



wwPDB X-ray Structure Validation Summary Report

Nov 13, 2023 – 12:31 PM JST

PDB ID : 5X7P
Title : Crystal structure of Paenibacillus sp. 598K alpha-1,6-glucosyltransferase complexed with acarbose
Authors : Fujimoto, Z.; Kishine, N.; Suzuki, N.; Momma, M.; Ichinose, H.; Kimura, A.; Funane, K.
Deposited on : 2017-02-27
Resolution : 2.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the  symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

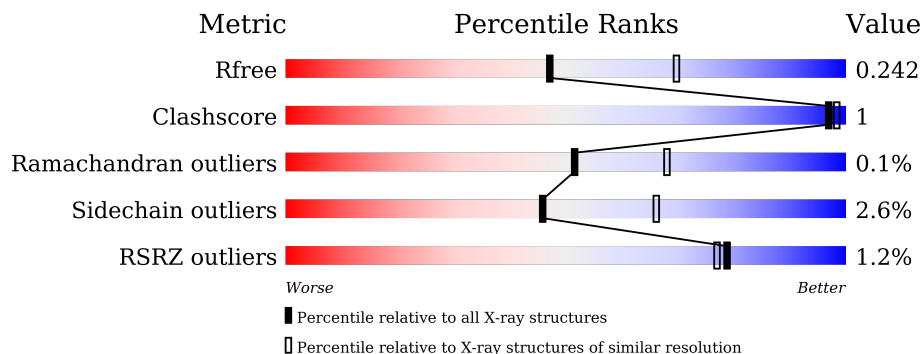
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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.



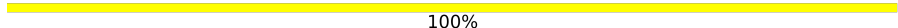

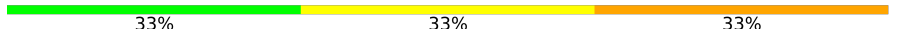
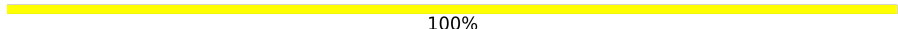


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	1263	 2% 94% 5%
1	B	1263	 2% 94% 5%
2	C	3	 100%
2	E	3	 33% 67%
2	G	3	 33% 33% 33%
2	H	3	 67% 33%

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Mol	Chain	Length	Quality of chain
2	I	3	 100%
2	J	3	 33% 67%
2	L	3	 33% 33% 33%
3	D	2	 100%
4	F	2	 50% 50%
4	K	2	 50% 50%

2 Entry composition i

There are 11 unique types of molecules in this entry. The entry contains 20523 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glycoside hydrolase family 31 alpha-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1247	9601	6023	1633	1923	22	0	0	0
1	B	1247	9612	6033	1634	1923	22	0	1	0

There are 34 discrepancies between the modelled and reference sequences:

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

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

- Molecule 2 is an oligosaccharide called 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
			Total	C	N	O			
2	C	3	44	25	1	18	0	0	0
2	E	3	33	19	1	13	0	0	1
2	G	3	33	19	1	13	0	0	1
2	H	3	44	25	1	18	0	0	0
2	I	3	33	18	1	14	0	0	0
2	J	3	33	19	1	13	0	0	1
2	L	3	33	19	1	13	0	0	1

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



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

- 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

e.

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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

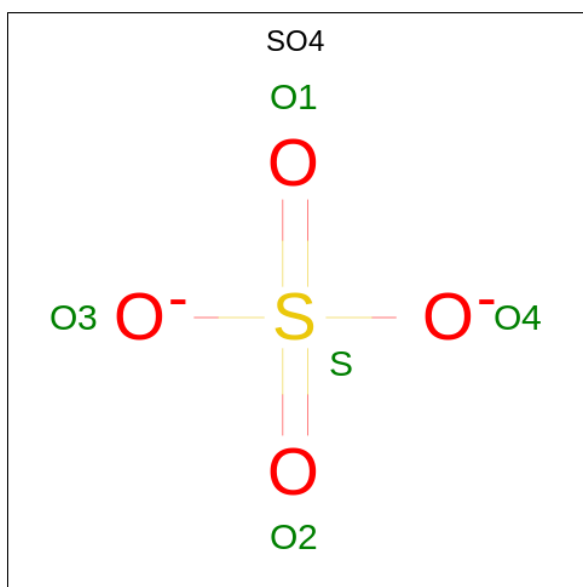
- Molecule 6 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

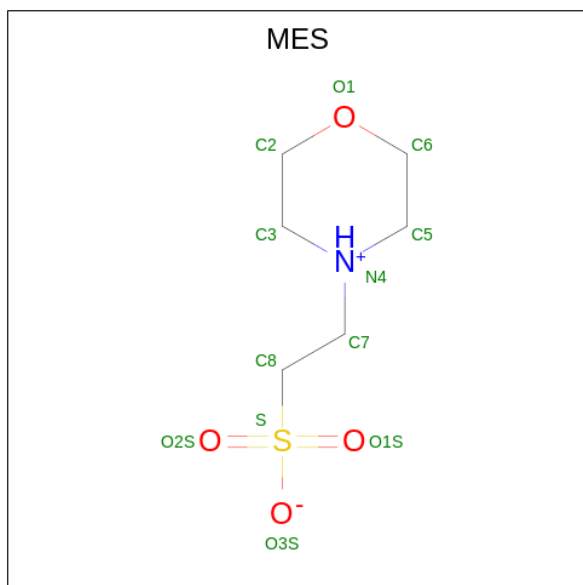
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	6	Total	Mg	0	0
			6	6		
7	B	6	Total	Mg	0	0
			6	6		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



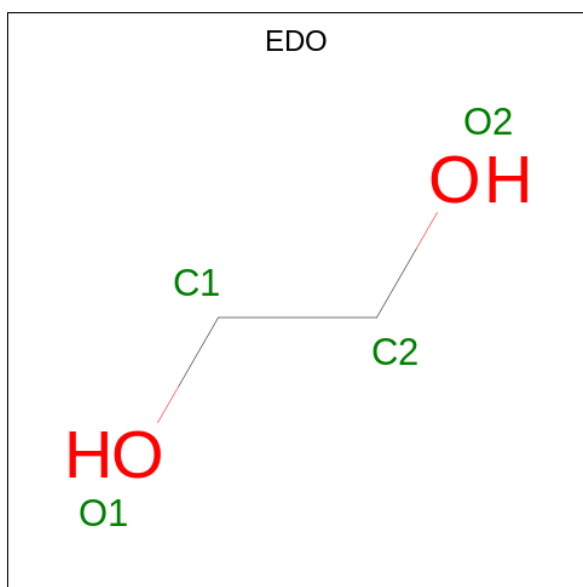
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total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

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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	B	1	Total C O 4 2 2	0	0
10	B	1	Total C O 4 2 2	0	0
10	B	1	Total C O 4 2 2	0	0
10	B	1	Total C O 4 2 2	0	0

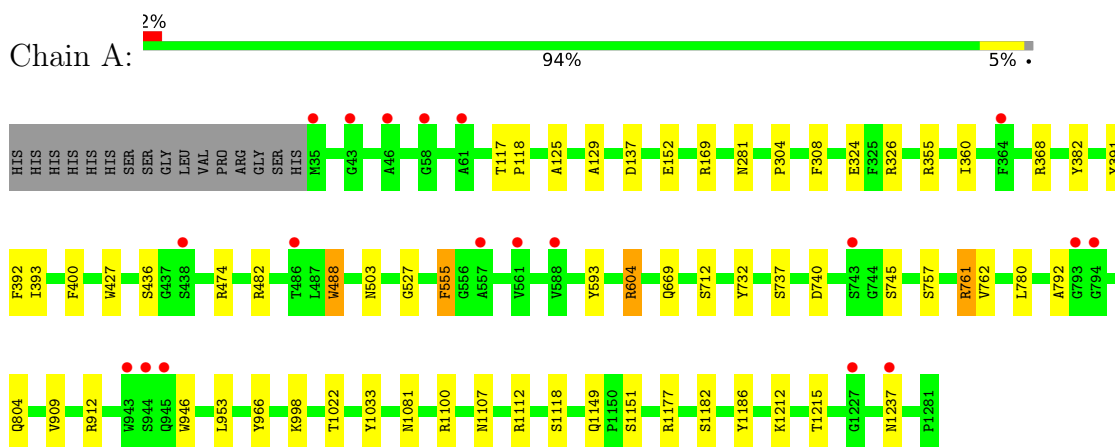
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	391	Total O 391 391	0	0
11	B	403	Total O 403 403	0	0

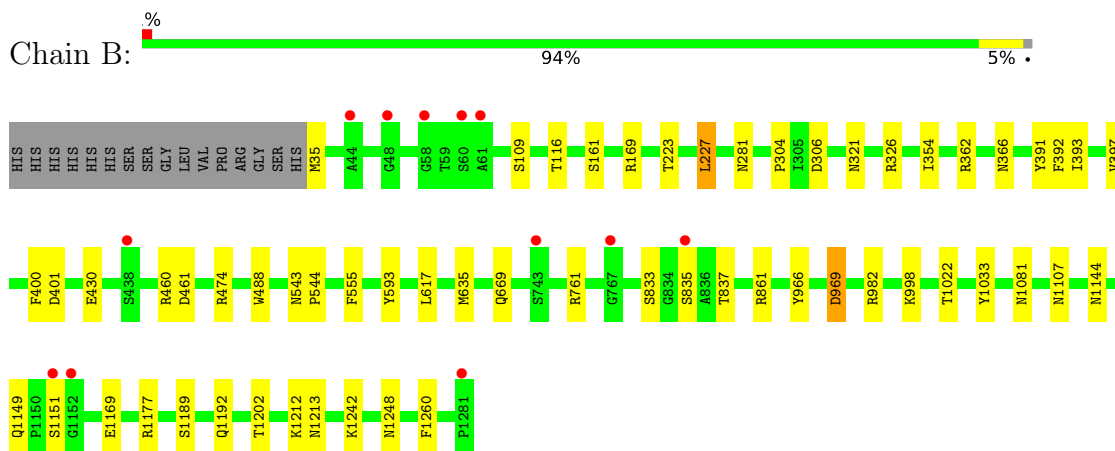
3 Residue-property plots [i](#)

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

- Molecule 1: Glycoside hydrolase family 31 alpha-glucosidase




- Molecule 1: Glycoside hydrolase family 31 alpha-glucosidase



- 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)-alpha-D-glucopyranose

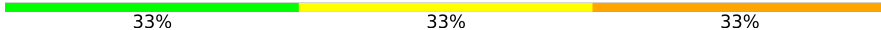


- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl}]\text{amino}\}$ - α -D-glucopyranose-(1-4)- α -D-glucopyranose-(1-4)- α -D-glucopyranose

Chain E:  33% 67%

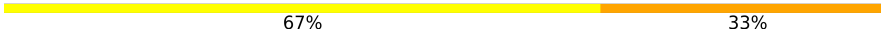

GLC1
GLC2
AC13

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

Chain G:  33% 33% 33%

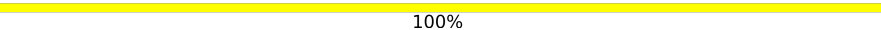

GLC1
GLC2
AC13

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

Chain H:  67% 33%


GLC1
GLC2
AC13

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

Chain I:  100%

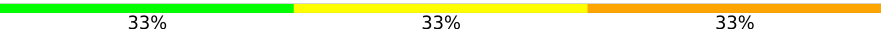

GLC1
GLC2
AC13

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

Chain J:  33% 67%


GLC1
GLC2
AC13

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

Chain L:  33% 33% 33%


GLC1
GLC2
AC13

- Molecule 3: α -D-glucopyranose-(1-4)- α -D-glucopyranose

Chain D:  100%

GLC1
GLC2

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

Chain F:  50% 50%GLC1
AC12

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

Chain K:  50% 50%GLC1
AC12

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	184.29Å 271.52Å 133.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.48 – 2.40 47.62 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.1 (152.48-2.40) 97.1 (47.62-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.64 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.180 , 0.237 0.189 , 0.242	Depositor DCC
R_{free} test set	6373 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	39.0	Xtrriage
Anisotropy	0.727	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20523	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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: NI, MG, CA, SO4, AC1, GLC, EDO, MES

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	0.72	0/9863	0.83	6/13473 (0.0%)
1	B	0.72	0/9879	0.84	7/13496 (0.1%)
All	All	0.72	0/19742	0.83	13/26969 (0.0%)

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	474	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	B	474	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	B	761	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	A	482	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	1112	ARG	NE-CZ-NH1	5.89	123.25	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9601	0	8954	22	1
1	B	9612	0	8964	20	0
2	C	44	0	30	0	0
2	E	33	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	33	0	19	1	0
2	H	44	0	30	1	0
2	I	33	0	21	0	0
2	J	33	0	19	0	0
2	L	33	0	19	1	0
3	D	23	0	21	0	0
4	F	22	0	10	0	0
4	K	22	0	10	0	1
5	A	3	0	0	0	0
5	B	3	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	6	0	0	0	0
7	B	6	0	0	0	0
8	A	25	0	0	0	0
8	B	35	0	0	0	0
9	A	24	0	26	0	0
9	B	60	0	65	0	0
10	A	16	0	24	0	0
10	B	16	0	24	0	0
11	A	391	0	0	0	0
11	B	403	0	0	0	0
All	All	20523	0	18255	35	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

The worst 5 of 35 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:362:ARG:HD3	1:B:366:ASN:OD1	2.06	0.54
1:B:161:SER:HB2	1:B:223:THR:O	2.10	0.52
1:A:360:ILE:HD13	1:B:397:VAL:HG12	1.93	0.51
1:A:909:VAL:HG21	1:A:953:LEU:HD12	1.91	0.51
1:B:430:GLU:OE2	2:H:3:AC1:O3	2.30	0.50

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1215:THR:OG1	4:K:2:AC1:O6B[6_555]	2.02	0.18

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1245/1263 (99%)	1207 (97%)	37 (3%)	1 (0%)	51 68
1	B	1246/1263 (99%)	1206 (97%)	39 (3%)	1 (0%)	51 68
All	All	2491/2526 (99%)	2413 (97%)	76 (3%)	2 (0%)	51 68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1213	ASN
1	A	792	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	997/1011 (99%)	970 (97%)	27 (3%)	44 65
1	B	998/1011 (99%)	973 (98%)	25 (2%)	47 67
All	All	1995/2022 (99%)	1943 (97%)	52 (3%)	46 66

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	109	SER
1	B	400	PHE
1	B	1151	SER
1	B	116	THR
1	B	281	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1107	ASN
1	B	1144	ASN
1	B	1213	ASN
1	A	1237	ASN
1	B	440	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

Of 27 monosaccharides modelled in this entry, 21 were used for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GLC	C	1	2	12,12,12	0.52	0	17,17,17	0.86	1 (5%)
2	GLC	C	2	2	11,11,12	0.74	0	15,15,17	1.17	1 (6%)
2	AC1	C	3	2	21,22,23	0.92	0	22,32,34	1.59	5 (22%)
3	GLC	D	1	3	12,12,12	0.77	0	17,17,17	1.44	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GLC	D	2	3	11,11,12	1.32	1 (9%)	15,15,17	1.93	3 (20%)
2	GLC	E	2	2	11,11,12	0.71	0	15,15,17	1.66	5 (33%)
2	AC1	E	3	2	21,22,23	1.57	3 (14%)	22,32,34	1.12	2 (9%)
4	AC1	F	2	4	21,22,23	1.00	1 (4%)	22,32,34	1.41	2 (9%)
2	GLC	G	2	2	11,11,12	0.63	0	15,15,17	1.70	5 (33%)
2	AC1	G	3	2	21,22,23	1.33	3 (14%)	22,32,34	1.60	6 (27%)
2	GLC	H	1	2	12,12,12	0.71	0	17,17,17	0.97	1 (5%)
2	GLC	H	2	2	11,11,12	0.62	0	15,15,17	1.08	1 (6%)
2	AC1	H	3	2	21,22,23	1.03	1 (4%)	22,32,34	1.78	7 (31%)
2	GLC	I	1	2	12,12,12	0.99	0	17,17,17	1.41	2 (11%)
2	GLC	I	2	2	11,11,12	0.81	0	15,15,17	1.43	2 (13%)
2	AC1	I	3	2	9,10,23	1.19	0	14,14,34	1.95	5 (35%)
2	GLC	J	2	2	11,11,12	0.75	0	15,15,17	1.57	3 (20%)
2	AC1	J	3	2	21,22,23	1.07	1 (4%)	22,32,34	1.44	5 (22%)
4	AC1	K	2	4	21,22,23	1.02	1 (4%)	22,32,34	1.67	3 (13%)
2	GLC	L	2	2	11,11,12	0.82	0	15,15,17	2.11	5 (33%)
2	AC1	L	3	2	21,22,23	0.80	0	22,32,34	1.09	1 (4%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	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	-	-	0/1/1/2
2	GLC	J	2	2	-	0/2/19/22	0/1/1/1
2	AC1	J	3	2	-	3/6/43/46	0/2/2/2
4	AC1	K	2	4	-	2/6/43/46	0/2/2/2
2	GLC	L	2	2	-	1/2/19/22	0/1/1/1
2	AC1	L	3	2	-	1/6/43/46	0/2/2/2

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3	AC1	C7B-C5B	4.18	1.38	1.32
2	E	3	AC1	C1B-C7B	2.98	1.54	1.50
2	G	3	AC1	C4A-C5B	2.91	1.53	1.51
2	H	3	AC1	C2B-C1B	2.80	1.56	1.52
2	J	3	AC1	C1B-C7B	2.71	1.54	1.50

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	2	GLC	C1-O5-C5	5.81	120.06	112.19
3	D	2	GLC	C1-O5-C5	5.00	118.97	112.19
4	K	2	AC1	C1-C2-C3	4.93	115.73	109.67
4	F	2	AC1	C1-C2-C3	4.53	115.23	109.67
2	I	3	AC1	C1-O5-C5	4.44	122.85	112.78

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

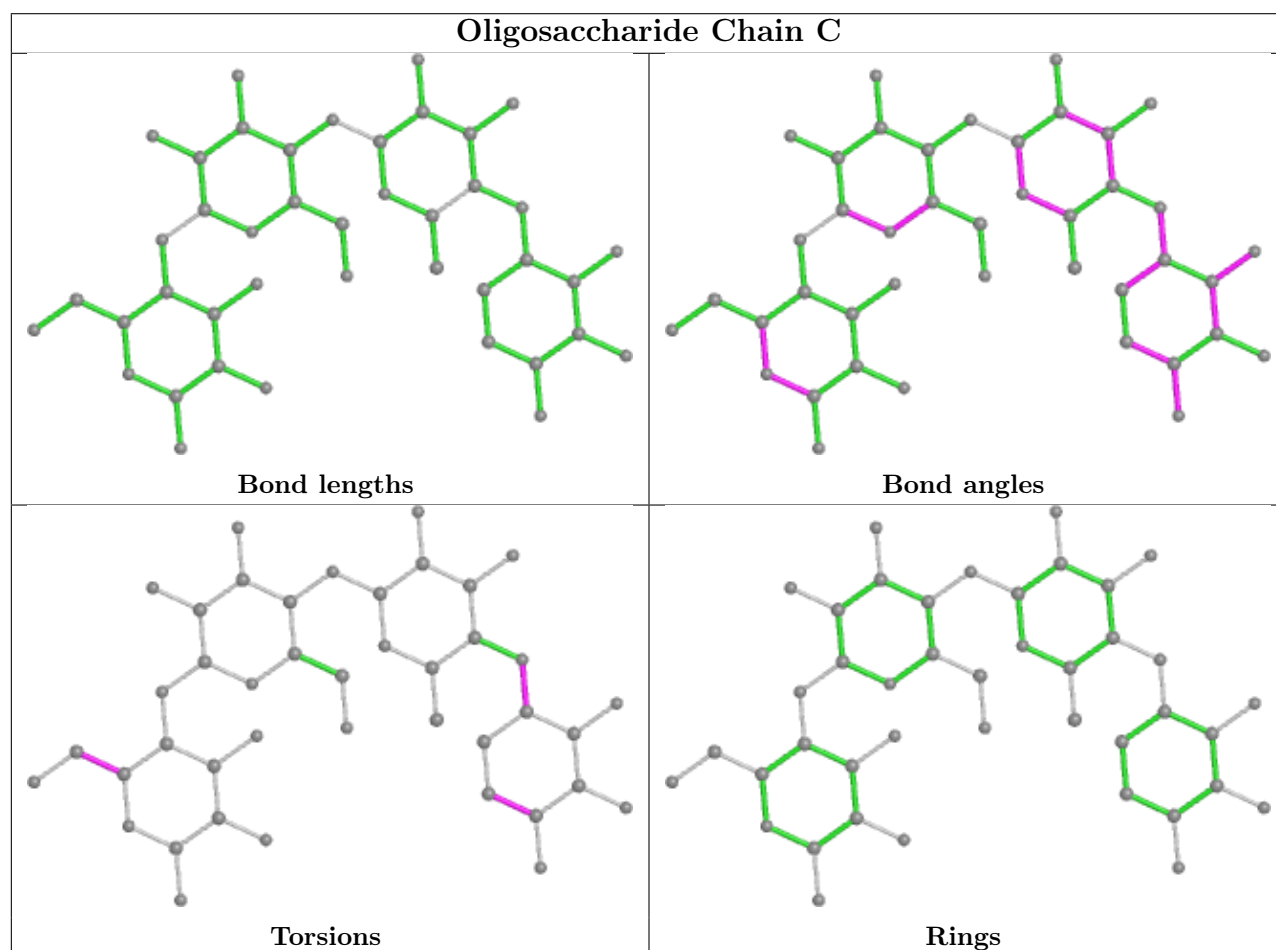
Mol	Chain	Res	Type	Atoms
2	C	3	AC1	C7B-C1B-N4A-C4
2	C	3	AC1	C4A-C5B-C6B-O6B
2	C	3	AC1	C7B-C5B-C6B-O6B
2	E	3	AC1	C4A-C5B-C6B-O6B
2	E	3	AC1	C7B-C5B-C6B-O6B

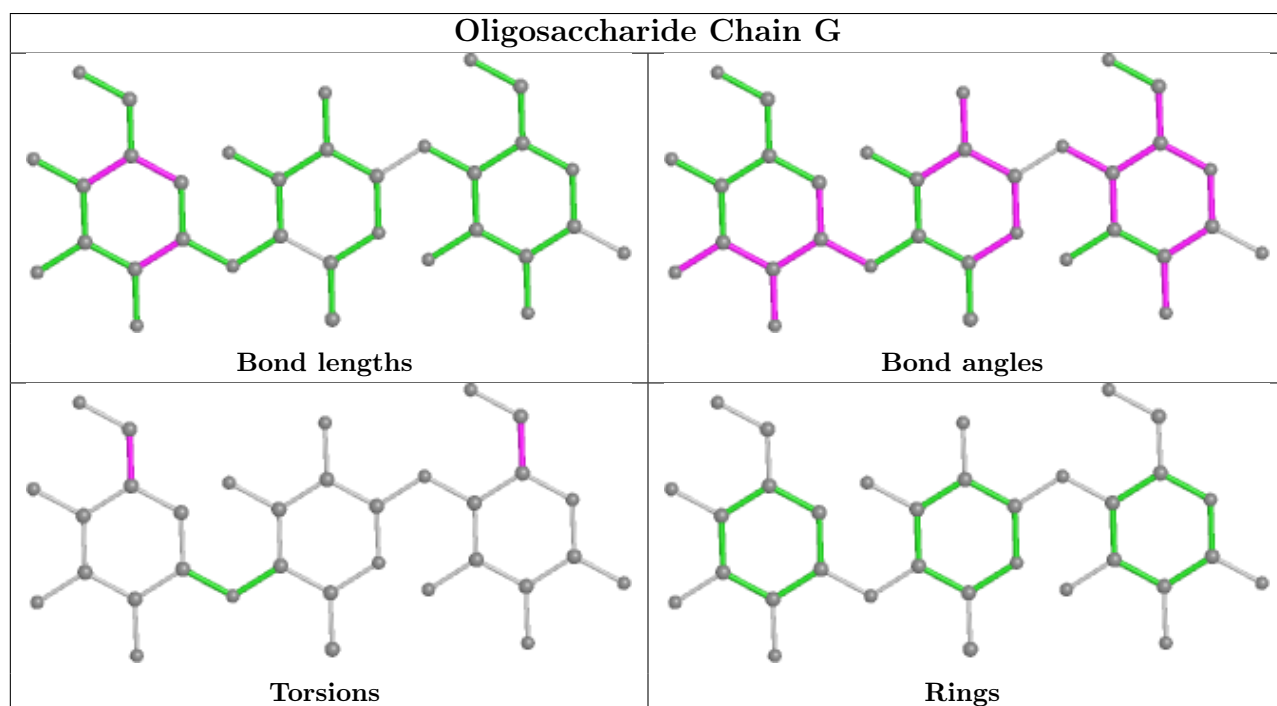
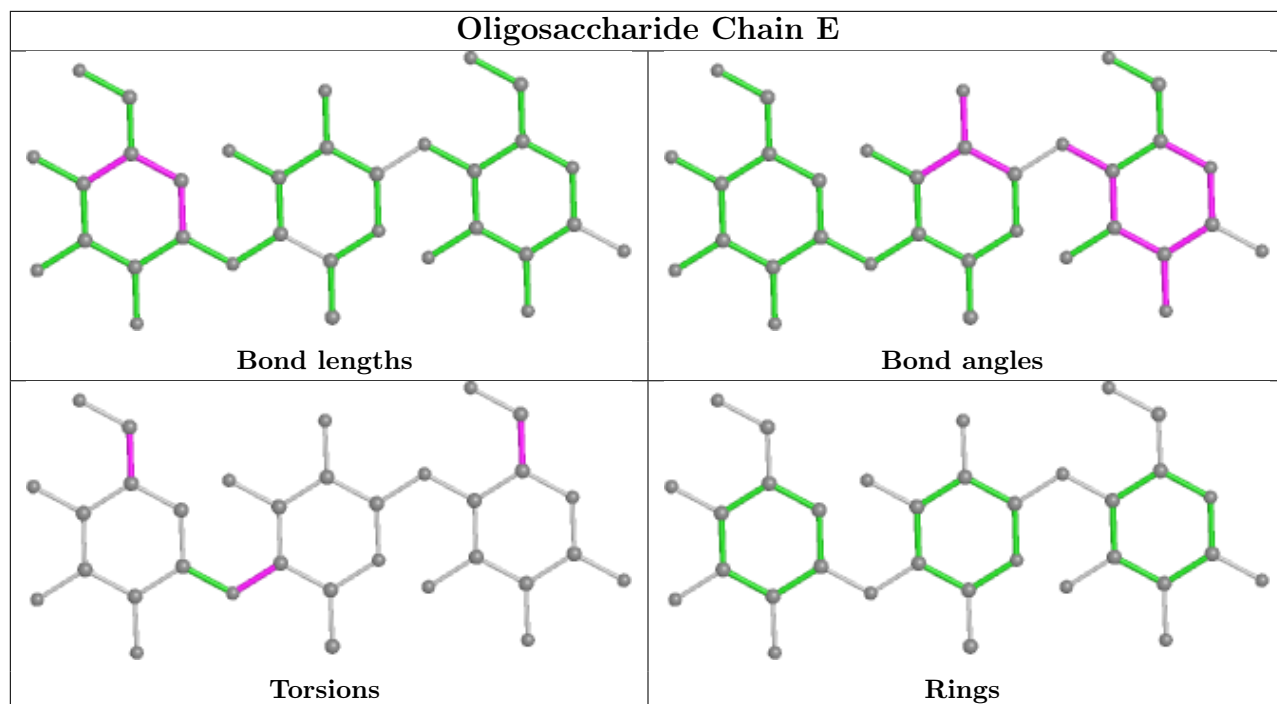
There are no ring outliers.

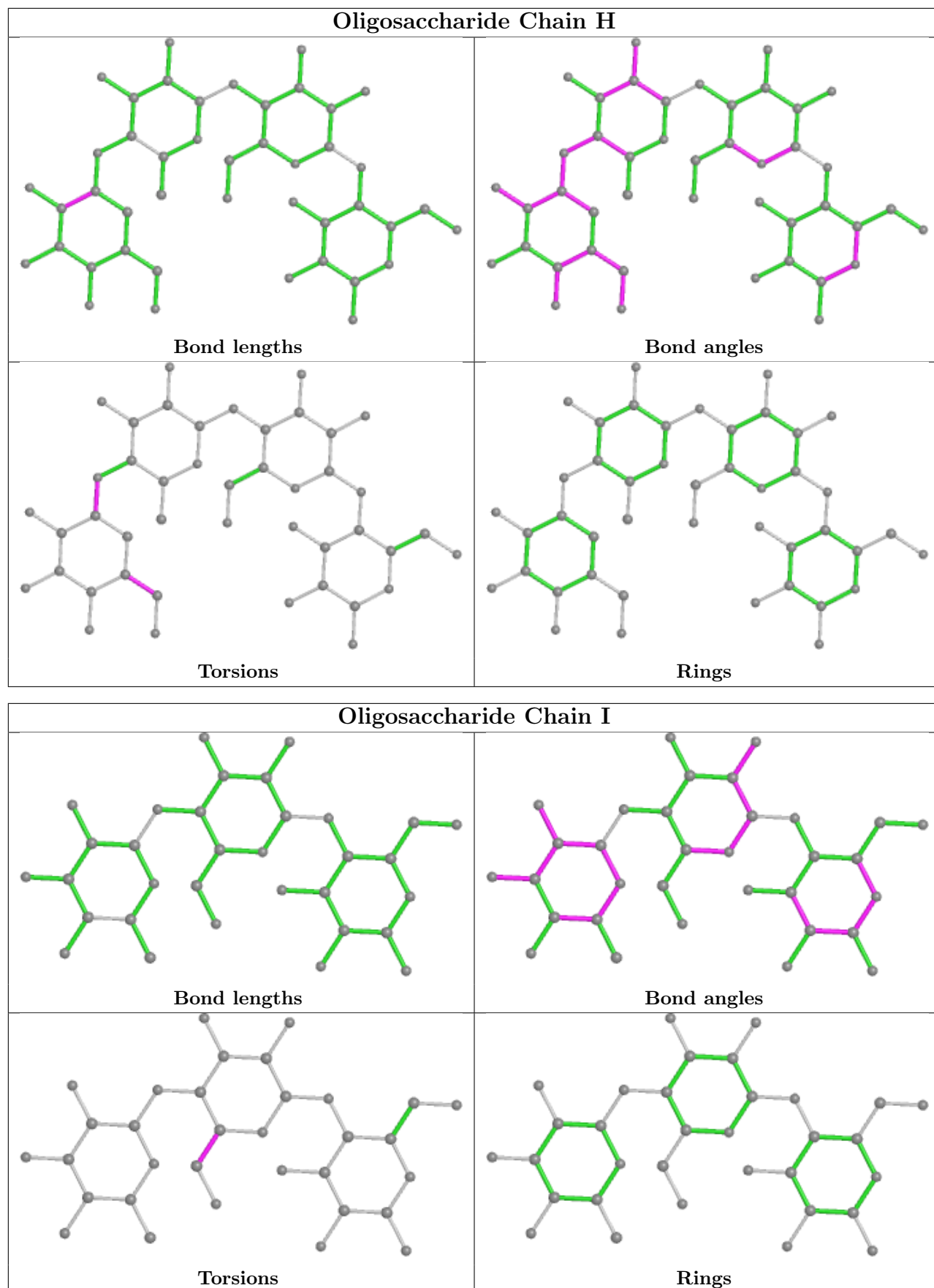
4 monomers are involved in 4 short contacts:

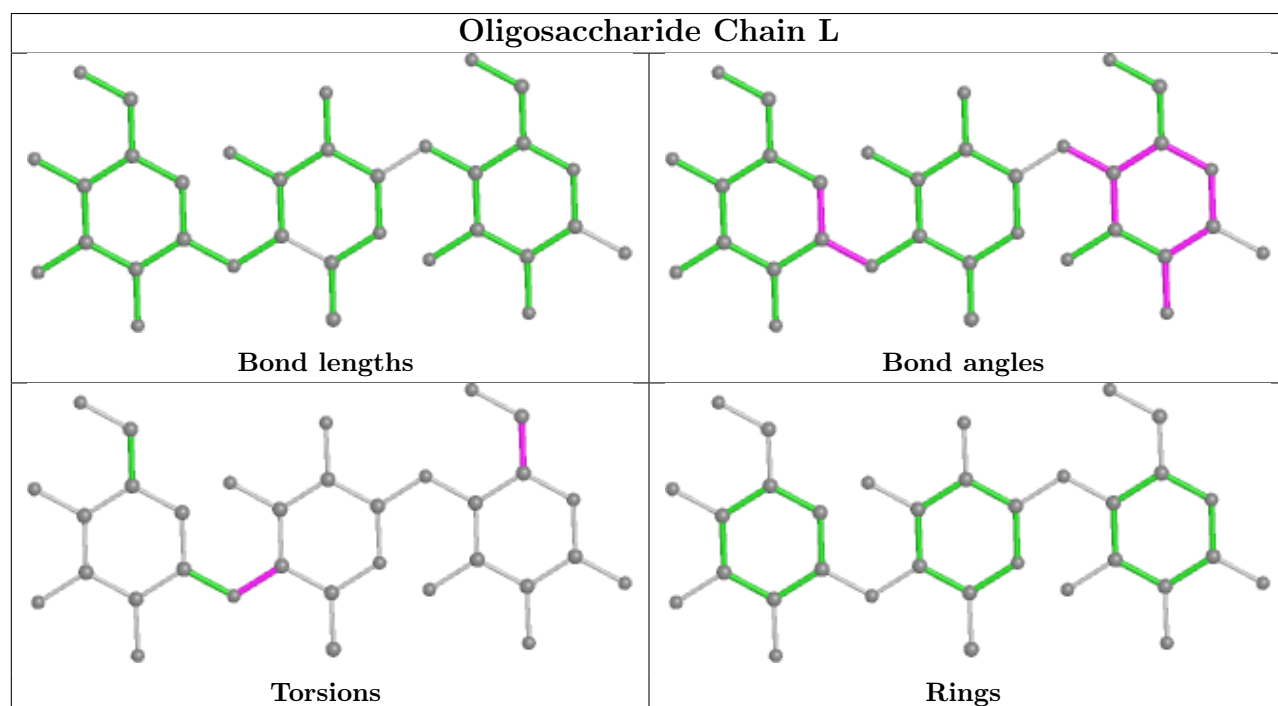
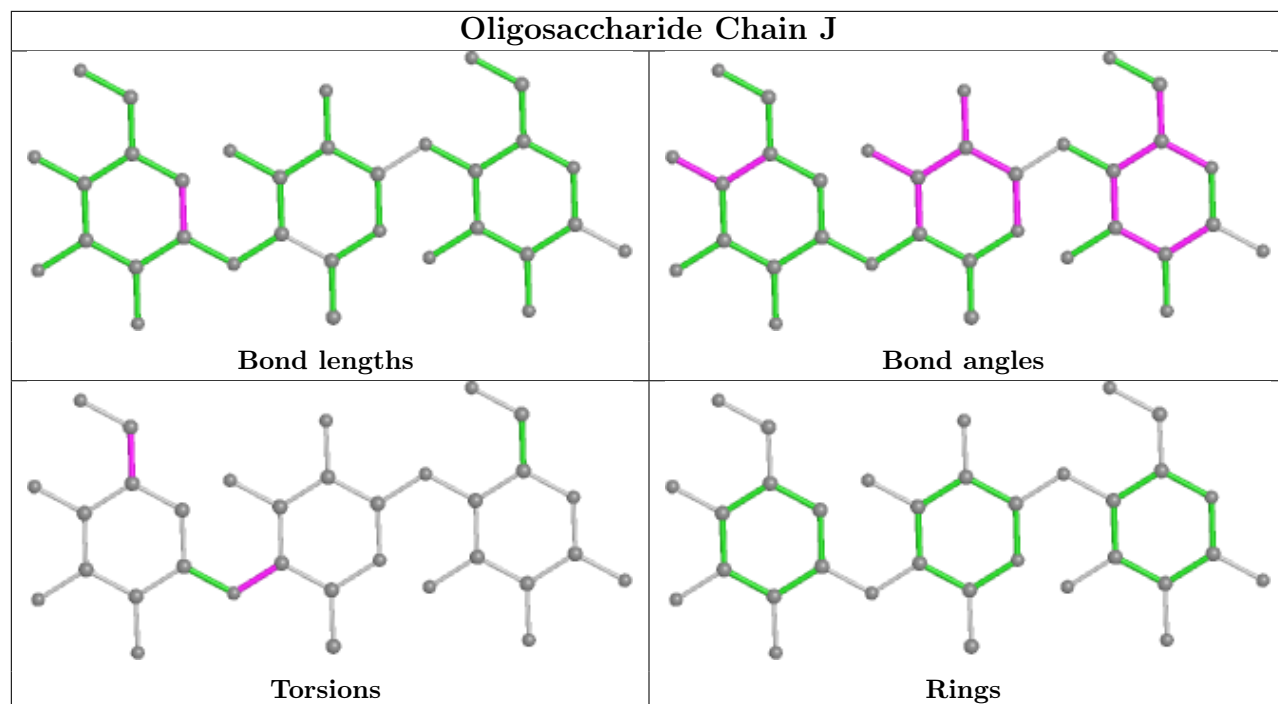
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	3	AC1	1	0
4	K	2	AC1	0	1
2	L	3	AC1	1	0
2	G	2	GLC	1	0

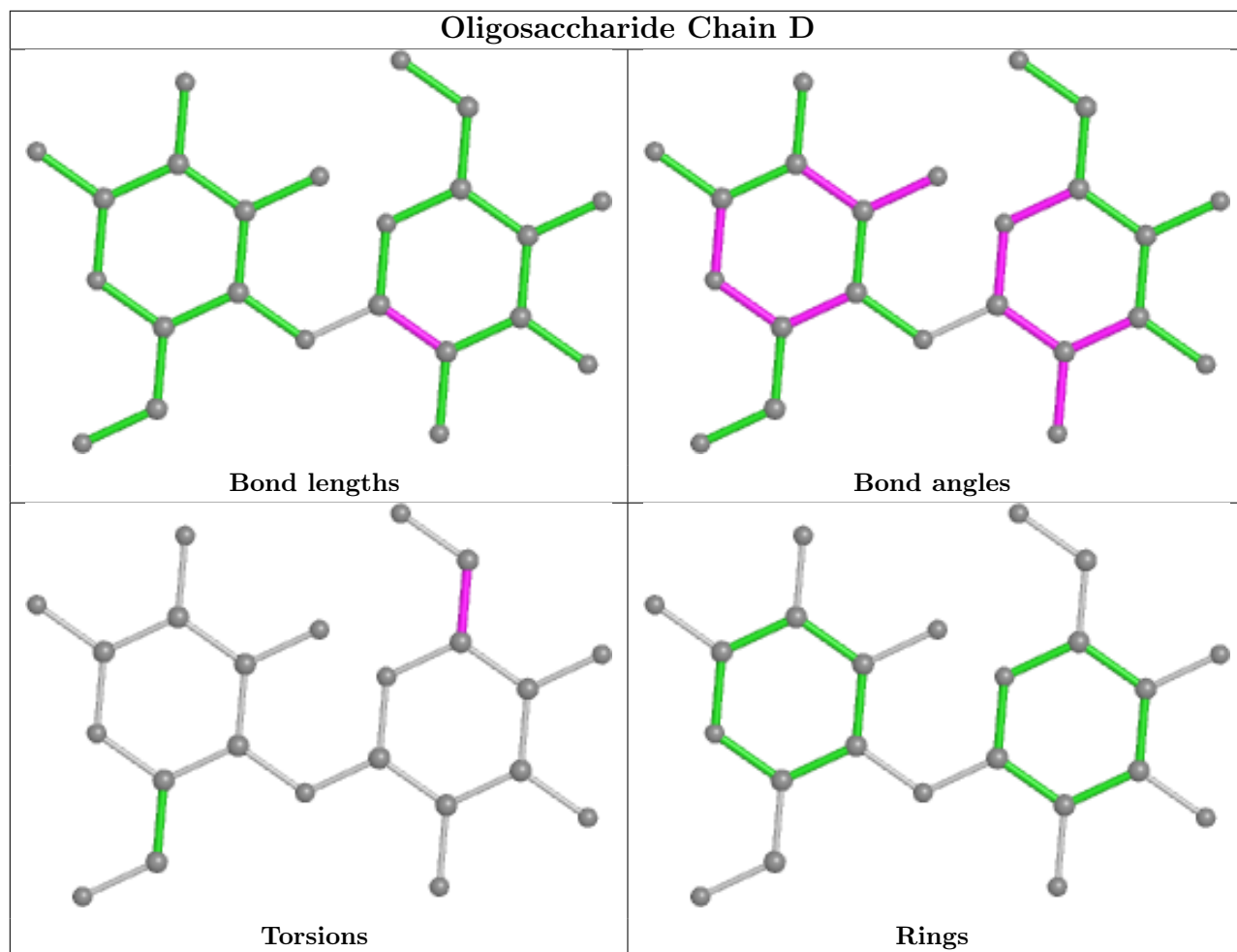
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

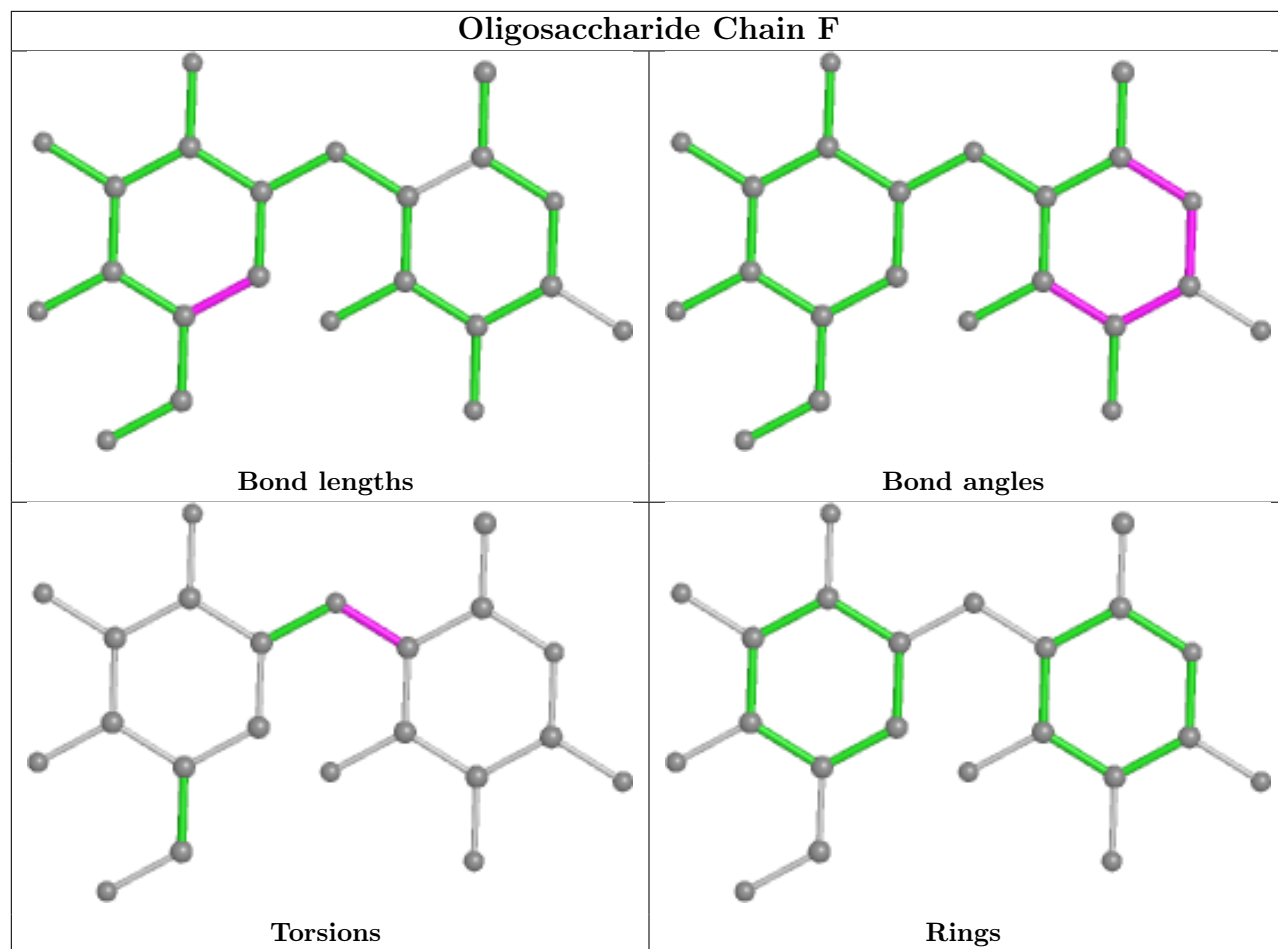


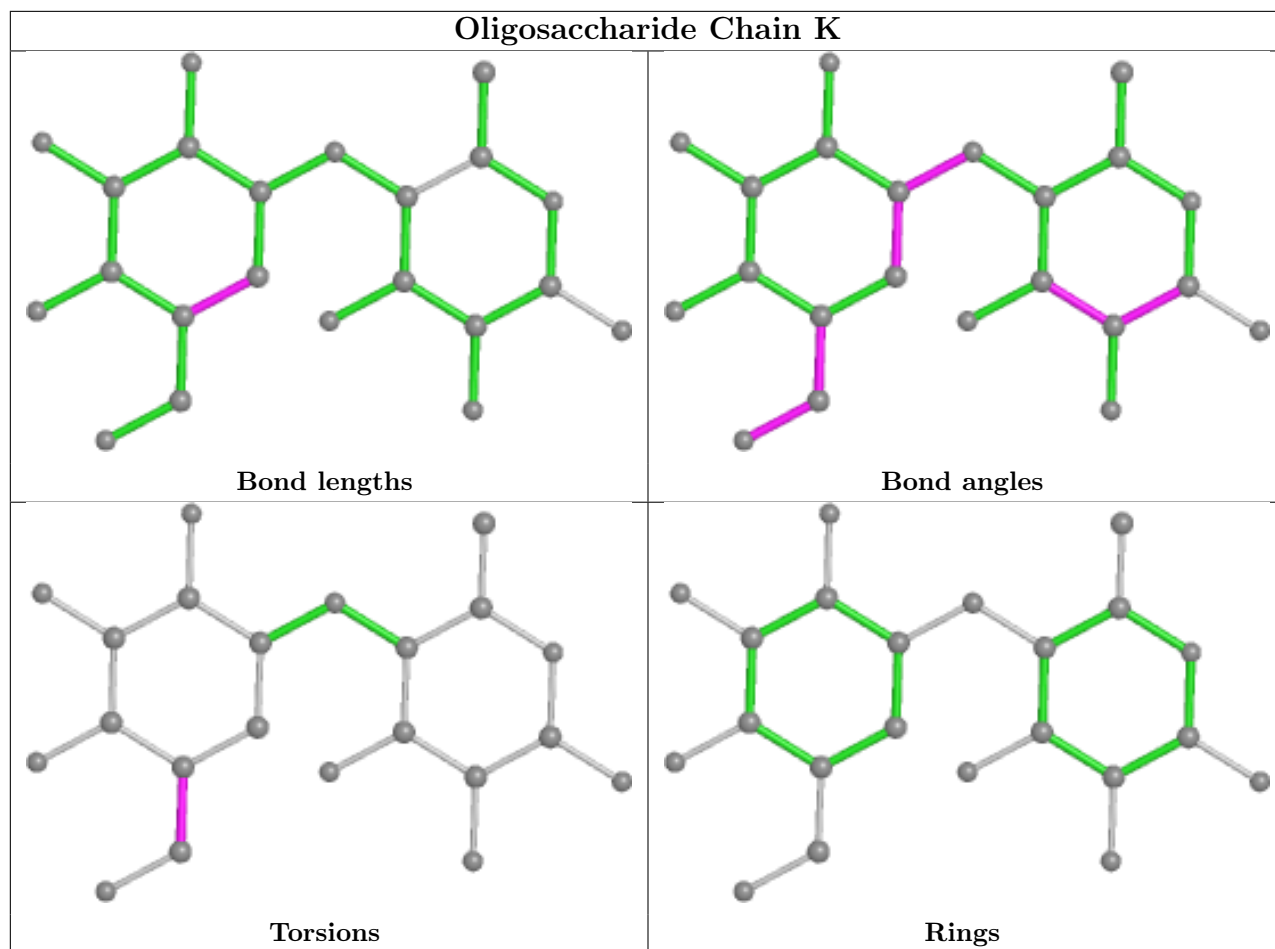












5.6 Ligand geometry [i](#)

Of 47 ligands modelled in this entry, 20 are monoatomic - leaving 27 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
8	SO4	B	1710	-	4,4,4	0.51	0	6,6,6	0.72	0
8	SO4	B	1707	-	4,4,4	0.38	0	6,6,6	0.81	0
8	SO4	A	1702	-	4,4,4	0.34	0	6,6,6	0.40	0
9	MES	B	1708	-	12,12,12	2.16	1 (8%)	14,16,16	1.13	1 (7%)
8	SO4	B	1706	-	4,4,4	0.40	0	6,6,6	0.40	0
9	MES	B	1709	-	12,12,12	2.20	1 (8%)	14,16,16	1.66	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	SO4	B	1702	-	4,4,4	0.50	0	6,6,6	0.52	0
10	EDO	B	1804	-	3,3,3	0.44	0	2,2,2	0.38	0
10	EDO	B	1803	-	3,3,3	0.20	0	2,2,2	0.71	0
8	SO4	A	1704	-	4,4,4	0.43	0	6,6,6	0.50	0
9	MES	A	1705	-	12,12,12	1.75	1 (8%)	14,16,16	2.64	5 (35%)
10	EDO	B	1802	-	3,3,3	0.43	0	2,2,2	0.71	0
8	SO4	A	1701	-	4,4,4	0.51	0	6,6,6	0.48	0
9	MES	B	1705	-	12,12,12	1.89	1 (8%)	14,16,16	2.54	4 (28%)
8	SO4	B	1704	-	4,4,4	0.43	0	6,6,6	0.47	0
8	SO4	B	1712	-	4,4,4	0.39	0	6,6,6	0.25	0
10	EDO	A	1801	-	3,3,3	0.65	0	2,2,2	0.46	0
10	EDO	A	1803	-	3,3,3	0.40	0	2,2,2	0.79	0
9	MES	A	1707	-	12,12,12	2.26	1 (8%)	14,16,16	1.96	4 (28%)
9	MES	B	1703	-	12,12,12	2.11	1 (8%)	14,16,16	2.23	5 (35%)
10	EDO	A	1802	-	3,3,3	0.37	0	2,2,2	0.24	0
9	MES	B	1711	-	12,12,12	2.23	1 (8%)	14,16,16	1.36	3 (21%)
10	EDO	B	1801	-	3,3,3	0.65	0	2,2,2	0.44	0
10	EDO	A	1804	-	3,3,3	0.62	0	2,2,2	0.73	0
8	SO4	B	1701	-	4,4,4	0.47	0	6,6,6	0.61	0
8	SO4	A	1703	-	4,4,4	0.53	0	6,6,6	0.64	0
8	SO4	A	1706	-	4,4,4	0.44	0	6,6,6	0.27	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
10	EDO	B	1804	-	-	1/1/1/1	-
10	EDO	B	1803	-	-	1/1/1/1	-
9	MES	B	1703	-	-	5/6/14/14	0/1/1/1
10	EDO	A	1801	-	-	0/1/1/1	-
10	EDO	A	1802	-	-	0/1/1/1	-
10	EDO	A	1803	-	-	0/1/1/1	-
9	MES	B	1711	-	-	0/6/14/14	0/1/1/1
10	EDO	B	1801	-	-	0/1/1/1	-
9	MES	A	1705	-	-	3/6/14/14	0/1/1/1
10	EDO	A	1804	-	-	0/1/1/1	-
10	EDO	B	1802	-	-	0/1/1/1	-
9	MES	A	1707	-	-	0/6/14/14	0/1/1/1
9	MES	B	1708	-	-	4/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MES	B	1705	-	-	0/6/14/14	0/1/1/1
9	MES	B	1709	-	-	2/6/14/14	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1707	MES	C8-S	-7.49	1.66	1.77
9	B	1709	MES	C8-S	-7.31	1.67	1.77
9	B	1711	MES	C8-S	-7.20	1.67	1.77
9	B	1703	MES	C8-S	-6.95	1.67	1.77
9	B	1708	MES	C8-S	-6.87	1.67	1.77

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1705	MES	O2S-S-C8	7.68	116.16	106.92
9	B	1705	MES	O1S-S-C8	6.61	114.88	106.92
9	B	1703	MES	C6-O1-C2	4.52	124.99	109.89
9	A	1707	MES	O3S-S-C8	4.02	112.27	105.77
9	B	1703	MES	O2S-S-C8	3.87	111.58	106.92

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1705	MES	C7-C8-S-O1S
9	A	1705	MES	C7-C8-S-O3S
9	B	1703	MES	C7-C8-S-O1S
9	B	1703	MES	C7-C8-S-O2S
9	B	1703	MES	C7-C8-S-O3S

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1247/1263 (98%)	-0.11	19 (1%) 73 72	28, 42, 61, 101	0
1	B	1247/1263 (98%)	-0.12	12 (0%) 82 80	29, 41, 59, 103	0
All	All	2494/2526 (98%)	-0.11	31 (1%) 79 77	28, 42, 60, 103	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1152	GLY	3.9
1	B	1281	PRO	3.9
1	B	1151	SER	3.4
1	A	1237	ASN	3.2
1	B	60	SER	2.8

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
4	GLC	F	1	1/12	0.13	0.24	68,68,68,68	0
4	GLC	K	1	1/12	0.46	0.25	66,66,66,66	0
2	AC1	I	3	10/22	0.59	0.35	88,101,112,116	0
3	GLC	D	2	11/12	0.75	0.27	65,79,85,86	0
2	GLC	J	1	1/12	0.80	0.29	77,77,77,77	0

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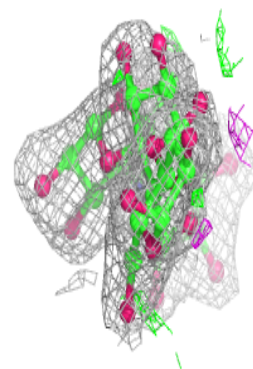
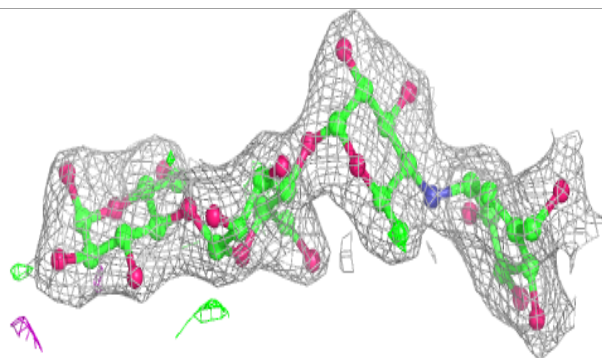
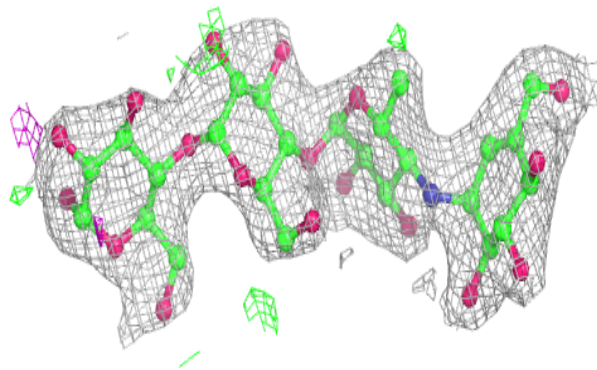
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GLC	I	1	12/12	0.82	0.42	75,83,86,87	0
2	GLC	G	2	11/12	0.82	0.21	69,82,89,93	0
3	GLC	D	1	12/12	0.85	0.43	72,86,92,92	0
2	GLC	E	1	1/12	0.85	0.18	71,71,71,71	0
2	GLC	J	2	11/12	0.85	0.45	72,89,98,101	0
2	GLC	L	2	11/12	0.85	0.18	71,86,95,98	0
2	GLC	I	2	11/12	0.86	0.30	70,80,87,87	0
2	GLC	E	2	11/12	0.87	0.39	65,81,88,89	0
2	AC1	E	3	21/22	0.88	0.25	46,57,68,73	0
2	GLC	H	1	12/12	0.88	0.21	61,68,71,72	0
2	GLC	G	1	1/12	0.89	0.68	106,106,106,106	0
2	GLC	L	1	1/12	0.91	0.35	104,104,104,104	0
4	AC1	F	2	21/22	0.91	0.23	49,61,77,82	0
2	AC1	G	3	21/22	0.91	0.19	46,62,74,78	0
2	AC1	L	3	21/22	0.92	0.17	48,61,73,74	0
2	GLC	C	2	11/12	0.92	0.13	51,61,70,70	0
4	AC1	K	2	21/22	0.93	0.16	44,58,70,71	0
2	AC1	C	3	21/22	0.94	0.16	40,42,45,46	0
2	GLC	C	1	12/12	0.94	0.16	52,60,65,66	0
2	AC1	J	3	21/22	0.94	0.27	40,50,61,63	0
2	GLC	H	2	11/12	0.94	0.12	49,60,67,72	0
2	AC1	H	3	21/22	0.96	0.12	38,43,51,52	0

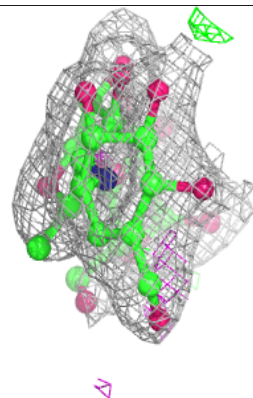
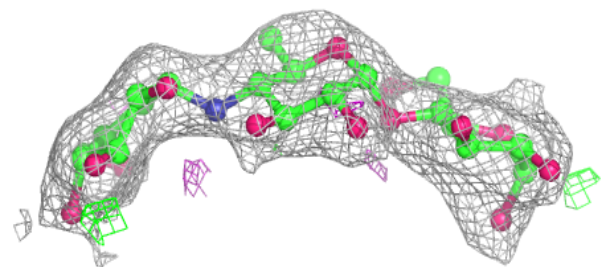
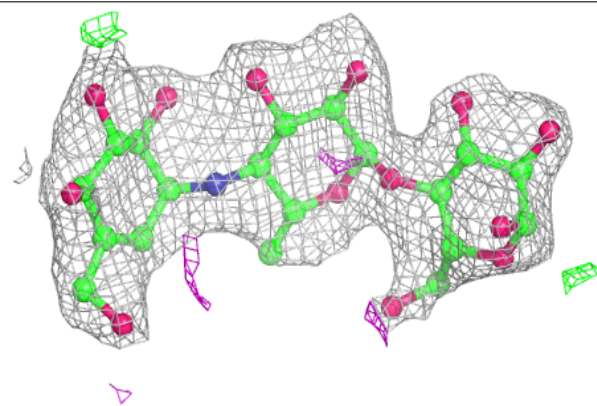
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

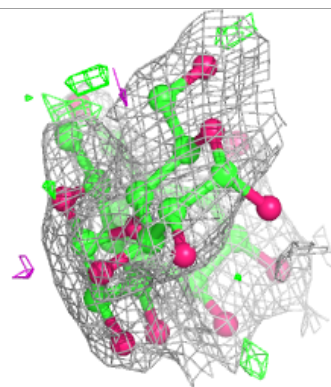
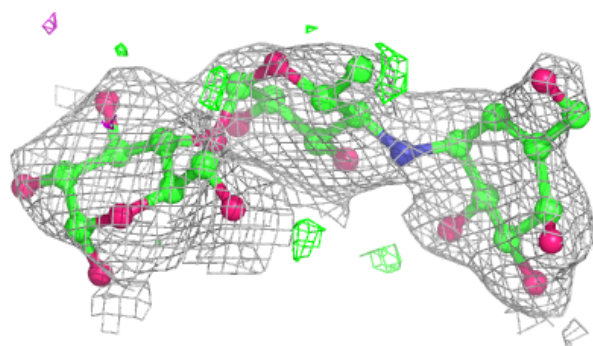
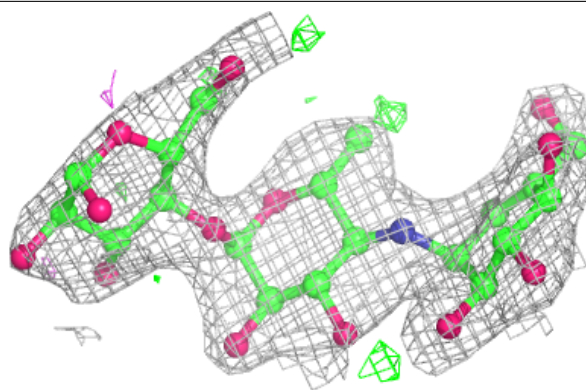
**Electron density around Chain E:**

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

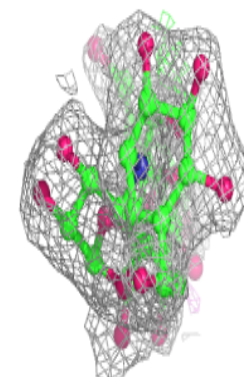
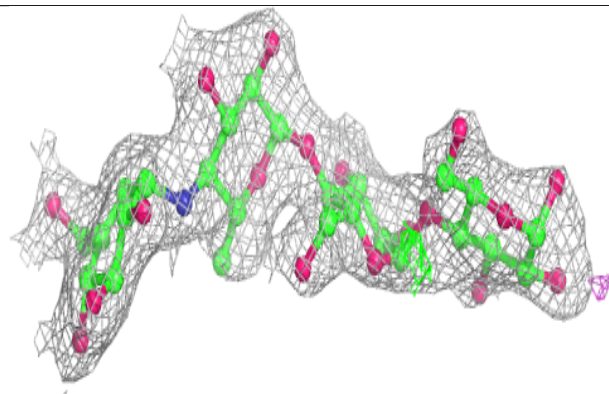
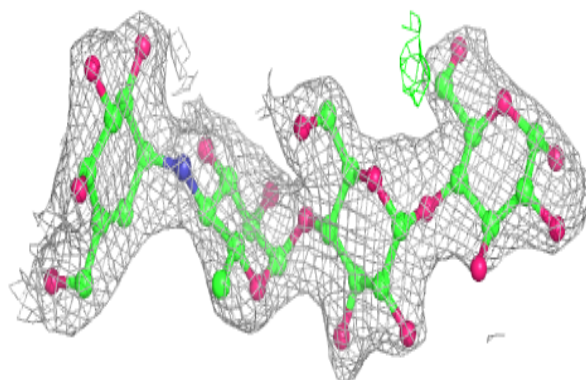


Electron density around Chain G:

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

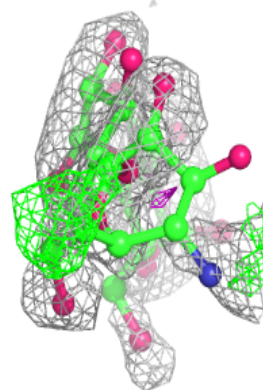
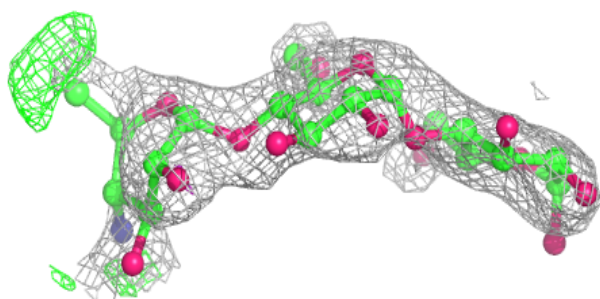
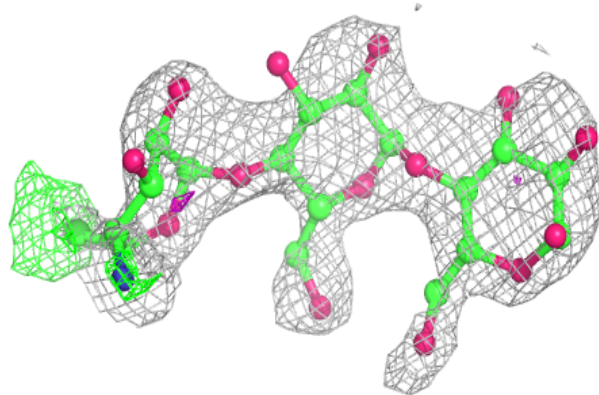
**Electron density around Chain H:**

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

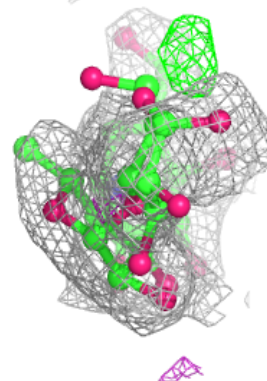
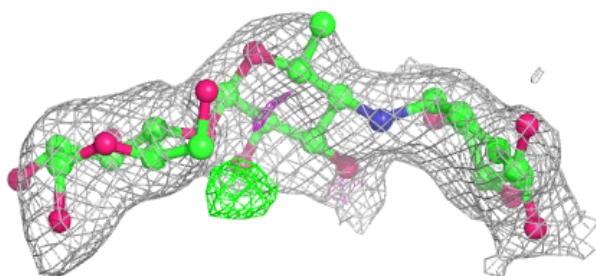
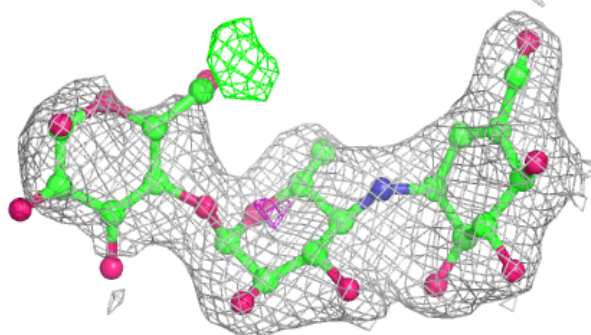


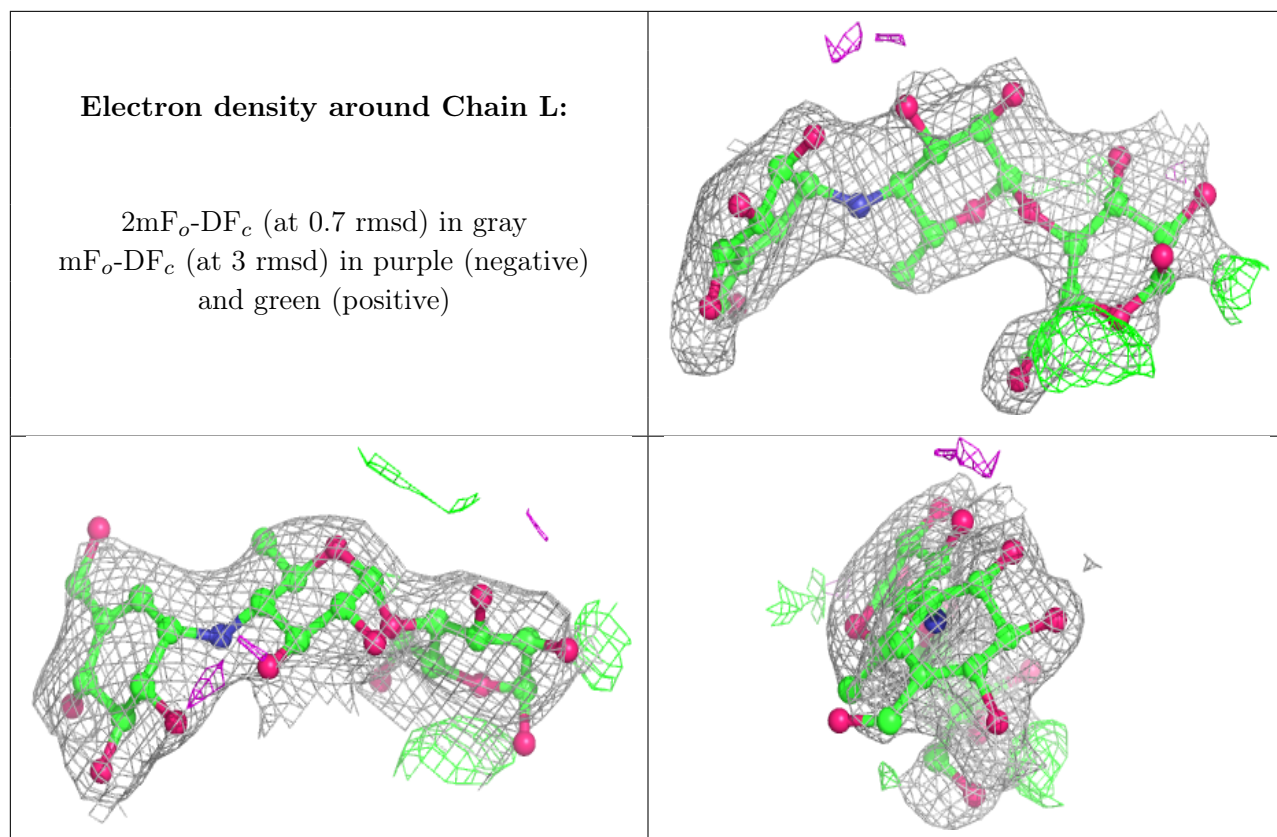
Electron density around Chain I:

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

**Electron density around Chain J:**

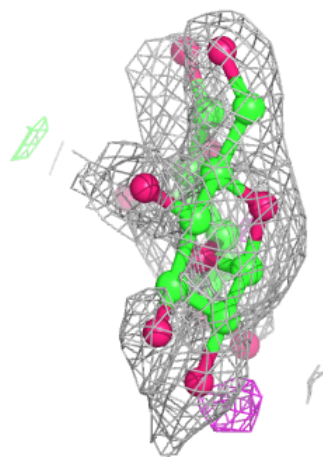
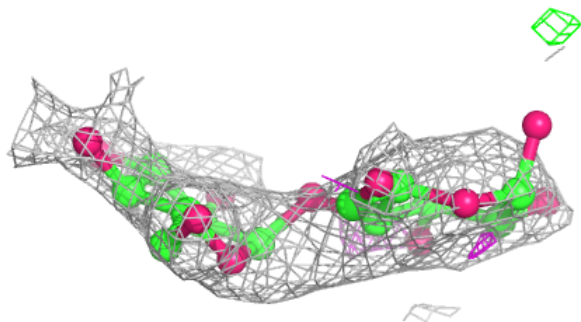
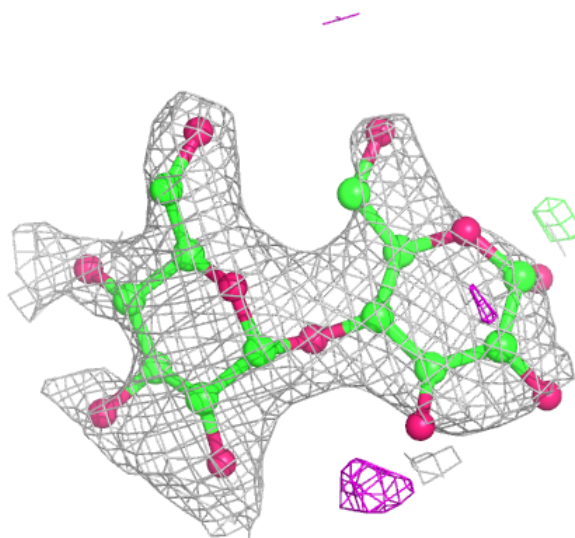
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





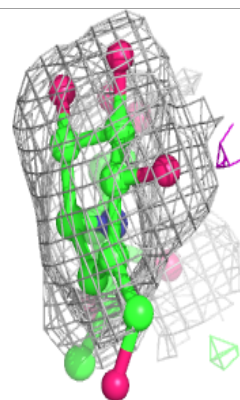
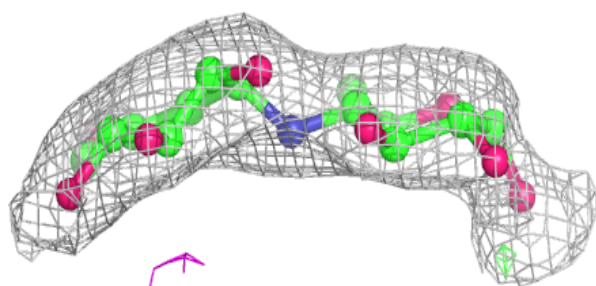
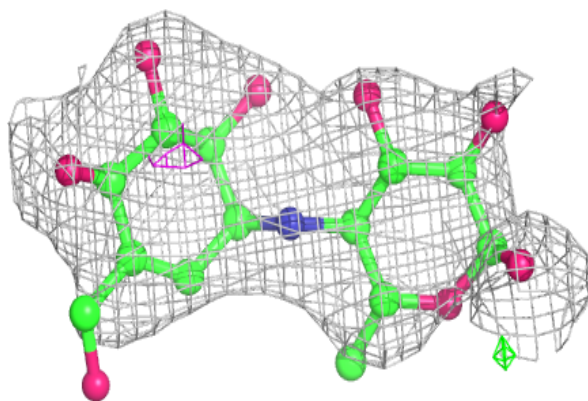
Electron density around Chain D:

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

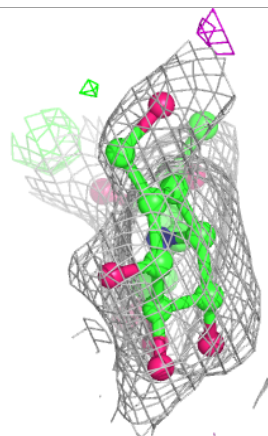
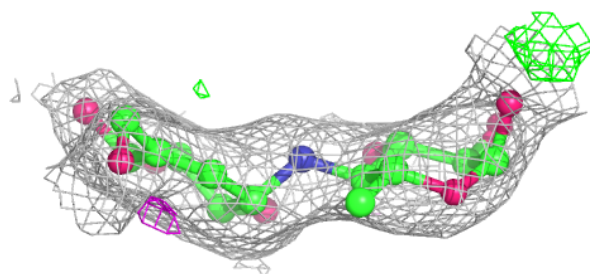
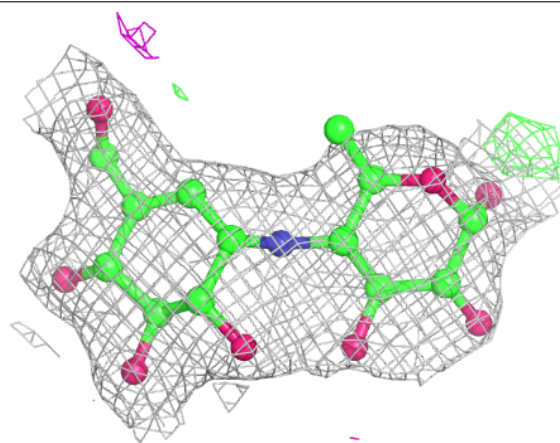


Electron density around Chain F:

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

**Electron density around Chain K:**

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



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MG	B	1605	1/1	0.83	0.15	71,71,71,71	0
9	MES	B	1703	12/12	0.85	0.34	71,79,96,96	0
9	MES	A	1705	12/12	0.88	0.24	61,83,88,90	0
8	SO4	B	1710	5/5	0.88	0.19	72,73,78,87	0
9	MES	B	1708	12/12	0.88	0.27	80,92,97,99	0
10	EDO	B	1803	4/4	0.89	0.24	52,59,61,67	0
7	MG	A	1602	1/1	0.90	0.05	61,61,61,61	0
9	MES	B	1709	12/12	0.91	0.21	78,85,89,94	0
10	EDO	A	1803	4/4	0.91	0.20	51,52,57,59	0
9	MES	B	1705	12/12	0.91	0.18	64,77,81,82	0
10	EDO	A	1804	4/4	0.92	0.20	40,47,47,52	0
8	SO4	A	1704	5/5	0.93	0.38	62,70,79,85	0
8	SO4	B	1706	5/5	0.93	0.26	75,77,84,87	0
7	MG	B	1603	1/1	0.93	0.06	57,57,57,57	0
10	EDO	B	1802	4/4	0.93	0.18	44,48,49,52	0
8	SO4	B	1712	5/5	0.93	0.34	73,74,80,83	0
8	SO4	A	1703	5/5	0.94	0.15	59,66,83,85	0
8	SO4	B	1702	5/5	0.94	0.25	60,61,69,69	0
10	EDO	B	1804	4/4	0.94	0.19	38,39,41,42	0
7	MG	A	1605	1/1	0.95	0.17	71,71,71,71	0
7	MG	A	1606	1/1	0.95	0.08	49,49,49,49	0
8	SO4	B	1704	5/5	0.95	0.13	70,72,80,81	0
10	EDO	A	1802	4/4	0.95	0.20	48,48,48,51	0
7	MG	B	1602	1/1	0.95	0.11	61,61,61,61	0
5	CA	A	1303	1/1	0.95	0.17	50,50,50,50	0
10	EDO	B	1801	4/4	0.95	0.18	38,38,40,41	0
7	MG	A	1603	1/1	0.95	0.05	61,61,61,61	0
8	SO4	A	1702	5/5	0.95	0.20	58,64,68,73	0
7	MG	A	1604	1/1	0.95	0.10	62,62,62,62	0
8	SO4	B	1701	5/5	0.96	0.24	53,58,67,71	0
8	SO4	A	1701	5/5	0.96	0.19	54,58,69,70	0
8	SO4	B	1707	5/5	0.97	0.12	51,54,58,63	0
7	MG	B	1604	1/1	0.97	0.14	51,51,51,51	0
5	CA	B	1302	1/1	0.97	0.07	59,59,59,59	0
6	NI	B	1501	1/1	0.98	0.03	63,63,63,63	0
9	MES	B	1711	12/12	0.98	0.10	42,44,48,50	0
10	EDO	A	1801	4/4	0.98	0.15	43,44,45,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	MG	A	1601	1/1	0.98	0.10	35,35,35,35	0
5	CA	A	1301	1/1	0.98	0.04	47,47,47,47	0
5	CA	A	1302	1/1	0.98	0.10	52,52,52,52	0
9	MES	A	1707	12/12	0.98	0.11	37,46,48,48	0
5	CA	B	1303	1/1	0.98	0.08	44,44,44,44	0
7	MG	B	1606	1/1	0.98	0.08	44,44,44,44	0
6	NI	A	1501	1/1	0.98	0.03	63,63,63,63	0
5	CA	B	1301	1/1	0.99	0.06	39,39,39,39	0
8	SO4	A	1706	5/5	0.99	0.12	50,51,55,56	0
7	MG	B	1601	1/1	0.99	0.08	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.