wwPDB X-ray Structure Validation Summary Report (i)

Jun 13, 2024 – 10:46 AM EDT

PDB ID	:	1PUU
Title	:	Mistletoe lectin I in complex with lactose
Authors	:	Krauspenhaar, R.; Voelter, W.; Stoeva, S.; Mikhailov, A.; Konareva, N.; Betzel, C.
Deposited on	:	2003-06-25
Resolution	:	2.30 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:

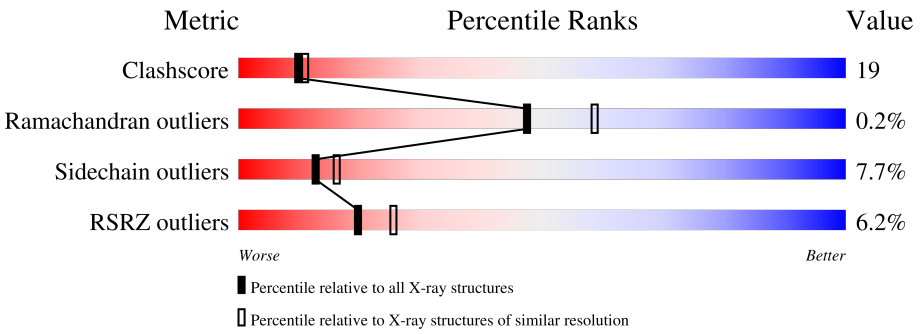
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.30 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))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	249	8%, 64%, 32%, •
2	B	263	5%, 80%, 16%, •
3	C	3	67%, 33%
4	D	2	50%, 50%
5	E	2	100%
5	F	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
10	SO4	A	2022	-	-	X	-
7	GOL	A	1021	-	X	-	-
7	GOL	A	1025	-	X	-	X
7	GOL	A	1031	-	X	X	X
7	GOL	A	1067	-	X	-	-
7	GOL	A	1069	-	X	-	-
7	GOL	A	1090	-	X	-	-
7	GOL	A	1096	-	X	-	-
7	GOL	A	1237	-	X	-	-
7	GOL	B	1041	-	X	-	X
7	GOL	B	1068	-	X	-	-
7	GOL	B	1070	-	X	-	-
7	GOL	B	1071	-	X	-	-
7	GOL	B	1088	-	X	-	-
7	GOL	B	1089	-	X	-	-
7	GOL	B	1091	-	X	-	-
7	GOL	B	1095	-	X	-	-
9	DIO	A	1830	-	-	-	X

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 4509 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.

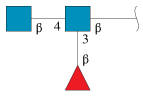
- Molecule 1 is a protein called lectin I A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	249	1921	1218	328	371	4	0	0	0

- Molecule 2 is a protein called lectin I B chain.

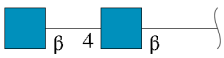
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	263	2000	1238	354	396	12	0	0	0

- Molecule 3 is an oligosaccharide called beta-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	3	38	22	2	14	0	0	0

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

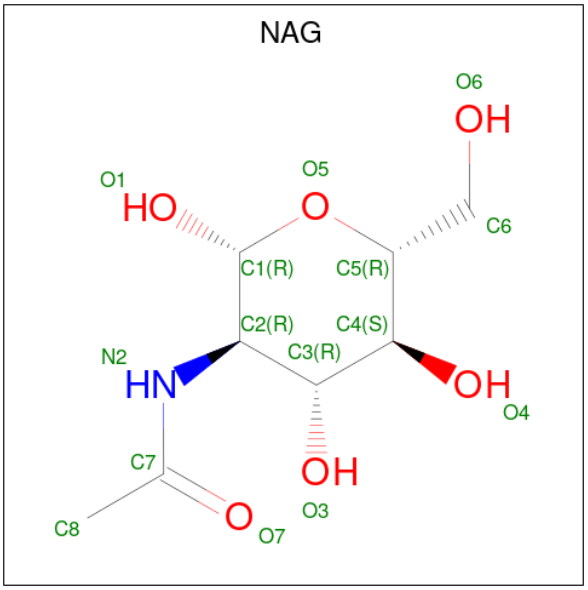


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	2	28	16	2	10	0	0	0

- Molecule 5 is an oligosaccharide called beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.

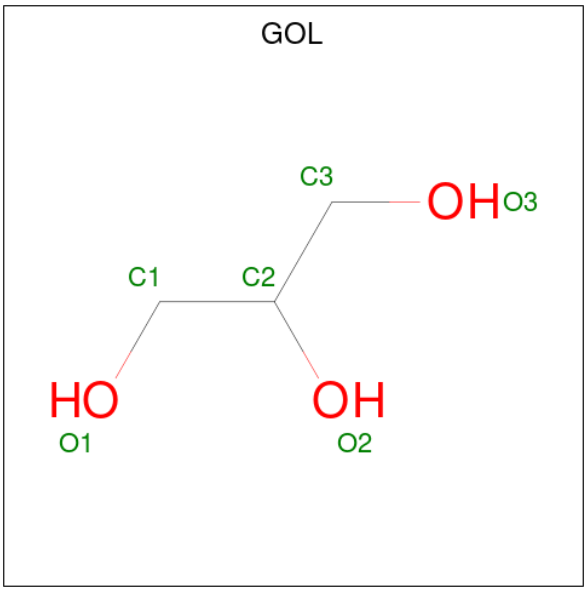
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	E	2	23	12		11	0	0	0
5	F	2	23	12		11	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	14	8	1	5	0	0
6	B	1	14	8	1	5	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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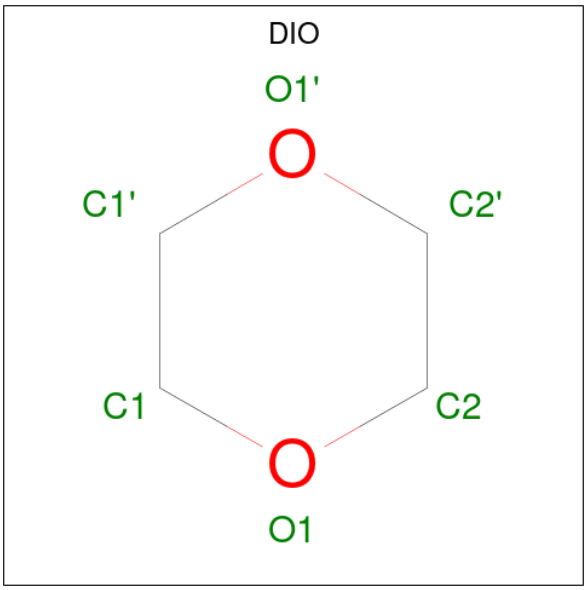
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	B	1	6	3	3	0	0
			Total	C	O		
7	B	1	6	3	3	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

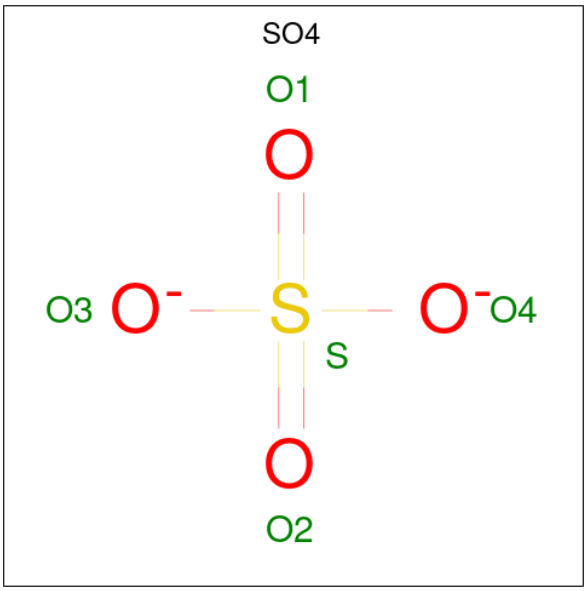
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
8	A	3	3	3	0	0

- Molecule 9 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: $C_4H_8O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	A	1	6	4	2	0	0

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 11 is water.

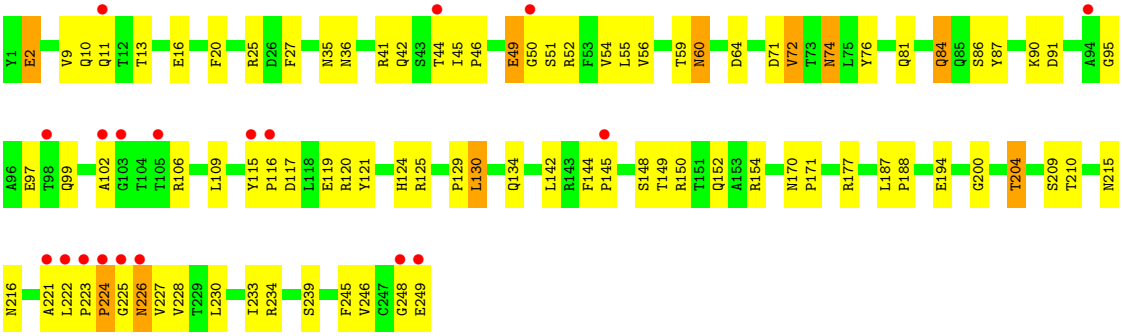
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	127	Total O 127 127	0	0
11	B	201	Total O 201 201	0	0

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.

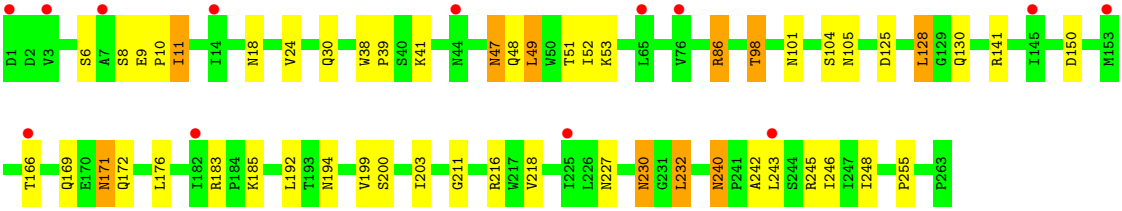
• Molecule 1: lectin I A chain

Chain A:



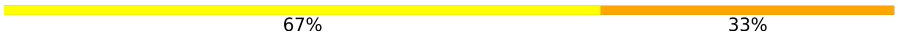
• Molecule 2: lectin I B chain

Chain B:



• Molecule 3: beta-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

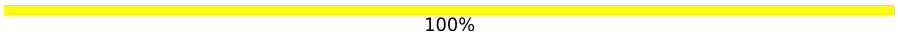
Chain C:



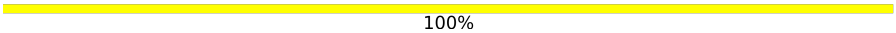
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

- Molecule 5: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain E: 

- Molecule 5: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain F: 

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	106.28Å 106.28Å 312.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.30 25.97 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (10.00-2.30) 99.8 (25.97-2.30)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	3.04 (at 2.31Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.207 , 0.232 0.198 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	40.3	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 53.7	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	0.95	EDS
Total number of atoms	4509	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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, SO4, FUL, BGC, GOL, NAG, DIO, GAL

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	0.46	0/1960	0.70	0/2670
2	B	0.49	0/2039	0.76	0/2782
All	All	0.47	0/3999	0.73	0/5452

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	1921	0	1899	97	0
2	B	2000	0	1931	58	0
3	C	38	0	34	4	0
4	D	28	0	25	2	0
5	E	23	0	21	0	0
5	F	23	0	21	0	0
6	A	14	0	13	1	0
6	B	14	0	13	0	0
7	A	48	0	32	11	0
7	B	48	0	33	4	0
8	A	3	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	6	0	8	1	0
10	A	15	0	0	3	0
11	A	127	0	0	2	0
11	B	201	0	0	5	0
All	All	4509	0	4030	158	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 19.

The worst 5 of 158 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:A:9:VAL:HG23	1:A:11:GLN:H	1.09	1.09
1:A:84:GLN:NE2	1:A:84:GLN:H	1.56	1.04
2:B:41:LYS:H	2:B:48:GLN:HE22	1.15	0.92
2:B:18:ASN:HD22	2:B:183:ARG:HH22	1.18	0.90
1:A:245:PHE:HE1	1:A:248:GLY:H	1.02	0.90

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	247/249 (99%)	239 (97%)	7 (3%)	1 (0%)	34 42
2	B	261/263 (99%)	252 (97%)	9 (3%)	0	100 100
All	All	508/512 (99%)	491 (97%)	16 (3%)	1 (0%)	47 58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	PRO

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	209/209 (100%)	191 (91%)	18 (9%)	10	12
2	B	219/219 (100%)	204 (93%)	15 (7%)	16	21
All	All	428/428 (100%)	395 (92%)	33 (8%)	13	16

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	192	LEU
2	B	218	VAL
2	B	240	ASN
1	A	187	LEU
1	A	142	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	30	GLN
2	B	240	ASN
2	B	101	ASN
2	B	227	ASN
2	B	48	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)

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	$\#\|Z\| > 2$
3	NAG	C	1	3,2	14,14,15	0.71	0	17,19,21	0.83	0
3	FUL	C	2	3	10,10,11	0.47	0	14,14,16	0.66	0
3	NAG	C	3	3	14,14,15	0.78	0	17,19,21	0.96	2 (11%)
4	NAG	D	1	2,4	14,14,15	0.38	0	17,19,21	0.89	0
4	NAG	D	2	4	14,14,15	0.52	0	17,19,21	0.73	1 (5%)
5	BGC	E	1	5	12,12,12	1.00	0	17,17,17	0.98	1 (5%)
5	GAL	E	2	5	11,11,12	1.39	2 (18%)	15,15,17	1.28	2 (13%)
5	BGC	F	1	5	12,12,12	0.87	0	17,17,17	0.84	1 (5%)
5	GAL	F	2	5	11,11,12	1.35	1 (9%)	15,15,17	1.41	3 (20%)

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	NAG	C	1	3,2	-	1/6/23/26	0/1/1/1
3	FUL	C	2	3	-	-	0/1/1/1
3	NAG	C	3	3	-	4/6/23/26	0/1/1/1
4	NAG	D	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	1/6/23/26	0/1/1/1
5	BGC	E	1	5	-	2/2/22/22	0/1/1/1
5	GAL	E	2	5	-	0/2/19/22	0/1/1/1
5	BGC	F	1	5	-	2/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GAL	F	2	5	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	2	GAL	O5-C5	3.20	1.49	1.43
5	E	2	GAL	O5-C5	2.84	1.49	1.43
5	E	2	GAL	O5-C1	2.06	1.47	1.43

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	2	GAL	O5-C5-C6	2.46	111.06	107.20
5	E	2	GAL	O2-C2-C1	2.39	114.04	109.15
5	F	2	GAL	O2-C2-C1	2.39	114.04	109.15
5	E	1	BGC	O3-C3-C2	-2.24	105.17	110.35
4	D	2	NAG	C2-N2-C7	-2.24	119.72	122.90

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	3	NAG	C8-C7-N2-C2
3	C	3	NAG	O7-C7-N2-C2
5	E	1	BGC	O5-C5-C6-O6
5	F	1	BGC	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6

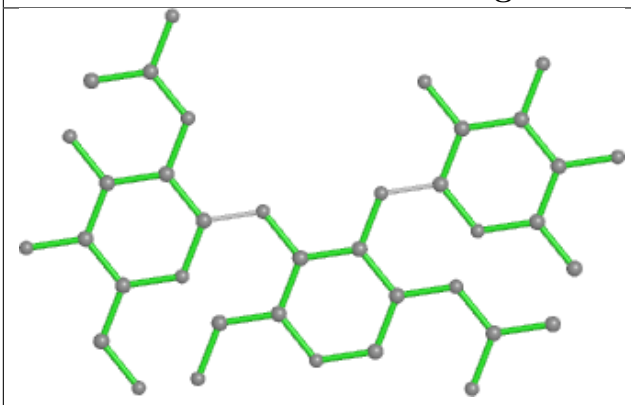
There are no ring outliers.

4 monomers are involved in 6 short contacts:

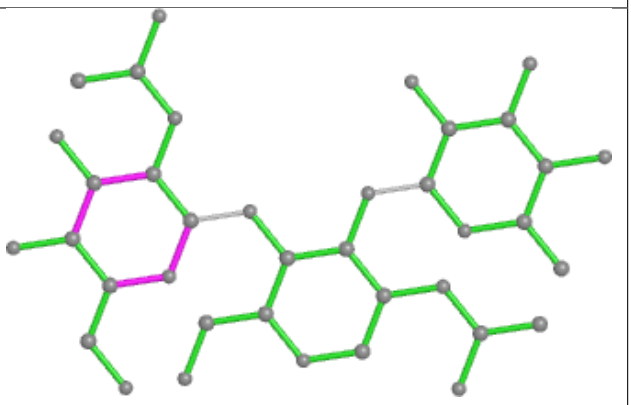
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2	FUL	2	0
4	D	2	NAG	2	0
3	C	3	NAG	3	0
3	C	1	NAG	2	0

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

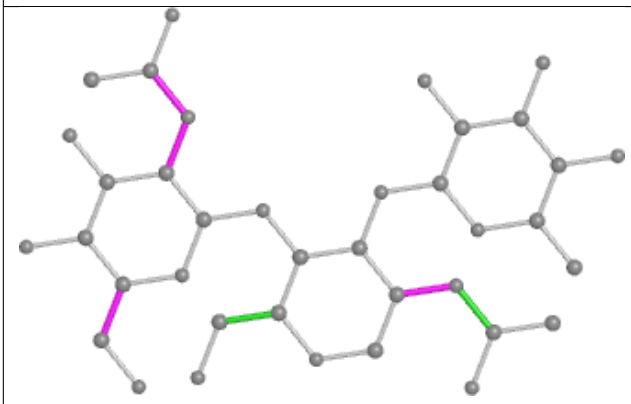
Oligosaccharide Chain C



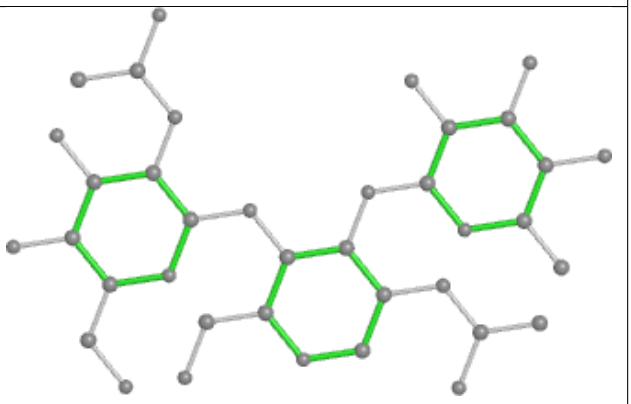
Bond lengths



Bond angles

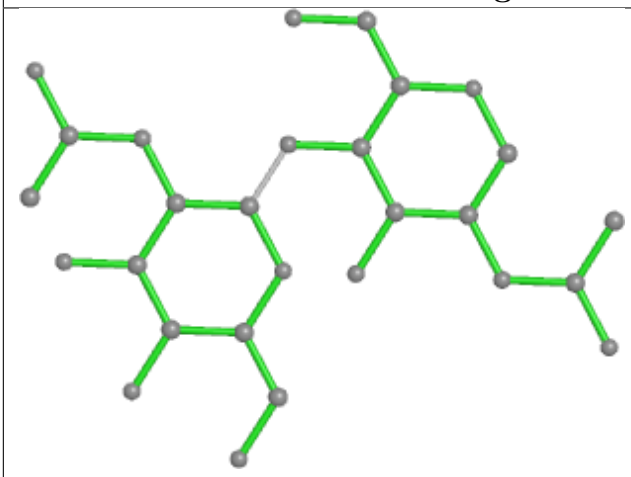


Torsions

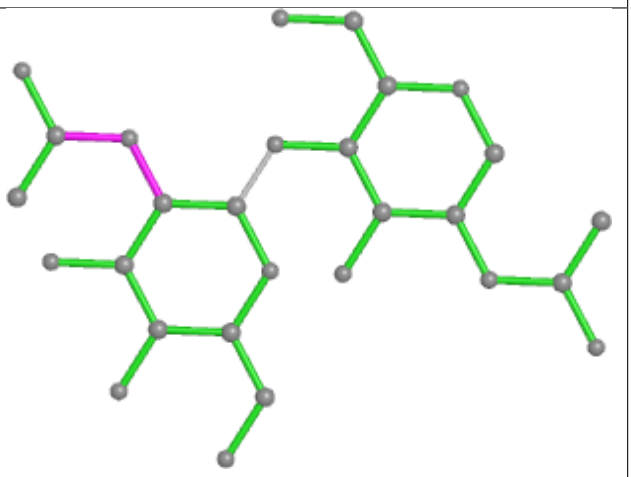


Rings

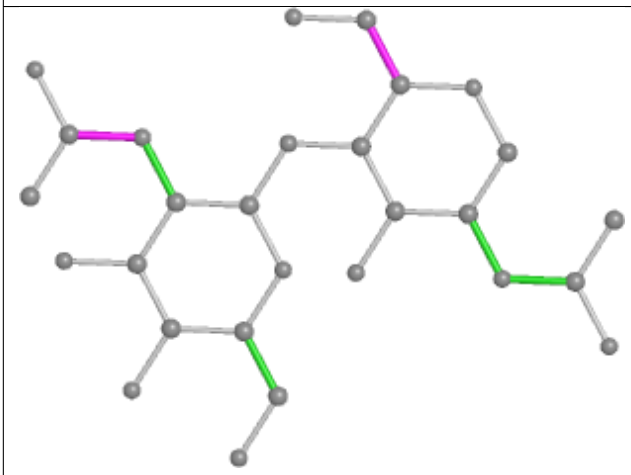
Oligosaccharide Chain D



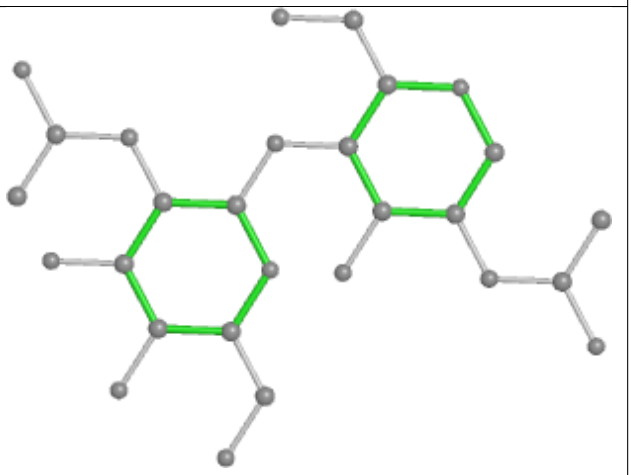
Bond lengths



Bond angles

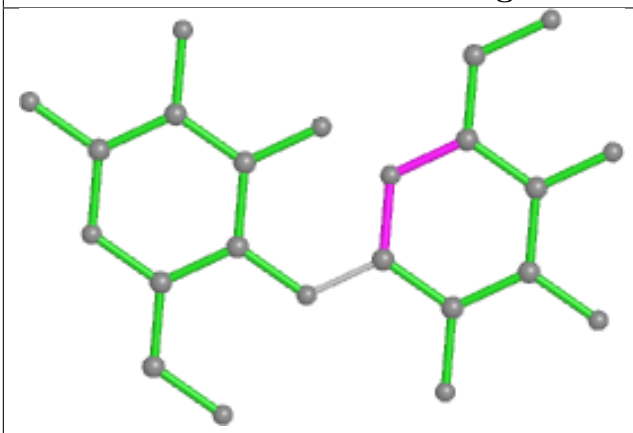


Torsions

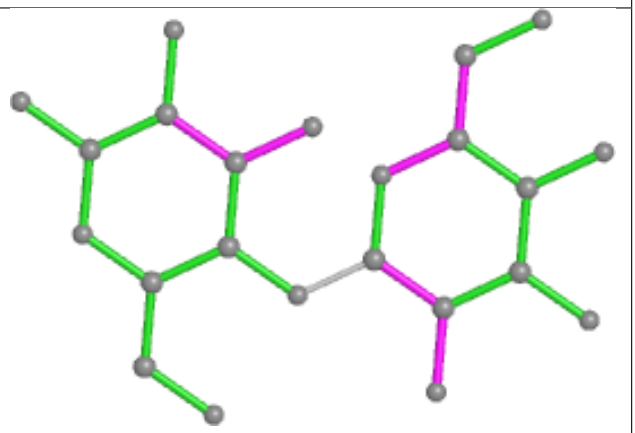


Rings

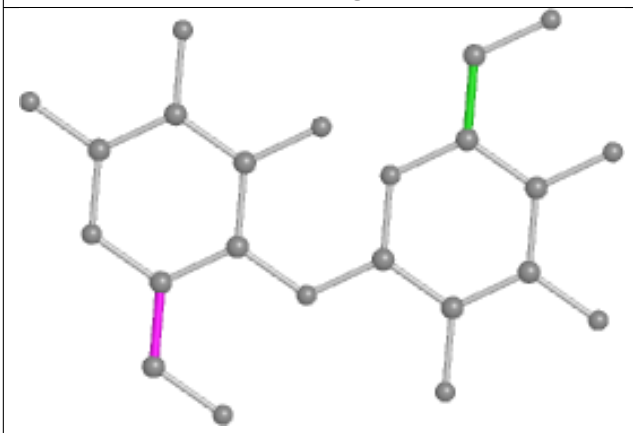
Oligosaccharide Chain E



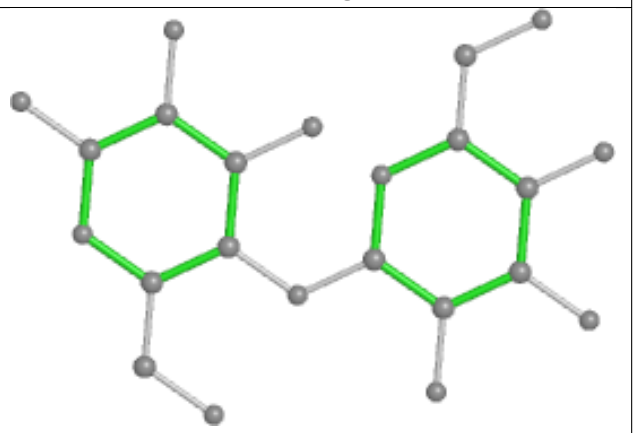
Bond lengths



Bond angles

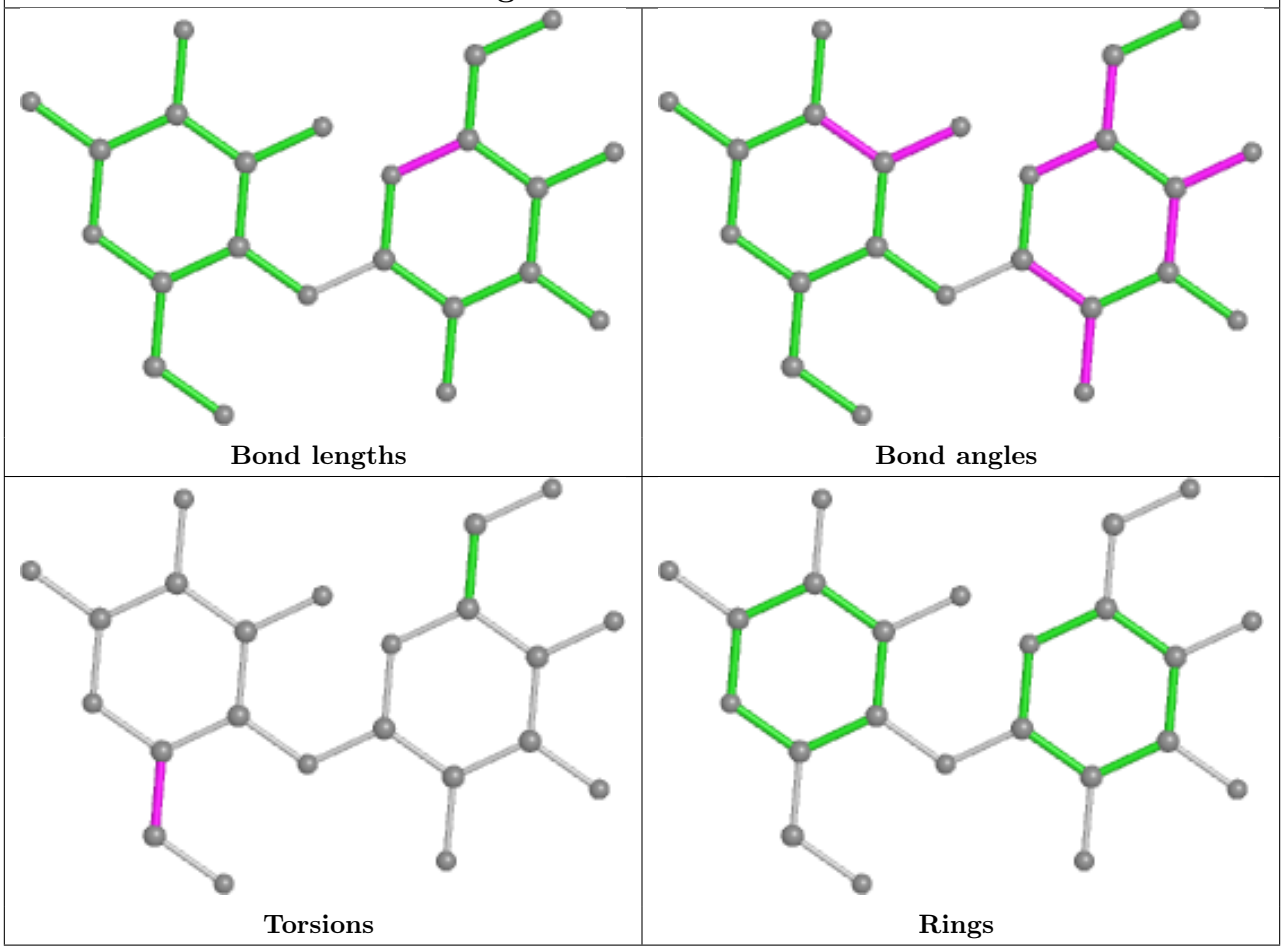


Torsions



Rings

Oligosaccharide Chain F



5.6 Ligand geometry (i)

Of 25 ligands modelled in this entry, 3 are monoatomic - leaving 22 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	$\#\|Z\| > 2$
10	SO4	A	2023	-	4,4,4	0.25	0	6,6,6	0.11	0
7	GOL	A	1067	-	5,5,5	4.59	5 (100%)	5,5,5	5.78	3 (60%)
7	GOL	B	1068	-	5,5,5	4.64	5 (100%)	5,5,5	5.79	3 (60%)
10	SO4	A	2032	-	4,4,4	0.29	0	6,6,6	0.15	0
7	GOL	B	1089	-	5,5,5	4.57	5 (100%)	5,5,5	5.73	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	GOL	A	1021	-	5,5,5	4.56	5 (100%)	5,5,5	5.75	3 (60%)
7	GOL	B	1088	-	5,5,5	4.59	5 (100%)	5,5,5	5.75	3 (60%)
7	GOL	B	1071	-	5,5,5	4.34	4 (80%)	5,5,5	5.89	3 (60%)
7	GOL	B	1070	-	5,5,5	4.48	5 (100%)	5,5,5	5.78	3 (60%)
10	SO4	A	2022	-	4,4,4	0.27	0	6,6,6	0.23	0
7	GOL	B	1095	-	5,5,5	4.52	5 (100%)	5,5,5	5.77	3 (60%)
7	GOL	A	1025	-	5,5,5	4.48	5 (100%)	5,5,5	5.78	3 (60%)
7	GOL	A	1090	-	5,5,5	4.62	5 (100%)	5,5,5	5.78	3 (60%)
6	NAG	A	703	1	14,14,15	0.71	0	17,19,21	0.93	1 (5%)
9	DIO	A	1830	-	6,6,6	1.72	1 (16%)	6,6,6	0.33	0
7	GOL	A	1096	-	5,5,5	4.51	5 (100%)	5,5,5	5.80	3 (60%)
7	GOL	A	1237	-	5,5,5	4.64	5 (100%)	5,5,5	5.79	3 (60%)
7	GOL	A	1031	-	5,5,5	4.75	5 (100%)	5,5,5	5.85	3 (60%)
7	GOL	B	1041	-	5,5,5	4.48	5 (100%)	5,5,5	5.78	3 (60%)
7	GOL	A	1069	-	5,5,5	4.56	5 (100%)	5,5,5	5.81	3 (60%)
7	GOL	B	1091	-	5,5,5	4.57	5 (100%)	5,5,5	5.81	3 (60%)
6	NAG	B	701	2	14,14,15	0.61	0	17,19,21	0.90	1 (5%)

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
7	GOL	A	1067	-	-	2/4/4/4	-
7	GOL	B	1068	-	-	2/4/4/4	-
7	GOL	B	1089	-	-	2/4/4/4	-
7	GOL	A	1021	-	-	2/4/4/4	-
7	GOL	B	1088	-	-	2/4/4/4	-
7	GOL	B	1071	-	-	2/4/4/4	-
7	GOL	B	1070	-	-	2/4/4/4	-
7	GOL	B	1095	-	-	2/4/4/4	-
7	GOL	A	1025	-	-	2/4/4/4	-
7	GOL	A	1090	-	-	3/4/4/4	-
6	NAG	A	703	1	-	4/6/23/26	0/1/1/1
9	DIO	A	1830	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	A	1096	-	-	3/4/4/4	-
7	GOL	A	1237	-	-	2/4/4/4	-
7	GOL	A	1031	-	-	2/4/4/4	-
7	GOL	B	1041	-	-	2/4/4/4	-
7	GOL	A	1069	-	-	2/4/4/4	-
7	GOL	B	1091	-	-	2/4/4/4	-
6	NAG	B	701	2	-	4/6/23/26	0/1/1/1

The worst 5 of 80 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1090	GOL	C3-C2	-7.91	1.19	1.51
7	A	1031	GOL	C3-C2	-7.88	1.19	1.51
7	B	1088	GOL	C3-C2	-7.69	1.20	1.51
7	A	1237	GOL	C3-C2	-7.67	1.20	1.51
7	B	1089	GOL	C3-C2	-7.64	1.20	1.51

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	1071	GOL	O3-C3-C2	10.96	162.75	110.20
7	A	1090	GOL	O3-C3-C2	10.72	161.61	110.20
7	B	1068	GOL	O3-C3-C2	10.61	161.09	110.20
7	A	1096	GOL	O3-C3-C2	10.60	161.03	110.20
7	A	1237	GOL	O3-C3-C2	10.57	160.88	110.20

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	703	NAG	C8-C7-N2-C2
6	A	703	NAG	O7-C7-N2-C2
7	A	1021	GOL	C1-C2-C3-O3
7	A	1025	GOL	O1-C1-C2-C3
7	A	1025	GOL	C1-C2-C3-O3

There are no ring outliers.

11 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	2032	SO4	1	0
7	A	1021	GOL	1	0
7	B	1088	GOL	1	0
10	A	2022	SO4	2	0
7	B	1095	GOL	1	0
6	A	703	NAG	1	0
9	A	1830	DIO	1	0
7	A	1237	GOL	2	0
7	A	1031	GOL	6	0
7	A	1069	GOL	2	0
7	B	1091	GOL	2	0

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	249/249 (100%)	0.31	19 (7%)	13	18	25, 38, 62, 70	6 (2%)
2	B	263/263 (100%)	0.04	13 (4%)	29	36	21, 30, 49, 64	0
All	All	512/512 (100%)	0.17	32 (6%)	20	25	21, 34, 57, 70	6 (1%)

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	PRO	7.2
1	A	248	GLY	6.1
1	A	115	TYR	5.4
2	B	1	ASP	3.8
1	A	222	LEU	3.6

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
3	NAG	C	3	14/15	0.72	0.31	67,68,70,71	14
3	NAG	C	1	14/15	0.81	0.33	58,64,66,67	0
3	FUL	C	2	10/11	0.84	0.34	67,67,68,68	10
5	BGC	F	1	12/12	0.84	0.50	67,74,76,78	0
4	NAG	D	2	14/15	0.85	0.32	54,56,61,62	0

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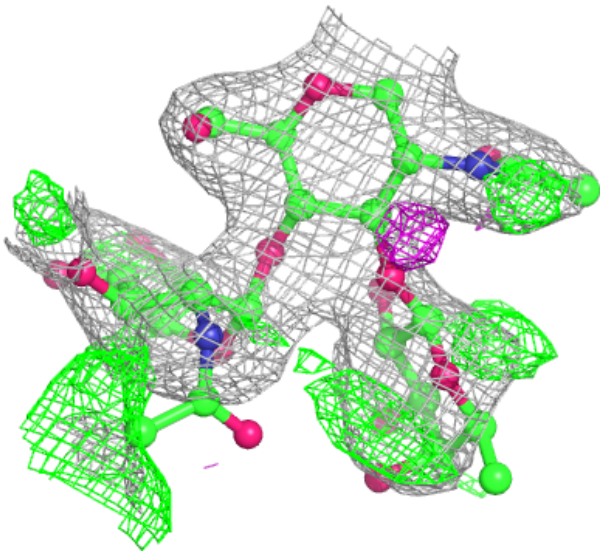
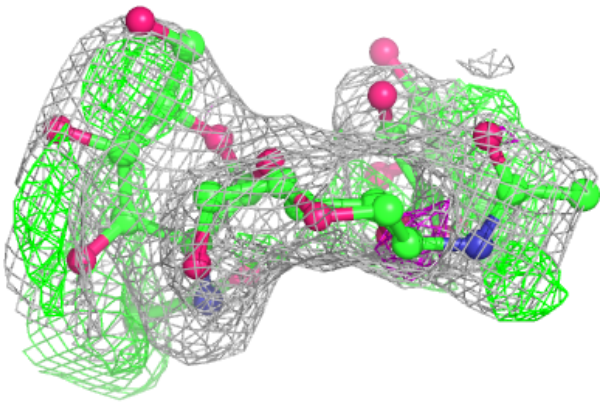
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GAL	F	2	11/12	0.87	0.23	51,57,60,61	0
5	BGC	E	1	12/12	0.90	0.32	51,59,62,64	0
5	GAL	E	2	11/12	0.92	0.13	31,40,44,47	0
4	NAG	D	1	14/15	0.95	0.13	31,38,48,51	0

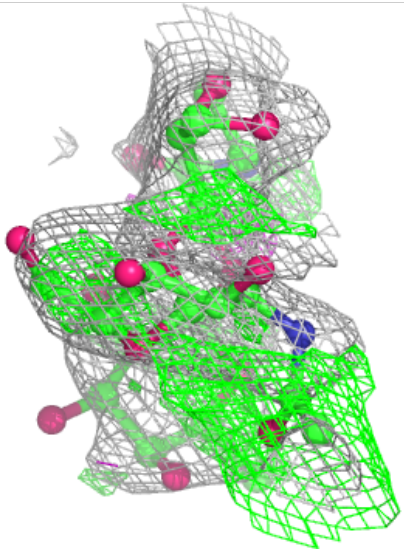
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

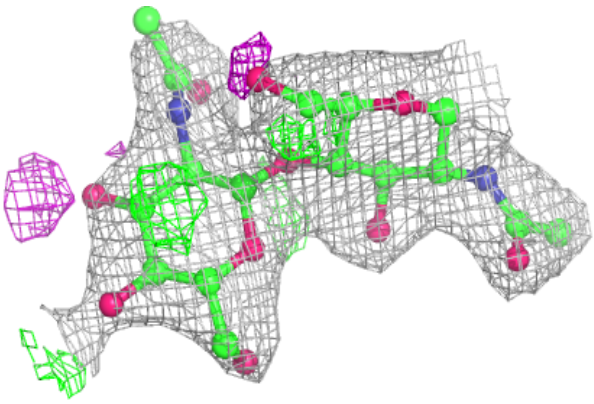


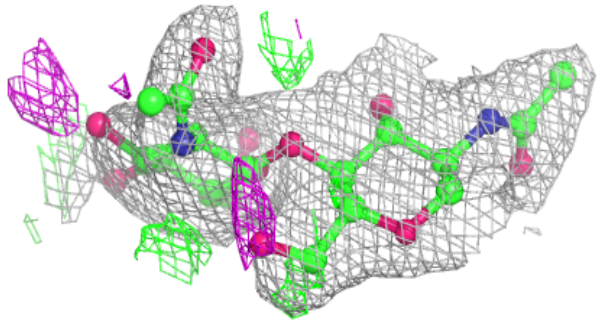


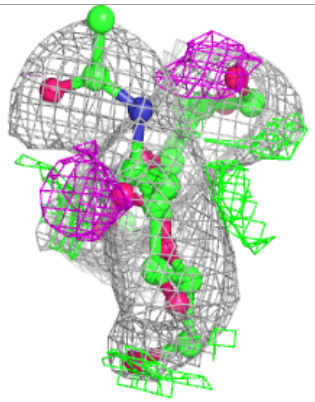


Electron density around Chain D:

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

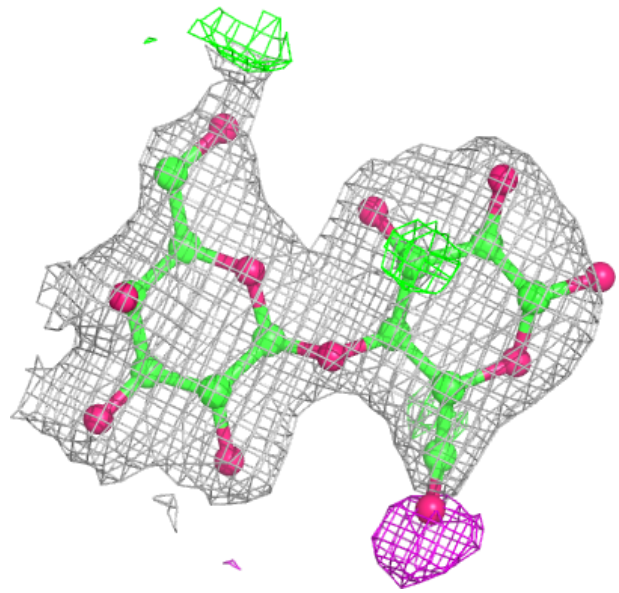


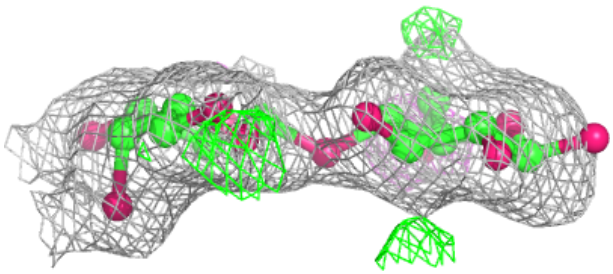


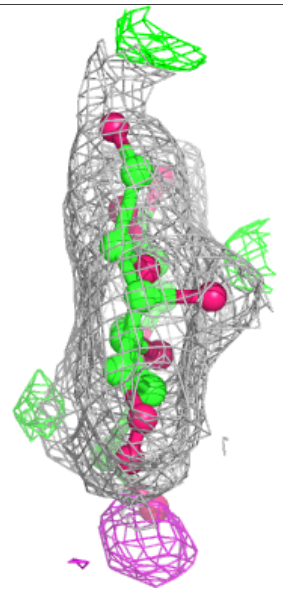


Electron density around Chain E:

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

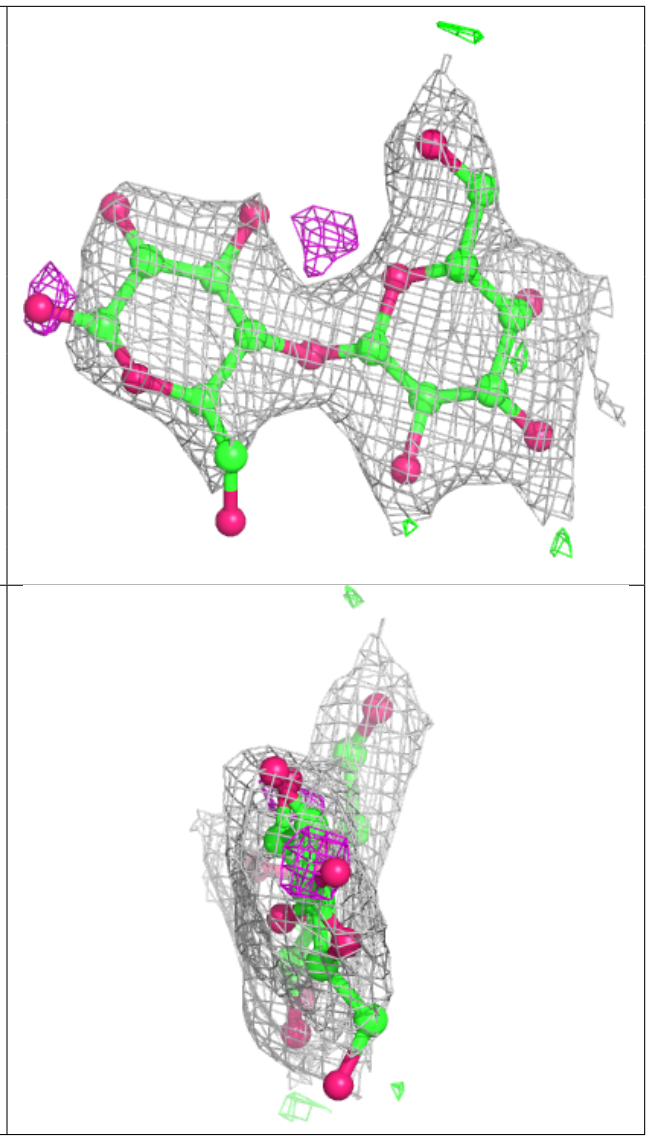






Electron density around Chain F:

$2mF_o$-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)

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
7	GOL	B	1041	6/6	0.43	0.48	84,86,86,86	0
7	GOL	A	1025	6/6	0.52	0.47	85,85,86,86	0
7	GOL	B	1095	6/6	0.59	0.29	76,77,78,79	0
7	GOL	B	1071	6/6	0.67	0.34	38,42,46,46	0
7	GOL	A	1021	6/6	0.71	0.27	87,88,89,89	0
7	GOL	A	1031	6/6	0.74	0.53	80,81,81,83	0
6	NAG	B	701	14/15	0.75	0.22	46,52,54,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	DIO	A	1830	6/6	0.75	0.48	95,95,95,96	0
7	GOL	B	1091	6/6	0.78	0.31	73,74,75,76	0
7	GOL	A	1237	6/6	0.80	0.27	88,89,89,89	0
7	GOL	B	1070	6/6	0.80	0.17	87,87,87,87	0
7	GOL	A	1096	6/6	0.82	0.24	60,63,65,67	0
6	NAG	A	703	14/15	0.82	0.36	71,75,76,76	0
7	GOL	B	1068	6/6	0.83	0.29	76,76,77,79	0
10	SO4	A	2032	5/5	0.83	0.27	90,90,90,91	0
7	GOL	A	1069	6/6	0.86	0.27	58,61,62,65	0
7	GOL	A	1090	6/6	0.88	0.24	42,44,45,48	0
7	GOL	B	1088	6/6	0.90	0.25	50,53,55,55	0
10	SO4	A	2023	5/5	0.91	0.17	99,99,100,100	0
7	GOL	A	1067	6/6	0.91	0.21	85,87,88,89	0
8	CL	A	1027	1/1	0.93	0.24	85,85,85,85	0
7	GOL	B	1089	6/6	0.94	0.20	39,50,52,53	0
10	SO4	A	2022	5/5	0.96	0.12	55,56,57,59	0
8	CL	A	1042	1/1	0.97	0.07	59,59,59,59	0
8	CL	A	1024	1/1	0.98	0.37	40,40,40,40	1

6.5 Other polymers (i)

There are no such residues in this entry.