



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 17, 2025 – 01:19 pm BST

PDB ID : 9FNH / pdb_00009fnh
Title : The glycoside hydrolase family 71 (GH71) member AnGH71C from *Aspergillus nidulans* in complex with nigerotetraose.
Authors : Mazurkewich, S.; Widen, T.; Branden, G.; Larsbrink, J.
Deposited on : 2024-06-10
Resolution : 1.92 Å(reported)

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

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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 Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

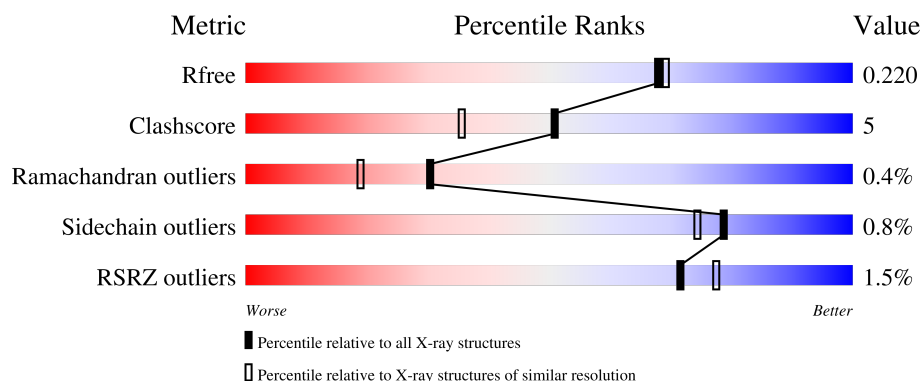
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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}	164625	1028 (1.92-1.92)
Clashscore	180529	1100 (1.92-1.92)
Ramachandran outliers	177936	1087 (1.92-1.92)
Sidechain outliers	177891	1087 (1.92-1.92)
RSRZ outliers	164620	1028 (1.92-1.92)

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	430	<div> <div></div> <div>79%13%8%</div> </div>
1	B	430	<div> <div></div> <div>81%10%8%</div> </div>
1	C	430	<div> <div></div> <div>79%13%8%</div> </div>
1	D	430	<div> <div></div> <div>79%13%7%</div> </div>
1	X	430	<div> <div></div> <div>97%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	4	 75% 25%
2	F	4	 100%
3	G	3	 33% 33% 33%
3	I	3	 33% 67%
3	J	3	 67% 33%
3	K	3	 67% 33%
4	H	4	 75% 25%
5	M	2	 50% 50%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13751 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 71.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	4	0
			3181	2035	512	621	13			
1	B	397	Total	C	N	O	S	0	0	0
			3147	2016	506	613	12			
1	C	397	Total	C	N	O	S	0	0	0
			3147	2016	506	613	12			
1	D	399	Total	C	N	O	S	0	1	0
			3173	2031	510	620	12			
1	X	12	Total	C	N	O		0	0	0
			92	60	16	16				

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MET	-	initiating methionine	UNP G5EB58
A	3	GLY	-	expression tag	UNP G5EB58
A	4	SER	-	expression tag	UNP G5EB58
A	5	SER	-	expression tag	UNP G5EB58
A	6	HIS	-	expression tag	UNP G5EB58
A	7	HIS	-	expression tag	UNP G5EB58
A	8	HIS	-	expression tag	UNP G5EB58
A	9	HIS	-	expression tag	UNP G5EB58
A	10	HIS	-	expression tag	UNP G5EB58
A	11	HIS	-	expression tag	UNP G5EB58
A	12	SER	-	expression tag	UNP G5EB58
A	13	SER	-	expression tag	UNP G5EB58
A	14	GLU	-	expression tag	UNP G5EB58
A	15	ASN	-	expression tag	UNP G5EB58
A	16	LEU	-	expression tag	UNP G5EB58
A	17	TYR	-	expression tag	UNP G5EB58
A	18	PHE	-	expression tag	UNP G5EB58
A	19	GLN	-	expression tag	UNP G5EB58
A	20	GLY	-	expression tag	UNP G5EB58

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Chain	Residue	Modelled	Actual	Comment	Reference
A	21	HIS	-	expression tag	UNP G5EB58
B	2	MET	-	initiating methionine	UNP G5EB58
B	3	GLY	-	expression tag	UNP G5EB58
B	4	SER	-	expression tag	UNP G5EB58
B	5	SER	-	expression tag	UNP G5EB58
B	6	HIS	-	expression tag	UNP G5EB58
B	7	HIS	-	expression tag	UNP G5EB58
B	8	HIS	-	expression tag	UNP G5EB58
B	9	HIS	-	expression tag	UNP G5EB58
B	10	HIS	-	expression tag	UNP G5EB58
B	11	HIS	-	expression tag	UNP G5EB58
B	12	SER	-	expression tag	UNP G5EB58
B	13	SER	-	expression tag	UNP G5EB58
B	14	GLU	-	expression tag	UNP G5EB58
B	15	ASN	-	expression tag	UNP G5EB58
B	16	LEU	-	expression tag	UNP G5EB58
B	17	TYR	-	expression tag	UNP G5EB58
B	18	PHE	-	expression tag	UNP G5EB58
B	19	GLN	-	expression tag	UNP G5EB58
B	20	GLY	-	expression tag	UNP G5EB58
B	21	HIS	-	expression tag	UNP G5EB58
C	2	MET	-	initiating methionine	UNP G5EB58
C	3	GLY	-	expression tag	UNP G5EB58
C	4	SER	-	expression tag	UNP G5EB58
C	5	SER	-	expression tag	UNP G5EB58
C	6	HIS	-	expression tag	UNP G5EB58
C	7	HIS	-	expression tag	UNP G5EB58
C	8	HIS	-	expression tag	UNP G5EB58
C	9	HIS	-	expression tag	UNP G5EB58
C	10	HIS	-	expression tag	UNP G5EB58
C	11	HIS	-	expression tag	UNP G5EB58
C	12	SER	-	expression tag	UNP G5EB58
C	13	SER	-	expression tag	UNP G5EB58
C	14	GLU	-	expression tag	UNP G5EB58
C	15	ASN	-	expression tag	UNP G5EB58
C	16	LEU	-	expression tag	UNP G5EB58
C	17	TYR	-	expression tag	UNP G5EB58
C	18	PHE	-	expression tag	UNP G5EB58
C	19	GLN	-	expression tag	UNP G5EB58
C	20	GLY	-	expression tag	UNP G5EB58
C	21	HIS	-	expression tag	UNP G5EB58
D	2	MET	-	initiating methionine	UNP G5EB58

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Chain	Residue	Modelled	Actual	Comment	Reference
D	3	GLY	-	expression tag	UNP G5EB58
D	4	SER	-	expression tag	UNP G5EB58
D	5	SER	-	expression tag	UNP G5EB58
D	6	HIS	-	expression tag	UNP G5EB58
D	7	HIS	-	expression tag	UNP G5EB58
D	8	HIS	-	expression tag	UNP G5EB58
D	9	HIS	-	expression tag	UNP G5EB58
D	10	HIS	-	expression tag	UNP G5EB58
D	11	HIS	-	expression tag	UNP G5EB58
D	12	SER	-	expression tag	UNP G5EB58
D	13	SER	-	expression tag	UNP G5EB58
D	14	GLU	-	expression tag	UNP G5EB58
D	15	ASN	-	expression tag	UNP G5EB58
D	16	LEU	-	expression tag	UNP G5EB58
D	17	TYR	-	expression tag	UNP G5EB58
D	18	PHE	-	expression tag	UNP G5EB58
D	19	GLN	-	expression tag	UNP G5EB58
D	20	GLY	-	expression tag	UNP G5EB58
D	21	HIS	-	expression tag	UNP G5EB58
X	-8	MET	-	initiating methionine	UNP G5EB58
X	-7	GLY	-	expression tag	UNP G5EB58
X	-6	SER	-	expression tag	UNP G5EB58
X	-5	SER	-	expression tag	UNP G5EB58
X	-4	HIS	-	expression tag	UNP G5EB58
X	-3	HIS	-	expression tag	UNP G5EB58
X	-2	HIS	-	expression tag	UNP G5EB58
X	-1	HIS	-	expression tag	UNP G5EB58
X	0	HIS	-	expression tag	UNP G5EB58
X	1	HIS	-	expression tag	UNP G5EB58
X	2	SER	-	expression tag	UNP G5EB58
X	3	SER	-	expression tag	UNP G5EB58
X	4	GLU	-	expression tag	UNP G5EB58
X	5	ASN	-	expression tag	UNP G5EB58
X	6	LEU	-	expression tag	UNP G5EB58
X	7	TYR	-	expression tag	UNP G5EB58
X	8	PHE	-	expression tag	UNP G5EB58
X	9	GLN	-	expression tag	UNP G5EB58
X	10	GLY	-	expression tag	UNP G5EB58
X	11	HIS	-	expression tag	UNP G5EB58

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose.



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

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



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

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



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

- Molecule 5 is an oligosaccharide called alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose.

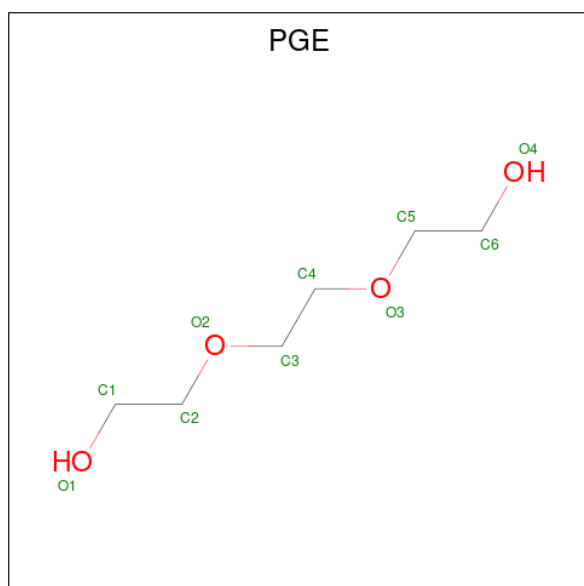


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	M	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

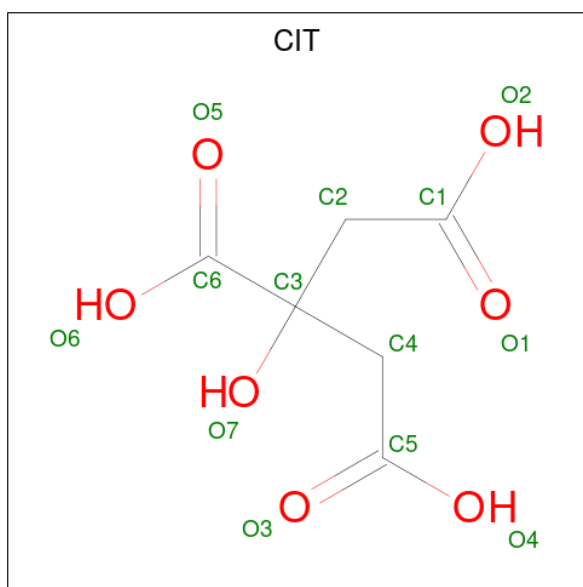
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Na	0	0
			1	1		
6	D	1	Total	Na	0	0
			1	1		

- Molecule 7 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



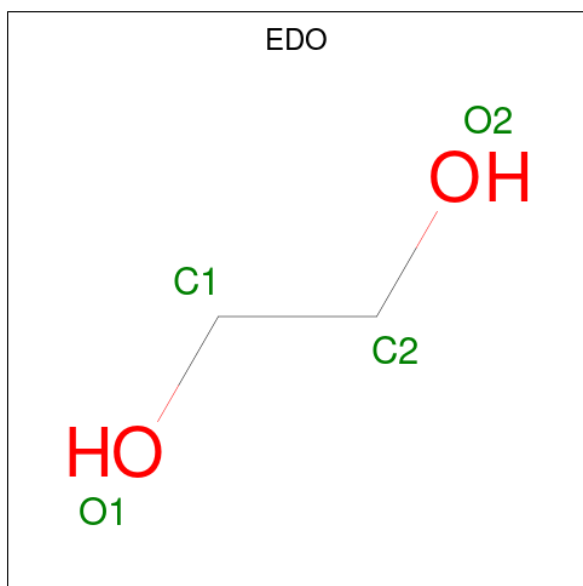
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			13	6	7		

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

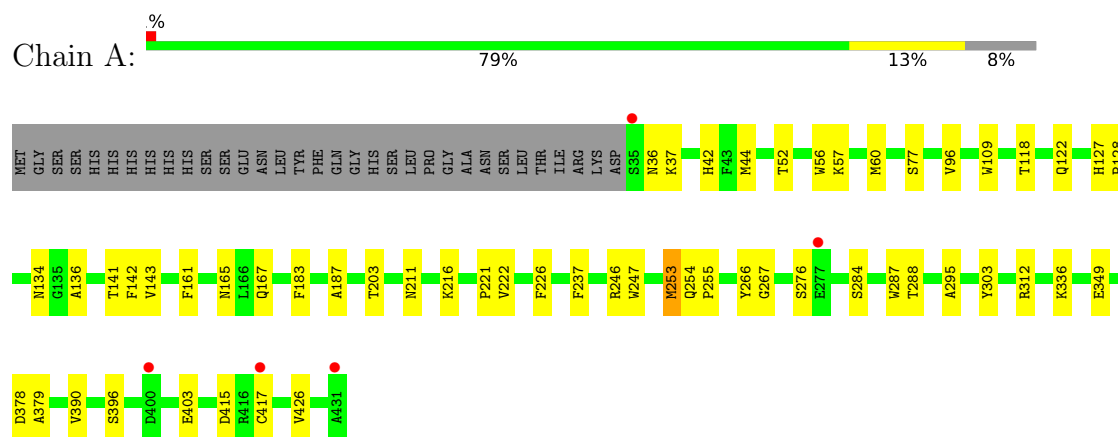
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	160	Total 160	O 160	0	0
10	B	154	Total 154	O 154	0	0
10	C	181	Total 181	O 181	0	0
10	D	184	Total 184	O 184	0	0
10	X	9	Total 9	O 9	0	0

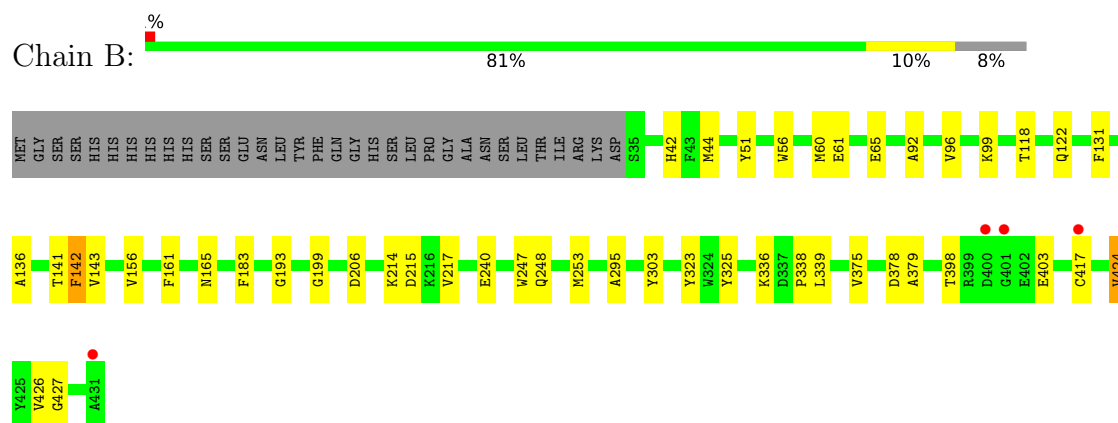
3 Residue-property plots [i](#)

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.

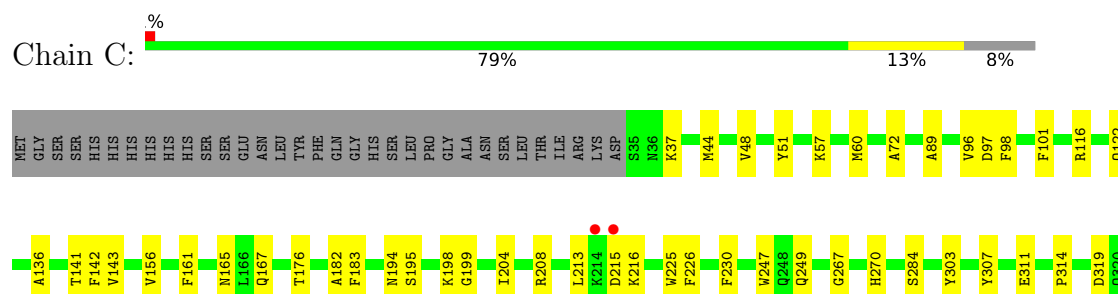
• Molecule 1: Glycoside hydrolase family 71

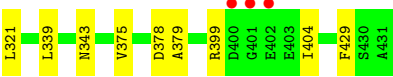


• Molecule 1: Glycoside hydrolase family 71

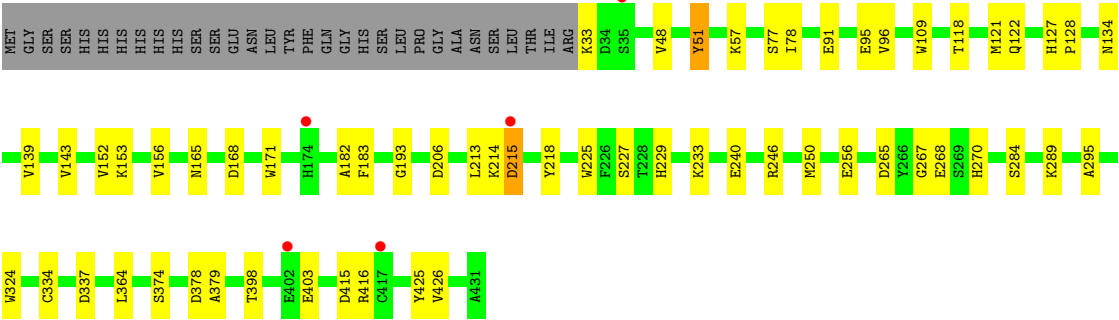
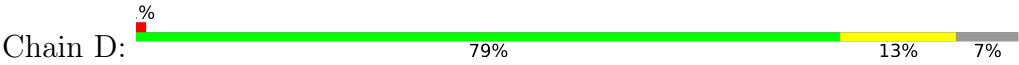


• Molecule 1: Glycoside hydrolase family 71

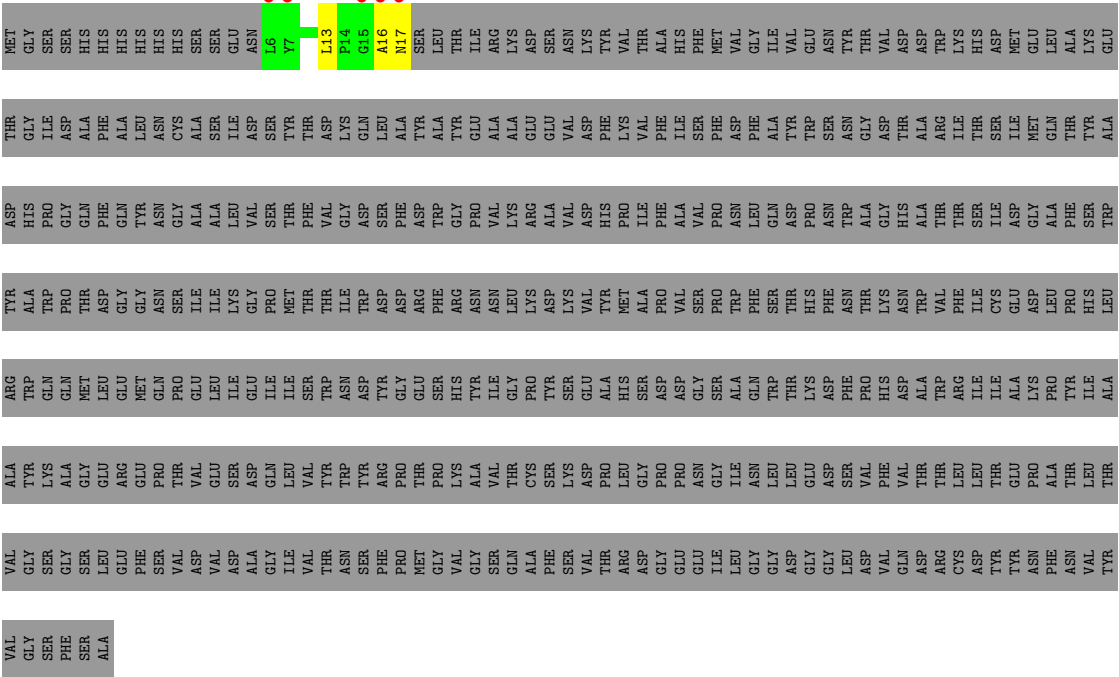




● Molecule 1: Glycoside hydrolase family 71



● Molecule 1: Glycoside hydrolase family 71



● Molecule 2: alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose




- Molecule 2: alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose

Chain F:  100%

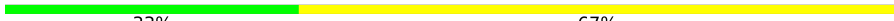
GLC1
GLC2
GLC3
GLC4

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

Chain G:  33% 33% 33%

GLC1
GLC2
GLC3

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

Chain I:  33% 67%

GLC1
GLC2
GLC3

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

Chain J:  67% 33%


GLC1
GLC2
GLC3

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

Chain K:  67% 33%

GLC1
GLC2
GLC3

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

Chain H:  75% 25%

BGC1
GLC2
GLC3
GLC4

- Molecule 5: alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose

Chain M:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	80.27Å 82.24Å 87.07Å 103.52° 105.64° 117.59°	Depositor
Resolution (Å)	41.70 – 1.92 41.70 – 1.92	Depositor EDS
% Data completeness (in resolution range)	62.5 (41.70-1.92) 62.9 (41.70-1.92)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 1.92Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.165 , 0.220 0.165 , 0.220	Depositor DCC
R_{free} test set	121725 reflections (7.55%)	wwPDB-VP
Wilson B-factor (Å ²)	24.7	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.038 for k,h,-h-k-l 0.000 for -k,-h,-l 0.000 for -h,-k,h+k+l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13751	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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: PGE, BGC, NA, CIT, EDO, 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	0.39	0/3282	0.64	2/4485 (0.0%)
1	B	0.38	0/3248	0.64	2/4439 (0.0%)
1	C	0.38	0/3248	0.65	2/4439 (0.0%)
1	D	0.40	0/3274	0.60	1/4473 (0.0%)
1	X	0.67	0/95	0.95	0/128
All	All	0.39	0/13147	0.63	7/17964 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	141	THR	CB-CA-C	-7.08	97.30	111.17
1	B	141	THR	CB-CA-C	-6.89	97.67	111.17
1	A	141	THR	CB-CA-C	-6.80	97.84	111.17
1	D	334	CYS	CA-CB-SG	5.92	128.03	114.40
1	A	142	PHE	N-CA-C	-5.78	99.82	109.24

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	3181	0	2940	34	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3147	0	2913	28	0
1	C	3147	0	2913	35	1
1	D	3173	0	2935	33	0
1	X	92	0	83	3	0
2	E	45	0	39	1	0
2	F	45	0	39	0	0
3	G	34	0	30	2	0
3	I	34	0	30	0	0
3	J	34	0	30	1	0
3	K	34	0	30	1	0
4	H	45	0	39	3	0
5	M	23	0	21	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	B	10	0	14	1	0
8	C	13	0	5	0	0
9	D	4	0	6	0	0
10	A	160	0	0	5	0
10	B	154	0	0	2	0
10	C	181	0	0	6	0
10	D	184	0	0	2	0
10	X	9	0	0	0	0
All	All	13751	0	12067	129	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 5.

The worst 5 of 129 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:THR:HB	1:X:17:ASN:HB3	1.70	0.74
1:A:211:ASN:ND2	10:A:501:HOH:O	2.20	0.74
1:D:215:ASP:OD1	1:D:215:ASP:N	2.23	0.71
1:A:36:ASN:HD21	1:A:134:ASN:HD21	1.43	0.65
1:A:203:THR:HG21	1:A:253[B]:MET:HE3	1.79	0.64

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:349:GLU:OE1	1:C:97:ASP:OD2[1_665]	2.19	0.01

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	399/430 (93%)	384 (96%)	14 (4%)	1 (0%)	37	26
1	B	395/430 (92%)	384 (97%)	9 (2%)	2 (0%)	25	13
1	C	395/430 (92%)	379 (96%)	15 (4%)	1 (0%)	37	26
1	D	398/430 (93%)	383 (96%)	12 (3%)	3 (1%)	16	6
1	X	10/430 (2%)	7 (70%)	3 (30%)	0	100	100
All	All	1597/2150 (74%)	1537 (96%)	53 (3%)	7 (0%)	30	19

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	VAL
1	B	143	VAL
1	C	143	VAL
1	D	143	VAL
1	B	240	GLU

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	339/364 (93%)	336 (99%)	3 (1%)	75	70
1	B	335/364 (92%)	330 (98%)	5 (2%)	60	49
1	C	335/364 (92%)	334 (100%)	1 (0%)	91	90
1	D	338/364 (93%)	335 (99%)	3 (1%)	75	70
1	X	9/364 (2%)	9 (100%)	0	100	100
All	All	1356/1820 (74%)	1344 (99%)	12 (1%)	79	70

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	424	VAL
1	C	375	VAL
1	D	215	ASP
1	D	51	TYR
1	B	51	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	414	GLN
1	D	248	GLN
1	B	231	ASN
1	D	212	ASN
1	B	211	ASN

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 ⓘ

26 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	E	1	2	12,12,12	0.54	0	17,17,17	1.65	5 (29%)
2	GLC	E	2	2	11,11,12	0.30	0	15,15,17	1.18	2 (13%)
2	GLC	E	3	2	11,11,12	0.47	0	15,15,17	1.21	2 (13%)
2	GLC	E	4	2	11,11,12	0.49	0	15,15,17	1.27	1 (6%)
2	GLC	F	1	2	12,12,12	0.64	0	17,17,17	1.60	6 (35%)
2	GLC	F	2	2	11,11,12	0.52	0	15,15,17	1.32	2 (13%)
2	GLC	F	3	2	11,11,12	0.45	0	15,15,17	1.44	2 (13%)
2	GLC	F	4	2	11,11,12	0.46	0	15,15,17	1.43	3 (20%)
3	GLC	G	1	3	12,12,12	0.57	0	17,17,17	2.05	6 (35%)
3	GLC	G	2	3	11,11,12	0.29	0	15,15,17	0.72	0
3	GLC	G	3	3	11,11,12	0.30	0	15,15,17	0.89	1 (6%)
4	BGC	H	1	4	12,12,12	0.90	1 (8%)	17,17,17	2.20	5 (29%)
4	GLC	H	2	4	11,11,12	0.29	0	15,15,17	1.14	1 (6%)
4	GLC	H	3	4	11,11,12	0.47	0	15,15,17	1.50	3 (20%)
4	GLC	H	4	4	11,11,12	0.35	0	15,15,17	1.26	1 (6%)
3	GLC	I	1	3	12,12,12	0.74	0	17,17,17	0.71	0
3	GLC	I	2	3	11,11,12	0.53	0	15,15,17	1.44	2 (13%)
3	GLC	I	3	3	11,11,12	0.32	0	15,15,17	1.75	3 (20%)
3	GLC	J	1	3	12,12,12	0.44	0	17,17,17	1.70	5 (29%)
3	GLC	J	2	3	11,11,12	0.52	0	15,15,17	1.39	3 (20%)
3	GLC	J	3	3	11,11,12	0.33	0	15,15,17	1.34	3 (20%)
3	GLC	K	1	3	12,12,12	0.53	0	17,17,17	1.92	4 (23%)
3	GLC	K	2	3	11,11,12	0.29	0	15,15,17	1.40	3 (20%)
3	GLC	K	3	3	11,11,12	0.44	0	15,15,17	1.09	1 (6%)
5	GLC	M	1	5	12,12,12	0.69	0	17,17,17	0.79	0
5	GLC	M	2	5	11,11,12	0.70	0	15,15,17	2.46	7 (46%)

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	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	GLC	E	3	2	-	2/2/19/22	0/1/1/1
2	GLC	E	4	2	-	0/2/19/22	0/1/1/1
2	GLC	F	1	2	-	1/2/22/22	0/1/1/1
2	GLC	F	2	2	-	0/2/19/22	0/1/1/1
2	GLC	F	3	2	-	2/2/19/22	0/1/1/1
2	GLC	F	4	2	-	2/2/19/22	0/1/1/1
3	GLC	G	1	3	-	0/2/22/22	0/1/1/1
3	GLC	G	2	3	-	0/2/19/22	0/1/1/1
3	GLC	G	3	3	-	0/2/19/22	0/1/1/1
4	BGC	H	1	4	-	1/2/22/22	0/1/1/1
4	GLC	H	2	4	-	0/2/19/22	0/1/1/1
4	GLC	H	3	4	-	2/2/19/22	0/1/1/1
4	GLC	H	4	4	-	2/2/19/22	0/1/1/1
3	GLC	I	1	3	-	0/2/22/22	0/1/1/1
3	GLC	I	2	3	-	2/2/19/22	0/1/1/1
3	GLC	I	3	3	-	0/2/19/22	0/1/1/1
3	GLC	J	1	3	-	0/2/22/22	0/1/1/1
3	GLC	J	2	3	-	0/2/19/22	0/1/1/1
3	GLC	J	3	3	-	0/2/19/22	0/1/1/1
3	GLC	K	1	3	-	0/2/22/22	0/1/1/1
3	GLC	K	2	3	-	0/2/19/22	0/1/1/1
3	GLC	K	3	3	-	0/2/19/22	0/1/1/1
5	GLC	M	1	5	-	1/2/22/22	0/1/1/1
5	GLC	M	2	5	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	BGC	O1-C1	2.45	1.47	1.39

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	2	GLC	C1-O5-C5	5.55	119.72	112.19
4	H	1	BGC	C1-O5-C5	5.36	123.78	113.66
3	I	3	GLC	C1-O5-C5	4.80	118.70	112.19
4	H	1	BGC	O5-C5-C4	4.68	118.18	109.69
3	G	1	GLC	C1-O5-C5	4.47	122.10	113.66

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

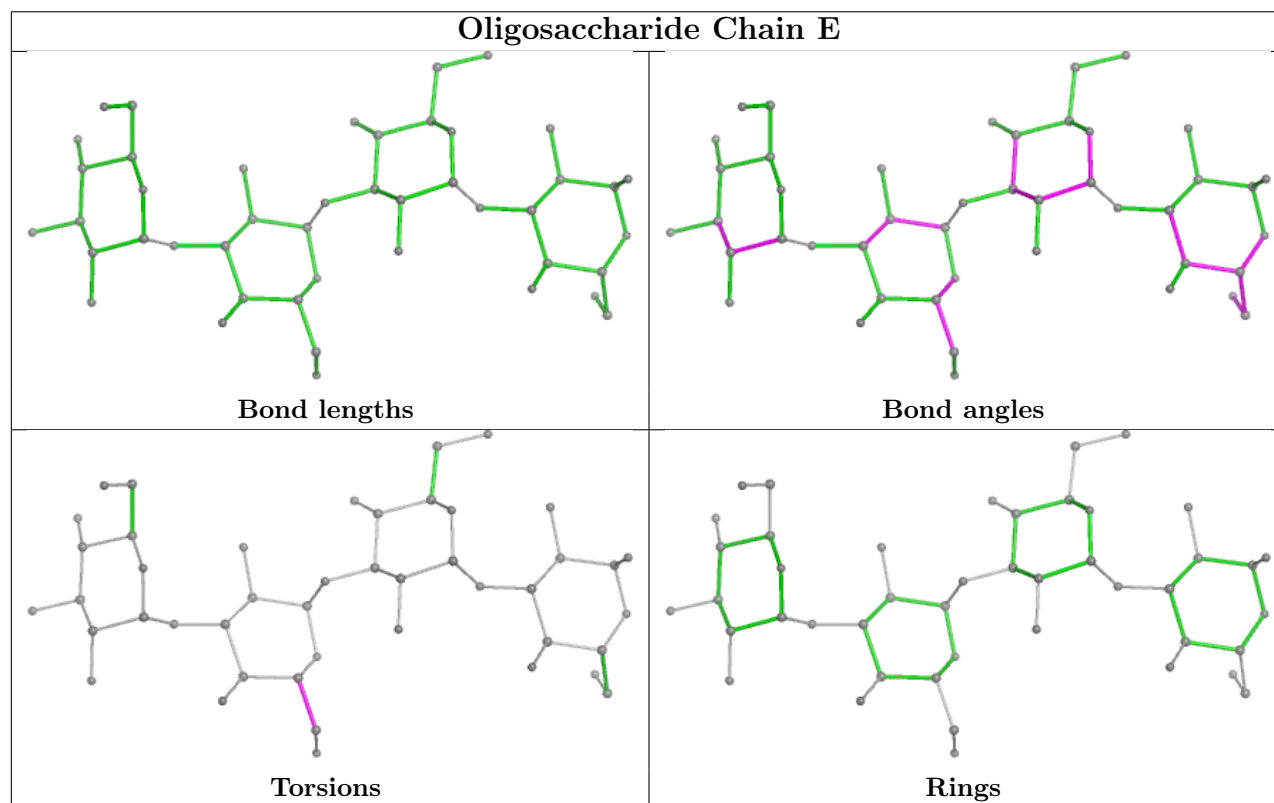
Mol	Chain	Res	Type	Atoms
2	F	4	GLC	O5-C5-C6-O6
3	I	2	GLC	C4-C5-C6-O6
3	I	2	GLC	O5-C5-C6-O6
2	F	4	GLC	C4-C5-C6-O6
5	M	2	GLC	C4-C5-C6-O6

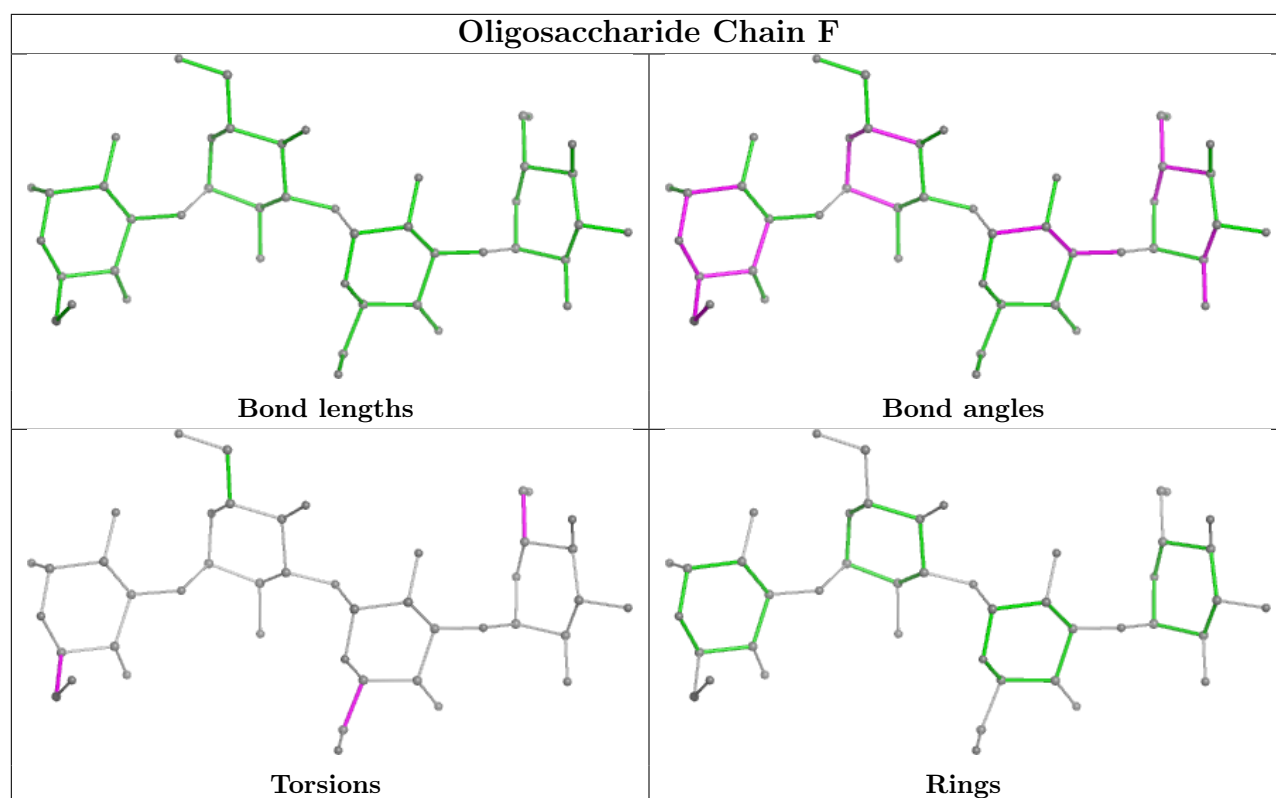
There are no ring outliers.

5 monomers are involved in 8 short contacts:

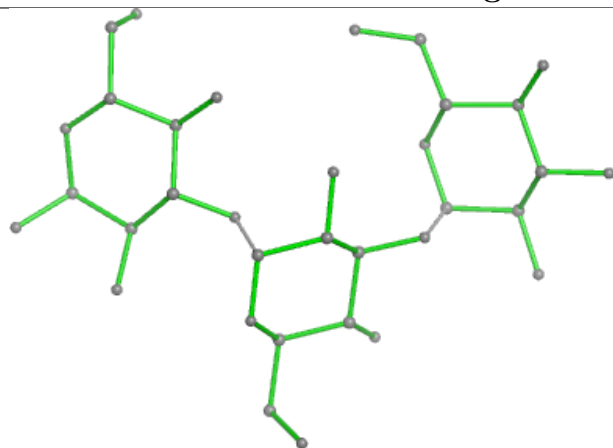
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	3	GLC	1	0
4	H	1	BGC	3	0
3	G	1	GLC	2	0
2	E	1	GLC	1	0
3	J	1	GLC	1	0

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

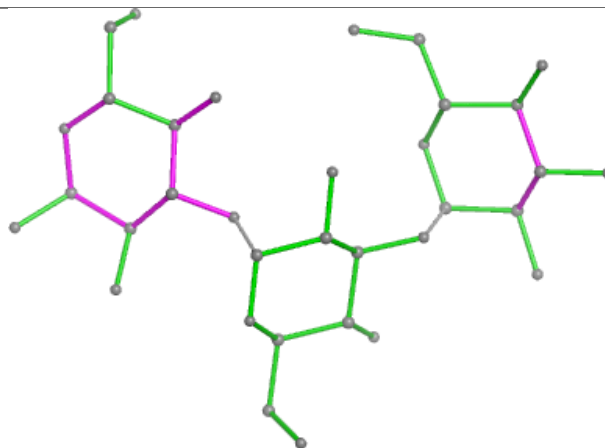




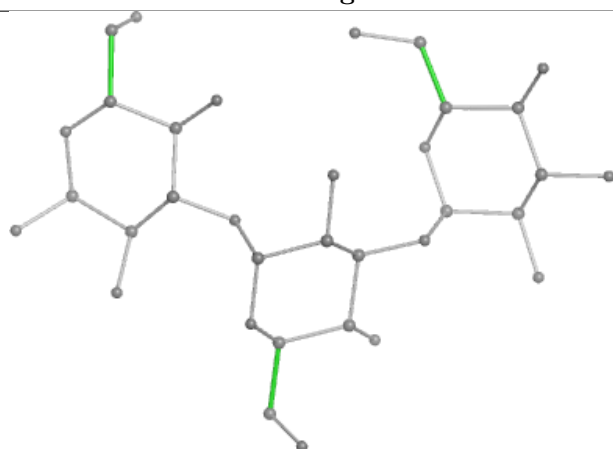
Oligosaccharide Chain G



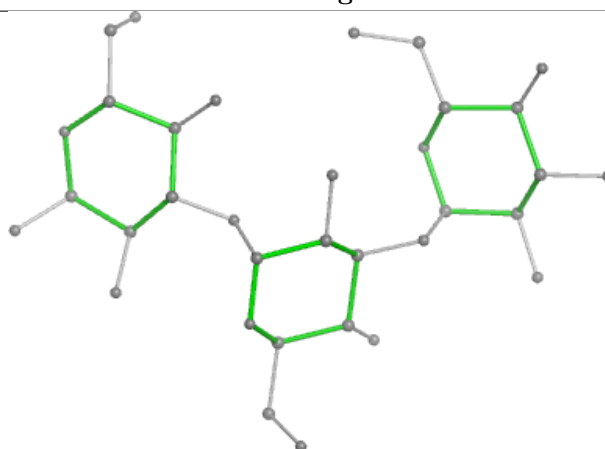
Bond lengths



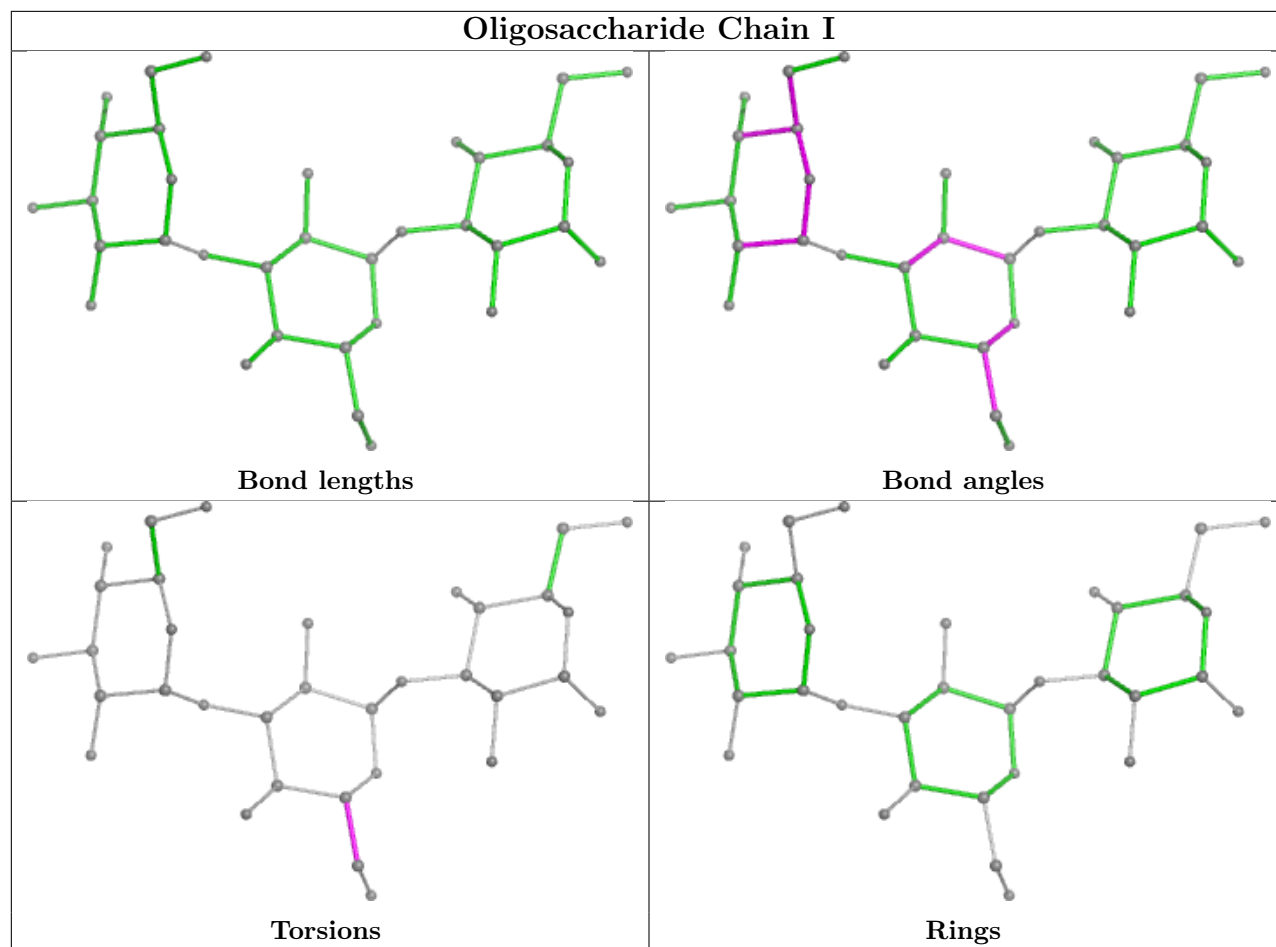
Bond angles



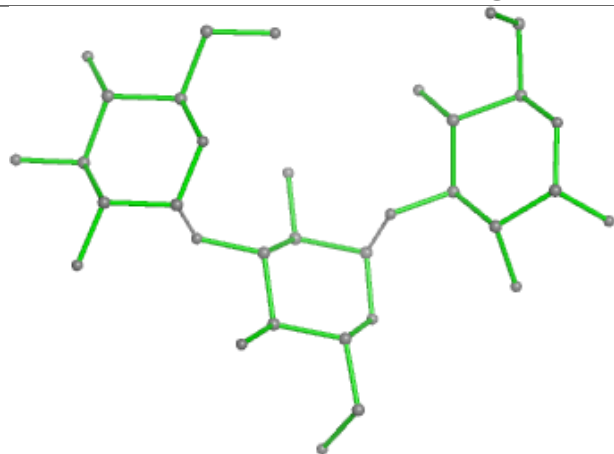
Torsions



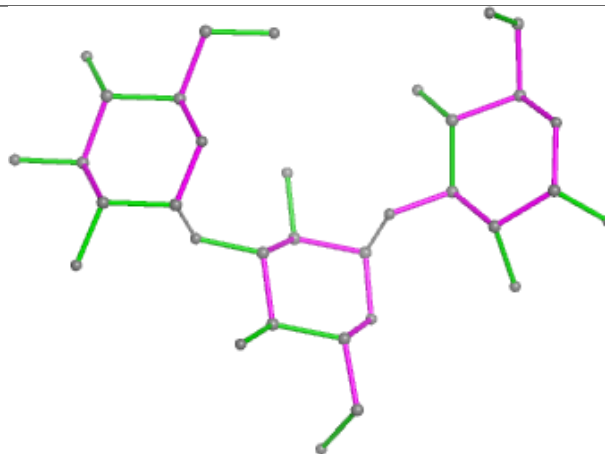
Rings



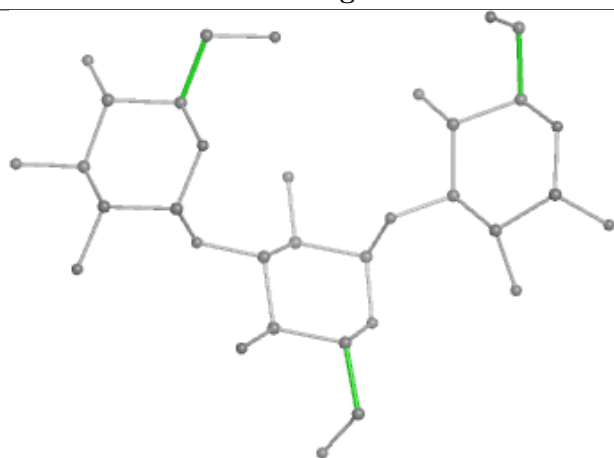
Oligosaccharide Chain J



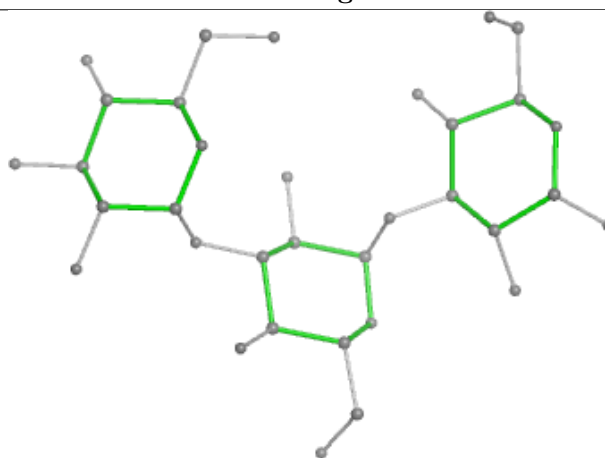
Bond lengths



Bond angles

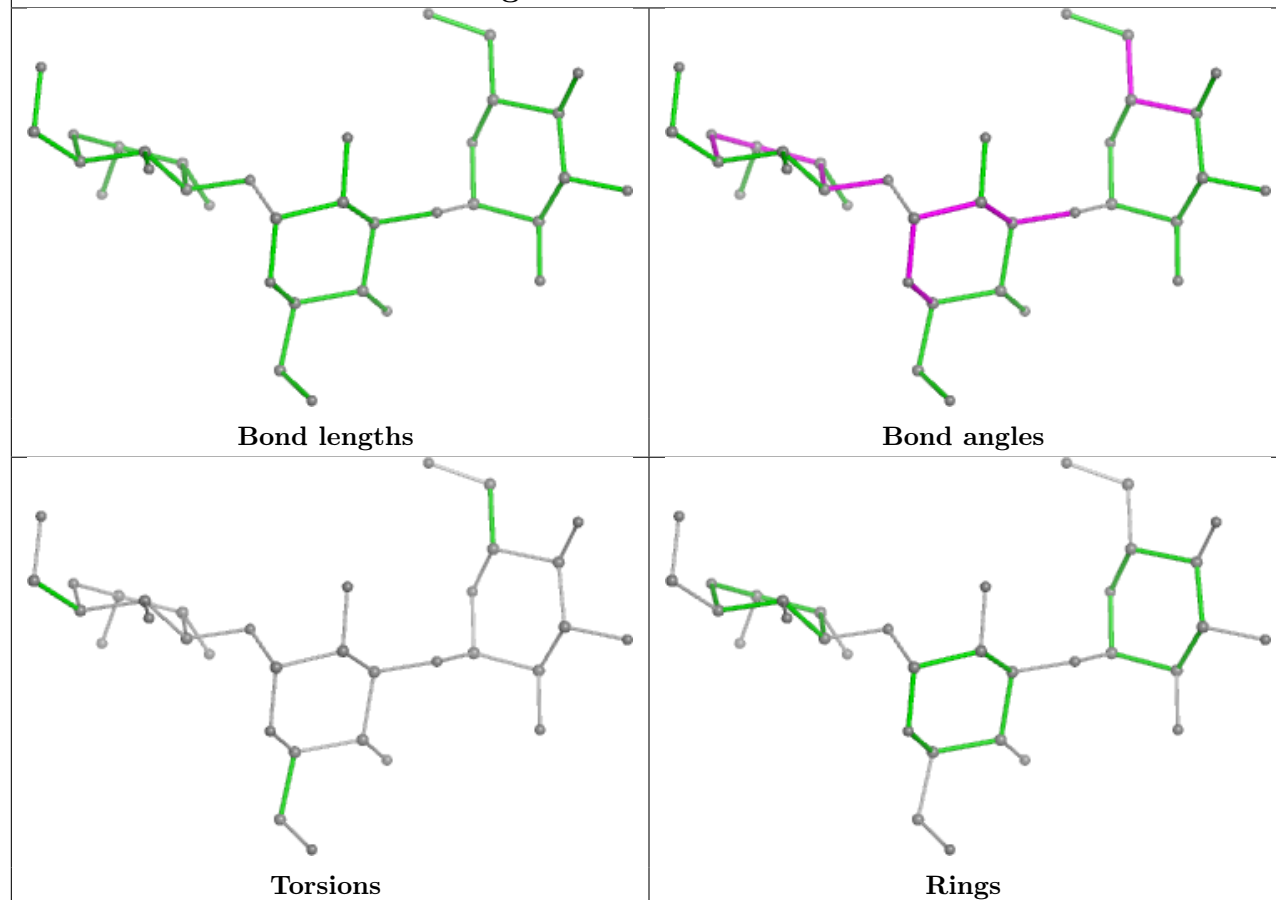


Torsions

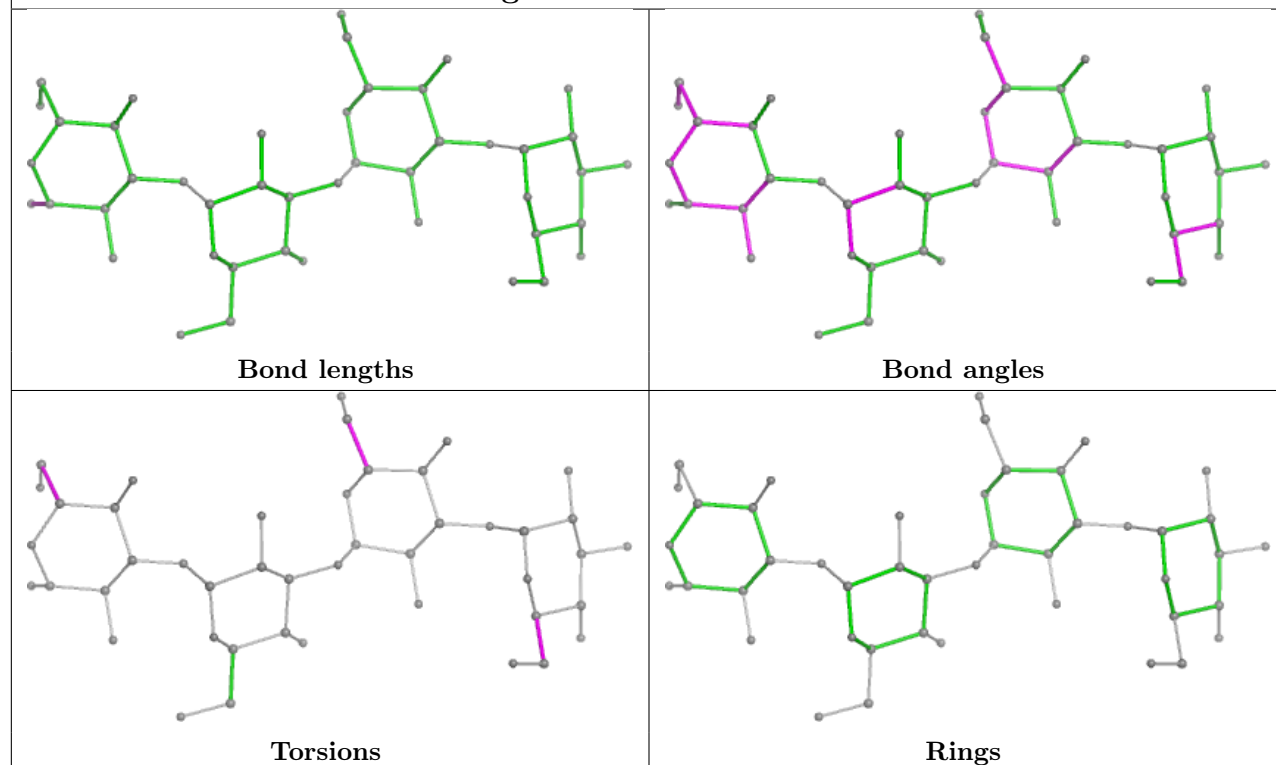


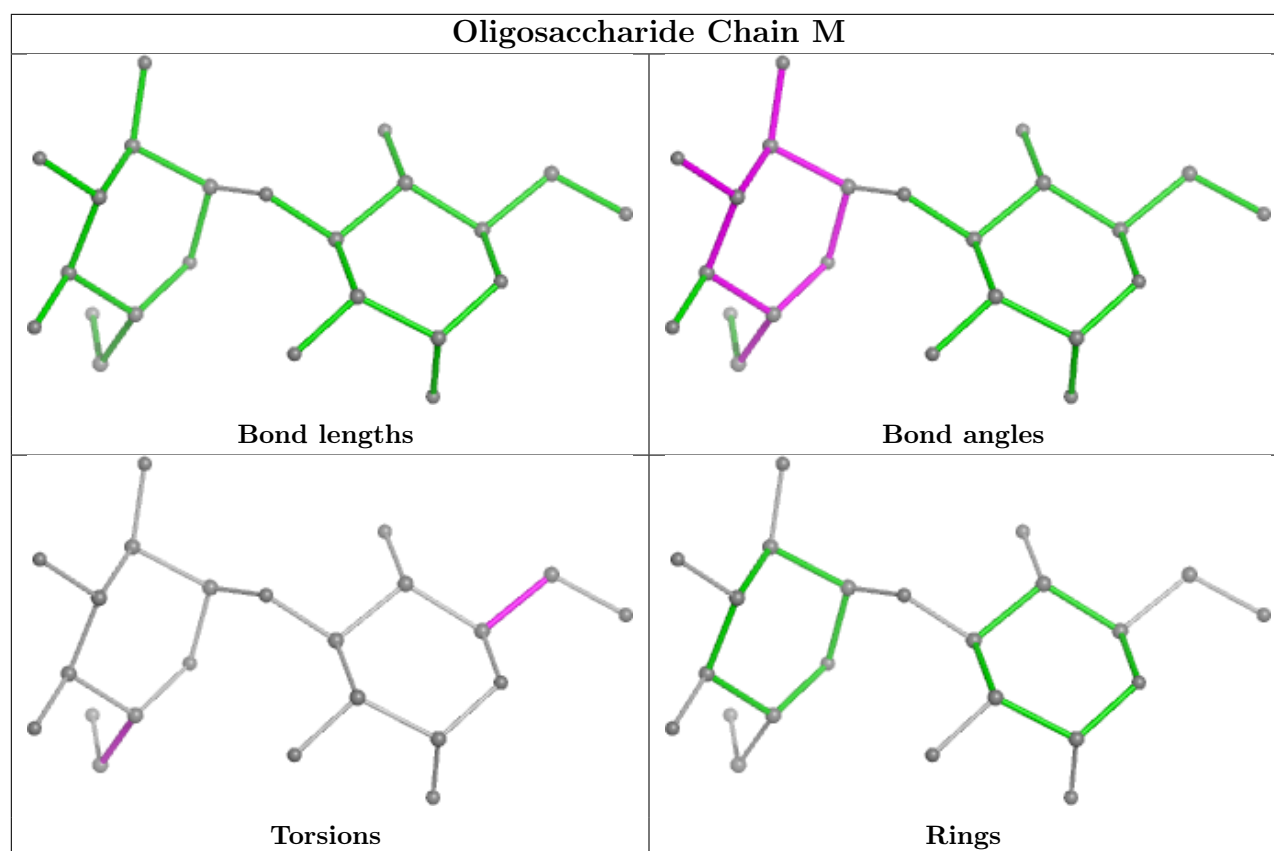
Rings

Oligosaccharide Chain K



Oligosaccharide Chain H





5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	D	501	-	3,3,3	0.54	0	2,2,2	0.29	0
7	PGE	B	502	-	9,9,9	0.38	0	8,8,8	0.36	0
8	CIT	C	501	-	12,12,12	1.04	0	17,17,17	1.73	4 (23%)

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	D	501	-	-	1/1/1/1	-
7	PGE	B	502	-	-	5/7/7/7	-
8	CIT	C	501	-	-	3/16/16/16	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	501	CIT	O6-C6-C3	4.48	120.82	113.05
8	C	501	CIT	O4-C5-C4	2.27	121.65	114.35
8	C	501	CIT	O4-C5-O3	-2.20	117.81	123.30
8	C	501	CIT	O5-C6-C3	-2.09	119.29	122.25

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	502	PGE	C4-C3-O2-C2
8	C	501	CIT	C1-C2-C3-C6
7	B	502	PGE	O1-C1-C2-O2
7	B	502	PGE	C3-C4-O3-C5
7	B	502	PGE	O3-C5-C6-O4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	502	PGE	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	397/430 (92%)	-0.28	5 (1%) 74 80	10, 25, 39, 57	4 (1%)
1	B	397/430 (92%)	-0.22	4 (1%) 79 84	16, 25, 42, 56	0
1	C	397/430 (92%)	-0.29	5 (1%) 74 80	18, 25, 42, 60	0
1	D	399/430 (92%)	-0.19	5 (1%) 74 80	17, 25, 41, 65	1 (0%)
1	X	12/430 (2%)	2.08	5 (41%) 1 1	36, 50, 55, 56	0
All	All	1602/2150 (74%)	-0.23	24 (1%) 71 77	10, 25, 42, 65	5 (0%)

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	16	ALA	4.9
1	D	417	CYS	4.4
1	X	17	ASN	3.3
1	X	6	LEU	3.2
1	B	417	CYS	3.2

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	GLC	E	1	12/12	-	-	21,25,33,34	0

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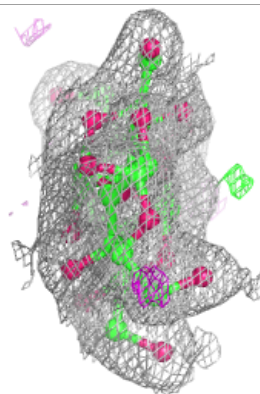
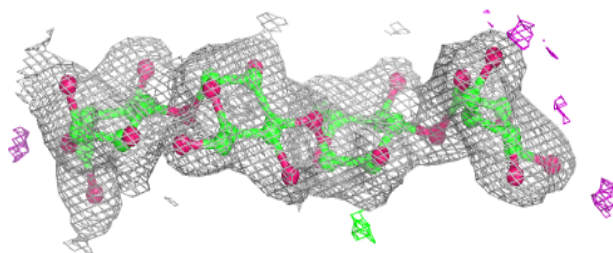
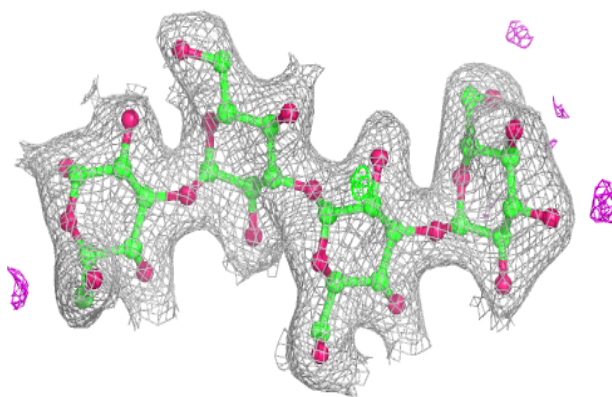
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GLC	E	2	11/12	-	-	15,19,22,23	0
2	GLC	E	3	11/12	-	-	18,20,24,26	0
2	GLC	E	4	11/12	-	-	25,28,33,34	0
5	GLC	M	1	12/12	0.86	0.09	28,39,45,45	0
5	GLC	M	2	11/12	0.86	0.11	34,43,47,48	0
3	GLC	G	1	12/12	0.93	0.09	18,23,26,26	0
3	GLC	J	3	11/12	0.93	0.08	18,20,23,25	0
2	GLC	F	4	11/12	0.94	0.07	21,25,32,41	0
3	GLC	K	1	12/12	0.95	0.07	25,33,43,43	0
4	GLC	H	2	11/12	0.95	0.06	17,24,26,27	0
3	GLC	I	1	12/12	-	-	19,22,25,27	0
3	GLC	I	2	11/12	0.96	0.06	20,23,26,26	0
3	GLC	I	3	11/12	0.96	0.06	28,31,38,43	0
3	GLC	J	1	12/12	0.96	0.05	23,27,31,32	0
2	GLC	F	1	12/12	0.96	0.06	20,26,30,30	0
3	GLC	G	3	11/12	0.97	0.04	16,20,22,24	0
2	GLC	F	2	11/12	0.97	0.05	16,19,23,23	0
3	GLC	K	2	11/12	0.97	0.06	22,23,27,29	0
3	GLC	K	3	11/12	0.97	0.05	24,26,29,30	0
4	BGC	H	1	12/12	-	-	24,29,33,35	0
2	GLC	F	3	11/12	0.97	0.04	18,22,26,26	0
4	GLC	H	3	11/12	0.97	0.05	20,24,26,27	0
4	GLC	H	4	11/12	-	-	25,30,36,43	0
3	GLC	G	2	11/12	0.97	0.06	18,22,26,26	0
3	GLC	J	2	11/12	0.97	0.04	22,26,28,31	0

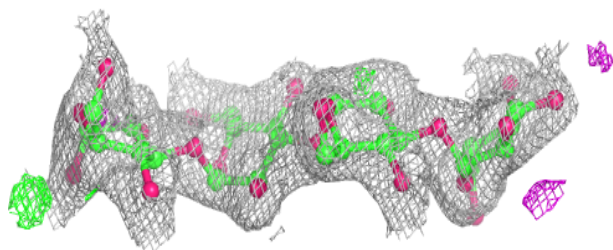
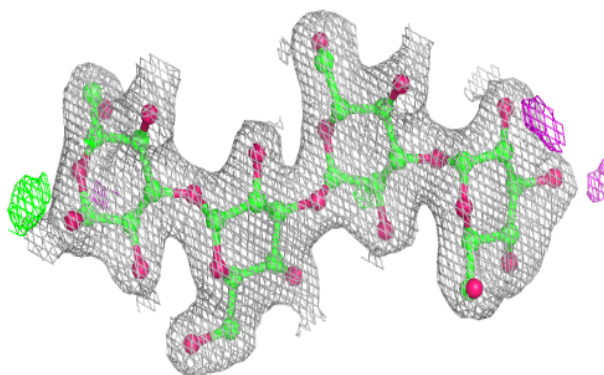
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

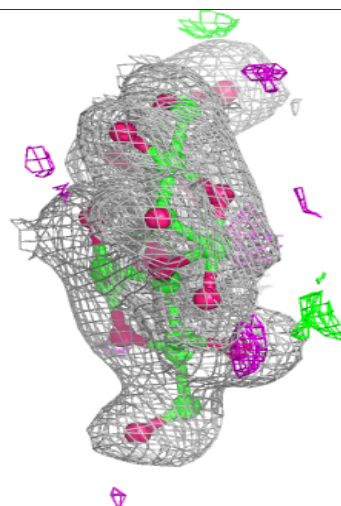
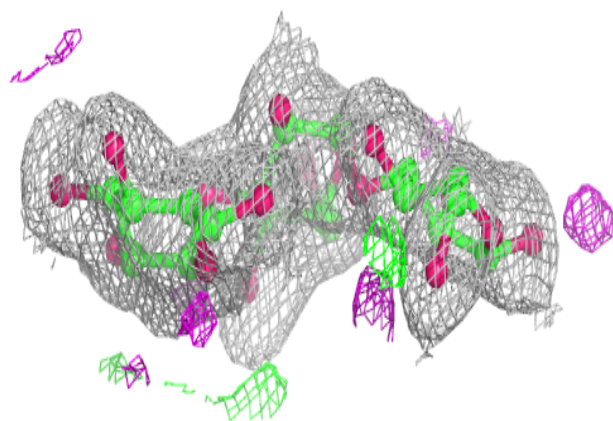
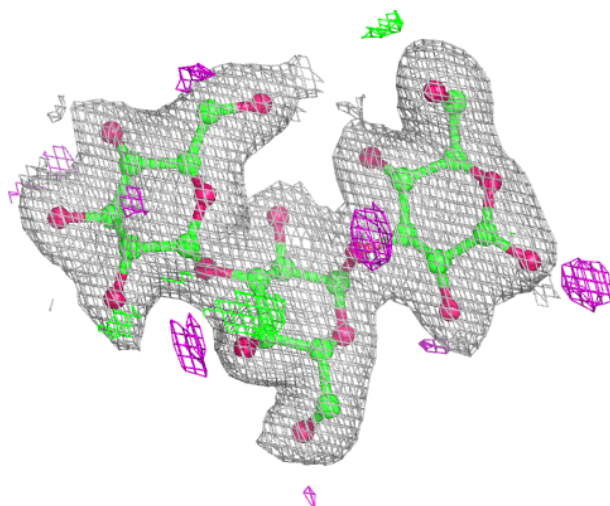
**Electron density around Chain F:**

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



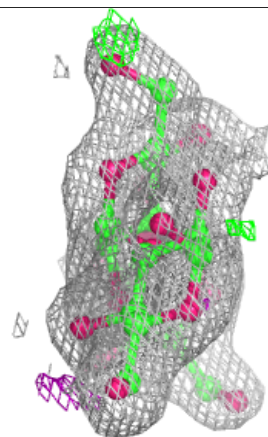
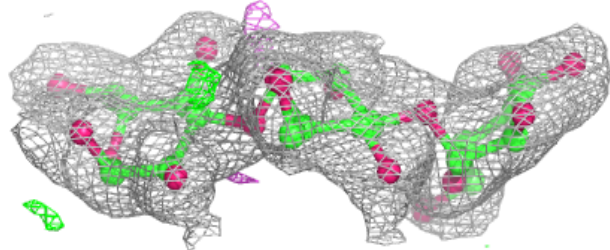
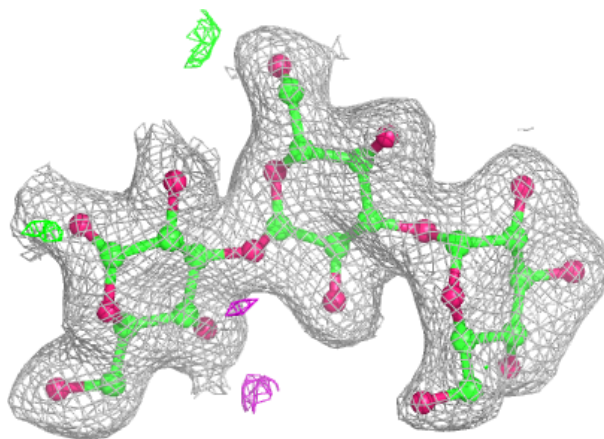
Electron density around Chain G:

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



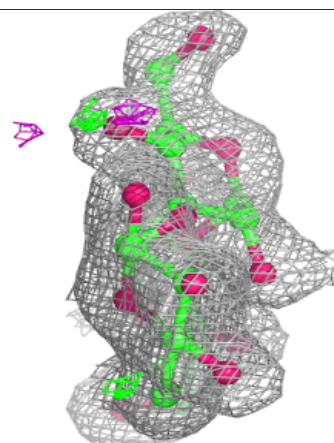
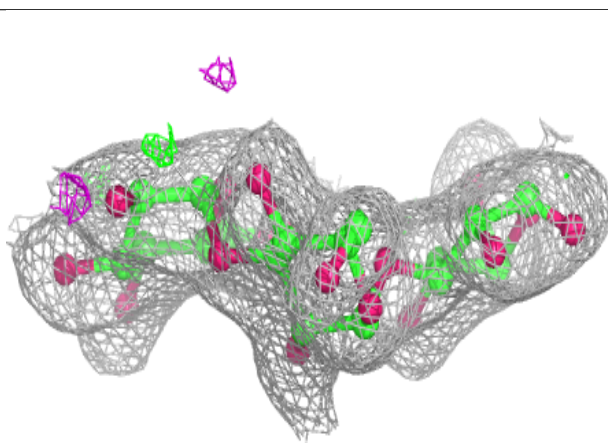
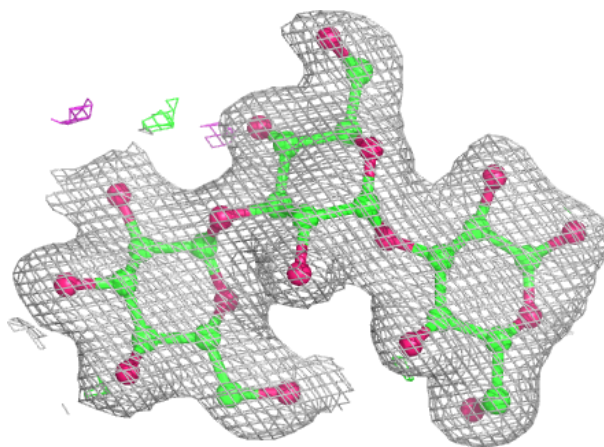
Electron density around Chain I:

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



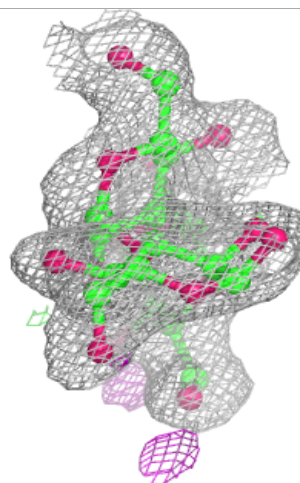
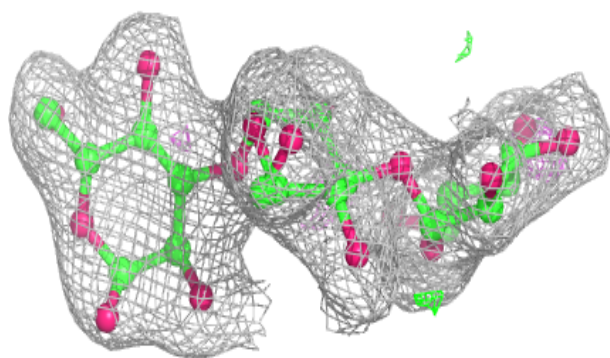
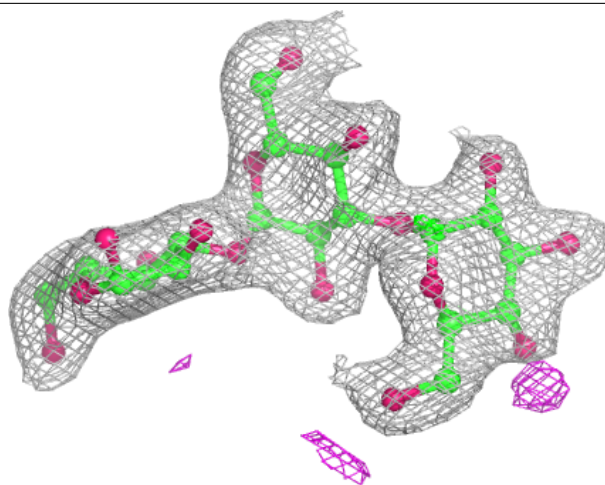
Electron density around Chain J:

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



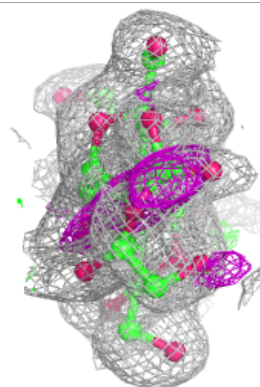
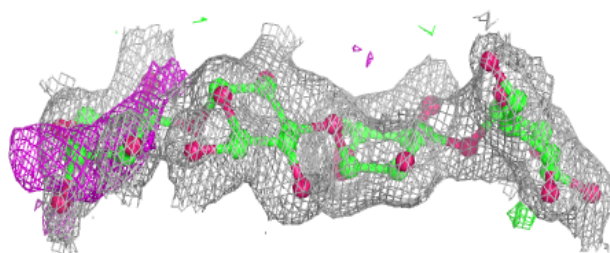
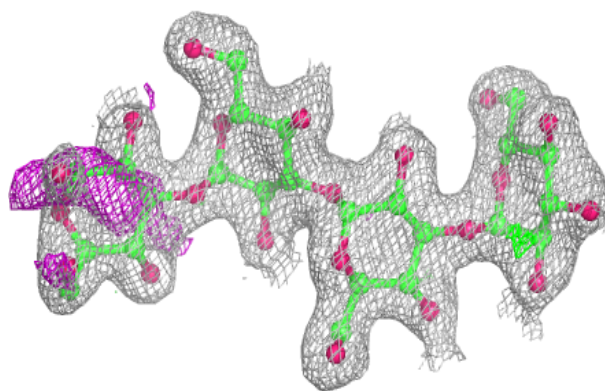
Electron density around Chain K:

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

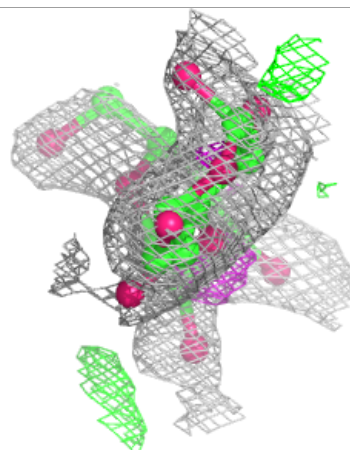
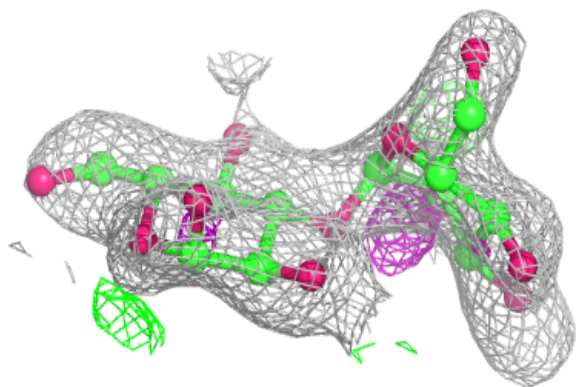
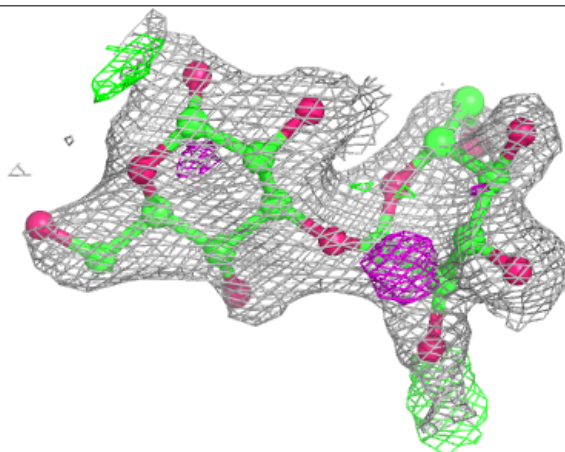


Electron density around Chain H:

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

**Electron density around Chain M:**

$2mF_o-DF_c$ (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	PGE	B	502	10/10	0.81	0.13	36,43,46,55	0
6	NA	D	502	1/1	0.84	0.14	39,39,39,39	0
9	EDO	D	501	4/4	0.85	0.14	36,37,39,40	0
8	CIT	C	501	13/13	0.88	0.10	27,39,47,48	0
6	NA	B	501	1/1	0.98	0.03	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.