



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:33 AM UTC

PDB ID : 6ZZ3 / pdb_00006zz3
Title : RBcell1 cellulase variant Y201F with cellotriose covalently bound
Authors : Collet, L.; Dutoit, R.
Deposited on : 2020-08-03
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

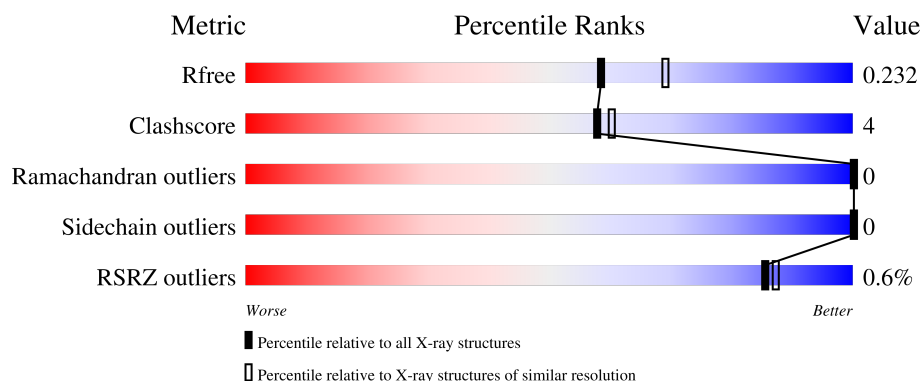
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

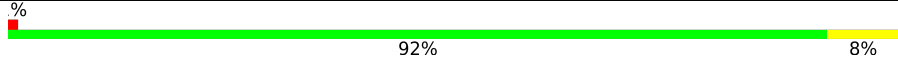
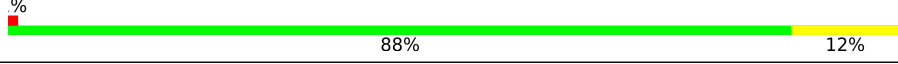
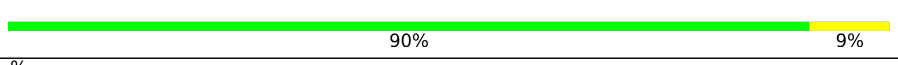
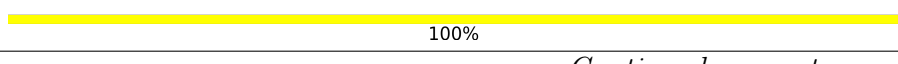
The reported resolution of this entry is 2.10 Å.

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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	320	
1	B	320	
1	C	320	
1	D	320	
2	E	3	

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

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10792 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.

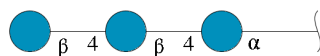
- Molecule 1 is a protein called Endoglucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	6	0
			2570	1657	429	475	9			
1	B	320	Total	C	N	O	S	0	3	1
			2521	1621	424	468	8			
1	C	319	Total	C	N	O	S	0	7	1
			2559	1648	426	476	9			
1	D	320	Total	C	N	O	S	0	2	0
			2535	1631	426	469	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	PHE	TYR	engineered mutation	UNP C1JI15
B	201	PHE	TYR	engineered mutation	UNP C1JI15
C	201	PHE	TYR	engineered mutation	UNP C1JI15
D	201	PHE	TYR	engineered mutation	UNP C1JI15

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



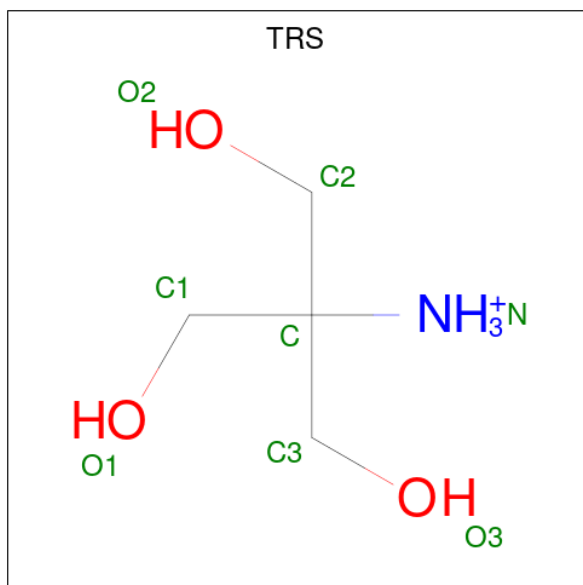
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	3	Total	C	O	0	0	0
			33	18	15			
2	F	3	Total	C	O	0	0	0
			33	18	15			
2	G	3	Total	C	O	0	0	0
			33	18	15			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	H	3	Total	C	O	0	0	0
			33	18	15			

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		

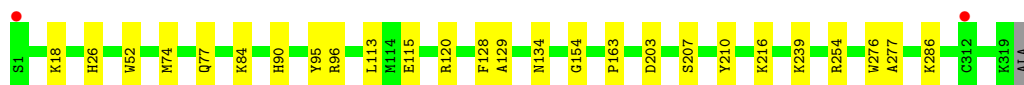
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	198	Total	O	0	0
			198	198		
4	B	61	Total	O	0	0
			61	61		
4	C	100	Total	O	0	0
			100	100		
4	D	108	Total	O	0	0
			108	108		

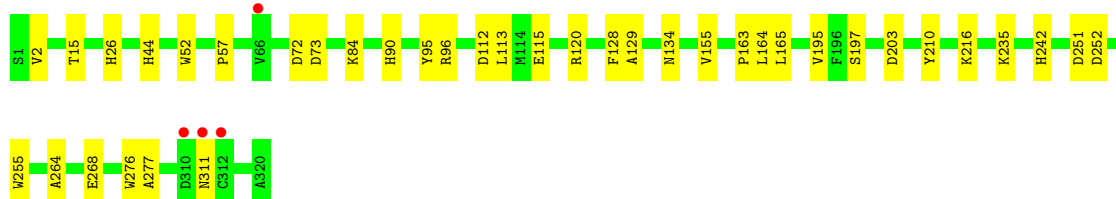
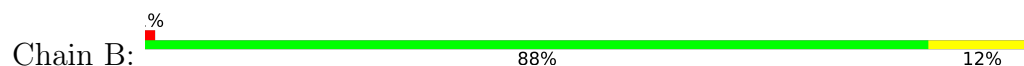
3 Residue-property plots

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: Endoglucanase



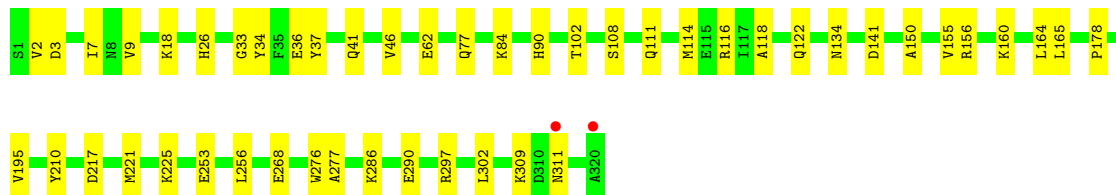
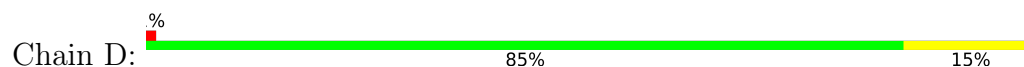
• Molecule 1: Endoglucanase



• Molecule 1: Endoglucanase



• Molecule 1: Endoglucanase



• Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-alpha-D-glucopyranos e

Chain E:  100%

GLC1
BGC2
BGC3

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

Chain F:  100%

GLC1
BGC2
BGC3

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

Chain G:  100%

GLC1
BGC2
BGC3

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

Chain H:  100%

GLC1
BGC2
BGC3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.00Å 61.89Å 177.26Å 90.00° 97.11° 90.00°	Depositor
Resolution (Å)	45.10 – 2.10 45.10 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (45.10-2.10) 99.5 (45.10-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.11-2563	Depositor
R, R_{free}	0.195 , 0.229 0.198 , 0.232	Depositor DCC
R_{free} test set	3607 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 32.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10792	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.98 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.6145e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, BGC, 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	0.31	0/2666	0.51	0/3613
1	B	0.29	1/2605 (0.0%)	0.49	0/3542
1	C	0.25	0/2655	0.49	1/3604 (0.0%)
1	D	0.27	0/2616	0.55	2/3553 (0.1%)
All	All	0.28	1/10542 (0.0%)	0.51	3/14312 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	216	LYS	CD-CE	5.58	1.69	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	179	ARG	NE-CZ-NH2	-9.21	110.91	119.20
1	D	309	LYS	CA-C-N	-6.03	113.43	122.47
1	D	309	LYS	C-N-CA	-6.03	113.43	122.47

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	179	ARG	Sidechain

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	2570	0	2479	18	0
1	B	2521	0	2379	22	0
1	C	2559	0	2444	19	0
1	D	2535	0	2412	33	0
2	E	33	0	28	0	0
2	F	33	0	28	0	0
2	G	33	0	28	0	0
2	H	33	0	28	0	0
3	A	8	0	12	1	0
4	A	198	0	0	4	0
4	B	61	0	0	3	1
4	C	100	0	0	3	0
4	D	108	0	0	9	1
All	All	10792	0	9838	90	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 4.

All (90) 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:D:108:SER:OG	4:D:401:HOH:O	1.90	0.89
1:B:73:ASP:OD2	4:B:402:HOH:O	1.93	0.87
1:C:96:ARG:NH2	4:C:402:HOH:O	2.07	0.86
1:D:62[A]:GLU:OE2	1:D:116:ARG:NH1	2.15	0.78
1:D:253:GLU:O	4:D:402:HOH:O	2.06	0.73
1:C:103:GLU:N	4:C:403:HOH:O	2.24	0.69
1:D:2:VAL:O	4:D:403:HOH:O	2.09	0.69
1:C:319:LYS:N	4:C:404:HOH:O	2.30	0.64
1:D:297:ARG:O	4:D:404:HOH:O	2.15	0.62
1:B:251:ASP:OD1	4:B:403:HOH:O	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:ASP:OD2	1:B:120:ARG:NH2	2.32	0.60
1:A:286:LYS:O	4:A:501:HOH:O	2.16	0.60
1:B:84:LYS:HB2	1:B:128:PHE:HB2	1.83	0.60
1:A:216:LYS:HE2	1:D:221[A]:MET:HE2	1.84	0.59
1:C:95:TYR:CE2	1:C:96:ARG:HG3	2.38	0.58
1:D:114:MET:HB3	1:D:155:VAL:HG23	1.86	0.58
1:C:84:LYS:HB3	1:C:128:PHE:HB2	1.87	0.57
1:D:141:ASP:OD2	4:D:405:HOH:O	2.17	0.57
1:C:264:ALA:O	1:C:268[B]:GLU:HG2	2.05	0.57
1:B:235:LYS:O	4:B:404:HOH:O	2.17	0.56
1:D:256:LEU:HD12	1:D:302:LEU:HD12	1.87	0.56
1:D:90:HIS:HA	1:D:134:ASN:HB3	1.87	0.55
1:D:311:ASN:OD1	1:D:311:ASN:N	2.40	0.54
1:D:34:TYR:OH	1:D:290:GLU:OE1	2.25	0.53
1:B:44:HIS:O	1:B:84:LYS:HG2	2.08	0.53
1:C:95:TYR:CD2	1:C:96:ARG:HG3	2.44	0.52
1:D:155:VAL:HG11	1:D:164:LEU:HD21	1.92	0.52
1:D:102:THR:O	4:D:407:HOH:O	2.19	0.51
1:C:90:HIS:HA	1:C:134:ASN:HB3	1.93	0.51
1:C:276:TRP:CD2	1:C:277:ALA:HB2	2.46	0.51
1:D:18:LYS:HG3	1:D:26:HIS:CD2	2.46	0.51
1:C:155:VAL:HG11	1:C:164:LEU:HD21	1.93	0.50
1:D:268:GLU:OE1	4:D:406:HOH:O	2.19	0.50
1:A:90:HIS:HA	1:A:134:ASN:HB3	1.92	0.50
1:A:84:LYS:HB3	1:A:128:PHE:HB2	1.94	0.50
1:A:239:LYS:NZ	4:A:505:HOH:O	2.24	0.49
1:D:156:ARG:O	1:D:160:LYS:HD3	2.12	0.49
1:A:18:LYS:HG3	1:A:26:HIS:CD2	2.48	0.49
1:A:207:SER:O	3:A:401:TRS:H21	2.12	0.49
1:C:231:VAL:HA	1:C:234:LEU:HD12	1.94	0.49
1:B:90:HIS:HA	1:B:134:ASN:HB3	1.94	0.49
1:D:3:ASP:OD2	1:D:84:LYS:NZ	2.41	0.49
1:C:240:LYS:NZ	1:C:315:PHE:O	2.35	0.48
1:B:203:ASP:HB3	1:B:210:TYR:CD1	2.49	0.48
1:A:203:ASP:HB3	1:A:210:TYR:CD2	2.49	0.47
1:B:197:SER:HA	1:B:242:HIS:O	2.14	0.47
1:C:114:MET:HB3	1:C:155:VAL:HG23	1.96	0.47
1:B:252:ASP:HB3	1:B:255:TRP:CD1	2.50	0.46
1:A:254:ARG:NH2	1:D:217:ASP:OD2	2.44	0.46
1:B:264:ALA:O	1:B:268[B]:GLU:HG3	2.15	0.46
1:C:197:SER:HA	1:C:242:HIS:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:TRP:CD2	1:D:277:ALA:HB2	2.52	0.45
1:A:115:GLU:HG3	1:A:154:GLY:HA2	1.99	0.45
1:D:210:TYR:O	1:D:286:LYS:NZ	2.51	0.44
1:B:95:TYR:CE2	1:B:96:ARG:HG3	2.52	0.44
1:B:155:VAL:HG11	1:B:164:LEU:HD21	1.98	0.44
1:B:276:TRP:CD2	1:B:277:ALA:HB2	2.52	0.44
1:D:9:VAL:O	1:D:9:VAL:HG23	2.17	0.44
1:D:33:GLY:H	1:D:77:GLN:NE2	2.14	0.44
1:B:52:TRP:CE2	1:B:113:LEU:HD22	2.53	0.44
1:C:74:MET:HE3	1:C:74:MET:HB3	1.83	0.43
1:C:285:TYR:CE2	1:C:287:LEU:HB2	2.53	0.43
1:D:111:GLN:HB2	1:D:150:ALA:HB1	1.99	0.43
1:B:203:ASP:OD1	1:B:203:ASP:N	2.48	0.43
1:A:129:ALA:HB2	1:A:163:PRO:HG2	2.01	0.43
1:A:276:TRP:CD2	1:A:277:ALA:HB2	2.53	0.43
1:B:129:ALA:HB2	1:B:163:PRO:HG2	2.01	0.43
1:A:77:GLN:HB2	4:A:538:HOH:O	2.18	0.42
1:A:95:TYR:CE2	1:A:96:ARG:HG3	2.54	0.42
1:B:2:VAL:O	1:B:311:ASN:ND2	2.52	0.42
1:D:221[A]:MET:HE3	1:D:225:LYS:HE3	2.00	0.42
1:C:176:ARG:O	1:C:179:ARG:HB2	2.18	0.42
1:D:118:ALA:O	1:D:122:GLN:HB2	2.20	0.42
1:B:165:LEU:HA	1:B:195:VAL:O	2.20	0.42
1:C:249:PRO:HG2	1:C:255:TRP:NE1	2.34	0.42
1:D:37:TYR:O	1:D:41:GLN:HG2	2.20	0.42
1:D:36:GLU:OE2	4:D:408:HOH:O	2.20	0.42
1:D:178:PRO:O	4:D:409:HOH:O	2.22	0.42
1:D:221[A]:MET:HE3	1:D:225:LYS:CE	2.50	0.42
1:B:112:ASP:O	1:B:115[B]:GLU:HG2	2.20	0.41
1:B:15:THR:HB	1:B:26:HIS:HB3	2.01	0.41
1:B:57:PRO:O	1:B:96:ARG:NH2	2.50	0.41
1:C:214:PRO:O	1:C:218:PHE:HB2	2.20	0.41
1:A:120:ARG:HD2	4:A:518:HOH:O	2.19	0.41
1:D:7:ILE:O	1:D:46:VAL:HA	2.21	0.41
1:D:165:LEU:HA	1:D:195:VAL:O	2.21	0.41
1:A:52:TRP:CE2	1:A:113:LEU:HD22	2.55	0.41
1:D:9:VAL:HG22	1:D:46:VAL:HG13	2.02	0.41
1:A:18:LYS:HA	1:A:18:LYS:HD3	1.81	0.40
1:A:74:MET:HE3	1:A:74:MET:HB3	1.94	0.40

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)
4:B:459:HOH:O	4:D:440:HOH:O[1_655]	2.07	0.13

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	323/320 (101%)	316 (98%)	7 (2%)	0	100	100
1	B	321/320 (100%)	314 (98%)	7 (2%)	0	100	100
1	C	324/320 (101%)	318 (98%)	6 (2%)	0	100	100
1	D	320/320 (100%)	315 (98%)	5 (2%)	0	100	100
All	All	1288/1280 (101%)	1263 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	263/263 (100%)	263 (100%)	0	100	100
1	B	251/263 (95%)	251 (100%)	0	100	100
1	C	259/263 (98%)	259 (100%)	0	100	100
1	D	254/263 (97%)	254 (100%)	0	100	100
All	All	1027/1052 (98%)	1027 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	269	ASN
1	A	274	ASN
1	B	60	ASN
1	B	274	ASN
1	C	60	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 ⓘ

12 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	1,2	11,11,12	1.52	3 (27%)	15,15,17	0.80	0
2	BGC	E	2	2	11,11,12	1.18	1 (9%)	15,15,17	0.72	0
2	BGC	E	3	2	11,11,12	1.64	3 (27%)	15,15,17	0.72	0
2	GLC	F	1	1,2	11,11,12	1.76	3 (27%)	15,15,17	0.84	0
2	BGC	F	2	2	11,11,12	1.28	1 (9%)	15,15,17	0.99	1 (6%)
2	BGC	F	3	2	11,11,12	1.58	3 (27%)	15,15,17	0.63	0
2	GLC	G	1	1,2	11,11,12	1.61	3 (27%)	15,15,17	0.69	0
2	BGC	G	2	2	11,11,12	1.35	2 (18%)	15,15,17	0.85	0
2	BGC	G	3	2	11,11,12	1.85	3 (27%)	15,15,17	1.08	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	H	1	1,2	11,11,12	1.59	3 (27%)	15,15,17	1.10	1 (6%)
2	BGC	H	2	2	11,11,12	1.19	1 (9%)	15,15,17	0.81	0
2	BGC	H	3	2	11,11,12	1.60	2 (18%)	15,15,17	1.12	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	GLC	E	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	E	2	2	-	1/2/19/22	0/1/1/1
2	BGC	E	3	2	-	0/2/19/22	0/1/1/1
2	GLC	F	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	F	2	2	-	0/2/19/22	0/1/1/1
2	BGC	F	3	2	-	1/2/19/22	0/1/1/1
2	GLC	G	1	1,2	-	1/2/19/22	0/1/1/1
2	BGC	G	2	2	-	0/2/19/22	0/1/1/1
2	BGC	G	3	2	-	2/2/19/22	0/1/1/1
2	GLC	H	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	H	2	2	-	0/2/19/22	0/1/1/1
2	BGC	H	3	2	-	2/2/19/22	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	3	BGC	O5-C1	4.29	1.50	1.43
2	F	1	GLC	O5-C1	4.06	1.50	1.43
2	E	3	BGC	O5-C1	3.96	1.50	1.43
2	H	3	BGC	O5-C1	3.96	1.50	1.43
2	H	1	GLC	O5-C1	3.64	1.49	1.43
2	F	3	BGC	O5-C1	3.58	1.49	1.43
2	G	1	GLC	O5-C1	3.34	1.49	1.43
2	G	3	BGC	C2-C3	-3.21	1.47	1.52
2	E	1	GLC	O5-C1	3.08	1.48	1.43
2	F	3	BGC	C2-C3	-2.95	1.48	1.52
2	F	1	GLC	C2-C3	-2.73	1.48	1.52
2	G	2	BGC	O5-C1	2.72	1.48	1.43
2	G	1	GLC	C2-C3	-2.70	1.48	1.52
2	E	3	BGC	C2-C3	-2.60	1.48	1.52
2	G	3	BGC	O5-C5	2.58	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	GLC	C2-C3	-2.55	1.48	1.52
2	F	2	BGC	O5-C1	2.49	1.47	1.43
2	H	3	BGC	C2-C3	-2.49	1.48	1.52
2	H	2	BGC	O5-C1	2.48	1.47	1.43
2	E	1	GLC	O5-C5	2.22	1.47	1.43
2	G	2	BGC	O5-C5	2.20	1.47	1.43
2	G	1	GLC	O5-C5	2.18	1.47	1.43
2	E	2	BGC	O5-C1	2.18	1.47	1.43
2	F	1	GLC	O5-C5	2.16	1.47	1.43
2	H	1	GLC	O5-C5	2.16	1.47	1.43
2	H	1	GLC	C2-C3	-2.12	1.49	1.52
2	F	3	BGC	O5-C5	2.09	1.47	1.43
2	E	3	BGC	O5-C5	2.02	1.47	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	GLC	C1-O5-C5	-2.82	108.41	112.19
2	F	2	BGC	C1-O5-C5	-2.56	108.75	112.19
2	G	3	BGC	C6-C5-C4	-2.43	107.05	113.02
2	H	3	BGC	C1-C2-C3	2.01	112.57	109.64

There are no chirality outliers.

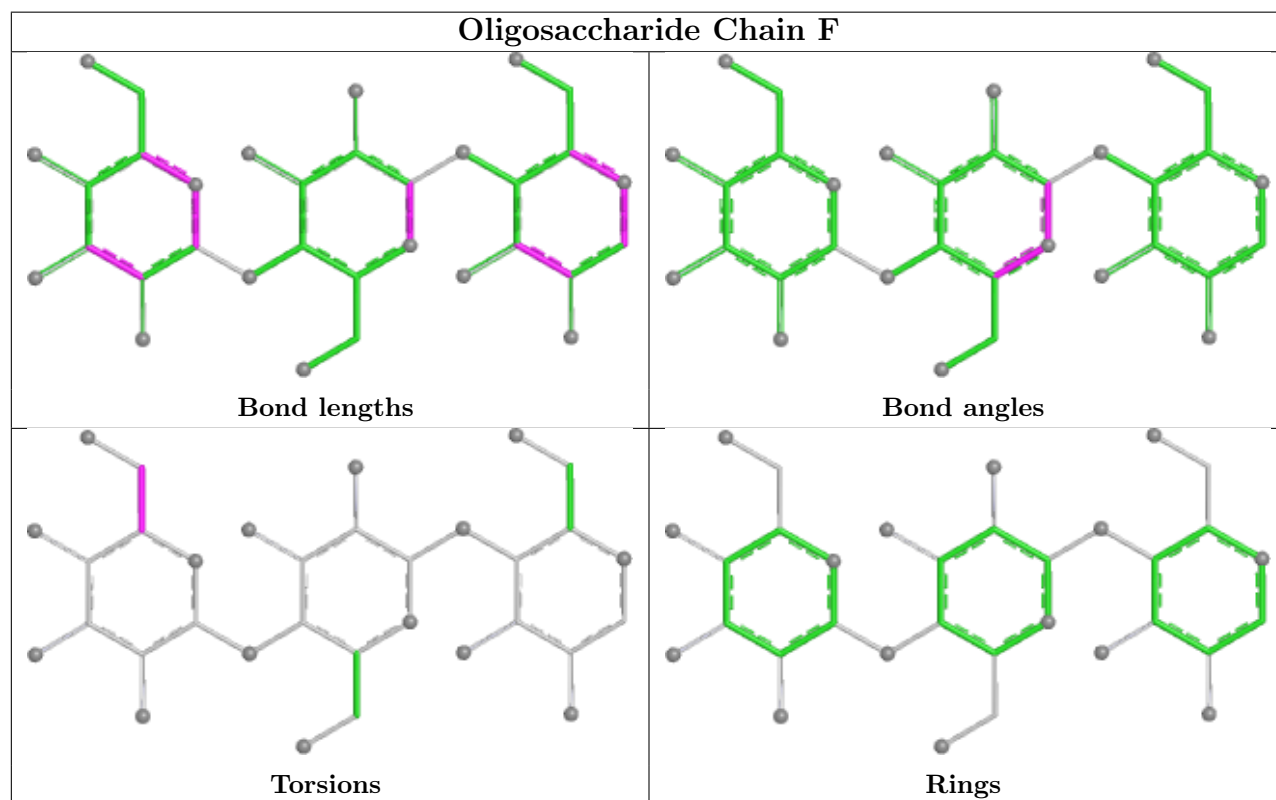
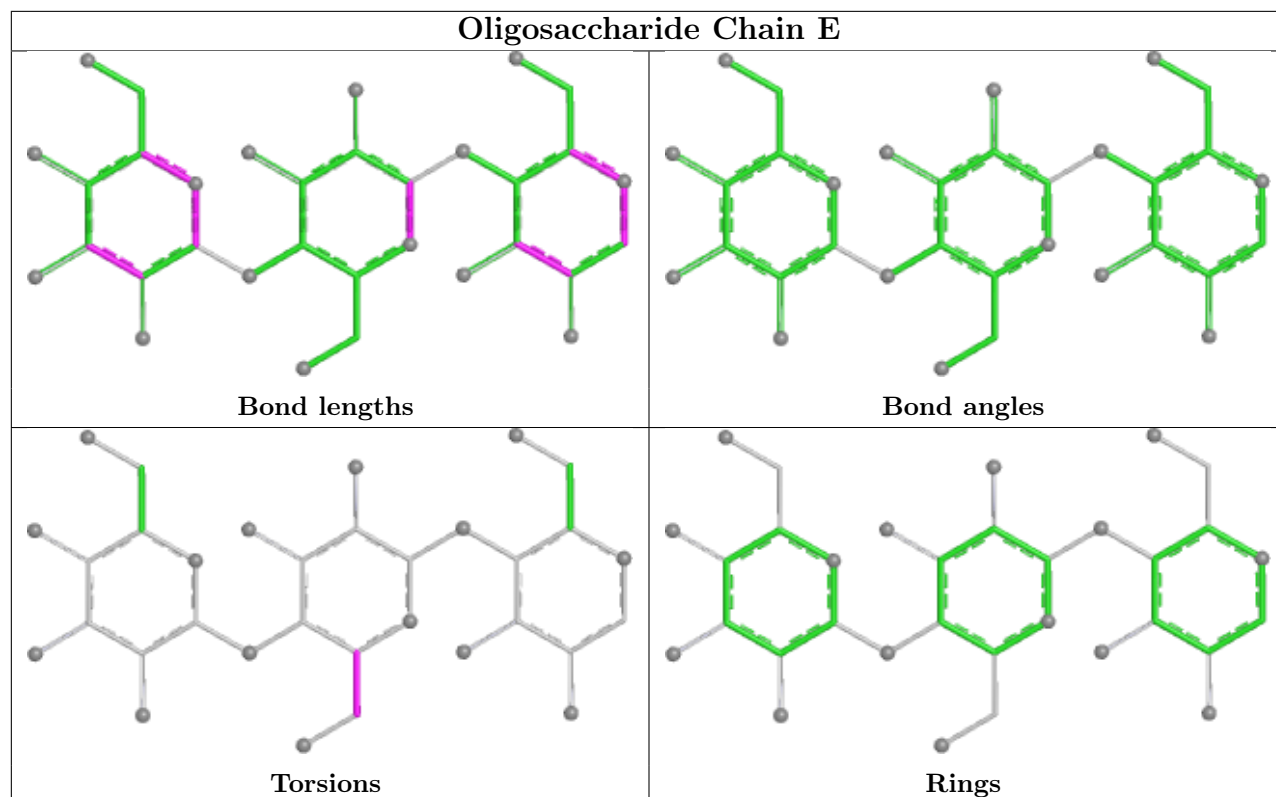
All (7) torsion outliers are listed below:

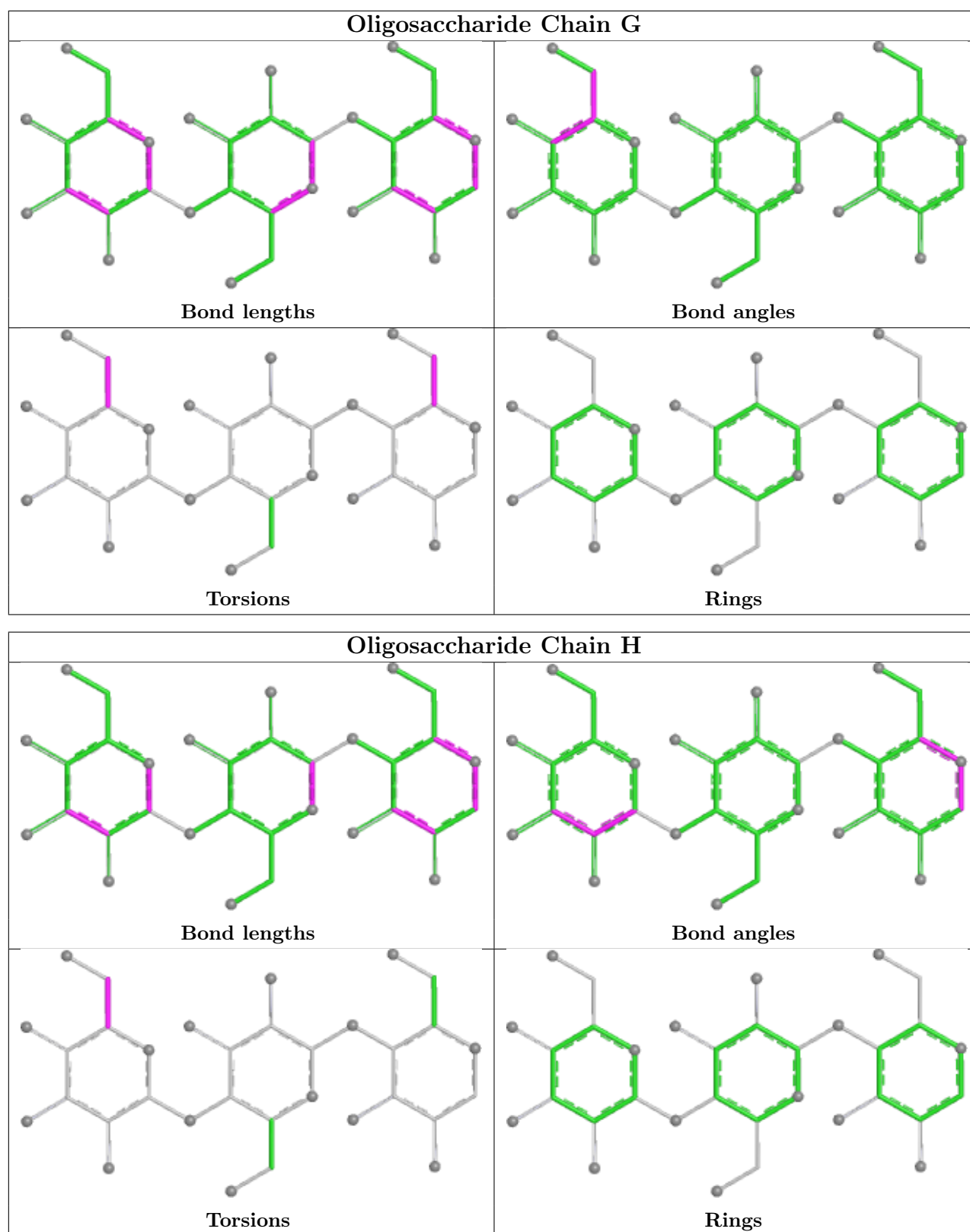
Mol	Chain	Res	Type	Atoms
2	G	3	BGC	O5-C5-C6-O6
2	G	1	GLC	O5-C5-C6-O6
2	H	3	BGC	C4-C5-C6-O6
2	G	3	BGC	C4-C5-C6-O6
2	E	2	BGC	O5-C5-C6-O6
2	F	3	BGC	O5-C5-C6-O6
2	H	3	BGC	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

1 ligand is 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	TRS	A	401	-	7,7,7	0.26	0	9,9,9	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TRS	A	401	-	-	8/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	TRS	C3-C-C1-O1
3	A	401	TRS	N-C-C1-O1
3	A	401	TRS	C2-C-C1-O1
3	A	401	TRS	C1-C-C2-O2
3	A	401	TRS	C3-C-C2-O2
3	A	401	TRS	N-C-C3-O3
3	A	401	TRS	N-C-C2-O2
3	A	401	TRS	C2-C-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	TRS	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	319/320 (99%)	-0.25	2 (0%) 85 87	24, 38, 55, 77	6 (1%)
1	B	320/320 (100%)	0.39	4 (1%) 75 77	31, 54, 73, 87	3 (0%)
1	C	319/320 (99%)	0.14	0 100 100	30, 50, 65, 74	7 (2%)
1	D	320/320 (100%)	0.17	2 (0%) 85 87	33, 49, 62, 86	2 (0%)
All	All	1278/1280 (99%)	0.11	8 (0%) 85 87	24, 48, 66, 87	18 (1%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	310	ASP	3.7
1	A	1	SER	3.1
1	D	320	ALA	2.6
1	B	312	CYS	2.6
1	B	311	ASN	2.3
1	D	311	ASN	2.2
1	A	312	CYS	2.2
1	B	66	VAL	2.1

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

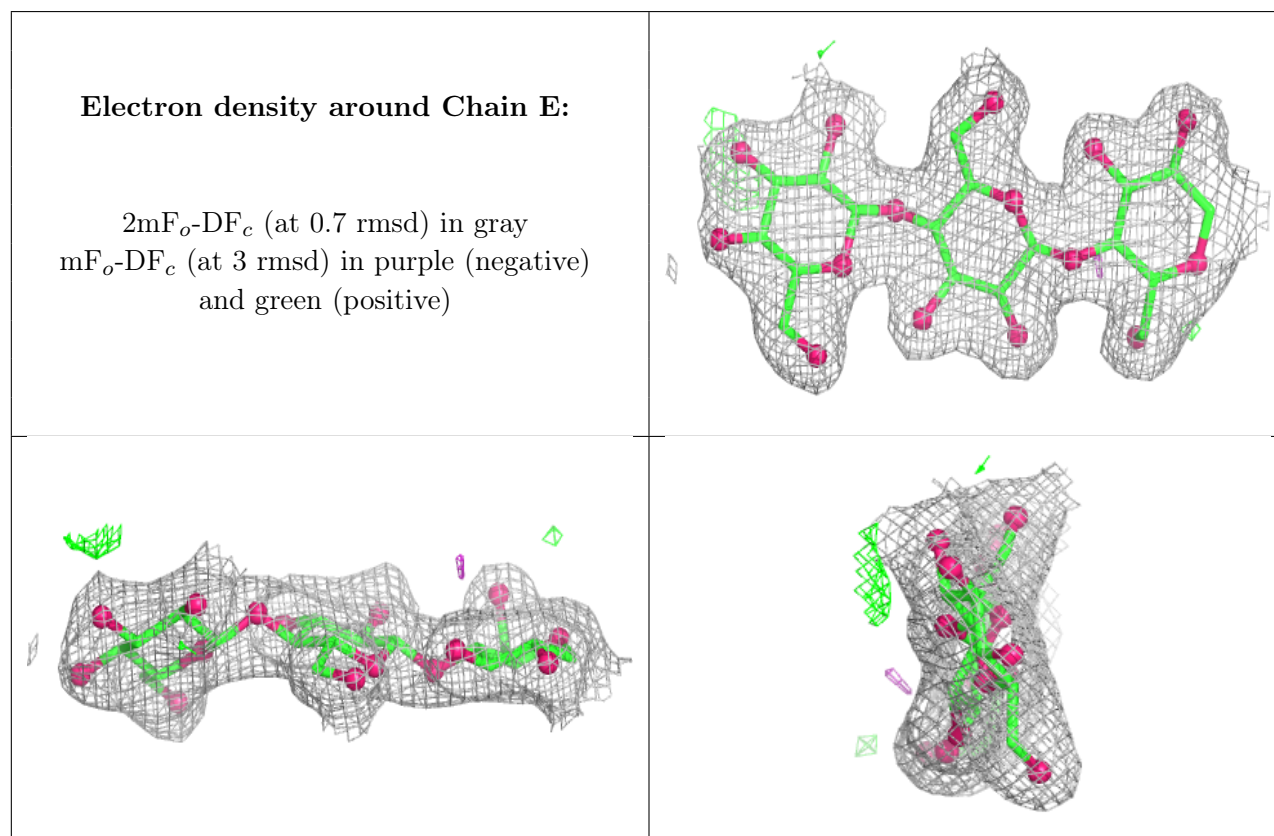
There are no non-standard protein/DNA/RNA residues in this entry.

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.

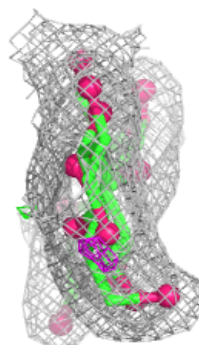
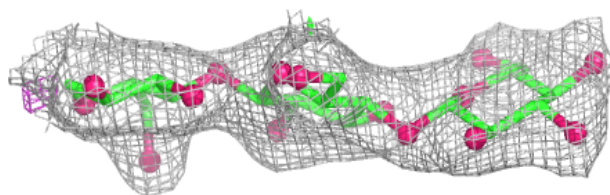
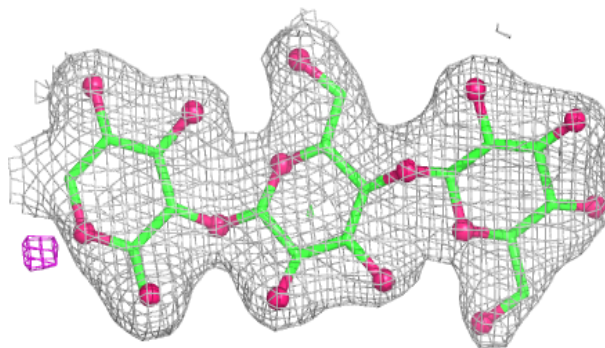
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BGC	G	3	11/12	0.90	0.08	47,51,57,57	0
2	GLC	H	1	11/12	0.90	0.11	38,43,44,45	0
2	GLC	G	1	11/12	0.91	0.08	43,47,50,60	0
2	BGC	H	3	11/12	0.91	0.08	46,49,54,57	0
2	BGC	F	3	11/12	0.92	0.08	50,54,58,58	0
2	BGC	G	2	11/12	0.93	0.07	45,46,50,51	0
2	GLC	F	1	11/12	0.93	0.07	38,43,48,52	0
2	BGC	E	3	11/12	0.94	0.07	36,41,45,46	0
2	BGC	F	2	11/12	0.94	0.07	42,48,51,51	0
2	BGC	H	2	11/12	0.95	0.06	40,41,49,51	0
2	GLC	E	1	11/12	0.96	0.06	32,33,39,41	0
2	BGC	E	2	11/12	0.97	0.05	32,36,40,40	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.

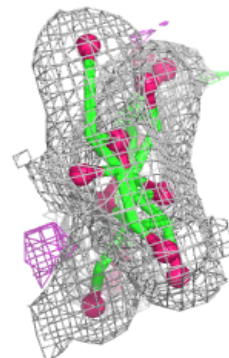
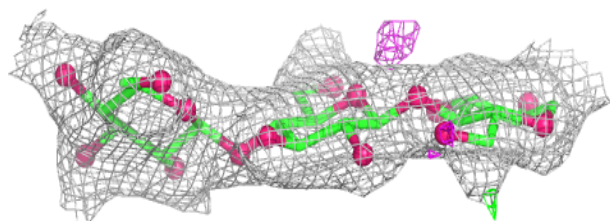
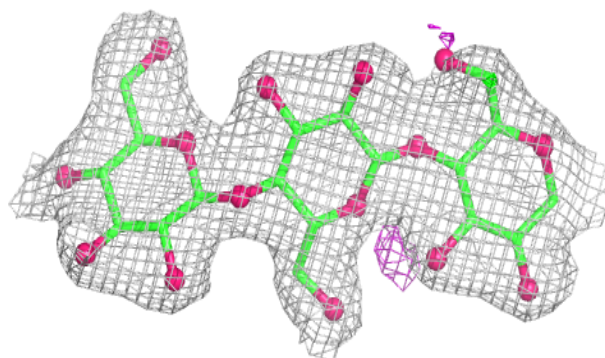


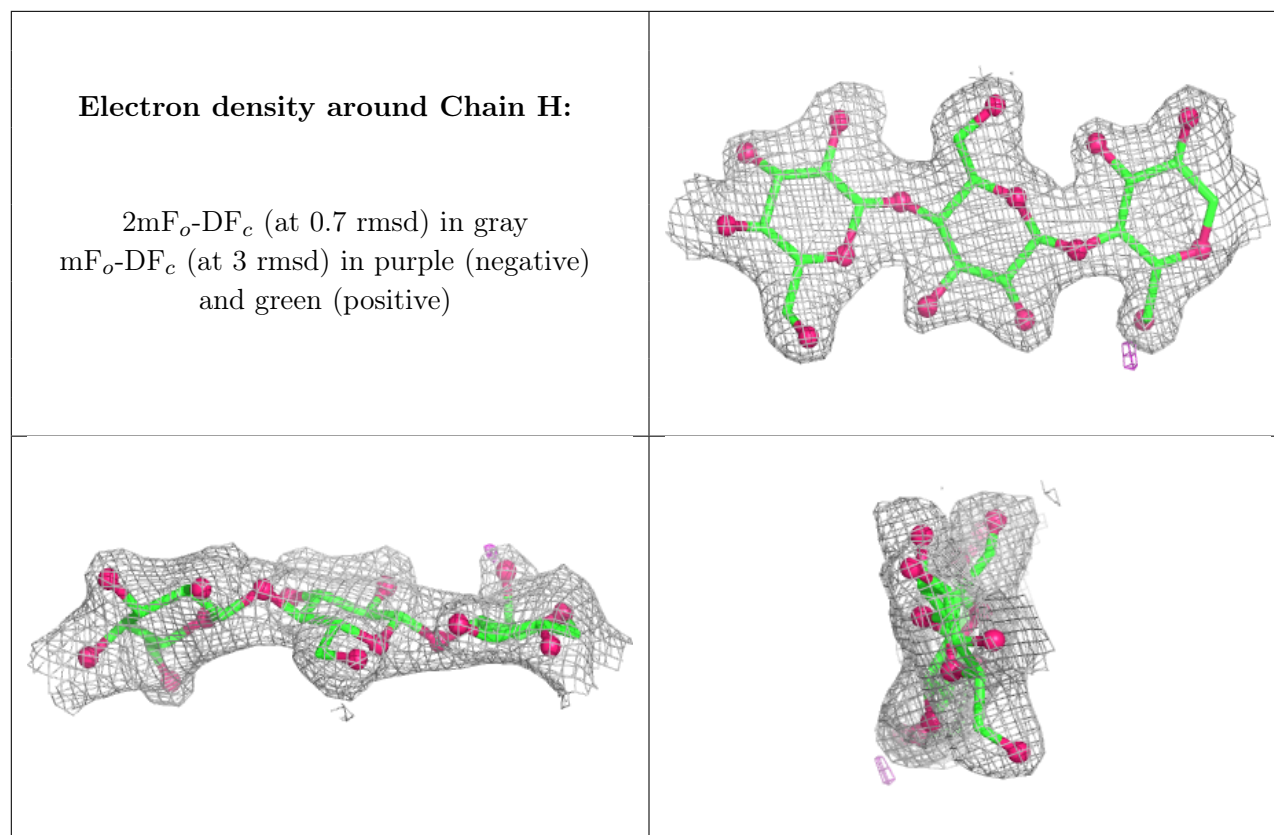
Electron density around Chain F:

$2mF_o-DF_c$ (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)





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
3	TRS	A	401	8/8	0.85	0.11	42,48,56,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.