Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2023 – 09:38 PM JST

PDB ID	:	6IDW
Title	:	GH6 Orpinomyces sp. Y102 enzyme
Authors	:	Tsai, L.C.; Huang, H.C.
Deposited on	:	2018-09-11
Resolution	:	2.78 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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:

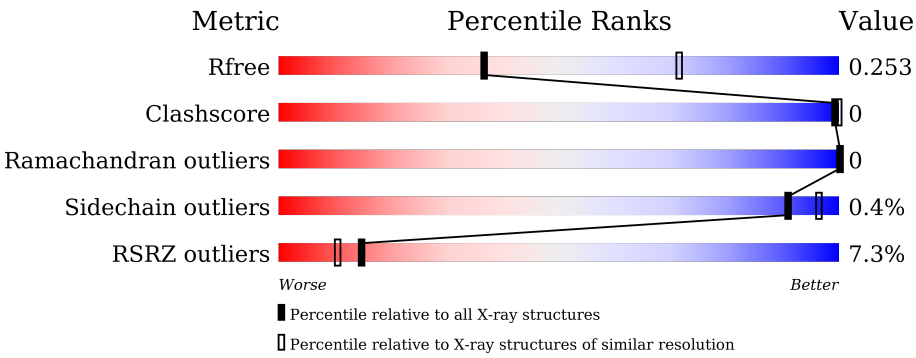
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.78 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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 >=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% 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	322	8% 100%
1	B	322	7% 100%
1	C	322	7% 100%
1	D	322	7% 99%
2	E	2	100%
2	F	2	100%

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Mol	Chain	Length	Quality of chain
2	G	2	100%
2	H	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	C	503	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 10479 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.

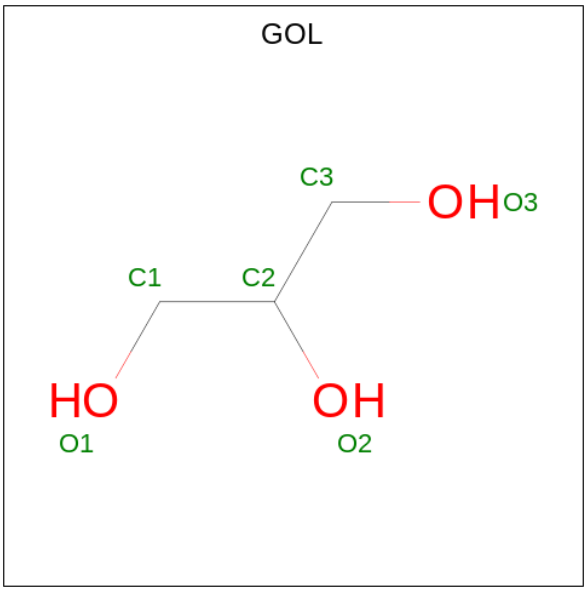
- Molecule 1 is a protein called Glucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	322	2498	1557	445	485	11	0	1	0
1	B	322	2494	1554	445	485	10	0	0	0
1	C	322	2498	1557	445	485	11	0	1	0
1	D	322	2494	1554	445	485	10	0	0	0

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-4)-beta-D-glucopyranose.

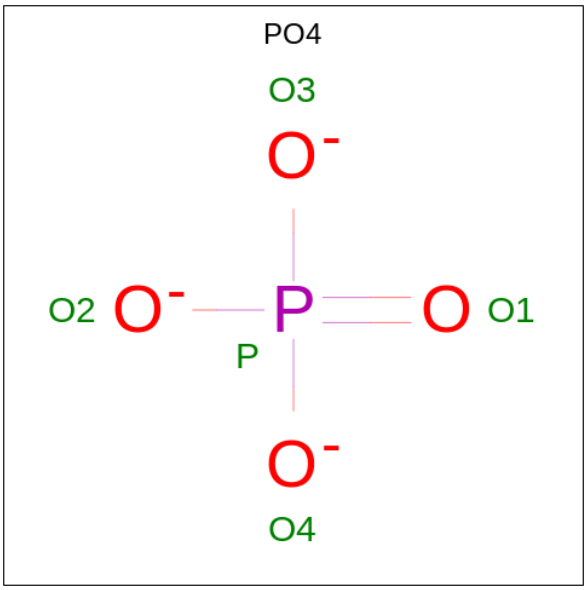
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	E	2	23	12	11	0	0	0
2	F	2	23	12	11	0	0	0
2	G	2	23	12	11	0	0	0
2	H	2	23	12	11	0	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



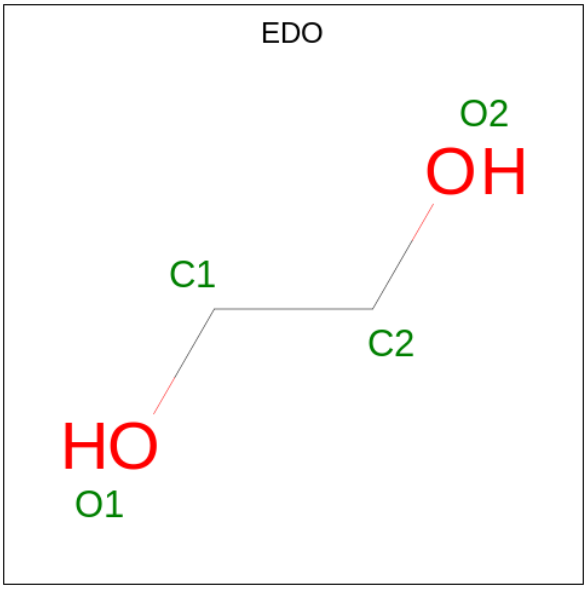
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	6	3	3	0	0
3	B	1	6	3	3	0	0
3	C	1	6	3	3	0	0
3	C	1	6	3	3	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



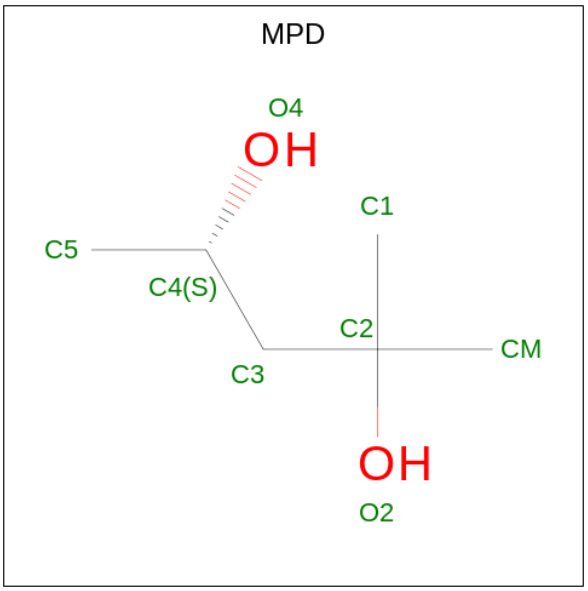
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
4	A	1	5	4	1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	B	1	8	6	2	0	0

- Molecule 7 is water.

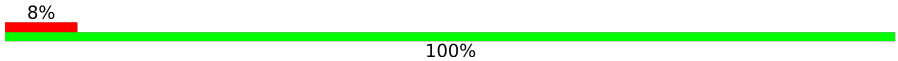
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	89	89	89	0	0
			Total	O		
7	B	102	102	102	0	0
			Total	O		
7	C	101	101	101	0	0
			Total	O		
7	D	58	58	58	0	0

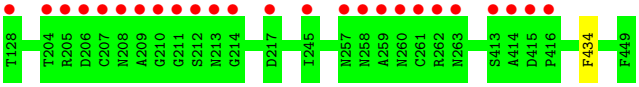
3 Residue-property plots (i)

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: Glucanase

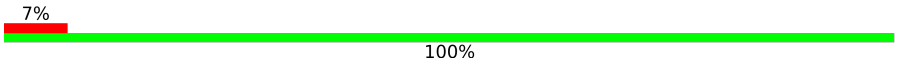
Chain A:

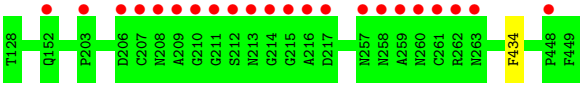




• Molecule 1: Glucanase

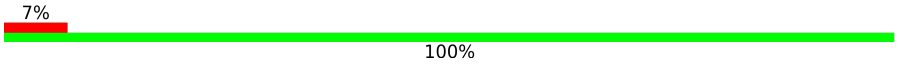
Chain B:

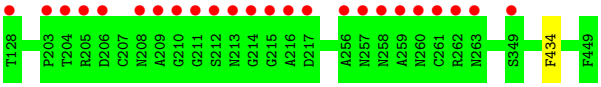




• Molecule 1: Glucanase

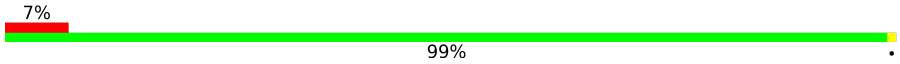
Chain C:

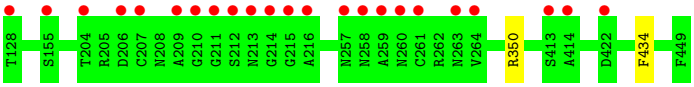




• Molecule 1: Glucanase

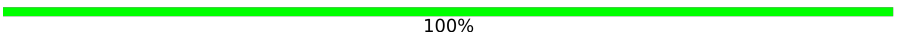
Chain D:





• Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain E:



• Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain F: 100%

BGC1
BGC2

• Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain G: 100%

BGC1
BGC2

• Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain H: 100%

BGC1
BGC2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	310.37Å 86.59Å 82.31Å 90.00° 93.67° 90.00°	Depositor
Resolution (Å)	154.87 – 2.78 26.34 – 2.78	Depositor EDS
% Data completeness (in resolution range)	92.0 (154.87-2.78) 92.1 (26.34-2.78)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.11 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.220 , 0.253 0.220 , 0.253	Depositor DCC
R_{free} test set	1934 reflections (3.82%)	wwPDB-VP
Wilson B-factor (Å^2)	27.5	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 32.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	10479	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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: BGC, PO4, EDO, GOL, MPD

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	0.80	0/2559	0.84	0/3479
1	B	0.86	0/2551	0.86	0/3469
1	C	0.86	0/2559	0.85	0/3479
1	D	0.77	0/2551	0.81	0/3469
All	All	0.82	0/10220	0.84	0/13896

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	2498	0	2390	0	0
1	B	2494	0	2385	0	0
1	C	2498	0	2390	0	0
1	D	2494	0	2385	1	0
2	E	23	0	21	0	0
2	F	23	0	21	0	0
2	G	23	0	21	0	0
2	H	23	0	21	0	0
3	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	8	0	0
3	C	12	0	16	0	0
4	A	5	0	0	0	0
5	A	4	0	6	0	0
5	B	8	0	12	0	0
5	C	4	0	6	0	0
6	B	8	0	14	0	0
7	A	89	0	0	0	0
7	B	102	0	0	0	0
7	C	101	0	0	0	0
7	D	58	0	0	1	0
All	All	10479	0	9704	1	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 0.

All (1) 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:D:350:ARG:NH1	7:D:601:HOH:O	2.39	0.53

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	321/322 (100%)	309 (96%)	12 (4%)	0	100	100
1	B	320/322 (99%)	308 (96%)	12 (4%)	0	100	100
1	C	321/322 (100%)	307 (96%)	14 (4%)	0	100	100
1	D	320/322 (99%)	309 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1282/1288 (100%)	1233 (96%)	49 (4%)	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	267/266 (100%)	266 (100%)	1 (0%)	91 96
1	B	266/266 (100%)	265 (100%)	1 (0%)	91 96
1	C	267/266 (100%)	266 (100%)	1 (0%)	91 96
1	D	266/266 (100%)	265 (100%)	1 (0%)	91 96
All	All	1066/1064 (100%)	1062 (100%)	4 (0%)	91 96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	434	PHE
1	B	434	PHE
1	C	434	PHE
1	D	434	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)

8 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	BGC	E	1	2	12,12,12	0.46	0	17,17,17	0.53	0
2	BGC	E	2	2	11,11,12	0.28	0	15,15,17	0.66	0
2	BGC	F	1	2	12,12,12	0.45	0	17,17,17	0.52	0
2	BGC	F	2	2	11,11,12	0.27	0	15,15,17	0.64	0
2	BGC	G	1	2	12,12,12	0.45	0	17,17,17	0.53	0
2	BGC	G	2	2	11,11,12	0.28	0	15,15,17	0.63	0
2	BGC	H	1	2	12,12,12	0.45	0	17,17,17	0.53	0
2	BGC	H	2	2	11,11,12	0.29	0	15,15,17	0.64	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	BGC	E	1	2	-	0/2/22/22	0/1/1/1
2	BGC	E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	F	1	2	-	0/2/22/22	0/1/1/1
2	BGC	F	2	2	-	1/2/19/22	0/1/1/1
2	BGC	G	1	2	-	0/2/22/22	0/1/1/1
2	BGC	G	2	2	-	0/2/19/22	0/1/1/1
2	BGC	H	1	2	-	0/2/22/22	0/1/1/1
2	BGC	H	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

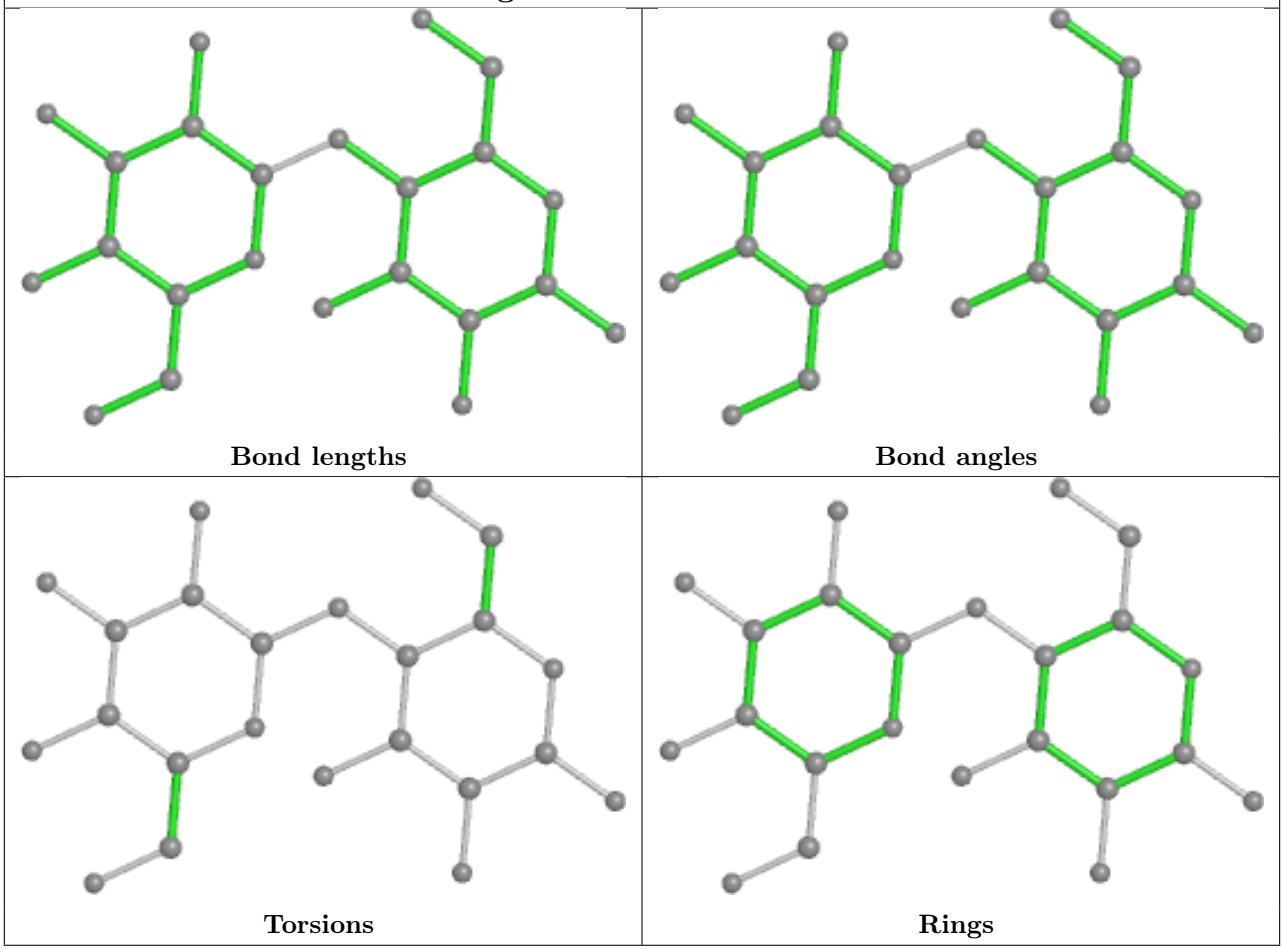
Mol	Chain	Res	Type	Atoms
2	F	2	BGC	C4-C5-C6-O6

There are no ring outliers.

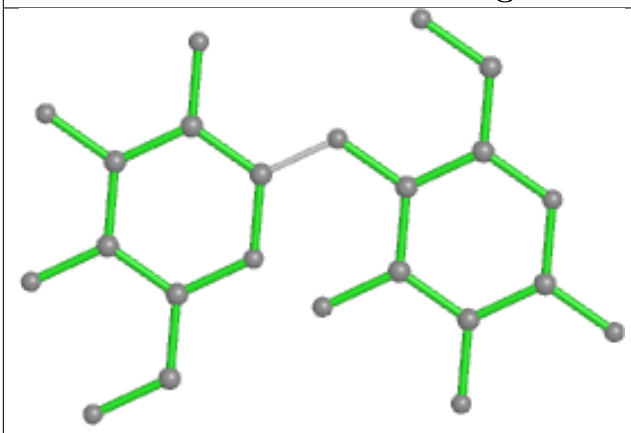
No monomer is involved in short contacts.

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

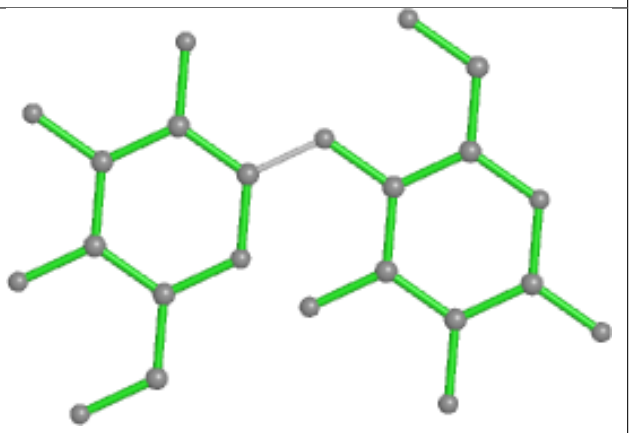
Oligosaccharide Chain E



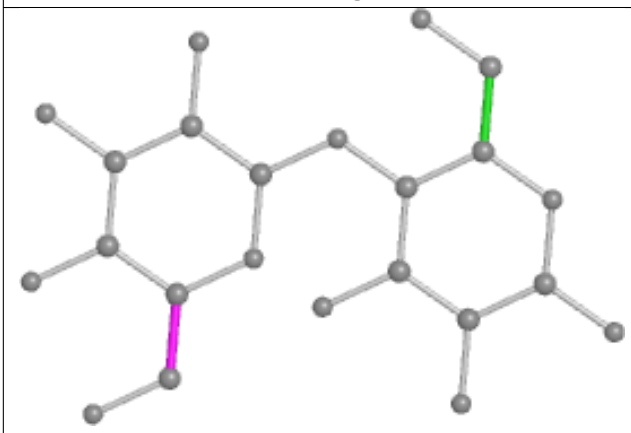
Oligosaccharide Chain F



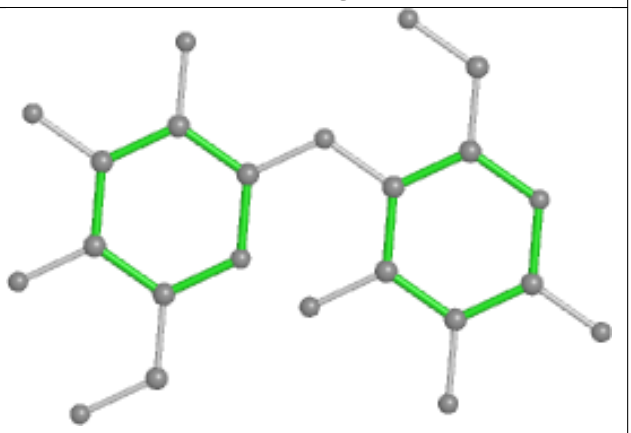
Bond lengths



Bond angles

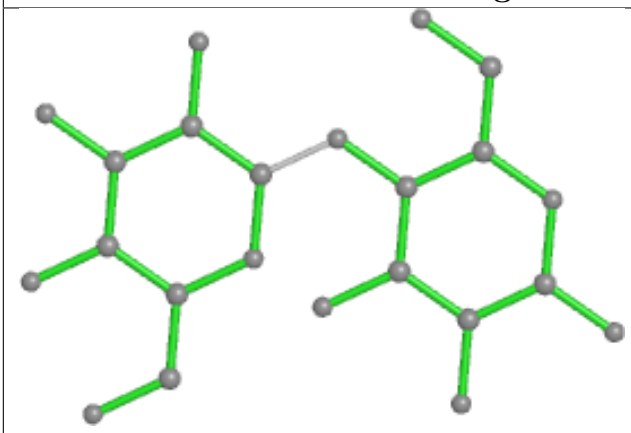


Torsions

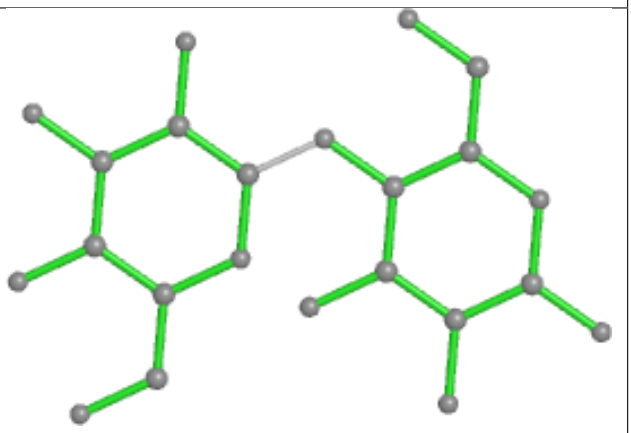


Rings

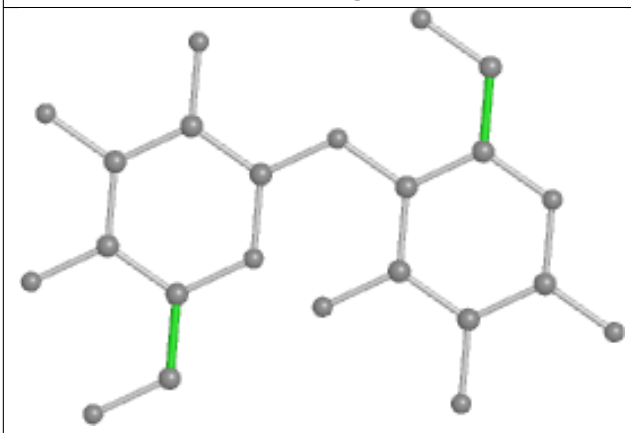
Oligosaccharide Chain G



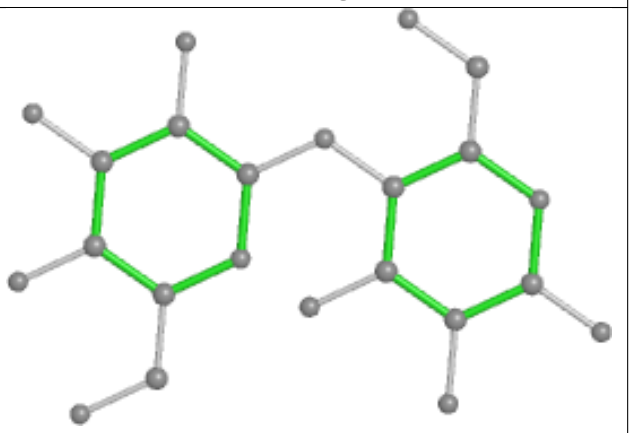
Bond lengths



Bond angles

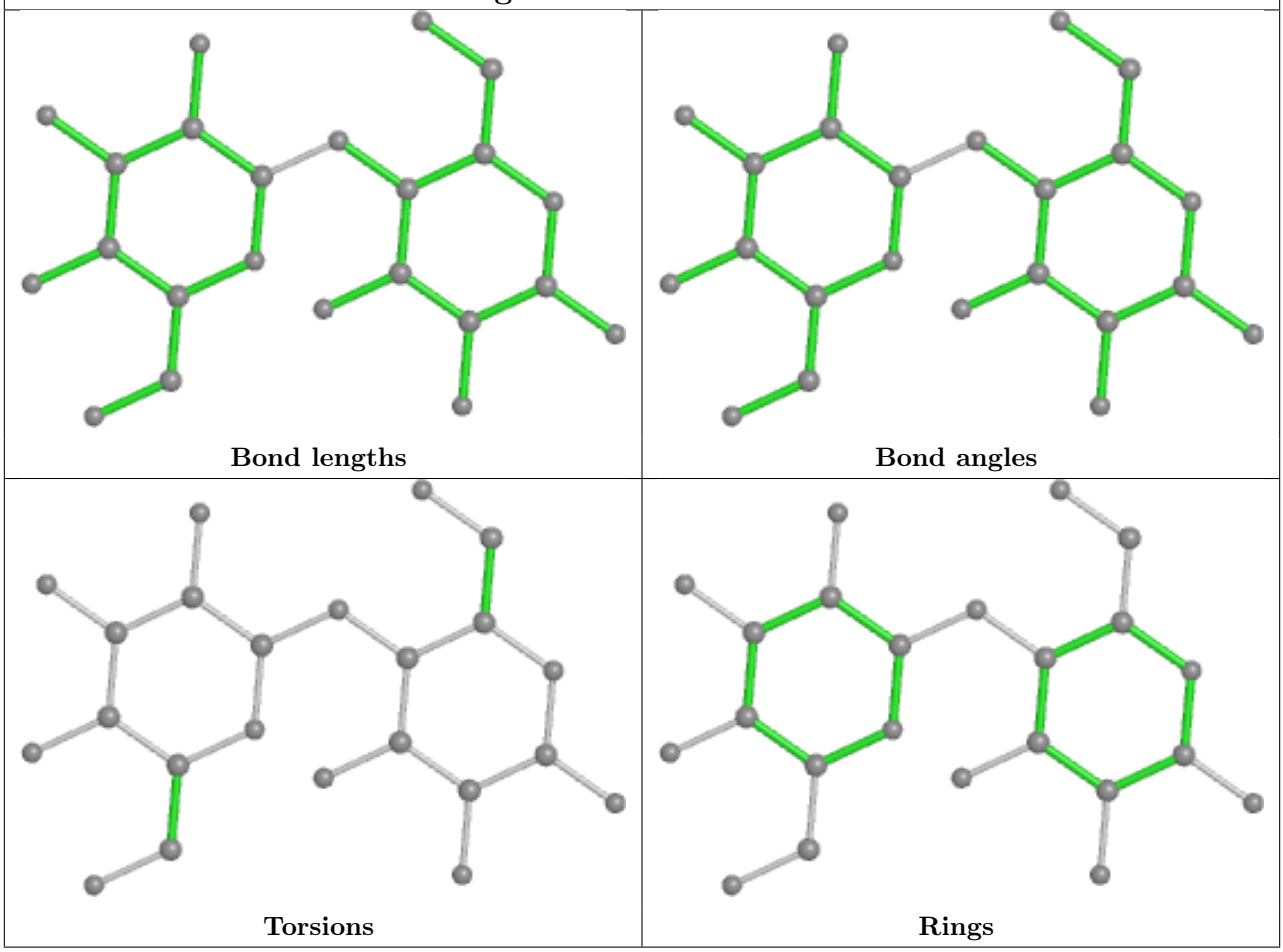


Torsions



Rings

Oligosaccharide Chain H



5.6 Ligand geometry (i)

10 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	$\#\|Z\| > 2$
3	GOL	C	503	-	5,5,5	0.27	0	5,5,5	0.28	0
3	GOL	B	502	-	5,5,5	0.42	0	5,5,5	0.64	0
4	PO4	A	503	-	4,4,4	0.86	0	6,6,6	0.44	0
3	GOL	C	502	-	5,5,5	0.35	0	5,5,5	0.85	0
5	EDO	B	505	-	3,3,3	0.34	0	2,2,2	0.04	0
5	EDO	B	503	-	3,3,3	0.31	0	2,2,2	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	A	502	-	5,5,5	0.27	0	5,5,5	0.29	0
5	EDO	C	504	-	3,3,3	0.30	0	2,2,2	0.42	0
5	EDO	A	504	-	3,3,3	0.45	0	2,2,2	0.34	0
6	MPD	B	504	-	7,7,7	0.25	0	9,10,10	0.21	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	C	503	-	-	0/4/4/4	-
3	GOL	B	502	-	-	4/4/4/4	-
3	GOL	C	502	-	-	2/4/4/4	-
5	EDO	B	505	-	-	0/1/1/1	-
5	EDO	B	503	-	-	1/1/1/1	-
3	GOL	A	502	-	-	0/4/4/4	-
5	EDO	C	504	-	-	1/1/1/1	-
5	EDO	A	504	-	-	0/1/1/1	-
6	MPD	B	504	-	-	0/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	GOL	O1-C1-C2-C3
3	B	502	GOL	C1-C2-C3-O3
3	C	502	GOL	C1-C2-C3-O3
3	B	502	GOL	O2-C2-C3-O3
5	B	503	EDO	O1-C1-C2-O2
3	C	502	GOL	O2-C2-C3-O3
3	B	502	GOL	O1-C1-C2-O2
5	C	504	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	322/322 (100%)	0.15	25 (7%)	13	9	16, 30, 59, 73	23 (7%)
1	B	322/322 (100%)	0.24	22 (6%)	17	12	11, 25, 64, 81	20 (6%)
1	C	322/322 (100%)	0.19	24 (7%)	14	10	9, 26, 64, 78	21 (6%)
1	D	322/322 (100%)	0.27	23 (7%)	16	11	20, 36, 61, 75	21 (6%)
All	All	1288/1288 (100%)	0.21	94 (7%)	15	10	9, 29, 63, 81	85 (6%)

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	215	GLY	18.1
1	B	212	SER	17.3
1	B	214	GLY	13.7
1	B	215	GLY	13.6
1	C	214	GLY	13.3
1	C	210	GLY	13.0
1	B	213	ASN	13.0
1	D	212	SER	13.0
1	C	211	GLY	12.9
1	B	216	ALA	11.4
1	A	211	GLY	11.3
1	D	213	ASN	10.8
1	A	210	GLY	10.6
1	A	258	ASN	10.4
1	B	210	GLY	9.9
1	D	214	GLY	9.4
1	C	260	ASN	9.3
1	D	259	ALA	9.2
1	C	259	ALA	9.0
1	A	212	SER	8.9
1	B	206	ASP	8.7

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Mol	Chain	Res	Type	RSRZ
1	B	209	ALA	8.5
1	A	213	ASN	8.4
1	A	206	ASP	8.3
1	A	259	ALA	8.0
1	B	211	GLY	7.7
1	C	209	ALA	7.4
1	C	213	ASN	7.3
1	A	208	ASN	7.2
1	C	212	SER	6.7
1	D	260	ASN	6.3
1	D	207	CYS	6.2
1	C	257	ASN	6.1
1	D	209	ALA	6.0
1	A	260	ASN	5.8
1	C	216	ALA	5.7
1	D	215	GLY	5.5
1	C	258	ASN	5.5
1	B	258	ASN	5.3
1	C	217	ASP	5.3
1	D	211	GLY	5.2
1	A	217	ASP	4.7
1	D	258	ASN	4.6
1	A	207	CYS	4.5
1	C	204	THR	4.5
1	D	257	ASN	4.5
1	C	263	ASN	4.4
1	B	257	ASN	4.1
1	B	263	ASN	4.1
1	C	206	ASP	4.0
1	B	262	ARG	3.9
1	A	262	ARG	3.7
1	B	207	CYS	3.5
1	B	217	ASP	3.5
1	A	263	ASN	3.4
1	A	204	THR	3.4
1	A	257	ASN	3.3
1	C	261	CYS	3.3
1	A	209	ALA	3.3
1	C	262	ARG	3.2
1	A	205	ARG	3.1
1	A	416	PRO	3.1
1	C	128	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	261	CYS	3.0
1	C	256	ALA	3.0
1	D	210	GLY	2.9
1	B	259	ALA	2.9
1	D	128	THR	2.8
1	B	203	PRO	2.8
1	B	208	ASN	2.8
1	A	414	ALA	2.7
1	A	413	SER	2.7
1	A	415	ASP	2.6
1	D	413	SER	2.6
1	A	128	THR	2.5
1	A	261	CYS	2.5
1	C	205	ARG	2.5
1	C	349	SER	2.5
1	C	208	ASN	2.4
1	D	206	ASP	2.4
1	B	260	ASN	2.3
1	D	414	ALA	2.3
1	B	261	CYS	2.3
1	A	245	ILE	2.3
1	B	448	PRO	2.3
1	D	264	VAL	2.3
1	B	152	GLN	2.2
1	D	216	ALA	2.2
1	D	155	SER	2.2
1	A	214	GLY	2.1
1	C	203	PRO	2.0
1	D	422	ASP	2.0
1	D	263	ASN	2.0
1	D	204	THR	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)

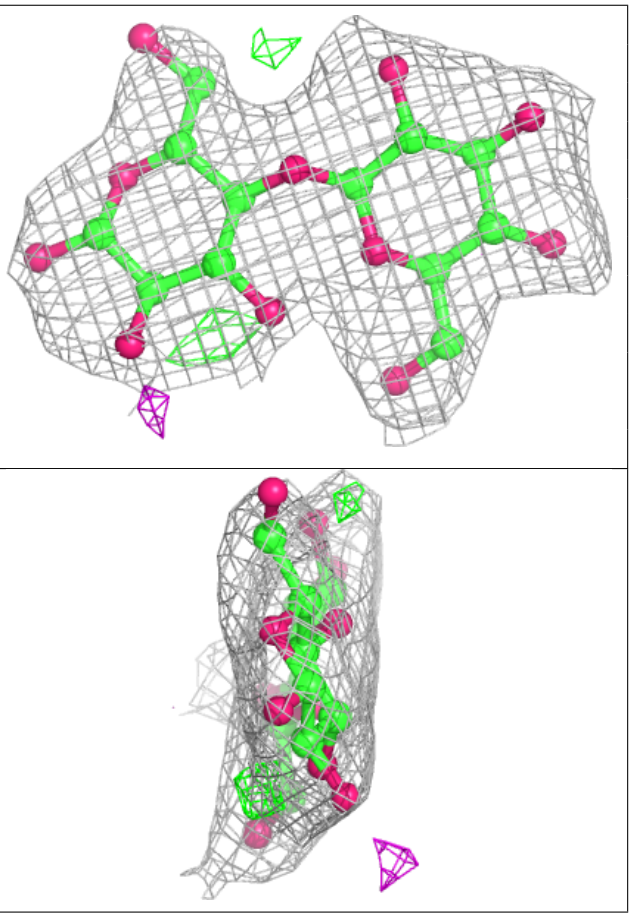
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BGC	G	1	12/12	0.91	0.22	30,37,46,47	0
2	BGC	E	1	12/12	0.92	0.19	27,36,39,43	0
2	BGC	F	2	11/12	0.94	0.16	23,25,27,27	0
2	BGC	H	1	12/12	0.94	0.17	43,49,52,60	0
2	BGC	H	2	11/12	0.94	0.14	37,39,41,41	0
2	BGC	F	1	12/12	0.95	0.16	27,32,34,38	0
2	BGC	E	2	11/12	0.97	0.11	20,22,24,25	0
2	BGC	G	2	11/12	0.97	0.11	21,24,25,26	0

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.

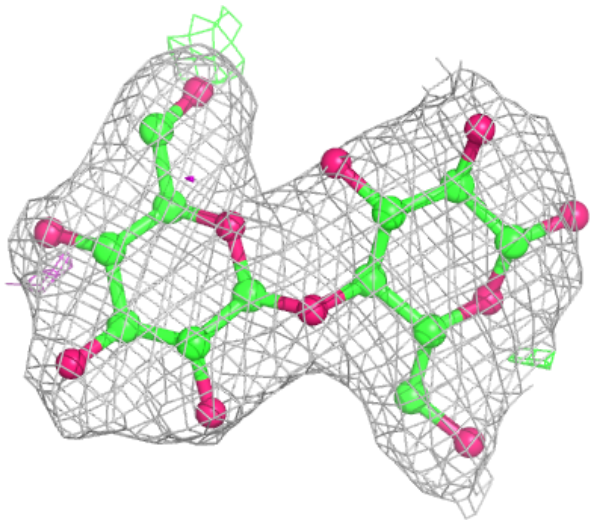
Electron density around Chain E:

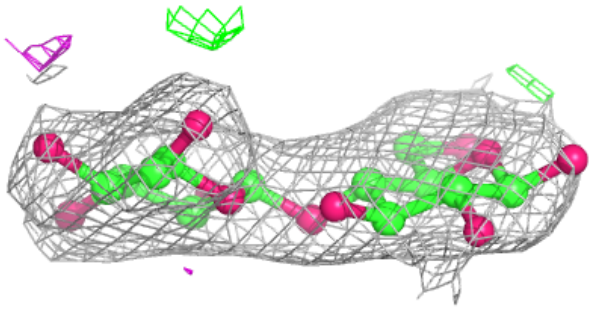
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

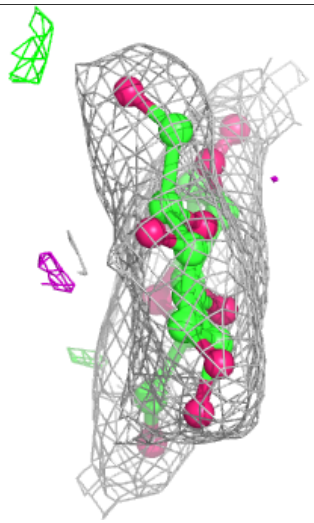


Electron density around Chain F:

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

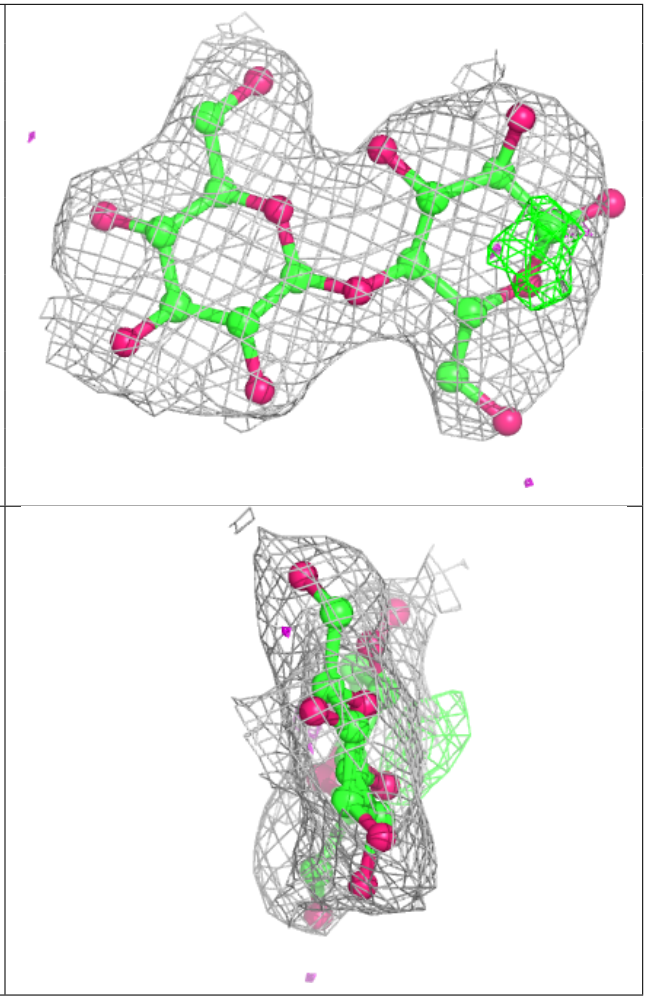






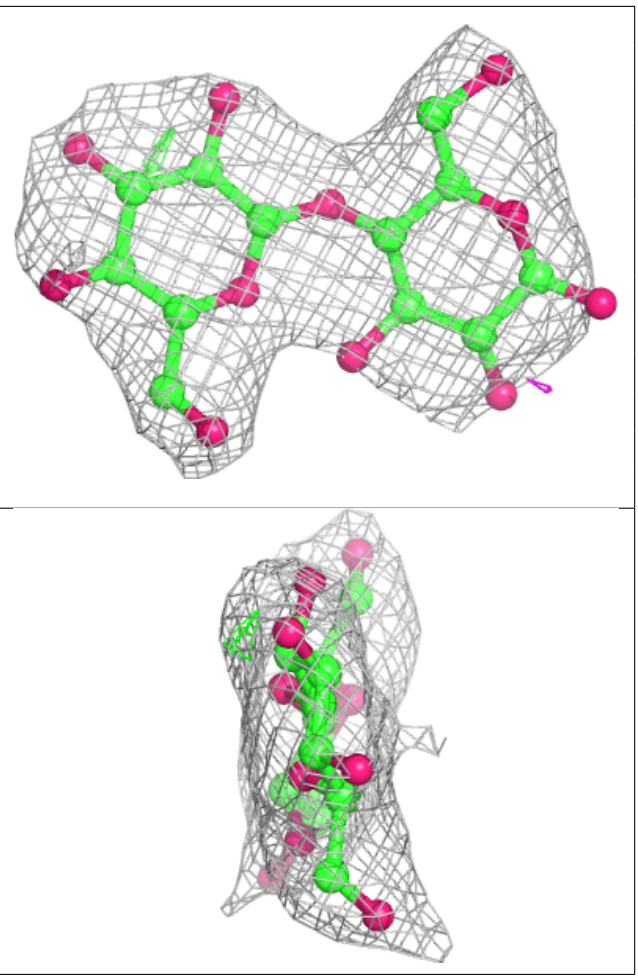
Electron density around Chain G:

$2mF_o$-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 H:

$2mF_o$-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)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	B	503	4/4	0.74	0.28	49,51,53,57	0
3	GOL	C	503	6/6	0.77	0.49	52,59,62,64	0
3	GOL	C	502	6/6	0.80	0.28	35,37,40,43	0
5	EDO	C	504	4/4	0.84	0.60	51,56,56,57	0
3	GOL	A	502	6/6	0.85	0.24	58,59,61,61	0
6	MPD	B	504	8/8	0.85	0.34	43,45,48,49	0
5	EDO	B	505	4/4	0.90	0.28	53,62,64,69	0
3	GOL	B	502	6/6	0.91	0.16	33,35,37,37	0
4	PO4	A	503	5/5	0.93	0.18	58,58,61,62	5
5	EDO	A	504	4/4	0.95	0.22	40,41,46,47	0

6.5 Other polymers (i)

There are no such residues in this entry.