



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 06:45 AM BST

PDB ID : 6UB1
Title : Crystal structure of a GH128 (subgroup III) curdlan-specific exo-beta-1,3-galactanase from *Blastomyces gilchristii* (BgGH128_III) in complex with laminaribiose at -3 and -2 subsites
Authors : Costa, P.A.C.R.; Santos, C.R.; Domingues, M.N.; Lima, E.A.; Mandelli, F.; Murakami, M.T.
Deposited on : 2019-09-11
Resolution : 1.60 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 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
buster-report : 1.1.7 (2018)
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

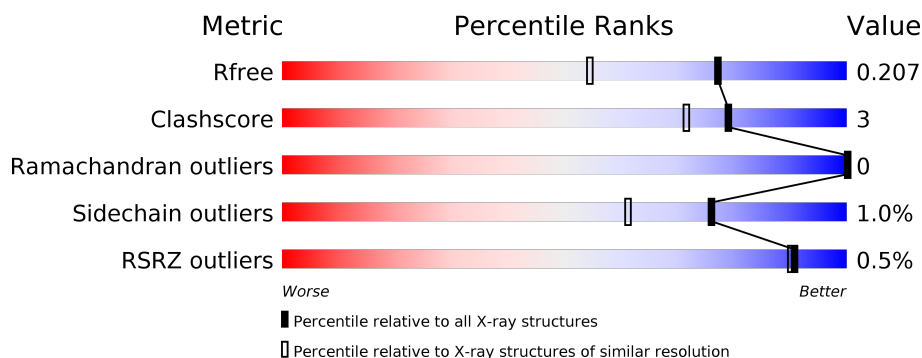
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 ≥ 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	261	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>5%</div> <div>12%</div> </div> </div>
1	B	261	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>7%</div> <div>12%</div> </div> </div>
1	C	261	<div> <div></div> <div> <div>80%</div> <div>7%</div> <div>12%</div> </div> </div>
1	D	261	<div> <div></div> <div> <div>83%</div> <div>5%</div> <div>12%</div> </div> </div>
2	E	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
2	F	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	2	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8197 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called GLYCOSIDE HYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	2	0
			1750	1120	295	329	6			
1	B	230	Total	C	N	O	S	0	2	0
			1755	1122	297	330	6			
1	C	230	Total	C	N	O	S	0	2	0
			1756	1123	296	331	6			
1	D	230	Total	C	N	O	S	0	3	0
			1759	1125	296	332	6			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MET	-	initiating methionine	UNP A0A179UGT5
A	3	GLY	-	expression tag	UNP A0A179UGT5
A	4	SER	-	expression tag	UNP A0A179UGT5
A	5	SER	-	expression tag	UNP A0A179UGT5
A	6	HIS	-	expression tag	UNP A0A179UGT5
A	7	HIS	-	expression tag	UNP A0A179UGT5
A	8	HIS	-	expression tag	UNP A0A179UGT5
A	9	HIS	-	expression tag	UNP A0A179UGT5
A	10	HIS	-	expression tag	UNP A0A179UGT5
A	11	HIS	-	expression tag	UNP A0A179UGT5
A	12	SER	-	expression tag	UNP A0A179UGT5
A	13	SER	-	expression tag	UNP A0A179UGT5
A	14	GLY	-	expression tag	UNP A0A179UGT5
A	15	LEU	-	expression tag	UNP A0A179UGT5
A	16	VAL	-	expression tag	UNP A0A179UGT5
A	17	PRO	-	expression tag	UNP A0A179UGT5
A	18	ALA	-	expression tag	UNP A0A179UGT5
A	19	GLY	-	expression tag	UNP A0A179UGT5
A	20	SER	-	expression tag	UNP A0A179UGT5
A	21	HIS	-	expression tag	UNP A0A179UGT5
A	22	MET	-	expression tag	UNP A0A179UGT5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	2	MET	-	initiating methionine	UNP A0A179UGT5
B	3	GLY	-	expression tag	UNP A0A179UGT5
B	4	SER	-	expression tag	UNP A0A179UGT5
B	5	SER	-	expression tag	UNP A0A179UGT5
B	6	HIS	-	expression tag	UNP A0A179UGT5
B	7	HIS	-	expression tag	UNP A0A179UGT5
B	8	HIS	-	expression tag	UNP A0A179UGT5
B	9	HIS	-	expression tag	UNP A0A179UGT5
B	10	HIS	-	expression tag	UNP A0A179UGT5
B	11	HIS	-	expression tag	UNP A0A179UGT5
B	12	SER	-	expression tag	UNP A0A179UGT5
B	13	SER	-	expression tag	UNP A0A179UGT5
B	14	GLY	-	expression tag	UNP A0A179UGT5
B	15	LEU	-	expression tag	UNP A0A179UGT5
B	16	VAL	-	expression tag	UNP A0A179UGT5
B	17	PRO	-	expression tag	UNP A0A179UGT5
B	18	ALA	-	expression tag	UNP A0A179UGT5
B	19	GLY	-	expression tag	UNP A0A179UGT5
B	20	SER	-	expression tag	UNP A0A179UGT5
B	21	HIS	-	expression tag	UNP A0A179UGT5
B	22	MET	-	expression tag	UNP A0A179UGT5
C	2	MET	-	initiating methionine	UNP A0A179UGT5
C	3	GLY	-	expression tag	UNP A0A179UGT5
C	4	SER	-	expression tag	UNP A0A179UGT5
C	5	SER	-	expression tag	UNP A0A179UGT5
C	6	HIS	-	expression tag	UNP A0A179UGT5
C	7	HIS	-	expression tag	UNP A0A179UGT5
C	8	HIS	-	expression tag	UNP A0A179UGT5
C	9	HIS	-	expression tag	UNP A0A179UGT5
C	10	HIS	-	expression tag	UNP A0A179UGT5
C	11	HIS	-	expression tag	UNP A0A179UGT5
C	12	SER	-	expression tag	UNP A0A179UGT5
C	13	SER	-	expression tag	UNP A0A179UGT5
C	14	GLY	-	expression tag	UNP A0A179UGT5
C	15	LEU	-	expression tag	UNP A0A179UGT5
C	16	VAL	-	expression tag	UNP A0A179UGT5
C	17	PRO	-	expression tag	UNP A0A179UGT5
C	18	ALA	-	expression tag	UNP A0A179UGT5
C	19	GLY	-	expression tag	UNP A0A179UGT5
C	20	SER	-	expression tag	UNP A0A179UGT5
C	21	HIS	-	expression tag	UNP A0A179UGT5
C	22	MET	-	expression tag	UNP A0A179UGT5

Continued on next page...

Continued from previous page...

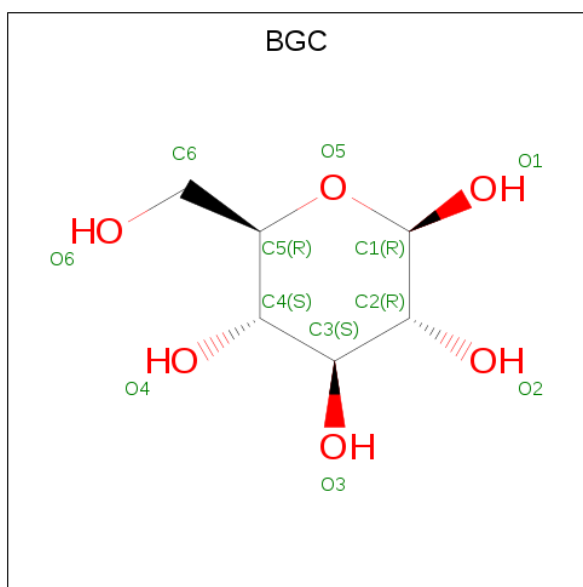
Chain	Residue	Modelled	Actual	Comment	Reference
D	2	MET	-	initiating methionine	UNP A0A179UGT5
D	3	GLY	-	expression tag	UNP A0A179UGT5
D	4	SER	-	expression tag	UNP A0A179UGT5
D	5	SER	-	expression tag	UNP A0A179UGT5
D	6	HIS	-	expression tag	UNP A0A179UGT5
D	7	HIS	-	expression tag	UNP A0A179UGT5
D	8	HIS	-	expression tag	UNP A0A179UGT5
D	9	HIS	-	expression tag	UNP A0A179UGT5
D	10	HIS	-	expression tag	UNP A0A179UGT5
D	11	HIS	-	expression tag	UNP A0A179UGT5
D	12	SER	-	expression tag	UNP A0A179UGT5
D	13	SER	-	expression tag	UNP A0A179UGT5
D	14	GLY	-	expression tag	UNP A0A179UGT5
D	15	LEU	-	expression tag	UNP A0A179UGT5
D	16	VAL	-	expression tag	UNP A0A179UGT5
D	17	PRO	-	expression tag	UNP A0A179UGT5
D	18	ALA	-	expression tag	UNP A0A179UGT5
D	19	GLY	-	expression tag	UNP A0A179UGT5
D	20	SER	-	expression tag	UNP A0A179UGT5
D	21	HIS	-	expression tag	UNP A0A179UGT5
D	22	MET	-	expression tag	UNP A0A179UGT5

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	2	Total	C	O	0	0	0
			23	12	11			
2	F	2	Total	C	O	0	0	0
			23	12	11			
2	G	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is beta-D-glucopyranose (three-letter code: BGC) (formula: C₆H₁₂O₆) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			12	6	6		

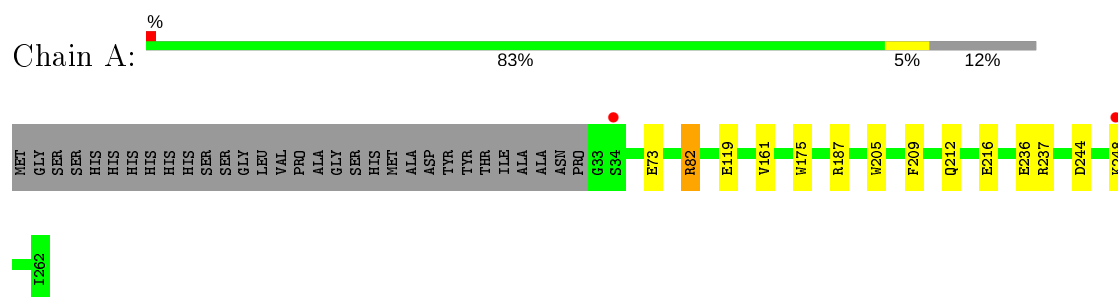
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	263	Total	O	0	0
			263	263		
4	B	273	Total	O	0	0
			273	273		
4	C	266	Total	O	0	0
			266	266		
4	D	294	Total	O	0	0
			294	294		

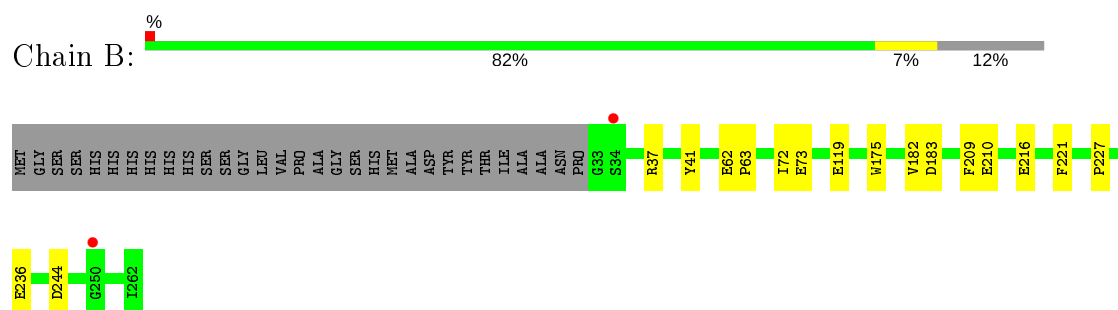
3 Residue-property plots [i](#)

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

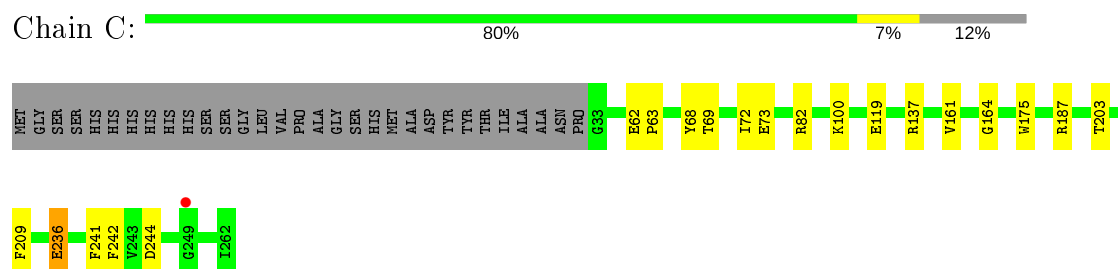
• Molecule 1: GLYCOSIDE HYDROLASE



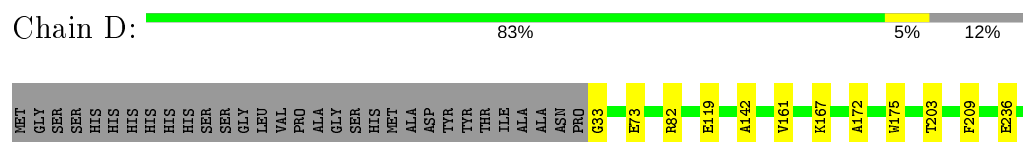
• Molecule 1: GLYCOSIDE HYDROLASE



• Molecule 1: GLYCOSIDE HYDROLASE



• Molecule 1: GLYCOSIDE HYDROLASE




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

Chain E:  50% 50%

BGC1
BGC2

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

Chain F:  50% 50%

BGC1
BGC2

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

Chain G:  50% 50%

BGC1
BGC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	56.32Å 60.80Å 63.55Å 69.67° 78.24° 77.86°	Depositor
Resolution (Å)	35.49 – 1.60 35.49 – 1.60	Depositor EDS
% Data completeness (in resolution range)	86.3 (35.49-1.60) 86.3 (35.49-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.60 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.160 , 0.197 0.172 , 0.207	Depositor DCC
R_{free} test set	4350 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	13.9	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.035 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8197	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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 90.48 % 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 2.2589e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.87	2/1806 (0.1%)	0.98	3/2456 (0.1%)
1	B	0.95	4/1807 (0.2%)	1.01	4/2457 (0.2%)
1	C	0.90	4/1808 (0.2%)	0.96	4/2458 (0.2%)
1	D	0.84	1/1815 (0.1%)	0.91	0/2468
All	All	0.89	11/7236 (0.2%)	0.97	11/9839 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	210	GLU	CD-OE1	11.34	1.38	1.25
1	B	236	GLU	CD-OE1	9.16	1.35	1.25
1	C	73	GLU	CD-OE1	-8.18	1.16	1.25
1	B	73	GLU	CD-OE1	-7.12	1.17	1.25
1	C	236[A]	GLU	CD-OE2	6.82	1.33	1.25
1	C	236[B]	GLU	CD-OE2	6.82	1.33	1.25
1	D	73	GLU	CD-OE1	-5.85	1.19	1.25
1	B	210	GLU	CD-OE2	-5.84	1.19	1.25
1	C	164	GLY	C-O	5.50	1.32	1.23
1	A	236	GLU	CD-OE1	5.38	1.31	1.25
1	A	73	GLU	CD-OE1	-5.34	1.19	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	187	ARG	NE-CZ-NH2	8.08	124.34	120.30
1	C	187	ARG	NE-CZ-NH1	-7.09	116.75	120.30
1	A	82	ARG	CB-CG-CD	6.79	129.25	111.60
1	B	119	GLU	CB-CA-C	6.66	123.72	110.40
1	C	68	TYR	CB-CG-CD1	-6.64	117.02	121.00
1	C	68	TYR	CB-CG-CD2	6.15	124.69	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	ARG	NE-CZ-NH2	6.07	123.33	120.30
1	B	41	TYR	CB-CG-CD1	5.73	124.44	121.00
1	B	37	ARG	CG-CD-NE	5.54	123.44	111.80
1	B	210	GLU	CG-CD-OE2	-5.11	108.08	118.30
1	A	187	ARG	CG-CD-NE	5.02	122.34	111.80

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	1750	0	1657	10	0
1	B	1755	0	1659	5	0
1	C	1756	0	1659	12	0
1	D	1759	0	1662	11	0
2	E	23	0	21	1	0
2	F	23	0	21	1	0
2	G	23	0	21	1	0
3	B	12	0	12	0	0
4	A	263	0	0	6	0
4	B	273	0	0	2	0
4	C	266	0	0	2	0
4	D	294	0	0	2	0
All	All	8197	0	6712	38	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 3.

All (38) 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:100:LYS:HE3	4:C:493:HOH:O	1.51	1.10
1:D:203:THR:HG21	1:D:236:GLU:OE2	1.63	0.98
1:C:203:THR:HG21	1:C:236[B]:GLU:OE2	1.64	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:GLN:HG3	4:A:573:HOH:O	1.81	0.80
1:D:82:ARG:NH2	2:G:2:BGC:O3	2.17	0.76
1:C:203:THR:OG1	1:C:236[B]:GLU:HG3	1.90	0.71
1:A:82:ARG:HG2	4:A:479:HOH:O	1.97	0.64
1:D:203:THR:HG21	1:D:236:GLU:CD	2.21	0.61
1:C:82:ARG:NH1	2:F:2:BGC:O3	2.33	0.59
1:D:203:THR:OG1	1:D:236:GLU:HG3	2.02	0.59
1:C:137:ARG:NH1	4:C:401:HOH:O	2.38	0.57
1:C:203:THR:HG21	1:C:236[B]:GLU:CD	2.27	0.56
1:A:216:GLU:HG3	4:A:557:HOH:O	2.07	0.55
1:A:119:GLU:HG3	4:A:404:HOH:O	2.07	0.54
1:B:182:VAL:HG22	1:B:221:PHE:CD1	2.42	0.54
1:A:82:ARG:NH2	2:E:2:BGC:O3	2.42	0.52
1:D:119[B]:GLU:HA	1:D:161:VAL:HG11	1.92	0.52
1:D:119[A]:GLU:HA	1:D:161:VAL:HG11	1.92	0.52
1:A:175:TRP:O	1:A:209:PHE:HA	2.10	0.52
1:D:33:GLY:N	4:D:407:HOH:O	2.44	0.51
1:C:175:TRP:O	1:C:209:PHE:HA	2.11	0.51
1:C:69:THR:HG21	1:C:72:ILE:HD12	1.95	0.49
1:B:175:TRP:O	1:B:209:PHE:HA	2.13	0.48
1:A:205:TRP:CZ2	1:A:237:ARG:HD2	2.49	0.48
1:D:175:TRP:O	1:D:209:PHE:HA	2.15	0.47
1:B:72:ILE:HD11	4:B:644:HOH:O	2.14	0.47
1:A:119:GLU:HA	1:A:161:VAL:HG11	1.97	0.46
1:C:62:GLU:HB3	1:C:63:PRO:HD2	1.98	0.46
1:C:69:THR:CG2	1:C:72:ILE:HD12	2.47	0.45
1:D:167:LYS:NZ	4:D:409:HOH:O	2.47	0.45
1:A:119:GLU:CG	4:A:404:HOH:O	2.65	0.45
1:C:241:PHE:HA	1:C:242:PHE:HB3	1.99	0.44
1:C:119:GLU:HA	1:C:161:VAL:HG11	2.01	0.42
1:B:216:GLU:HG2	4:B:530:HOH:O	2.19	0.41
1:D:142:ALA:HA	1:D:172:ALA:O	2.21	0.41
1:B:62:GLU:HB3	1:B:63:PRO:HD2	2.03	0.41
1:D:203:THR:HG21	1:D:236:GLU:CG	2.51	0.41
1:A:119:GLU:OE1	4:A:401:HOH:O	2.22	0.41

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	229/261 (88%)	223 (97%)	6 (3%)	0	100	100
1	B	229/261 (88%)	223 (97%)	6 (3%)	0	100	100
1	C	229/261 (88%)	224 (98%)	5 (2%)	0	100	100
1	D	230/261 (88%)	224 (97%)	6 (3%)	0	100	100
All	All	917/1044 (88%)	894 (98%)	23 (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	171/194 (88%)	169 (99%)	2 (1%)	71	54
1	B	171/194 (88%)	168 (98%)	3 (2%)	59	36
1	C	171/194 (88%)	170 (99%)	1 (1%)	86	77
1	D	172/194 (89%)	171 (99%)	1 (1%)	86	77
All	All	685/776 (88%)	678 (99%)	7 (1%)	76	61

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	244	ASP
1	A	248	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	183	ASP
1	B	227	PRO
1	B	244	ASP
1	C	244	ASP
1	D	244	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	GLN
1	B	42	ASN
1	D	42	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 ⓘ

6 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	E	1	2	12,12,12	1.58	2 (16%)	17,17,17	2.03	5 (29%)
2	BGC	E	2	2	11,11,12	0.62	0	15,15,17	2.24	8 (53%)
2	BGC	F	1	2	12,12,12	1.25	2 (16%)	17,17,17	1.96	7 (41%)
2	BGC	F	2	2	11,11,12	1.13	1 (9%)	15,15,17	2.66	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	G	1	2	12,12,12	1.81	2 (16%)	17,17,17	3.19	11 (64%)
2	BGC	G	2	2	11,11,12	0.87	0	15,15,17	1.96	4 (26%)

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	E	1	2	-	0/2/22/22	0/1/1/1
2	BGC	E	2	2	-	1/2/19/22	0/1/1/1
2	BGC	F	1	2	-	0/2/22/22	0/1/1/1
2	BGC	F	2	2	-	2/2/19/22	0/1/1/1
2	BGC	G	1	2	-	1/2/22/22	0/1/1/1
2	BGC	G	2	2	-	2/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	BGC	O2-C2	3.94	1.52	1.43
2	E	1	BGC	O1-C1	3.90	1.52	1.39
2	G	1	BGC	O1-C1	3.46	1.50	1.39
2	E	1	BGC	O2-C2	3.00	1.50	1.43
2	F	1	BGC	O2-C2	2.67	1.49	1.43
2	F	2	BGC	O5-C1	-2.52	1.39	1.43
2	F	1	BGC	O1-C1	2.41	1.47	1.39

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	BGC	O5-C1-C2	-6.45	98.77	110.28
2	F	2	BGC	O2-C2-C3	5.73	121.62	110.14
2	F	2	BGC	C1-O5-C5	5.41	119.53	112.19
2	G	2	BGC	C2-C3-C4	-4.46	103.17	110.89
2	G	1	BGC	O1-C1-C2	4.35	121.28	109.03
2	G	1	BGC	C4-C3-C2	4.35	118.42	110.82
2	E	1	BGC	O2-C2-C1	4.21	118.93	109.16
2	E	2	BGC	O3-C3-C2	-3.98	102.37	109.99
2	F	2	BGC	O4-C4-C3	3.92	119.41	110.35
2	G	1	BGC	C6-C5-C4	3.73	121.75	113.00
2	G	1	BGC	O4-C4-C5	3.65	118.36	109.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	BGC	O1-C1-C2	3.50	118.90	109.03
2	F	1	BGC	O4-C4-C5	3.49	117.96	109.30
2	G	1	BGC	O3-C3-C2	-3.41	102.47	110.35
2	E	1	BGC	O2-C2-C3	-3.38	102.55	110.35
2	G	1	BGC	C3-C4-C5	-3.37	104.23	110.24
2	E	1	BGC	C4-C3-C2	3.26	116.52	110.82
2	G	1	BGC	O3-C3-C4	-3.26	102.81	110.35
2	E	2	BGC	O2-C2-C1	3.21	115.71	109.15
2	F	1	BGC	O3-C3-C4	-3.18	102.99	110.35
2	G	2	BGC	C1-C2-C3	-3.11	105.85	109.67
2	E	1	BGC	O3-C3-C4	-2.99	103.44	110.35
2	E	2	BGC	O5-C5-C4	-2.96	103.62	110.83
2	G	1	BGC	O2-C2-C1	2.95	116.01	109.16
2	F	2	BGC	C1-C2-C3	-2.86	106.14	109.67
2	G	1	BGC	O1-C1-O5	2.79	118.76	110.38
2	F	1	BGC	O2-C2-C1	2.75	115.54	109.16
2	G	1	BGC	O4-C4-C3	-2.74	104.02	110.35
2	F	1	BGC	O4-C4-C3	-2.73	104.03	110.35
2	G	2	BGC	O5-C1-C2	-2.63	106.71	110.77
2	E	2	BGC	O2-C2-C3	2.63	115.40	110.14
2	E	2	BGC	O4-C4-C3	-2.57	104.41	110.35
2	F	1	BGC	O1-C1-O5	-2.53	102.79	110.38
2	E	2	BGC	C2-C3-C4	-2.52	106.53	110.89
2	G	2	BGC	O5-C5-C4	-2.32	105.19	110.83
2	F	1	BGC	O5-C1-C2	2.32	114.42	110.28
2	E	2	BGC	O4-C4-C5	2.30	115.00	109.30
2	E	2	BGC	C1-C2-C3	-2.23	106.93	109.67
2	F	1	BGC	O3-C3-C2	-2.18	105.30	110.35
2	F	2	BGC	O5-C5-C6	-2.03	104.03	107.20

There are no chirality outliers.

All (6) torsion outliers are listed below:

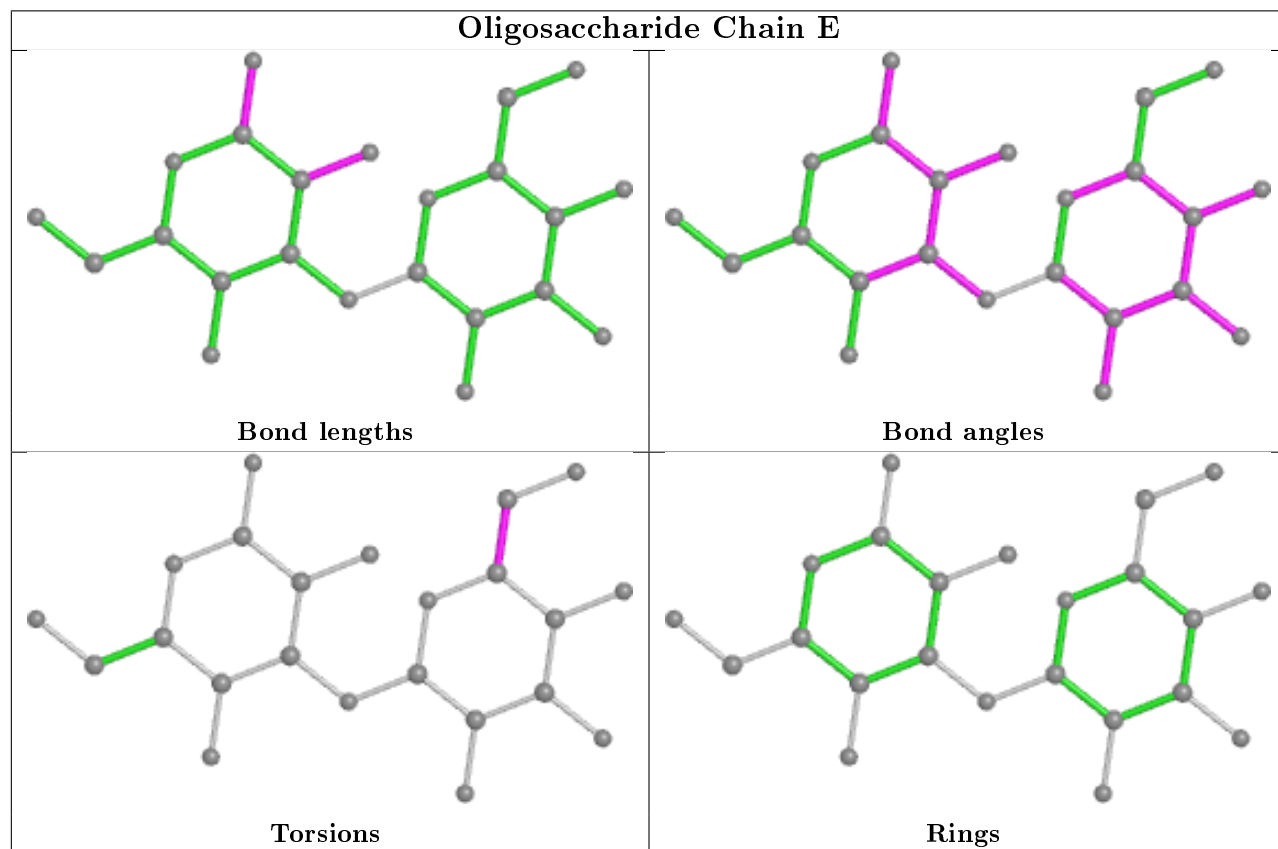
Mol	Chain	Res	Type	Atoms
2	F	2	BGC	O5-C5-C6-O6
2	F	2	BGC	C4-C5-C6-O6
2	G	2	BGC	O5-C5-C6-O6
2	G	2	BGC	C4-C5-C6-O6
2	E	2	BGC	O5-C5-C6-O6
2	G	1	BGC	C4-C5-C6-O6

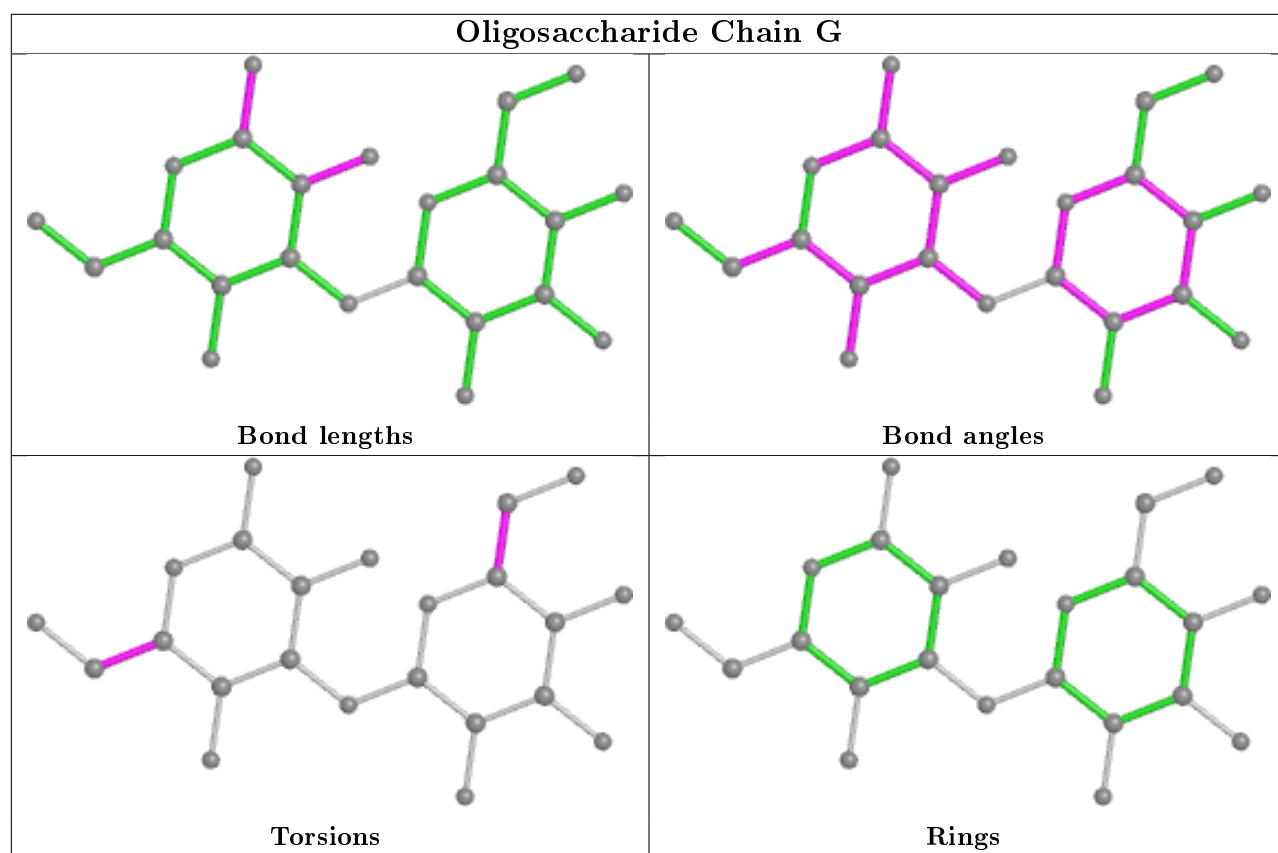
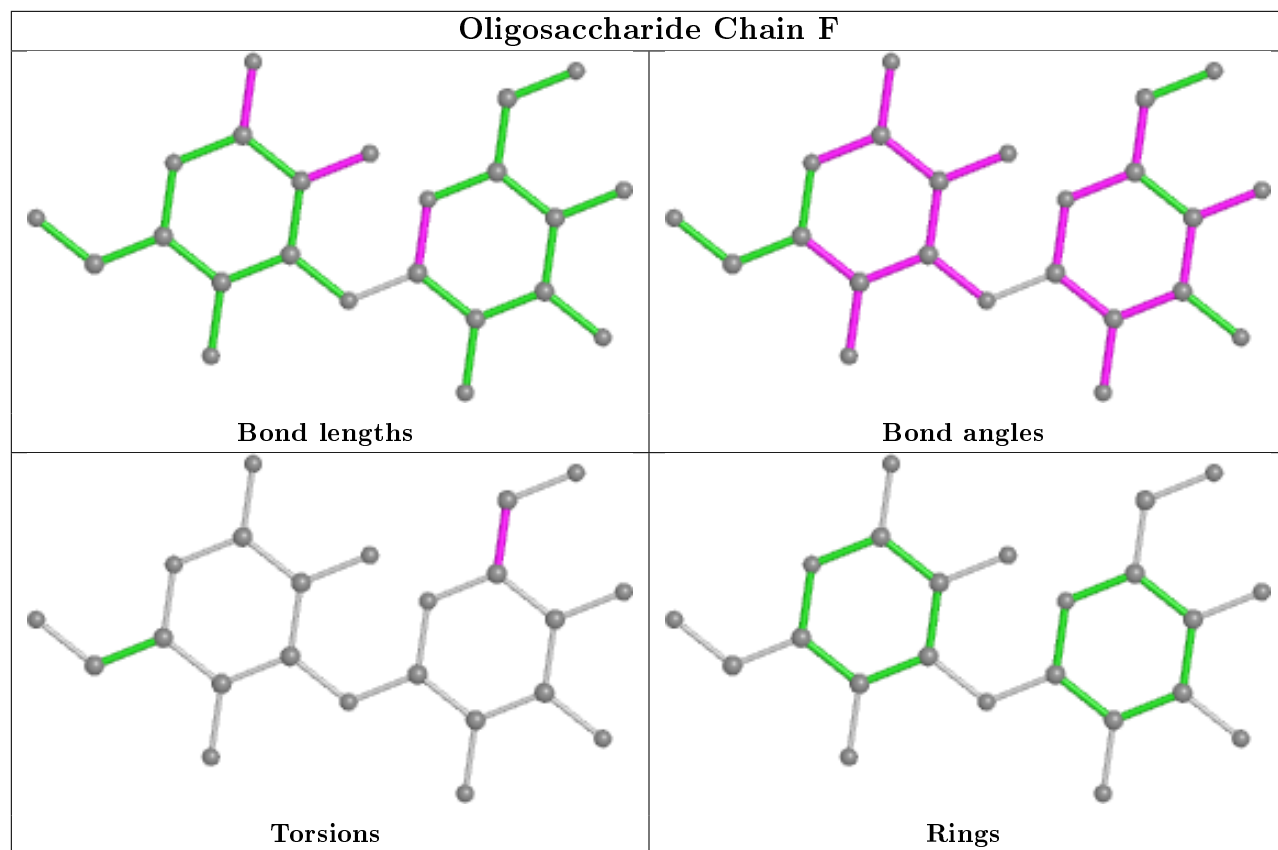
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	BGC	1	0
2	G	2	BGC	1	0
2	F	2	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

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	BGC	B	301	-	12,12,12	1.00	0	17,17,17	2.37	7 (41%)

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	BGC	B	301	-	-	2/2/22/22	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	BGC	O4-C4-C3	-5.14	98.47	110.35
3	B	301	BGC	O2-C2-C1	3.23	116.66	109.16
3	B	301	BGC	C1-C2-C3	3.12	116.80	110.31
3	B	301	BGC	O1-C1-O5	-2.97	101.47	110.38
3	B	301	BGC	O5-C1-C2	2.93	115.52	110.28
3	B	301	BGC	C1-O5-C5	-2.59	108.77	113.66
3	B	301	BGC	O4-C4-C5	2.42	115.31	109.30

There are no chirality outliers.

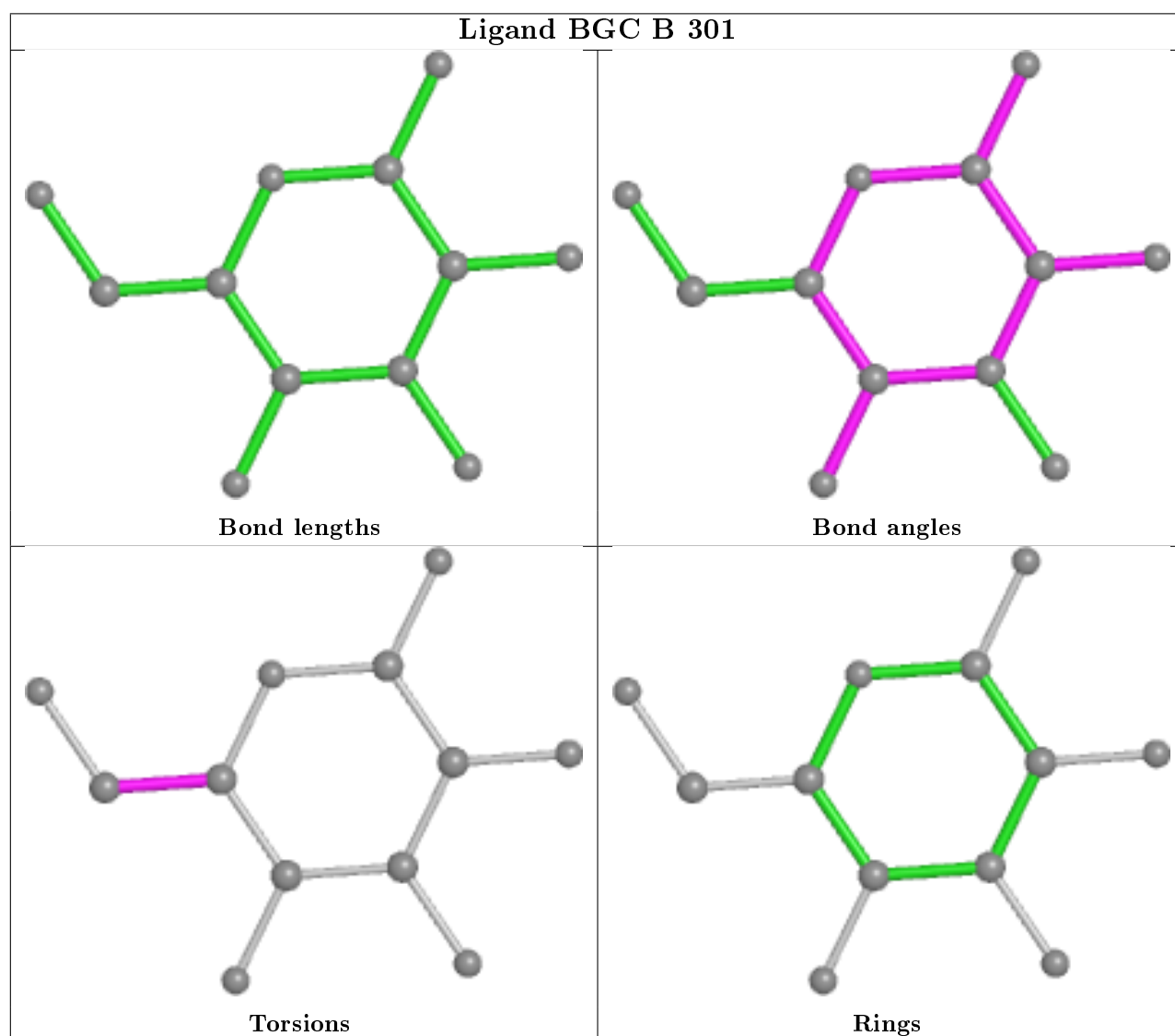
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	301	BGC	O5-C5-C6-O6
3	B	301	BGC	C4-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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	230/261 (88%)	-0.39	2 (0%) 84 84	10, 17, 28, 45	0
1	B	230/261 (88%)	-0.37	2 (0%) 84 84	9, 15, 26, 40	0
1	C	230/261 (88%)	-0.44	1 (0%) 92 92	9, 16, 24, 38	0
1	D	230/261 (88%)	-0.46	0 100 100	10, 16, 24, 32	0
All	All	920/1044 (88%)	-0.41	5 (0%) 91 90	9, 16, 26, 45	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	249	GLY	3.8
1	A	34	SER	2.9
1	B	250	GLY	2.5
1	A	248	LYS	2.4
1	B	34	SER	2.3

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BGC	F	2	11/12	0.87	0.17	25,31,33,36	0
2	BGC	E	1	12/12	0.89	0.10	19,23,24,25	0

Continued on next page...

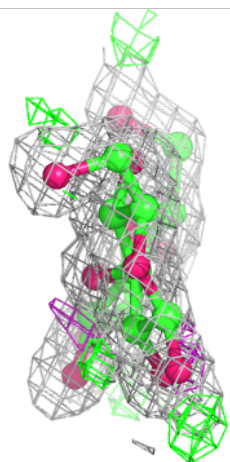
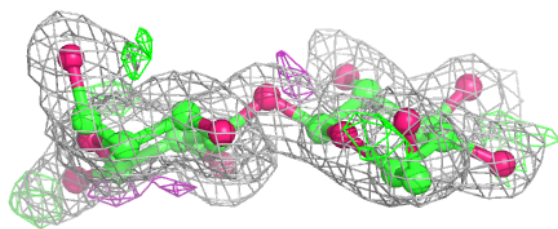
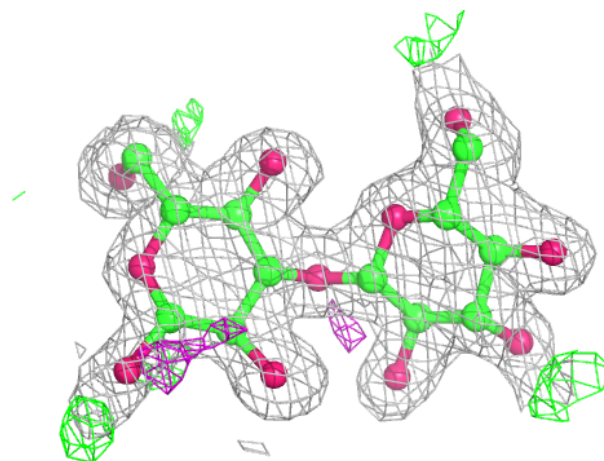
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BGC	G	2	11/12	0.90	0.13	28,36,43,43	0
2	BGC	G	1	12/12	0.91	0.10	19,24,28,33	0
2	BGC	F	1	12/12	0.92	0.10	18,23,27,28	0
2	BGC	E	2	11/12	0.93	0.09	21,25,29,30	0

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

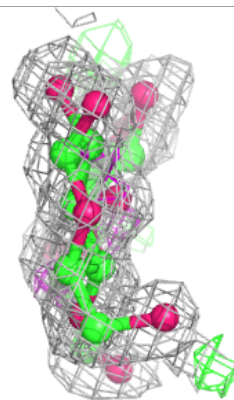
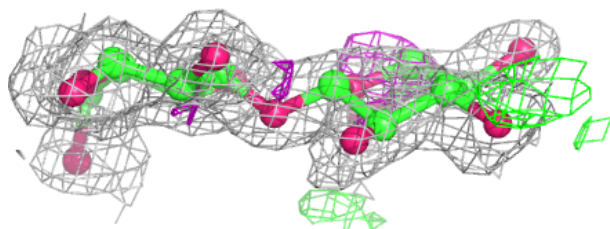
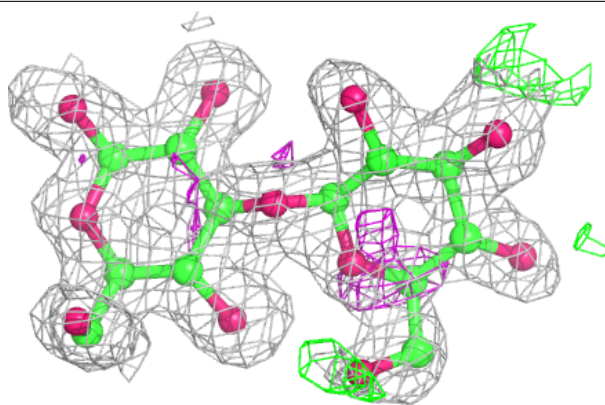
Electron density around Chain E:

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

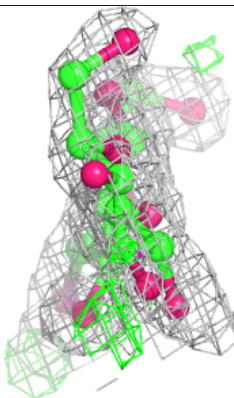
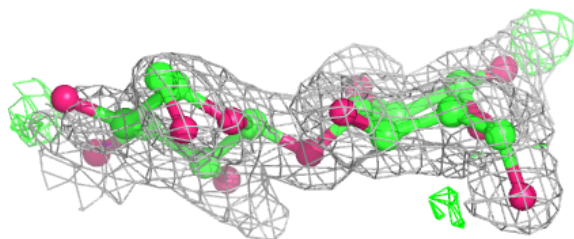
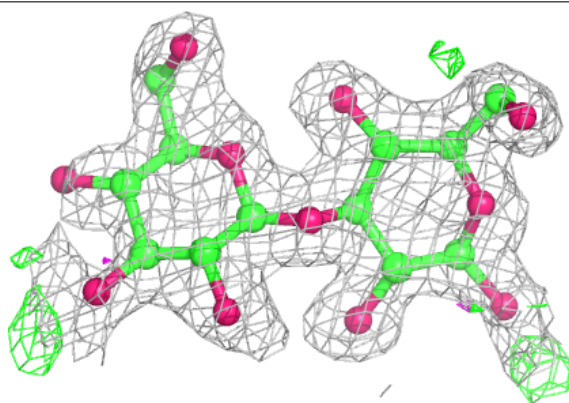


Electron density around Chain F:

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

**Electron density around Chain G:**

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



6.4 Ligands

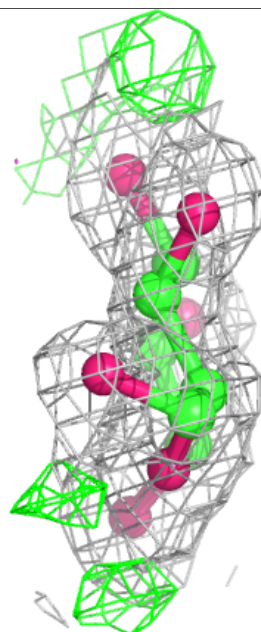
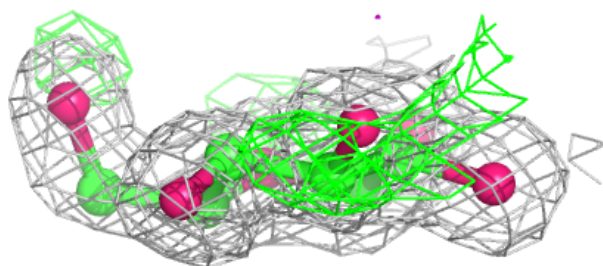
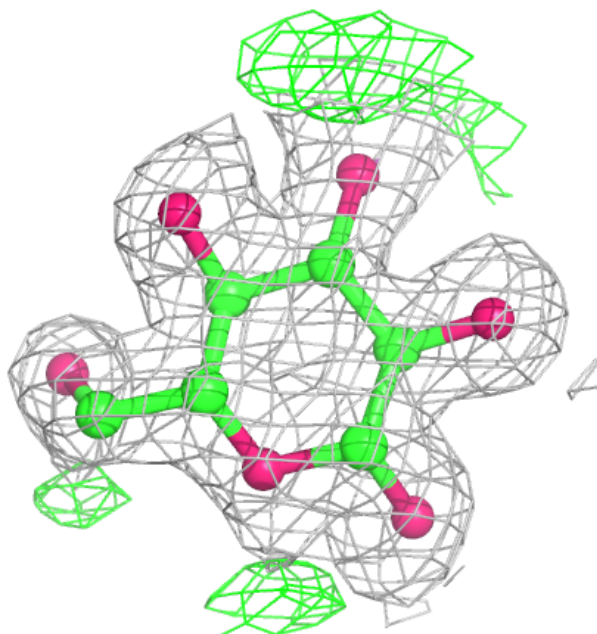
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	BGC	B	301	12/12	0.92	0.10	18,23,26,28	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around BGC B 301:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.