Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 12:31 PM JST

PDB ID	:	5X7Q
Title	:	Crystal structure of Paenibacillus sp. 598K alpha-1,6-glucosyltransferase complexed with maltohexaose
Authors	:	Fujimoto, Z.; Kishine, N.; Suzuki, N.; Momma, M.; Ichinose, H.; Kimura, A.; Funane, K.
Deposited on	:	2017-02-27
Resolution	:	1.95 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 ⓘ 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 ⓘ) were used in the production of this report:

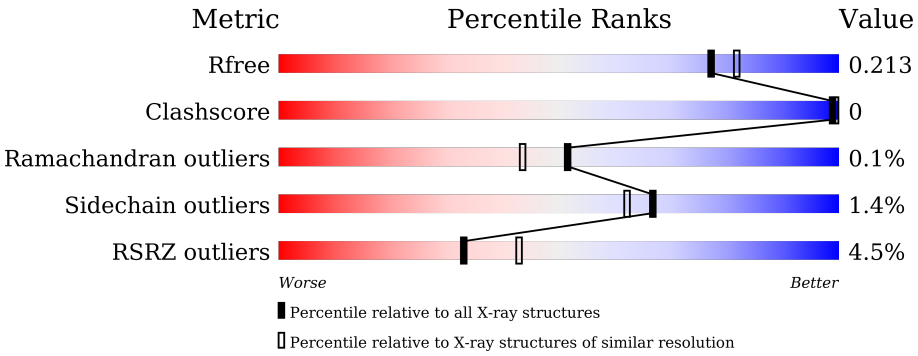
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	1263	5% 96%
1	B	1263	4% 96%
2	C	5	40% 60%
3	D	2	100%
3	H	2	50% 50%
4	E	4	25% 75%

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Mol	Chain	Length	Quality of chain
4	G	4	50% 50%
5	F	4	50% 25% 25%
5	J	4	25% 75%
6	I	3	67% 33%
7	K	2	50% 50%
7	L	2	50% 50%

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
2	GLC	C	5	-	-	-	X

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 21372 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 Glycoside hydrolase family 31 alpha-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1247	Total	C	N	O	S	0	0	0
			9601	6023	1633	1923	22			
1	B	1247	Total	C	N	O	S	0	1	0
			9611	6032	1634	1923	22			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	HIS	-	expression tag	UNP A0A193PKW5
A	20	HIS	-	expression tag	UNP A0A193PKW5
A	21	HIS	-	expression tag	UNP A0A193PKW5
A	22	HIS	-	expression tag	UNP A0A193PKW5
A	23	HIS	-	expression tag	UNP A0A193PKW5
A	24	HIS	-	expression tag	UNP A0A193PKW5
A	25	SER	-	expression tag	UNP A0A193PKW5
A	26	SER	-	expression tag	UNP A0A193PKW5
A	27	GLY	-	expression tag	UNP A0A193PKW5
A	28	LEU	-	expression tag	UNP A0A193PKW5
A	29	VAL	-	expression tag	UNP A0A193PKW5
A	30	PRO	-	expression tag	UNP A0A193PKW5
A	31	ARG	-	expression tag	UNP A0A193PKW5
A	32	GLY	-	expression tag	UNP A0A193PKW5
A	33	SER	-	expression tag	UNP A0A193PKW5
A	34	HIS	-	expression tag	UNP A0A193PKW5
A	35	MET	-	expression tag	UNP A0A193PKW5
B	19	HIS	-	expression tag	UNP A0A193PKW5
B	20	HIS	-	expression tag	UNP A0A193PKW5
B	21	HIS	-	expression tag	UNP A0A193PKW5
B	22	HIS	-	expression tag	UNP A0A193PKW5
B	23	HIS	-	expression tag	UNP A0A193PKW5
B	24	HIS	-	expression tag	UNP A0A193PKW5
B	25	SER	-	expression tag	UNP A0A193PKW5
B	26	SER	-	expression tag	UNP A0A193PKW5

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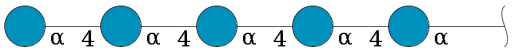
Chain	Residue	Modelled	Actual	Comment	Reference
B	27	GLY	-	expression tag	UNP A0A193PKW5
B	28	LEU	-	expression tag	UNP A0A193PKW5
B	29	VAL	-	expression tag	UNP A0A193PKW5
B	30	PRO	-	expression tag	UNP A0A193PKW5
B	31	ARG	-	expression tag	UNP A0A193PKW5
B	32	GLY	-	expression tag	UNP A0A193PKW5
B	33	SER	-	expression tag	UNP A0A193PKW5
B	34	HIS	-	expression tag	UNP A0A193PKW5
B	35	MET	-	expression tag	UNP A0A193PKW5

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	C	5	Total C O 56 30 26	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	D	2	Total C O 23 12 11	0	0	0
3	H	2	Total C O 23 12 11	0	0	0

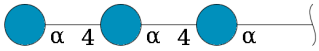
- Molecule 4 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	E	4	Total C O 45 24 21	0	0	0
4	G	4	Total C O 45 24 21	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	F	4	Total C O 45 24 21	0	0	0
5	J	4	Total C O 45 24 21	0	0	0

- Molecule 6 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	I	3	Total C O 34 18 16	0	0	0

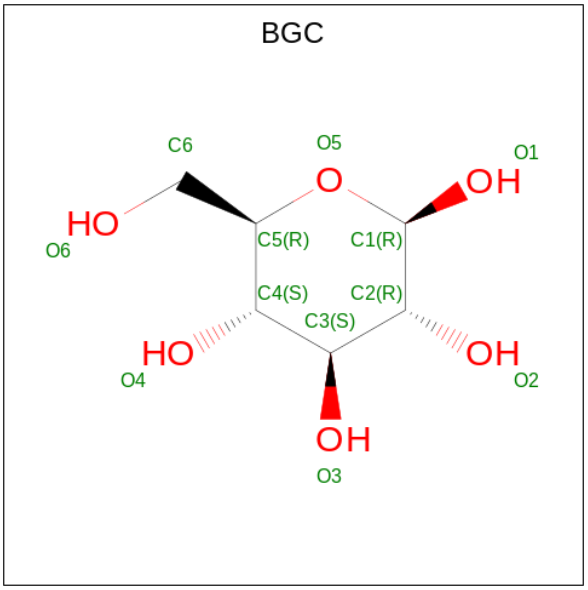
- Molecule 7 is an oligosaccharide called 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	K	2	Total C N O 22 13 1 8	0	0	1
7	L	2	Total C N O 22 13 1 8	0	0	1

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

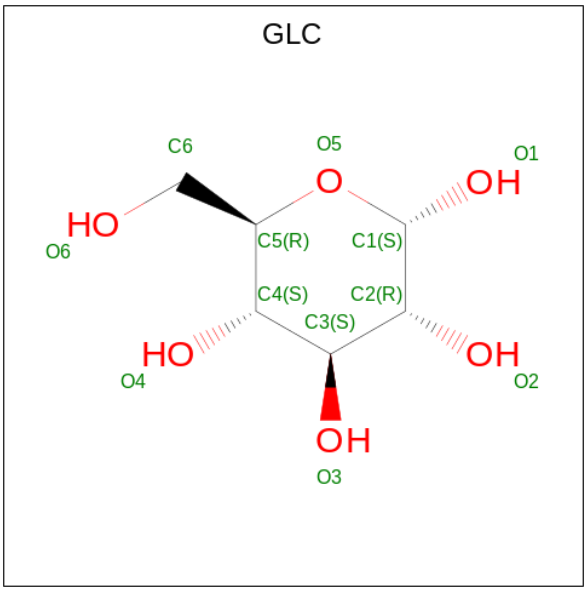
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	3	Total Ca 3 3	0	0
8	B	3	Total Ca 3 3	0	0

- Molecule 9 is beta-D-glucopyranose (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 12 6 6	0	0
9	B	1	Total C O 12 6 6	0	0

- Molecule 10 is alpha-D-glucopyranose (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 12 6 6	0	0
10	B	1	Total C O 12 6 6	0	0

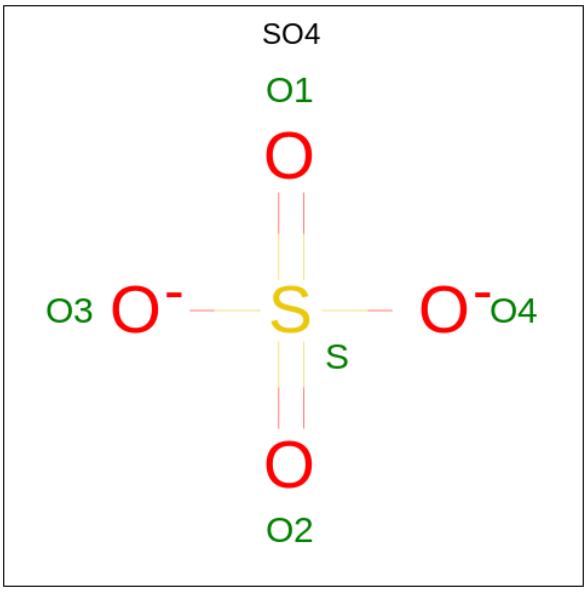
- Molecule 11 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total Ni 1 1	0	0
11	B	1	Total Ni 1 1	0	0

- Molecule 12 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	6	Total Mg 6 6	0	0
12	B	6	Total Mg 6 6	0	0

- Molecule 13 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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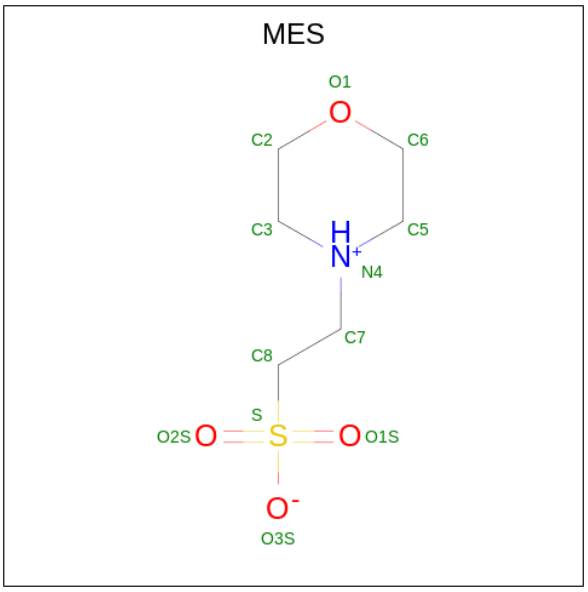
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	1	Total O S 5 4 1	0	0
13	B	1	Total O S 5 4 1	0	0
13	B	1	Total O S 5 4 1	0	0

- Molecule 14 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	1	Total C N O S 12 6 1 4 1	0	0
14	A	1	Total C N O S 12 6 1 4 1	0	0
14	A	1	Total C N O S 12 6 1 4 1	0	0
14	A	1	Total C N O S 12 6 1 4 1	0	0
14	B	1	Total C N O S 12 6 1 4 1	0	0
14	B	1	Total C N O S 12 6 1 4 1	0	0
14	B	1	Total C N O S 12 6 1 4 1	0	0
14	B	1	Total C N O S 12 6 1 4 1	0	0

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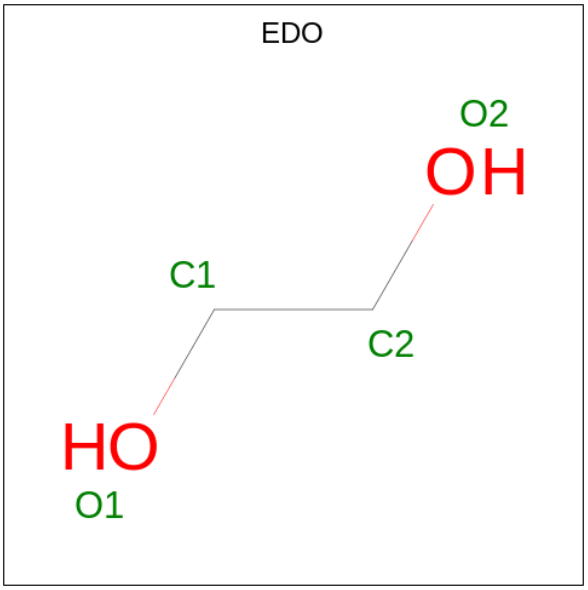
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 15 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 16 is water.

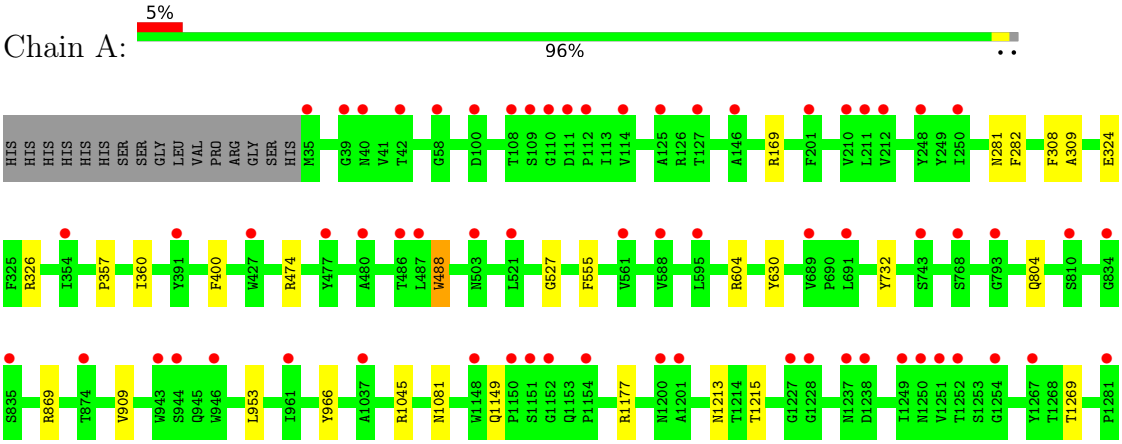
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	730	Total O 730 730	0	0
16	B	769	Total O 769 769	0	0

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.

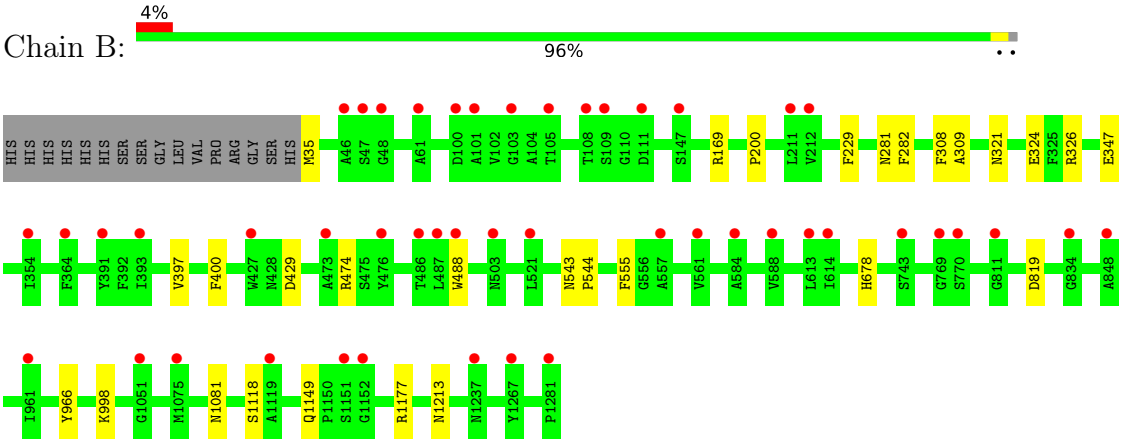
• Molecule 1: Glycoside hydrolase family 31 alpha-glucosidase

Chain A:



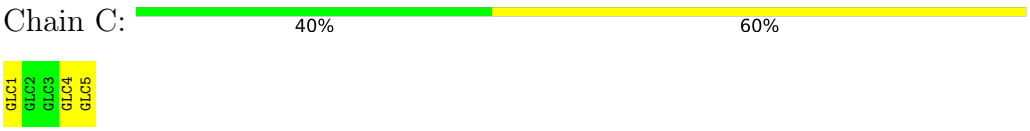
• Molecule 1: Glycoside hydrolase family 31 alpha-glucosidase

Chain B:



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

Chain C:



• Molecule 3: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose

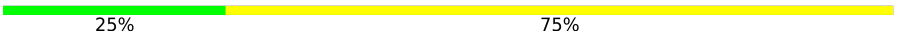
Chain D:

• Molecule 3: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose

Chain H:

• Molecule 4: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain E:



• Molecule 4: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

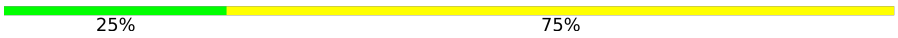
Chain G:

• Molecule 5: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain F:

• Molecule 5: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain J:



• Molecule 6: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain I:

• Molecule 7: 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

Chain K:

• Molecule 7: 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

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	184.27Å 271.76Å 133.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.51 – 1.95 38.47 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.3 (152.51-1.95) 99.4 (38.47-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.59 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.176 , 0.205 0.186 , 0.213	Depositor DCC
R_{free} test set	12050 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	27.8	Xtriage
Anisotropy	0.713	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 44.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	21372	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AC1, EDO, BGC, GLC, CA, MES, MG, NI, SO4

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	0.45	0/9863	0.69	3/13473 (0.0%)
1	B	0.45	0/9879	0.68	1/13496 (0.0%)
All	All	0.45	0/19742	0.68	4/26969 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	474	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	869	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	1045	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	474	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	9601	0	8954	9	1
1	B	9611	0	8960	9	0
2	C	56	0	48	0	0
3	D	23	0	21	0	0
3	H	23	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	45	0	39	0	0
4	G	45	0	39	0	0
5	F	45	0	39	1	0
5	J	45	0	39	0	0
6	I	34	0	30	0	0
7	K	22	0	10	0	0
7	L	22	0	10	0	1
8	A	3	0	0	0	0
8	B	3	0	0	0	0
9	A	12	0	12	0	0
9	B	12	0	12	0	0
10	A	12	0	12	0	0
10	B	12	0	12	0	0
11	A	1	0	0	0	0
11	B	1	0	0	0	0
12	A	6	0	0	0	0
12	B	6	0	0	0	0
13	A	35	0	0	0	0
13	B	50	0	0	0	0
14	A	48	0	52	0	0
14	B	60	0	65	1	0
15	A	20	0	30	0	0
15	B	20	0	30	0	0
16	A	730	0	0	1	0
16	B	769	0	0	0	0
All	All	21372	0	18435	15	1

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 (15) 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:360:ILE:HD13	1:B:397:VAL:HG12	1.76	0.68
1:A:604:ARG:HD2	1:A:732:TYR:CE1	2.37	0.60
1:A:360:ILE:HD13	1:B:397:VAL:CG1	2.37	0.55
1:A:630:TYR:OH	16:A:2001:HOH:O	2.20	0.48
1:B:543:ASN:HB3	1:B:544:PRO:HD2	1.96	0.47
1:A:282:PHE:CG	1:A:309:ALA:HB3	2.52	0.44
1:B:321:ASN:O	1:B:326:ARG:NH1	2.49	0.44
1:B:819:ASP:HB2	14:B:1708:MES:O3S	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:678:HIS:ND1	1:B:998:LYS:HD3	2.33	0.44
1:A:357:PRO:HD3	1:B:429:ASP:O	2.20	0.42
1:A:1269:THR:HG21	5:F:2:GLC:O3	2.19	0.41
1:B:200:PRO:HB3	1:B:229:PHE:CE1	2.54	0.41
1:B:282:PHE:CG	1:B:309:ALA:HB3	2.54	0.41
1:A:909:VAL:HG21	1:A:953:LEU:HD12	2.01	0.41
1:A:488:TRP:HA	1:A:527:GLY:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1215:THR:OG1	7:L:2:AC1:O6B[6_555]	2.17	0.03

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	1245/1263 (99%)	1219 (98%)	25 (2%)	1 (0%)	51 43
1	B	1246/1263 (99%)	1221 (98%)	24 (2%)	1 (0%)	51 43
All	All	2491/2526 (99%)	2440 (98%)	49 (2%)	2 (0%)	51 43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1213	ASN
1	B	1213	ASN

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	997/1011 (99%)	984 (99%)	13 (1%)	69	65
1	B	998/1011 (99%)	984 (99%)	14 (1%)	67	62
All	All	1995/2022 (99%)	1968 (99%)	27 (1%)	67	62

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	ARG
1	A	281	ASN
1	A	308	PHE
1	A	324	GLU
1	A	326	ARG
1	A	400	PHE
1	A	488	TRP
1	A	555	PHE
1	A	804	GLN
1	A	966	TYR
1	A	1081	ASN
1	A	1149	GLN
1	A	1177	ARG
1	B	35	MET
1	B	169	ARG
1	B	281	ASN
1	B	308	PHE
1	B	324	GLU
1	B	347	GLU
1	B	400	PHE
1	B	488	TRP
1	B	555	PHE
1	B	966	TYR
1	B	1081	ASN
1	B	1118	SER
1	B	1149	GLN
1	B	1177	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	654	GLN
1	A	1226	HIS
1	B	440	GLN
1	B	1226	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

Of 32 monosaccharides modelled in this entry, 30 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	GLC	C	1	2	12,12,12	0.45	0	17,17,17	1.13	2 (11%)
2	GLC	C	2	2	11,11,12	0.47	0	15,15,17	0.71	0
2	GLC	C	3	2	11,11,12	0.34	0	15,15,17	0.72	0
2	GLC	C	4	2	11,11,12	0.43	0	15,15,17	0.95	1 (6%)
2	GLC	C	5	2	11,11,12	0.51	0	15,15,17	1.66	1 (6%)
3	GLC	D	1	3	12,12,12	0.59	0	17,17,17	0.89	0
3	GLC	D	2	3	11,11,12	0.53	0	15,15,17	0.77	0
4	GLC	E	1	4	12,12,12	0.57	0	17,17,17	0.86	0
4	GLC	E	2	4	11,11,12	0.47	0	15,15,17	0.84	1 (6%)
4	GLC	E	3	4	11,11,12	0.32	0	15,15,17	1.29	2 (13%)
4	GLC	E	4	4	11,11,12	0.53	0	15,15,17	0.96	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	BGC	F	1	5	12,12,12	0.36	0	17,17,17	1.55	4 (23%)
5	GLC	F	2	5	11,11,12	0.44	0	15,15,17	1.00	1 (6%)
5	GLC	F	3	5	11,11,12	0.25	0	15,15,17	0.75	0
5	GLC	F	4	5	11,11,12	0.55	0	15,15,17	0.72	0
4	GLC	G	1	4	12,12,12	0.51	0	17,17,17	1.20	2 (11%)
4	GLC	G	2	4	11,11,12	0.33	0	15,15,17	0.85	0
4	GLC	G	3	4	11,11,12	0.36	0	15,15,17	0.47	0
4	GLC	G	4	4	11,11,12	0.50	0	15,15,17	1.72	3 (20%)
3	GLC	H	1	3	12,12,12	0.67	0	17,17,17	1.03	0
3	GLC	H	2	3	11,11,12	0.39	0	15,15,17	1.00	2 (13%)
6	GLC	I	1	6	12,12,12	0.59	0	17,17,17	0.96	1 (5%)
6	GLC	I	2	6	11,11,12	0.40	0	15,15,17	0.89	0
6	GLC	I	3	6	11,11,12	0.30	0	15,15,17	0.82	0
5	BGC	J	1	5	12,12,12	0.45	0	17,17,17	1.27	1 (5%)
5	GLC	J	2	5	11,11,12	0.66	0	15,15,17	1.19	1 (6%)
5	GLC	J	3	5	11,11,12	0.40	0	15,15,17	0.80	0
5	GLC	J	4	5	11,11,12	0.46	0	15,15,17	1.01	2 (13%)
7	AC1	K	2	7	21,22,23	0.72	0	22,32,34	0.89	1 (4%)
7	AC1	L	2	7	21,22,23	0.79	1 (4%)	22,32,34	1.05	2 (9%)

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	GLC	C	1	2	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	C	3	2	-	0/2/19/22	0/1/1/1
2	GLC	C	4	2	-	0/2/19/22	0/1/1/1
2	GLC	C	5	2	-	0/2/19/22	0/1/1/1
3	GLC	D	1	3	-	0/2/22/22	0/1/1/1
3	GLC	D	2	3	-	0/2/19/22	0/1/1/1
4	GLC	E	1	4	-	2/2/22/22	0/1/1/1
4	GLC	E	2	4	-	0/2/19/22	0/1/1/1
4	GLC	E	3	4	-	0/2/19/22	0/1/1/1
4	GLC	E	4	4	-	2/2/19/22	0/1/1/1
5	BGC	F	1	5	-	0/2/22/22	0/1/1/1
5	GLC	F	2	5	-	0/2/19/22	0/1/1/1
5	GLC	F	3	5	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GLC	F	4	5	-	0/2/19/22	0/1/1/1
4	GLC	G	1	4	-	0/2/22/22	0/1/1/1
4	GLC	G	2	4	-	0/2/19/22	0/1/1/1
4	GLC	G	3	4	-	0/2/19/22	0/1/1/1
4	GLC	G	4	4	-	2/2/19/22	0/1/1/1
3	GLC	H	1	3	-	0/2/22/22	0/1/1/1
3	GLC	H	2	3	-	0/2/19/22	0/1/1/1
6	GLC	I	1	6	-	2/2/22/22	0/1/1/1
6	GLC	I	2	6	-	0/2/19/22	0/1/1/1
6	GLC	I	3	6	-	0/2/19/22	0/1/1/1
5	BGC	J	1	5	-	0/2/22/22	0/1/1/1
5	GLC	J	2	5	-	0/2/19/22	0/1/1/1
5	GLC	J	3	5	-	0/2/19/22	0/1/1/1
5	GLC	J	4	5	-	0/2/19/22	0/1/1/1
7	AC1	K	2	7	-	1/6/43/46	0/2/2/2
7	AC1	L	2	7	-	1/6/43/46	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	2	AC1	C7B-C5B	2.07	1.35	1.32

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	5	GLC	C1-O5-C5	5.53	119.69	112.19
4	G	4	GLC	C1-O5-C5	5.13	119.14	112.19
4	G	1	GLC	C1-O5-C5	3.19	119.68	113.66
5	J	1	BGC	O5-C1-C2	-3.08	104.78	110.28
4	G	4	GLC	O5-C5-C6	3.01	111.92	107.20
5	J	2	GLC	C1-O5-C5	2.98	116.23	112.19
7	L	2	AC1	C7B-C1B-N4A	-2.95	106.25	110.68
5	F	1	BGC	C3-C4-C5	2.88	115.37	110.24
7	L	2	AC1	C1-C2-C3	2.83	113.14	109.67
5	F	2	GLC	C1-O5-C5	2.66	115.79	112.19
5	F	1	BGC	C1-C2-C3	-2.57	104.98	110.31
4	E	4	GLC	C1-O5-C5	2.57	115.67	112.19
4	E	3	GLC	O4-C4-C3	-2.40	104.80	110.35
5	F	1	BGC	O5-C1-C2	-2.38	106.05	110.28
7	K	2	AC1	C2-C3-C4	-2.36	108.55	110.63
4	E	2	GLC	C1-O5-C5	2.33	115.34	112.19
2	C	4	GLC	C1-O5-C5	2.31	115.32	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	4	GLC	C1-O5-C5	2.26	115.26	112.19
2	C	1	GLC	C1-O5-C5	2.26	117.92	113.66
2	C	1	GLC	C6-C5-C4	-2.22	107.80	113.00
3	H	2	GLC	C1-O5-C5	2.16	115.12	112.19
4	E	3	GLC	O5-C5-C6	2.16	110.59	107.20
4	G	4	GLC	C6-C5-C4	-2.13	108.01	113.00
4	G	1	GLC	C6-C5-C4	-2.13	108.01	113.00
3	H	2	GLC	O5-C5-C6	2.12	110.53	107.20
6	I	1	GLC	O5-C5-C6	2.11	111.68	106.44
5	F	1	BGC	O5-C5-C6	2.10	111.66	106.44
5	J	4	GLC	C2-C3-C4	-2.02	107.40	110.89

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1	GLC	O5-C5-C6-O6
4	G	4	GLC	O5-C5-C6-O6
4	E	1	GLC	C4-C5-C6-O6
4	G	4	GLC	C4-C5-C6-O6
6	I	1	GLC	O5-C5-C6-O6
4	E	4	GLC	C4-C5-C6-O6
6	I	1	GLC	C4-C5-C6-O6
4	E	4	GLC	O5-C5-C6-O6
7	K	2	AC1	C5-C4-N4A-C1B
5	F	3	GLC	C4-C5-C6-O6
7	L	2	AC1	C5-C4-N4A-C1B

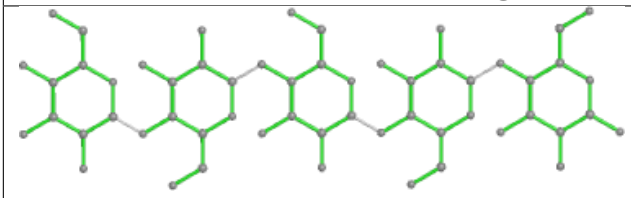
There are no ring outliers.

2 monomers are involved in 2 short contacts:

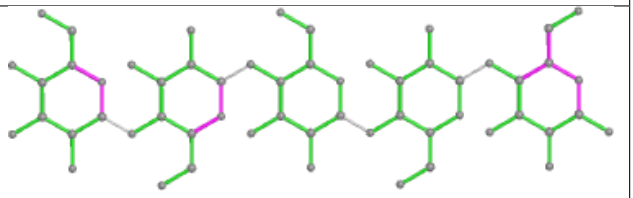
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	2	AC1	0	1
5	F	2	GLC	1	0

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

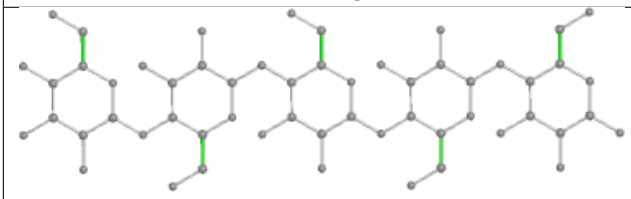
Oligosaccharide Chain C



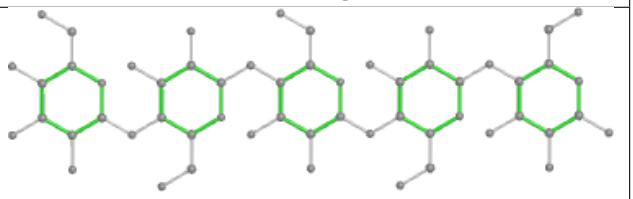
Bond lengths



Bond angles

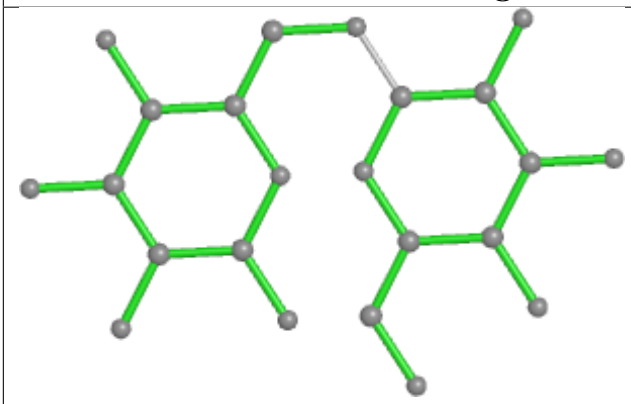


Torsions

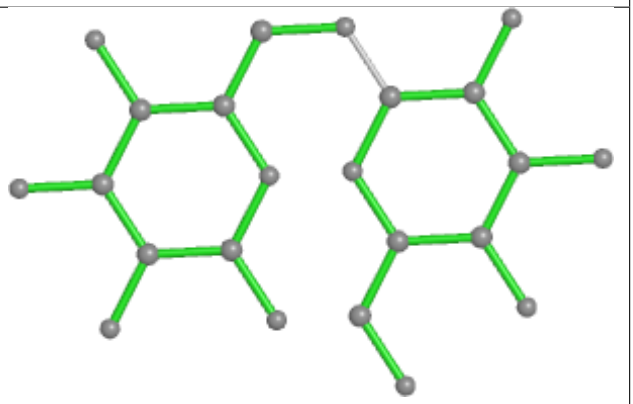


Rings

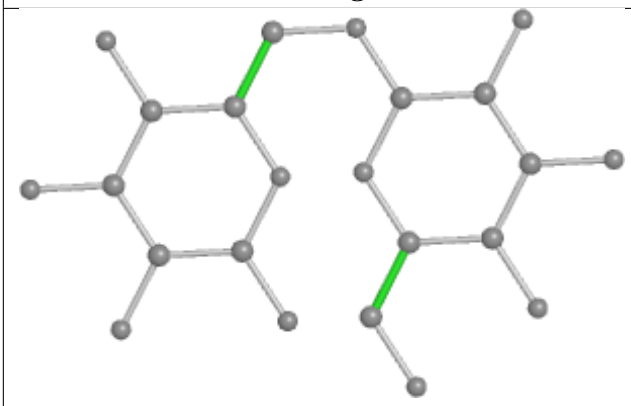
Oligosaccharide Chain D



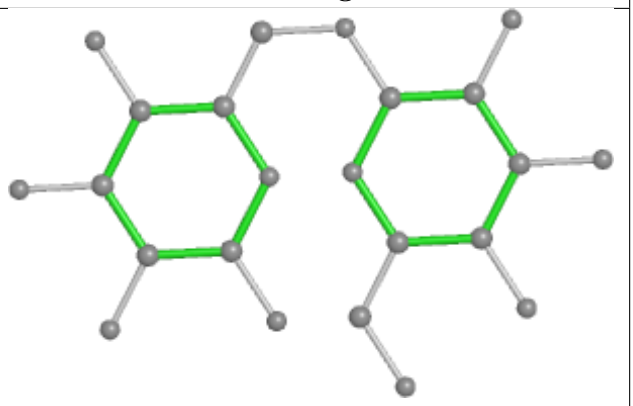
Bond lengths



Bond angles

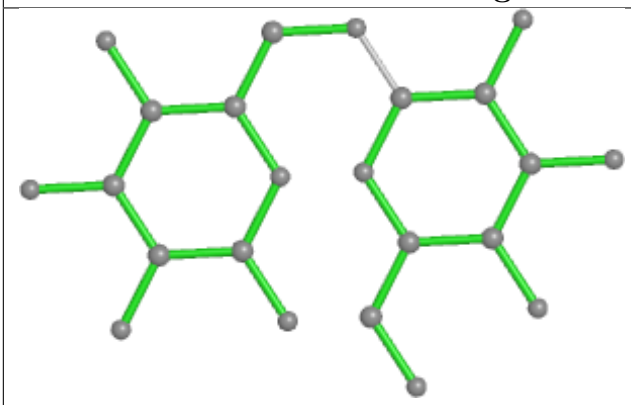


Torsions

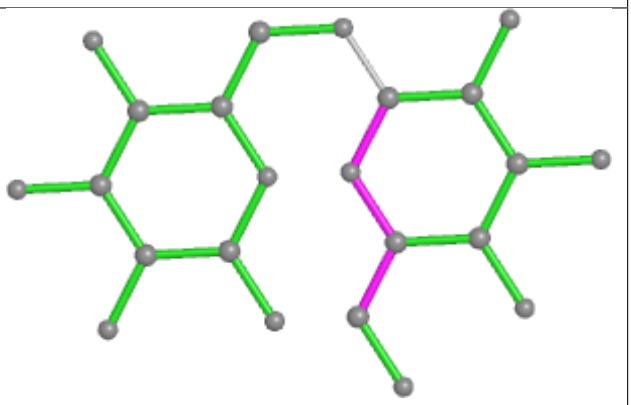


Rings

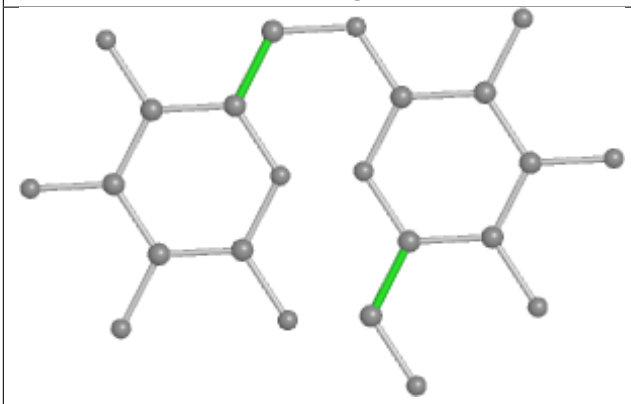
Oligosaccharide Chain H



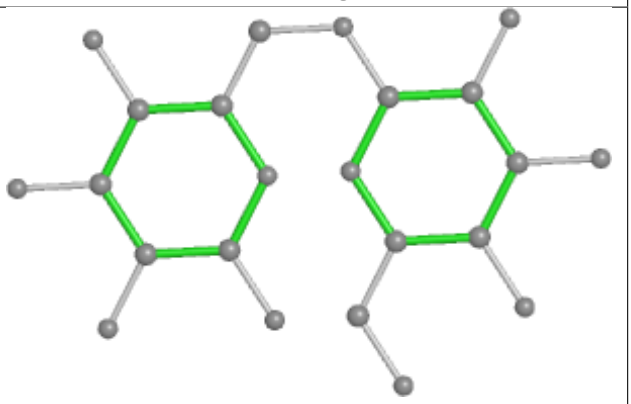
Bond lengths



Bond angles

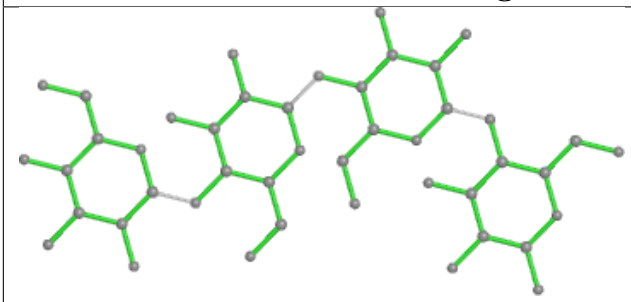


Torsions

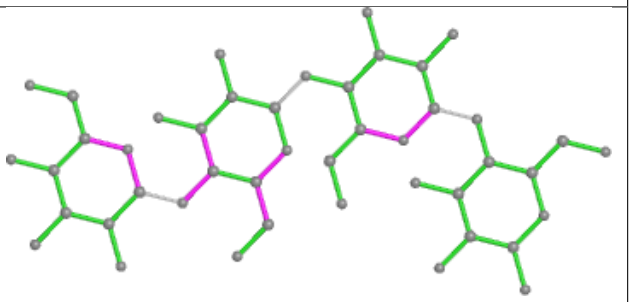


Rings

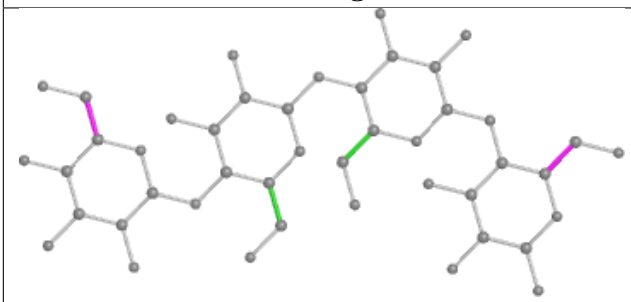
Oligosaccharide Chain E



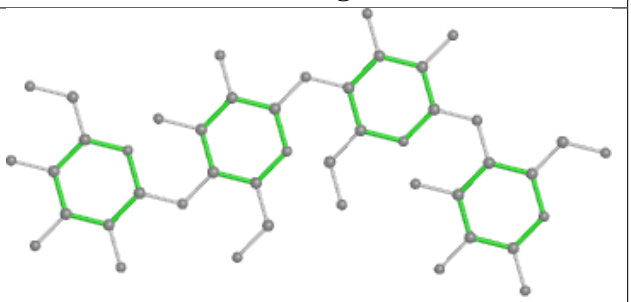
Bond lengths



Bond angles

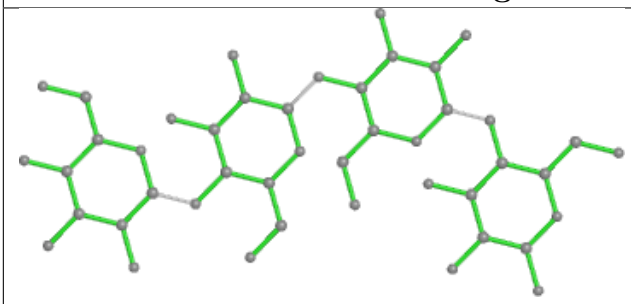


Torsions

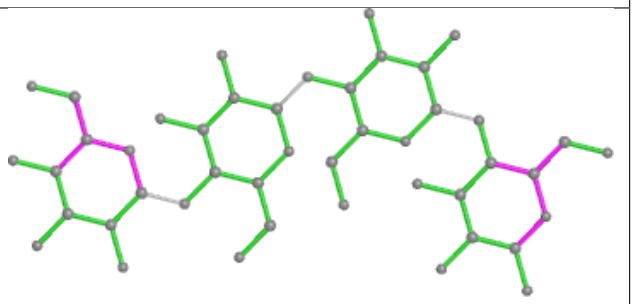


Rings

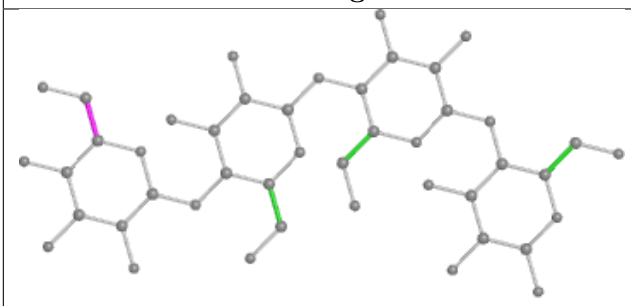
Oligosaccharide Chain G



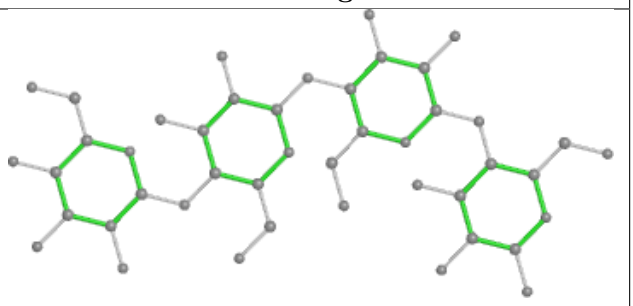
Bond lengths



Bond angles

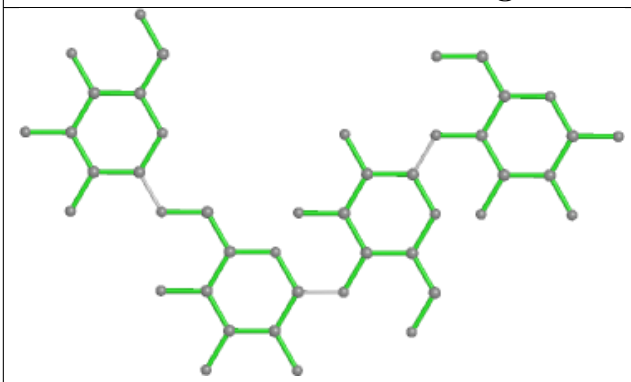


Torsions

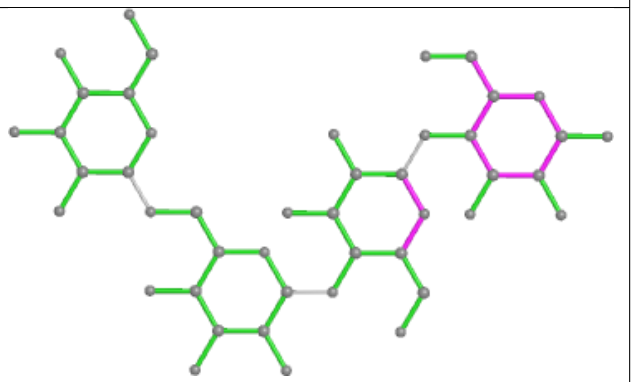


Rings

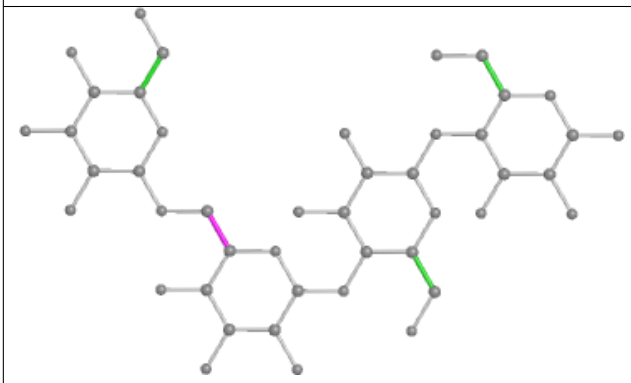
Oligosaccharide Chain F



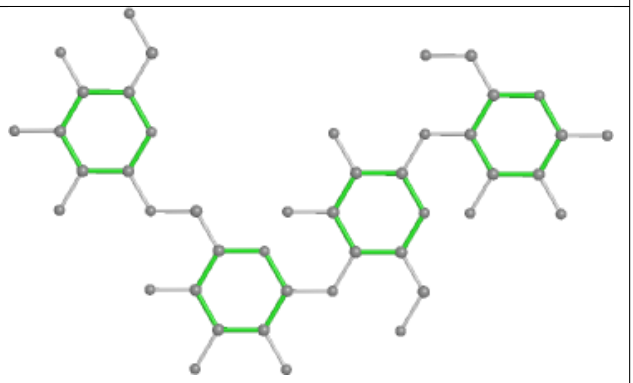
Bond lengths



Bond angles

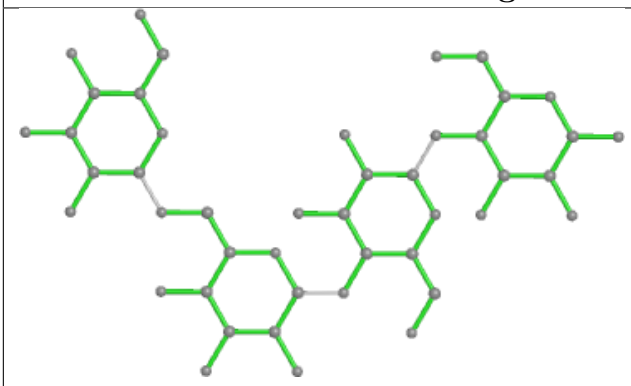


Torsions

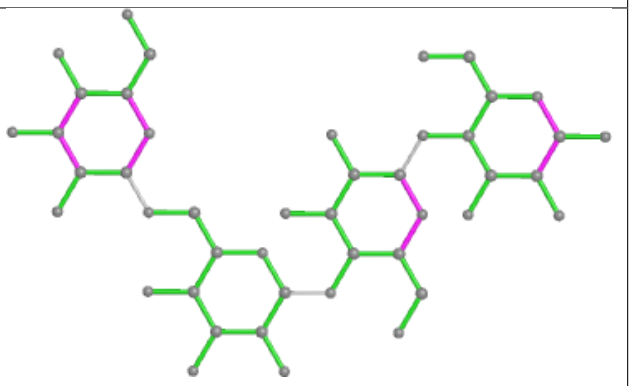


Rings

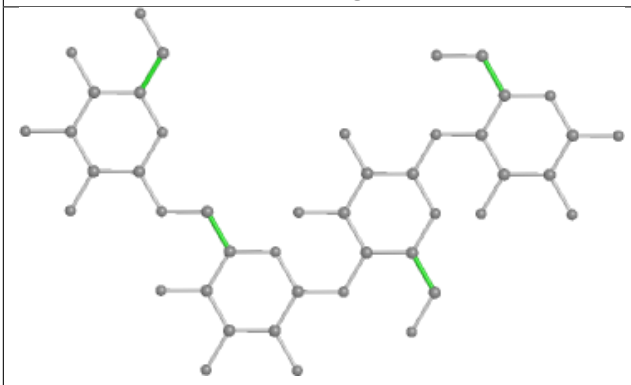
Oligosaccharide Chain J



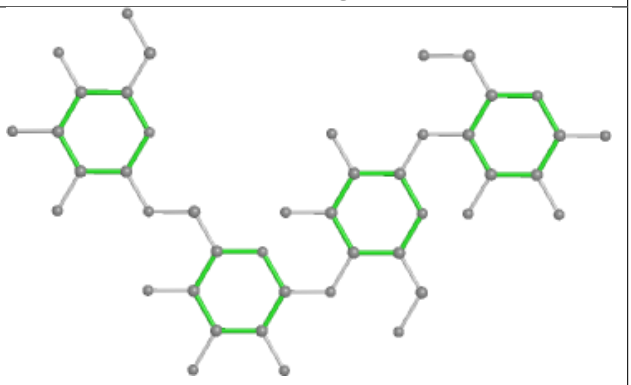
Bond lengths



Bond angles

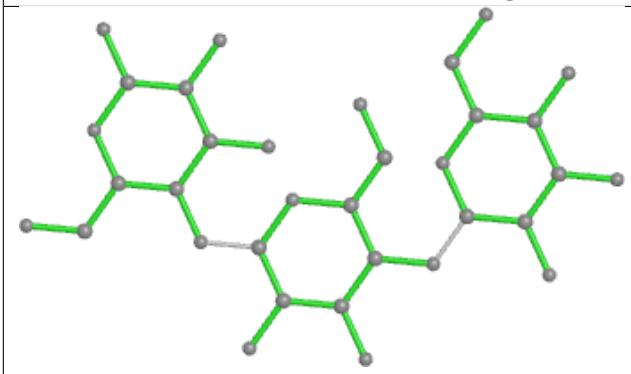


Torsions

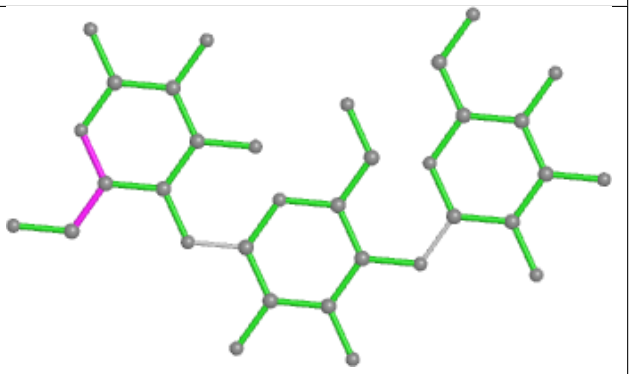


Rings

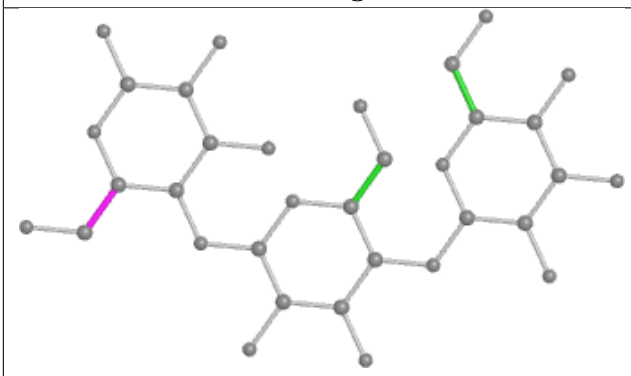
Oligosaccharide Chain I



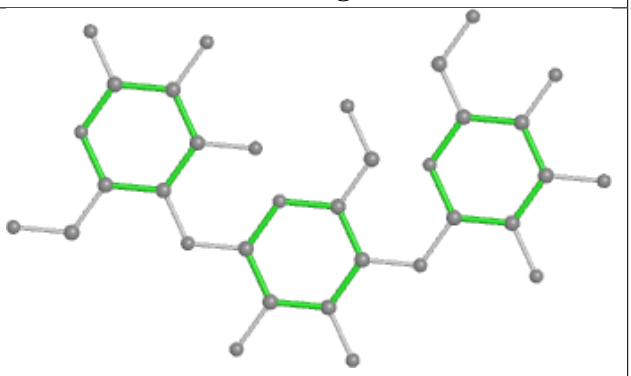
Bond lengths



Bond angles

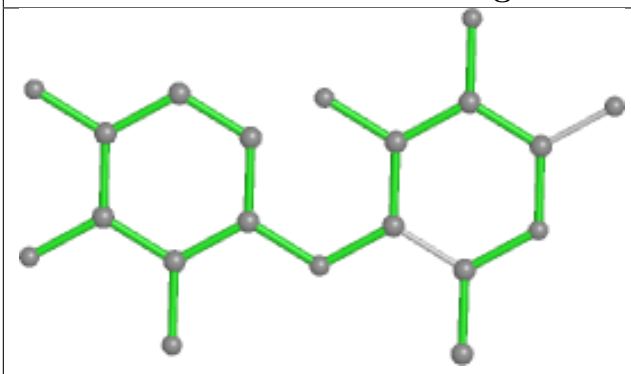


Torsions

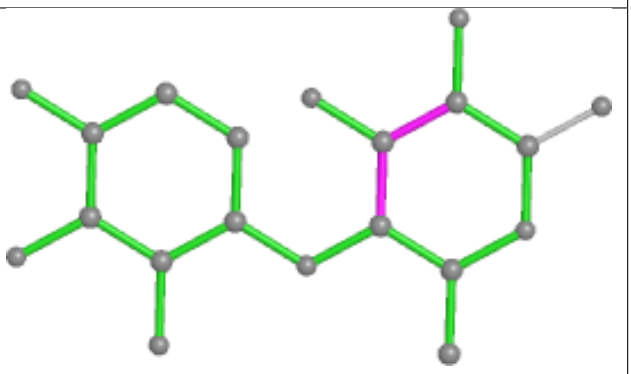


Rings

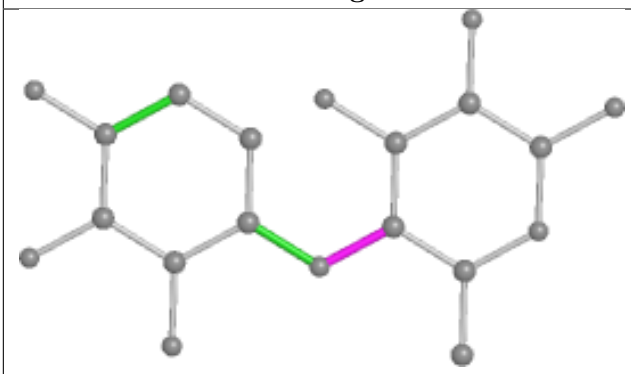
Oligosaccharide Chain K



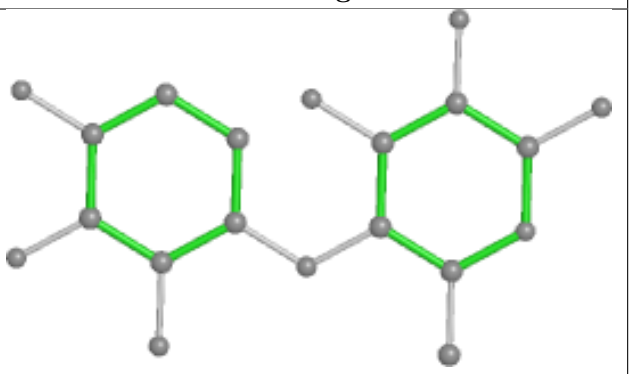
Bond lengths



Bond angles

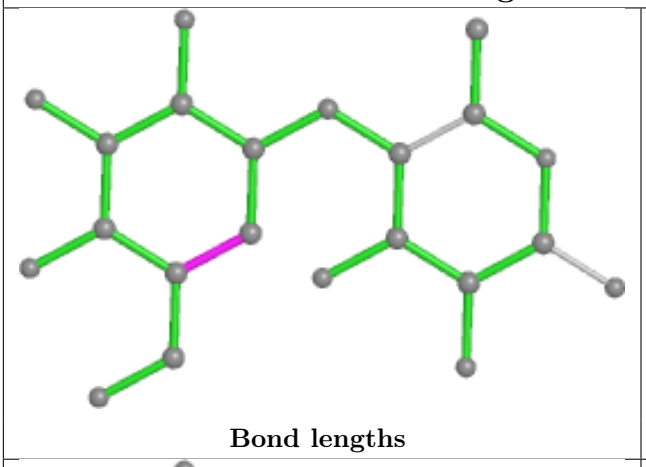


Torsions

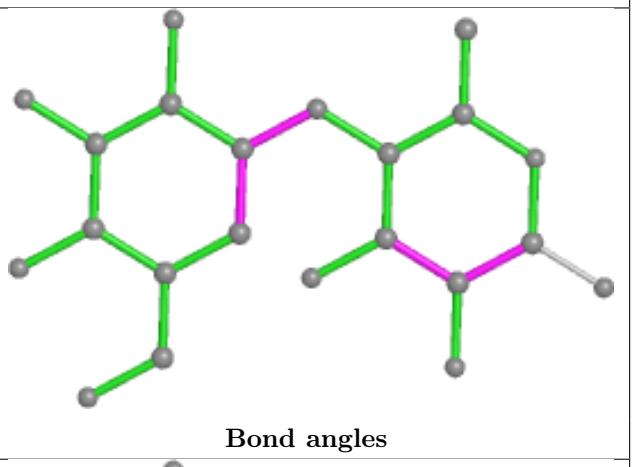


Rings

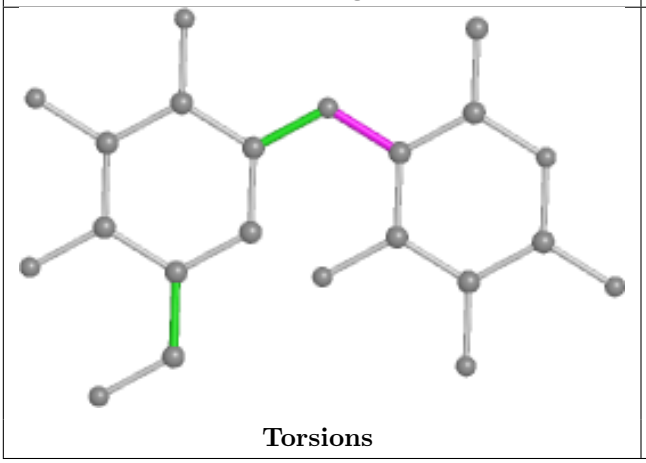
Oligosaccharide Chain L



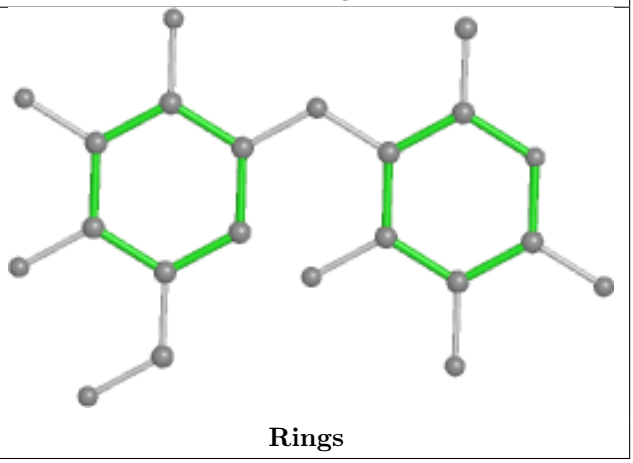
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 60 ligands modelled in this entry, 20 are monoatomic - leaving 40 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	$\#\|Z\| > 2$
13	SO4	A	1705	-	4,4,4	0.33	0	6,6,6	0.18	0
13	SO4	A	1703	-	4,4,4	0.41	0	6,6,6	0.32	0
15	EDO	A	1801	-	3,3,3	0.44	0	2,2,2	0.21	0
13	SO4	B	1706	-	4,4,4	0.33	0	6,6,6	0.18	0
13	SO4	B	1701	-	4,4,4	0.37	0	6,6,6	0.20	0
14	MES	B	1709	-	12,12,12	2.20	1 (8%)	14,16,16	1.47	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	SO4	B	1713	-	4,4,4	0.36	0	6,6,6	0.29	0
14	MES	A	1707	-	12,12,12	2.03	1 (8%)	14,16,16	1.68	1 (7%)
14	MES	B	1705	-	12,12,12	1.96	1 (8%)	14,16,16	2.02	4 (28%)
13	SO4	B	1714	-	4,4,4	0.38	0	6,6,6	0.17	0
15	EDO	B	1801	-	3,3,3	0.54	0	2,2,2	0.24	0
10	GLC	A	1451	-	12,12,12	0.69	0	17,17,17	0.77	0
13	SO4	B	1715	-	4,4,4	0.35	0	6,6,6	0.14	0
13	SO4	A	1702	-	4,4,4	0.34	0	6,6,6	0.23	0
15	EDO	A	1802	-	3,3,3	0.41	0	2,2,2	0.36	0
9	BGC	A	1401	-	12,12,12	0.54	0	17,17,17	0.63	0
15	EDO	A	1804	-	3,3,3	0.45	0	2,2,2	0.67	0
15	EDO	A	1805	-	3,3,3	0.59	0	2,2,2	0.16	0
15	EDO	A	1803	-	3,3,3	0.37	0	2,2,2	0.23	0
13	SO4	B	1704	-	4,4,4	0.32	0	6,6,6	0.11	0
15	EDO	B	1803	-	3,3,3	0.26	0	2,2,2	0.61	0
14	MES	A	1709	-	12,12,12	2.05	1 (8%)	14,16,16	1.54	3 (21%)
10	GLC	B	1451	-	12,12,12	0.63	0	17,17,17	0.72	0
14	MES	A	1710	-	12,12,12	2.30	1 (8%)	14,16,16	1.04	2 (14%)
14	MES	A	1704	-	12,12,12	1.95	1 (8%)	14,16,16	2.07	2 (14%)
13	SO4	B	1707	-	4,4,4	0.30	0	6,6,6	0.33	0
13	SO4	B	1702	-	4,4,4	0.31	0	6,6,6	0.16	0
14	MES	B	1708	-	12,12,12	2.33	1 (8%)	14,16,16	1.38	3 (21%)
15	EDO	B	1805	-	3,3,3	0.63	0	2,2,2	0.25	0
13	SO4	A	1711	-	4,4,4	0.37	0	6,6,6	0.17	0
13	SO4	B	1710	-	4,4,4	0.49	0	6,6,6	0.26	0
13	SO4	A	1701	-	4,4,4	0.35	0	6,6,6	0.17	0
13	SO4	A	1706	-	4,4,4	0.32	0	6,6,6	0.17	0
13	SO4	A	1708	-	4,4,4	0.31	0	6,6,6	0.39	0
13	SO4	B	1711	-	4,4,4	0.45	0	6,6,6	0.30	0
15	EDO	B	1804	-	3,3,3	0.40	0	2,2,2	0.57	0
14	MES	B	1712	-	12,12,12	2.17	1 (8%)	14,16,16	1.26	1 (7%)
14	MES	B	1703	-	12,12,12	2.11	1 (8%)	14,16,16	1.56	2 (14%)
15	EDO	B	1802	-	3,3,3	0.40	0	2,2,2	0.09	0
9	BGC	B	1401	-	12,12,12	0.60	0	17,17,17	0.59	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
15	EDO	A	1801	-	-	0/1/1/1	-
14	MES	B	1709	-	-	4/6/14/14	0/1/1/1
14	MES	A	1707	-	-	3/6/14/14	0/1/1/1
14	MES	B	1705	-	-	0/6/14/14	0/1/1/1
15	EDO	B	1801	-	-	0/1/1/1	-
10	GLC	A	1451	-	-	0/2/22/22	0/1/1/1
15	EDO	A	1802	-	-	0/1/1/1	-
9	BGC	A	1401	-	-	0/2/22/22	0/1/1/1
15	EDO	A	1804	-	-	0/1/1/1	-
15	EDO	A	1805	-	-	1/1/1/1	-
15	EDO	A	1803	-	-	1/1/1/1	-
15	EDO	B	1803	-	-	1/1/1/1	-
14	MES	A	1709	-	-	4/6/14/14	0/1/1/1
10	GLC	B	1451	-	-	0/2/22/22	0/1/1/1
14	MES	A	1710	-	-	0/6/14/14	0/1/1/1
14	MES	A	1704	-	-	5/6/14/14	0/1/1/1
14	MES	B	1708	-	-	0/6/14/14	0/1/1/1
15	EDO	B	1805	-	-	0/1/1/1	-
15	EDO	B	1804	-	-	0/1/1/1	-
14	MES	B	1712	-	-	0/6/14/14	0/1/1/1
14	MES	B	1703	-	-	3/6/14/14	0/1/1/1
15	EDO	B	1802	-	-	0/1/1/1	-
9	BGC	B	1401	-	-	0/2/22/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1708	MES	C8-S	-7.65	1.66	1.77
14	A	1710	MES	C8-S	-7.58	1.66	1.77
14	B	1709	MES	C8-S	-7.30	1.67	1.77
14	B	1712	MES	C8-S	-7.20	1.67	1.77
14	B	1703	MES	C8-S	-6.95	1.67	1.77
14	A	1709	MES	C8-S	-6.68	1.68	1.77
14	A	1707	MES	C8-S	-6.59	1.68	1.77
14	A	1704	MES	C8-S	-6.22	1.68	1.77
14	B	1705	MES	C8-S	-6.18	1.68	1.77

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1704	MES	O2S-S-C8	6.54	114.79	106.92
14	B	1705	MES	O1S-S-C8	5.27	113.26	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1707	MES	O2S-S-C8	4.79	112.68	106.92
14	B	1703	MES	O1S-S-C8	3.97	111.69	106.92
14	B	1712	MES	O1S-S-C8	3.32	110.91	106.92
14	A	1709	MES	O3S-S-C8	3.14	110.85	105.77
14	B	1709	MES	O3S-S-C8	3.02	110.66	105.77
14	B	1708	MES	O3S-S-C8	2.86	110.39	105.77
14	A	1709	MES	O2S-S-C8	2.70	110.17	106.92
14	A	1710	MES	O3S-S-C8	2.60	109.97	105.77
14	A	1704	MES	O3S-S-C8	2.60	109.97	105.77
14	B	1708	MES	O3S-S-O2S	-2.41	105.39	111.27
14	B	1708	MES	O1S-S-C8	2.29	109.67	106.92
14	A	1709	MES	O1S-S-C8	2.25	109.63	106.92
14	B	1705	MES	O3S-S-C8	2.21	109.34	105.77
14	B	1709	MES	O1S-S-C8	2.05	109.38	106.92
14	B	1705	MES	O2S-S-C8	2.04	109.37	106.92
14	A	1710	MES	O1-C6-C5	-2.03	107.32	111.80
14	B	1705	MES	O3S-S-O1S	-2.02	106.35	111.27
14	B	1703	MES	O2S-S-C8	2.01	109.33	106.92

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	1704	MES	C7-C8-S-O1S
14	A	1704	MES	C7-C8-S-O3S
14	A	1707	MES	C7-C8-S-O1S
14	A	1709	MES	N4-C7-C8-S
14	A	1709	MES	C7-C8-S-O2S
14	B	1703	MES	C7-C8-S-O1S
14	B	1703	MES	C7-C8-S-O2S
14	B	1709	MES	N4-C7-C8-S
14	B	1709	MES	C7-C8-S-O1S
14	A	1709	MES	C7-C8-S-O3S
14	B	1703	MES	C7-C8-S-O3S
14	B	1709	MES	C7-C8-S-O3S
15	A	1803	EDO	O1-C1-C2-O2
15	A	1805	EDO	O1-C1-C2-O2
15	B	1803	EDO	O1-C1-C2-O2
14	A	1707	MES	C7-C8-S-O3S
14	A	1704	MES	C7-C8-S-O2S
14	A	1707	MES	C7-C8-S-O2S
14	A	1709	MES	C7-C8-S-O1S

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Mol	Chain	Res	Type	Atoms
14	B	1709	MES	C7-C8-S-O2S
14	A	1704	MES	C8-C7-N4-C5
14	A	1704	MES	C8-C7-N4-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	1708	MES	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, 95^{th} 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	1247/1263 (98%)	0.30	65 (5%)	27	37	22, 33, 48, 80	0
1	B	1247/1263 (98%)	0.20	47 (3%)	40	50	22, 32, 50, 81	0
All	All	2494/2526 (98%)	0.25	112 (4%)	33	43	22, 32, 49, 81	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1281	PRO	6.0
1	A	1281	PRO	5.2
1	A	58	GLY	4.8
1	B	1237	ASN	4.3
1	A	1237	ASN	4.2
1	A	1227	GLY	4.0
1	B	503	ASN	3.8
1	A	743	SER	3.7
1	B	103	GLY	3.7
1	A	1154	PRO	3.5
1	A	1151	SER	3.5
1	A	1152	GLY	3.5
1	B	109	SER	3.4
1	A	211	LEU	3.4
1	A	793	GLY	3.3
1	A	1250	ASN	3.3
1	B	427	TRP	3.2
1	B	561	VAL	3.2
1	B	1075	MET	3.2
1	A	109	SER	3.2
1	B	487	LEU	3.1
1	B	105	THR	3.1
1	A	588	VAL	3.1
1	A	487	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	1151	SER	2.9
1	A	212	VAL	2.9
1	A	691	LEU	2.9
1	B	46	ALA	2.9
1	A	125	ALA	2.9
1	A	521	LEU	2.8
1	B	834	GLY	2.8
1	A	503	ASN	2.8
1	A	127	THR	2.8
1	A	835	SER	2.8
1	A	108	THR	2.7
1	B	1267	TYR	2.7
1	B	521	LEU	2.7
1	A	946	TRP	2.7
1	A	810	SER	2.7
1	A	1251	VAL	2.7
1	B	48	GLY	2.7
1	A	112	PRO	2.6
1	A	768	SER	2.6
1	B	61	ALA	2.6
1	B	1051	GLY	2.6
1	B	743	SER	2.6
1	B	364	PHE	2.5
1	B	476	TYR	2.5
1	A	1252	THR	2.5
1	A	146	ALA	2.5
1	A	1228	GLY	2.5
1	B	1152	GLY	2.5
1	A	1150	PRO	2.5
1	A	354	ILE	2.5
1	A	248	TYR	2.5
1	B	47	SER	2.5
1	B	100	ASP	2.4
1	B	211	LEU	2.4
1	B	391	TYR	2.4
1	A	39	GLY	2.4
1	A	111	ASP	2.4
1	B	769	GLY	2.4
1	A	42	THR	2.4
1	A	944	SER	2.4
1	B	613	LEU	2.4
1	A	486	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	614	ILE	2.4
1	A	1267	TYR	2.4
1	B	961	ILE	2.4
1	A	1254	GLY	2.4
1	A	1148	TRP	2.4
1	B	488	TRP	2.4
1	A	561	VAL	2.4
1	A	35	MET	2.3
1	A	1201	ALA	2.3
1	A	201	PHE	2.3
1	A	391	TYR	2.3
1	B	354	ILE	2.3
1	B	811	GLY	2.3
1	B	584	ALA	2.3
1	A	689	VAL	2.3
1	A	110	GLY	2.2
1	B	473	ALA	2.2
1	A	480	ALA	2.2
1	A	250	ILE	2.2
1	A	943	TRP	2.2
1	B	486	THR	2.2
1	B	1119	ALA	2.2
1	B	111	ASP	2.2
1	B	557	ALA	2.2
1	B	848	ALA	2.2
1	A	114	VAL	2.2
1	A	595	LEU	2.1
1	A	834	GLY	2.1
1	A	100	ASP	2.1
1	A	427	TRP	2.1
1	A	210	VAL	2.1
1	B	108	THR	2.1
1	B	101	ALA	2.1
1	B	147	SER	2.1
1	A	1249	ILE	2.1
1	A	1238	ASP	2.1
1	A	477	TYR	2.1
1	A	1037	ALA	2.1
1	A	1200	ASN	2.1
1	A	961	ILE	2.1
1	B	212	VAL	2.0
1	B	588	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	874	THR	2.0
1	B	770	SER	2.0
1	A	40	ASN	2.0
1	B	393	ILE	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, 95^{th} 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	GLC	C	5	11/12	0.39	0.49	83,90,94,95	0
4	GLC	E	4	11/12	0.58	0.33	67,74,77,78	0
7	GLC	K	1	1/12	0.62	0.39	66,66,66,66	0
5	GLC	J	4	11/12	0.79	0.39	57,61,64,67	0
5	GLC	F	4	11/12	0.81	0.27	49,53,59,61	0
3	GLC	H	1	12/12	0.83	0.29	41,52,54,56	0
4	GLC	E	1	12/12	0.84	0.30	62,73,76,78	0
7	AC1	L	2	21/22	0.84	0.17	38,49,58,60	0
3	GLC	D	1	12/12	0.85	0.32	49,59,63,63	0
7	AC1	K	2	21/22	0.87	0.21	39,46,61,61	0
2	GLC	C	4	11/12	0.87	0.30	61,67,75,78	0
6	GLC	I	1	12/12	0.88	0.30	49,55,58,59	0
4	GLC	G	4	11/12	0.88	0.27	58,64,65,67	0
4	GLC	E	2	11/12	0.89	0.23	44,49,57,62	0
2	GLC	C	3	11/12	0.90	0.16	43,45,48,54	0
5	BGC	F	1	12/12	0.91	0.12	39,40,43,48	0
3	GLC	D	2	11/12	0.92	0.16	38,44,48,49	0
5	BGC	J	1	12/12	0.92	0.15	41,45,48,50	0
6	GLC	I	2	11/12	0.92	0.19	39,42,46,50	0
4	GLC	G	3	11/12	0.93	0.20	45,48,51,54	0
4	GLC	G	1	12/12	0.93	0.18	44,48,50,53	0
7	GLC	L	1	1/12	0.93	0.11	56,56,56,56	0
6	GLC	I	3	11/12	0.93	0.13	34,39,42,43	0
5	GLC	J	3	11/12	0.94	0.10	32,33,41,47	0

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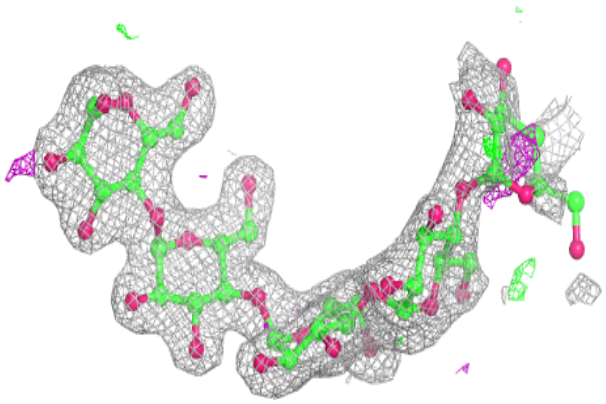
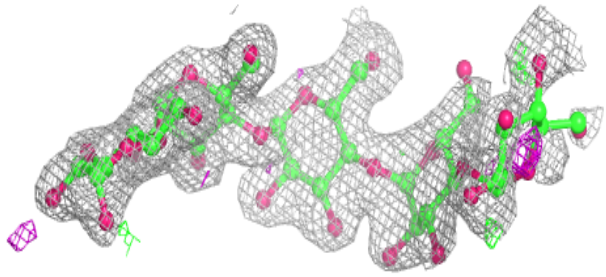
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GLC	G	2	11/12	0.94	0.15	41,44,46,47	0
4	GLC	E	3	11/12	0.94	0.11	37,43,46,57	0
5	GLC	F	3	11/12	0.95	0.10	30,33,37,40	0
2	GLC	C	1	12/12	0.95	0.18	41,44,47,50	0
5	GLC	F	2	11/12	0.95	0.08	33,36,38,39	0
5	GLC	J	2	11/12	0.96	0.10	33,35,36,37	0
2	GLC	C	2	11/12	0.96	0.15	36,40,42,43	0
3	GLC	H	2	11/12	0.97	0.12	31,34,37,38	0

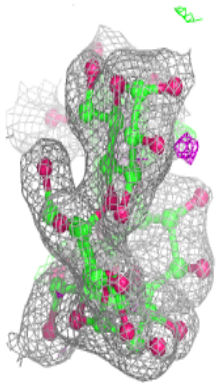
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

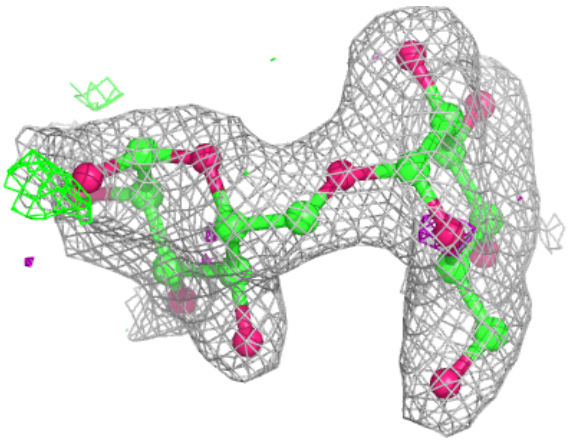


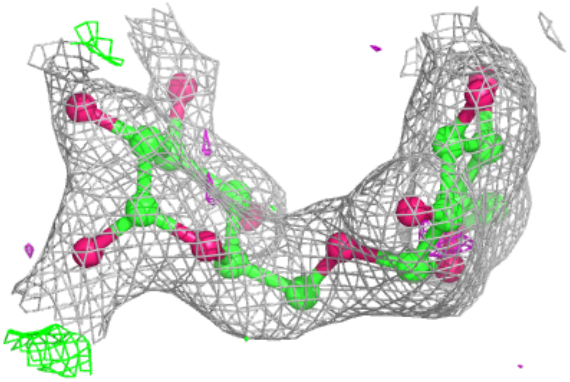


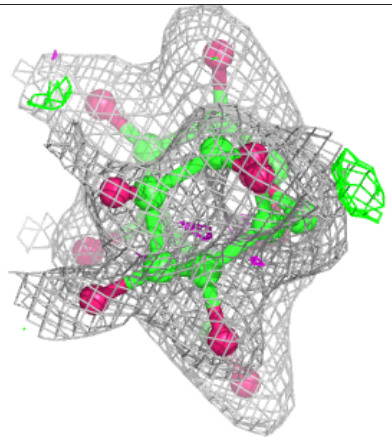


Electron density around Chain D:

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

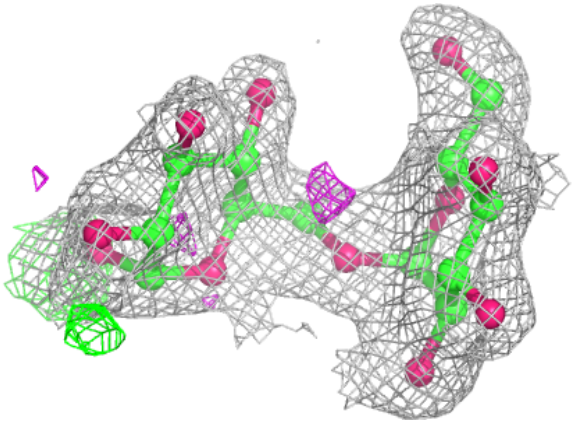


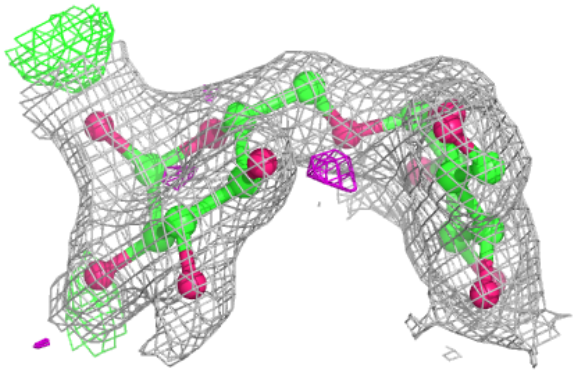


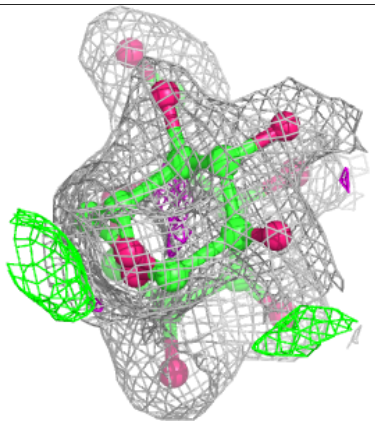


Electron density around Chain H:

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

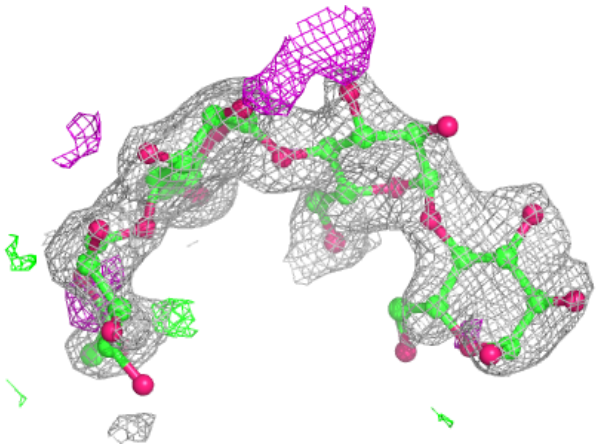


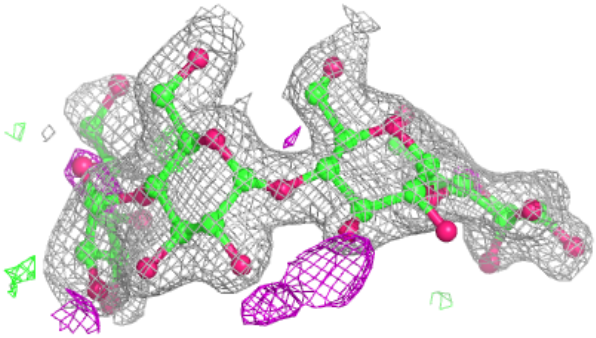


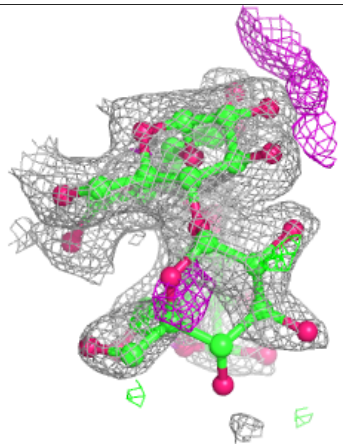


Electron density around Chain E:

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

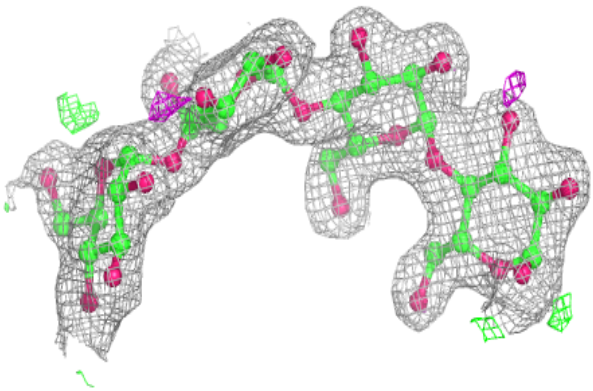


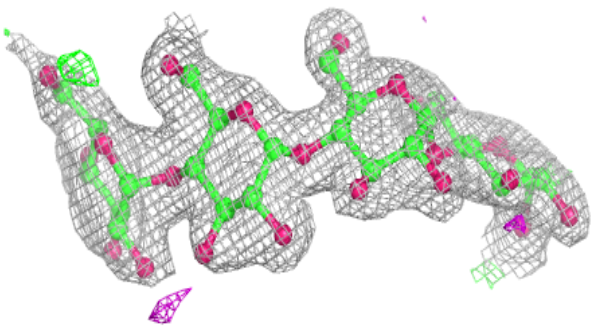


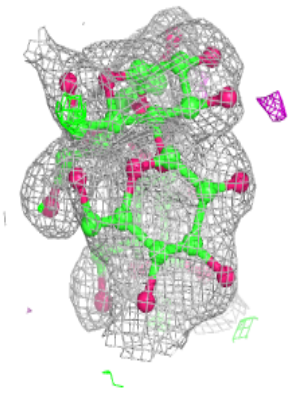


Electron density around Chain G:

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

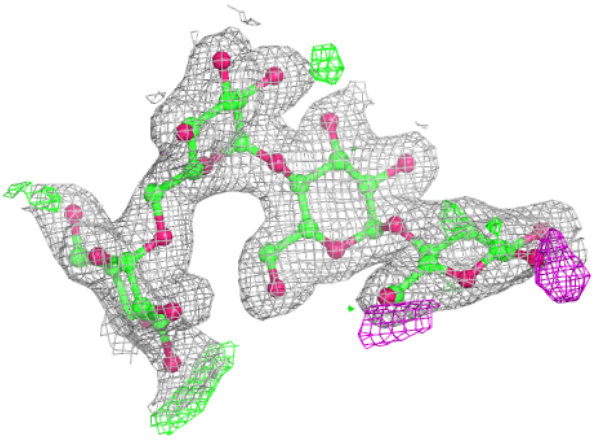


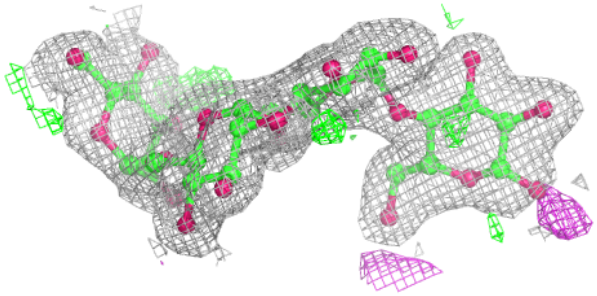


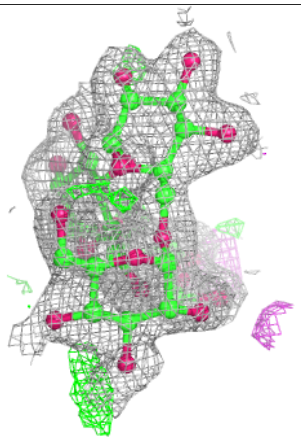


Electron density around Chain F:

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

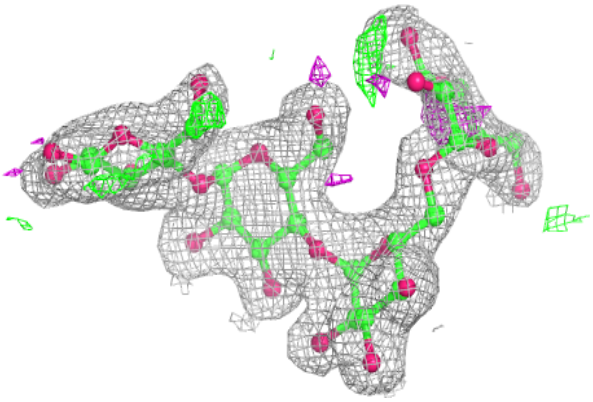


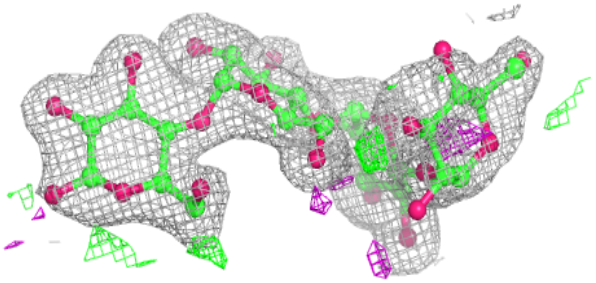


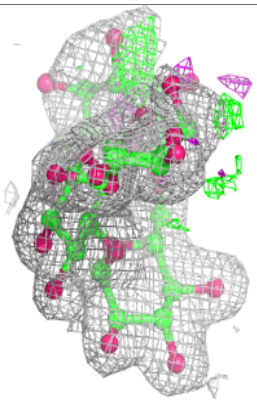


Electron density around Chain J:

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

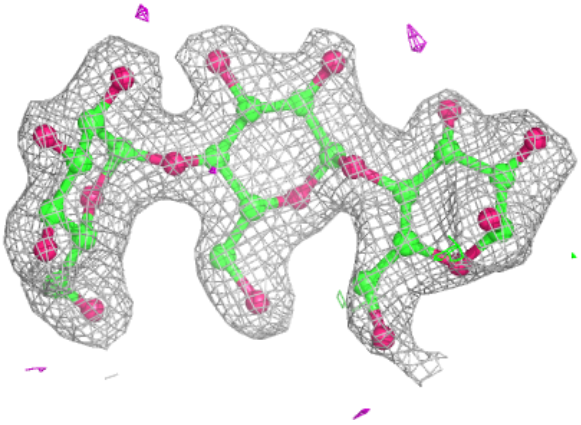


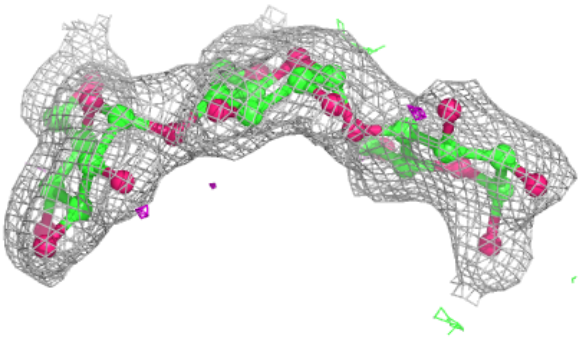


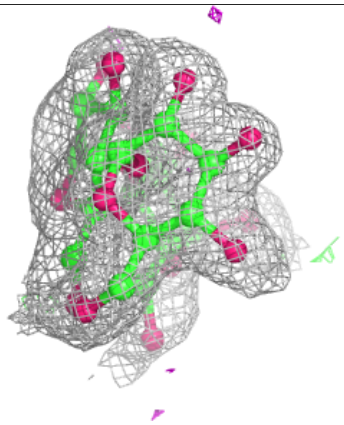


Electron density around Chain I:

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

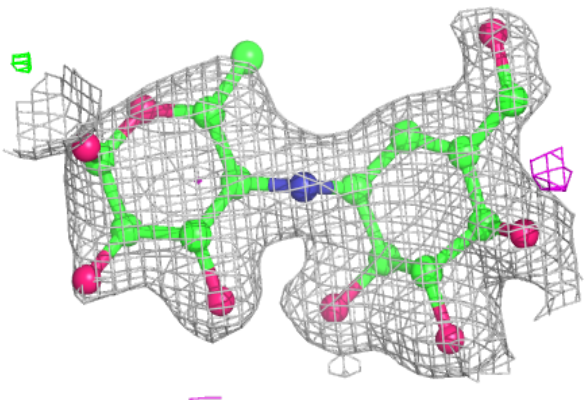


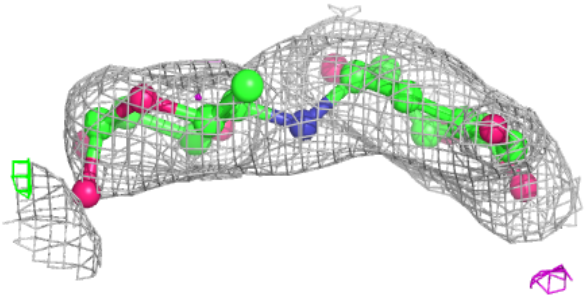


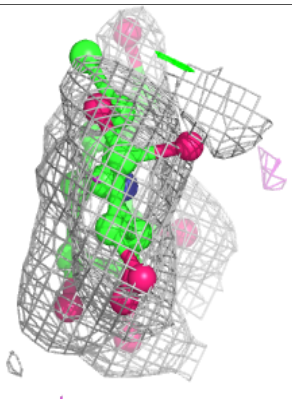


Electron density around Chain K:

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

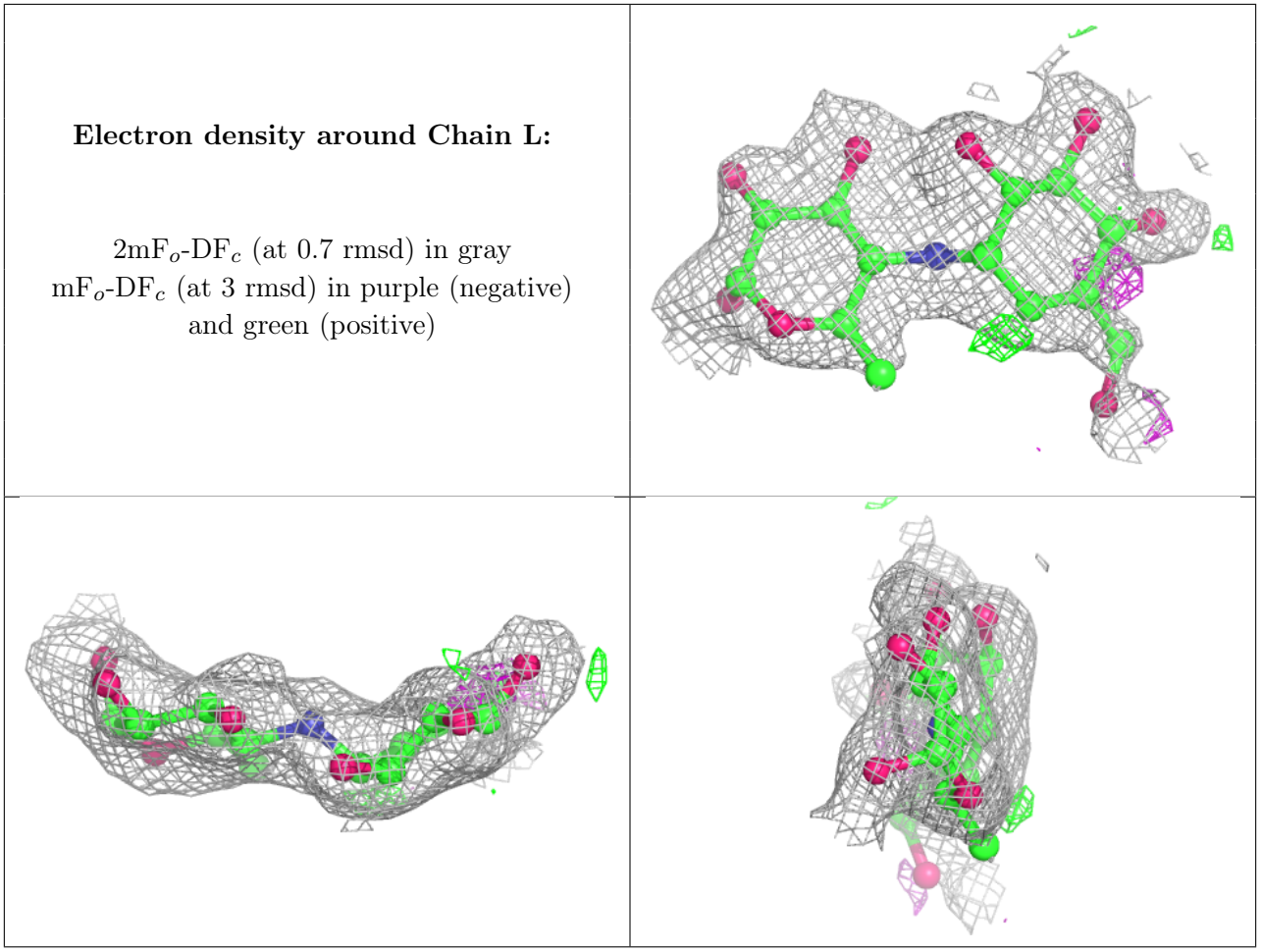






Electron density around Chain L:

$2mF_o$-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, 95^{th} 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
14	MES	A	1709	12/12	0.72	0.39	75,83,90,92	0
14	MES	B	1708	12/12	0.77	0.26	74,77,81,83	0
14	MES	A	1707	12/12	0.79	0.35	59,71,80,84	0
12	MG	A	1605	1/1	0.80	0.26	69,69,69,69	0
15	EDO	B	1805	4/4	0.80	0.17	41,44,46,49	0
14	MES	A	1704	12/12	0.81	0.36	54,68,82,84	0
14	MES	B	1709	12/12	0.82	0.33	73,80,85,89	0
14	MES	B	1703	12/12	0.82	0.34	62,66,83,89	0
13	SO4	A	1711	5/5	0.83	0.28	86,88,91,91	0
13	SO4	B	1714	5/5	0.84	0.43	77,80,83,84	0
12	MG	B	1605	1/1	0.84	0.29	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	GLC	A	1451	12/12	0.84	0.20	46,52,54,56	0
13	SO4	B	1710	5/5	0.84	0.32	56,62,70,73	0
14	MES	B	1705	12/12	0.86	0.23	46,62,69,69	0
13	SO4	B	1715	5/5	0.86	0.28	82,84,87,88	0
13	SO4	A	1703	5/5	0.87	0.35	61,65,74,75	0
13	SO4	B	1711	5/5	0.87	0.24	53,59,66,67	0
10	GLC	B	1451	12/12	0.87	0.24	41,48,51,52	0
15	EDO	A	1804	4/4	0.88	0.17	31,36,37,41	0
15	EDO	A	1802	4/4	0.89	0.15	44,45,45,46	0
15	EDO	B	1803	4/4	0.90	0.18	48,48,49,51	0
13	SO4	B	1706	5/5	0.90	0.22	72,77,78,80	0
12	MG	A	1602	1/1	0.91	0.04	43,43,43,43	0
15	EDO	A	1805	4/4	0.91	0.15	42,45,46,47	0
12	MG	A	1604	1/1	0.92	0.24	60,60,60,60	0
13	SO4	B	1713	5/5	0.92	0.25	61,63,64,70	0
15	EDO	A	1803	4/4	0.93	0.14	42,48,49,50	0
15	EDO	B	1804	4/4	0.93	0.14	29,31,33,37	0
15	EDO	B	1801	4/4	0.93	0.09	35,35,35,36	0
13	SO4	B	1701	5/5	0.94	0.15	53,55,59,62	0
13	SO4	A	1706	5/5	0.94	0.20	64,65,69,71	0
8	CA	A	1302	1/1	0.95	0.06	41,41,41,41	0
13	SO4	A	1701	5/5	0.95	0.12	53,55,58,61	0
12	MG	B	1604	1/1	0.95	0.32	57,57,57,57	0
13	SO4	B	1702	5/5	0.95	0.23	58,59,63,63	0
13	SO4	A	1705	5/5	0.95	0.22	66,70,72,72	0
12	MG	B	1602	1/1	0.96	0.11	48,48,48,48	0
13	SO4	A	1702	5/5	0.96	0.24	55,56,59,59	0
13	SO4	B	1704	5/5	0.96	0.20	62,65,67,67	0
9	BGC	B	1401	12/12	0.97	0.19	24,25,26,26	0
12	MG	B	1603	1/1	0.97	0.09	60,60,60,60	0
8	CA	A	1303	1/1	0.97	0.07	33,33,33,33	0
9	BGC	A	1401	12/12	0.97	0.14	25,26,27,28	0
15	EDO	B	1802	4/4	0.97	0.10	39,39,40,40	0
12	MG	B	1606	1/1	0.97	0.07	40,40,40,40	0
14	MES	B	1712	12/12	0.97	0.09	35,37,39,43	0
13	SO4	A	1708	5/5	0.97	0.12	45,47,51,51	0
14	MES	A	1710	12/12	0.98	0.07	37,41,43,43	0
12	MG	A	1601	1/1	0.98	0.06	28,28,28,28	0
12	MG	A	1606	1/1	0.98	0.09	38,38,38,38	0
8	CA	A	1301	1/1	0.98	0.04	36,36,36,36	0
13	SO4	B	1707	5/5	0.98	0.10	44,45,46,48	0
12	MG	A	1603	1/1	0.98	0.16	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	EDO	A	1801	4/4	0.98	0.10	32,34,34,34	0
8	CA	B	1302	1/1	0.98	0.05	40,40,40,40	0
12	MG	B	1601	1/1	0.99	0.06	25,25,25,25	0
8	CA	B	1303	1/1	0.99	0.07	34,34,34,34	0
11	NI	A	1501	1/1	0.99	0.05	45,45,45,45	0
8	CA	B	1301	1/1	1.00	0.07	30,30,30,30	0
11	NI	B	1501	1/1	1.00	0.04	45,45,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.