



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 10:05 AM BST

PDB ID : 5GM4  
Title : Crystal structure of FI-CMCase from *Aspergillus aculeatus* F-50 in complex with cellotetrose  
Authors : Huang, J.W.; Liu, W.D.; Zheng, Y.Y.; Chen, C.C.; Guo, R.T.  
Deposited on : 2016-07-12  
Resolution : 1.92 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](mailto: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.

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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 : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

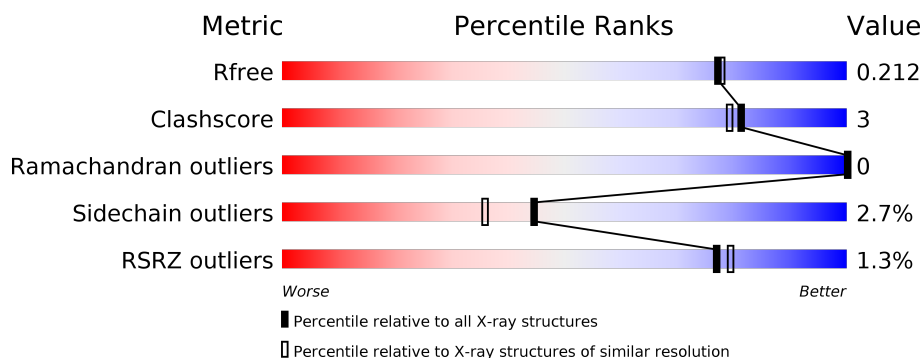
# 1 Overall quality at a glance

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))
$R_{free}$	130704	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	219	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>
1	B	219	<div> <div></div> <div> <div>92%</div> <div>7%</div> <div>.</div> </div> </div>
1	C	219	<div> <div>%</div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>
1	D	219	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>8%</div> </div> </div>
1	E	219	<div> <div>%</div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>
1	F	219	<div> <div>%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	219	<div><div></div><div>3%87%11%</div></div>
2	H	4	<div><div></div><div>25%75%</div></div>
2	I	4	<div><div></div><div>75%25%</div></div>
2	J	4	<div><div></div><div>25%50%25%</div></div>
2	K	4	<div><div></div><div>25%50%25%</div></div>
2	L	4	<div><div></div><div>25%75%</div></div>
2	M	4	<div><div></div><div>100%</div></div>
2	N	4	<div><div></div><div>25%75%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13282 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 Endoglucanase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1680	1065	277	335	3			
1	B	218	Total	C	N	O	S	0	0	0
			1675	1062	276	334	3			
1	C	219	Total	C	N	O	S	0	0	0
			1680	1065	277	335	3			
1	D	218	Total	C	N	O	S	0	0	0
			1675	1062	276	334	3			
1	E	219	Total	C	N	O	S	0	0	0
			1680	1065	277	335	3			
1	F	218	Total	C	N	O	S	0	0	0
			1675	1062	276	334	3			
1	G	218	Total	C	N	O	S	0	0	0
			1675	1062	276	334	3			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	ALA	GLU	engineered mutation	UNP P22669
B	202	ALA	GLU	engineered mutation	UNP P22669
C	202	ALA	GLU	engineered mutation	UNP P22669
D	202	ALA	GLU	engineered mutation	UNP P22669
E	202	ALA	GLU	engineered mutation	UNP P22669
F	202	ALA	GLU	engineered mutation	UNP P22669
G	202	ALA	GLU	engineered mutation	UNP P22669

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	H	4	Total C O 45 24 21	0	0	0
2	I	4	Total C O 45 24 21	0	0	0
2	J	4	Total C O 45 24 21	0	0	0
2	K	4	Total C O 45 24 21	0	0	0
2	L	4	Total C O 45 24 21	0	0	0
2	M	4	Total C O 45 24 21	0	0	0
2	N	4	Total C O 45 24 21	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	183	Total	O	0	0
			183	183		
4	B	202	Total	O	0	0
			202	202		
4	C	186	Total	O	0	0
			186	186		
4	D	166	Total	O	0	0
			166	166		
4	E	159	Total	O	0	0
			159	159		
4	F	161	Total	O	0	0
			161	161		
4	G	130	Total	O	0	0
			130	130		

### 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: Endoglucanase-1



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- Molecule 1: Endoglucanase-1



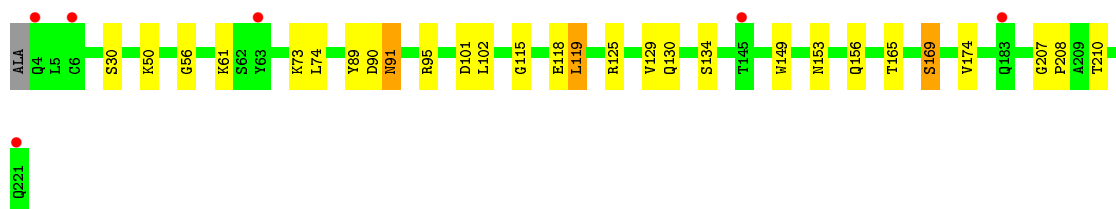
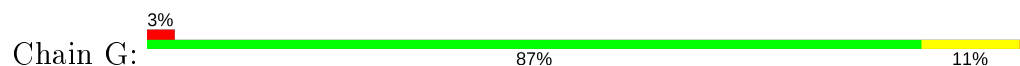
- Molecule 1: Endoglucanase-1



- Molecule 1: Endoglucanase-1



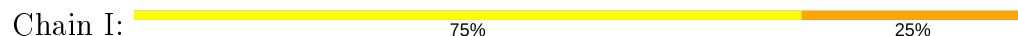
- Molecule 1: Endoglucanase-1



- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



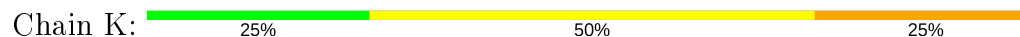
- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



Chain L:  25% 75%

BGC1  
BGC2  
BGC3  
BGC4

- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain M:  100%

BGC1  
BGC2  
BGC3  
BGC4

- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain N:  25% 75%

BGC1  
BGC2  
BGC3  
BGC4

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.91Å 85.28Å 106.03Å 90.00° 92.47° 90.00°	Depositor
Resolution (Å)	25.00 – 1.92 24.96 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.8 (25.00-1.92) 99.9 (24.96-1.92)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.38 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.156 , 0.207 0.166 , 0.212	Depositor DCC
$R_{free}$ test set	5636 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.5	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.007 for k,h,-l 0.005 for -k,-h,-l 0.018 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	13282	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.56	0/1729	0.77	0/2366
1	B	0.56	0/1724	0.76	4/2359 (0.2%)
1	C	0.58	0/1729	0.75	1/2366 (0.0%)
1	D	0.52	0/1724	0.74	2/2359 (0.1%)
1	E	0.55	0/1729	0.72	0/2366
1	F	0.51	0/1724	0.72	0/2359
1	G	0.50	0/1724	0.70	2/2359 (0.1%)
All	All	0.54	0/12083	0.74	9/16534 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	G	95	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	125	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	D	86	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	C	107	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	B	107	ASP	CB-CG-OD1	5.54	123.29	118.30
1	D	125	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	G	119	LEU	CA-CB-CG	5.05	126.91	115.30
1	B	95	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1680	0	1561	10	0
1	B	1675	0	1556	9	0
1	C	1680	0	1561	13	0
1	D	1675	0	1556	6	0
1	E	1680	0	1561	9	0
1	F	1675	0	1556	6	0
1	G	1675	0	1556	13	0
2	H	45	0	39	0	0
2	I	45	0	39	1	0
2	J	45	0	39	1	0
2	K	45	0	39	1	0
2	L	45	0	39	0	0
2	M	45	0	39	0	0
2	N	45	0	39	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	15	0	0	0	0
3	G	5	0	0	0	0
4	A	183	0	0	2	1
4	B	202	0	0	1	2
4	C	186	0	0	2	0
4	D	166	0	0	0	0
4	E	159	0	0	3	0
4	F	161	0	0	1	3
4	G	130	0	0	1	0
All	All	13282	0	11180	60	3

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 3.

All (60) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:ASN:HD22	1:C:153:ASN:C	1.81	0.81
1:C:130:GLN:HG2	4:C:487:HOH:O	1.88	0.74
1:B:130:GLN:HE21	1:C:72:LYS:NZ	1.86	0.73
1:E:77:GLN:OE1	4:E:401:HOH:O	2.10	0.69
1:C:153:ASN:ND2	1:C:153:ASN:C	2.44	0.68
1:B:130:GLN:HE21	1:C:72:LYS:HZ3	1.44	0.65
1:E:20:ASN:HB3	4:E:502:HOH:O	2.00	0.60
1:A:147:GLU:OE2	4:A:401:HOH:O	2.17	0.59
1:G:125:ARG:NH1	1:G:129:VAL:O	2.35	0.59
1:E:19:ILE:HD12	1:E:19:ILE:N	2.18	0.59
1:F:11:THR:HG21	1:G:134:SER:OG	2.04	0.58
1:A:115:GLY:H	1:A:156:GLN:HE21	1.53	0.56
1:G:90:ASP:OD1	1:G:91:ASN:N	2.39	0.55
1:B:135:GLN:O	2:J:4:BGC:H6C2	2.07	0.54
1:A:19:ILE:N	1:A:19:ILE:HD12	2.23	0.54
1:E:115:GLY:H	1:E:156:GLN:HE21	1.56	0.53
1:G:56:GLY:O	1:G:61:LYS:NZ	2.38	0.53
1:B:86:ARG:HD3	1:B:215:ASN:HB3	1.91	0.52
1:G:50:LYS:HG3	1:G:210:THR:OG1	2.09	0.52
1:C:153:ASN:HD21	1:C:156:GLN:H	1.57	0.51
1:B:115:GLY:H	1:B:156:GLN:HE21	1.59	0.51
1:A:135:GLN:O	2:K:4:BGC:H6C2	2.11	0.49
1:D:86:ARG:HD3	1:D:215:ASN:HB3	1.95	0.49
1:B:130:GLN:NE2	1:C:112:THR:HG21	2.28	0.49
1:F:46:SER:HB2	1:F:214:SER:O	2.13	0.49
1:D:80:GLN:HG3	1:D:82:PRO:HD3	1.96	0.48
1:A:101:ASP:OD1	1:A:118:GLU:OE2	2.31	0.47
1:E:95:ARG:NH2	4:E:406:HOH:O	2.47	0.47
1:E:153:ASN:OD1	1:E:153:ASN:C	2.53	0.47
1:C:153:ASN:ND2	1:C:156:GLN:H	2.13	0.47
1:G:115:GLY:H	1:G:156:GLN:HE21	1.61	0.46
1:E:48:SER:HA	1:E:211:LEU:O	2.15	0.46
1:G:207:GLY:HA2	1:G:208:PRO:C	2.35	0.46
1:E:52:ASN:HD22	1:E:52:ASN:C	2.19	0.46
1:F:104:THR:HA	1:F:193:TYR:O	2.16	0.46
1:A:135:GLN:NE2	4:A:403:HOH:O	2.46	0.45
1:F:4:GLN:N	4:F:410:HOH:O	2.50	0.45
1:A:207:GLY:HA2	1:A:208:PRO:C	2.36	0.45
1:C:95:ARG:NH2	4:C:407:HOH:O	2.48	0.45
1:D:101:ASP:OD1	1:D:118:GLU:OE2	2.36	0.44
1:F:112:THR:HG21	1:G:130:GLN:HE22	1.83	0.44
2:I:1:BGC:H6C2	2:I:2:BGC:O5	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:GLN:NE2	4:B:407:HOH:O	2.50	0.44
1:G:169:SER:HB3	4:G:440:HOH:O	2.17	0.43
1:C:153:ASN:HD22	1:C:154:GLY:N	2.12	0.43
1:A:130:GLN:HE21	1:D:72:LYS:NZ	2.16	0.42
1:F:125:ARG:HD2	1:F:129:VAL:O	2.19	0.42
1:D:115:GLY:H	1:D:156:GLN:HE21	1.68	0.42
1:E:207:GLY:HA2	1:E:208:PRO:C	2.40	0.42
1:C:115:GLY:H	1:C:156:GLN:HE21	1.66	0.42
1:A:153:ASN:C	1:A:153:ASN:OD1	2.56	0.42
1:B:11:THR:HA	1:B:19:ILE:O	2.20	0.42
1:A:104:THR:HA	1:A:193:TYR:O	2.20	0.42
1:G:102:LEU:HD21	1:G:174:VAL:HG11	2.02	0.41
1:G:134:SER:HA	1:G:149:TRP:CE3	2.56	0.41
1:B:104:THR:HA	1:B:193:TYR:O	2.20	0.41
1:C:153:ASN:ND2	1:C:155:SER:H	2.19	0.41
1:D:104:THR:OG1	1:D:117:TYR:HB2	2.21	0.41
1:G:101:ASP:OD1	1:G:118:GLU:OE2	2.39	0.41
1:C:86:ARG:NE	1:G:74:LEU:HD11	2.36	0.40

All (3) 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)
4:B:488:HOH:O	4:F:473:HOH:O[2_644]	2.02	0.18
4:A:525:HOH:O	4:F:467:HOH:O[2_645]	2.11	0.09
4:B:516:HOH:O	4:F:473:HOH:O[2_644]	2.18	0.02

## 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	217/219 (99%)	213 (98%)	4 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	216/219 (99%)	209 (97%)	7 (3%)	0	100	100
1	C	217/219 (99%)	215 (99%)	2 (1%)	0	100	100
1	D	216/219 (99%)	210 (97%)	6 (3%)	0	100	100
1	E	217/219 (99%)	213 (98%)	4 (2%)	0	100	100
1	F	216/219 (99%)	212 (98%)	4 (2%)	0	100	100
1	G	216/219 (99%)	211 (98%)	5 (2%)	0	100	100
All	All	1515/1533 (99%)	1483 (98%)	32 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	177/177 (100%)	173 (98%)	4 (2%)	50	43
1	B	177/177 (100%)	172 (97%)	5 (3%)	43	34
1	C	177/177 (100%)	173 (98%)	4 (2%)	50	43
1	D	177/177 (100%)	170 (96%)	7 (4%)	31	21
1	E	177/177 (100%)	174 (98%)	3 (2%)	60	55
1	F	177/177 (100%)	174 (98%)	3 (2%)	60	55
1	G	177/177 (100%)	169 (96%)	8 (4%)	27	17
All	All	1239/1239 (100%)	1205 (97%)	34 (3%)	44	36

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	73	LYS
1	A	89	TYR
1	A	130	GLN
1	B	89	TYR

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Mol	Chain	Res	Type
1	B	125	ARG
1	B	130	GLN
1	B	171	GLN
1	B	183	GLN
1	C	52	ASN
1	C	73	LYS
1	C	89	TYR
1	C	153	ASN
1	D	30	SER
1	D	73	LYS
1	D	86	ARG
1	D	89	TYR
1	D	144	GLN
1	D	145	THR
1	D	171	GLN
1	E	52	ASN
1	E	89	TYR
1	E	155	SER
1	F	89	TYR
1	F	130	GLN
1	F	171	GLN
1	G	30	SER
1	G	73	LYS
1	G	89	TYR
1	G	91	ASN
1	G	119	LEU
1	G	153	ASN
1	G	165	THR
1	G	169	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	38	ASN
1	A	130	GLN
1	A	135	GLN
1	A	156	GLN
1	A	192	GLN
1	A	221	GLN
1	B	4	GLN
1	B	38	ASN

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Mol	Chain	Res	Type
1	B	130	GLN
1	B	135	GLN
1	B	156	GLN
1	B	192	GLN
1	B	221	GLN
1	C	4	GLN
1	C	38	ASN
1	C	153	ASN
1	C	156	GLN
1	C	192	GLN
1	C	221	GLN
1	D	38	ASN
1	D	135	GLN
1	D	156	GLN
1	D	192	GLN
1	E	4	GLN
1	E	52	ASN
1	E	80	GLN
1	E	135	GLN
1	E	156	GLN
1	E	192	GLN
1	E	215	ASN
1	E	221	GLN
1	F	38	ASN
1	F	135	GLN
1	F	192	GLN
1	F	215	ASN
1	G	38	ASN
1	G	130	GLN
1	G	135	GLN
1	G	153	ASN
1	G	156	GLN
1	G	192	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 ⓘ

28 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	H	1	2	12,12,12	0.47	0	17,17,17	1.57	2 (11%)
2	BGC	H	2	2	11,11,12	0.47	0	15,15,17	0.96	0
2	BGC	H	3	2	11,11,12	0.52	0	15,15,17	1.10	2 (13%)
2	BGC	H	4	2	11,11,12	0.80	0	15,15,17	2.59	5 (33%)
2	BGC	I	1	2	12,12,12	0.49	0	17,17,17	1.77	6 (35%)
2	BGC	I	2	2	11,11,12	0.41	0	15,15,17	0.95	0
2	BGC	I	3	2	11,11,12	0.56	0	15,15,17	1.08	1 (6%)
2	BGC	I	4	2	11,11,12	0.38	0	15,15,17	1.21	1 (6%)
2	BGC	J	1	2	12,12,12	0.39	0	17,17,17	1.11	1 (5%)
2	BGC	J	2	2	11,11,12	0.37	0	15,15,17	0.80	0
2	BGC	J	3	2	11,11,12	0.59	0	15,15,17	1.54	2 (13%)
2	BGC	J	4	2	11,11,12	0.32	0	15,15,17	1.08	1 (6%)
2	BGC	K	1	2	12,12,12	0.46	0	17,17,17	1.02	1 (5%)
2	BGC	K	2	2	11,11,12	0.50	0	15,15,17	0.99	0
2	BGC	K	3	2	11,11,12	0.50	0	15,15,17	1.33	2 (13%)
2	BGC	K	4	2	11,11,12	0.46	0	15,15,17	1.36	3 (20%)
2	BGC	L	1	2	12,12,12	0.48	0	17,17,17	1.19	2 (11%)
2	BGC	L	2	2	11,11,12	0.56	0	15,15,17	0.93	0
2	BGC	L	3	2	11,11,12	0.70	0	15,15,17	1.26	1 (6%)
2	BGC	L	4	2	11,11,12	0.34	0	15,15,17	1.32	1 (6%)
2	BGC	M	1	2	12,12,12	0.42	0	17,17,17	1.74	3 (17%)
2	BGC	M	2	2	11,11,12	0.63	0	15,15,17	0.96	1 (6%)
2	BGC	M	3	2	11,11,12	0.45	0	15,15,17	1.61	4 (26%)
2	BGC	M	4	2	11,11,12	0.48	0	15,15,17	1.54	3 (20%)
2	BGC	N	1	2	12,12,12	0.52	0	17,17,17	1.59	4 (23%)
2	BGC	N	2	2	11,11,12	0.55	0	15,15,17	0.68	0
2	BGC	N	3	2	11,11,12	0.46	0	15,15,17	1.08	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	BGC	N	4	2	11,11,12	0.37	0	15,15,17	1.19	2 (13%)

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	H	1	2	-	1/2/22/22	0/1/1/1
2	BGC	H	2	2	-	0/2/19/22	0/1/1/1
2	BGC	H	3	2	-	0/2/19/22	0/1/1/1
2	BGC	H	4	2	-	2/2/19/22	0/1/1/1
2	BGC	I	1	2	-	1/2/22/22	0/1/1/1
2	BGC	I	2	2	-	0/2/19/22	0/1/1/1
2	BGC	I	3	2	-	0/2/19/22	0/1/1/1
2	BGC	I	4	2	-	0/2/19/22	0/1/1/1
2	BGC	J	1	2	-	0/2/22/22	0/1/1/1
2	BGC	J	2	2	-	0/2/19/22	0/1/1/1
2	BGC	J	3	2	-	2/2/19/22	0/1/1/1
2	BGC	J	4	2	-	1/2/19/22	0/1/1/1
2	BGC	K	1	2	-	1/2/22/22	0/1/1/1
2	BGC	K	2	2	-	0/2/19/22	0/1/1/1
2	BGC	K	3	2	-	0/2/19/22	0/1/1/1
2	BGC	K	4	2	-	1/2/19/22	0/1/1/1
2	BGC	L	1	2	-	2/2/22/22	0/1/1/1
2	BGC	L	2	2	-	0/2/19/22	0/1/1/1
2	BGC	L	3	2	-	0/2/19/22	0/1/1/1
2	BGC	L	4	2	-	0/2/19/22	0/1/1/1
2	BGC	M	1	2	-	0/2/22/22	0/1/1/1
2	BGC	M	2	2	-	0/2/19/22	0/1/1/1
2	BGC	M	3	2	-	0/2/19/22	0/1/1/1
2	BGC	M	4	2	-	1/2/19/22	0/1/1/1
2	BGC	N	1	2	-	2/2/22/22	0/1/1/1
2	BGC	N	2	2	-	0/2/19/22	0/1/1/1
2	BGC	N	3	2	-	0/2/19/22	0/1/1/1
2	BGC	N	4	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	4	BGC	O3-C3-C2	-5.76	98.97	109.99
2	M	1	BGC	O5-C1-C2	-5.14	101.12	110.28
2	H	4	BGC	O5-C1-C2	-4.94	103.14	110.77
2	H	1	BGC	O6-C6-C5	-4.47	95.95	111.29
2	N	1	BGC	O5-C1-C2	-3.90	103.33	110.28
2	J	3	BGC	C6-C5-C4	3.67	121.61	113.00
2	L	4	BGC	C1-C2-C3	-3.52	105.34	109.67
2	I	1	BGC	C1-O5-C5	-3.23	107.57	113.66
2	M	4	BGC	C6-C5-C4	-3.22	105.46	113.00
2	M	1	BGC	C1-O5-C5	-3.11	107.79	113.66
2	H	4	BGC	O5-C5-C6	3.07	112.02	107.20
2	J	3	BGC	O3-C3-C4	3.05	117.41	110.35
2	M	3	BGC	C1-O5-C5	-3.03	108.09	112.19
2	M	4	BGC	O5-C1-C2	-2.95	106.21	110.77
2	M	3	BGC	O5-C5-C6	2.94	111.81	107.20
2	I	1	BGC	O5-C1-C2	-2.84	105.21	110.28
2	M	4	BGC	O5-C5-C6	2.84	111.66	107.20
2	K	4	BGC	C2-C3-C4	-2.83	106.01	110.89
2	I	1	BGC	C1-C2-C3	-2.80	104.50	110.31
2	I	1	BGC	C4-C3-C2	-2.76	106.00	110.82
2	N	1	BGC	C1-C2-C3	-2.75	104.61	110.31
2	J	4	BGC	C1-C2-C3	-2.65	106.40	109.67
2	L	3	BGC	O5-C5-C6	2.61	111.30	107.20
2	L	1	BGC	C1-O5-C5	2.59	118.54	113.66
2	M	3	BGC	C6-C5-C4	-2.56	107.02	113.00
2	K	4	BGC	C1-C2-C3	-2.52	106.56	109.67
2	H	4	BGC	O2-C2-C3	2.52	115.19	110.14
2	I	4	BGC	O5-C5-C6	2.49	111.10	107.20
2	K	1	BGC	O1-C1-C2	-2.48	102.05	109.03
2	I	1	BGC	O2-C2-C1	2.33	114.57	109.16
2	I	1	BGC	C3-C4-C5	2.33	114.39	110.24
2	J	1	BGC	O3-C3-C4	2.32	115.70	110.35
2	H	1	BGC	C1-O5-C5	-2.28	109.36	113.66
2	I	3	BGC	O5-C5-C6	2.24	110.72	107.20
2	N	1	BGC	O4-C4-C3	-2.24	105.16	110.35
2	M	1	BGC	C1-C2-C3	-2.20	105.74	110.31
2	H	4	BGC	C1-O5-C5	2.20	115.17	112.19
2	K	3	BGC	O2-C2-C3	-2.19	105.75	110.14
2	N	4	BGC	O4-C4-C5	2.17	114.68	109.30
2	K	3	BGC	O6-C6-C5	-2.13	103.99	111.29
2	N	3	BGC	O4-C4-C5	-2.11	104.05	109.30
2	N	3	BGC	C6-C5-C4	-2.09	108.10	113.00
2	L	1	BGC	O6-C6-C5	-2.07	104.18	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	1	BGC	O3-C3-C4	2.07	115.14	110.35
2	N	4	BGC	C1-O5-C5	-2.05	109.42	112.19
2	M	2	BGC	O3-C3-C2	2.05	113.92	109.99
2	H	3	BGC	C1-O5-C5	2.05	114.96	112.19
2	M	3	BGC	O3-C3-C4	-2.04	105.63	110.35
2	H	3	BGC	O4-C4-C5	-2.03	104.25	109.30
2	K	4	BGC	O5-C1-C2	-2.02	107.66	110.77

There are no chirality outliers.

All (16) torsion outliers are listed below:

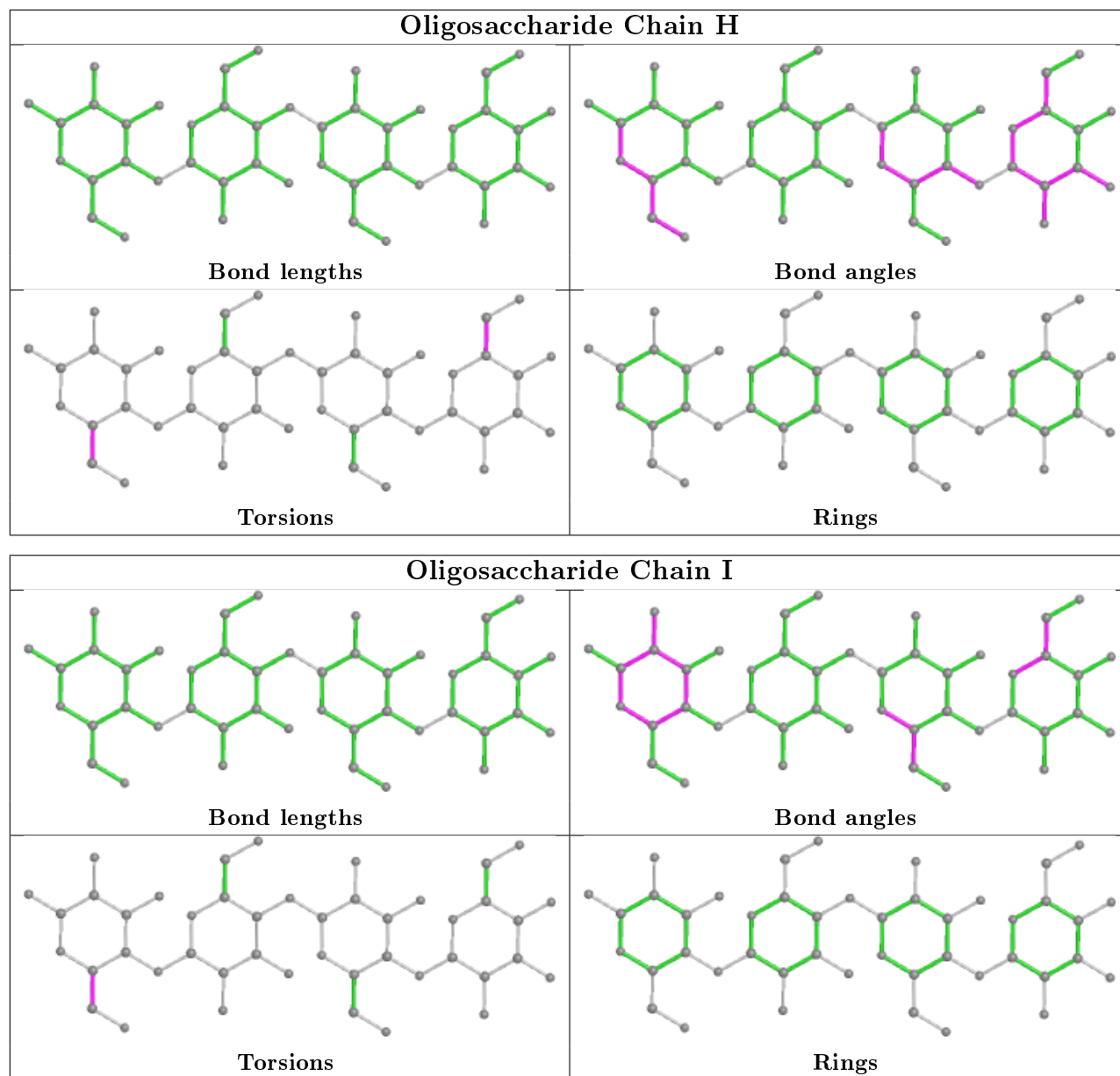
Mol	Chain	Res	Type	Atoms
2	N	4	BGC	O5-C5-C6-O6
2	J	3	BGC	C4-C5-C6-O6
2	J	3	BGC	O5-C5-C6-O6
2	N	4	BGC	C4-C5-C6-O6
2	H	4	BGC	O5-C5-C6-O6
2	L	1	BGC	O5-C5-C6-O6
2	N	1	BGC	C4-C5-C6-O6
2	H	4	BGC	C4-C5-C6-O6
2	H	1	BGC	O5-C5-C6-O6
2	I	1	BGC	C4-C5-C6-O6
2	M	4	BGC	O5-C5-C6-O6
2	L	1	BGC	C4-C5-C6-O6
2	J	4	BGC	O5-C5-C6-O6
2	K	1	BGC	O5-C5-C6-O6
2	K	4	BGC	O5-C5-C6-O6
2	N	1	BGC	O5-C5-C6-O6

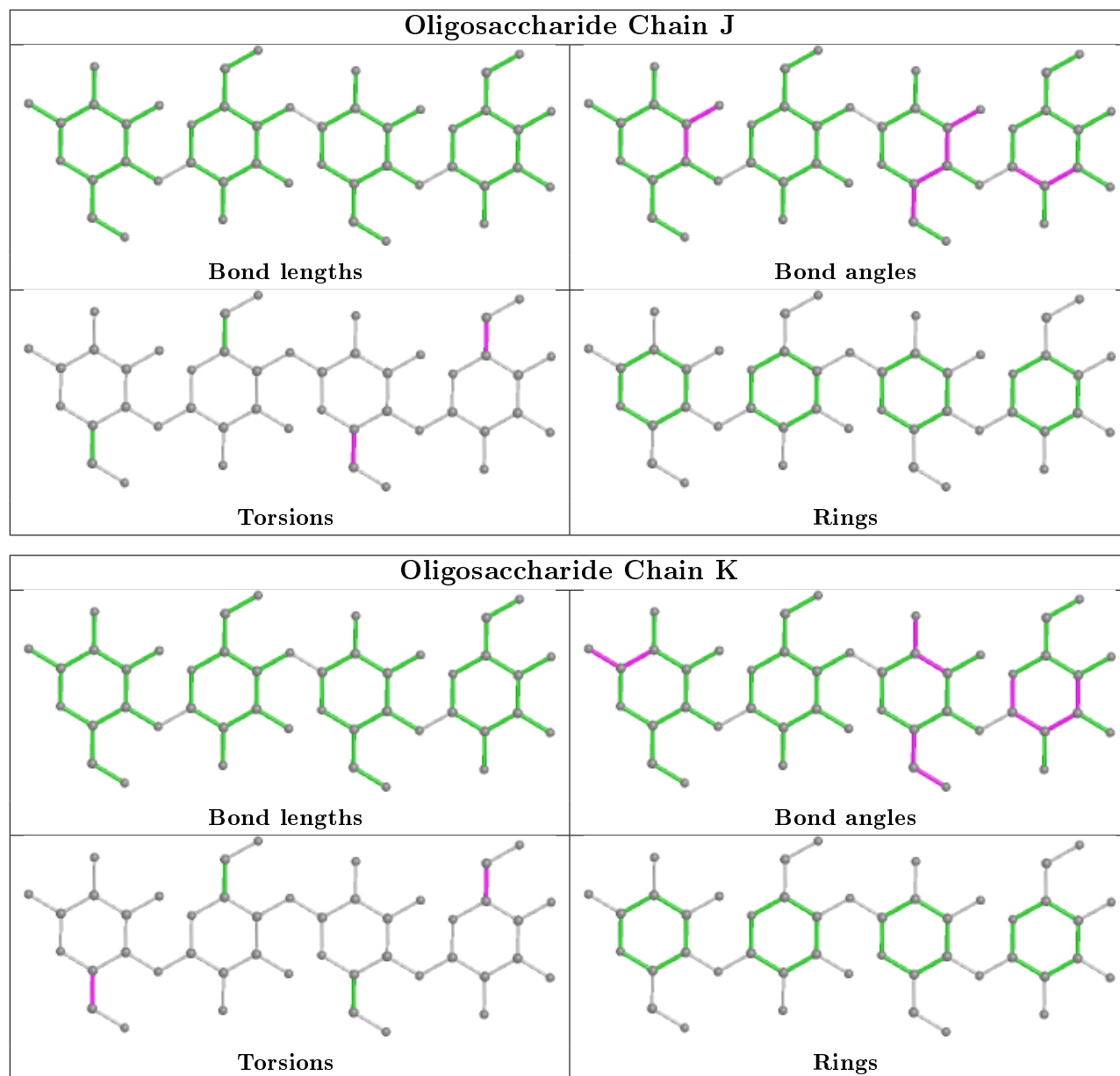
There are no ring outliers.

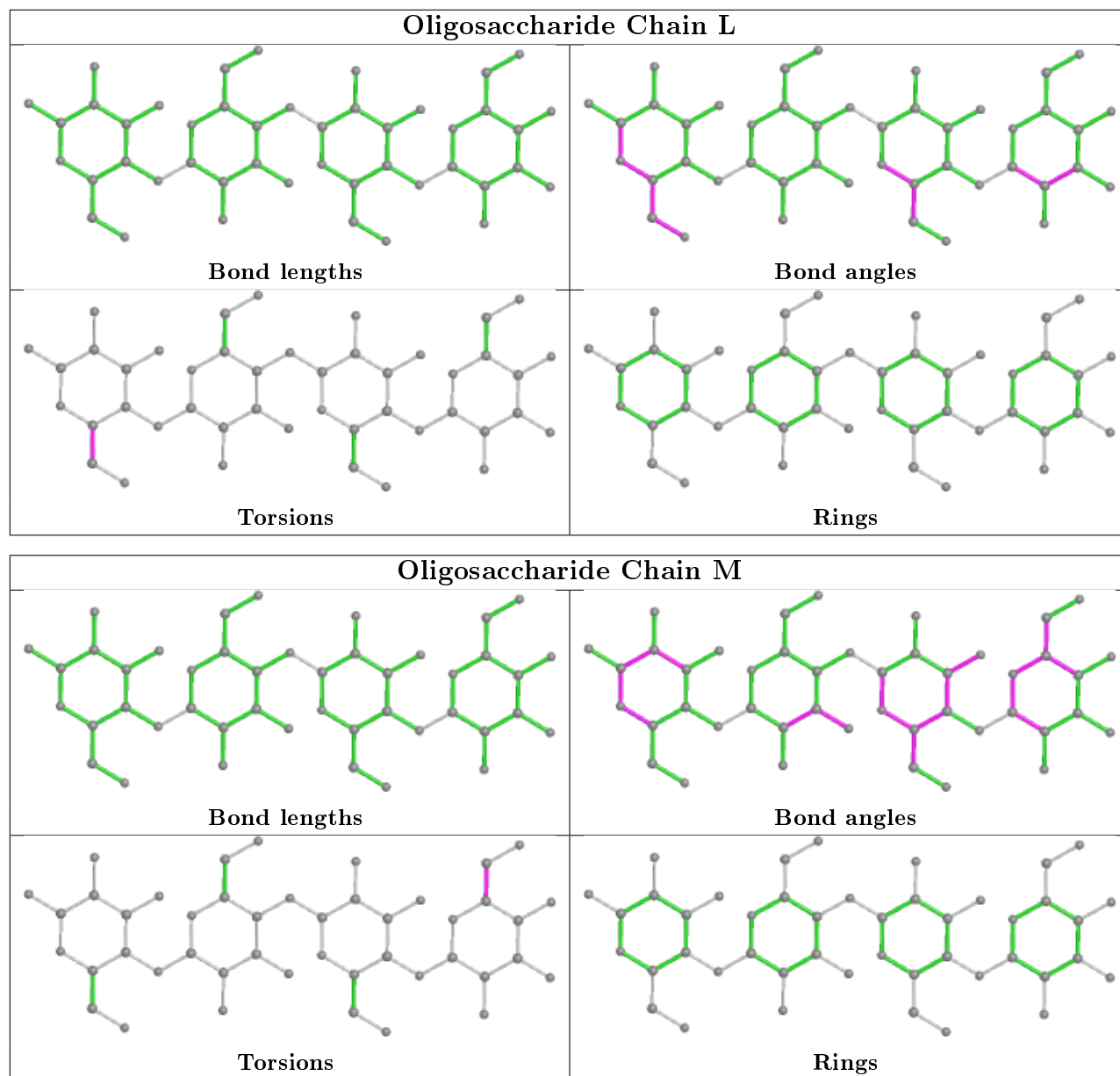
4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	4	BGC	1	0
2	I	1	BGC	1	0
2	I	2	BGC	1	0
2	J	4	BGC	1	0

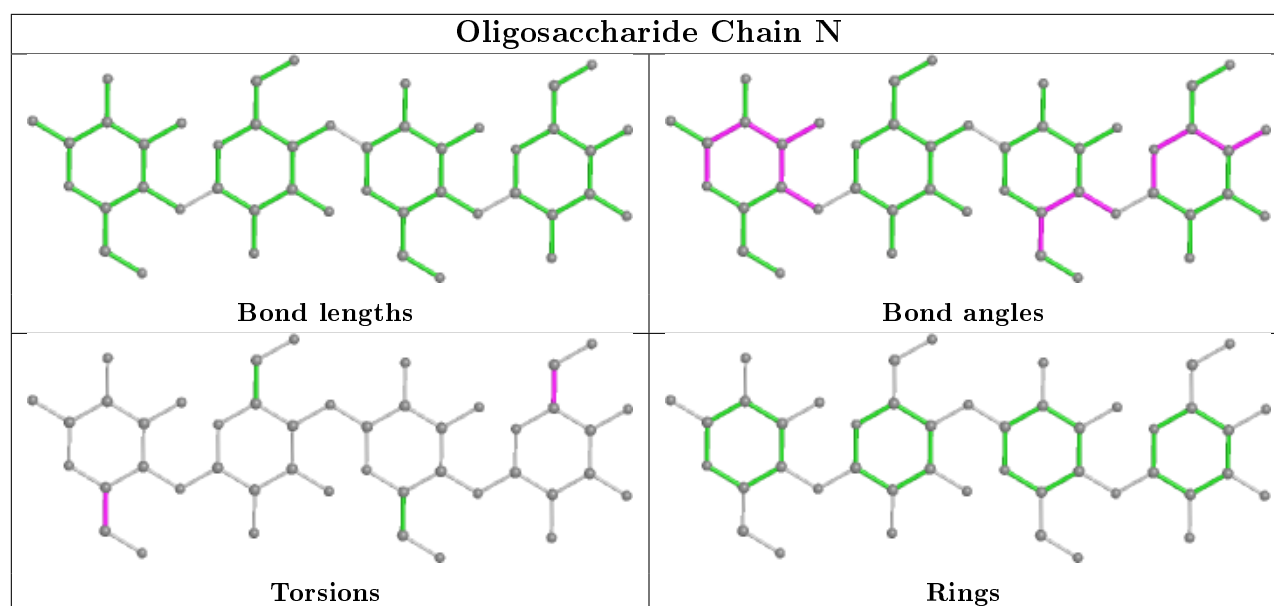
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

8 ligands 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	$\# Z  > 2$
3	SO4	A	301	-	4,4,4	0.42	0	6,6,6	0.33	0
3	SO4	D	301	-	4,4,4	0.37	0	6,6,6	0.40	0
3	SO4	G	301	-	4,4,4	0.38	0	6,6,6	0.23	0
3	SO4	B	301	-	4,4,4	0.42	0	6,6,6	0.29	0
3	SO4	C	301	-	4,4,4	0.37	0	6,6,6	0.20	0
3	SO4	E	302	-	4,4,4	0.40	0	6,6,6	0.19	0
3	SO4	E	301	-	4,4,4	0.40	0	6,6,6	0.20	0
3	SO4	E	303	-	4,4,4	0.39	0	6,6,6	0.31	0

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	219/219 (100%)	-0.10	3 (1%) 75 77	18, 26, 40, 60	0
1	B	218/219 (99%)	-0.18	1 (0%) 91 92	17, 24, 37, 53	0
1	C	219/219 (100%)	-0.16	2 (0%) 84 85	19, 26, 41, 54	0
1	D	218/219 (99%)	-0.17	3 (1%) 75 77	20, 28, 43, 56	0
1	E	219/219 (100%)	-0.12	3 (1%) 75 77	19, 28, 43, 53	0
1	F	218/219 (99%)	-0.00	2 (0%) 84 85	21, 29, 45, 70	0
1	G	218/219 (99%)	0.20	6 (2%) 53 56	23, 35, 48, 62	0
All	All	1529/1533 (99%)	-0.08	20 (1%) 77 79	17, 28, 44, 70	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	154	GLY	4.2
1	F	143	GLY	4.2
1	E	154	GLY	3.8
1	C	3	ALA	3.4
1	E	3	ALA	3.1
1	G	63	TYR	3.1
1	D	155	SER	2.9
1	D	154	GLY	2.7
1	F	144	GLN	2.6
1	G	4	GLN	2.4
1	A	102	LEU	2.4
1	G	6	CYS	2.4
1	A	197	LEU	2.3
1	B	143	GLY	2.2
1	C	28	ALA	2.1
1	G	221	GLN	2.1
1	E	155	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	64	ALA	2.0
1	G	145	THR	2.0
1	G	183	GLN	2.0

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

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

## 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

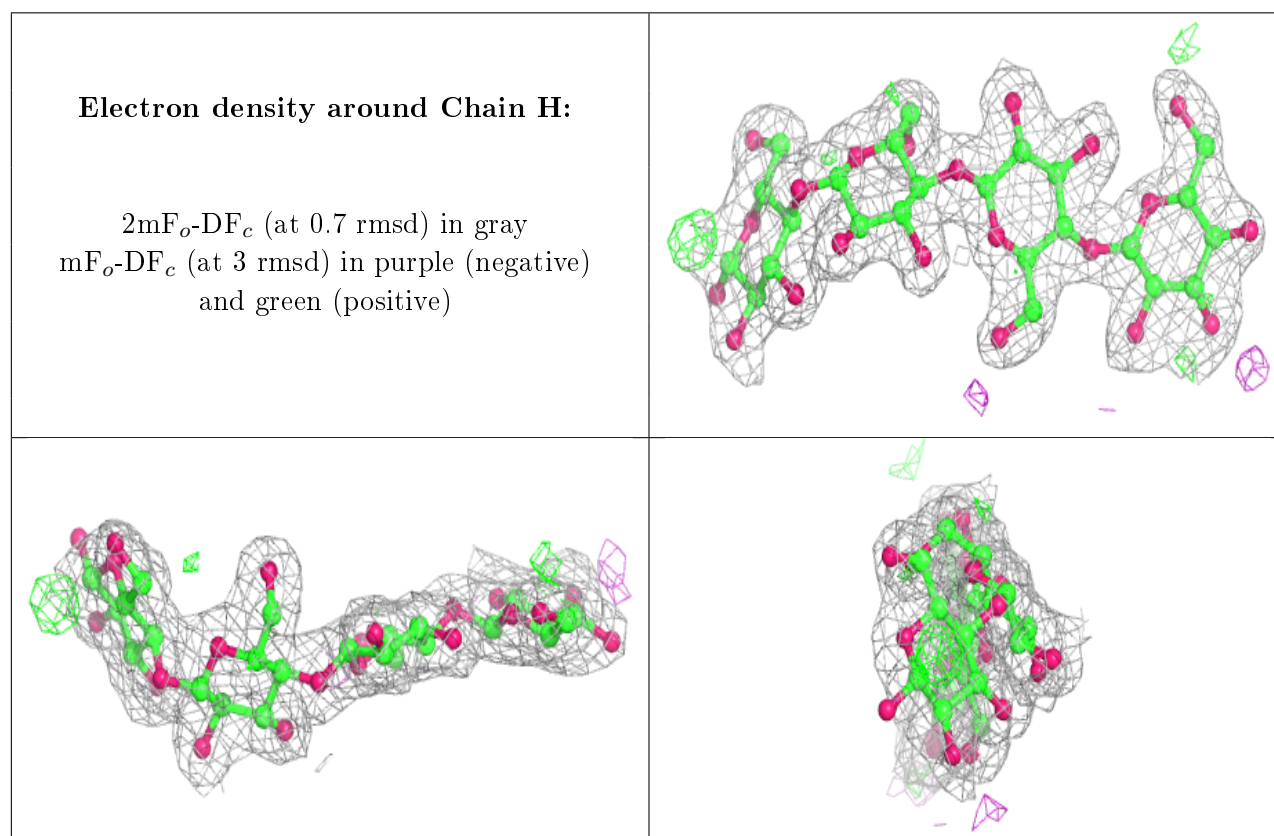
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	BGC	N	1	12/12	0.89	0.14	29,40,51,59	0
2	BGC	K	1	12/12	0.93	0.11	24,35,39,46	0
2	BGC	N	3	11/12	0.93	0.10	27,29,34,37	0
2	BGC	H	4	11/12	0.93	0.11	28,34,39,39	0
2	BGC	L	1	12/12	0.94	0.12	25,32,37,51	0
2	BGC	M	1	12/12	0.94	0.11	23,30,38,54	0
2	BGC	J	1	12/12	0.94	0.14	26,33,45,46	0
2	BGC	N	2	11/12	0.95	0.10	25,28,31,32	0
2	BGC	K	4	11/12	0.95	0.10	30,37,41,41	0
2	BGC	K	3	11/12	0.95	0.10	23,25,29,31	0
2	BGC	L	3	11/12	0.95	0.08	21,23,26,30	0
2	BGC	J	4	11/12	0.95	0.08	29,32,38,43	0
2	BGC	H	3	11/12	0.95	0.10	20,23,26,28	0
2	BGC	I	4	11/12	0.95	0.08	26,29,35,37	0
2	BGC	J	3	11/12	0.95	0.08	23,25,35,53	0
2	BGC	L	4	11/12	0.95	0.09	22,28,35,35	0
2	BGC	H	1	12/12	0.95	0.10	20,31,38,56	0
2	BGC	M	4	11/12	0.95	0.09	29,31,35,47	0
2	BGC	M	3	11/12	0.95	0.09	23,27,29,29	0
2	BGC	I	1	12/12	0.95	0.14	23,35,53,65	0
2	BGC	I	3	11/12	0.96	0.07	21,23,26,27	0
2	BGC	N	4	11/12	0.96	0.09	33,40,49,51	0
2	BGC	K	2	11/12	0.96	0.10	23,25,29,30	0
2	BGC	I	2	11/12	0.97	0.12	20,21,23,23	0
2	BGC	H	2	11/12	0.97	0.09	19,21,26,28	0

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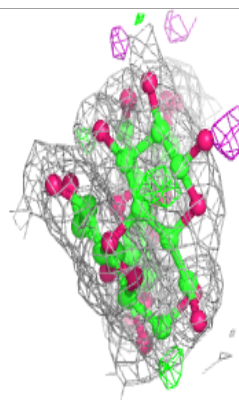
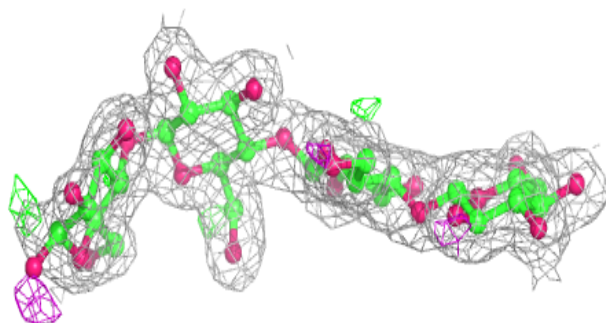
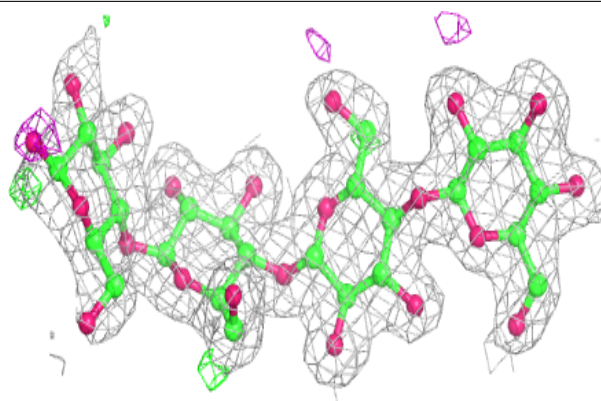
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BGC	J	2	11/12	0.98	0.09	22,24,26,27	0
2	BGC	L	2	11/12	0.98	0.09	22,24,25,26	0
2	BGC	M	2	11/12	0.98	0.08	21,22,24,25	0

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.

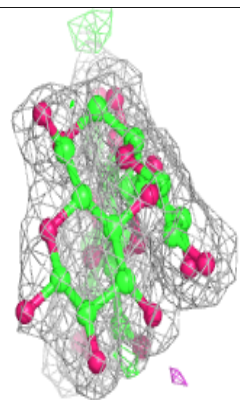
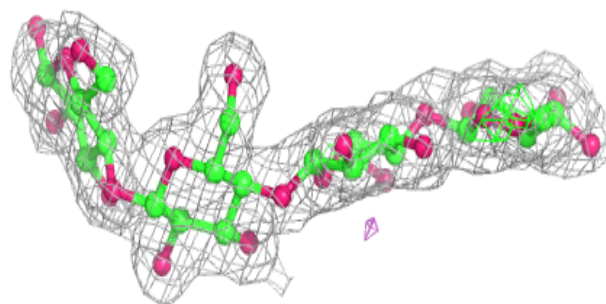
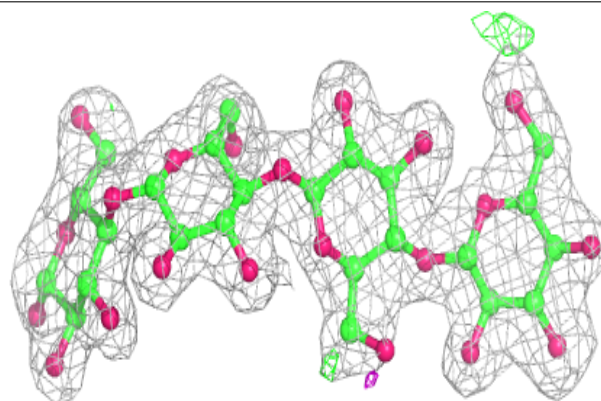


**Electron density around Chain I:**

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

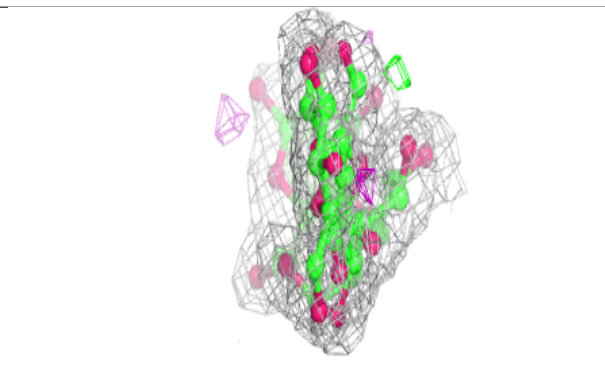
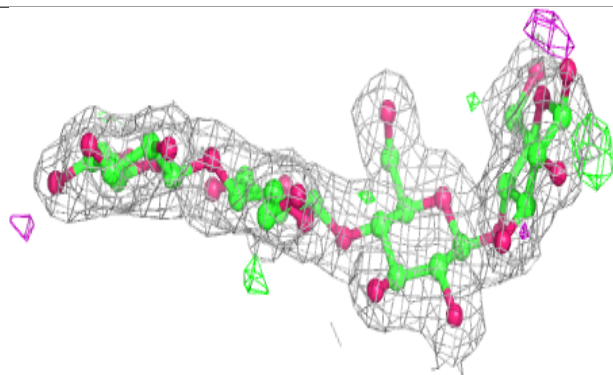
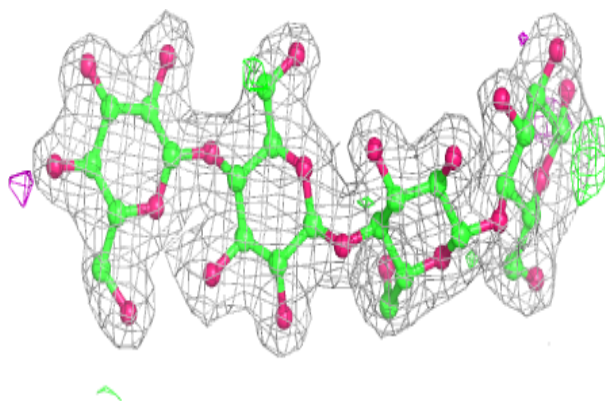
**Electron density around Chain J:**

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

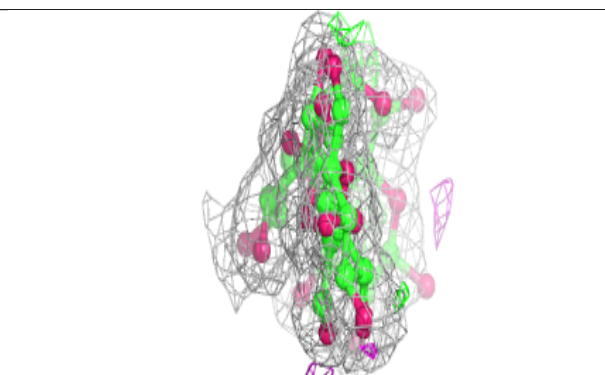
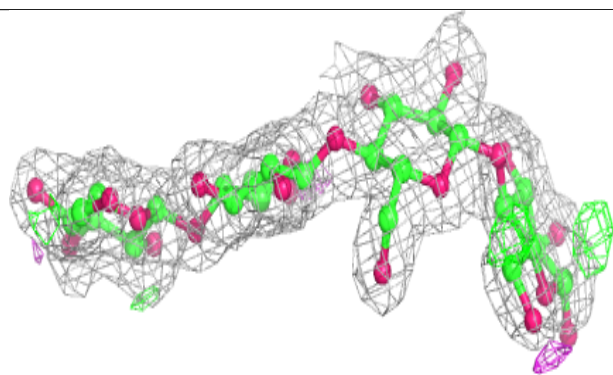
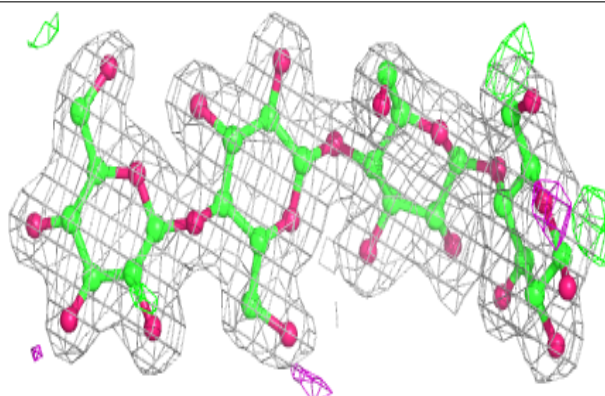


**Electron density around Chain K:**

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

**Electron density around Chain L:**

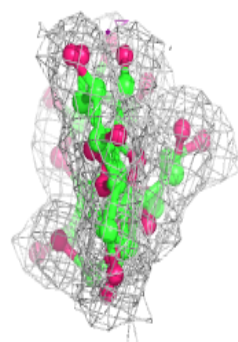
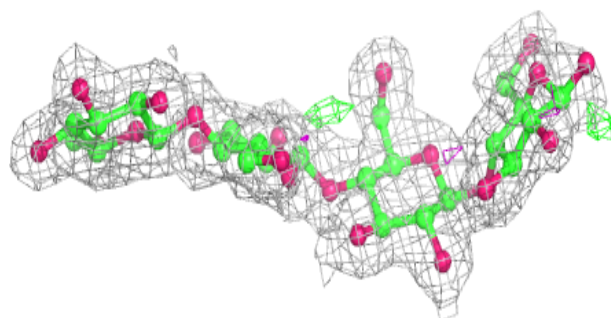
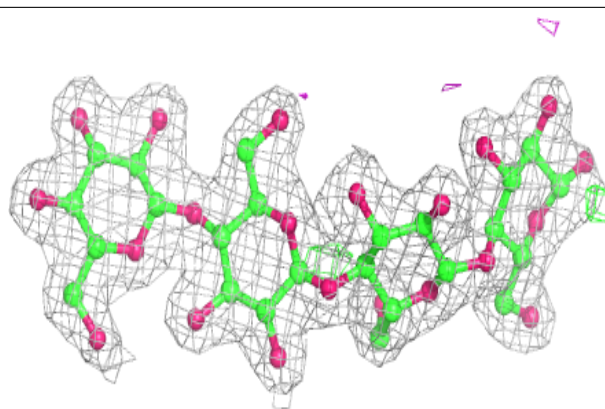
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



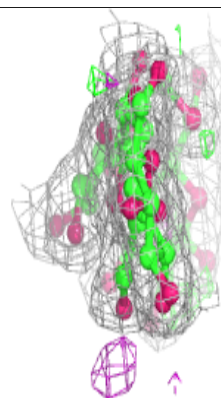
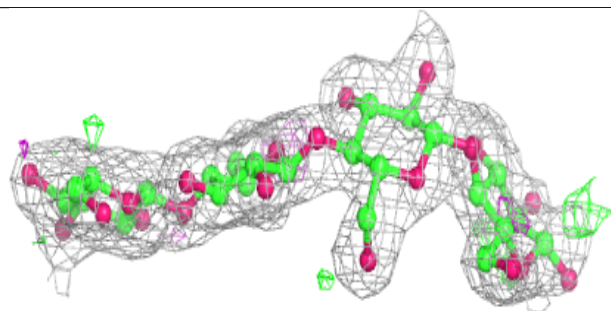
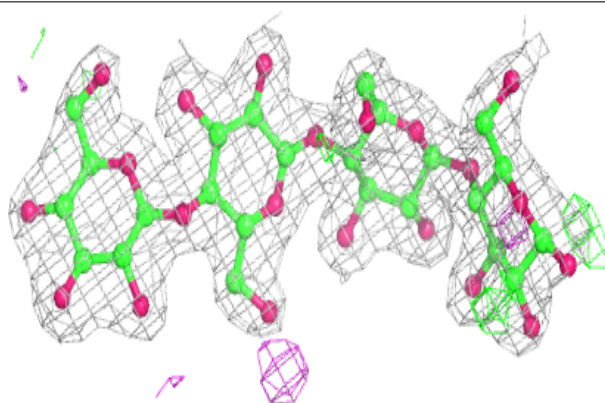


**Electron density around Chain M:**

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

**Electron density around Chain N:**

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





## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	SO4	E	301	5/5	0.69	0.29	92,93,94,99	0
3	SO4	E	303	5/5	0.89	0.22	52,62,86,94	0
3	SO4	A	301	5/5	0.92	0.27	58,65,70,75	0
3	SO4	C	301	5/5	0.92	0.32	70,75,96,111	0
3	SO4	B	301	5/5	0.94	0.31	52,60,78,93	0
3	SO4	D	301	5/5	0.94	0.35	75,77,98,107	0
3	SO4	G	301	5/5	0.95	0.27	66,79,82,95	0
3	SO4	E	302	5/5	0.97	0.28	57,61,71,80	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.