



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:52 AM UTC

PDB ID : 9US4 / pdb_00009us4
Title : Klebsiella pneumoniae maltohexaose-producing alpha-amylase in complex with acarbose
Authors : Fujimoto, Z.; Kishine, N.; Momma, M.
Deposited on : 2025-05-01
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:

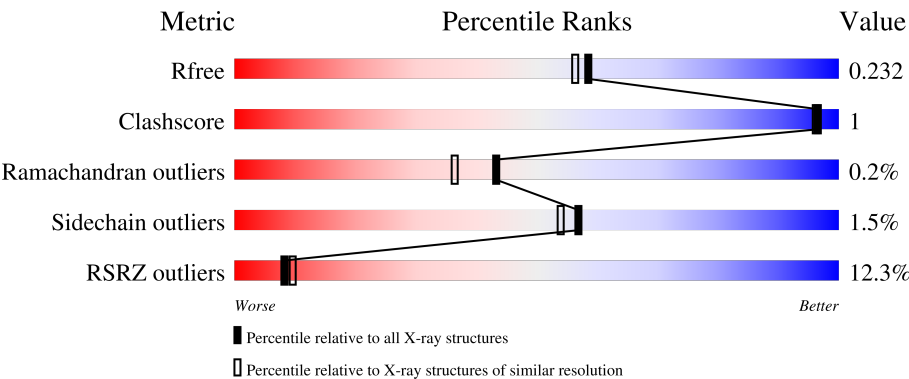
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	660	3% 96% ..
1	B	660	21% 94% 5% .
2	C	3	67% 33%
2	E	3	33% 67%
2	I	3	67% 33%

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Mol	Chain	Length	Quality of chain
3	D	3	 100%
3	G	3	 100%
3	H	3	 100%
4	F	2	 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11746 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 Maltohexaose-producing amylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	650	Total	C	N	O	S	0	2	0
			5178	3286	894	974	24			
1	B	652	Total	C	N	O	S	0	0	0
			5186	3290	898	974	24			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	E	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	I	3	Total	C	N	O	0	0	0
			44	25	1	18			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	3	Total	C	N	O	0	0	0
			44	25	1	18			
3	G	3	Total	C	N	O	0	0	0
			44	25	1	18			
3	H	3	Total	C	N	O	0	0	0
			44	25	1	18			

- Molecule 4 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
4	F	2	Total	C	N	O	0	0	0
			33	19	1	13			

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Ca	0	0
			2	2		
5	B	2	Total	Ca	0	0
			2	2		

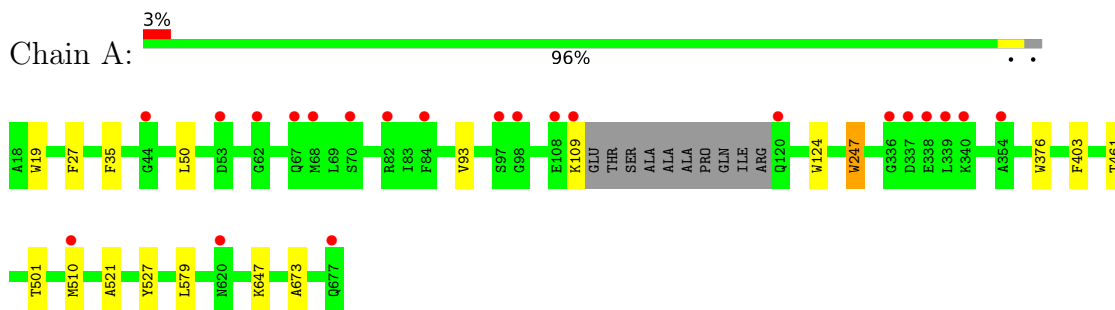
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	698	Total	O	0	0
			698	698		
6	B	383	Total	O	0	0
			383	383		

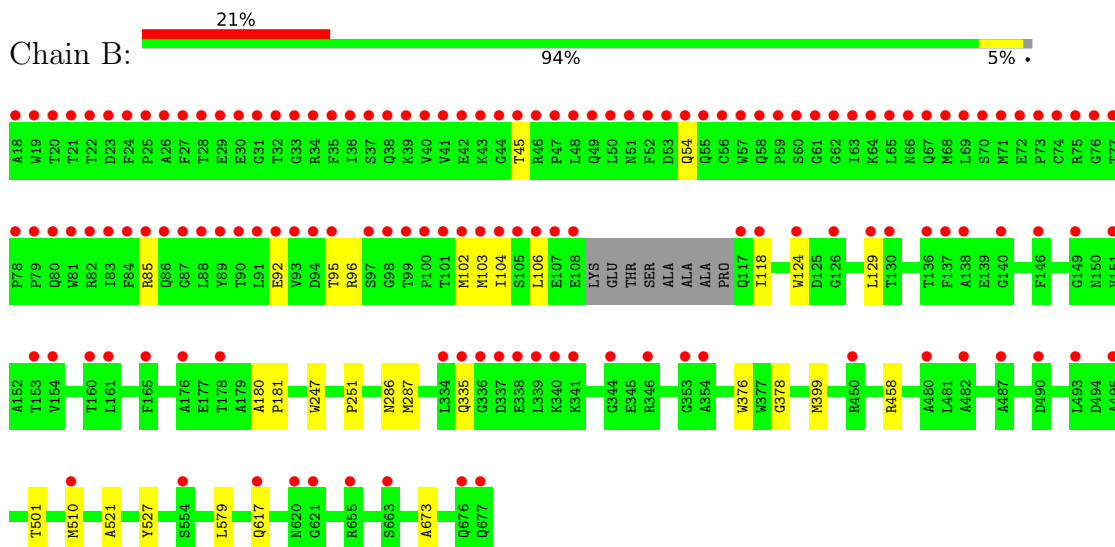
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

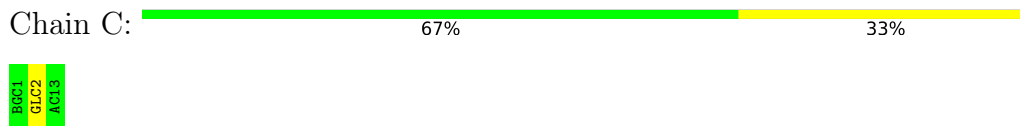
- Molecule 1: Maltohexaose-producing amylase



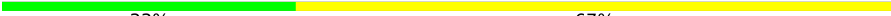
- Molecule 1: Maltohexaose-producing amylase



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



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

Chain E:  33% 67%



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

Chain I:  67% 33%



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

Chain D:  100%



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

Chain G:  100%



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

Chain H:  100%



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

Chain F:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.91Å 108.24Å 82.28Å 90.00° 96.77° 90.00°	Depositor
Resolution (Å)	29.68 – 1.95 29.68 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.5 (29.68-1.95) 97.5 (29.68-1.95)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.189 , 0.227 0.196 , 0.232	Depositor DCC
R_{free} test set	4624 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11746	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 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.97	0/5333	1.30	0/7231
1	B	0.99	0/5334	1.33	1/7233 (0.0%)
All	All	0.98	0/10667	1.32	1/14464 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	378	GLY	CA-C-O	-5.12	118.69	122.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5178	0	4917	11	0
1	B	5186	0	4926	14	0
2	C	44	0	30	0	0
2	E	44	0	30	0	0
2	I	44	0	30	0	0
3	D	44	0	30	0	0
3	G	44	0	30	0	0
3	H	44	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	33	0	21	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	698	0	0	0	0
6	B	383	0	0	0	0
All	All	11746	0	10044	21	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 1.

All (21) 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:B:129:LEU:HD11	1:B:673:ALA:HB2	1.80	0.64
1:A:403:PHE:CZ	1:B:399:MET:HE3	2.42	0.55
1:B:102:MET:HE2	1:B:104:ILE:HG13	1.90	0.54
1:B:180:ALA:HB1	1:B:181:PRO:HD2	1.93	0.51
1:A:501:THR:HA	1:A:521:ALA:O	2.11	0.50
1:B:501:THR:HA	1:B:521:ALA:O	2.14	0.48
1:B:247:TRP:CD1	1:B:247:TRP:C	2.94	0.46
1:B:124:TRP:CD1	1:B:673:ALA:HB1	2.52	0.44
1:A:403:PHE:CZ	1:B:399:MET:CE	3.01	0.44
1:A:527:TYR:OH	1:A:579:LEU:O	2.31	0.43
1:A:247:TRP:C	1:A:247:TRP:CD1	2.95	0.43
1:B:458:ARG:HD3	1:B:458:ARG:C	2.44	0.43
1:A:19:TRP:HB2	1:A:27:PHE:HB2	2.01	0.43
1:B:251:PRO:HA	1:B:287:MET:HG3	2.01	0.42
1:A:403:PHE:HZ	1:B:399:MET:CE	2.32	0.42
1:B:92:GLU:HB2	1:B:103:MET:HB3	2.01	0.41
1:A:50:LEU:HD13	1:A:93:VAL:CG1	2.51	0.41
1:A:403:PHE:HZ	1:B:399:MET:HE3	1.86	0.41
1:A:35:PHE:HB2	1:A:93:VAL:HG22	2.03	0.41
1:B:527:TYR:OH	1:B:579:LEU:O	2.19	0.40
1:A:124:TRP:CG	1:A:673:ALA:HB1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	648/660 (98%)	629 (97%)	18 (3%)	1 (0%)	43	36
1	B	648/660 (98%)	623 (96%)	24 (4%)	1 (0%)	43	36
All	All	1296/1320 (98%)	1252 (97%)	42 (3%)	2 (0%)	43	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	TRP
1	B	376	TRP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	535/540 (99%)	530 (99%)	5 (1%)	70	70
1	B	535/540 (99%)	524 (98%)	11 (2%)	47	41
All	All	1070/1080 (99%)	1054 (98%)	16 (2%)	57	54

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	LYS
1	A	247	TRP
1	A	461	THR
1	A	510	MET

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Mol	Chain	Res	Type
1	A	647	LYS
1	B	45	THR
1	B	54	GLN
1	B	85	ARG
1	B	95	THR
1	B	96	ARG
1	B	106	LEU
1	B	118	ILE
1	B	286	ASN
1	B	335	GLN
1	B	510	MET
1	B	617	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	GLN
1	A	362	ASN
1	A	553	GLN
1	B	55	GLN
1	B	120	GLN
1	B	162	GLN
1	B	208	ASN
1	B	335	GLN
1	B	362	ASN
1	B	423	HIS
1	B	553	GLN
1	B	675	GLN
1	B	677	GLN

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

20 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	C	1	2	12,12,12	0.50	0	17,17,17	0.64	0
2	GLC	C	2	2	11,11,12	0.23	0	15,15,17	0.84	1 (6%)
2	AC1	C	3	2	21,22,23	0.28	0	22,32,34	0.52	0
3	GLC	D	1	3	12,12,12	0.52	0	17,17,17	0.42	0
3	GLC	D	2	3	11,11,12	0.38	0	15,15,17	0.70	0
3	AC1	D	3	3	21,22,23	0.30	0	22,32,34	0.50	0
2	BGC	E	1	2	12,12,12	0.55	0	17,17,17	0.69	0
2	GLC	E	2	2	11,11,12	0.35	0	15,15,17	0.83	1 (6%)
2	AC1	E	3	2	21,22,23	0.41	0	22,32,34	0.98	1 (4%)
4	GLC	F	1	4	12,12,12	0.52	0	17,17,17	0.58	0
4	AC1	F	2	4	21,22,23	0.30	0	22,32,34	0.50	0
3	GLC	G	1	3	12,12,12	0.52	0	17,17,17	0.75	0
3	GLC	G	2	3	11,11,12	0.27	0	15,15,17	0.76	0
3	AC1	G	3	3	21,22,23	0.27	0	22,32,34	0.50	0
3	GLC	H	1	3	12,12,12	0.52	0	17,17,17	0.68	0
3	GLC	H	2	3	11,11,12	0.30	0	15,15,17	0.65	0
3	AC1	H	3	3	21,22,23	0.31	0	22,32,34	0.44	0
2	BGC	I	1	2	12,12,12	0.55	0	17,17,17	0.86	0
2	GLC	I	2	2	11,11,12	0.29	0	15,15,17	0.77	1 (6%)
2	AC1	I	3	2	21,22,23	0.38	0	22,32,34	0.67	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	C	1	2	-	2/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	AC1	C	3	2	-	1/6/43/46	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
3	AC1	D	3	3	-	1/6/43/46	0/2/2/2
2	BGC	E	1	2	-	0/2/22/22	0/1/1/1
2	GLC	E	2	2	-	0/2/19/22	0/1/1/1
2	AC1	E	3	2	-	0/6/43/46	0/2/2/2
4	GLC	F	1	4	-	0/2/22/22	0/1/1/1
4	AC1	F	2	4	-	1/6/43/46	0/2/2/2
3	GLC	G	1	3	-	2/2/22/22	0/1/1/1
3	GLC	G	2	3	-	0/2/19/22	0/1/1/1
3	AC1	G	3	3	-	1/6/43/46	0/2/2/2
3	GLC	H	1	3	-	2/2/22/22	0/1/1/1
3	GLC	H	2	3	-	0/2/19/22	0/1/1/1
3	AC1	H	3	3	-	0/6/43/46	0/2/2/2
2	BGC	I	1	2	-	0/2/22/22	0/1/1/1
2	GLC	I	2	2	-	2/2/19/22	0/1/1/1
2	AC1	I	3	2	-	1/6/43/46	0/2/2/2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	AC1	C7B-C1B-N4A	-2.93	106.37	110.68
2	C	2	GLC	C1-O5-C5	2.48	115.51	112.19
2	E	2	GLC	C1-O5-C5	2.42	115.43	112.19
2	I	2	GLC	C1-O5-C5	2.13	115.04	112.19

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	1	GLC	C4-C5-C6-O6
3	H	1	GLC	O5-C5-C6-O6
3	G	1	GLC	O5-C5-C6-O6
2	C	1	BGC	O5-C5-C6-O6
3	H	1	GLC	C4-C5-C6-O6
2	C	1	BGC	C4-C5-C6-O6
2	I	2	GLC	C4-C5-C6-O6
2	I	2	GLC	O5-C5-C6-O6
2	I	3	AC1	C7B-C1B-N4A-C4

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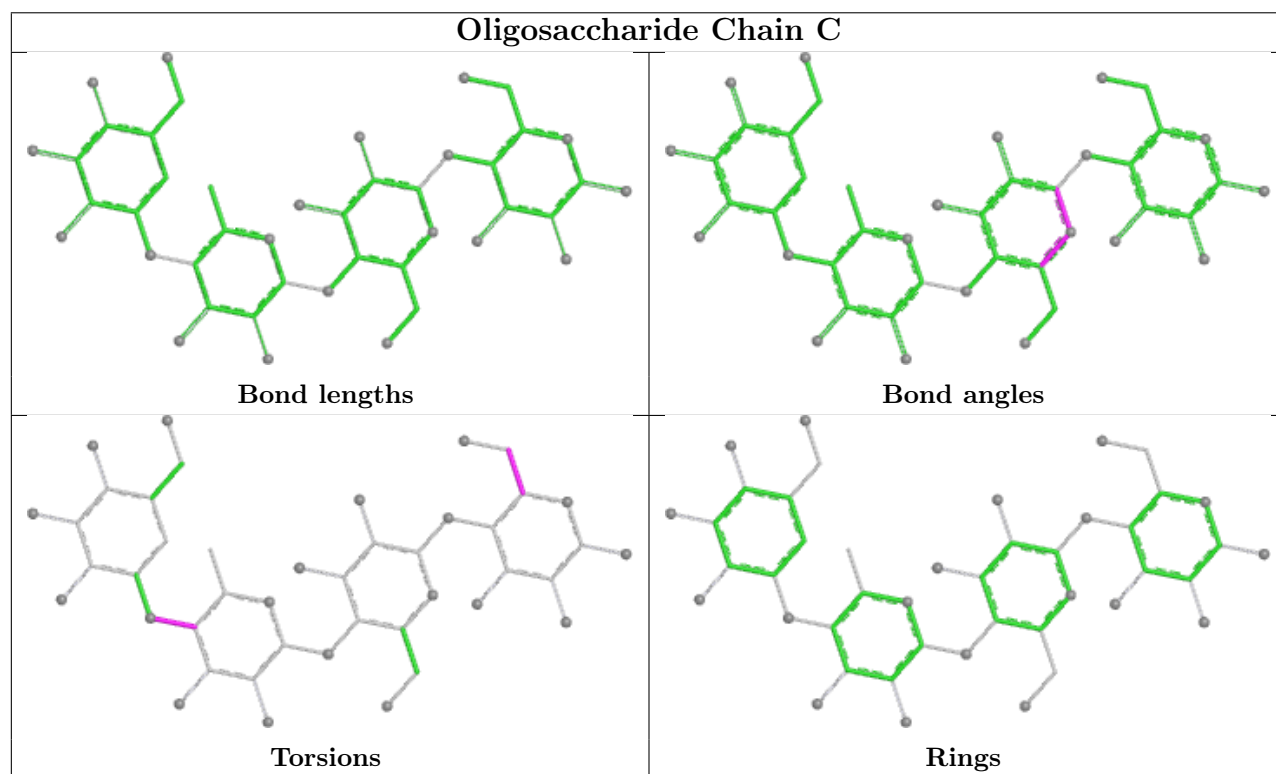
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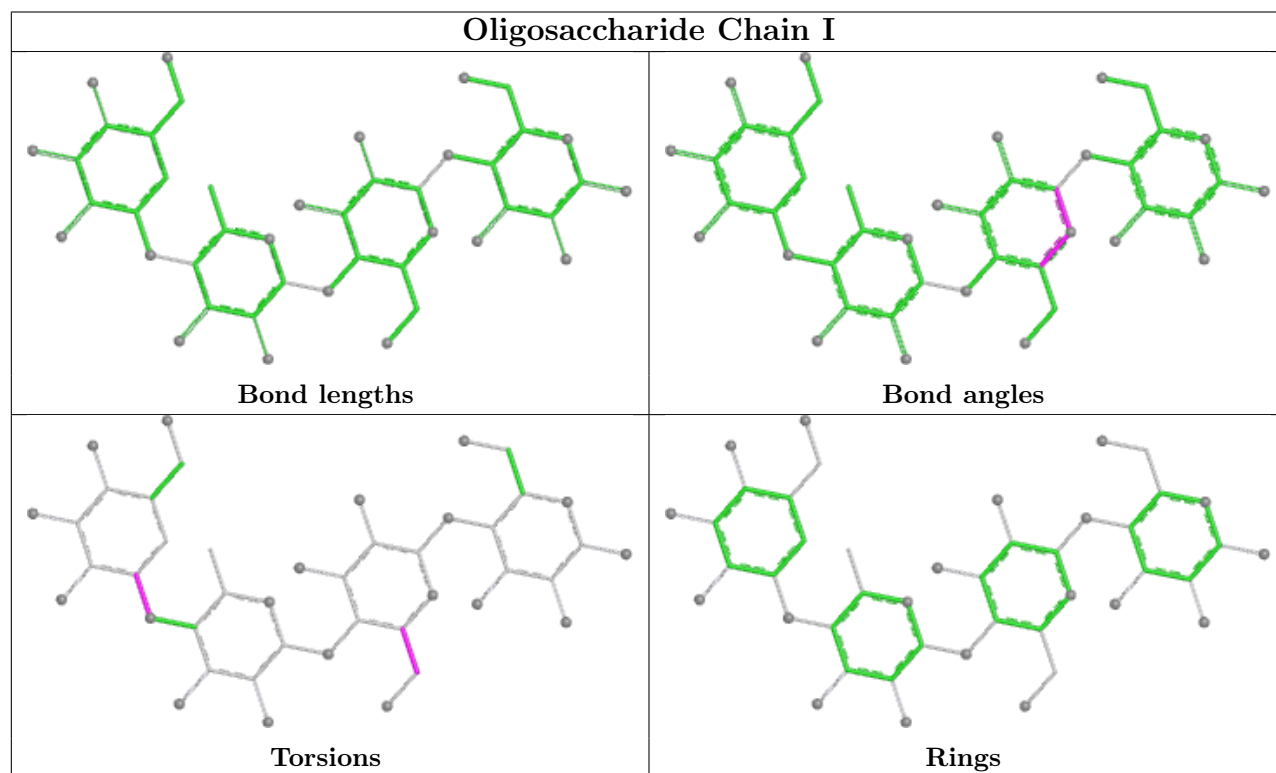
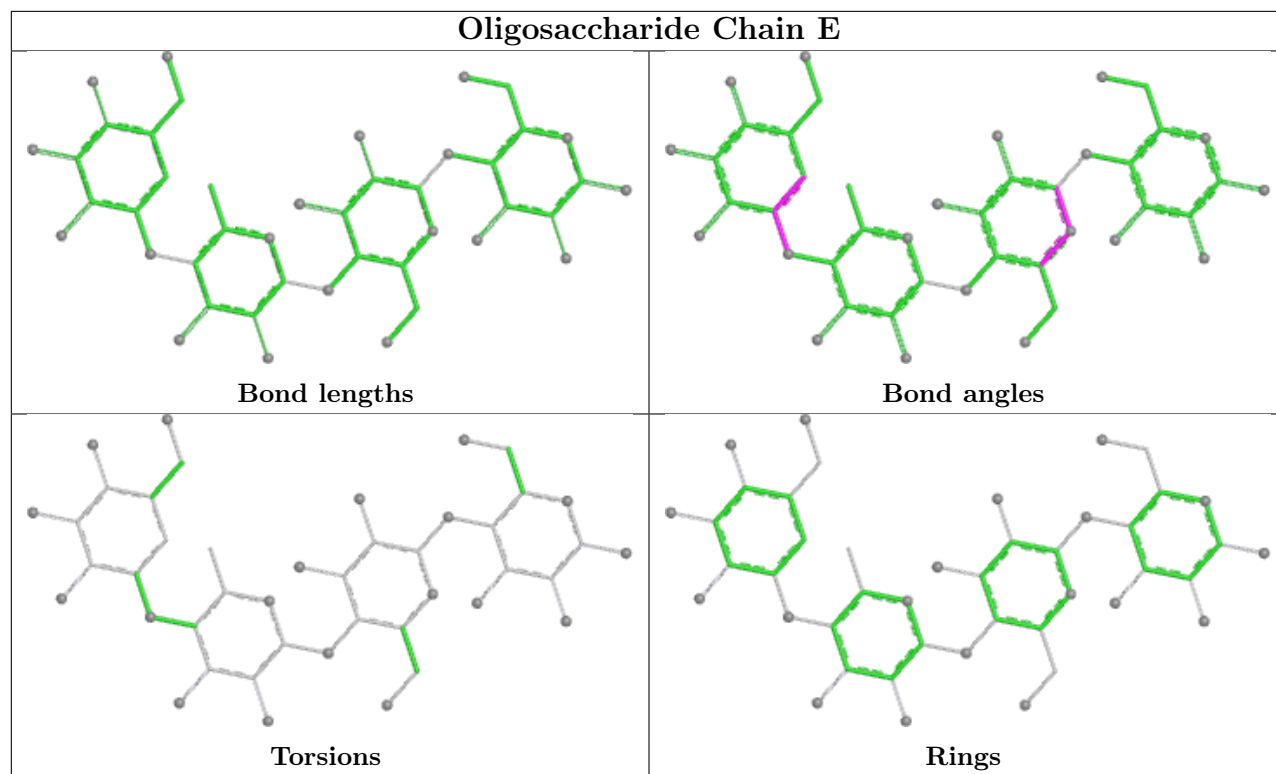
Mol	Chain	Res	Type	Atoms
2	C	3	AC1	C5-C4-N4A-C1B
3	D	3	AC1	C5-C4-N4A-C1B
3	G	3	AC1	C5-C4-N4A-C1B
4	F	2	AC1	C5-C4-N4A-C1B

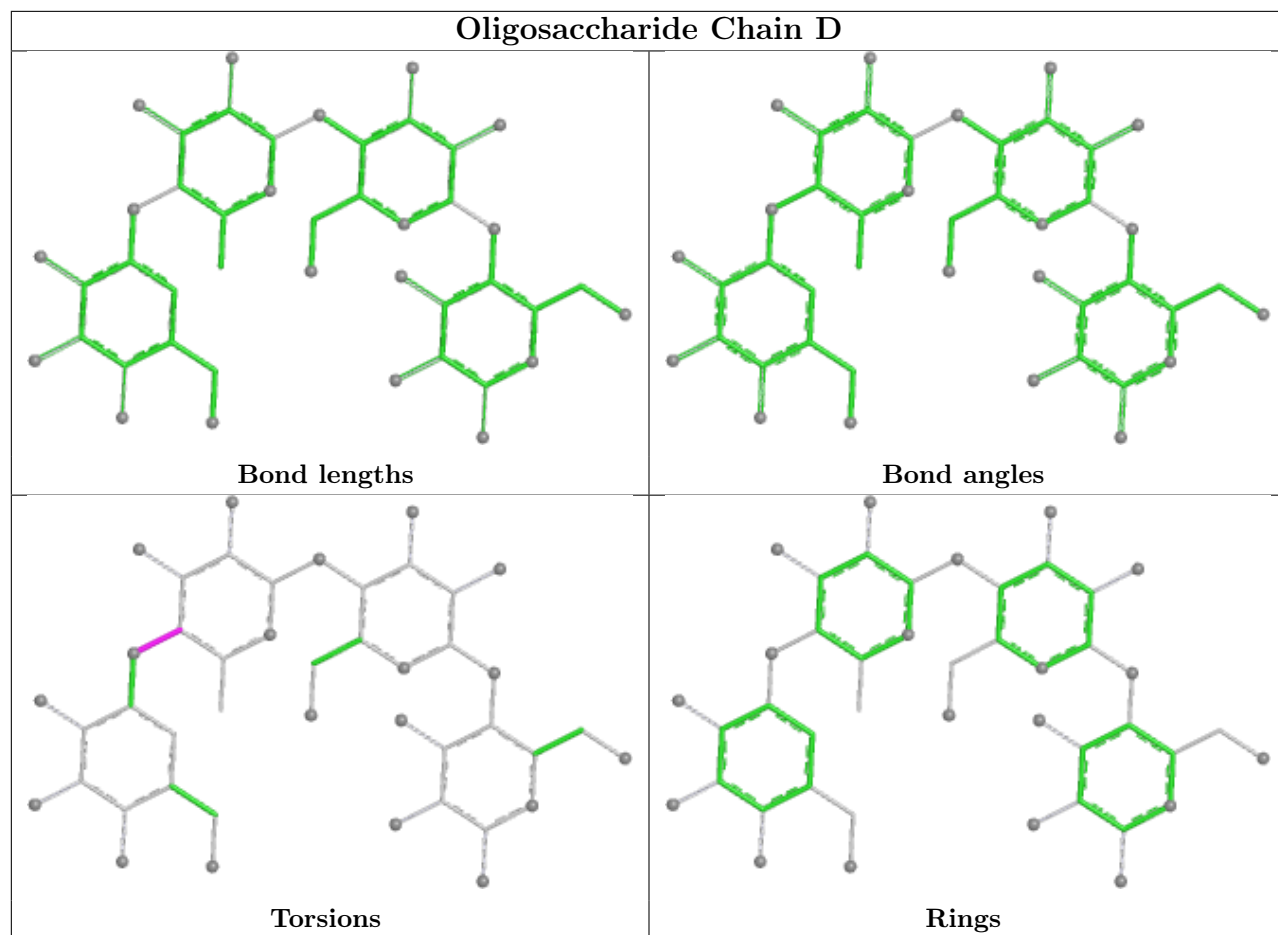
There are no ring outliers.

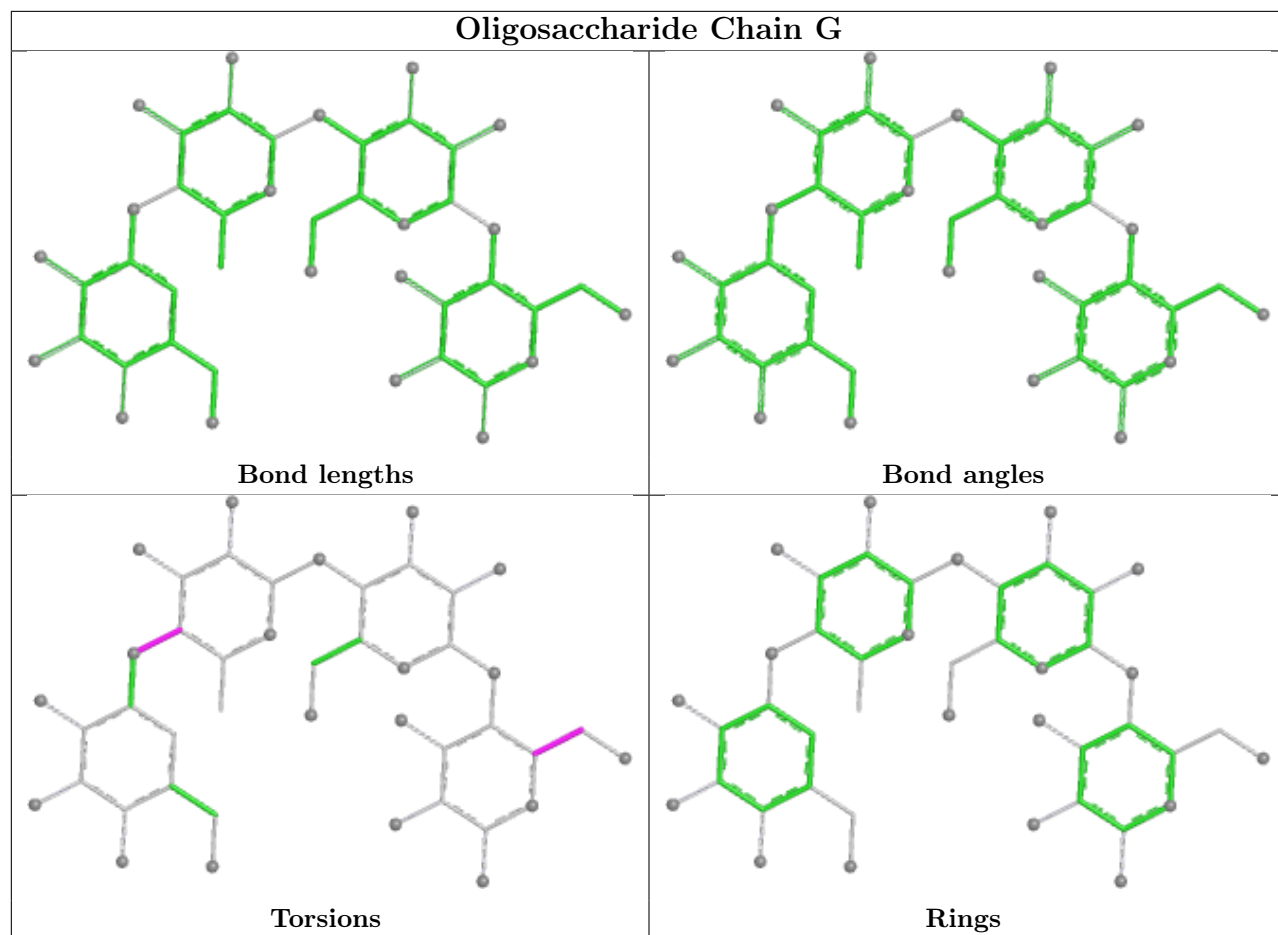
No monomer is involved in short contacts.

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

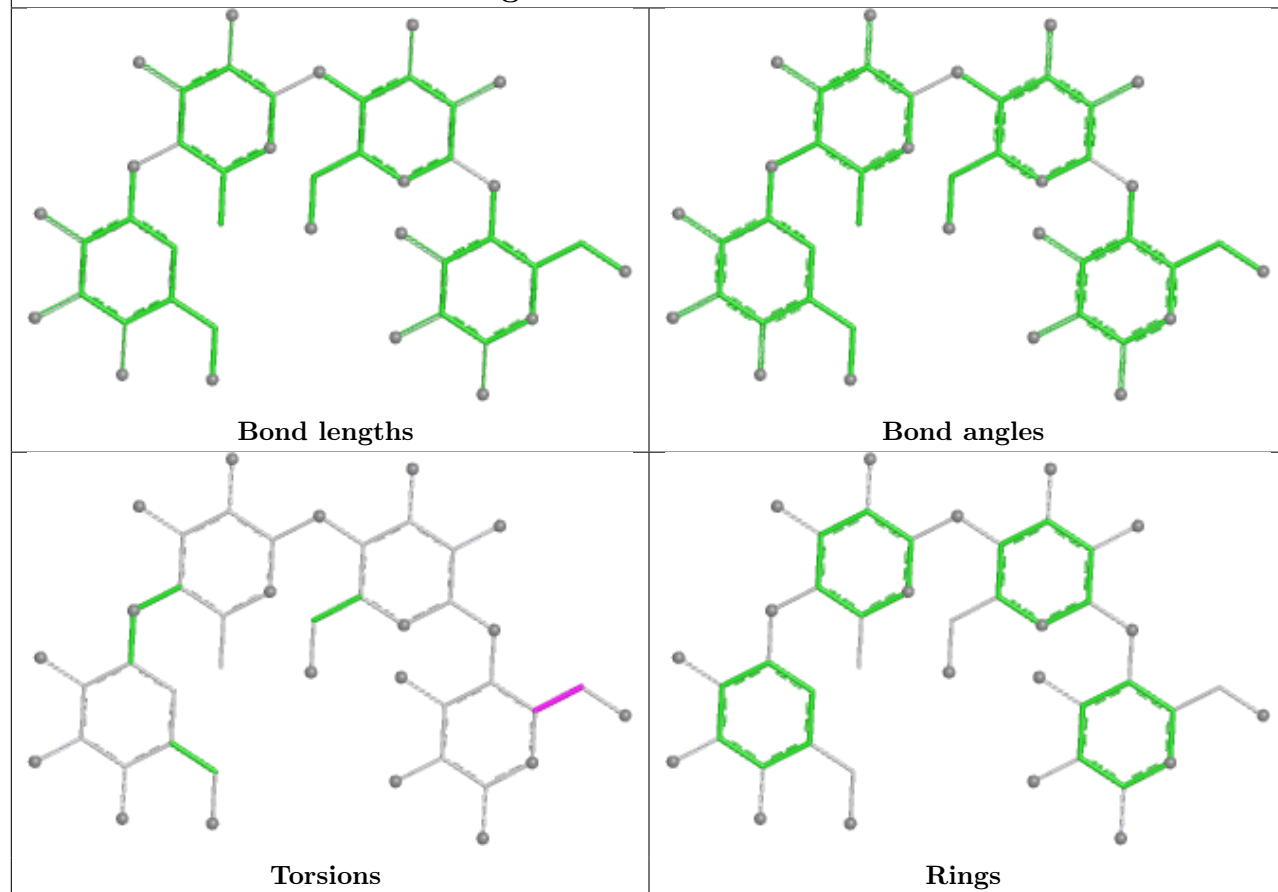




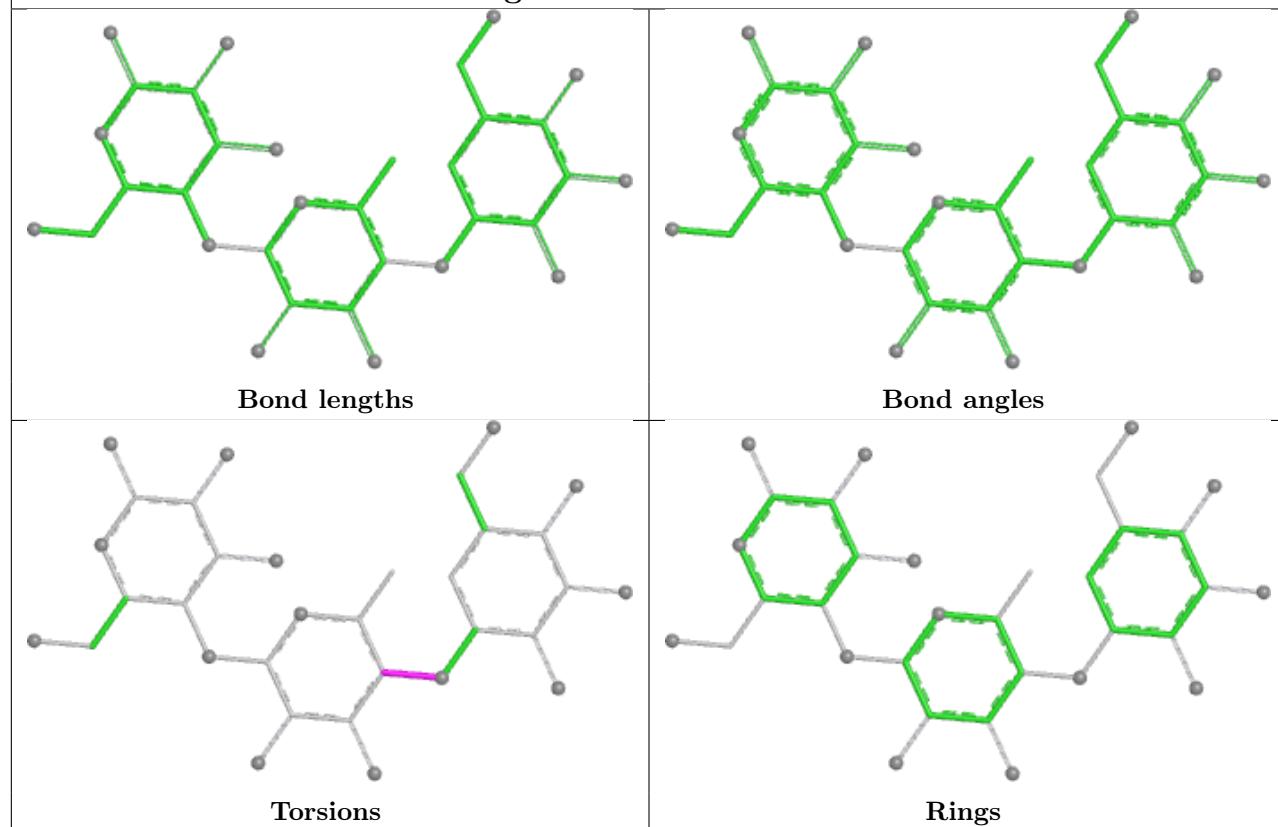




Oligosaccharide Chain H



Oligosaccharide Chain F



5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	650/660 (98%)	0.02	22 (3%) 48 54	10, 16, 35, 55	2 (0%)
1	B	652/660 (98%)	1.07	138 (21%) 2 2	15, 27, 100, 110	0
All	All	1302/1320 (98%)	0.55	160 (12%) 8 9	10, 21, 93, 110	2 (0%)

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	81	TRP	6.7
1	B	48	LEU	6.6
1	B	41	VAL	6.3
1	B	26	ALA	6.3
1	B	50	LEU	6.2
1	B	99	THR	6.1
1	B	36	ILE	6.0
1	B	40	VAL	5.8
1	B	65	LEU	5.7
1	B	77	THR	5.6
1	B	91	LEU	5.4
1	B	83	ILE	5.4
1	B	87	GLY	5.2
1	B	73	PRO	5.2
1	B	84	PHE	5.0
1	B	19	TRP	5.0
1	B	93	VAL	5.0
1	B	79	PRO	4.9
1	B	78	PRO	4.8
1	B	31	GLY	4.8
1	B	63	ILE	4.8
1	B	104	ILE	4.8
1	B	102	MET	4.7
1	B	22	THR	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	101	THR	4.7
1	B	106	LEU	4.7
1	B	88	LEU	4.6
1	B	69	LEU	4.6
1	B	90	THR	4.5
1	B	59	PRO	4.5
1	B	74	CYS	4.5
1	B	57	TRP	4.4
1	B	45	THR	4.4
1	B	52	PHE	4.4
1	B	89	TYR	4.4
1	B	47	PRO	4.4
1	B	103	MET	4.4
1	B	95	THR	4.3
1	B	27	PHE	4.2
1	B	100	PRO	4.2
1	B	35	PHE	4.1
1	B	24	PHE	4.1
1	B	20	THR	4.0
1	B	32	THR	4.0
1	A	62	GLY	4.0
1	B	44	GLY	3.9
1	B	98	GLY	3.9
1	B	92	GLU	3.8
1	A	337	ASP	3.8
1	B	76	GLY	3.8
1	B	68	MET	3.8
1	A	339	LEU	3.7
1	B	61	GLY	3.7
1	B	53	ASP	3.7
1	B	30	GLU	3.6
1	B	18	ALA	3.6
1	B	56	CYS	3.6
1	B	37	SER	3.6
1	B	105	SER	3.6
1	B	28	THR	3.6
1	B	67	GLN	3.5
1	B	60	SER	3.5
1	B	335	GLN	3.5
1	B	46	ARG	3.4
1	A	510	MET	3.4
1	B	51	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	49	GLN	3.3
1	B	336	GLY	3.3
1	B	510	MET	3.2
1	B	97	SER	3.2
1	B	138	ALA	3.2
1	B	70	SER	3.1
1	B	339	LEU	3.1
1	B	64	LYS	3.1
1	B	117	GLN	3.1
1	B	677	GLN	3.1
1	B	107	GLU	3.1
1	A	354	ALA	3.1
1	B	34	ARG	3.0
1	B	66	ASN	3.0
1	A	338	GLU	3.0
1	B	21	THR	3.0
1	B	55	GLN	3.0
1	B	29	GLU	3.0
1	B	124	TRP	3.0
1	B	126	GLY	2.9
1	B	25	PRO	2.9
1	B	620	ASN	2.9
1	B	176	ALA	2.9
1	B	75	ARG	2.9
1	B	137	PHE	2.9
1	B	80	GLN	2.8
1	B	38	GLN	2.8
1	B	154	VAL	2.8
1	B	62	GLY	2.8
1	B	86	GLN	2.8
1	B	621	GLY	2.8
1	B	118	ILE	2.8
1	A	84	PHE	2.7
1	A	53	ASP	2.7
1	B	94	ASP	2.7
1	B	54	GLN	2.7
1	B	72	GLU	2.7
1	B	487	ALA	2.7
1	B	178	THR	2.7
1	B	140	GLY	2.6
1	B	340	LYS	2.6
1	B	495	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	161	LEU	2.6
1	B	82	ARG	2.6
1	B	338	GLU	2.6
1	B	165	PHE	2.6
1	B	33	GLY	2.6
1	B	354	ALA	2.6
1	B	136	THR	2.6
1	A	108	GLU	2.5
1	A	44	GLY	2.5
1	A	620	ASN	2.5
1	B	85	ARG	2.5
1	B	482	ALA	2.5
1	B	71	MET	2.5
1	B	617	GLN	2.4
1	B	334	LEU	2.4
1	A	97	SER	2.4
1	B	346	ARG	2.3
1	B	42	GLU	2.3
1	B	676	GLN	2.3
1	A	68	MET	2.3
1	B	337	ASP	2.3
1	B	153	THR	2.3
1	B	353	GLY	2.3
1	B	490	ASP	2.3
1	A	120	GLN	2.2
1	A	109	LYS	2.2
1	B	341	LYS	2.2
1	B	160	THR	2.2
1	A	67	GLN	2.2
1	A	70	SER	2.2
1	B	23	ASP	2.2
1	B	39	LYS	2.2
1	B	43	LYS	2.2
1	B	655	ARG	2.2
1	A	336	GLY	2.2
1	B	58	GLN	2.1
1	B	554	SER	2.1
1	B	129	LEU	2.1
1	B	493	LEU	2.1
1	B	151	VAL	2.1
1	B	480	ALA	2.1
1	B	146	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	130	THR	2.1
1	B	450	ARG	2.1
1	A	340	LYS	2.0
1	B	108	GLU	2.0
1	B	663	SER	2.0
1	A	98	GLY	2.0
1	A	82	ARG	2.0
1	A	677	GLN	2.0
1	B	149	GLY	2.0
1	B	344	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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

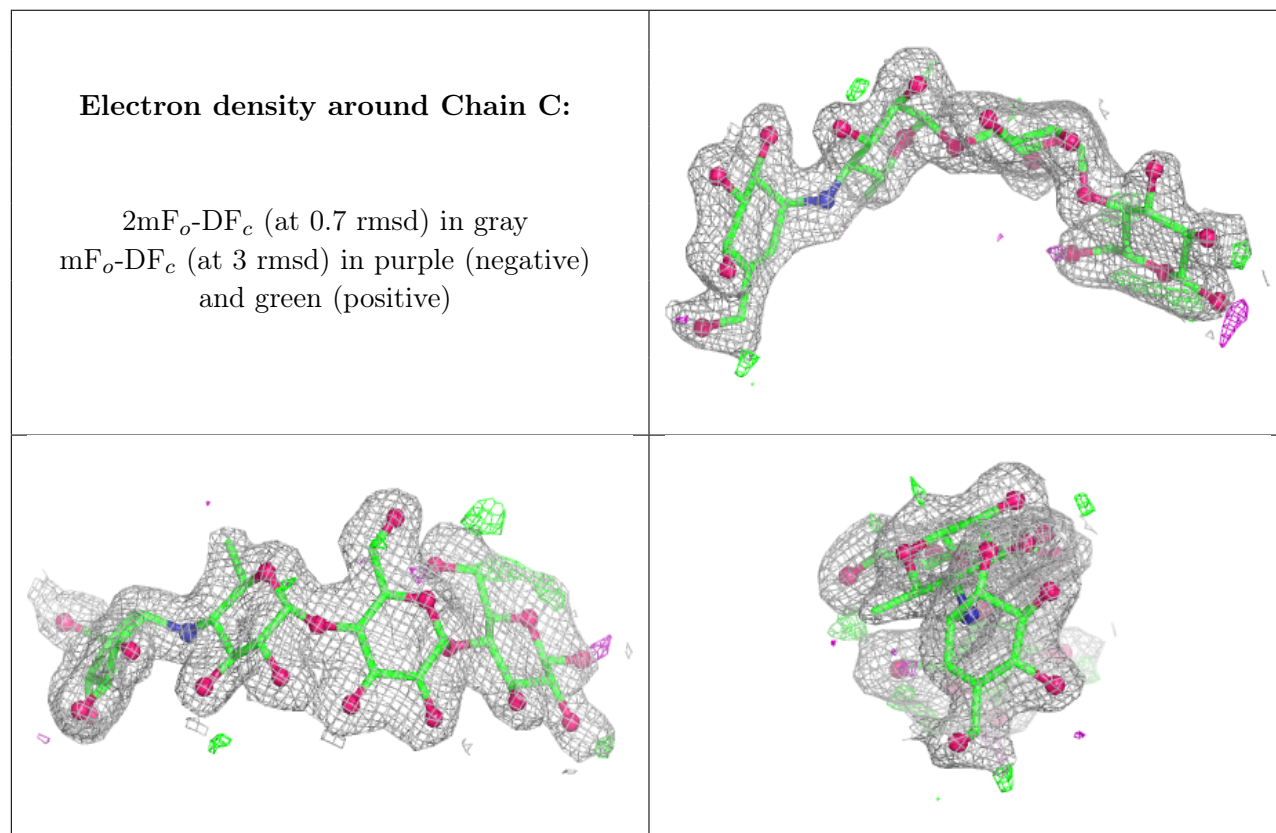
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	AC1	E	3	21/22	0.51	0.16	50,59,66,67	0
2	AC1	I	3	21/22	0.58	0.15	58,65,71,71	0
3	GLC	H	1	12/12	0.61	0.14	43,49,50,51	0
4	GLC	F	1	12/12	0.68	0.15	44,47,49,49	0
3	GLC	D	1	12/12	0.69	0.14	41,48,49,49	0
3	GLC	G	1	12/12	0.76	0.16	31,35,37,37	0
2	BGC	I	1	12/12	0.78	0.13	46,47,48,49	0
3	AC1	H	3	21/22	0.79	0.12	28,31,33,34	0
2	GLC	I	2	11/12	0.80	0.13	47,49,51,54	0
2	BGC	C	1	12/12	0.82	0.12	27,30,31,31	0
4	AC1	F	2	21/22	0.82	0.12	34,36,41,43	0
2	BGC	E	1	12/12	0.83	0.10	38,40,41,41	0
2	GLC	E	2	11/12	0.83	0.12	40,42,44,47	0
3	GLC	H	2	11/12	0.86	0.10	36,38,39,40	0
3	AC1	D	3	21/22	0.87	0.10	29,30,30,30	0
3	GLC	D	2	11/12	0.89	0.10	31,33,35,36	0
3	GLC	G	2	11/12	0.91	0.09	25,26,28,28	0
2	AC1	C	3	21/22	0.91	0.09	22,25,28,28	0

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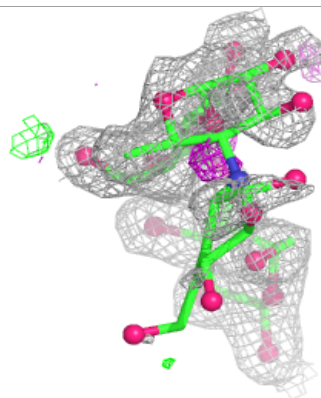
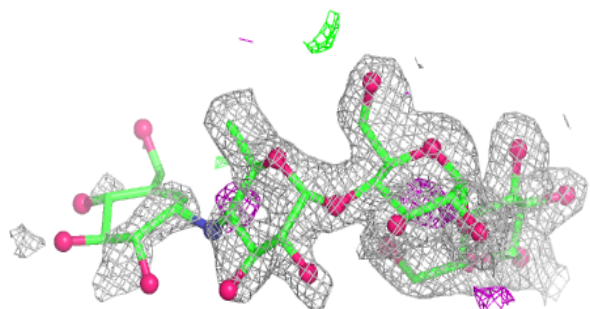
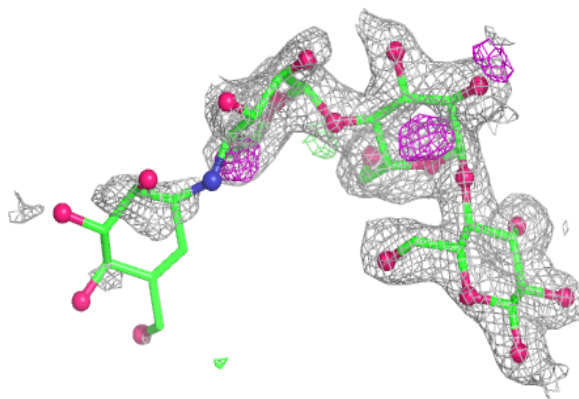
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	C	2	11/12	0.92	0.08	23,24,25,25	0
3	AC1	G	3	21/22	0.93	0.07	24,24,26,27	0

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

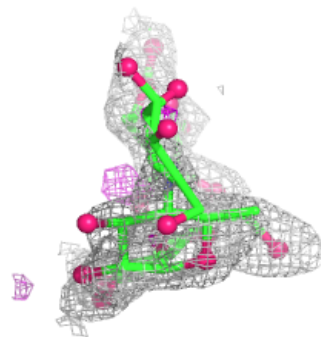
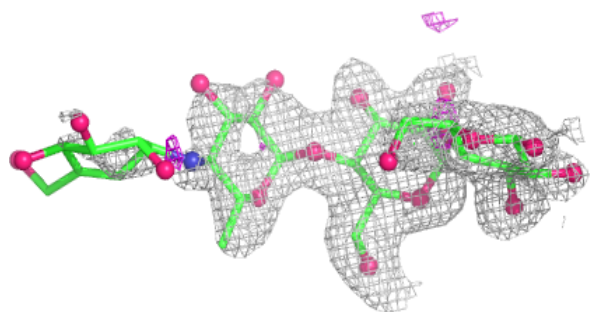
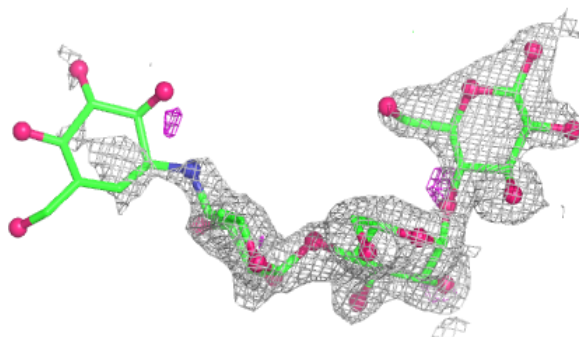


Electron density around Chain E:

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

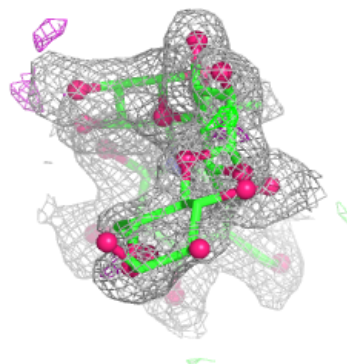
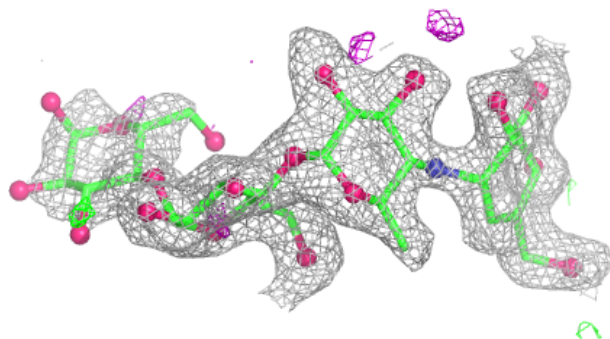
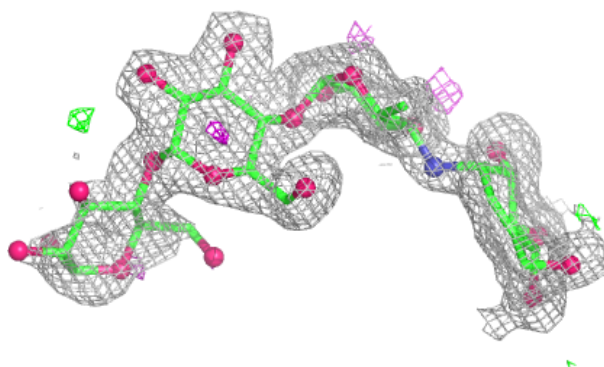
**Electron density around Chain I:**

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

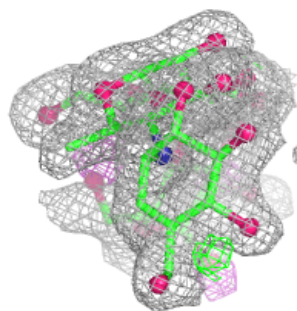
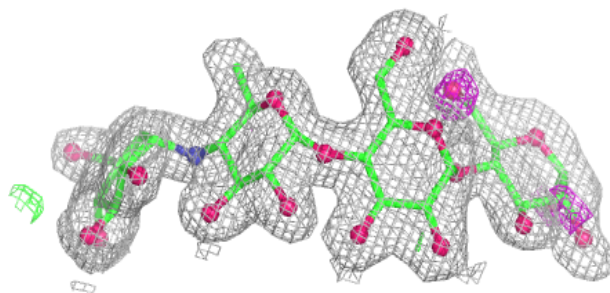
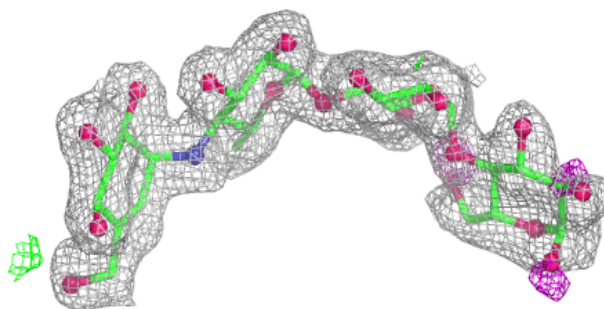


Electron density around Chain D:

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

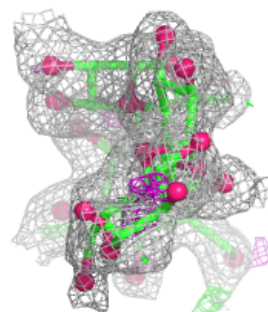
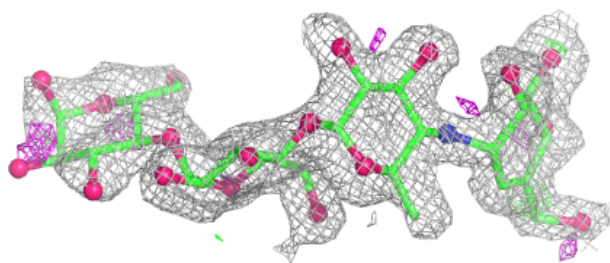
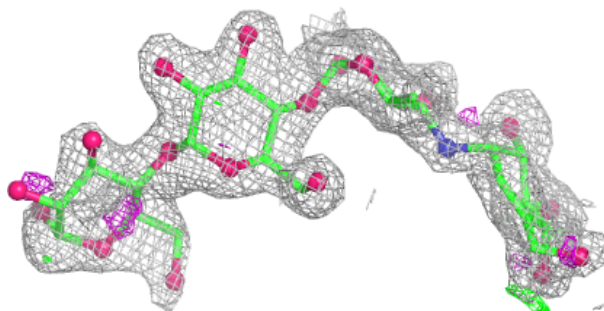
**Electron density around Chain G:**

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

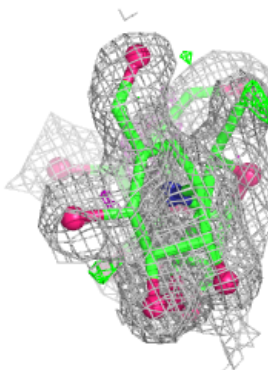
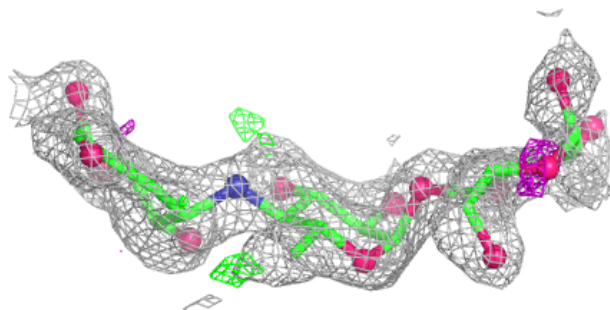
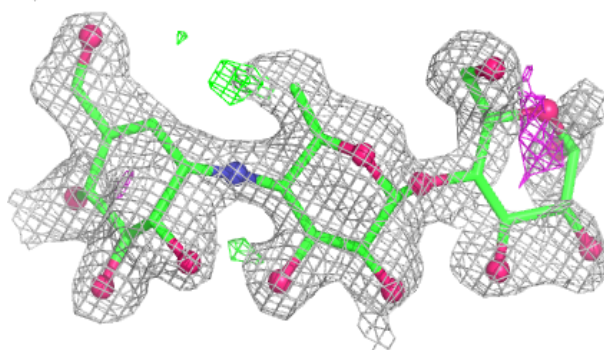


Electron density around Chain H:

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

**Electron density around Chain F:**

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



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	CA	A	702	1/1	0.99	0.02	12,12,12,12	0
5	CA	B	701	1/1	0.99	0.02	15,15,15,15	0
5	CA	B	702	1/1	0.99	0.03	15,15,15,15	0
5	CA	A	701	1/1	1.00	0.01	11,11,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.