



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 21, 2020 – 05:11 PM BST

PDB ID : 2X2I
Title : Crystal structure of the Gracilariopsis lemaneiformis alpha-1,4- glucan lyase with acarbose
Authors : Rozeboom, H.J.; Yu, S.; Madrid, S.; Kalk, K.H.; Dijkstra, B.W.
Deposited on : 2010-01-13
Resolution : 2.60 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 ⓘ symbol.

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	:	2.14.6
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)	:	2.14.6

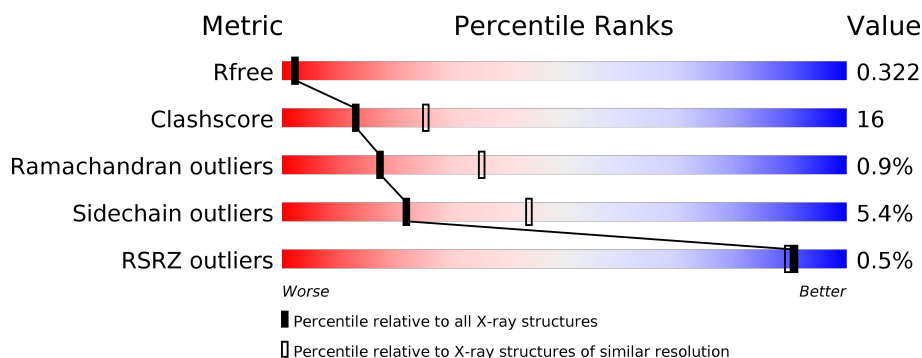
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1027	<div> <div style="width: 67%;"></div> <div style="width: 31%;"></div> <div style="width: 2%;"></div> </div>
1	B	1027	<div> <div style="width: 66%;"></div> <div style="width: 31%;"></div> <div style="width: 3%;"></div> </div>
1	C	1027	<div> <div style="width: 69%;"></div> <div style="width: 29%;"></div> <div style="width: 2%;"></div> </div>
1	D	1027	<div> <div style="width: 65%;"></div> <div style="width: 32%;"></div> <div style="width: 3%;"></div> </div>
2	E	3	<div> <div style="width: 67%;"></div> <div style="width: 33%;"></div> </div>
2	F	3	<div> <div style="width: 33%;"></div> <div style="width: 67%;"></div> </div>

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Mol	Chain	Length	Quality of chain
2	G	3	<div><div></div><div>33%</div><div>33%</div><div>33%</div></div>
2	H	3	<div><div></div><div>33%</div><div>33%</div><div>33%</div></div>
2	I	3	<div><div></div><div>33%</div><div>33%</div><div>33%</div></div>
2	J	3	<div><div></div><div>33%</div><div>33%</div><div>33%</div></div>
2	K	3	<div><div></div><div>33%</div><div>67%</div></div>
2	L	3	<div><div></div><div>33%</div><div>67%</div></div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 33852 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 ALPHA-1,4-GLUCAN LYASE ISOZYME 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1025	Total	C	N	O	S	0	1	0
			8171	5143	1385	1596	47			
1	B	1025	Total	C	N	O	S	0	0	0
			8162	5135	1385	1595	47			
1	C	1025	Total	C	N	O	S	0	1	0
			8171	5143	1385	1596	47			
1	D	1025	Total	C	N	O	S	0	0	0
			8162	5135	1385	1595	47			

- Molecule 2 is an oligosaccharide called 4,6-dideoxy-4-[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	F	3	Total	C	N	O	0	0	1
			33	19	1	13			
2	G	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	H	3	Total	C	N	O	0	0	1
			33	19	1	13			
2	I	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	J	3	Total	C	N	O	0	0	1
			33	19	1	13			
2	K	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	L	3	Total	C	N	O	0	0	1
			33	19	1	13			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

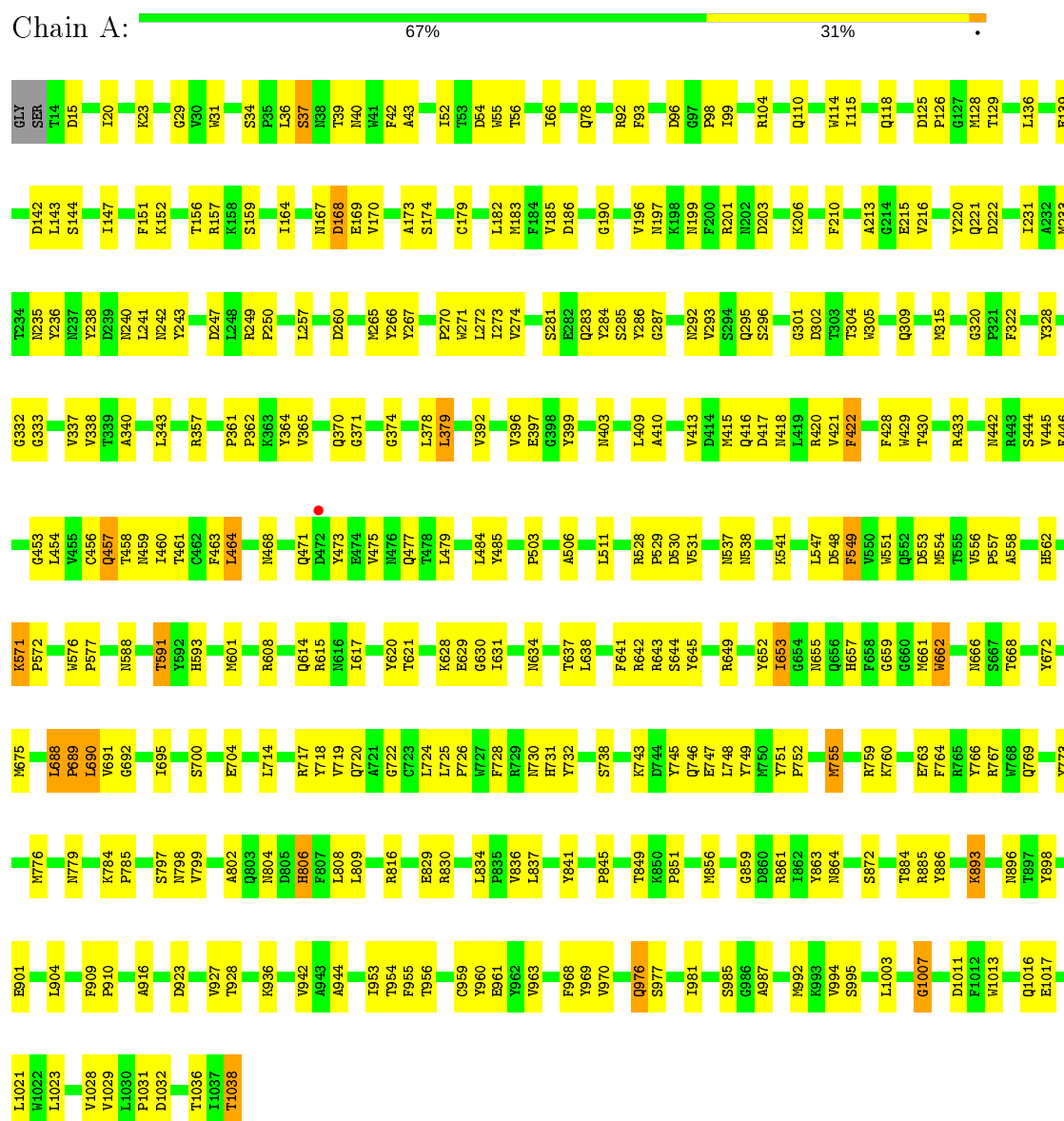
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	239	Total	O	0	0
			239	239		
4	B	178	Total	O	0	0
			178	178		
4	C	274	Total	O	0	0
			274	274		
4	D	145	Total	O	0	0
			145	145		

3 Residue-property plots

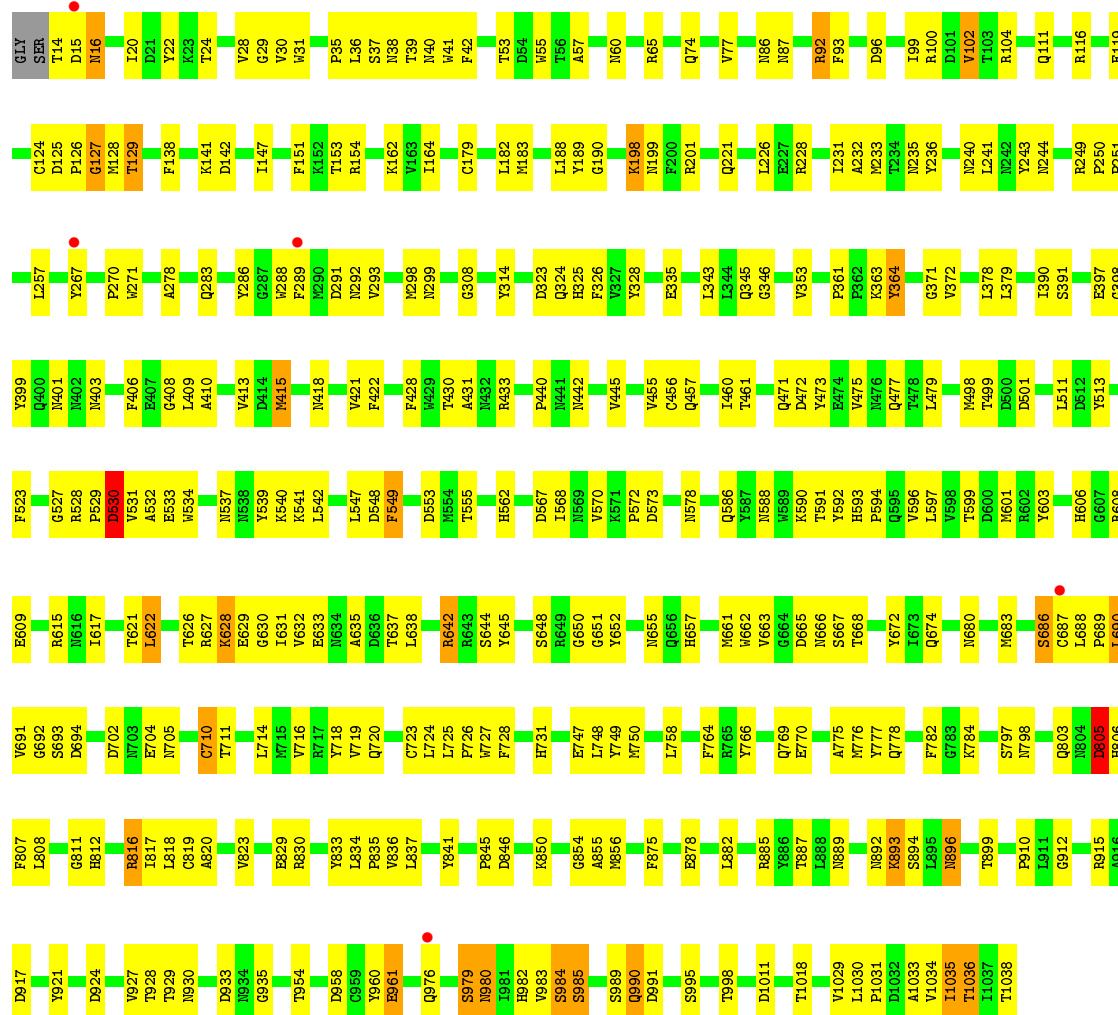
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ALPHA-1,4-GLUCAN LYASE ISOZYME 1



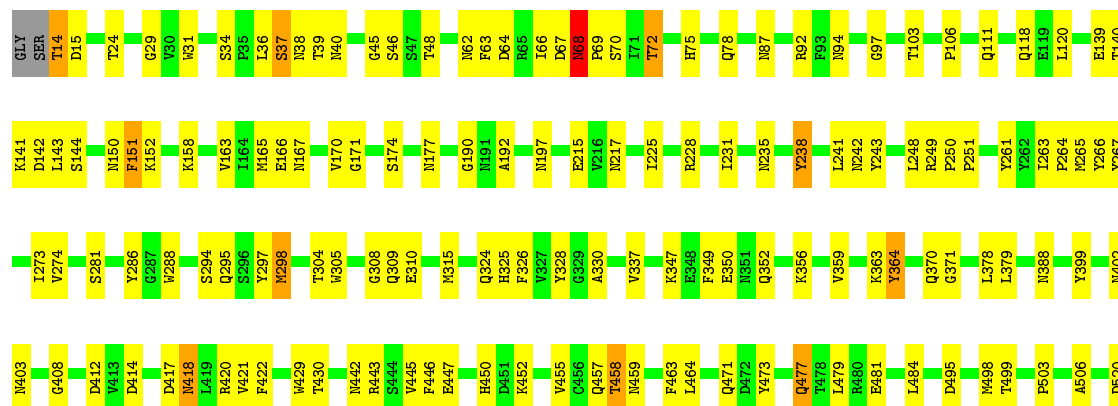
- Molecule 1: ALPHA-1,4-GLUCAN LYASE ISOZYME 1

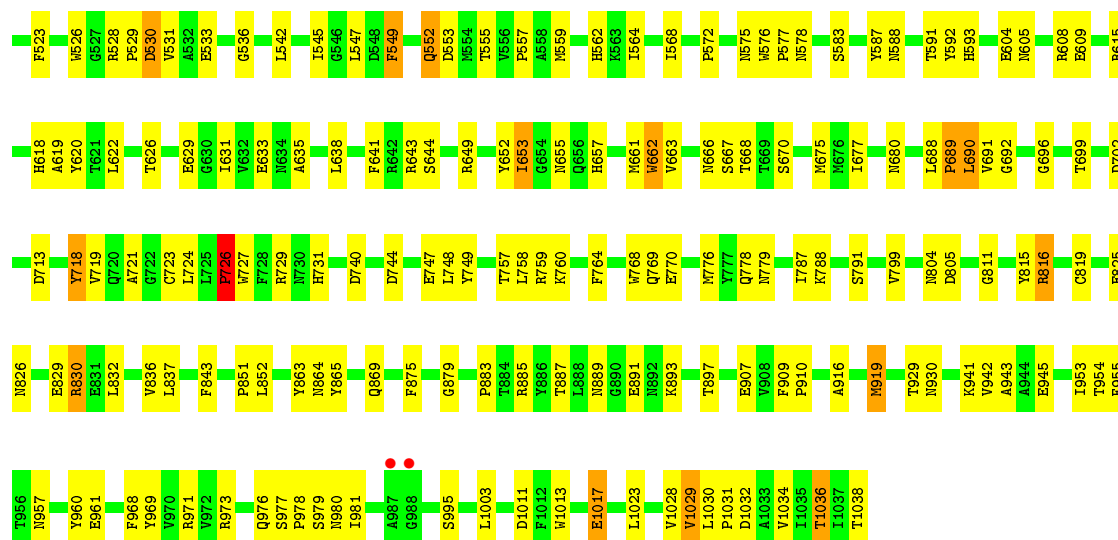
Chain B:  66% 31%



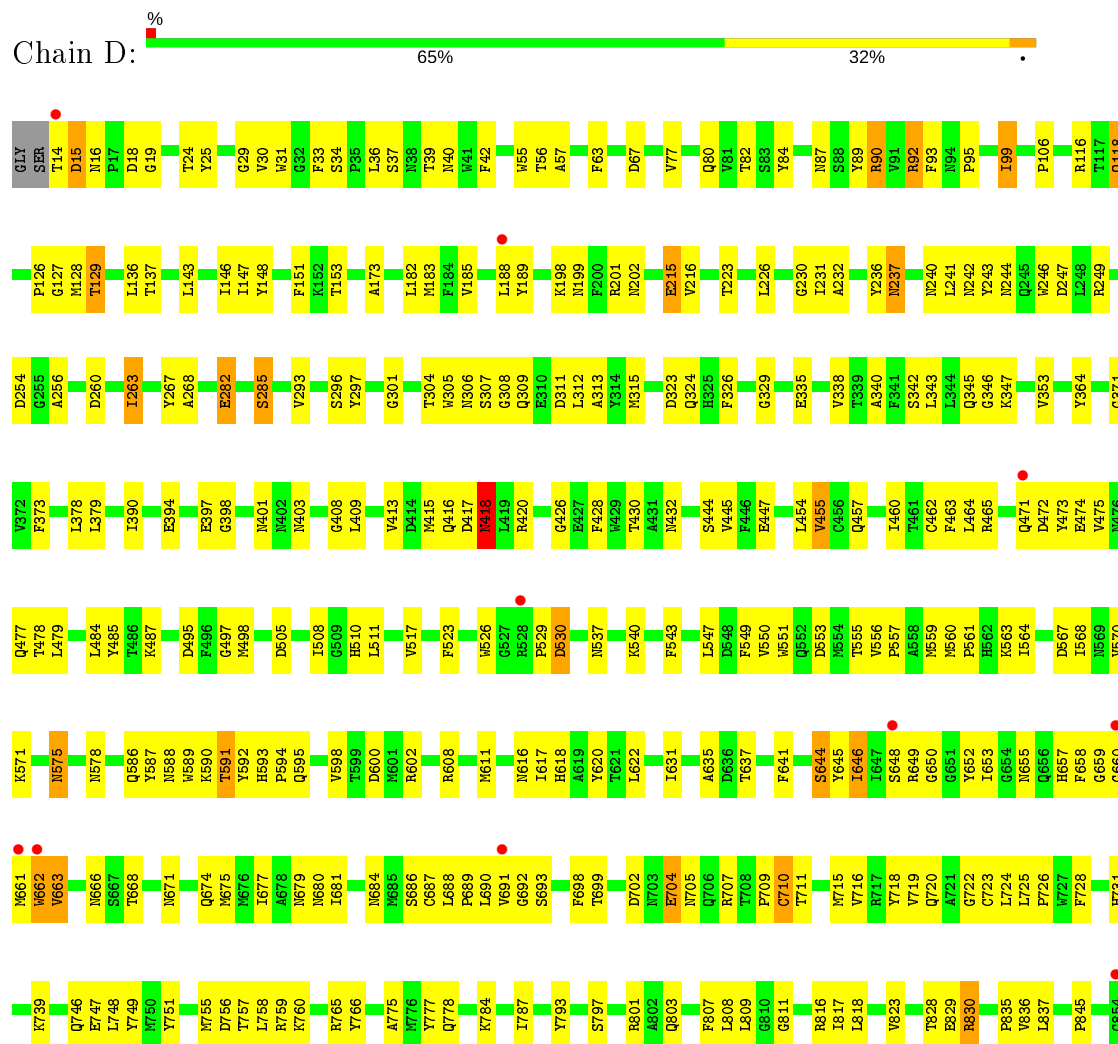
• Molecule 1: ALPHA-1,4-GLUCAN LYASE ISOZYME 1

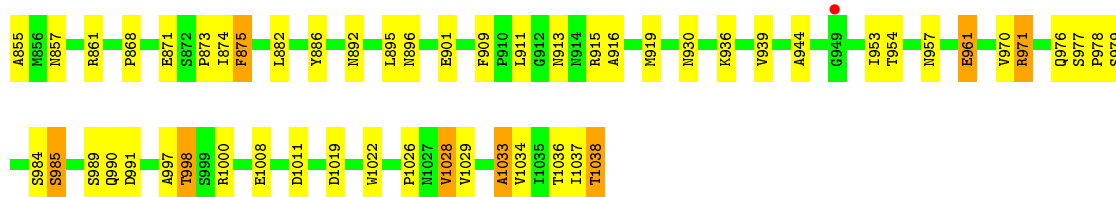
Chain C:  69% 29%





• Molecule 1: ALPHA-1,4-GLUCAN LYASE ISOZYME 1





- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino\}$ - α -D-glucopyranose-(1-4)- α -D-glucopyranose-(1-4)- β -D-glucopyranose

Chain E: 67% 33%



- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino\}$ - α -D-glucopyranose-(1-4)- α -D-glucopyranose-(1-4)- β -D-glucopyranose

Chain F: 33% 67%



- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino\}$ - α -D-glucopyranose-(1-4)- α -D-glucopyranose-(1-4)- β -D-glucopyranose

Chain G: 33% 33% 33%



- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino\}$ - α -D-glucopyranose-(1-4)- α -D-glucopyranose-(1-4)- β -D-glucopyranose

Chain H: 33% 33% 33%



- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino\}$ - α -D-glucopyranose-(1-4)- α -D-glucopyranose-(1-4)- β -D-glucopyranose

Chain I: 33% 33% 33%



- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino\}$ - α -D-glucopyranose-(1-4)- α -D-glucopyranose-(1-4)- β -D-glucopyranose

Chain J: 33% 33% 33%



- Molecule 2: 4,6-dideoxy-4-[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain K:



- Molecule 2: 4,6-dideoxy-4-[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain L:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	134.86Å 91.80Å 193.35Å 90.00° 99.34° 90.00°	Depositor
Resolution (Å)	41.85 – 2.60 41.84 – 2.60	Depositor EDS
% Data completeness (in resolution range)	82.2 (41.85-2.60) 82.2 (41.84-2.60)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.229 , 0.320 0.233 , 0.322	Depositor DCC
R_{free} test set	5895 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	33852	wwPDB-VP
Average B, all atoms (Å ²)	40.0	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 54.12 % 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 3.8208e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GLC, GOL, CSO, BGC, AC1

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	0.50	0/8387	0.65	1/11407 (0.0%)
1	B	0.47	0/8374	0.62	0/11389
1	C	0.50	0/8387	0.64	0/11407
1	D	0.46	0/8374	0.62	0/11389
All	All	0.49	0/33522	0.63	1/45592 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	ASP	CB-CG-OD1	5.45	123.21	118.30

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	8171	0	7615	256	0
1	B	8162	0	7606	263	0
1	C	8171	0	7615	256	0
1	D	8162	0	7606	267	0
2	E	44	0	30	1	0
2	F	33	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	44	0	30	2	0
2	H	33	0	19	2	0
2	I	44	0	30	3	0
2	J	33	0	19	2	0
2	K	44	0	30	4	0
2	L	33	0	19	3	0
3	A	24	0	32	4	0
3	C	12	0	16	1	0
3	D	6	0	8	1	0
4	A	239	0	0	32	0
4	B	178	0	0	31	0
4	C	274	0	0	22	0
4	D	145	0	0	30	0
All	All	33852	0	30694	1043	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 16.

The worst 5 of 1043 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:118:GLN:HB3	4:A:2029:HOH:O	1.39	1.19
1:B:766:TYR:O	1:B:769:GLN:HG2	1.44	1.17
1:B:14:THR:HG23	1:B:15:ASP:H	1.11	1.10
1:C:34:SER:O	1:C:37:SER:HB2	1.52	1.09
1:A:34:SER:O	1:A:37:SER:HB2	1.53	1.09

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	1023/1027 (100%)	936 (92%)	80 (8%)	7 (1%)	22	43
1	B	1022/1027 (100%)	912 (89%)	101 (10%)	9 (1%)	17	35
1	C	1023/1027 (100%)	932 (91%)	84 (8%)	7 (1%)	22	43
1	D	1022/1027 (100%)	913 (89%)	94 (9%)	15 (2%)	10	21
All	All	4090/4108 (100%)	3693 (90%)	359 (9%)	38 (1%)	17	35

5 of 38 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	653	ILE
1	B	985	SER
1	C	68	ASN
1	D	173	ALA
1	A	422	PHE

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	878/878 (100%)	836 (95%)	42 (5%)	25	49
1	B	877/878 (100%)	824 (94%)	53 (6%)	19	39
1	C	878/878 (100%)	834 (95%)	44 (5%)	24	47
1	D	877/878 (100%)	826 (94%)	51 (6%)	20	40
All	All	3510/3512 (100%)	3320 (95%)	190 (5%)	22	44

5 of 190 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	958	ASP
1	C	359	VAL
1	D	828	THR
1	B	984	SER
1	C	37	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	930	ASN
1	C	325	HIS
1	D	826	ASN
1	B	934	ASN
1	C	177	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CSO	B	336	1	3,6,7	0.67	0	0,6,8	0.00	-
1	CSO	D	336	1	3,6,7	0.63	0	0,6,8	0.00	-
1	CSO	A	336	1	3,6,7	0.74	0	0,6,8	0.00	-
1	CSO	C	336	1	3,6,7	0.71	0	0,6,8	0.00	-

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
1	CSO	B	336	1	-	0/1/5/7	-
1	CSO	D	336	1	-	0/1/5/7	-
1	CSO	A	336	1	-	0/1/5/7	-
1	CSO	C	336	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

Of 24 monosaccharides modelled in this entry, 20 were used 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	$\# Z > 2$
2	BGC	E	1	2	12,12,12	0.60	0	17,17,17	1.30	2 (11%)
2	GLC	E	2	2	11,11,12	0.54	0	15,15,17	1.10	2 (13%)
2	AC1	E	3	2	21,22,23	0.56	0	22,32,34	1.57	4 (18%)
2	GLC	F	2	2	11,11,12	0.71	0	15,15,17	1.79	3 (20%)
2	AC1	F	3	2	21,22,23	2.59	1 (4%)	22,32,34	1.23	2 (9%)
2	BGC	G	1	2	12,12,12	0.45	0	17,17,17	0.61	0
2	GLC	G	2	2	11,11,12	0.41	0	15,15,17	1.31	1 (6%)
2	AC1	G	3	2	21,22,23	0.55	0	22,32,34	1.17	2 (9%)
2	GLC	H	2	2	11,11,12	0.63	0	15,15,17	1.18	2 (13%)
2	AC1	H	3	2	21,22,23	2.57	1 (4%)	22,32,34	1.61	5 (22%)
2	BGC	I	1	2	12,12,12	0.59	0	17,17,17	1.18	2 (11%)
2	GLC	I	2	2	11,11,12	0.23	0	15,15,17	1.07	0
2	AC1	I	3	2	21,22,23	0.74	0	22,32,34	2.02	7 (31%)
2	GLC	J	2	2	11,11,12	0.84	0	15,15,17	1.69	2 (13%)
2	AC1	J	3	2	21,22,23	2.58	1 (4%)	22,32,34	1.59	6 (27%)
2	BGC	K	1	2	12,12,12	0.54	0	17,17,17	0.92	0
2	GLC	K	2	2	11,11,12	0.26	0	15,15,17	1.14	2 (13%)
2	AC1	K	3	2	21,22,23	0.72	1 (4%)	22,32,34	1.60	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	L	2	2	11,11,12	0.53	0	15,15,17	1.40	2 (13%)
2	AC1	L	3	2	21,22,23	1.35	1 (4%)	22,32,34	1.43	4 (18%)

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	GLC	E	2	2	-	0/2/19/22	0/1/1/1
2	AC1	E	3	2	-	4/6/43/46	0/2/2/2
2	GLC	F	2	2	-	2/2/19/22	0/1/1/1
2	AC1	F	3	2	-	1/6/43/46	0/2/2/2
2	BGC	G	1	2	-	0/2/22/22	0/1/1/1
2	GLC	G	2	2	-	2/2/19/22	0/1/1/1
2	AC1	G	3	2	-	5/6/43/46	0/2/2/2
2	GLC	H	2	2	-	2/2/19/22	0/1/1/1
2	AC1	H	3	2	-	1/6/43/46	0/2/2/2
2	BGC	I	1	2	-	2/2/22/22	0/1/1/1
2	GLC	I	2	2	-	1/2/19/22	0/1/1/1
2	AC1	I	3	2	-	4/6/43/46	0/2/2/2
2	GLC	J	2	2	-	0/2/19/22	0/1/1/1
2	AC1	J	3	2	-	1/6/43/46	0/2/2/2
2	BGC	K	1	2	-	0/2/22/22	0/1/1/1
2	GLC	K	2	2	-	0/2/19/22	0/1/1/1
2	AC1	K	3	2	-	2/6/43/46	0/2/2/2
2	GLC	L	2	2	-	2/2/19/22	0/1/1/1
2	AC1	L	3	2	-	2/6/43/46	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	3	AC1	C4-N4A	-11.54	1.27	1.47
2	H	3	AC1	C4-N4A	-11.45	1.28	1.47
2	J	3	AC1	C4-N4A	-11.33	1.28	1.47
2	L	3	AC1	C4-N4A	-4.74	1.39	1.47
2	K	3	AC1	C4A-C5B	-2.43	1.49	1.51

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	GLC	C1-C2-C3	5.35	116.25	109.67
2	K	3	AC1	C2-C3-C4	-5.21	106.04	110.63
2	J	2	GLC	C1-O5-C5	4.76	118.64	112.19
2	E	3	AC1	C2-C3-C4	-4.53	106.63	110.63
2	I	3	AC1	O3B-C3B-C4A	-4.39	101.29	109.68

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

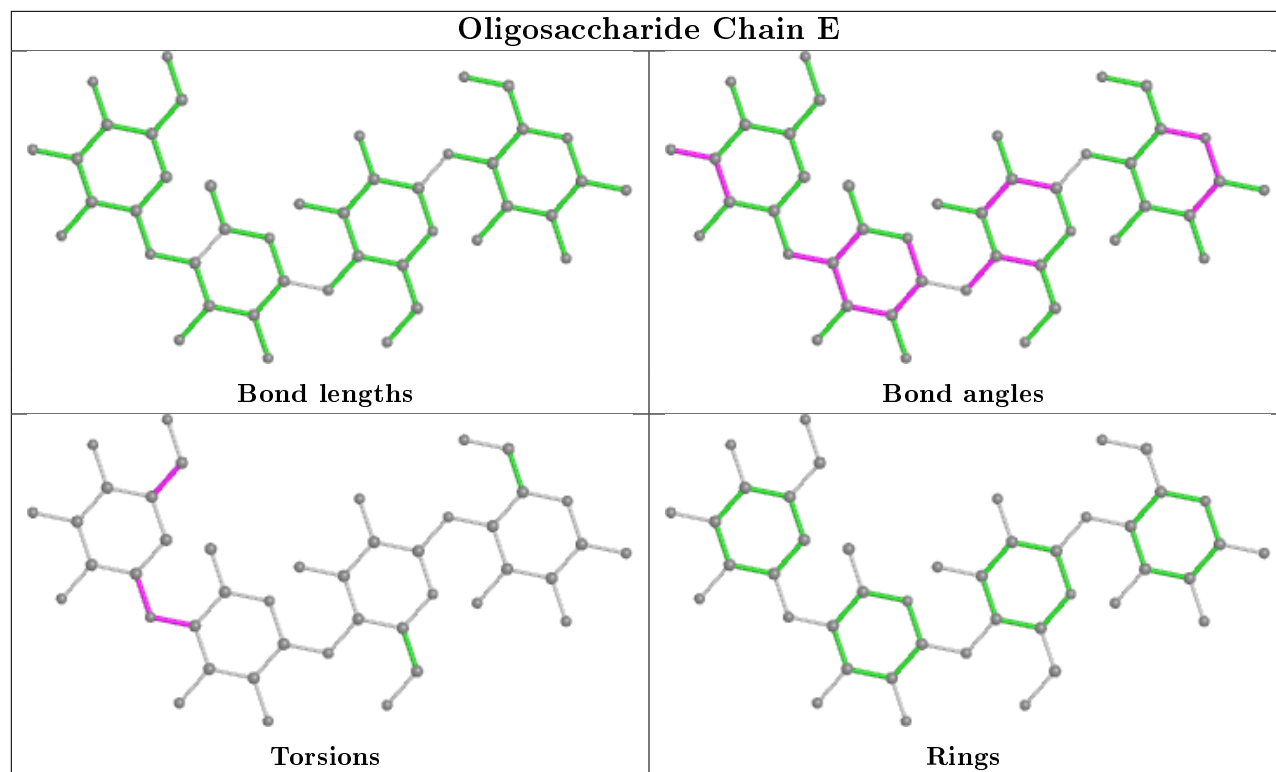
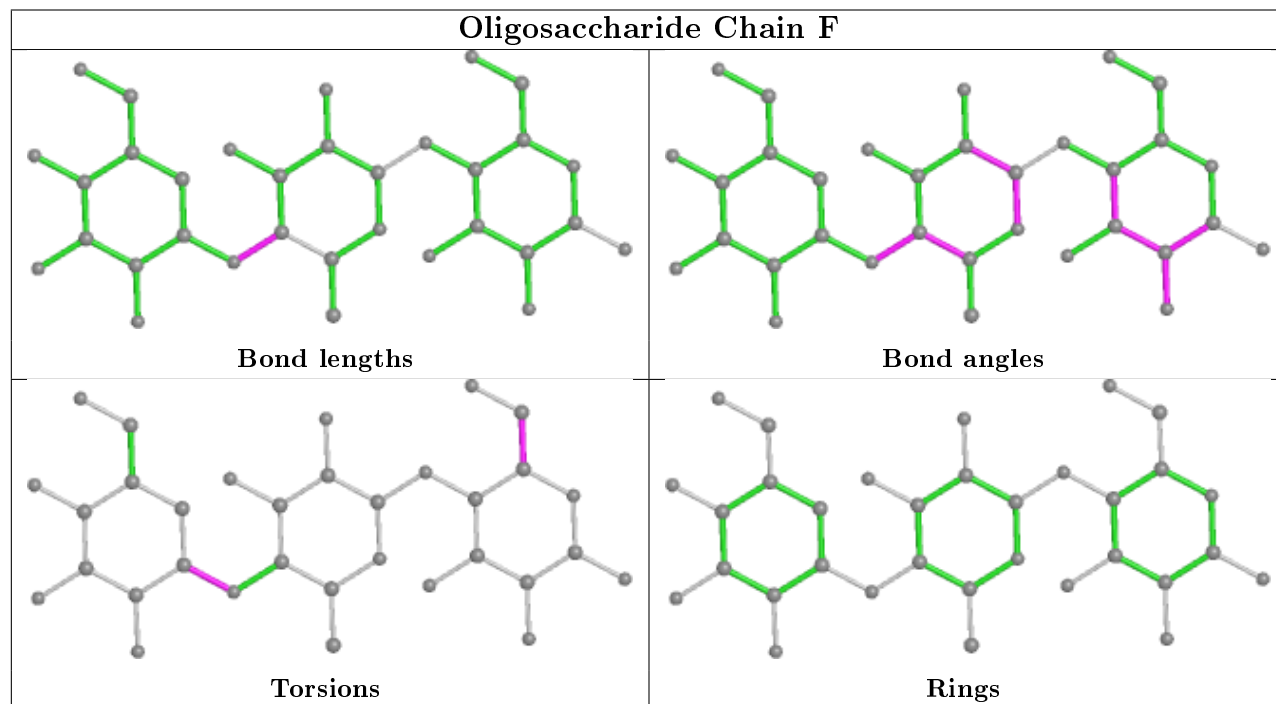
Mol	Chain	Res	Type	Atoms
2	L	3	AC1	C7B-C1B-N4A-C4
2	L	3	AC1	C7B-C5B-C6B-O6B
2	I	3	AC1	C7B-C1B-N4A-C4
2	I	3	AC1	C7B-C5B-C6B-O6B
2	H	3	AC1	C7B-C1B-N4A-C4

There are no ring outliers.

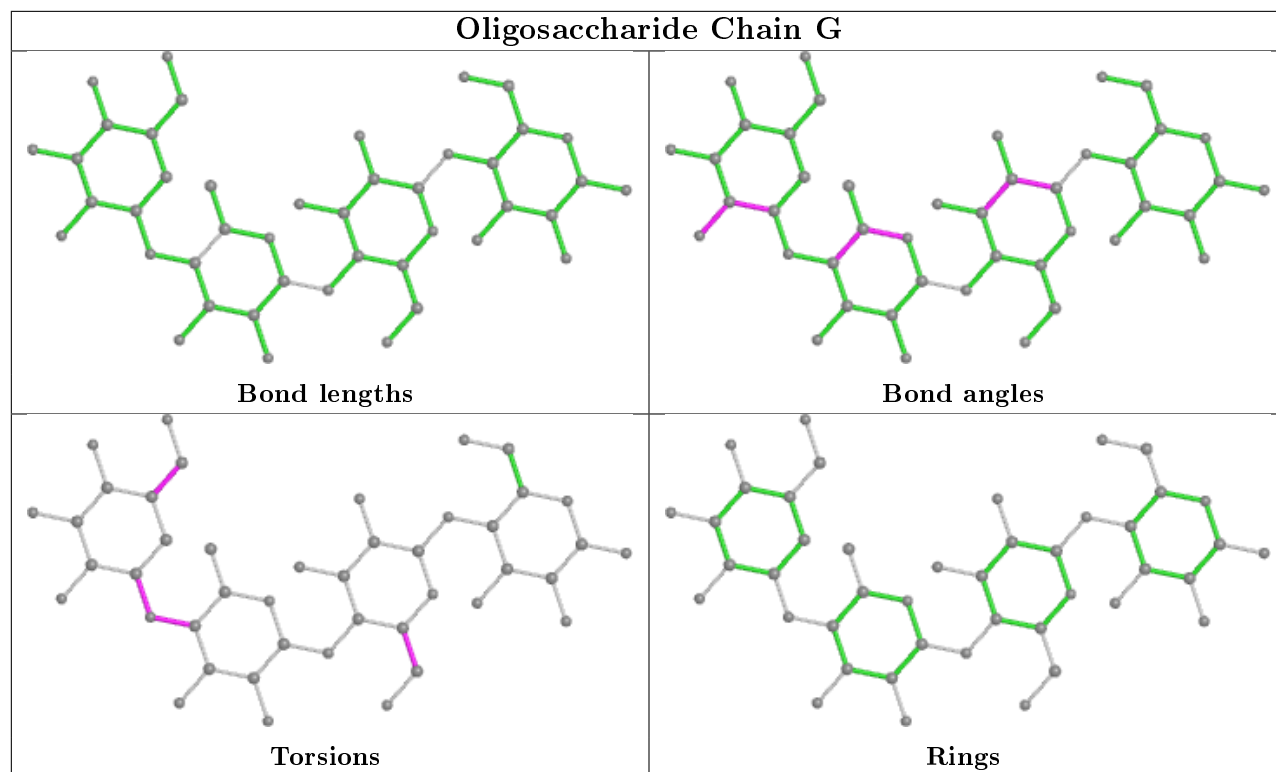
9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	3	AC1	2	0
2	J	3	AC1	2	0
2	H	3	AC1	2	0
2	K	2	GLC	1	0
2	L	2	GLC	1	0
2	E	3	AC1	1	0
2	I	3	AC1	3	0
2	K	3	AC1	3	0
2	L	3	AC1	2	0

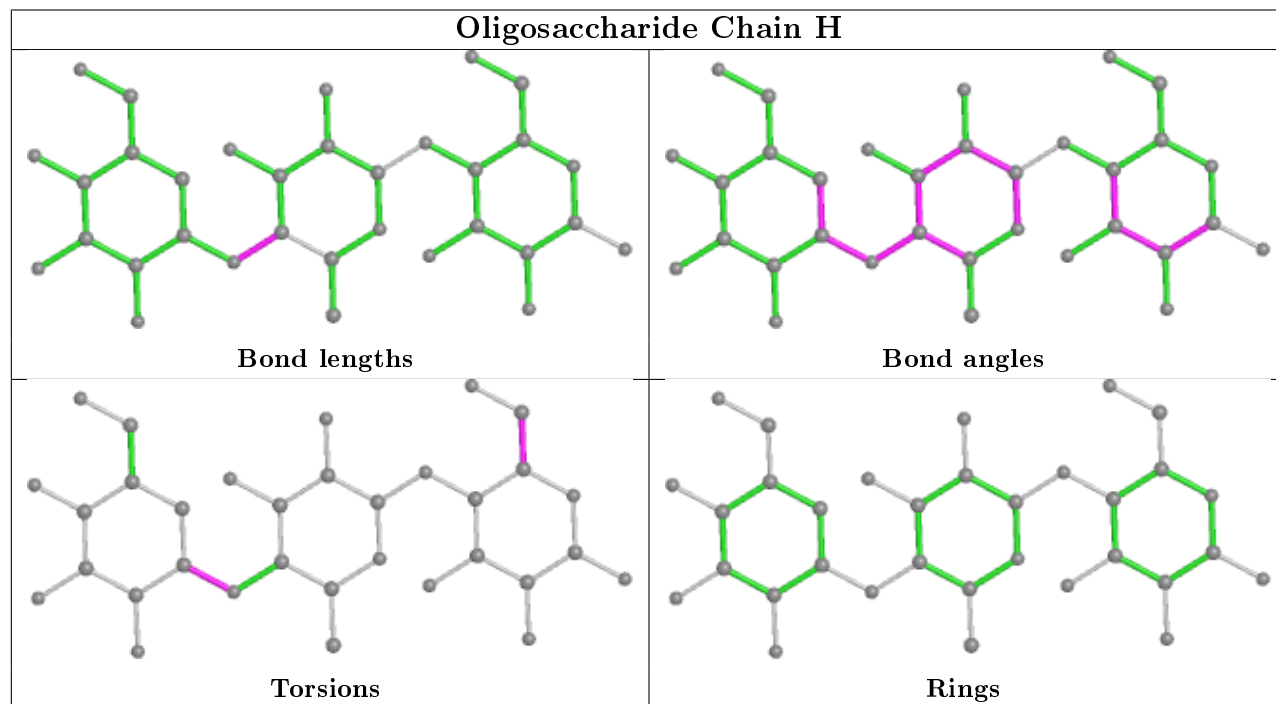
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

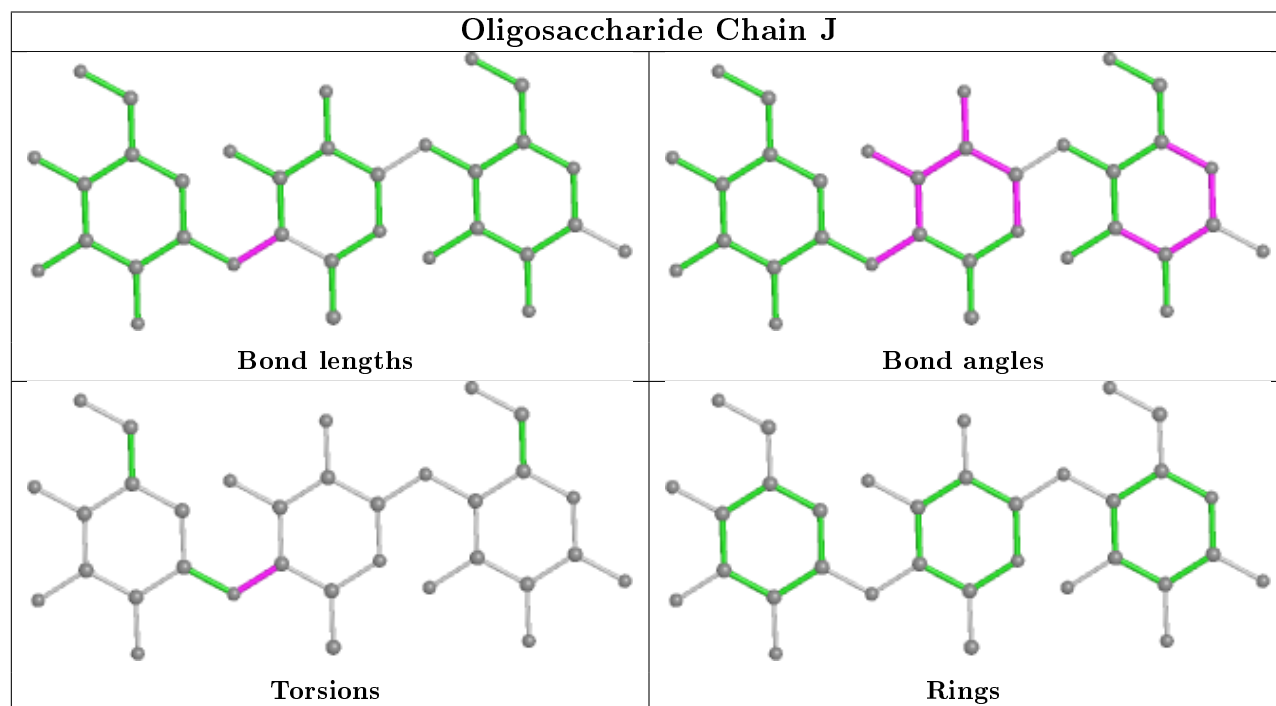
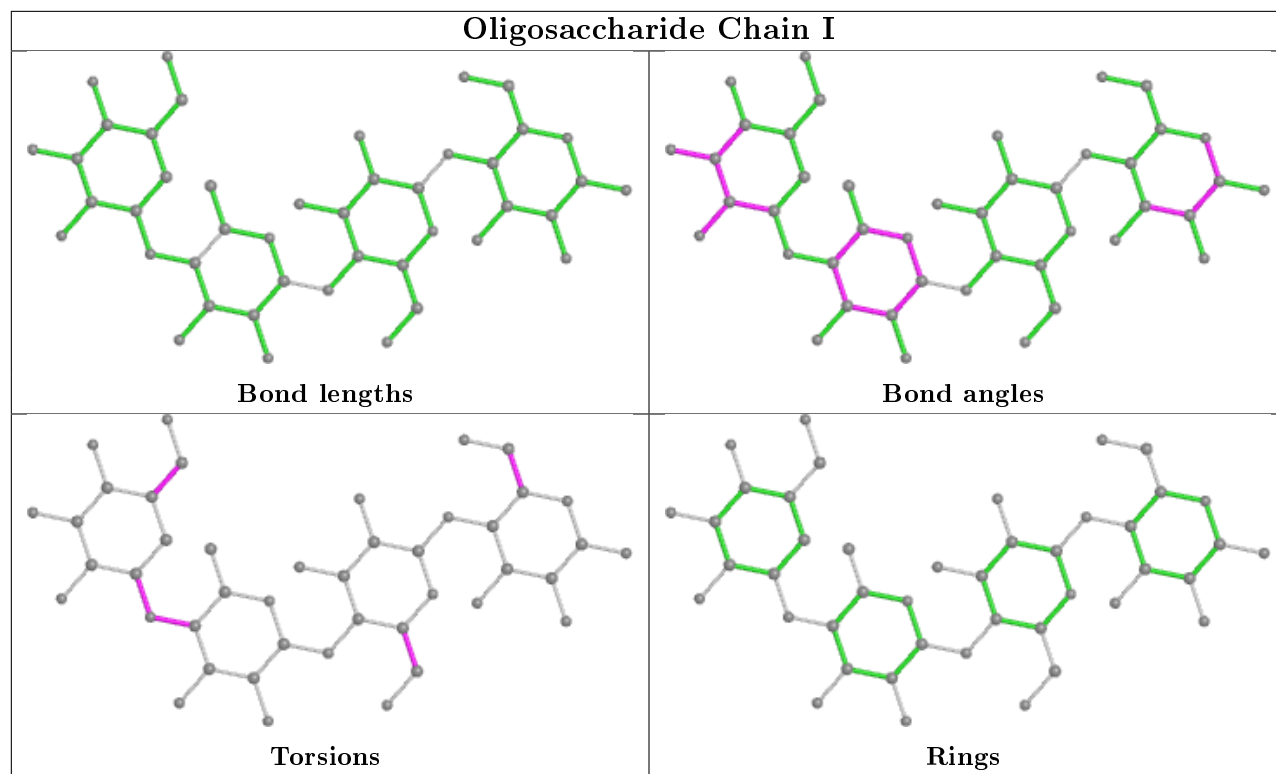
Oligosaccharide Chain E**Oligosaccharide Chain F**

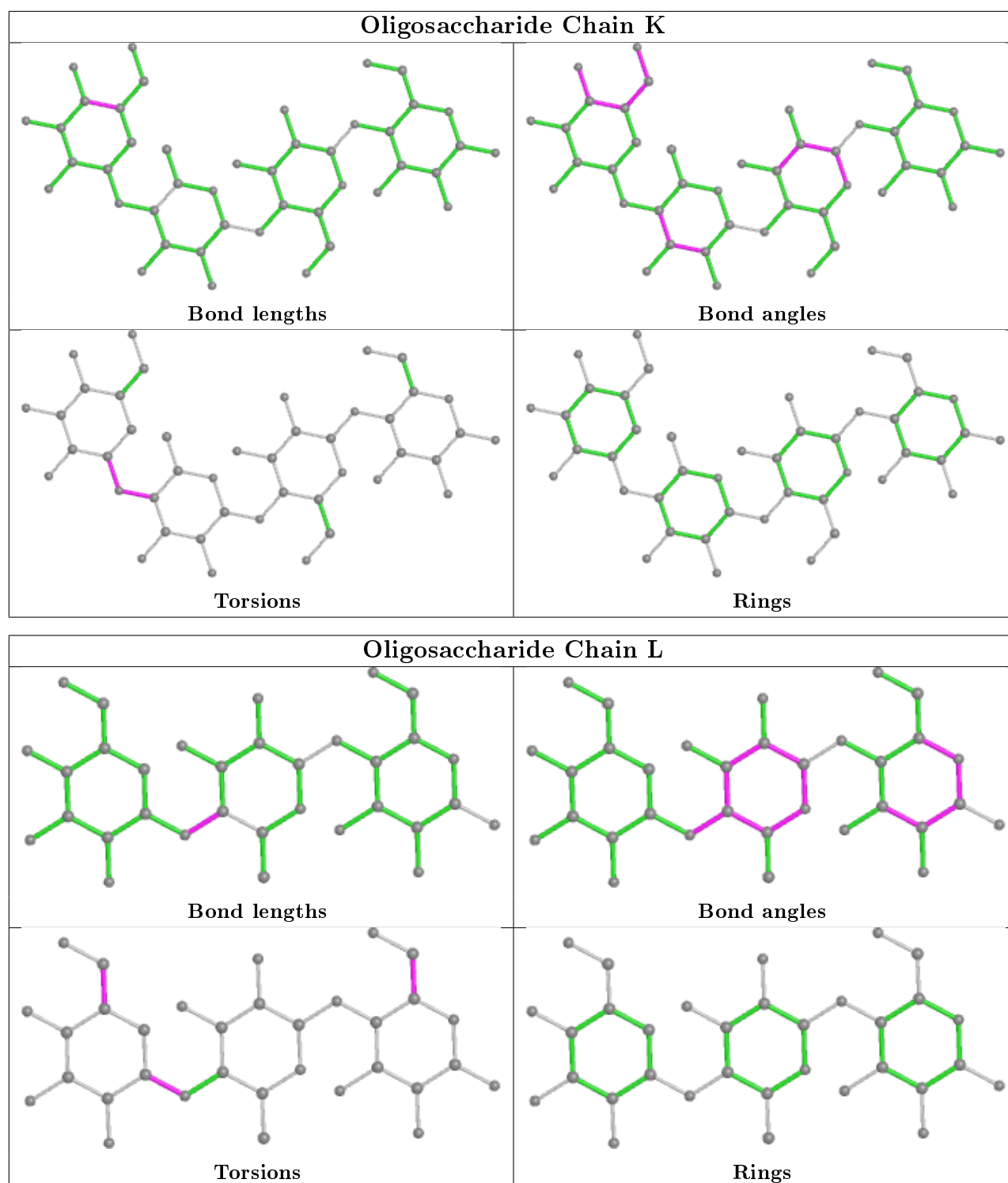
Oligosaccharide Chain G



Oligosaccharide Chain H







5.6 Ligand geometry [i](#)

7 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	1539	-	5,5,5	0.44	0	5,5,5	0.39	0
3	GOL	A	1539	-	5,5,5	0.47	0	5,5,5	0.58	0
3	GOL	A	1541	-	5,5,5	0.46	0	5,5,5	0.31	0
3	GOL	A	1542	-	5,5,5	0.48	0	5,5,5	0.35	0
3	GOL	D	1539	-	5,5,5	0.41	0	5,5,5	0.26	0
3	GOL	C	1540	-	5,5,5	0.45	0	5,5,5	0.33	0
3	GOL	A	1540	-	5,5,5	0.46	0	5,5,5	0.49	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	1539	-	-	2/4/4/4	-
3	GOL	A	1539	-	-	2/4/4/4	-
3	GOL	A	1541	-	-	0/4/4/4	-
3	GOL	A	1542	-	-	4/4/4/4	-
3	GOL	D	1539	-	-	2/4/4/4	-
3	GOL	C	1540	-	-	4/4/4/4	-
3	GOL	A	1540	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1539	GOL	O1-C1-C2-O2
3	C	1539	GOL	O1-C1-C2-C3
3	A	1539	GOL	O2-C2-C3-O3
3	A	1542	GOL	C1-C2-C3-O3
3	D	1539	GOL	C1-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1539	GOL	1	0
3	A	1541	GOL	1	0
3	A	1542	GOL	2	0
3	D	1539	GOL	1	0
3	C	1540	GOL	1	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	1024/1027 (99%)	-0.43	1 (0%) 95 95	24, 37, 51, 65	0
1	B	1024/1027 (99%)	-0.22	5 (0%) 91 89	25, 42, 55, 69	0
1	C	1024/1027 (99%)	-0.47	2 (0%) 95 95	22, 36, 49, 65	0
1	D	1024/1027 (99%)	-0.16	11 (1%) 80 78	28, 44, 56, 73	0
All	All	4096/4108 (99%)	-0.32	19 (0%) 91 89	22, 40, 54, 73	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	188	LEU	3.4
1	C	987	ALA	3.3
1	D	14	THR	3.0
1	D	691	VAL	2.9
1	A	472	ASP	2.9

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

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
1	CSO	B	336	7/8	0.96	0.10	41,42,43,43	0
1	CSO	D	336	7/8	0.96	0.11	39,41,41,42	0
1	CSO	A	336	7/8	0.96	0.16	31,33,34,35	0
1	CSO	C	336	7/8	0.98	0.15	31,31,32,32	0

6.3 Carbohydrates ⓘ

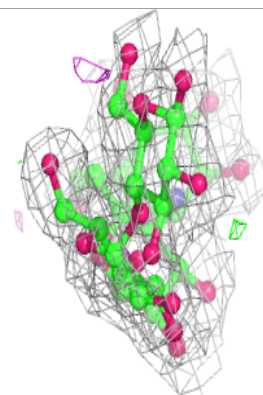
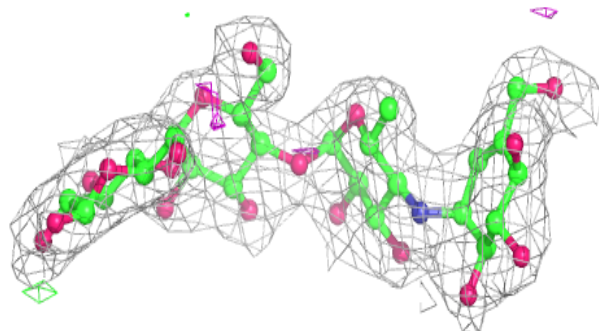
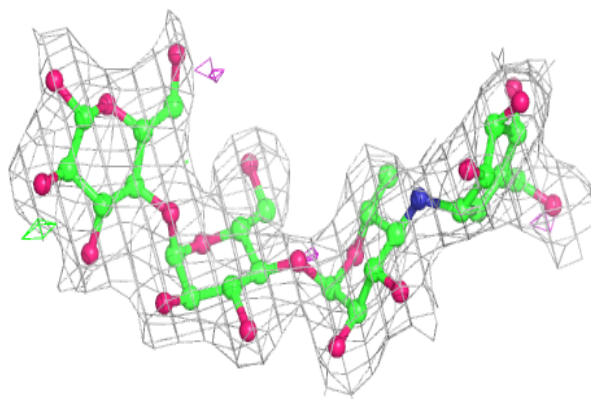
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	F	1	1/12	0.64	0.15	56,56,56,56	0
2	AC1	L	3	21/22	0.71	0.24	71,72,75,75	0
2	GLC	H	2	11/12	0.84	0.28	70,72,72,72	0
2	GLC	L	2	11/12	0.86	0.25	76,76,77,77	0
2	BGC	H	1	1/12	0.86	0.27	72,72,72,72	0
2	AC1	H	3	21/22	0.89	0.16	60,61,69,69	0
2	GLC	J	2	11/12	0.90	0.19	47,49,50,50	0
2	GLC	F	2	11/12	0.90	0.21	53,56,57,57	0
2	AC1	J	3	21/22	0.91	0.14	30,34,44,45	0
2	AC1	F	3	21/22	0.91	0.14	44,45,50,51	0
2	BGC	J	1	1/12	0.92	0.20	50,50,50,50	0
2	BGC	E	1	12/12	0.92	0.14	40,41,42,43	0
2	BGC	I	1	12/12	0.92	0.14	41,42,43,44	0
2	BGC	K	1	12/12	0.93	0.15	38,38,40,40	0
2	GLC	E	2	11/12	0.93	0.15	37,38,38,38	0
2	AC1	G	3	21/22	0.93	0.16	41,42,42,42	0
2	AC1	E	3	21/22	0.94	0.20	32,34,36,36	0
2	BGC	L	1	1/12	0.95	0.20	76,76,76,76	0
2	AC1	I	3	21/22	0.95	0.20	37,39,41,42	0
2	AC1	K	3	21/22	0.95	0.15	37,38,39,40	0
2	GLC	G	2	11/12	0.95	0.10	40,41,41,42	0
2	BGC	G	1	12/12	0.96	0.10	40,41,41,41	0
2	GLC	K	2	11/12	0.97	0.12	35,37,37,38	0
2	GLC	I	2	11/12	0.97	0.15	38,39,40,40	0

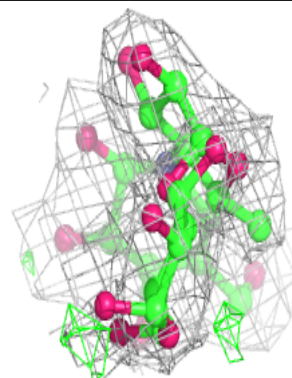
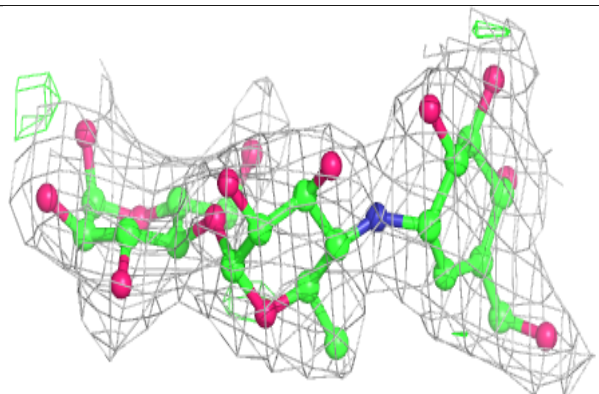
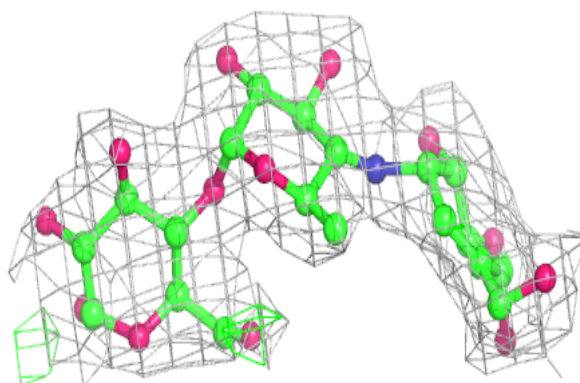
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

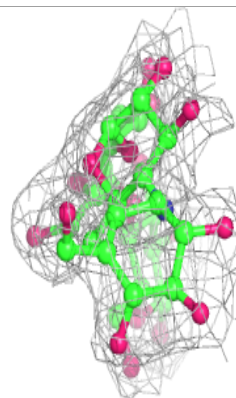
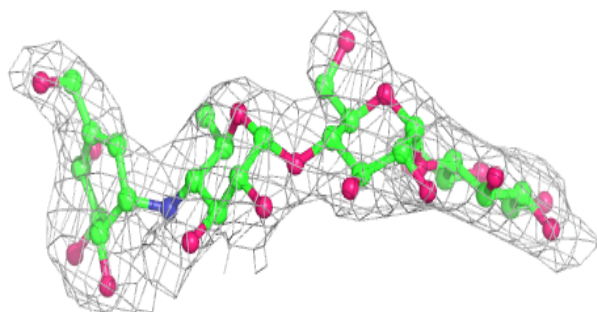
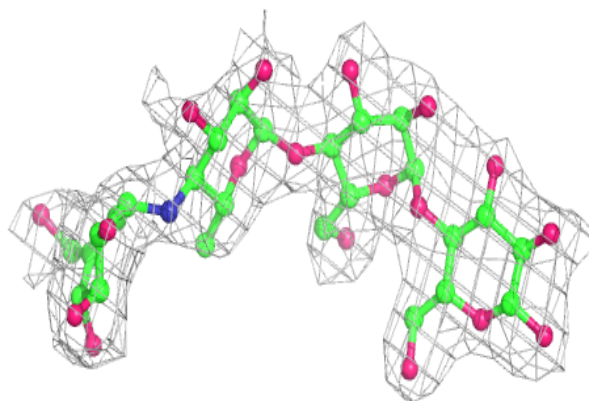
**Electron density around Chain F:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

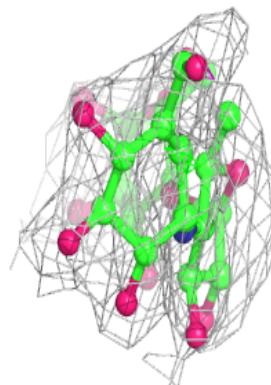
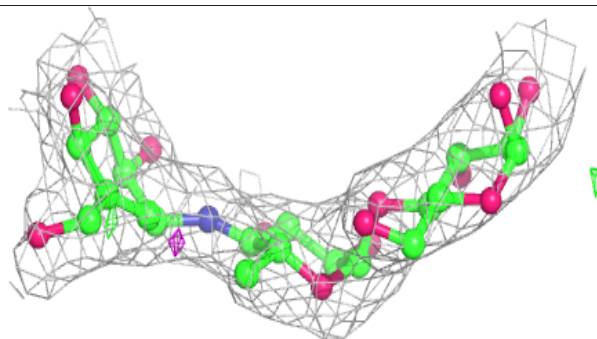
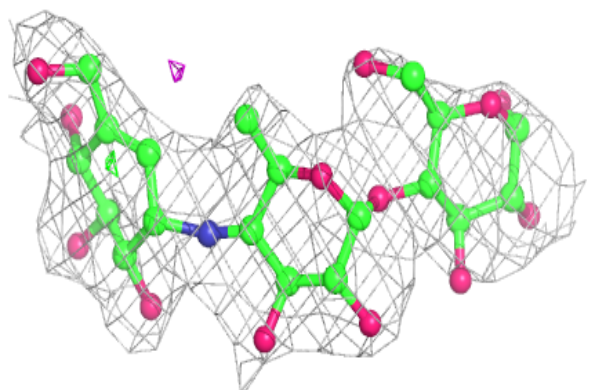


Electron density around Chain G:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

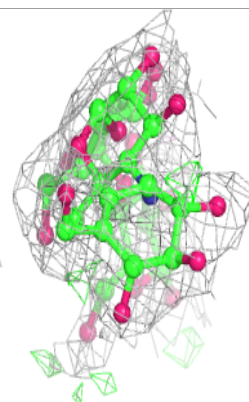
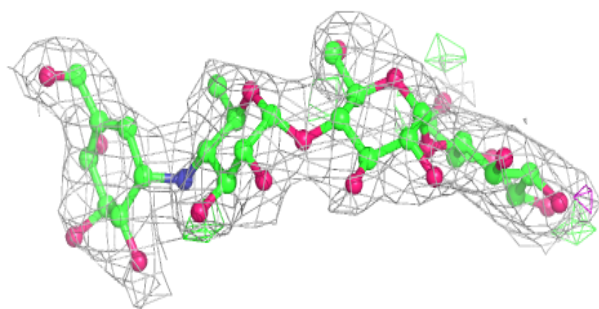
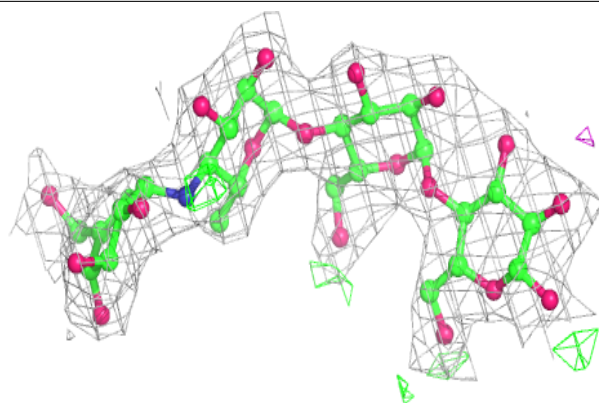
**Electron density around Chain H:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

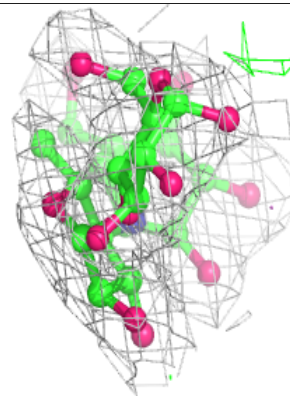
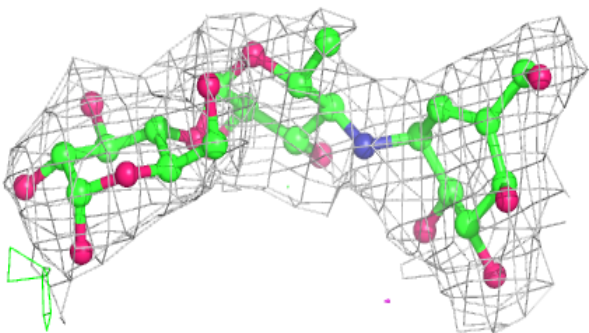
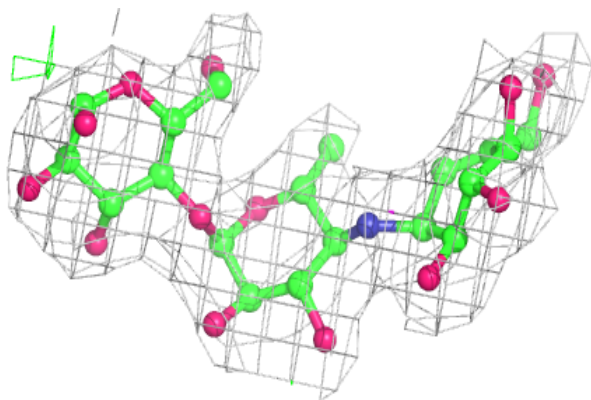


Electron density around Chain I:

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

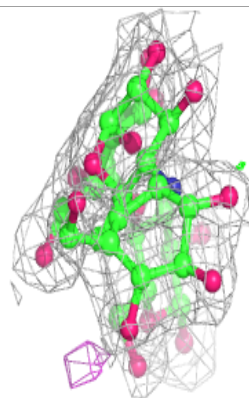
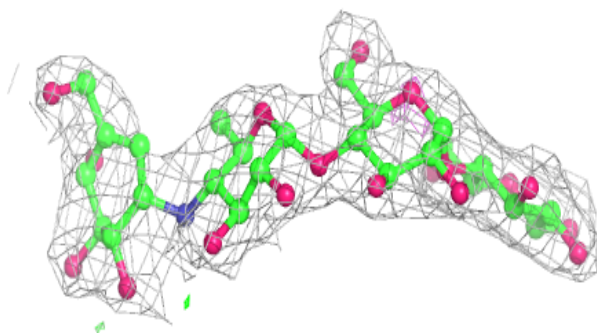
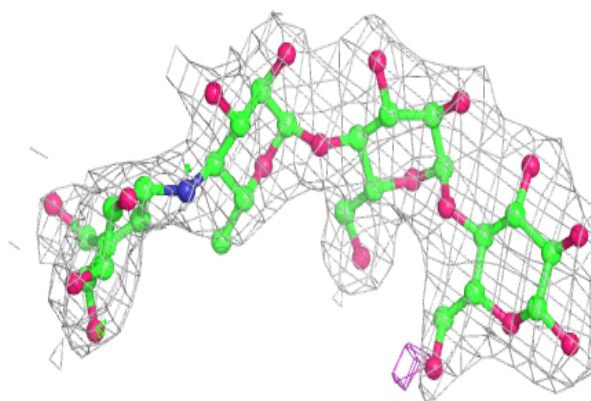
**Electron density around Chain J:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

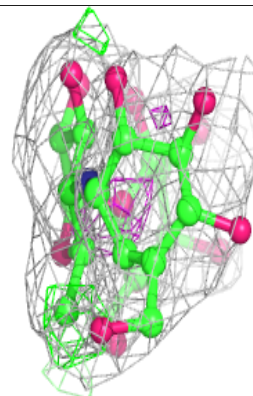
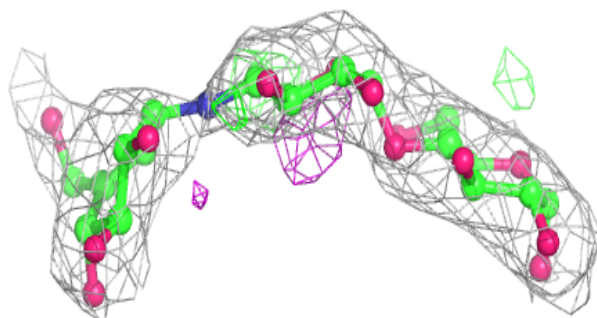
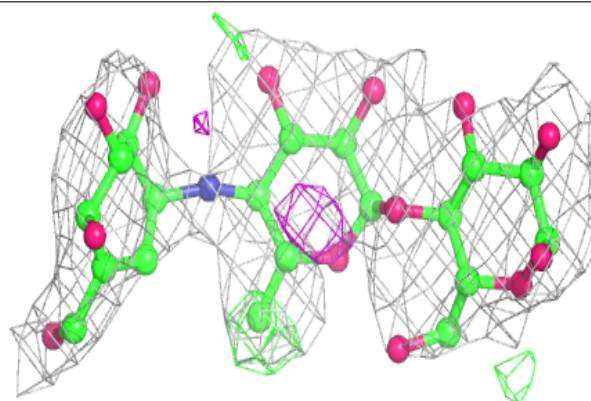


Electron density around Chain K:

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

**Electron density around Chain L:**

$2mF_o-DF_c$ (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(\AA^2)	Q<0.9
3	GOL	A	1542	6/6	0.81	0.25	57,57,58,58	0
3	GOL	D	1539	6/6	0.84	0.25	53,53,54,54	0
3	GOL	C	1539	6/6	0.90	0.18	42,43,43,44	0
3	GOL	A	1539	6/6	0.92	0.17	27,30,30,31	0
3	GOL	A	1540	6/6	0.93	0.20	46,46,46,47	0
3	GOL	A	1541	6/6	0.94	0.15	48,48,49,49	0
3	GOL	C	1540	6/6	0.96	0.12	40,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.