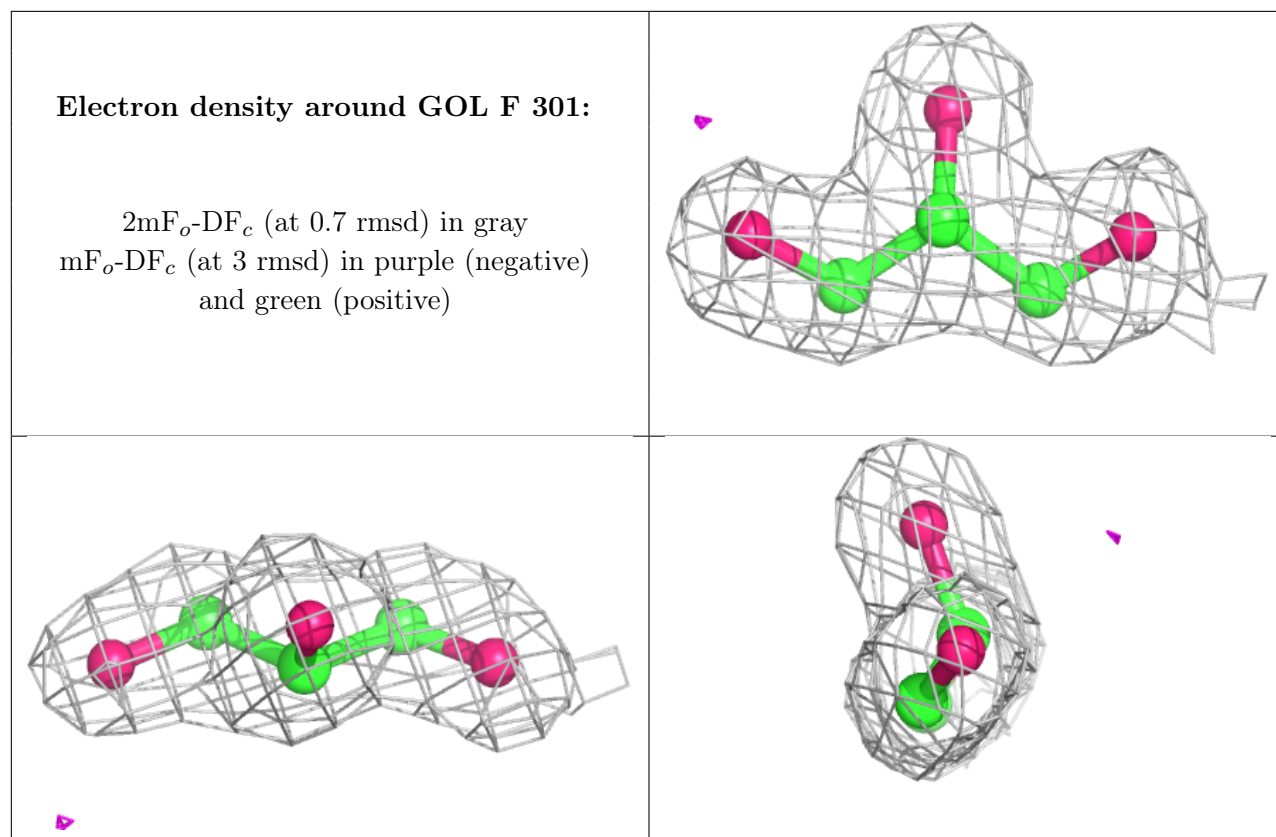
**Electron density around GOL B 301:**

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

**Electron density around GOL 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.