wwPDB X-ray Structure Validation Summary Report (i)

Sep 11, 2023 – 11:59 AM EDT

PDB ID	:	8DL1
Title	:	BoGH13ASus-E523Q from Bacteroides ovatus bound to maltoheptaose
Authors	:	Brown, H.A.; DeVeaux, A.L.; Koropatkin, N.M.
Deposited on	:	2022-07-06
Resolution	:	2.09 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

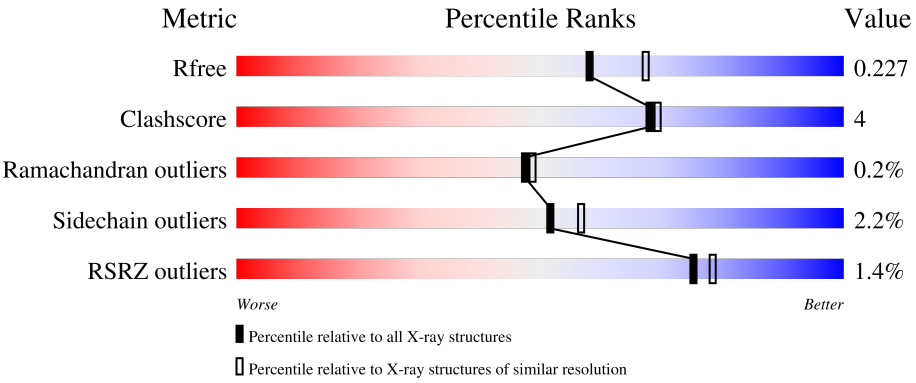
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.09 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	738	88% 7%
1	B	738	% 89% 7%
1	C	738	2% 87% 8%
1	D	738	2% 87% 8%
2	G	5	100%

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Mol	Chain	Length	Quality of chain
2	H	5	20% 80%
2	I	5	20% 80%
2	J	5	20% 80%
2	K	5	80% 20%
3	L	3	67% 33%
3	M	3	100%
4	N	4	75% 25%
5	O	7	86% 14%
6	P	7	100%
7	Q	6	17% 83%
8	R	5	20% 80%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	ACT	D	805	-	-	X	-
13	1PE	C	2301	-	-	X	-
9	EDO	A	2316	-	-	X	-

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 25543 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.

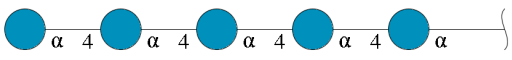
- Molecule 1 is a protein called Alpha amylase, catalytic domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total	C	N	O	S	0	1	0
			5726	3652	943	1108	23			
1	B	708	Total	C	N	O	S	0	2	0
			5664	3613	932	1096	23			
1	C	712	Total	C	N	O	S	0	0	0
			5698	3635	940	1101	22			
1	D	706	Total	C	N	O	S	0	1	0
			5613	3586	925	1080	22			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLY	-	expression tag	UNP A7M087
A	523	GLN	GLU	engineered mutation	UNP A7M087
B	21	GLY	-	expression tag	UNP A7M087
B	523	GLN	GLU	engineered mutation	UNP A7M087
C	21	GLY	-	expression tag	UNP A7M087
C	523	GLN	GLU	engineered mutation	UNP A7M087
D	21	GLY	-	expression tag	UNP A7M087
D	523	GLN	GLU	engineered mutation	UNP A7M087

- 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	G	5	Total	C	O	0	0	0
			56	30	26			

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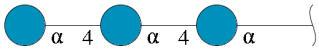
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	H	5	Total C O 56 30 26	0	0	0
2	I	5	Total C O 56 30 26	0	0	0
2	J	5	Total C O 56 30 26	0	0	0
2	K	5	Total C O 56 30 26	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

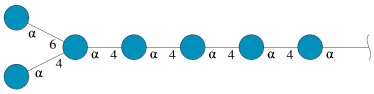


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	L	3	Total C O 34 18 16	0	0	0
3	M	3	Total C O 34 18 16	0	0	0

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

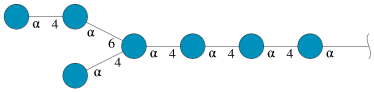
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	N	4	Total C O 45 24 21	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]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
5	O	7	Total C O 78 42 36	0	0	0

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

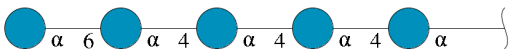


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	P	7	Total C O 78 42 36	0	0	0

- Molecule 7 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

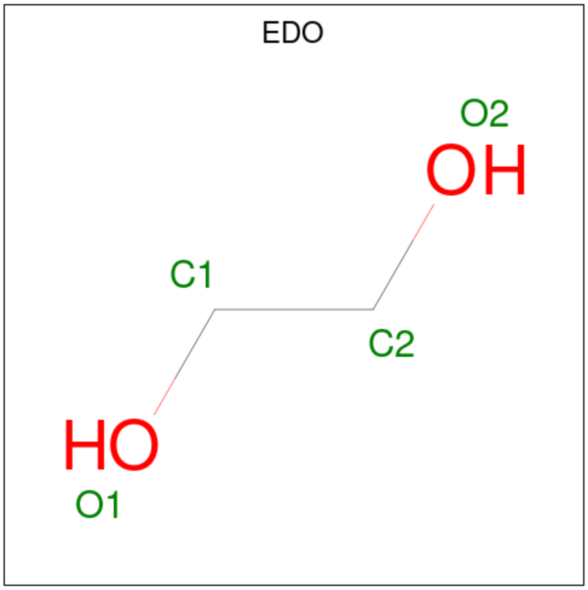
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	Q	6	Total C O 67 36 31	0	0	0

- Molecule 8 is an oligosaccharide called alpha-D-glucopyranose-(1-6)-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
8	R	5	Total C O 56 30 26	0	0	0

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

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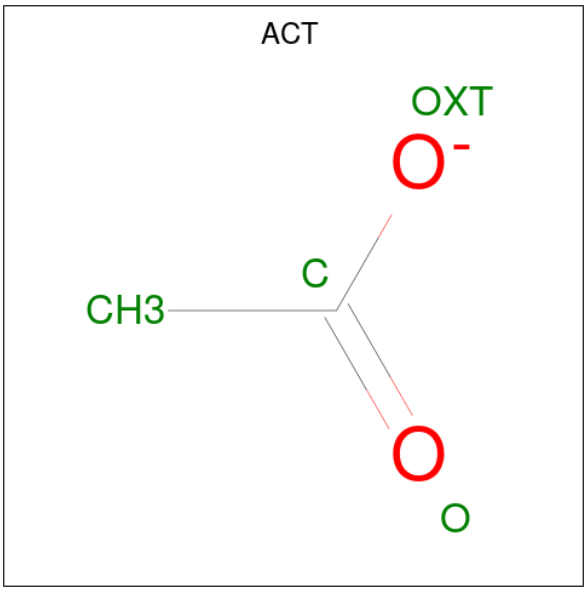
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	C	1	Total C O 4 2 2	0	0
9	C	1	Total C O 4 2 2	0	0
9	C	1	Total C O 4 2 2	0	0
9	C	1	Total C O 4 2 2	0	0
9	C	1	Total C O 4 2 2	0	0
9	C	1	Total C O 4 2 2	0	0
9	C	1	Total C O 4 2 2	0	0
9	C	1	Total C O 4 2 2	0	0
9	C	1	Total C O 4 2 2	0	0
9	C	1	Total C O 4 2 2	0	0
9	C	1	Total C O 4 2 2	0	0
9	C	1	Total C O 4 2 2	0	0
9	C	1	Total C O 4 2 2	0	0
9	D	1	Total C O 4 2 2	0	0
9	D	1	Total C O 4 2 2	0	0
9	D	1	Total C O 4 2 2	0	0
9	D	1	Total C O 4 2 2	0	0
9	D	1	Total C O 4 2 2	0	0

- Molecule 10 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 4 2 2	0	0
10	A	1	Total C O 4 2 2	0	0
10	A	1	Total C O 4 2 2	0	0
10	A	1	Total C O 4 2 2	0	0
10	D	1	Total C O 4 2 2	0	0

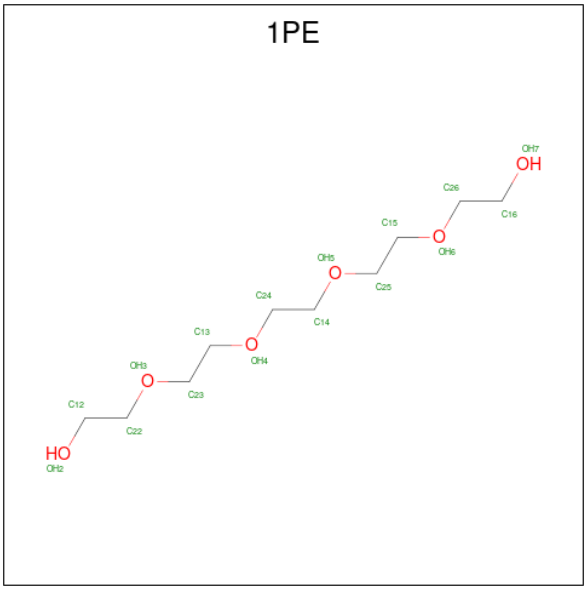
- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 12 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

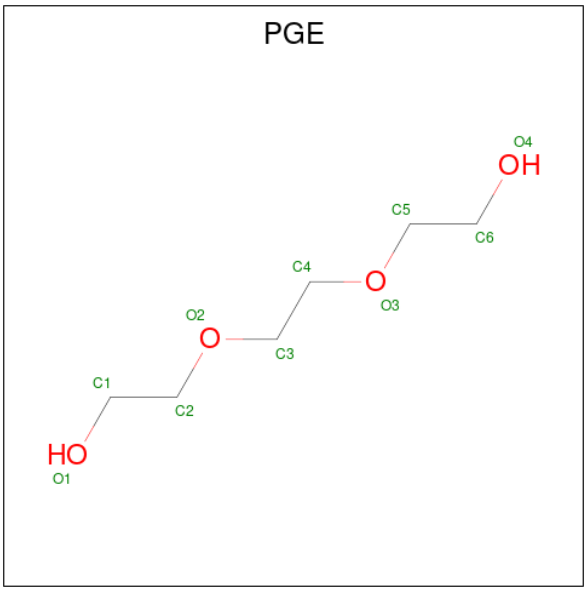
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total Mn 1 1	0	0
12	B	1	Total Mn 1 1	0	0
12	C	1	Total Mn 1 1	0	0
12	D	1	Total Mn 1 1	0	0

- Molecule 13 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	C	1	Total C O 16 10 6	0	0

- Molecule 14 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).

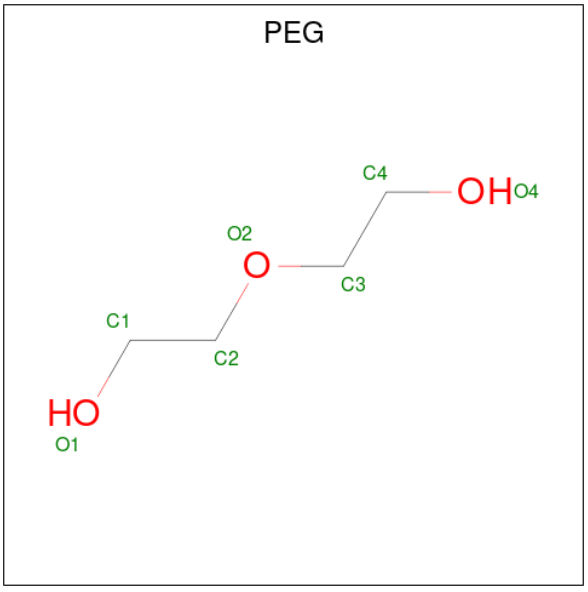


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	C	1	Total C O 10 6 4	0	0

- Molecule 15 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	C	1	Total Na 1 1	0	0

- Molecule 16 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	C	1	Total C O 7 4 3	0	0

- Molecule 17 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	D	1	Total Cl 1 1	0	0

- Molecule 18 is water.

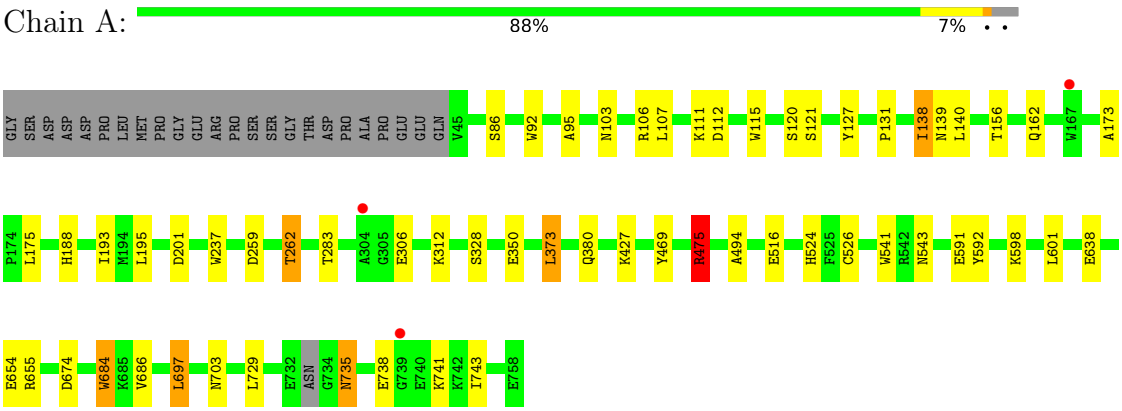
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	587	Total O 587 587	0	0
18	B	488	Total O 488 488	0	0
18	C	462	Total O 462 462	0	0
18	D	350	Total O 350 350	0	0

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.

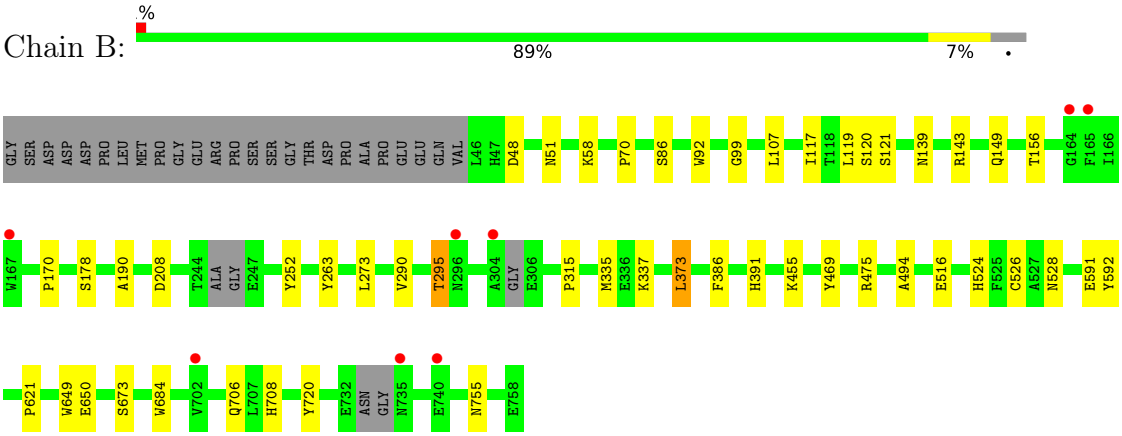
• Molecule 1: Alpha amylase, catalytic domain protein

Chain A:



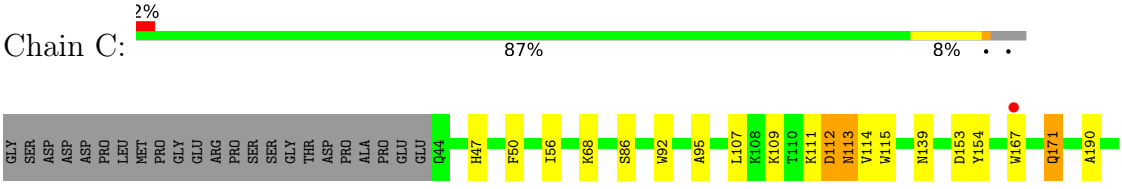
• Molecule 1: Alpha amylase, catalytic domain protein

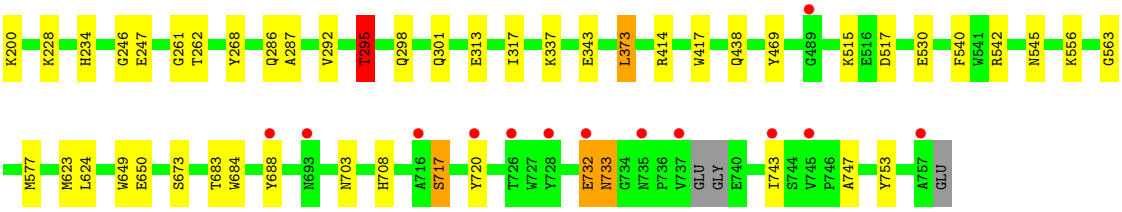
Chain B:



• Molecule 1: Alpha amylase, catalytic domain protein

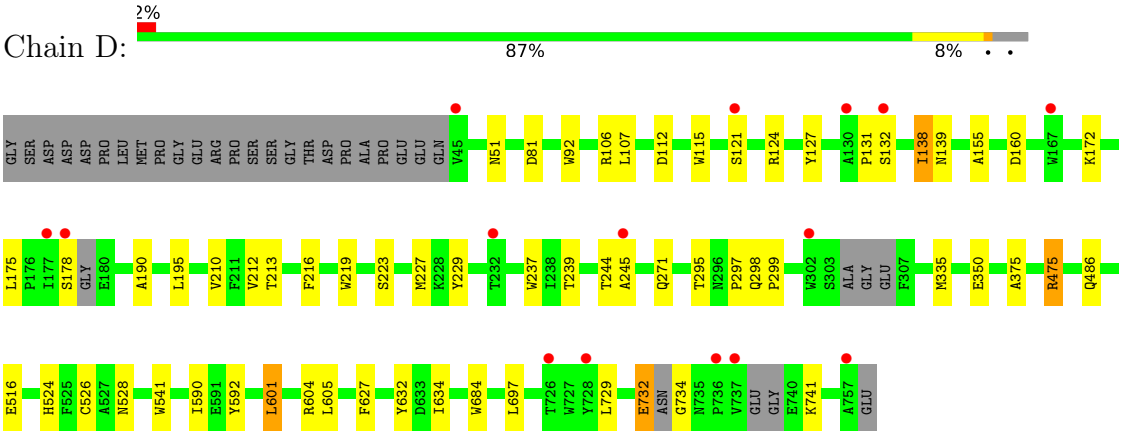
Chain C:





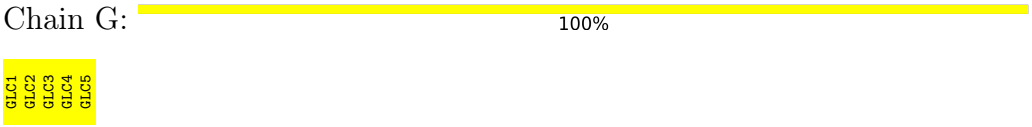
• Molecule 1: Alpha amylase, catalytic domain protein

Chain D:



• 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 G:



• 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 H:

• 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

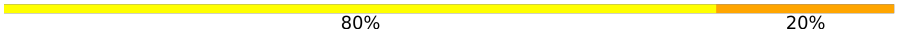
Chain I:

• 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 J:

• 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 K:

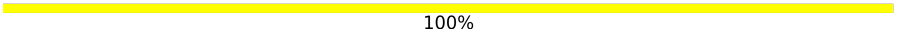


• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain L:

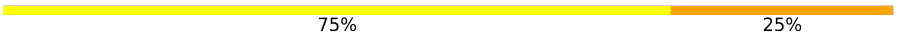
• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain M:



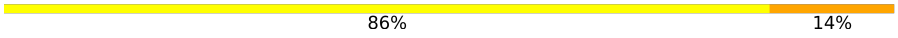
• Molecule 4: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

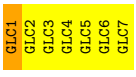
Chain N:



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

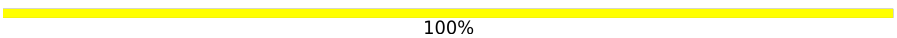
Chain O:

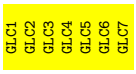




• Molecule 6: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-6)-[alpha-D-glucopyranose-(1-4)]alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

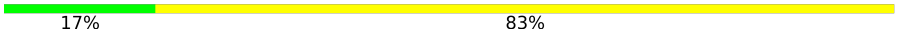
Chain P:

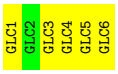




• Molecule 7: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain Q:





• Molecule 8: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain R:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	99.68Å 128.64Å 149.76Å 90.00° 105.37° 90.00°	Depositor
Resolution (Å)	47.93 – 2.09 47.89 – 2.09	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.93-2.09) 98.8 (47.89-2.09)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.177 , 0.223 0.185 , 0.227	Depositor DCC
R_{free} test set	10581 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	20.8	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 53.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	25543	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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: CA, GLC, PEG, EDO, 1PE, NA, MN, PGE, CL, ACT

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	0.70	0/5895	0.84	1/8021 (0.0%)
1	B	0.69	0/5832	0.84	0/7939
1	C	0.68	0/5864	0.83	1/7986 (0.0%)
1	D	0.68	0/5779	0.80	0/7875
All	All	0.69	0/23370	0.83	2/31821 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	475	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	C	295	THR	N-CA-CB	-5.08	100.65	110.30

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	5726	0	5357	37	0
1	B	5664	0	5266	38	0
1	C	5698	0	5310	55	0
1	D	5613	0	5186	36	0
2	G	56	0	48	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	56	0	48	0	0
2	I	56	0	48	0	0
2	J	56	0	48	0	0
2	K	56	0	48	1	0
3	L	34	0	30	0	0
3	M	34	0	30	0	0
4	N	45	0	39	1	0
5	O	78	0	66	1	0
6	P	78	0	66	0	0
7	Q	67	0	57	0	0
8	R	56	0	48	0	0
9	A	68	0	102	7	0
9	B	80	0	120	10	0
9	C	52	0	78	6	0
9	D	20	0	30	2	0
10	A	16	0	12	0	0
10	D	4	0	3	2	0
11	A	1	0	0	0	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
11	D	1	0	0	0	0
12	A	1	0	0	0	0
12	B	1	0	0	0	0
12	C	1	0	0	0	0
12	D	1	0	0	0	0
13	C	16	0	22	19	0
14	C	10	0	14	1	0
15	C	1	0	0	0	0
16	C	7	0	10	2	0
17	D	1	0	0	0	0
18	A	587	0	0	4	0
18	B	488	0	0	9	0
18	C	462	0	0	8	0
18	D	350	0	0	2	0
All	All	25543	0	22086	174	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 4.

The worst 5 of 174 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:TRP:HE1	13:C:2301:1PE:H162	1.27	0.97
1:B:190:ALA:O	1:B:295:THR:HG21	1.72	0.90
1:C:50:PHE:H	16:C:2312:PEG:H21	1.46	0.79
1:D:271:GLN:HG3	10:D:805:ACT:H1	1.66	0.77
1:C:92:TRP:NE1	13:C:2301:1PE:H162	2.00	0.76

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	710/738 (96%)	681 (96%)	27 (4%)	2 (0%)	41	41
1	B	702/738 (95%)	664 (95%)	38 (5%)	0	100	100
1	C	708/738 (96%)	678 (96%)	29 (4%)	1 (0%)	51	54
1	D	697/738 (94%)	658 (94%)	36 (5%)	3 (0%)	34	32
All	All	2817/2952 (95%)	2681 (95%)	130 (5%)	6 (0%)	47	49

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	733	ASN
1	A	306	GLU
1	A	121	SER
1	D	298	GLN
1	D	245	ALA

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	611/639 (96%)	592 (97%)	19 (3%)	40	43
1	B	601/639 (94%)	593 (99%)	8 (1%)	69	75
1	C	605/639 (95%)	594 (98%)	11 (2%)	59	65
1	D	589/639 (92%)	574 (98%)	15 (2%)	47	52
All	All	2406/2556 (94%)	2353 (98%)	53 (2%)	52	57

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	112	ASP
1	C	684	TRP
1	D	601	LEU
1	C	113	ASN
1	C	298	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	298	GLN
1	C	408	ASN
1	D	408	ASN
1	C	113	ASN
1	A	546	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

60 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GLC	G	1	2	12,12,12	0.71	0	17,17,17	1.84	4 (23%)
2	GLC	G	2	2	11,11,12	0.80	0	15,15,17	1.34	3 (20%)
2	GLC	G	3	2	11,11,12	0.79	0	15,15,17	1.00	1 (6%)
2	GLC	G	4	2	11,11,12	0.60	0	15,15,17	1.34	2 (13%)
2	GLC	G	5	2	11,11,12	0.55	0	15,15,17	1.35	1 (6%)
2	GLC	H	1	2	12,12,12	0.72	0	17,17,17	1.47	4 (23%)
2	GLC	H	2	2	11,11,12	0.65	0	15,15,17	1.49	4 (26%)
2	GLC	H	3	2	11,11,12	0.73	0	15,15,17	0.90	0
2	GLC	H	4	2	11,11,12	0.70	0	15,15,17	1.36	2 (13%)
2	GLC	H	5	2	11,11,12	0.87	1 (9%)	15,15,17	2.31	9 (60%)
2	GLC	I	1	2	12,12,12	0.63	0	17,17,17	1.81	5 (29%)
2	GLC	I	2	2	11,11,12	0.64	0	15,15,17	1.15	1 (6%)
2	GLC	I	3	2	11,11,12	0.74	0	15,15,17	0.75	0
2	GLC	I	4	2	11,11,12	0.64	0	15,15,17	1.05	1 (6%)
2	GLC	I	5	2	11,11,12	0.49	0	15,15,17	1.20	1 (6%)
2	GLC	J	1	2	12,12,12	0.63	0	17,17,17	1.38	3 (17%)
2	GLC	J	2	2	11,11,12	1.03	1 (9%)	15,15,17	1.65	3 (20%)
2	GLC	J	3	2	11,11,12	0.86	0	15,15,17	1.30	2 (13%)
2	GLC	J	4	2	11,11,12	0.50	0	15,15,17	0.79	0
2	GLC	J	5	2	11,11,12	0.72	0	15,15,17	1.28	2 (13%)
2	GLC	K	1	2	12,12,12	0.73	0	17,17,17	1.27	2 (11%)
2	GLC	K	2	2	11,11,12	0.90	0	15,15,17	1.57	3 (20%)
2	GLC	K	3	2	11,11,12	0.57	0	15,15,17	1.63	5 (33%)
2	GLC	K	4	2	11,11,12	0.57	0	15,15,17	1.52	2 (13%)
2	GLC	K	5	2	11,11,12	0.68	0	15,15,17	1.36	3 (20%)
3	GLC	L	1	3	12,12,12	0.37	0	17,17,17	1.12	0
3	GLC	L	2	3	11,11,12	0.94	1 (9%)	15,15,17	1.59	3 (20%)
3	GLC	L	3	3	11,11,12	0.65	0	15,15,17	0.85	0
3	GLC	M	1	3	12,12,12	0.66	0	17,17,17	1.22	2 (11%)
3	GLC	M	2	3	11,11,12	0.28	0	15,15,17	1.24	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GLC	M	3	3	11,11,12	0.47	0	15,15,17	1.16	1 (6%)
4	GLC	N	1	4	12,12,12	0.77	0	17,17,17	1.16	2 (11%)
4	GLC	N	2	4	11,11,12	0.63	0	15,15,17	1.47	3 (20%)
4	GLC	N	3	4	11,11,12	0.71	0	15,15,17	1.01	1 (6%)
4	GLC	N	4	4	11,11,12	0.50	0	15,15,17	1.49	2 (13%)
5	GLC	O	1	5	12,12,12	0.94	0	17,17,17	1.17	3 (17%)
5	GLC	O	2	5	11,11,12	0.83	1 (9%)	15,15,17	1.81	5 (33%)
5	GLC	O	3	5	11,11,12	0.98	0	15,15,17	1.30	1 (6%)
5	GLC	O	4	5	11,11,12	0.85	0	15,15,17	1.85	3 (20%)
5	GLC	O	5	5	11,11,12	0.92	0	15,15,17	1.65	5 (33%)
5	GLC	O	6	5	11,11,12	0.46	0	15,15,17	2.26	5 (33%)
5	GLC	O	7	5	11,11,12	1.32	2 (18%)	15,15,17	1.89	4 (26%)
6	GLC	P	1	6	12,12,12	0.70	0	17,17,17	2.23	5 (29%)
6	GLC	P	2	6	11,11,12	0.92	1 (9%)	15,15,17	1.29	2 (13%)
6	GLC	P	3	6	11,11,12	0.94	0	15,15,17	2.08	7 (46%)
6	GLC	P	4	6	11,11,12	0.65	0	15,15,17	1.60	3 (20%)
6	GLC	P	5	6	11,11,12	1.03	0	15,15,17	1.63	3 (20%)
6	GLC	P	6	6	11,11,12	0.60	0	15,15,17	1.39	2 (13%)
6	GLC	P	7	6	11,11,12	0.86	0	15,15,17	2.20	4 (26%)
7	GLC	Q	1	7	12,12,12	0.78	0	17,17,17	1.79	3 (17%)
7	GLC	Q	2	7	11,11,12	0.46	0	15,15,17	0.82	0
7	GLC	Q	3	7	11,11,12	0.94	0	15,15,17	1.95	4 (26%)
7	GLC	Q	4	7	11,11,12	0.85	0	15,15,17	1.86	3 (20%)
7	GLC	Q	5	7	11,11,12	1.33	2 (18%)	15,15,17	1.38	2 (13%)
7	GLC	Q	6	7	11,11,12	0.94	1 (9%)	15,15,17	2.06	3 (20%)
8	GLC	R	1	8	12,12,12	0.73	0	17,17,17	0.72	0
8	GLC	R	2	8	11,11,12	0.83	0	15,15,17	1.21	1 (6%)
8	GLC	R	3	8	11,11,12	0.57	0	15,15,17	1.96	3 (20%)
8	GLC	R	4	8	11,11,12	0.99	0	15,15,17	1.23	2 (13%)
8	GLC	R	5	8	11,11,12	1.43	2 (18%)	15,15,17	1.67	4 (26%)

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	G	1	2	-	2/2/22/22	0/1/1/1
2	GLC	G	2	2	-	0/2/19/22	0/1/1/1
2	GLC	G	3	2	-	0/2/19/22	0/1/1/1
2	GLC	G	4	2	-	0/2/19/22	0/1/1/1
2	GLC	G	5	2	-	0/2/19/22	0/1/1/1
2	GLC	H	1	2	-	0/2/22/22	0/1/1/1
2	GLC	H	2	2	-	0/2/19/22	0/1/1/1
2	GLC	H	3	2	-	0/2/19/22	0/1/1/1
2	GLC	H	4	2	-	0/2/19/22	0/1/1/1
2	GLC	H	5	2	-	0/2/19/22	0/1/1/1
2	GLC	I	1	2	-	0/2/22/22	0/1/1/1
2	GLC	I	2	2	-	0/2/19/22	0/1/1/1
2	GLC	I	3	2	-	0/2/19/22	0/1/1/1
2	GLC	I	4	2	-	0/2/19/22	0/1/1/1
2	GLC	I	5	2	-	0/2/19/22	0/1/1/1
2	GLC	J	1	2	-	2/2/22/22	0/1/1/1
2	GLC	J	2	2	-	0/2/19/22	0/1/1/1
2	GLC	J	3	2	-	0/2/19/22	0/1/1/1
2	GLC	J	4	2	-	0/2/19/22	0/1/1/1
2	GLC	J	5	2	-	2/2/19/22	0/1/1/1
2	GLC	K	1	2	-	0/2/22/22	0/1/1/1
2	GLC	K	2	2	-	2/2/19/22	0/1/1/1
2	GLC	K	3	2	-	0/2/19/22	0/1/1/1
2	GLC	K	4	2	-	0/2/19/22	0/1/1/1
2	GLC	K	5	2	-	2/2/19/22	0/1/1/1
3	GLC	L	1	3	-	2/2/22/22	0/1/1/1
3	GLC	L	2	3	-	0/2/19/22	0/1/1/1
3	GLC	L	3	3	-	0/2/19/22	0/1/1/1
3	GLC	M	1	3	-	2/2/22/22	0/1/1/1
3	GLC	M	2	3	-	0/2/19/22	0/1/1/1
3	GLC	M	3	3	-	0/2/19/22	0/1/1/1
4	GLC	N	1	4	-	0/2/22/22	0/1/1/1
4	GLC	N	2	4	-	0/2/19/22	0/1/1/1
4	GLC	N	3	4	-	2/2/19/22	0/1/1/1
4	GLC	N	4	4	-	0/2/19/22	0/1/1/1
5	GLC	O	1	5	-	0/2/22/22	0/1/1/1
5	GLC	O	2	5	-	0/2/19/22	0/1/1/1
5	GLC	O	3	5	-	0/2/19/22	0/1/1/1
5	GLC	O	4	5	-	2/2/19/22	0/1/1/1
5	GLC	O	5	5	-	0/2/19/22	0/1/1/1
5	GLC	O	6	5	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GLC	O	7	5	-	0/2/19/22	0/1/1/1
6	GLC	P	1	6	-	2/2/22/22	0/1/1/1
6	GLC	P	2	6	-	0/2/19/22	0/1/1/1
6	GLC	P	3	6	-	2/2/19/22	0/1/1/1
6	GLC	P	4	6	-	0/2/19/22	0/1/1/1
6	GLC	P	5	6	-	0/2/19/22	0/1/1/1
6	GLC	P	6	6	-	2/2/19/22	0/1/1/1
6	GLC	P	7	6	-	2/2/19/22	0/1/1/1
7	GLC	Q	1	7	-	2/2/22/22	0/1/1/1
7	GLC	Q	2	7	-	0/2/19/22	0/1/1/1
7	GLC	Q	3	7	-	1/2/19/22	0/1/1/1
7	GLC	Q	4	7	-	0/2/19/22	0/1/1/1
7	GLC	Q	5	7	-	0/2/19/22	0/1/1/1
7	GLC	Q	6	7	-	0/2/19/22	0/1/1/1
8	GLC	R	1	8	-	0/2/22/22	0/1/1/1
8	GLC	R	2	8	-	1/2/19/22	0/1/1/1
8	GLC	R	3	8	-	1/2/19/22	0/1/1/1
8	GLC	R	4	8	-	0/2/19/22	0/1/1/1
8	GLC	R	5	8	-	0/2/19/22	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	2	GLC	O5-C1	-2.55	1.39	1.43
7	Q	5	GLC	C2-C3	2.39	1.56	1.52
5	O	7	GLC	O5-C5	2.23	1.48	1.43
8	R	5	GLC	O5-C1	2.17	1.47	1.43
6	P	2	GLC	O5-C1	-2.15	1.40	1.43

The worst 5 of 156 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	Q	6	GLC	C1-O5-C5	5.95	120.25	112.19
6	P	7	GLC	O5-C5-C6	5.47	115.78	107.20
7	Q	4	GLC	O5-C1-C2	-5.34	102.53	110.77
6	P	1	GLC	C1-O5-C5	4.64	122.42	113.66
6	P	1	GLC	O1-C1-C2	4.62	122.05	109.03

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

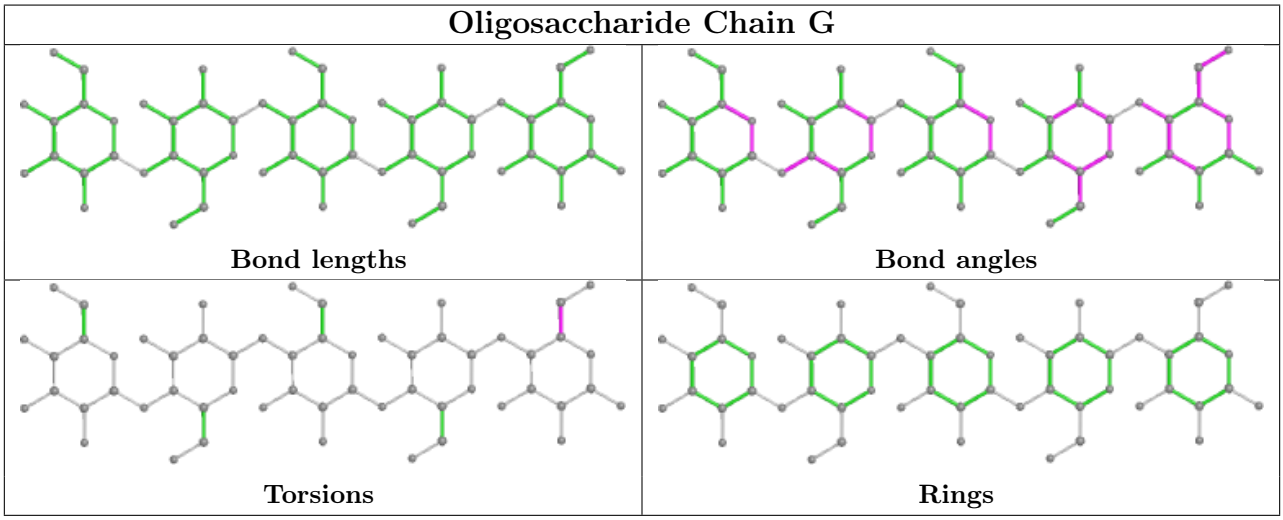
Mol	Chain	Res	Type	Atoms
4	N	3	GLC	O5-C5-C6-O6
2	K	5	GLC	O5-C5-C6-O6
6	P	6	GLC	C4-C5-C6-O6
6	P	1	GLC	O5-C5-C6-O6
6	P	7	GLC	O5-C5-C6-O6

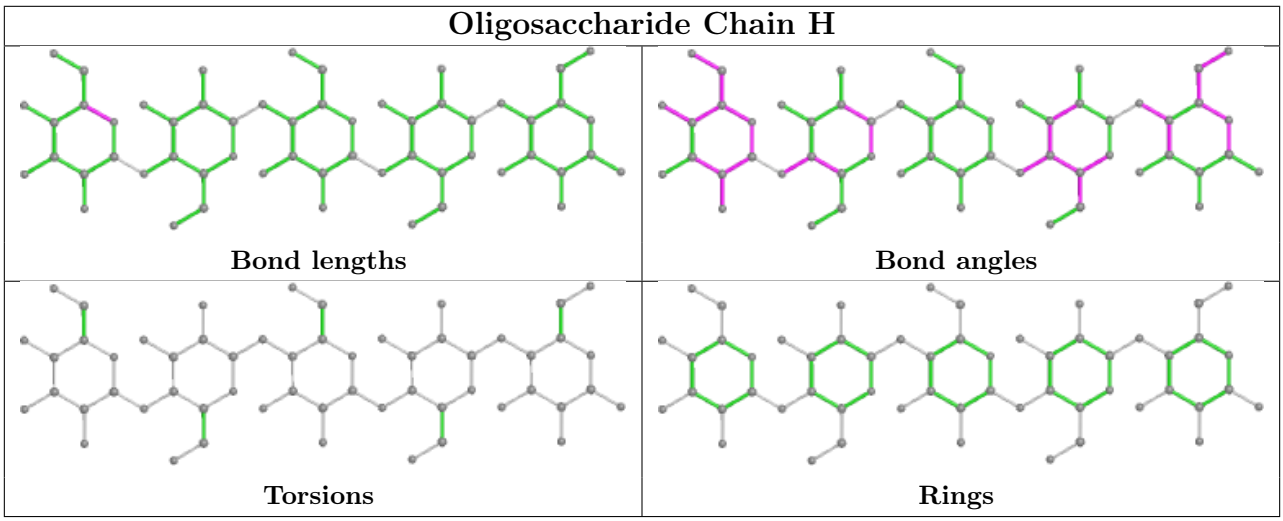
There are no ring outliers.

3 monomers are involved in 3 short contacts:

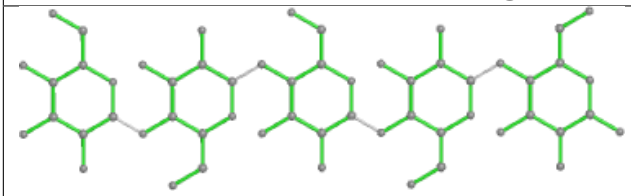
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	2	GLC	1	0
5	O	1	GLC	1	0
4	N	1	GLC	1	0

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

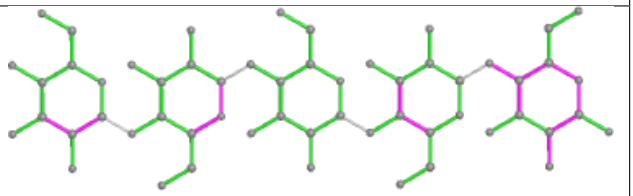




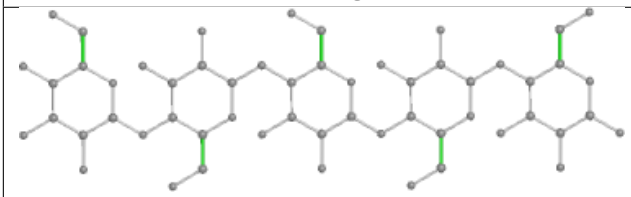
Oligosaccharide Chain I



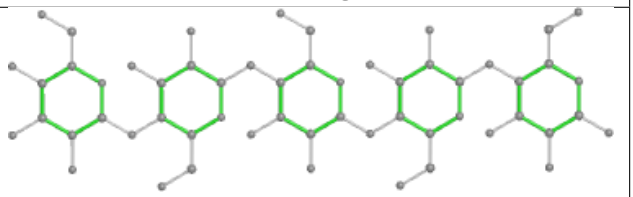
Bond lengths



Bond angles

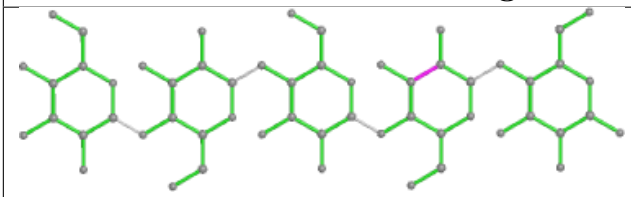


Torsions

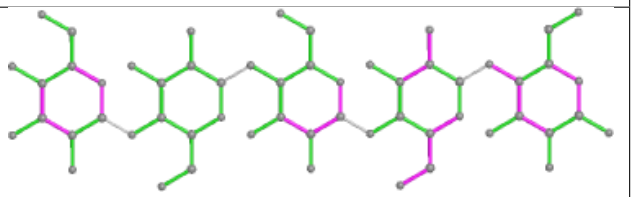


Rings

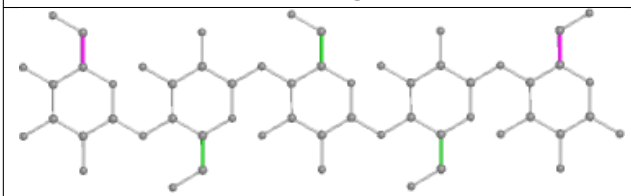
Oligosaccharide Chain J



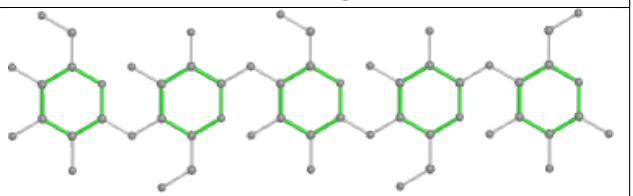
Bond lengths



Bond angles

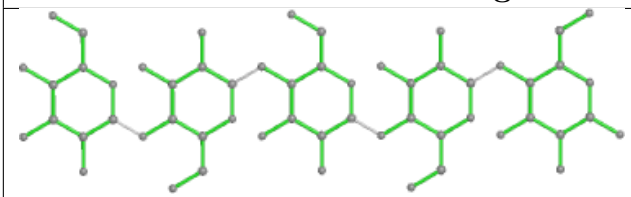


Torsions

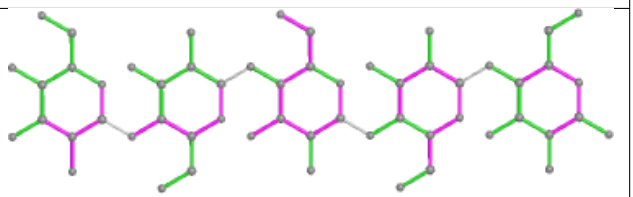


Rings

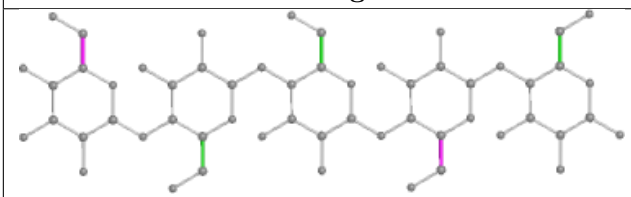
Oligosaccharide Chain K



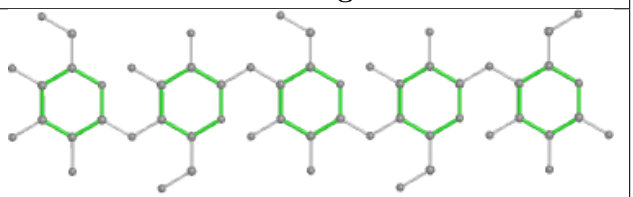
Bond lengths



Bond angles

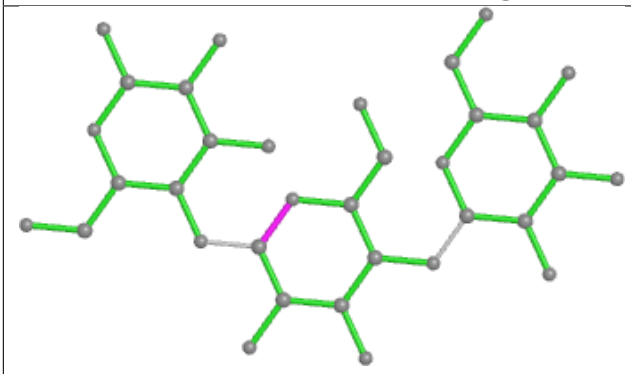


Torsions

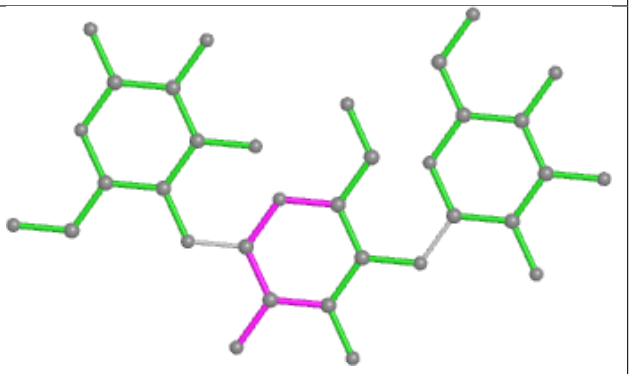


Rings

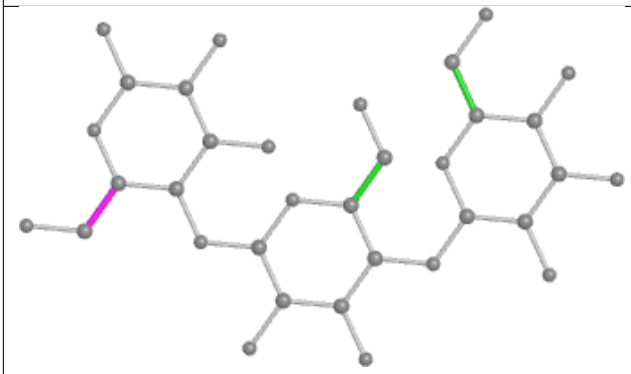
Oligosaccharide Chain L



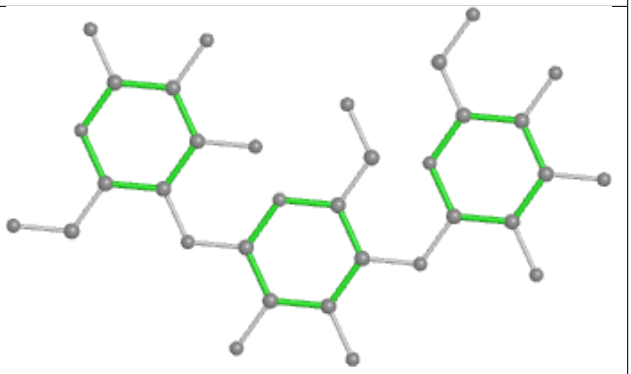
Bond lengths



Bond angles

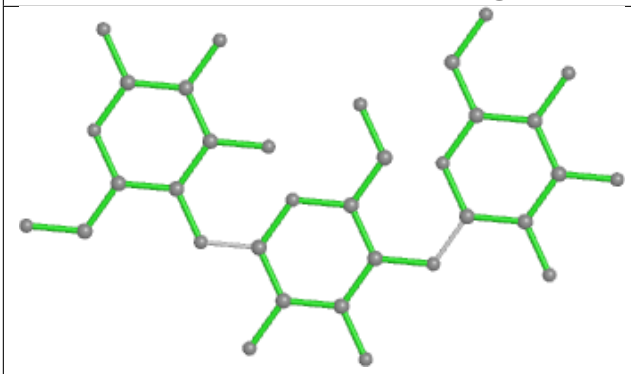


Torsions

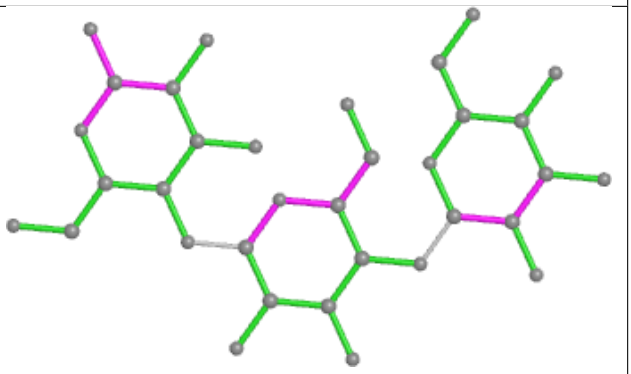


Rings

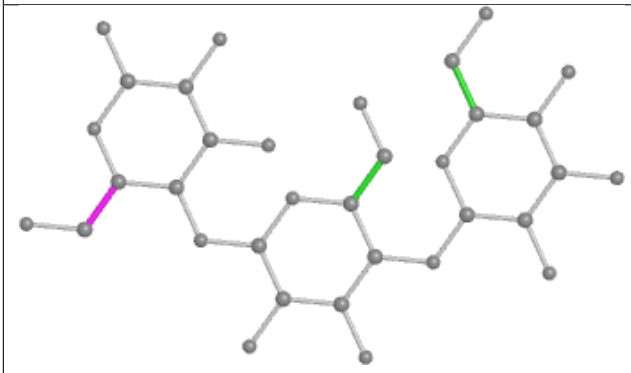
Oligosaccharide Chain M



Bond lengths



Bond angles



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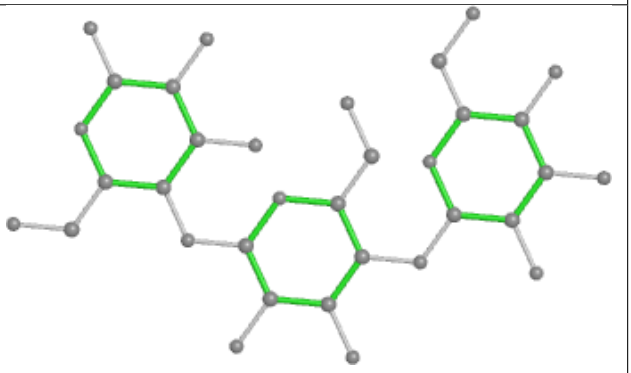
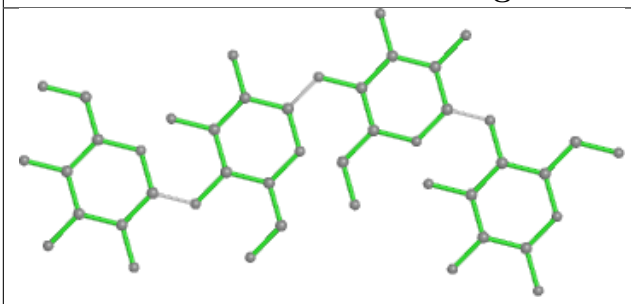
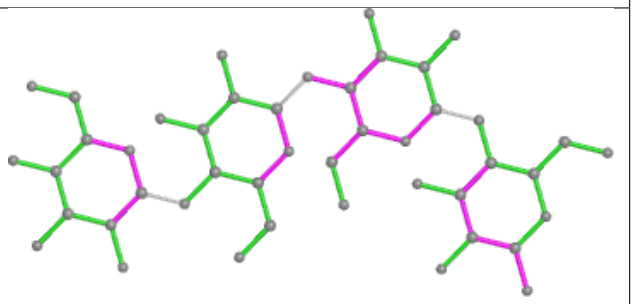


Rings

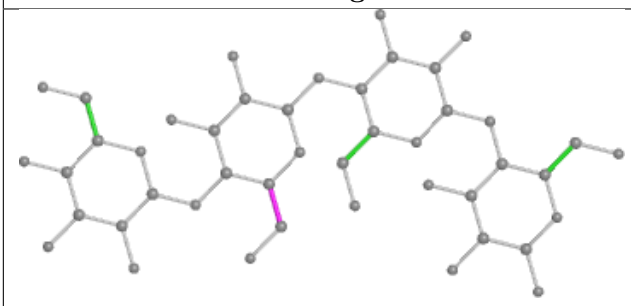
Oligosaccharide Chain N



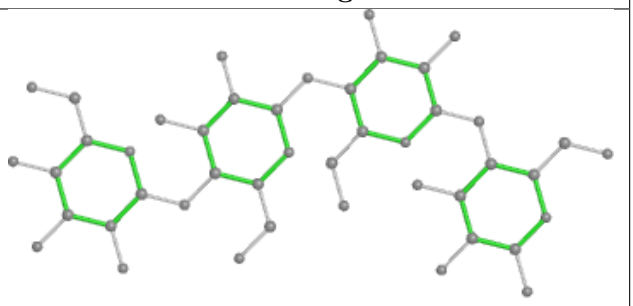
Bond lengths



Bond angles

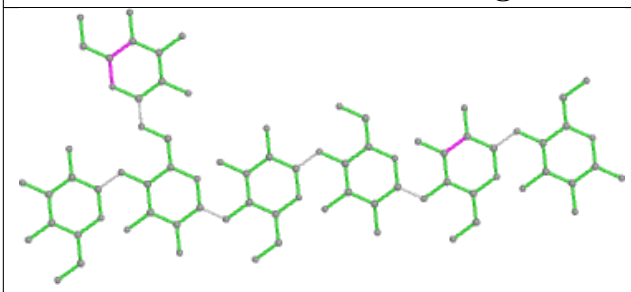


Torsions

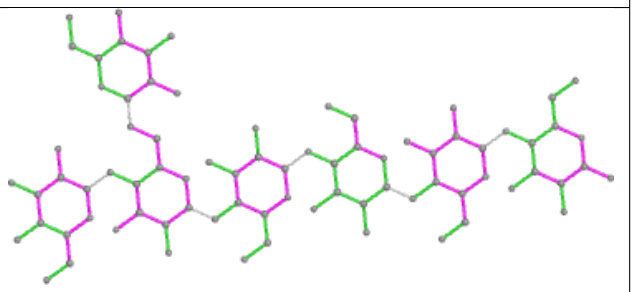


Rings

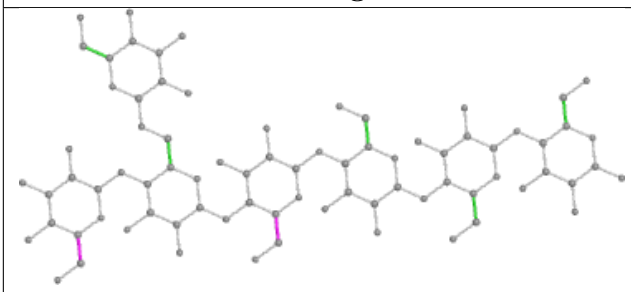
Oligosaccharide Chain O



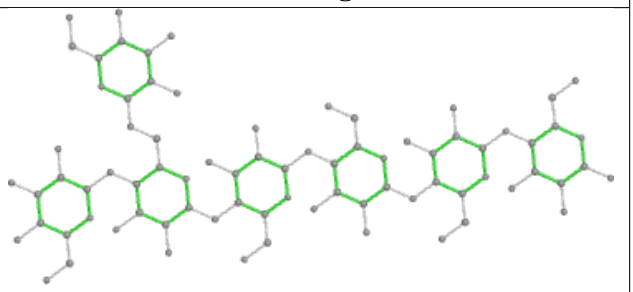
Bond lengths



Bond angles

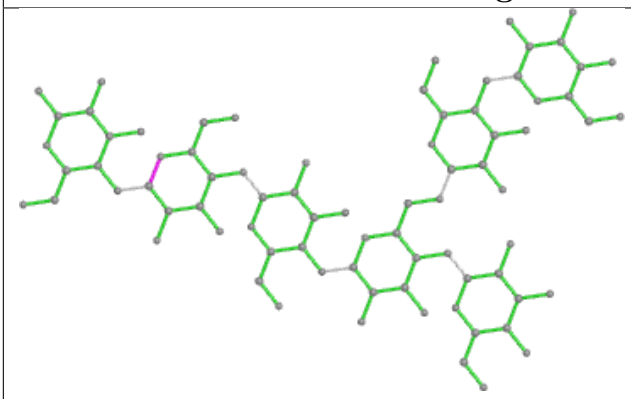


Torsions

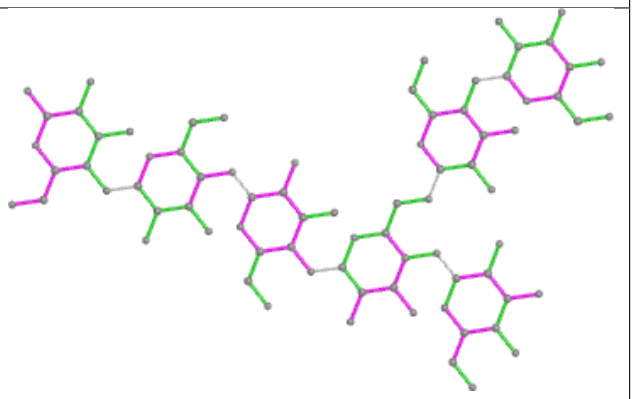


Rings

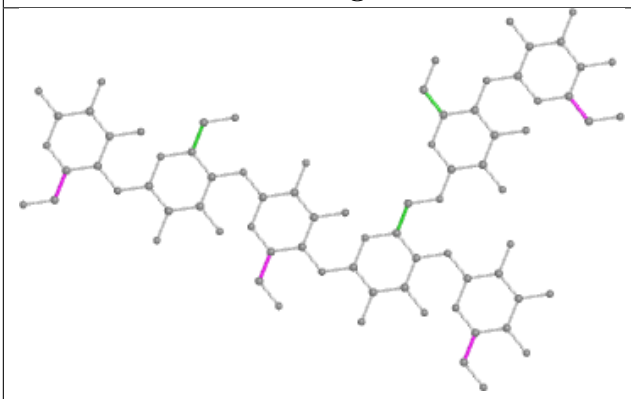
Oligosaccharide Chain P



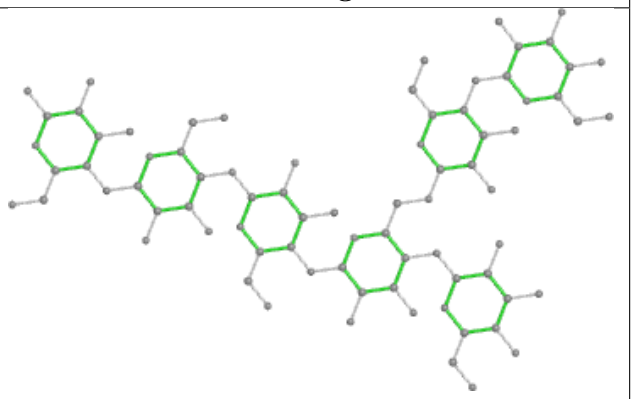
Bond lengths



Bond angles

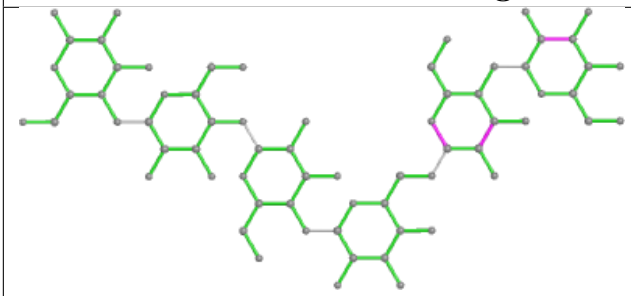


Torsions

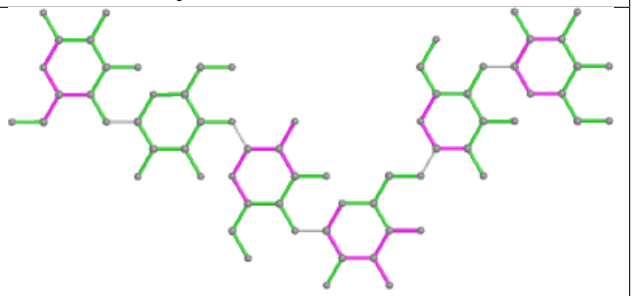


Rings

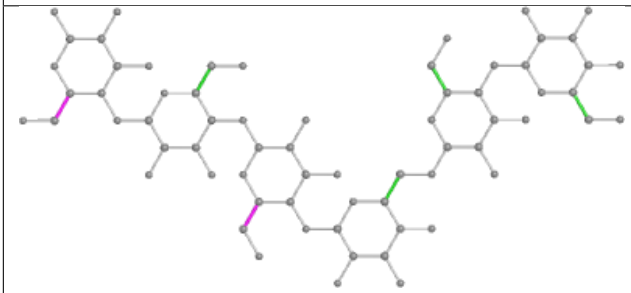
Oligosaccharide Chain Q



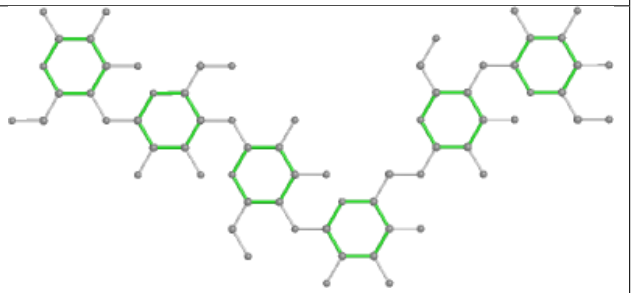
Bond lengths



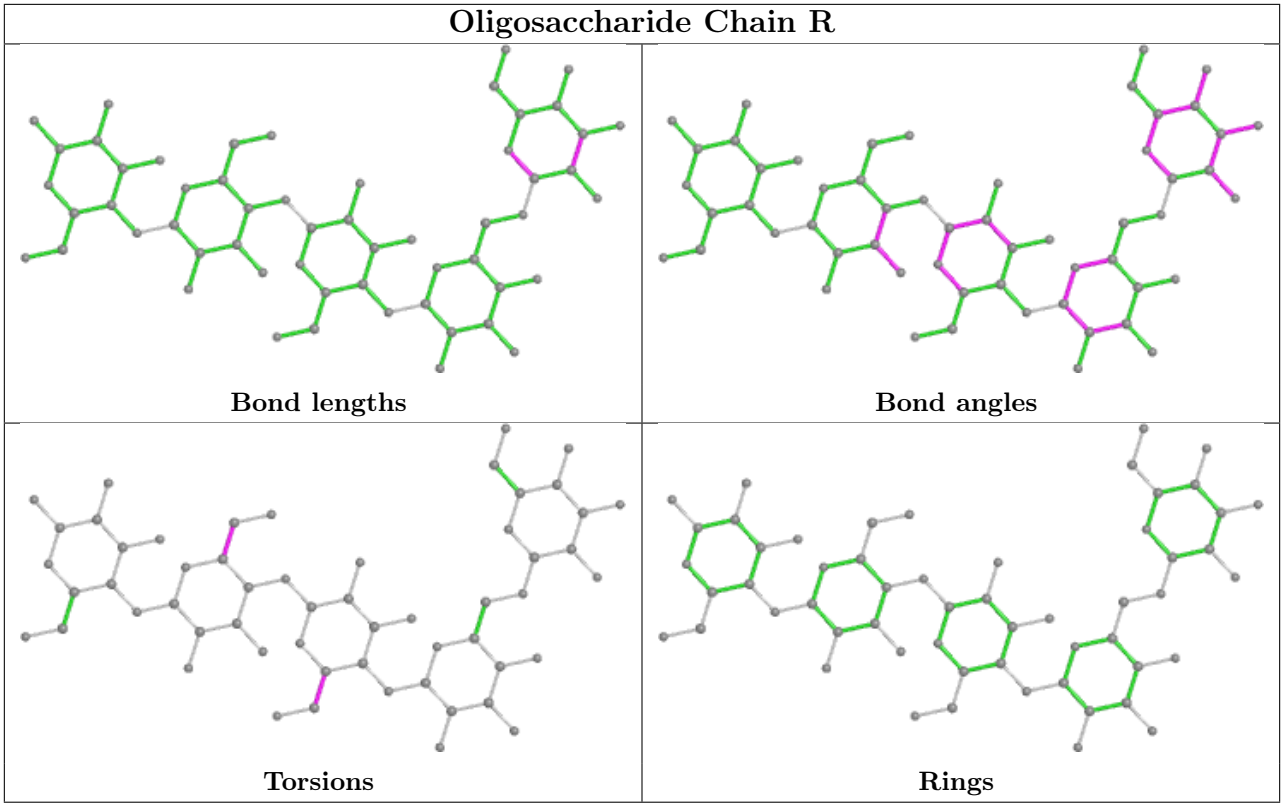
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 73 ligands modelled in this entry, 10 are monoatomic - leaving 63 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	$\#\|Z\| > 2$
9	EDO	A	2307	-	3,3,3	0.04	0	2,2,2	0.22	0
9	EDO	B	3318	-	3,3,3	0.12	0	2,2,2	0.30	0
10	ACT	D	805	-	3,3,3	0.85	0	3,3,3	1.03	0
9	EDO	B	3308	-	3,3,3	0.07	0	2,2,2	0.46	0
10	ACT	A	2320	-	3,3,3	1.04	0	3,3,3	0.68	0
9	EDO	A	2308	-	3,3,3	0.18	0	2,2,2	0.33	0
9	EDO	C	2303	-	3,3,3	0.24	0	2,2,2	0.52	0
9	EDO	B	3304	-	3,3,3	0.28	0	2,2,2	0.12	0
9	EDO	B	3321	-	3,3,3	0.10	0	2,2,2	0.15	0
9	EDO	C	2313	-	3,3,3	0.40	0	2,2,2	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	EDO	C	2306	-	3,3,3	0.18	0	2,2,2	0.12	0
9	EDO	D	806	-	3,3,3	0.05	0	2,2,2	0.13	0
9	EDO	B	3312	-	3,3,3	0.12	0	2,2,2	0.28	0
9	EDO	B	3320	-	3,3,3	0.14	0	2,2,2	0.60	0
9	EDO	B	3306	-	3,3,3	0.07	0	2,2,2	0.34	0
9	EDO	A	2316	-	3,3,3	0.57	0	2,2,2	0.71	0
9	EDO	B	3313	-	3,3,3	0.20	0	2,2,2	0.15	0
9	EDO	C	2305	-	3,3,3	0.17	0	2,2,2	0.28	0
14	PGE	C	2302	-	9,9,9	0.24	0	8,8,8	0.16	0
9	EDO	A	2314	-	3,3,3	0.28	0	2,2,2	0.33	0
9	EDO	A	2318	-	3,3,3	0.14	0	2,2,2	0.30	0
9	EDO	B	3301	-	3,3,3	0.09	0	2,2,2	0.11	0
9	EDO	B	3302	-	3,3,3	0.22	0	2,2,2	0.41	0
16	PEG	C	2312	-	6,6,6	0.62	0	5,5,5	0.48	0
9	EDO	C	2307	-	3,3,3	0.32	0	2,2,2	0.55	0
9	EDO	C	2317	-	3,3,3	0.20	0	2,2,2	0.20	0
9	EDO	C	2311	-	3,3,3	0.07	0	2,2,2	0.18	0
9	EDO	A	2303	-	3,3,3	0.21	0	2,2,2	0.12	0
9	EDO	B	3317	-	3,3,3	0.19	0	2,2,2	0.07	0
9	EDO	B	3303	-	3,3,3	0.13	0	2,2,2	0.28	0
9	EDO	C	2318	-	3,3,3	0.15	0	2,2,2	0.22	0
9	EDO	A	2306	-	3,3,3	0.09	0	2,2,2	0.25	0
10	ACT	A	2302	-	3,3,3	1.23	0	3,3,3	0.50	0
9	EDO	A	2309	-	3,3,3	0.08	0	2,2,2	0.37	0
9	EDO	D	807	-	3,3,3	0.11	0	2,2,2	0.15	0
9	EDO	A	2323	-	3,3,3	0.16	0	2,2,2	0.19	0
9	EDO	D	804	-	3,3,3	0.10	0	2,2,2	0.34	0
9	EDO	B	3307	-	3,3,3	0.30	0	2,2,2	0.58	0
9	EDO	B	3316	-	3,3,3	0.13	0	2,2,2	0.50	0
9	EDO	C	2314	-	3,3,3	0.19	0	2,2,2	0.47	0
9	EDO	B	3315	-	3,3,3	0.11	0	2,2,2	0.34	0
9	EDO	C	2315	-	3,3,3	0.39	0	2,2,2	0.24	0
9	EDO	C	2304	-	3,3,3	0.24	0	2,2,2	0.40	0
9	EDO	A	2301	-	3,3,3	0.16	0	2,2,2	0.18	0
9	EDO	C	2319	-	3,3,3	0.13	0	2,2,2	0.21	0
9	EDO	D	809	-	3,3,3	0.21	0	2,2,2	0.19	0
9	EDO	A	2321	-	3,3,3	0.12	0	2,2,2	0.31	0
9	EDO	A	2305	-	3,3,3	0.29	0	2,2,2	0.53	0
9	EDO	D	808	-	3,3,3	0.18	0	2,2,2	0.13	0
9	EDO	A	2315	-	3,3,3	0.60	0	2,2,2	0.83	0
9	EDO	B	3319	-	3,3,3	0.11	0	2,2,2	0.44	0
13	1PE	C	2301	-	15,15,15	0.35	0	14,14,14	0.35	0
9	EDO	B	3314	-	3,3,3	0.30	0	2,2,2	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	EDO	A	2317	-	3,3,3	0.10	0	2,2,2	0.22	0
9	EDO	A	2311	-	3,3,3	0.17	0	2,2,2	0.72	0
9	EDO	B	3322	-	3,3,3	0.11	0	2,2,2	0.02	0
9	EDO	B	3305	-	3,3,3	0.09	0	2,2,2	0.18	0
10	ACT	A	2322	-	3,3,3	1.02	0	3,3,3	0.84	0
10	ACT	A	2319	-	3,3,3	1.19	0	3,3,3	0.81	0
9	EDO	A	2310	-	3,3,3	0.23	0	2,2,2	0.17	0
9	EDO	B	3311	-	3,3,3	0.17	0	2,2,2	0.33	0
9	EDO	A	2304	-	3,3,3	0.15	0	2,2,2	0.25	0
9	EDO	C	2316	-	3,3,3	0.08	0	2,2,2	0.22	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
9	EDO	A	2307	-	-	1/1/1/1	-
9	EDO	B	3318	-	-	0/1/1/1	-
9	EDO	B	3308	-	-	1/1/1/1	-
9	EDO	A	2308	-	-	1/1/1/1	-
9	EDO	C	2303	-	-	1/1/1/1	-
9	EDO	B	3304	-	-	1/1/1/1	-
9	EDO	B	3321	-	-	1/1/1/1	-
9	EDO	C	2313	-	-	1/1/1/1	-
9	EDO	C	2306	-	-	0/1/1/1	-
9	EDO	D	806	-	-	0/1/1/1	-
9	EDO	B	3312	-	-	1/1/1/1	-
9	EDO	B	3320	-	-	1/1/1/1	-
9	EDO	B	3306	-	-	0/1/1/1	-
9	EDO	A	2316	-	-	0/1/1/1	-
9	EDO	B	3313	-	-	1/1/1/1	-
9	EDO	C	2305	-	-	1/1/1/1	-
14	PGE	C	2302	-	-	5/7/7/7	-
9	EDO	A	2314	-	-	0/1/1/1	-
9	EDO	A	2318	-	-	1/1/1/1	-
9	EDO	B	3301	-	-	1/1/1/1	-
9	EDO	B	3302	-	-	0/1/1/1	-
16	PEG	C	2312	-	-	1/4/4/4	-
9	EDO	C	2307	-	-	1/1/1/1	-
9	EDO	C	2317	-	-	1/1/1/1	-
9	EDO	C	2311	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EDO	A	2303	-	-	1/1/1/1	-
9	EDO	B	3317	-	-	0/1/1/1	-
9	EDO	B	3303	-	-	1/1/1/1	-
9	EDO	C	2318	-	-	1/1/1/1	-
9	EDO	A	2306	-	-	1/1/1/1	-
9	EDO	A	2309	-	-	1/1/1/1	-
9	EDO	D	807	-	-	1/1/1/1	-
9	EDO	A	2323	-	-	0/1/1/1	-
9	EDO	D	804	-	-	0/1/1/1	-
9	EDO	B	3307	-	-	0/1/1/1	-
9	EDO	B	3316	-	-	0/1/1/1	-
9	EDO	C	2314	-	-	1/1/1/1	-
9	EDO	B	3315	-	-	0/1/1/1	-
9	EDO	C	2315	-	-	1/1/1/1	-
9	EDO	C	2304	-	-	0/1/1/1	-
9	EDO	A	2301	-	-	1/1/1/1	-
9	EDO	C	2319	-	-	1/1/1/1	-
9	EDO	D	809	-	-	0/1/1/1	-
9	EDO	A	2321	-	-	0/1/1/1	-
9	EDO	A	2305	-	-	1/1/1/1	-
9	EDO	D	808	-	-	1/1/1/1	-
9	EDO	A	2315	-	-	1/1/1/1	-
9	EDO	B	3319	-	-	1/1/1/1	-
13	1PE	C	2301	-	-	7/13/13/13	-
9	EDO	B	3314	-	-	1/1/1/1	-
9	EDO	A	2317	-	-	0/1/1/1	-
9	EDO	A	2311	-	-	1/1/1/1	-
9	EDO	B	3322	-	-	1/1/1/1	-
9	EDO	B	3305	-	-	1/1/1/1	-
9	EDO	A	2310	-	-	1/1/1/1	-
9	EDO	B	3311	-	-	1/1/1/1	-
9	EDO	A	2304	-	-	1/1/1/1	-
9	EDO	C	2316	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	C	2301	1PE	OH4-C13-C23-OH3

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Mol	Chain	Res	Type	Atoms
14	C	2302	PGE	O2-C3-C4-O3
13	C	2301	1PE	OH5-C14-C24-OH4
13	C	2301	1PE	OH7-C16-C26-OH6
16	C	2312	PEG	O1-C1-C2-O2

There are no ring outliers.

15 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	805	ACT	2	0
9	B	3304	EDO	2	0
9	B	3320	EDO	1	0
9	A	2316	EDO	5	0
9	B	3313	EDO	1	0
14	C	2302	PGE	1	0
16	C	2312	PEG	2	0
9	C	2318	EDO	2	0
9	D	804	EDO	2	0
9	B	3307	EDO	3	0
9	B	3316	EDO	3	0
9	C	2314	EDO	2	0
9	C	2315	EDO	2	0
9	A	2315	EDO	2	0
13	C	2301	1PE	19	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	713/738 (96%)	-0.46	3 (0%)	92	93	10, 19, 43, 62	0
1	B	708/738 (95%)	-0.29	8 (1%)	80	84	11, 22, 48, 64	0
1	C	712/738 (96%)	-0.09	14 (1%)	65	69	11, 26, 52, 84	0
1	D	706/738 (95%)	-0.05	15 (2%)	63	68	18, 34, 59, 80	0
All	All	2839/2952 (96%)	-0.22	40 (1%)	75	78	10, 25, 51, 84	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	757	ALA	4.5
1	D	737	VAL	4.1
1	A	167	TRP	3.7
1	C	728	TYR	3.5
1	B	164	GLY	3.5

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

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

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, 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
6	GLC	P	7	11/12	0.71	0.30	65,75,85,91	0
2	GLC	K	1	12/12	0.78	0.25	35,58,63,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	GLC	Q	6	11/12	0.80	0.17	42,56,59,60	0
5	GLC	O	6	11/12	0.83	0.19	51,59,65,69	0
2	GLC	I	1	12/12	0.84	0.17	29,43,53,54	0
4	GLC	N	4	11/12	0.85	0.31	52,55,63,65	0
2	GLC	J	1	12/12	0.85	0.15	38,54,57,67	0
8	GLC	R	5	11/12	0.86	0.17	34,44,46,47	0
2	GLC	H	5	11/12	0.87	0.14	34,39,43,56	0
5	GLC	O	7	11/12	0.87	0.17	25,34,38,38	0
8	GLC	R	4	11/12	0.87	0.11	32,36,41,42	0
6	GLC	P	6	11/12	0.87	0.19	46,51,55,56	0
7	GLC	Q	1	12/12	0.89	0.16	33,36,43,45	0
2	GLC	G	1	12/12	0.89	0.12	21,35,43,49	0
5	GLC	O	1	12/12	0.90	0.15	32,46,55,56	0
2	GLC	H	1	12/12	0.90	0.14	21,37,41,43	0
7	GLC	Q	4	11/12	0.90	0.10	28,33,35,36	0
3	GLC	M	3	11/12	0.91	0.27	47,55,58,58	0
2	GLC	J	5	11/12	0.91	0.16	45,49,53,56	0
3	GLC	M	1	12/12	0.91	0.23	43,48,52,58	0
6	GLC	P	5	11/12	0.92	0.13	21,35,41,43	0
3	GLC	M	2	11/12	0.92	0.18	38,44,46,50	0
2	GLC	J	2	11/12	0.93	0.12	23,26,30,31	0
7	GLC	Q	5	11/12	0.93	0.11	25,33,38,45	0
6	GLC	P	1	12/12	0.93	0.10	21,24,25,30	0
2	GLC	K	5	11/12	0.93	0.13	33,40,51,58	0
7	GLC	Q	3	11/12	0.93	0.11	24,29,29,32	0
7	GLC	Q	2	11/12	0.94	0.15	30,35,36,42	0
2	GLC	I	5	11/12	0.94	0.12	38,44,47,49	0
6	GLC	P	4	11/12	0.94	0.10	25,29,35,47	0
2	GLC	G	5	11/12	0.94	0.11	26,29,32,37	0
5	GLC	O	5	11/12	0.94	0.10	20,25,34,37	0
3	GLC	L	3	11/12	0.94	0.18	30,32,38,42	0
4	GLC	N	1	12/12	0.94	0.16	29,33,37,40	0
8	GLC	R	1	12/12	0.95	0.09	27,33,36,36	0
8	GLC	R	2	11/12	0.95	0.09	29,32,38,40	0
2	GLC	J	3	11/12	0.95	0.09	22,29,30,31	0
5	GLC	O	2	11/12	0.95	0.11	20,25,31,31	0
6	GLC	P	3	11/12	0.96	0.10	16,21,23,24	0
4	GLC	N	3	11/12	0.96	0.16	30,36,44,50	0
3	GLC	L	1	12/12	0.96	0.14	23,28,36,39	0
8	GLC	R	3	11/12	0.96	0.09	20,26,28,32	0
2	GLC	K	2	11/12	0.96	0.10	19,25,30,34	0
2	GLC	J	4	11/12	0.96	0.08	31,33,35,37	0

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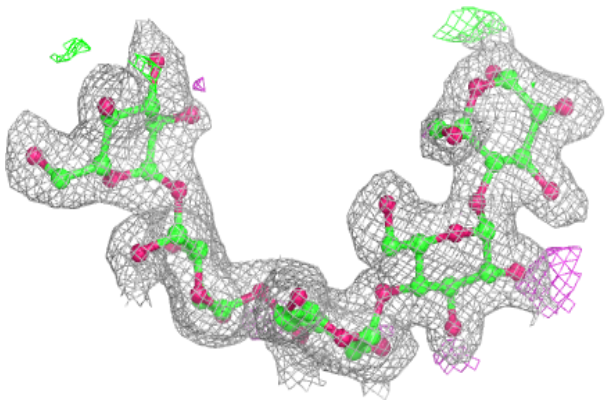
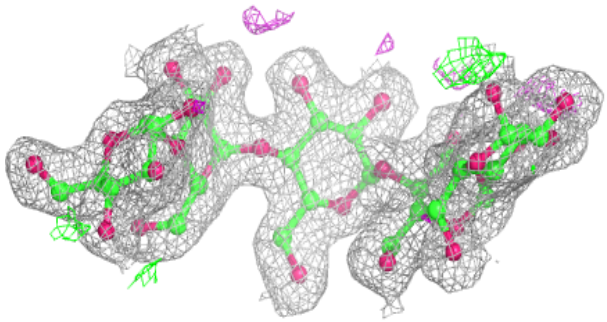
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GLC	L	2	11/12	0.97	0.11	21,23,26,27	0
2	GLC	I	2	11/12	0.97	0.07	17,18,22,25	0
2	GLC	I	4	11/12	0.97	0.08	20,22,24,29	0
4	GLC	N	2	11/12	0.97	0.14	22,29,36,42	0
5	GLC	O	3	11/12	0.97	0.08	18,20,21,22	0
2	GLC	G	4	11/12	0.98	0.07	16,17,18,21	0
6	GLC	P	2	11/12	0.98	0.08	18,20,22,23	0
2	GLC	H	2	11/12	0.98	0.08	13,14,15,17	0
2	GLC	K	3	11/12	0.98	0.07	13,16,21,22	0
2	GLC	K	4	11/12	0.98	0.07	19,21,24,28	0
5	GLC	O	4	11/12	0.98	0.07	15,18,19,20	0
2	GLC	I	3	11/12	0.98	0.07	15,16,17,18	0
2	GLC	H	4	11/12	0.98	0.07	20,21,25,26	0
2	GLC	G	2	11/12	0.98	0.10	11,14,15,17	0
2	GLC	G	3	11/12	0.99	0.08	9,11,12,13	0
2	GLC	H	3	11/12	0.99	0.07	13,15,16,17	0

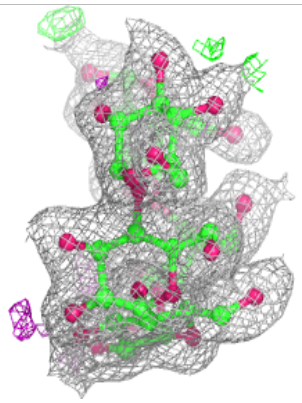
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

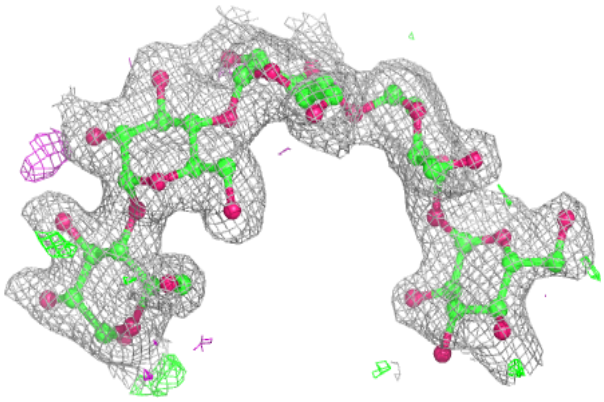


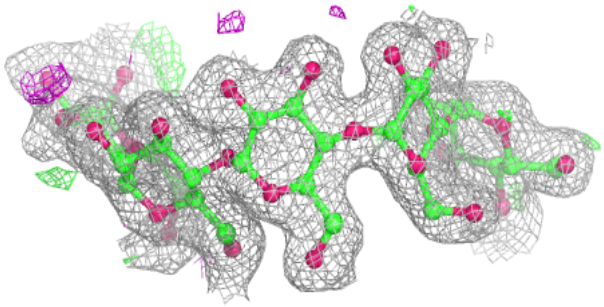




Electron density around Chain H:

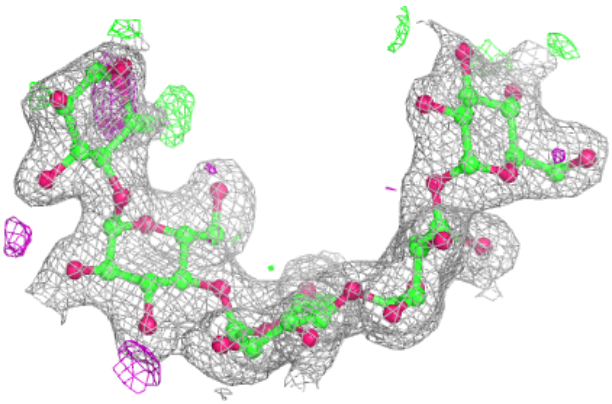
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

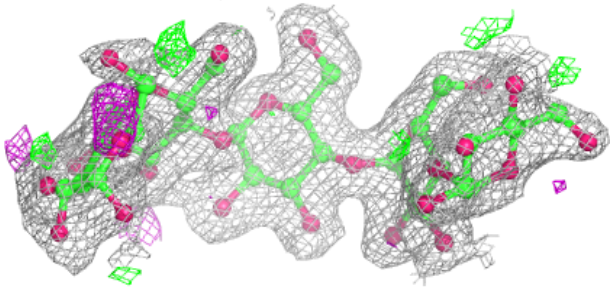


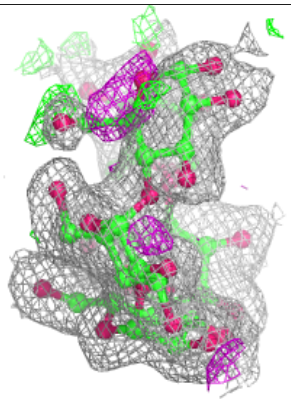


Electron density around Chain I:

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

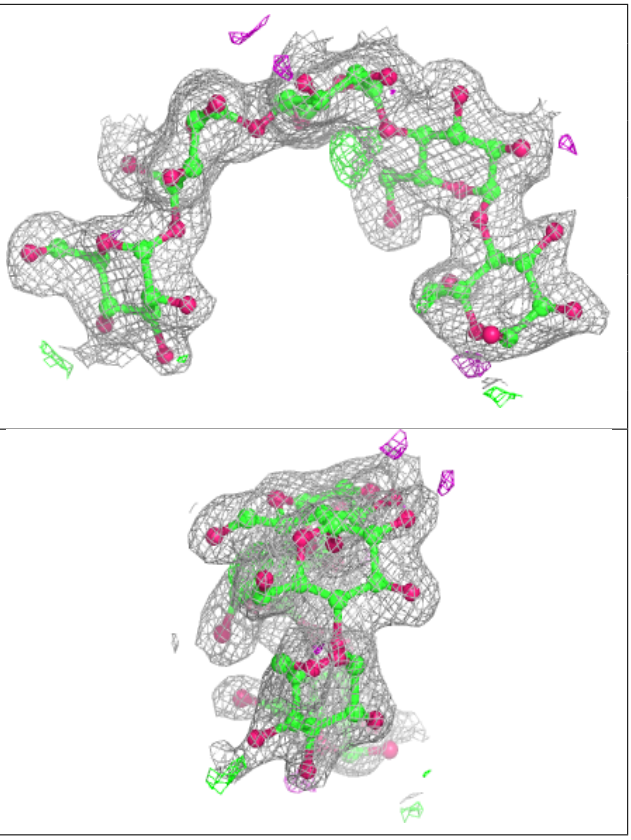






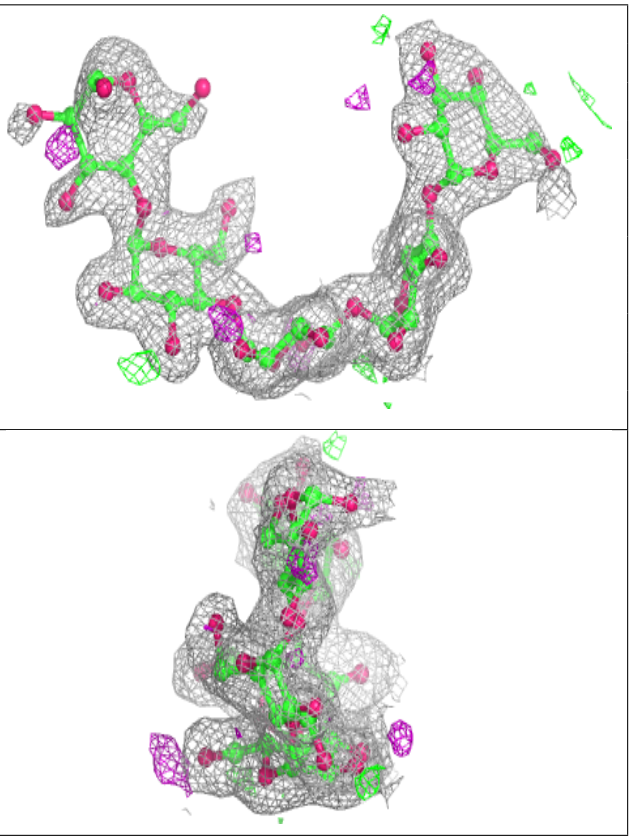
Electron density around Chain J:

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



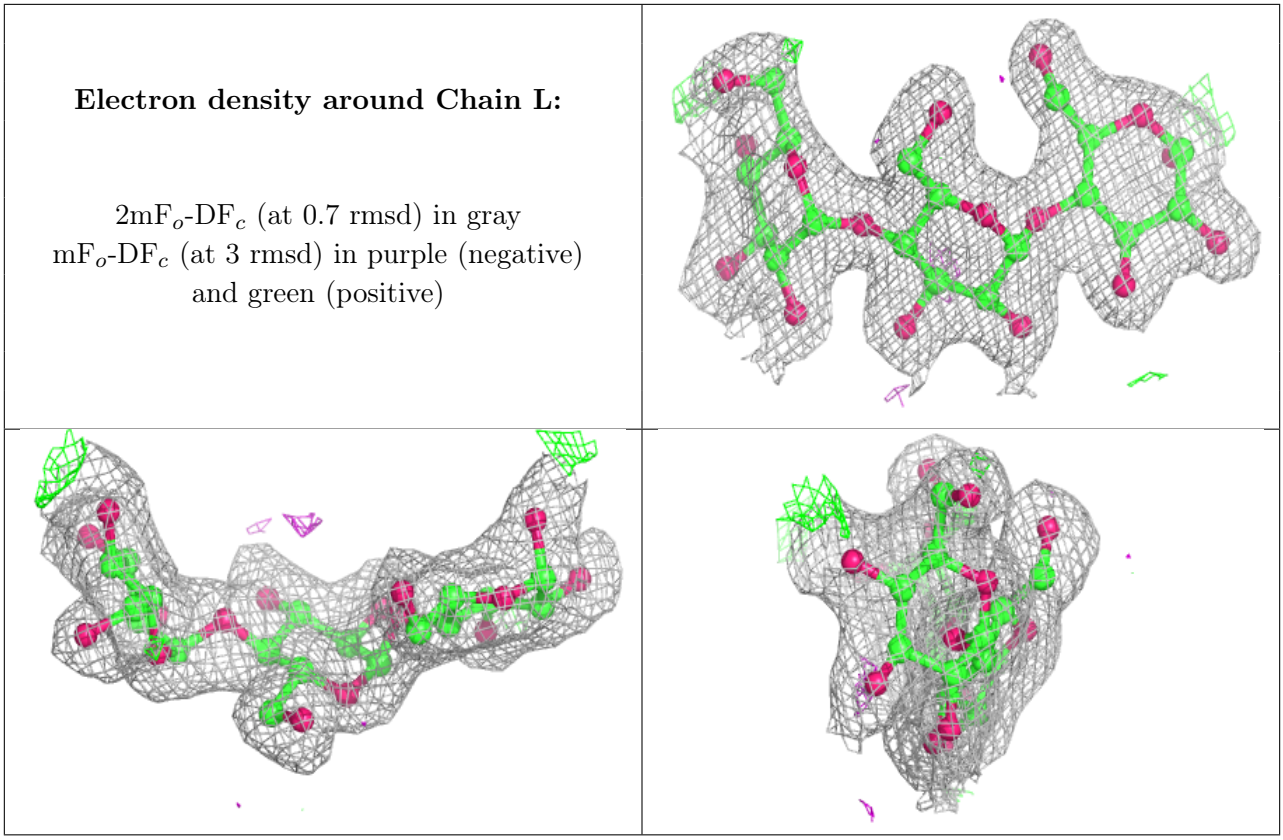
Electron density around Chain K:

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



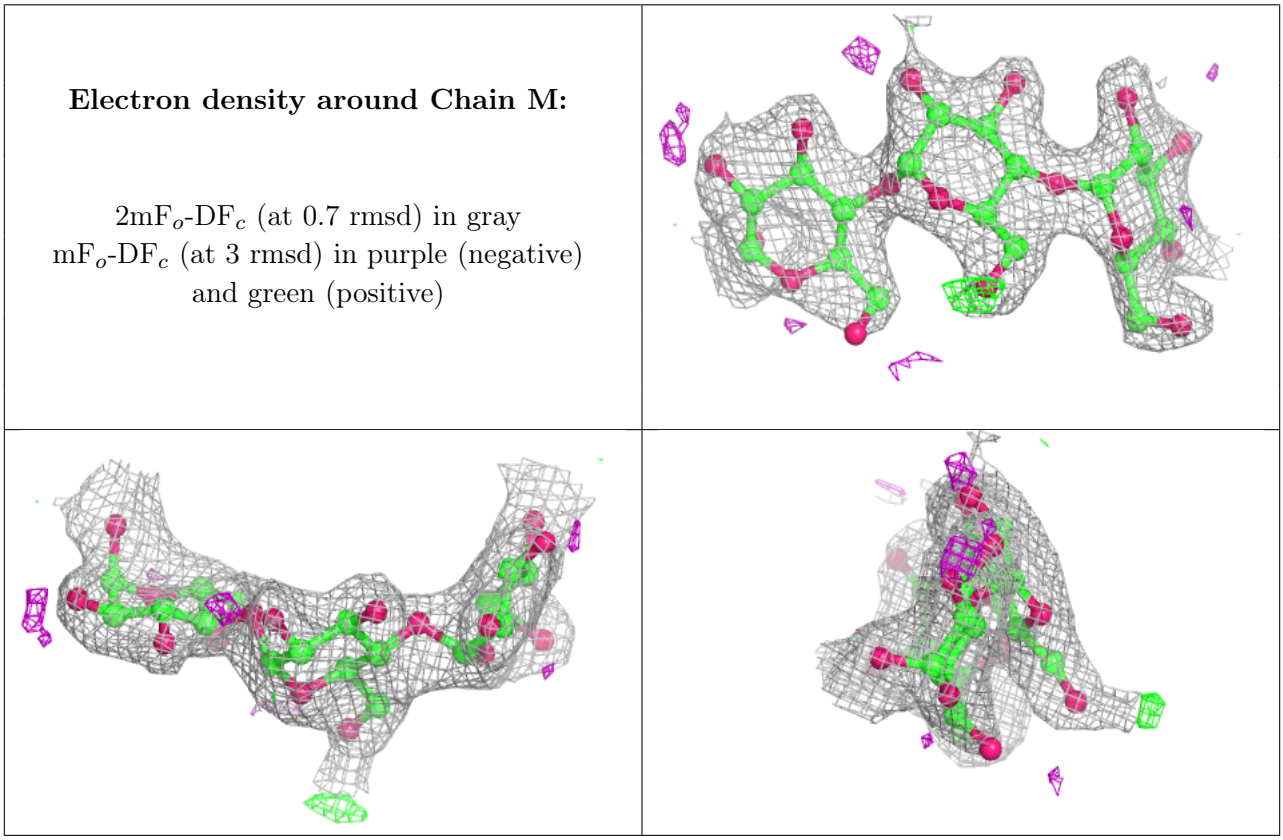
Electron density around Chain L:

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



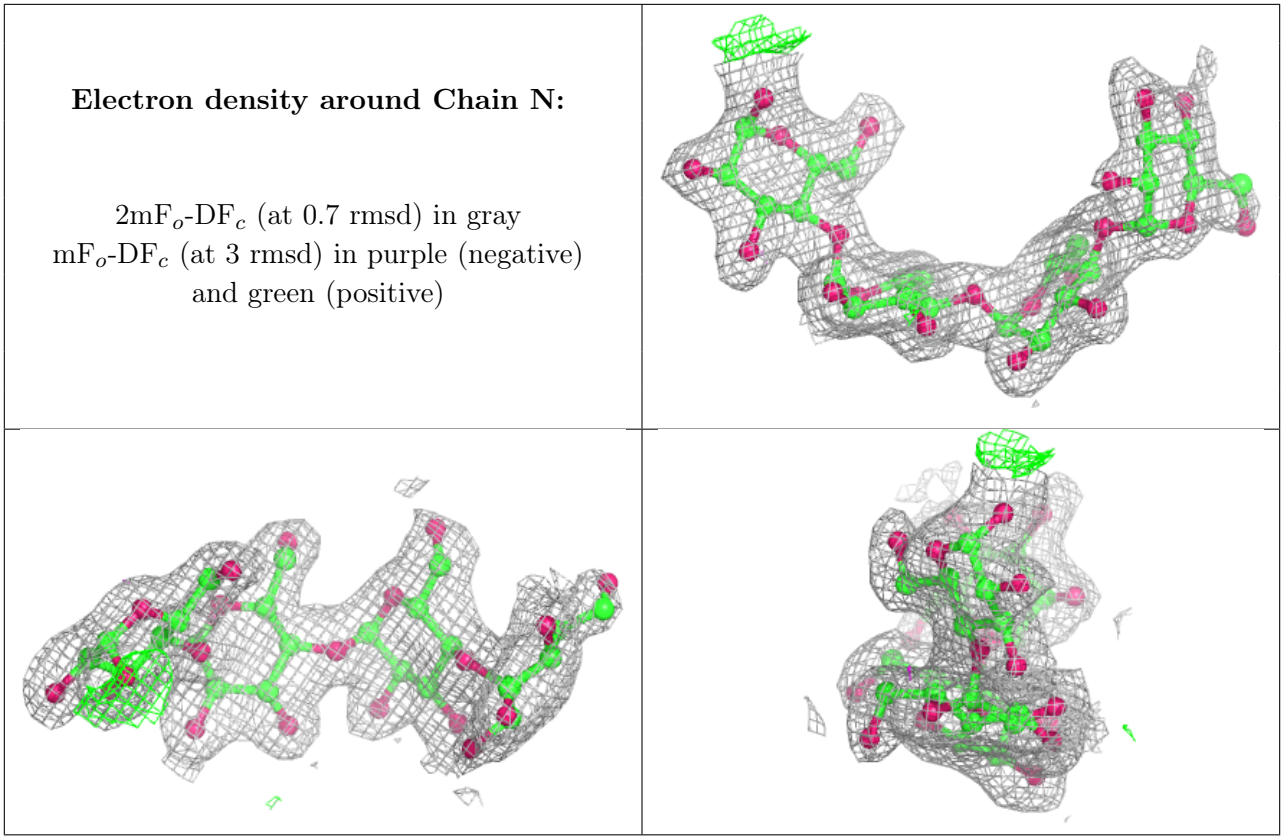
Electron density around Chain M:

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



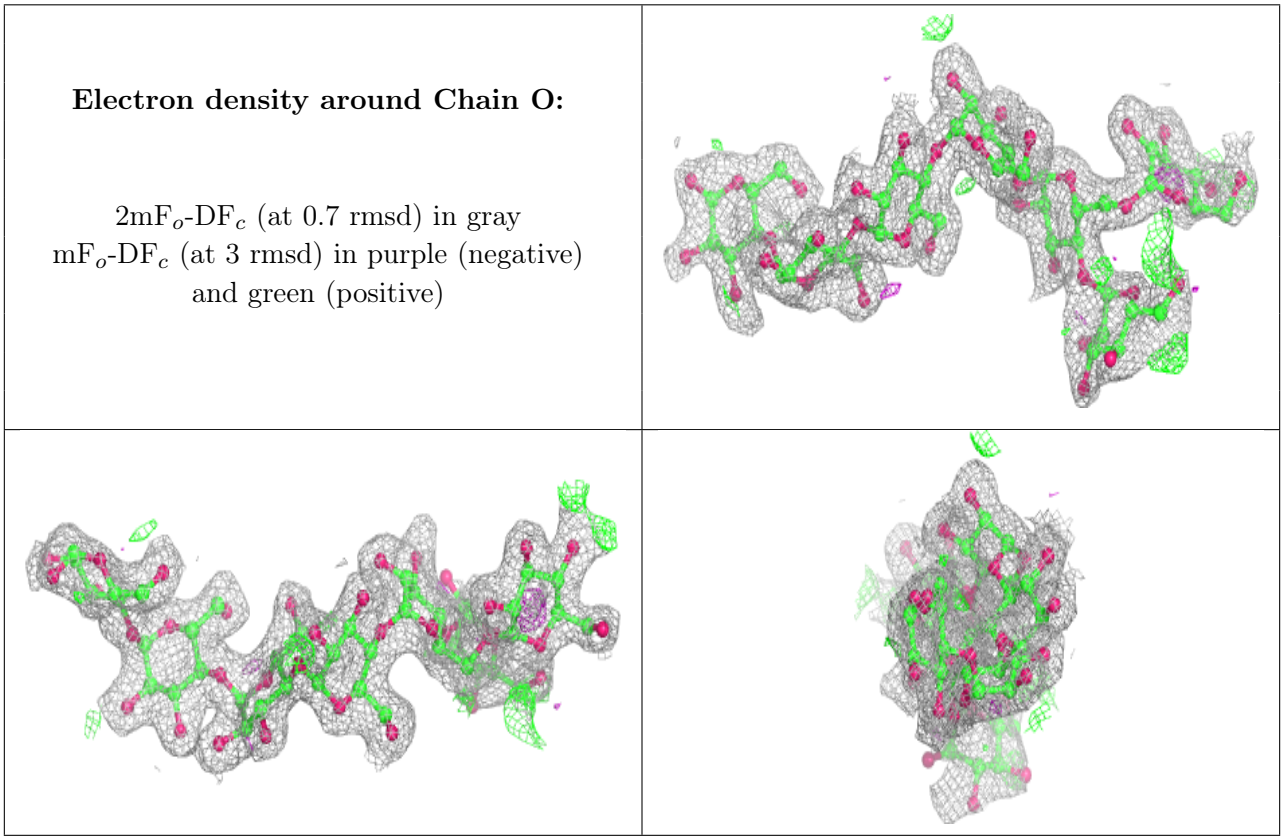
Electron density around Chain N:

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



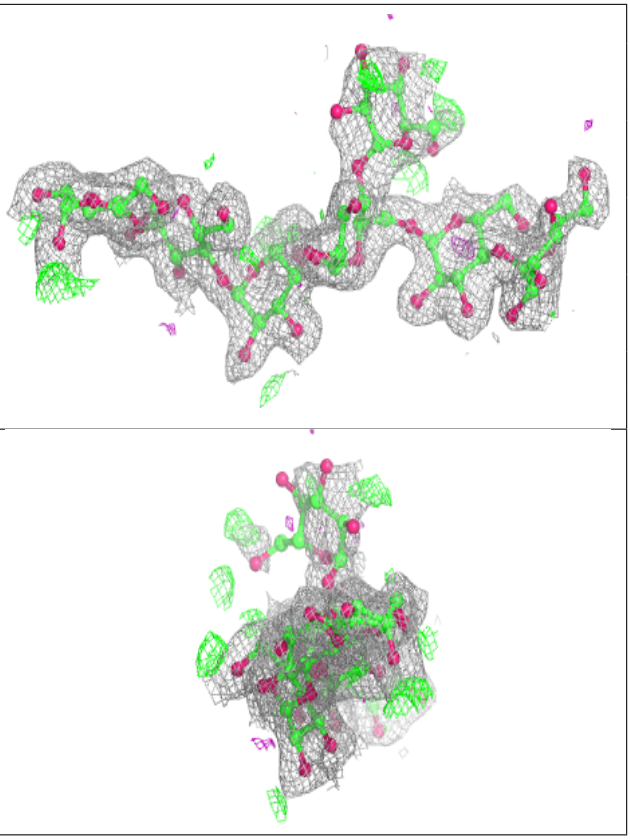
Electron density around Chain O:

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



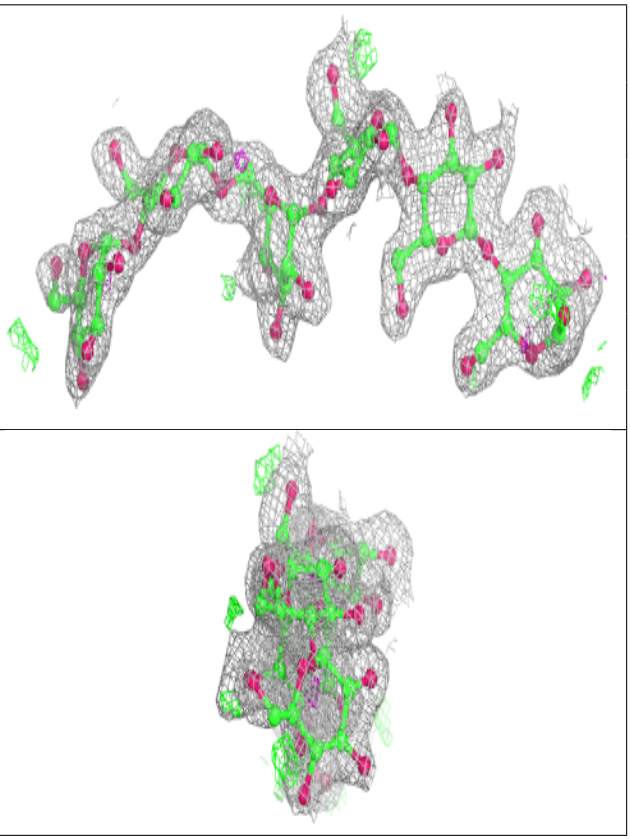
Electron density around Chain P:

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



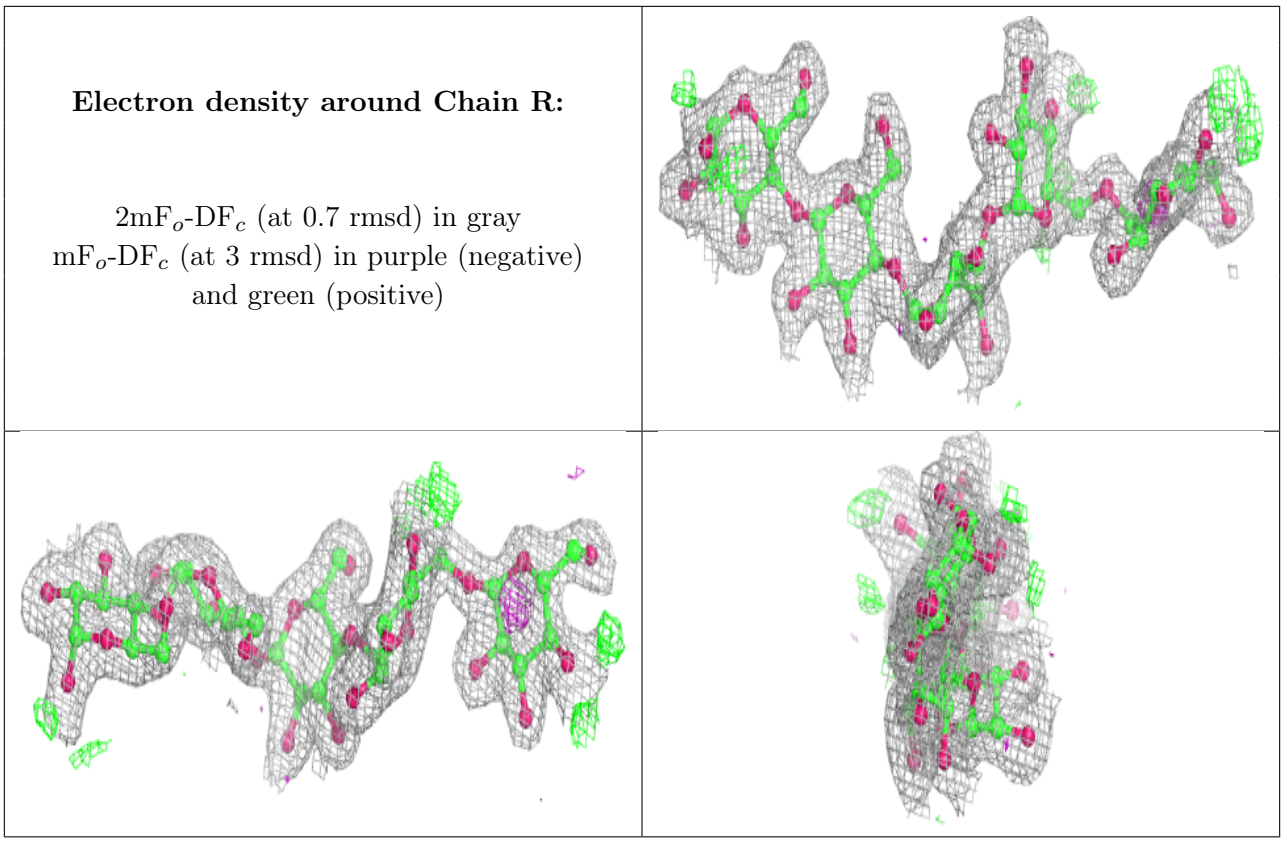
Electron density around Chain Q:

$2mF_o$-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 R:

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



6.4 Ligands

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
9	EDO	B	3320	4/4	0.60	0.36	55,56,60,60	0
9	EDO	B	3321	4/4	0.67	0.29	65,67,68,69	0
9	EDO	D	806	4/4	0.67	0.24	65,65,66,71	0
9	EDO	C	2304	4/4	0.69	0.36	49,59,62,62	0
9	EDO	A	2303	4/4	0.70	0.35	52,54,57,65	0
9	EDO	B	3301	4/4	0.72	0.27	60,63,67,68	0
9	EDO	A	2314	4/4	0.74	0.26	56,57,60,61	0
9	EDO	A	2310	4/4	0.74	0.21	46,55,56,56	0
9	EDO	A	2316	4/4	0.75	0.37	34,37,39,42	0
9	EDO	A	2315	4/4	0.77	0.19	42,46,46,47	0
9	EDO	C	2307	4/4	0.79	0.12	50,50,51,53	0
9	EDO	B	3311	4/4	0.79	0.18	51,52,53,58	0
14	PGE	C	2302	10/10	0.79	0.29	50,66,68,72	0
16	PEG	C	2312	7/7	0.79	0.26	43,51,54,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	EDO	B	3307	4/4	0.80	0.22	45,52,53,55	0
9	EDO	A	2305	4/4	0.81	0.18	44,50,51,54	0
9	EDO	D	808	4/4	0.81	0.34	62,62,64,65	0
9	EDO	C	2311	4/4	0.81	0.16	51,52,54,55	0
9	EDO	C	2314	4/4	0.81	0.20	49,50,51,51	0
17	CL	D	803	1/1	0.81	0.20	68,68,68,68	0
10	ACT	D	805	4/4	0.82	0.30	58,59,61,63	0
9	EDO	B	3306	4/4	0.82	0.18	56,56,58,59	0
9	EDO	C	2316	4/4	0.82	0.26	50,53,53,58	0
10	ACT	A	2302	4/4	0.82	0.20	43,44,44,47	0
9	EDO	C	2313	4/4	0.83	0.15	35,38,40,40	0
9	EDO	D	807	4/4	0.83	0.32	54,65,66,68	0
9	EDO	C	2318	4/4	0.84	0.17	47,48,48,50	0
10	ACT	A	2322	4/4	0.84	0.23	49,58,58,62	0
9	EDO	B	3318	4/4	0.85	0.27	53,55,57,59	0
15	NA	C	2310	1/1	0.85	0.11	49,49,49,49	0
9	EDO	A	2308	4/4	0.86	0.41	52,54,54,58	0
9	EDO	B	3302	4/4	0.86	0.21	50,51,53,53	0
9	EDO	C	2303	4/4	0.86	0.21	51,52,52,54	0
9	EDO	A	2317	4/4	0.86	0.18	46,53,55,58	0
9	EDO	C	2305	4/4	0.86	0.13	40,45,49,49	0
10	ACT	A	2319	4/4	0.86	0.20	40,41,47,49	0
9	EDO	B	3303	4/4	0.87	0.22	51,52,53,55	0
9	EDO	B	3322	4/4	0.88	0.21	52,52,53,54	0
9	EDO	B	3317	4/4	0.88	0.17	47,51,52,53	0
9	EDO	C	2315	4/4	0.88	0.21	46,46,47,51	0
9	EDO	B	3313	4/4	0.88	0.15	44,47,48,49	0
9	EDO	B	3315	4/4	0.89	0.33	54,57,57,63	0
9	EDO	B	3305	4/4	0.89	0.26	53,53,54,55	0
9	EDO	B	3314	4/4	0.89	0.17	39,40,44,45	0
9	EDO	C	2317	4/4	0.89	0.13	39,39,40,42	0
9	EDO	A	2307	4/4	0.90	0.16	53,58,60,62	0
9	EDO	A	2304	4/4	0.90	0.13	37,43,44,49	0
9	EDO	A	2321	4/4	0.90	0.19	46,49,50,53	0
9	EDO	A	2309	4/4	0.90	0.20	42,43,46,46	0
13	1PE	C	2301	16/16	0.91	0.27	25,43,52,52	0
9	EDO	C	2306	4/4	0.92	0.17	50,51,54,56	0
9	EDO	A	2306	4/4	0.92	0.29	47,48,49,53	0
9	EDO	D	809	4/4	0.92	0.15	47,49,51,51	0
9	EDO	B	3304	4/4	0.92	0.13	41,44,44,49	0
9	EDO	A	2323	4/4	0.92	0.15	48,50,53,54	0
9	EDO	B	3316	4/4	0.92	0.16	41,44,45,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	EDO	D	804	4/4	0.93	0.28	41,47,47,50	0
10	ACT	A	2320	4/4	0.93	0.12	35,36,38,43	0
9	EDO	B	3308	4/4	0.93	0.20	39,46,46,47	0
9	EDO	A	2301	4/4	0.94	0.15	51,53,54,54	0
9	EDO	A	2318	4/4	0.94	0.27	35,43,45,49	0
9	EDO	C	2319	4/4	0.94	0.15	52,58,59,60	0
9	EDO	B	3312	4/4	0.95	0.12	33,42,43,45	0
9	EDO	B	3319	4/4	0.95	0.24	41,47,48,49	0
9	EDO	A	2311	4/4	0.95	0.15	53,55,55,56	0
11	CA	D	801	1/1	0.99	0.05	23,23,23,23	0
12	MN	A	2313	1/1	0.99	0.04	36,36,36,36	0
12	MN	B	3310	1/1	0.99	0.04	33,33,33,33	0
12	MN	C	2309	1/1	0.99	0.04	41,41,41,41	0
12	MN	D	802	1/1	0.99	0.04	47,47,47,47	0
11	CA	B	3309	1/1	1.00	0.08	14,14,14,14	0
11	CA	C	2308	1/1	1.00	0.10	15,15,15,15	0
11	CA	A	2312	1/1	1.00	0.09	11,11,11,11	0

6.5 Other polymers (i)

There are no such residues in this entry.