wwPDB X-ray Structure Validation Summary Report (i)

Oct 15, 2023 – 11:30 PM EDT

PDB ID	:	8EW1
Title	:	Structure of Bacple_01703-E145L
Authors	:	Ulaganathan, T.; Cygler, M.
Deposited on	:	2022-10-21
Resolution	:	1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

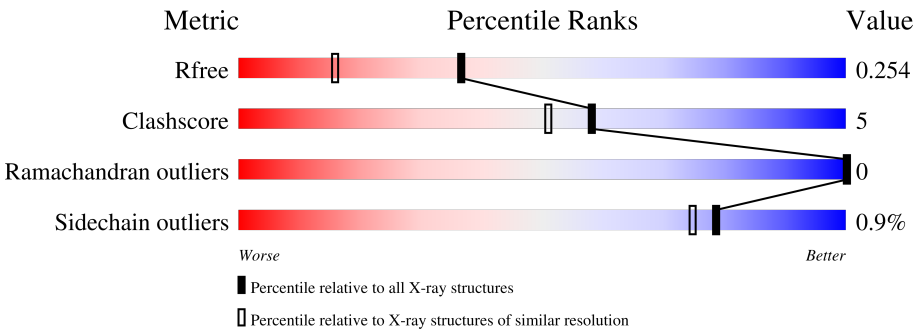
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	267	90% 9% ·
1	B	267	90% 10% ·
1	C	267	78% 18% ·
2	D	3	100%
2	E	3	100%
2	F	3	67% 33%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7341 atoms, of which 94 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 Glycosyl hydrolase family 16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	264	2223	1430	388	398	7	0	1	0
1	B	265	2248	1447	392	402	7	0	2	0
1	C	259	2139	1387	365	380	7	0	1	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP B5CYA6
A	2	GLY	-	expression tag	UNP B5CYA6
A	3	SER	-	expression tag	UNP B5CYA6
A	4	SER	-	expression tag	UNP B5CYA6
A	5	HIS	-	expression tag	UNP B5CYA6
A	6	HIS	-	expression tag	UNP B5CYA6
A	7	HIS	-	expression tag	UNP B5CYA6
A	8	HIS	-	expression tag	UNP B5CYA6
A	9	HIS	-	expression tag	UNP B5CYA6
A	10	HIS	-	expression tag	UNP B5CYA6
A	11	GLY	-	expression tag	UNP B5CYA6
A	145	LEU	GLU	engineered mutation	UNP B5CYA6
B	1	MET	-	initiating methionine	UNP B5CYA6
B	2	GLY	-	expression tag	UNP B5CYA6
B	3	SER	-	expression tag	UNP B5CYA6
B	4	SER	-	expression tag	UNP B5CYA6
B	5	HIS	-	expression tag	UNP B5CYA6
B	6	HIS	-	expression tag	UNP B5CYA6
B	7	HIS	-	expression tag	UNP B5CYA6
B	8	HIS	-	expression tag	UNP B5CYA6
B	9	HIS	-	expression tag	UNP B5CYA6
B	10	HIS	-	expression tag	UNP B5CYA6
B	11	GLY	-	expression tag	UNP B5CYA6

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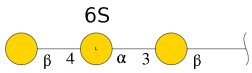
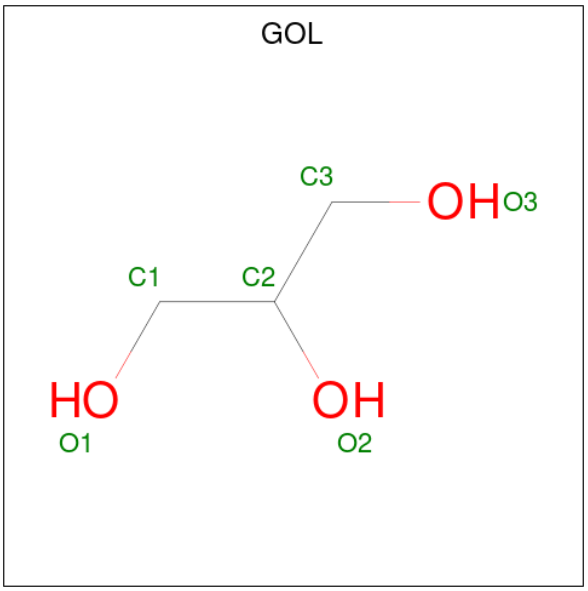
Chain	Residue	Modelled	Actual	Comment	Reference
B	145	LEU	GLU	engineered mutation	UNP B5CYA6
C	1	MET	-	initiating methionine	UNP B5CYA6
C	2	GLY	-	expression tag	UNP B5CYA6
C	3	SER	-	expression tag	UNP B5CYA6
C	4	SER	-	expression tag	UNP B5CYA6
C	5	HIS	-	expression tag	UNP B5CYA6
C	6	HIS	-	expression tag	UNP B5CYA6
C	7	HIS	-	expression tag	UNP B5CYA6
C	8	HIS	-	expression tag	UNP B5CYA6
C	9	HIS	-	expression tag	UNP B5CYA6
C	10	HIS	-	expression tag	UNP B5CYA6
C	11	GLY	-	expression tag	UNP B5CYA6
C	145	LEU	GLU	engineered mutation	UNP B5CYA6

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-4)-6-O-sulfo-alpha-L-galactopyranose-(1-3)-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	O	S			
2	D	3	68	18	31	18	1	0	0	0
			Total	C	H	O	S			
2	E	3	68	18	31	18	1	0	0	0
			Total	C	H	O	S			
2	F	3	68	18	31	18	1	0	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0

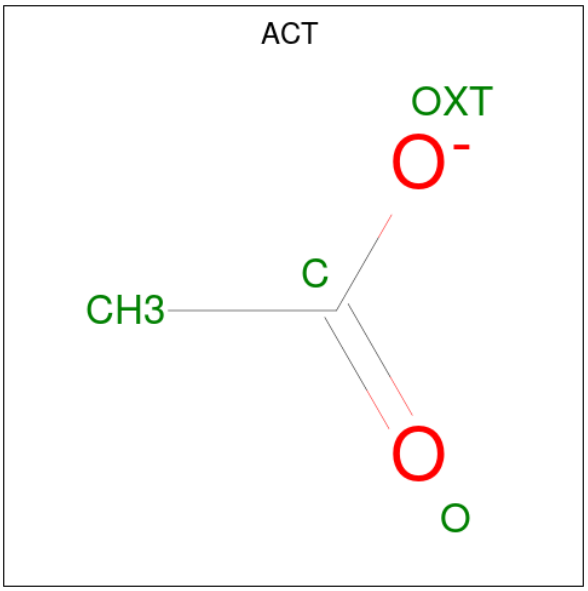
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0
4	B	1	Total Ca 1 1	0	0
4	C	1	Total Ca 1 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H O 5 2 1 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0

- Molecule 7 is water.

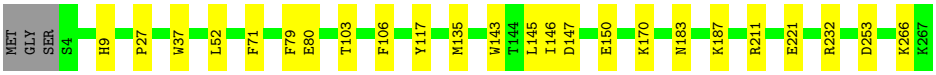
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	210	Total O 210 210	0	0
7	B	215	Total O 215 215	0	0
7	C	79	Total O 79 79	0	0

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. 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. 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: Glycosyl hydrolase family 16

Chain A:

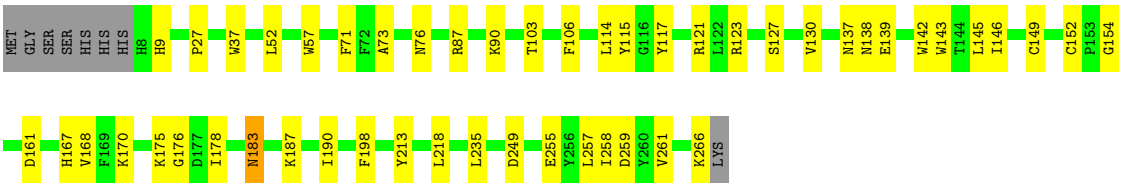


• Molecule 1: Glycosyl hydrolase family 16

Chain B:

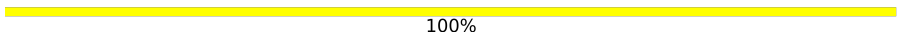
• Molecule 1: Glycosyl hydrolase family 16

Chain C:



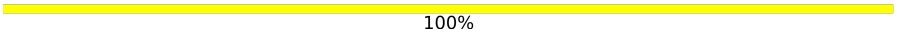
• Molecule 2: beta-D-galactopyranose-(1-4)-6-O-sulfo-alpha-L-galactopyranose-(1-3)-beta-D-galactopyranose

Chain D:



• Molecule 2: beta-D-galactopyranose-(1-4)-6-O-sulfo-alpha-L-galactopyranose-(1-3)-beta-D-galactopyranose

Chain E:



• Molecule 2: beta-D-galactopyranose-(1-4)-6-O-sulfo-alpha-L-galactopyranose-(1-3)-beta-D-galactopyranose

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	85.72Å 85.72Å 112.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.80 – 1.80 44.80 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.80-1.80) 100.0 (44.80-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.227 , 0.255 0.226 , 0.254	Depositor DCC
R_{free} test set	4282 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	25.4	Xtriage
Anisotropy	0.547	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 29.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.277 for -h,-k,l 0.370 for h,-h-k,-l 0.240 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7341	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CL, CA, ACT, GAL, GOL, L6S

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	0.27	0/2302	0.51	0/3122
1	B	0.27	0/2329	0.52	0/3159
1	C	0.25	0/2220	0.48	0/3022
All	All	0.26	0/6851	0.50	0/9303

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	2223	0	2079	11	1
1	B	2248	0	2101	16	0
1	C	2139	0	1961	34	0
2	D	37	31	28	0	0
2	E	37	31	28	0	0
2	F	37	31	28	1	0
3	A	6	0	8	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
6	A	4	1	3	0	0
6	B	4	0	3	0	0
6	C	4	0	3	0	0
7	A	210	0	0	0	0
7	B	215	0	0	2	1
7	C	79	0	0	6	1
All	All	7247	94	6242	62	2

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 5.

The worst 5 of 62 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:149:CYS:SG	7:C:533:HOH:O	2.43	0.77
1:C:139:GLU:OE2	7:C:501:HOH:O	2.11	0.69
3:A:301:GOL:H12	1:B:98:GLU:H	1.62	0.63
2:F:2:L6S:O3	2:F:3:GAL:O5	2.14	0.62
3:A:301:GOL:C1	1:B:98:GLU:H	2.15	0.60

All (2) 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)
7:B:594:HOH:O	7:B:655:HOH:O[2_655]	1.93	0.27
1:A:253:ASP:O	7:C:502:HOH:O[3_664]	2.18	0.02

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	263/267 (98%)	257 (98%)	6 (2%)	0	100	100
1	B	265/267 (99%)	260 (98%)	5 (2%)	0	100	100
1	C	258/267 (97%)	253 (98%)	5 (2%)	0	100	100
All	All	786/801 (98%)	770 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	235/239 (98%)	233 (99%)	2 (1%)	78	75
1	B	238/239 (100%)	236 (99%)	2 (1%)	81	78
1	C	217/239 (91%)	215 (99%)	2 (1%)	78	75
All	All	690/717 (96%)	684 (99%)	6 (1%)	78	75

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	183	ASN
1	C	106	PHE
1	C	183	ASN
1	A	183	ASN
1	A	106	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

9 monosaccharides 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	GAL	D	1	2	12,12,12	0.79	1 (8%)	17,17,17	1.21	1 (5%)
2	L6S	D	2	2	15,15,16	0.85	2 (13%)	20,22,24	1.47	4 (20%)
2	GAL	D	3	2	10,10,12	0.79	1 (10%)	12,13,17	0.95	0
2	GAL	E	1	2	12,12,12	0.78	1 (8%)	17,17,17	1.00	1 (5%)
2	L6S	E	2	2	15,15,16	0.91	2 (13%)	20,22,24	1.47	2 (10%)
2	GAL	E	3	2	10,10,12	0.83	1 (10%)	12,13,17	0.80	0
2	GAL	F	1	2	12,12,12	0.79	1 (8%)	17,17,17	1.00	1 (5%)
2	L6S	F	2	2	15,15,16	0.91	2 (13%)	20,22,24	1.23	2 (10%)
2	GAL	F	3	2	10,10,12	0.32	0	12,13,17	0.82	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	GAL	D	1	2	-	0/2/22/22	0/1/1/1
2	L6S	D	2	2	-	3/6/23/26	0/1/1/1
2	GAL	D	3	2	-	2/2/15/22	0/1/1/1
2	GAL	E	1	2	-	0/2/22/22	0/1/1/1
2	L6S	E	2	2	-	4/6/23/26	0/1/1/1
2	GAL	E	3	2	-	2/2/15/22	0/1/1/1
2	GAL	F	1	2	-	0/2/22/22	0/1/1/1
2	L6S	F	2	2	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	F	3	2	-	2/2/15/22	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3	GAL	C1-C2	2.49	1.53	1.51
2	D	3	GAL	C1-C2	2.37	1.53	1.51
2	F	2	L6S	O4-C4	-2.24	1.37	1.43
2	F	2	L6S	O3S-S1	2.21	1.64	1.50
2	E	2	L6S	O4-C4	-2.20	1.37	1.43

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2	L6S	C1-C2-C3	4.20	114.82	109.67
2	D	2	L6S	C1-C2-C3	3.99	114.57	109.67
2	F	2	L6S	O4-C4-C3	3.50	118.44	110.35
2	D	1	GAL	O3-C3-C4	2.90	117.06	110.35
2	D	2	L6S	O6-C6-C5	2.81	112.86	107.62

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3	GAL	O5-C5-C6-O6
2	E	3	GAL	O5-C5-C6-O6
2	D	3	GAL	C4-C5-C6-O6
2	F	3	GAL	C4-C5-C6-O6
2	E	3	GAL	C4-C5-C6-O6

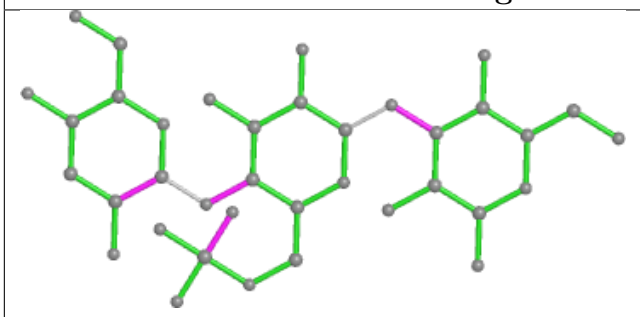
There are no ring outliers.

2 monomers are involved in 1 short contact:

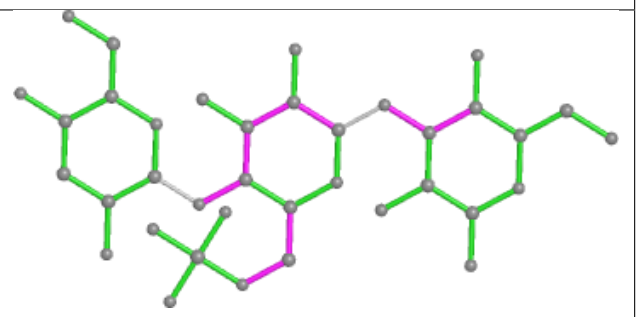
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	3	GAL	1	0
2	F	2	L6S	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

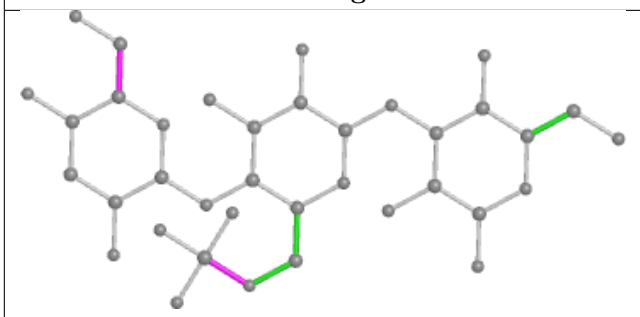
Oligosaccharide Chain D



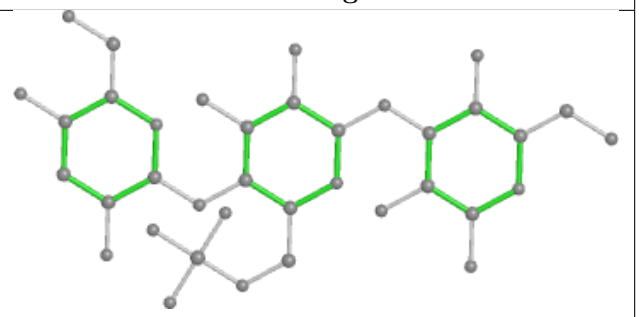
Bond lengths



Bond angles

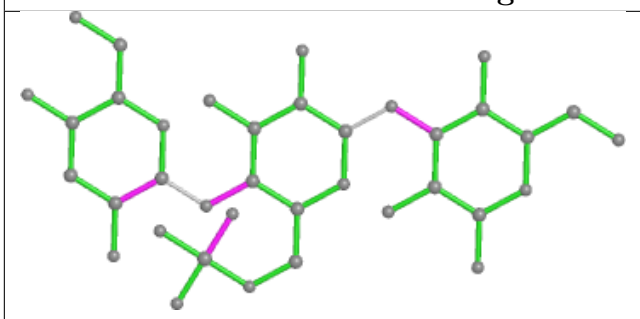


Torsions

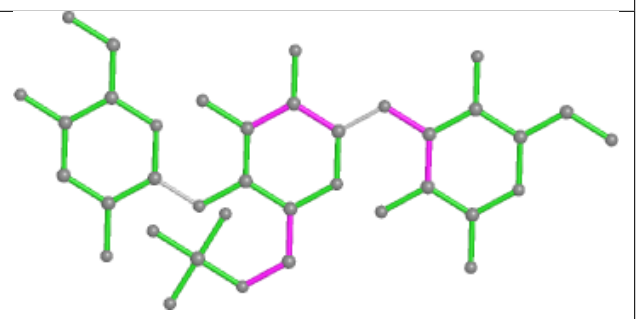


Rings

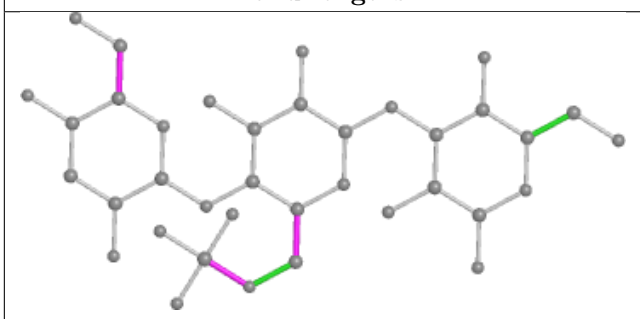
Oligosaccharide Chain E



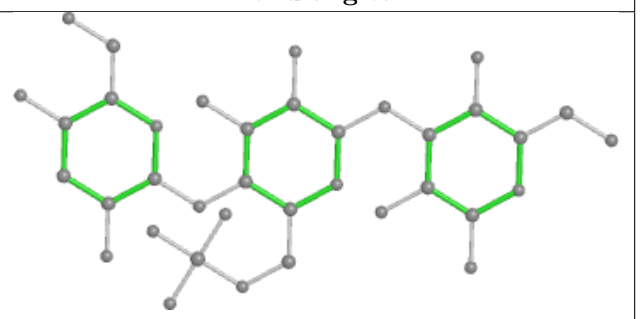
Bond lengths



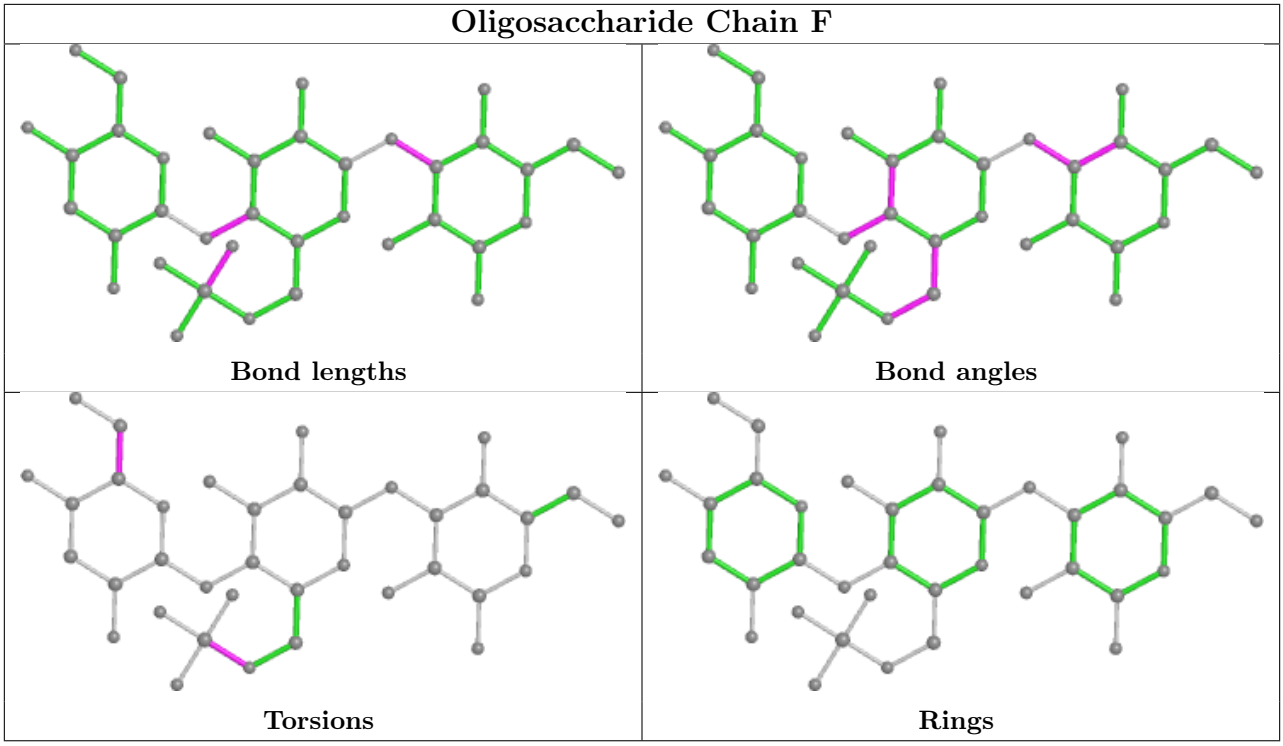
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	ACT	B	402	-	3,3,3	0.91	0	3,3,3	0.81	0
3	GOL	A	301	-	5,5,5	0.90	0	5,5,5	1.00	0
6	ACT	A	304	-	3,3,3	0.90	0	3,3,3	0.88	0
6	ACT	C	402	-	3,3,3	0.92	0	3,3,3	0.79	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
3	GOL	A	301	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

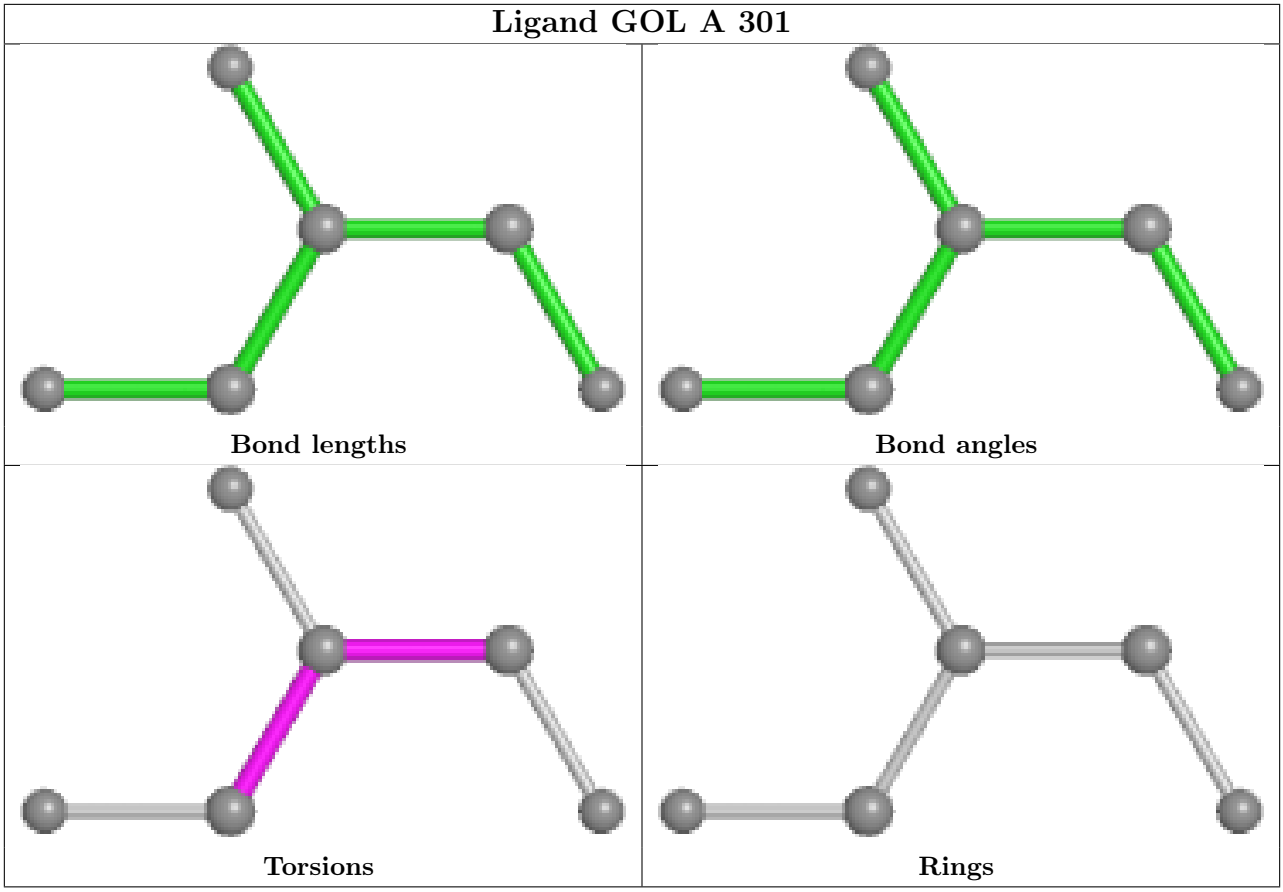
Mol	Chain	Res	Type	Atoms
3	A	301	GOL	O1-C1-C2-C3
3	A	301	GOL	C1-C2-C3-O3
3	A	301	GOL	O1-C1-C2-O2
3	A	301	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	GOL	2	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 then 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)

Unable to reproduce the depositors R factor - this section is therefore empty.

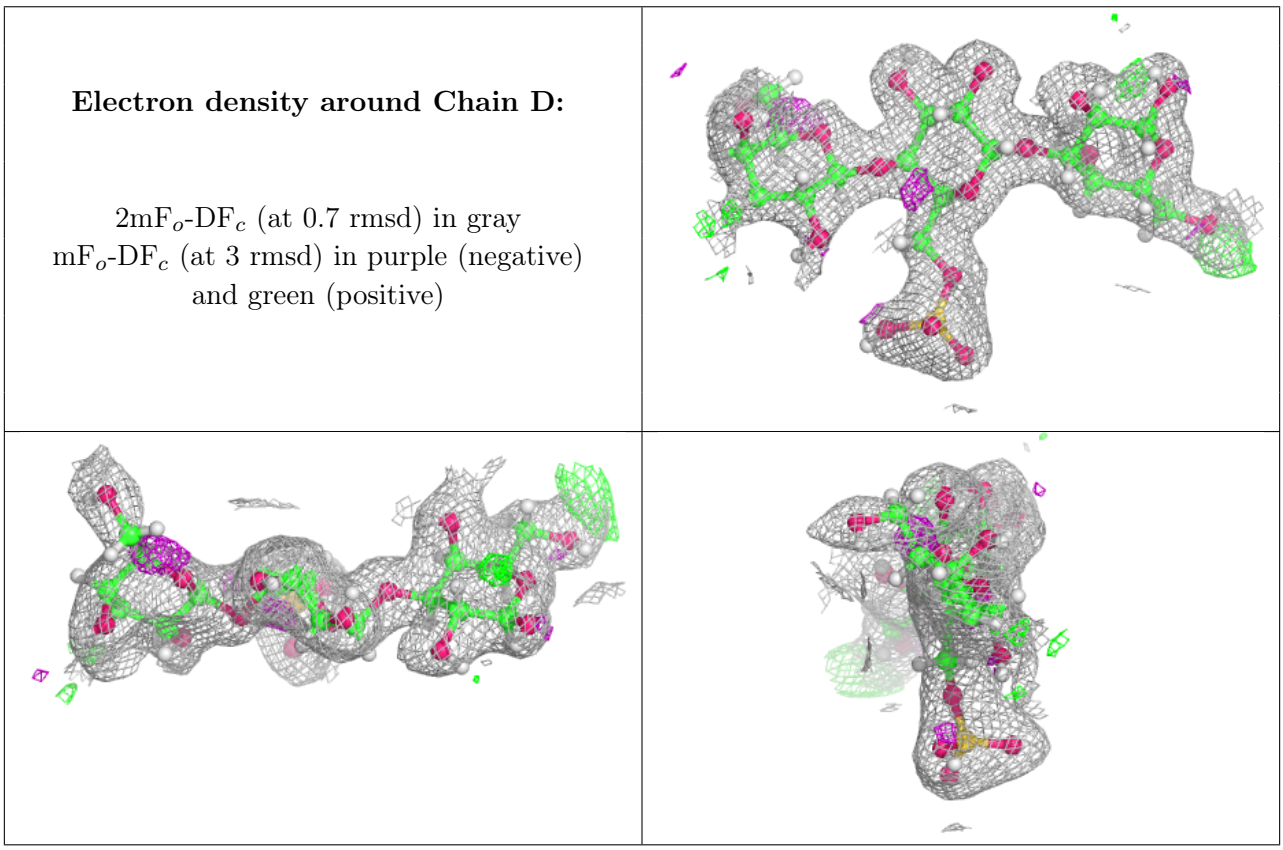
6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

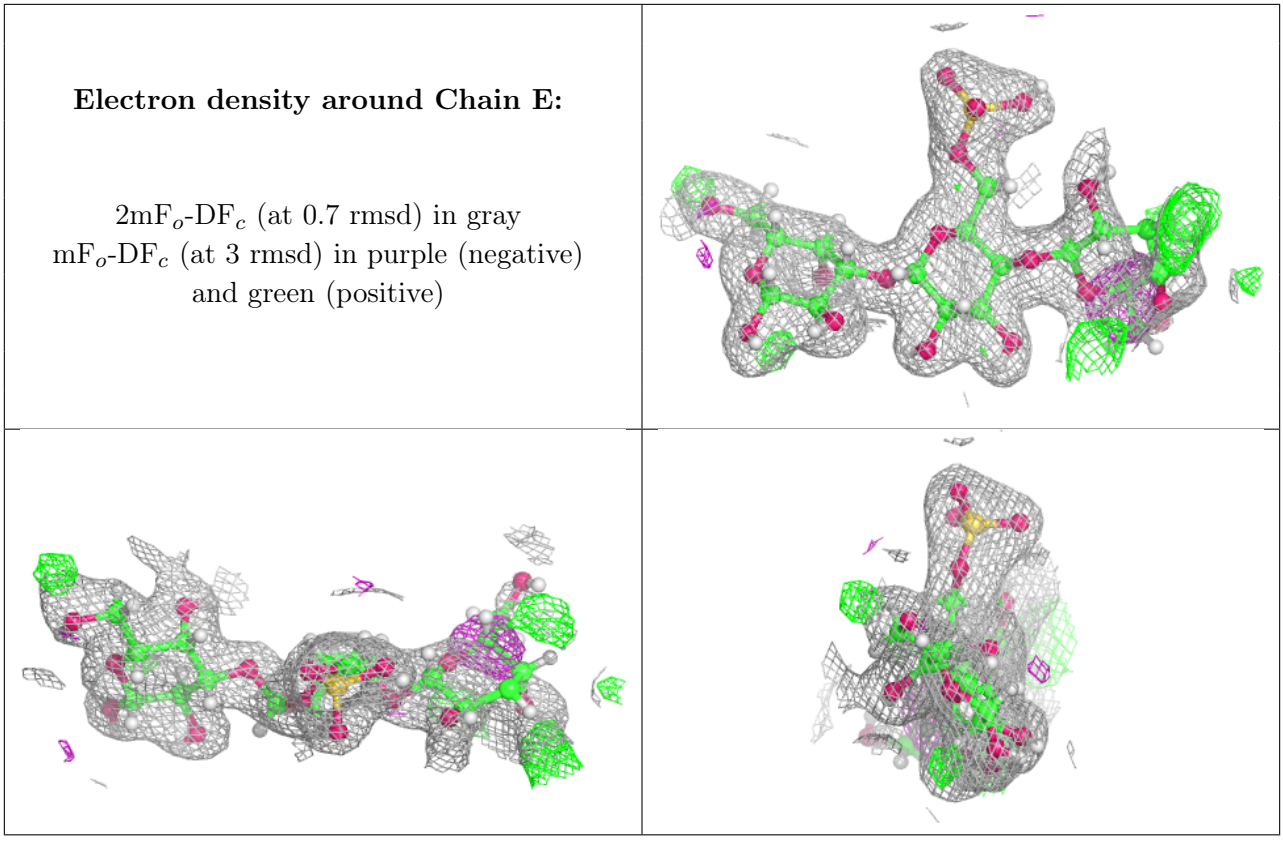
Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



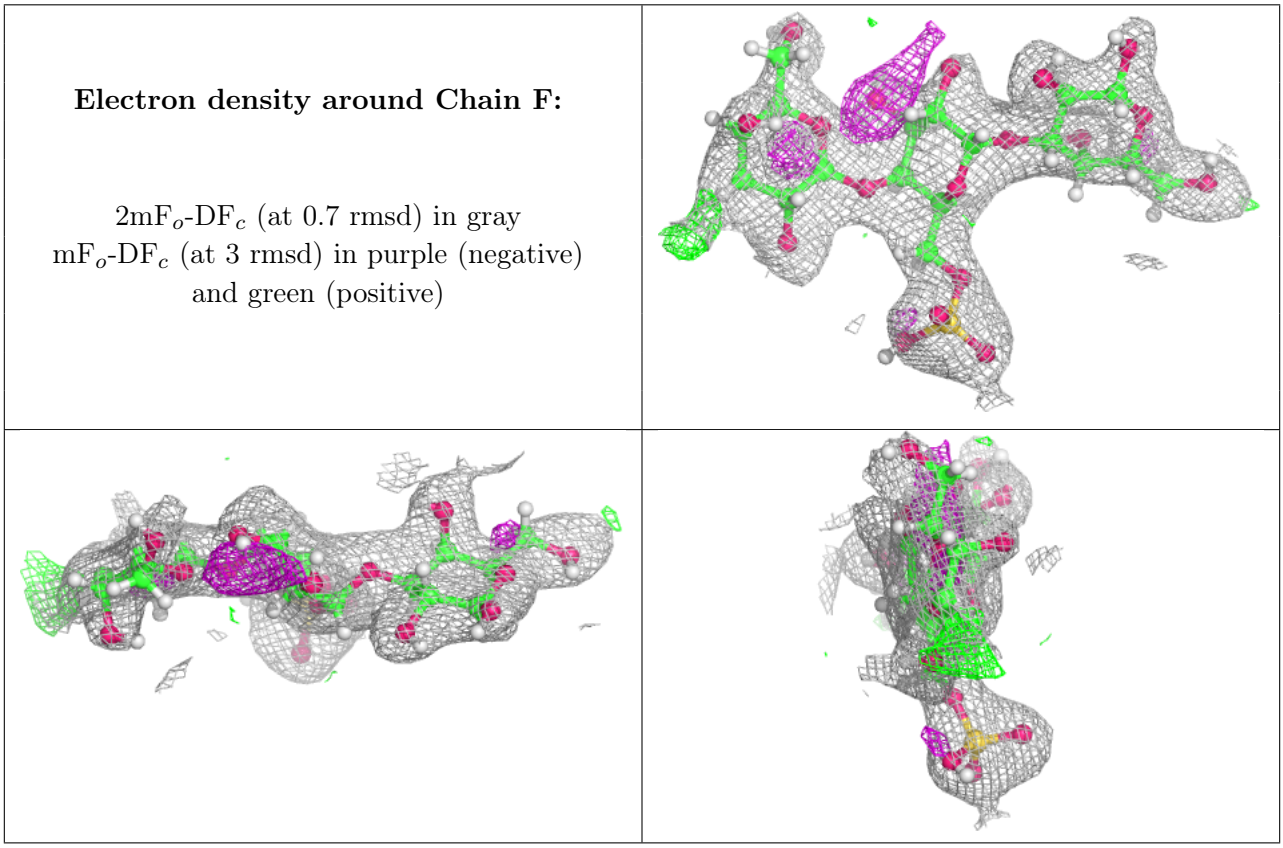
Electron density around Chain E:

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



Electron density around Chain F:

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



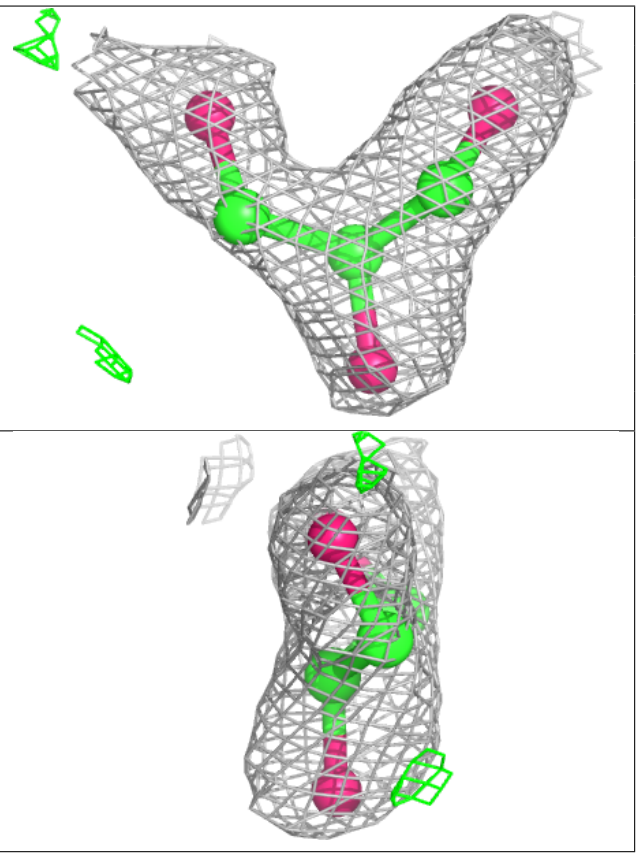
6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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 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)



6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.