



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 03:16 AM UTC

PDB ID : 8B48 / pdb_00008b48
Title : Structure of Lentithecium fluviatile carbohydrate esterase from the CE15 family (LfCE15C)
Authors : Scholzen, K.; Mazurkewich, S.; Poulsen, J.C.N.; Larsbrink, J.; Lo Leggio, L.
Deposited on : 2022-09-20
Resolution : 2.65 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

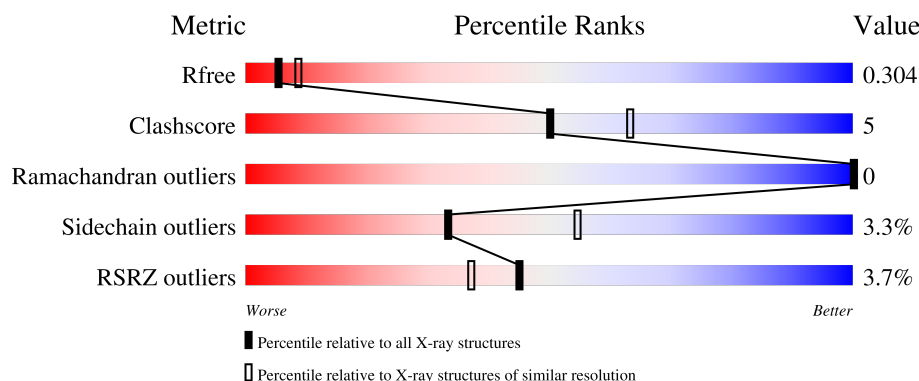
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



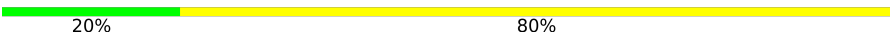
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	394	 3% 80% 13% • 6%
1	B	394	 3% 79% 14% • 6%
1	C	394	 3% 82% 12% 6%
1	D	394	 6% 81% 12% 6%
2	E	4	 75% 25%

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Mol	Chain	Length	Quality of chain
3	F	5	 20%80%
3	H	5	 20%80%
4	G	6	 67%33%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11960 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 Carbohydrate esterase family 15 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	2	0
			2853	1813	492	533	15			
1	B	370	Total	C	N	O	S	0	3	0
			2866	1823	496	534	13			
1	C	370	Total	C	N	O	S	0	0	0
			2847	1809	492	533	13			
1	D	369	Total	C	N	O	S	0	0	0
			2841	1806	491	531	13			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	388	GLY	-	expression tag	UNP A0A6G1IIU9
A	389	LEU	-	expression tag	UNP A0A6G1IIU9
A	390	GLU	-	expression tag	UNP A0A6G1IIU9
A	391	GLN	-	expression tag	UNP A0A6G1IIU9
A	392	LYS	-	expression tag	UNP A0A6G1IIU9
A	393	LEU	-	expression tag	UNP A0A6G1IIU9
A	394	ILE	-	expression tag	UNP A0A6G1IIU9
A	395	SER	-	expression tag	UNP A0A6G1IIU9
A	396	GLU	-	expression tag	UNP A0A6G1IIU9
A	397	GLU	-	expression tag	UNP A0A6G1IIU9
A	398	ASP	-	expression tag	UNP A0A6G1IIU9
A	399	LEU	-	expression tag	UNP A0A6G1IIU9
A	400	ASN	-	expression tag	UNP A0A6G1IIU9
A	401	SER	-	expression tag	UNP A0A6G1IIU9
A	402	ALA	-	expression tag	UNP A0A6G1IIU9
A	403	VAL	-	expression tag	UNP A0A6G1IIU9
A	404	ASP	-	expression tag	UNP A0A6G1IIU9
A	405	HIS	-	expression tag	UNP A0A6G1IIU9
A	406	HIS	-	expression tag	UNP A0A6G1IIU9
A	407	HIS	-	expression tag	UNP A0A6G1IIU9
A	408	HIS	-	expression tag	UNP A0A6G1IIU9

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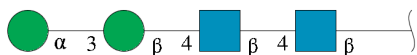
Chain	Residue	Modelled	Actual	Comment	Reference
A	409	HIS	-	expression tag	UNP A0A6G1IIU9
A	410	HIS	-	expression tag	UNP A0A6G1IIU9
B	388	GLY	-	expression tag	UNP A0A6G1IIU9
B	389	LEU	-	expression tag	UNP A0A6G1IIU9
B	390	GLU	-	expression tag	UNP A0A6G1IIU9
B	391	GLN	-	expression tag	UNP A0A6G1IIU9
B	392	LYS	-	expression tag	UNP A0A6G1IIU9
B	393	LEU	-	expression tag	UNP A0A6G1IIU9
B	394	ILE	-	expression tag	UNP A0A6G1IIU9
B	395	SER	-	expression tag	UNP A0A6G1IIU9
B	396	GLU	-	expression tag	UNP A0A6G1IIU9
B	397	GLU	-	expression tag	UNP A0A6G1IIU9
B	398	ASP	-	expression tag	UNP A0A6G1IIU9
B	399	LEU	-	expression tag	UNP A0A6G1IIU9
B	400	ASN	-	expression tag	UNP A0A6G1IIU9
B	401	SER	-	expression tag	UNP A0A6G1IIU9
B	402	ALA	-	expression tag	UNP A0A6G1IIU9
B	403	VAL	-	expression tag	UNP A0A6G1IIU9
B	404	ASP	-	expression tag	UNP A0A6G1IIU9
B	405	HIS	-	expression tag	UNP A0A6G1IIU9
B	406	HIS	-	expression tag	UNP A0A6G1IIU9
B	407	HIS	-	expression tag	UNP A0A6G1IIU9
B	408	HIS	-	expression tag	UNP A0A6G1IIU9
B	409	HIS	-	expression tag	UNP A0A6G1IIU9
B	410	HIS	-	expression tag	UNP A0A6G1IIU9
C	388	GLY	-	expression tag	UNP A0A6G1IIU9
C	389	LEU	-	expression tag	UNP A0A6G1IIU9
C	390	GLU	-	expression tag	UNP A0A6G1IIU9
C	391	GLN	-	expression tag	UNP A0A6G1IIU9
C	392	LYS	-	expression tag	UNP A0A6G1IIU9
C	393	LEU	-	expression tag	UNP A0A6G1IIU9
C	394	ILE	-	expression tag	UNP A0A6G1IIU9
C	395	SER	-	expression tag	UNP A0A6G1IIU9
C	396	GLU	-	expression tag	UNP A0A6G1IIU9
C	397	GLU	-	expression tag	UNP A0A6G1IIU9
C	398	ASP	-	expression tag	UNP A0A6G1IIU9
C	399	LEU	-	expression tag	UNP A0A6G1IIU9
C	400	ASN	-	expression tag	UNP A0A6G1IIU9
C	401	SER	-	expression tag	UNP A0A6G1IIU9
C	402	ALA	-	expression tag	UNP A0A6G1IIU9
C	403	VAL	-	expression tag	UNP A0A6G1IIU9
C	404	ASP	-	expression tag	UNP A0A6G1IIU9

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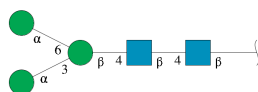
Chain	Residue	Modelled	Actual	Comment	Reference
C	405	HIS	-	expression tag	UNP A0A6G1IIU9
C	406	HIS	-	expression tag	UNP A0A6G1IIU9
C	407	HIS	-	expression tag	UNP A0A6G1IIU9
C	408	HIS	-	expression tag	UNP A0A6G1IIU9
C	409	HIS	-	expression tag	UNP A0A6G1IIU9
C	410	HIS	-	expression tag	UNP A0A6G1IIU9
D	388	GLY	-	expression tag	UNP A0A6G1IIU9
D	389	LEU	-	expression tag	UNP A0A6G1IIU9
D	390	GLU	-	expression tag	UNP A0A6G1IIU9
D	391	GLN	-	expression tag	UNP A0A6G1IIU9
D	392	LYS	-	expression tag	UNP A0A6G1IIU9
D	393	LEU	-	expression tag	UNP A0A6G1IIU9
D	394	ILE	-	expression tag	UNP A0A6G1IIU9
D	395	SER	-	expression tag	UNP A0A6G1IIU9
D	396	GLU	-	expression tag	UNP A0A6G1IIU9
D	397	GLU	-	expression tag	UNP A0A6G1IIU9
D	398	ASP	-	expression tag	UNP A0A6G1IIU9
D	399	LEU	-	expression tag	UNP A0A6G1IIU9
D	400	ASN	-	expression tag	UNP A0A6G1IIU9
D	401	SER	-	expression tag	UNP A0A6G1IIU9
D	402	ALA	-	expression tag	UNP A0A6G1IIU9
D	403	VAL	-	expression tag	UNP A0A6G1IIU9
D	404	ASP	-	expression tag	UNP A0A6G1IIU9
D	405	HIS	-	expression tag	UNP A0A6G1IIU9
D	406	HIS	-	expression tag	UNP A0A6G1IIU9
D	407	HIS	-	expression tag	UNP A0A6G1IIU9
D	408	HIS	-	expression tag	UNP A0A6G1IIU9
D	409	HIS	-	expression tag	UNP A0A6G1IIU9
D	410	HIS	-	expression tag	UNP A0A6G1IIU9

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



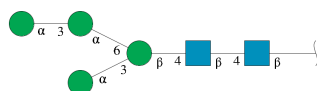
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



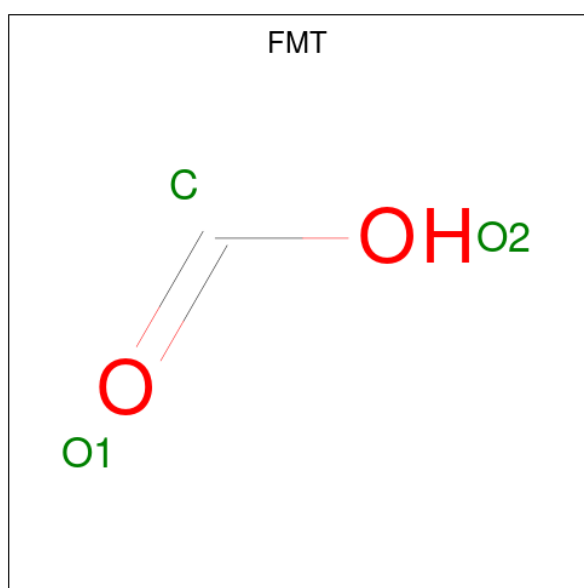
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	H	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 5 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	1	2		
5	D	1	Total	C	O	0	0
			3	1	2		

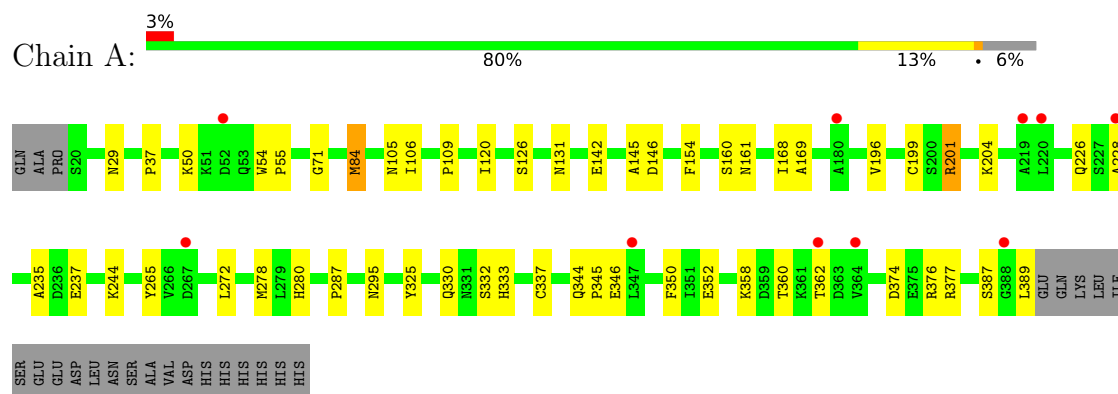
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	78	Total	O	0	0
			78	78		
6	B	80	Total	O	0	0
			80	80		
6	C	76	Total	O	0	0
			76	76		
6	D	69	Total	O	0	0
			69	69		

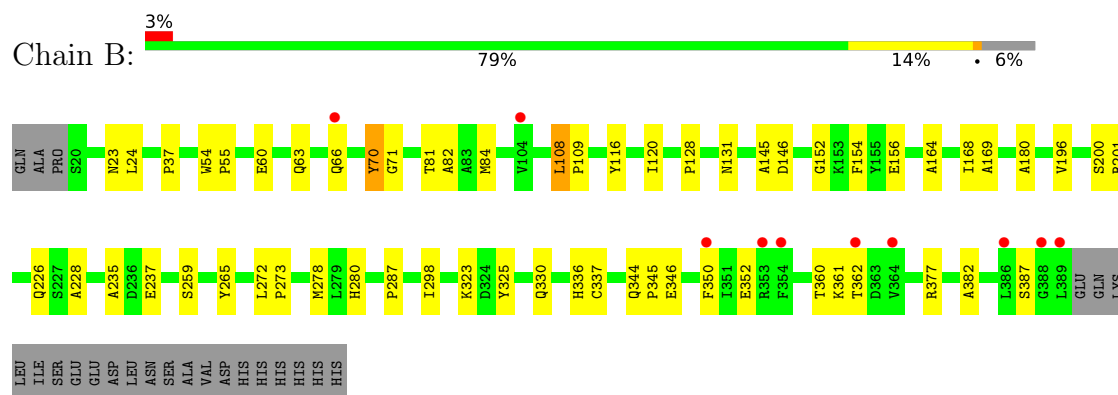
3 Residue-property plots

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

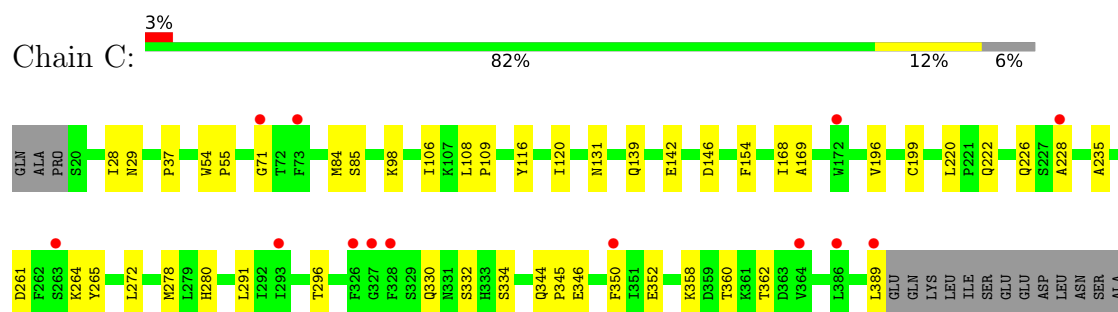
- Molecule 1: Carbohydrate esterase family 15 protein



- Molecule 1: Carbohydrate esterase family 15 protein



- Molecule 1: Carbohydrate esterase family 15 protein



VAL
ASP
HIS
HIS
HIS
HIS
HIS

- Molecule 1: Carbohydrate esterase family 15 protein

Chain D: 

GLN ALA PRO SER C21 P22 N23 L24 I28 N29 P37 D38 P39 F40 W54 P55 E59 Y70 G71 R76 P77 M84 S85 G86 I106 K107 L108 P109 Y116 I120 A121 Y122 P128 N131 T132 E142 K151 F154 M167 I168 A169 V196

CL99 Q222 Q226 S227 A228 A229 C231 L234 A235 M253 D261 K264 Y265 L272 M278 L279 H280 Y283 D324 Q330 S332 H333 S334 Q344 P345 E346 F350 T351 E352 K358 D359 T360 K361 T362 L386 S387 Q388 L389 GLU GLN LYS LEU

TLE SER GLU GLU LEU ASN SER ALA VAL ASP HIS HIS HIS HIS HIS

- Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 

MAG1
MAG2
BMA3
MAN4

- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 

MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 

MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 4: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	70.74Å 79.57Å 86.01Å 113.32° 98.53° 94.44°	Depositor
Resolution (Å)	47.25 – 2.65 47.25 – 2.65	Depositor EDS
% Data completeness (in resolution range)	97.6 (47.25-2.65) 97.6 (47.25-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.238 , 0.298 0.241 , 0.304	Depositor DCC
R_{free} test set	2294 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11960	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% 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: MAN, FMT, NAG, BMA

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	1.00	0/2937	1.36	3/3992 (0.1%)
1	B	1.00	0/2954	1.38	2/4014 (0.0%)
1	C	1.00	0/2925	1.37	1/3976 (0.0%)
1	D	0.99	0/2919	1.36	1/3968 (0.0%)
All	All	1.00	0/11735	1.37	7/15950 (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	D	71	GLY	CA-C-O	-7.29	116.76	122.52
1	A	71	GLY	CA-C-O	-6.97	117.01	122.52
1	C	71	GLY	CA-C-O	-6.51	117.38	122.52
1	B	145	ALA	CA-C-N	5.15	127.44	120.65
1	B	145	ALA	C-N-CA	5.15	127.44	120.65

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	2853	0	2783	32	0
1	B	2866	0	2801	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2847	0	2773	25	0
1	D	2841	0	2768	23	0
2	E	50	0	43	1	0
3	F	61	0	52	0	0
3	H	61	0	52	0	0
4	G	72	0	61	1	0
5	A	3	0	1	0	0
5	D	3	0	1	0	0
6	A	78	0	0	3	0
6	B	80	0	0	7	0
6	C	76	0	0	2	0
6	D	69	0	0	3	0
All	All	11960	0	11335	121	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 121 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:298:ILE:HD12	1:B:336[A]:HIS:CE1	2.18	0.77
1:B:273:PRO:O	6:B:501:HOH:O	2.11	0.68
1:B:200:SER:HB2	1:B:336[B]:HIS:NE2	2.09	0.66
1:C:139:GLN:HB3	1:C:142:GLU:OE1	1.94	0.66
1:A:201:ARG:HG2	1:A:201:ARG:HH11	1.60	0.66

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	370/394 (94%)	347 (94%)	23 (6%)	0	100	100
1	B	371/394 (94%)	348 (94%)	23 (6%)	0	100	100
1	C	368/394 (93%)	348 (95%)	20 (5%)	0	100	100
1	D	367/394 (93%)	345 (94%)	22 (6%)	0	100	100
All	All	1476/1576 (94%)	1388 (94%)	88 (6%)	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	301/321 (94%)	291 (97%)	10 (3%)	33	55
1	B	302/321 (94%)	295 (98%)	7 (2%)	44	66
1	C	299/321 (93%)	291 (97%)	8 (3%)	39	61
1	D	298/321 (93%)	283 (95%)	15 (5%)	22	37
All	All	1200/1284 (94%)	1160 (97%)	40 (3%)	33	55

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	76	ARG
1	D	332	SER
1	D	85	SER
1	D	151	LYS
1	D	346	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	226	GLN
1	D	330	GLN
1	C	306	ASN

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Mol	Chain	Res	Type
1	D	306	ASN
1	C	280	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

20 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	E	1	1,2	14,14,15	1.21	2 (14%)	17,19,21	2.20	5 (29%)
2	NAG	E	2	2	14,14,15	0.54	0	17,19,21	1.14	1 (5%)
2	BMA	E	3	2	11,11,12	0.43	0	15,15,17	1.99	4 (26%)
2	MAN	E	4	2	11,11,12	0.51	0	15,15,17	1.41	3 (20%)
3	NAG	F	1	1,3	14,14,15	0.46	0	17,19,21	2.90	10 (58%)
3	NAG	F	2	3	14,14,15	0.58	0	17,19,21	2.51	6 (35%)
3	BMA	F	3	3	11,11,12	0.39	0	15,15,17	1.00	2 (13%)
3	MAN	F	4	3	11,11,12	0.32	0	15,15,17	1.20	2 (13%)
3	MAN	F	5	3	11,11,12	0.32	0	15,15,17	0.79	0
4	NAG	G	1	1,4	14,14,15	0.46	0	17,19,21	2.05	2 (11%)
4	NAG	G	2	4	14,14,15	0.41	0	17,19,21	1.63	4 (23%)
4	BMA	G	3	4	11,11,12	0.37	0	15,15,17	1.44	2 (13%)
4	MAN	G	4	4	11,11,12	0.59	0	15,15,17	1.60	3 (20%)
4	MAN	G	5	4	11,11,12	0.34	0	15,15,17	1.40	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	G	6	4	11,11,12	0.49	0	15,15,17	1.31	1 (6%)
3	NAG	H	1	1,3	14,14,15	0.56	0	17,19,21	2.21	4 (23%)
3	NAG	H	2	3	14,14,15	0.54	0	17,19,21	0.96	0
3	BMA	H	3	3	11,11,12	0.24	0	15,15,17	1.80	6 (40%)
3	MAN	H	4	3	11,11,12	0.39	0	15,15,17	1.01	1 (6%)
3	MAN	H	5	3	11,11,12	0.53	0	15,15,17	1.13	1 (6%)

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	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	1/6/23/26	0/1/1/1
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1
2	MAN	E	4	2	-	2/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	5/6/23/26	0/1/1/1
3	BMA	F	3	3	-	2/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	MAN	F	5	3	-	0/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	2/2/19/22	0/1/1/1
4	MAN	G	4	4	-	0/2/19/22	0/1/1/1
4	MAN	G	5	4	-	1/2/19/22	0/1/1/1
4	MAN	G	6	4	-	0/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	BMA	H	3	3	-	2/2/19/22	0/1/1/1
3	MAN	H	4	3	-	2/2/19/22	0/1/1/1
3	MAN	H	5	3	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	NAG	O5-C5	-2.57	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	NAG	C2-N2	-2.28	1.42	1.46

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	NAG	C1-O5-C5	7.54	122.29	112.19
3	F	1	NAG	C1-O5-C5	7.38	122.08	112.19
4	G	1	NAG	C1-O5-C5	6.58	121.00	112.19
3	F	2	NAG	C1-O5-C5	-5.20	105.22	112.19
2	E	3	BMA	C1-O5-C5	5.06	118.96	112.19

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	2	NAG	O5-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
4	G	3	BMA	C4-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6

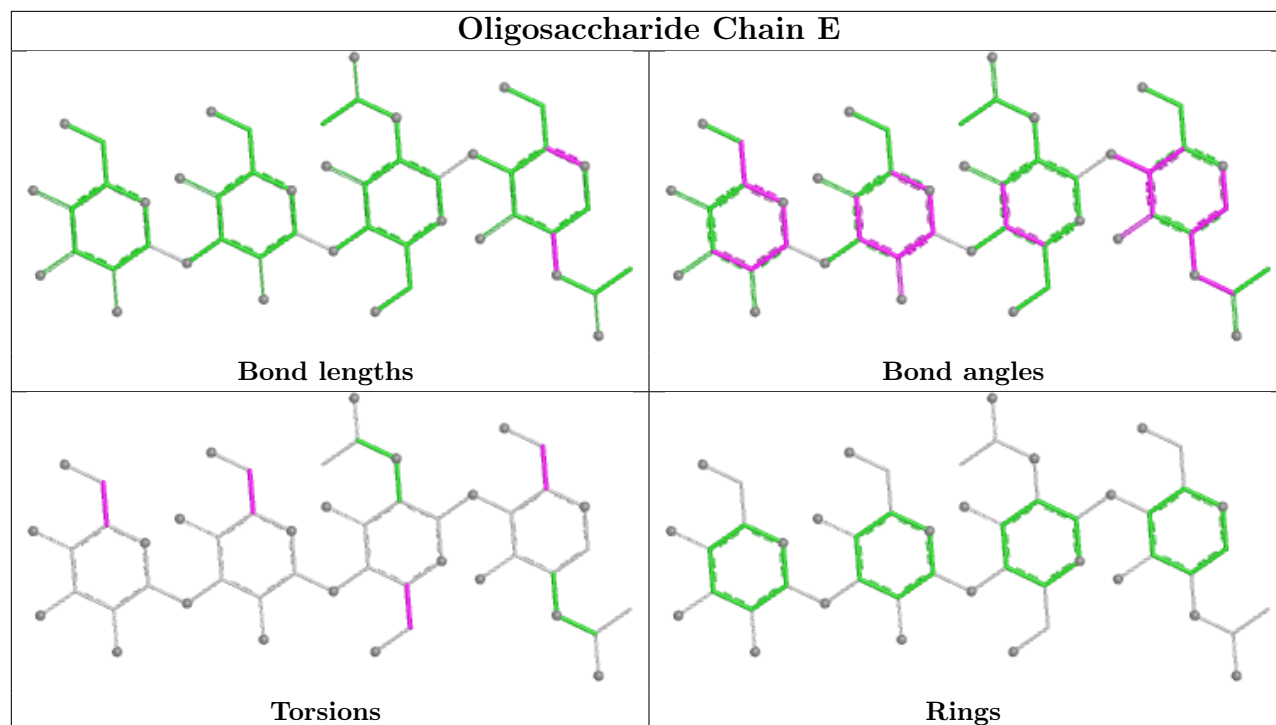
There are no ring outliers.

3 monomers are involved in 2 short contacts:

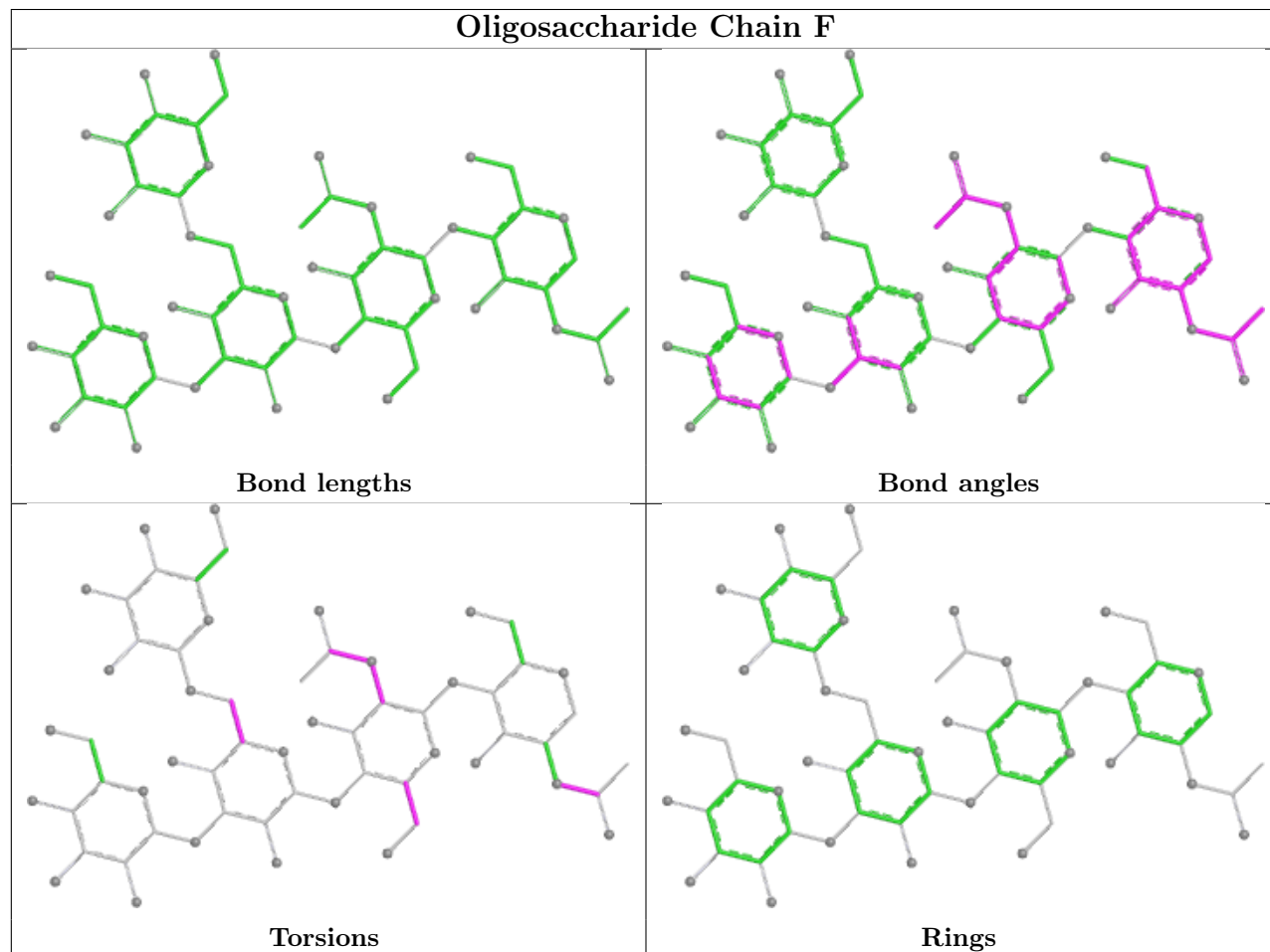
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	6	MAN	1	0
4	G	3	BMA	1	0
2	E	1	NAG	1	0

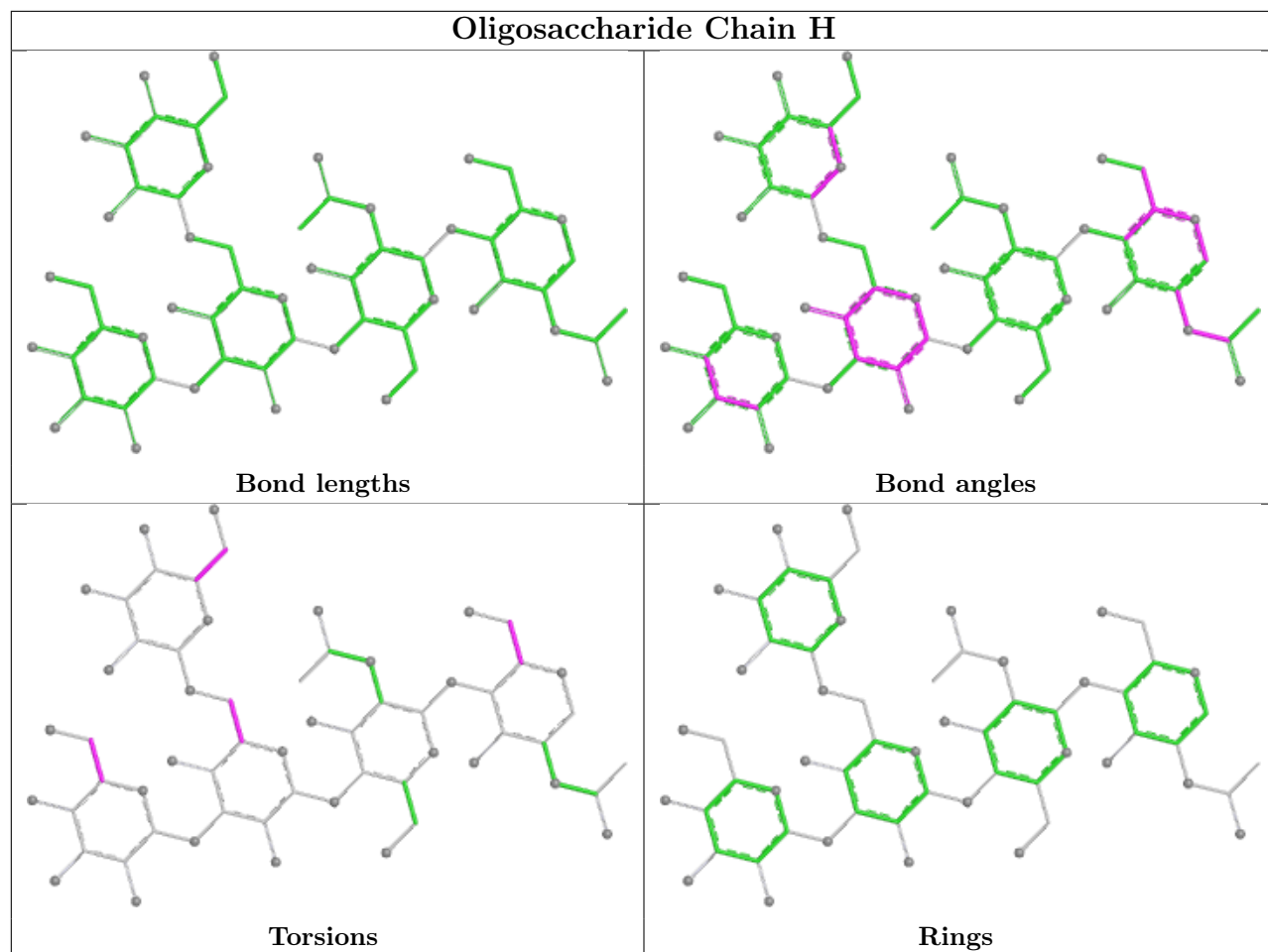
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

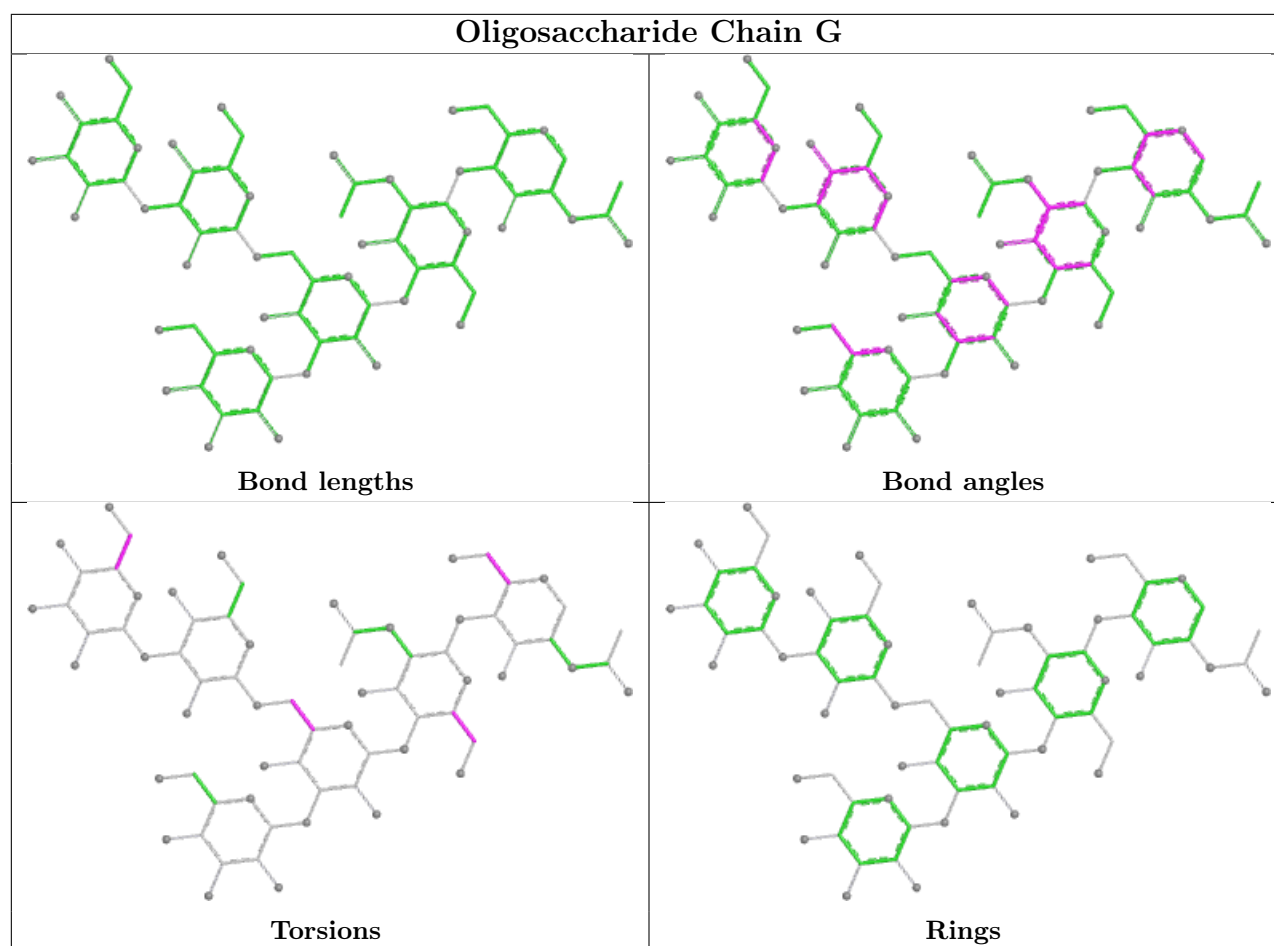
Oligosaccharide Chain E



Oligosaccharide Chain F







5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
5	FMT	D	501	-	2,2,2	0.36	0	1,1,1	0.12	0
5	FMT	A	501	-	2,2,2	0.32	0	1,1,1	0.16	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 [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	370/394 (93%)	0.53	10 (2%) 56 49	40, 61, 84, 107	2 (0%)
1	B	370/394 (93%)	0.41	10 (2%) 56 49	35, 56, 77, 129	3 (0%)
1	C	370/394 (93%)	0.54	13 (3%) 47 38	39, 59, 87, 144	0
1	D	369/394 (93%)	0.70	22 (5%) 27 21	41, 67, 94, 162	0
All	All	1479/1576 (93%)	0.55	55 (3%) 45 37	35, 60, 88, 162	5 (0%)

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	326	PHE	5.1
1	C	293	ILE	4.4
1	B	362	THR	4.0
1	D	389	LEU	3.8
1	D	235	ALA	3.7

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
3	MAN	H	5	11/12	0.41	0.15	121,144,152,155	0
3	BMA	F	3	11/12	0.48	0.12	138,175,185,200	0

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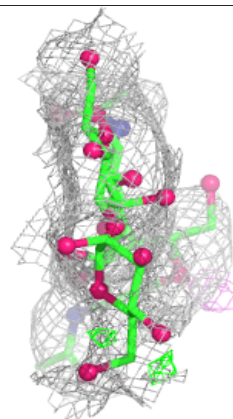
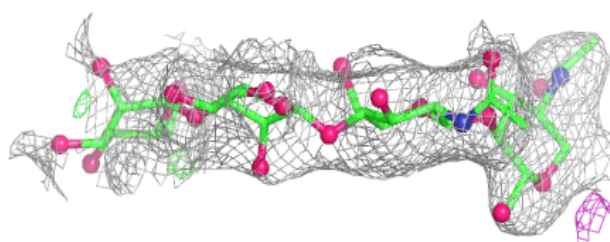
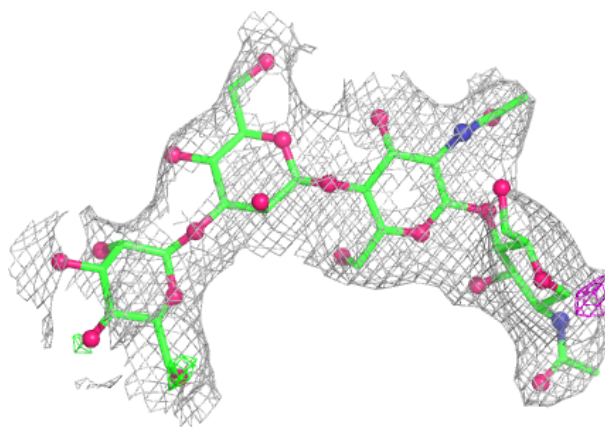
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MAN	G	5	11/12	0.48	0.11	104,143,165,174	0
2	MAN	E	4	11/12	0.52	0.14	128,173,182,191	0
4	MAN	G	6	11/12	0.52	0.14	107,140,155,164	0
3	MAN	F	4	11/12	0.53	0.12	153,172,190,195	0
3	MAN	F	5	11/12	0.54	0.14	115,157,181,181	0
3	BMA	H	3	11/12	0.54	0.10	125,135,149,161	0
3	MAN	H	4	11/12	0.54	0.13	122,145,161,163	0
4	BMA	G	3	11/12	0.55	0.10	121,143,163,168	0
4	MAN	G	4	11/12	0.58	0.12	71,126,148,181	0
2	BMA	E	3	11/12	0.65	0.09	105,129,138,144	0
2	NAG	E	2	14/15	0.85	0.10	62,74,90,90	0
3	NAG	H	2	14/15	0.86	0.13	82,99,107,116	0
4	NAG	G	2	14/15	0.86	0.10	76,83,94,113	0
3	NAG	F	2	14/15	0.87	0.11	85,95,106,121	0
3	NAG	F	1	14/15	0.89	0.11	58,70,78,81	0
4	NAG	G	1	14/15	0.90	0.09	46,65,69,75	0
2	NAG	E	1	14/15	0.90	0.11	59,71,86,90	0
3	NAG	H	1	14/15	0.92	0.10	49,56,68,69	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.

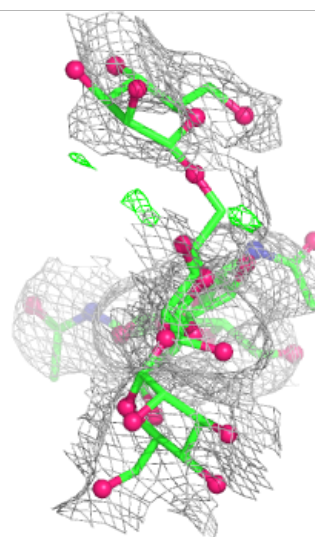
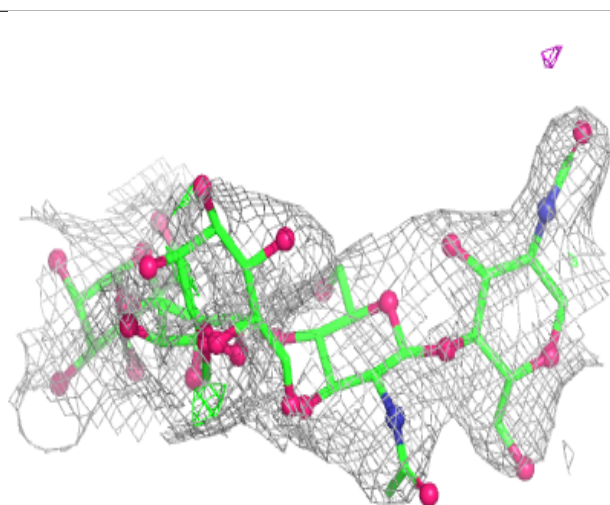
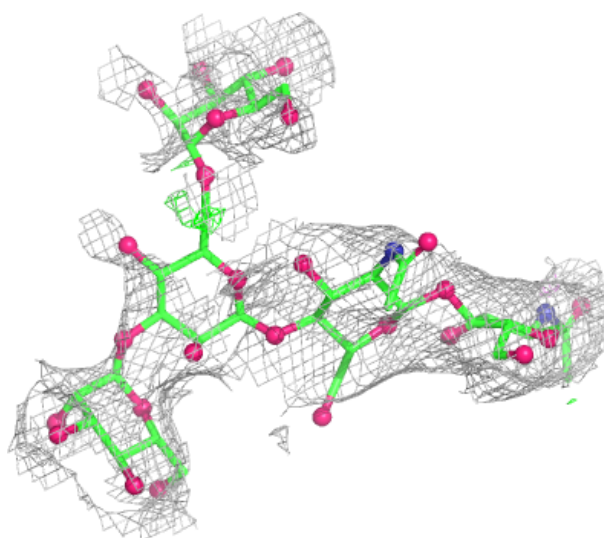
Electron density around Chain E:

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



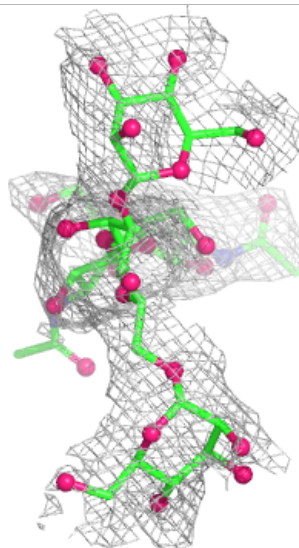
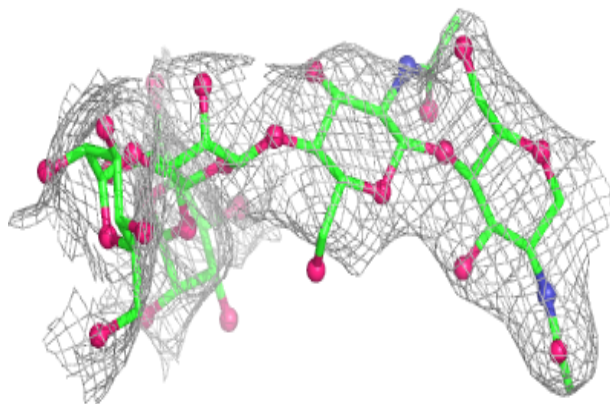
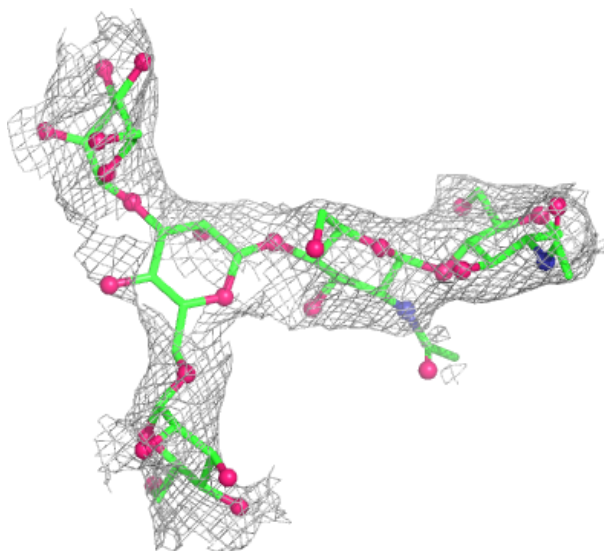
Electron density around Chain F:

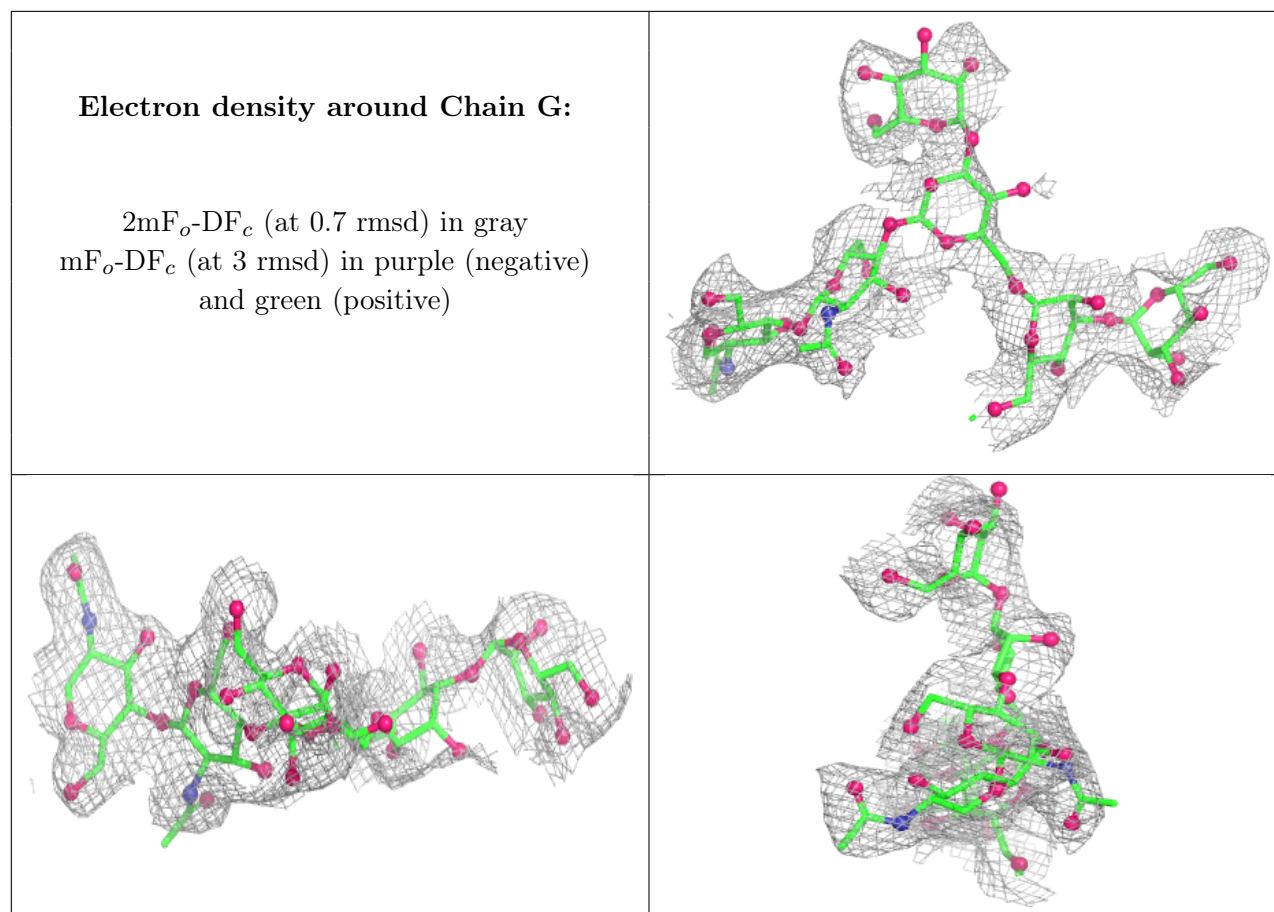
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain H:

$2mF_o-DF_c$ (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($\text{\AA}^2$)	Q<0.9
5	FMT	A	501	3/3	0.69	0.16	69,69,73,74	0
5	FMT	D	501	3/3	0.73	0.13	60,60,61,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.