



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 09:33 PM BST

PDB ID : 6A0K  
Title : Cyclic alpha-maltosyl-(1-->6)-maltose hydrolase from *Arthrobacter globiformis*, complex with panose  
Authors : Kohno, M.; Arakawa, T.; Mori, T.; Nishimoto, T.; Fushinobu, S.  
Deposited on : 2018-06-05  
Resolution : 1.94 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

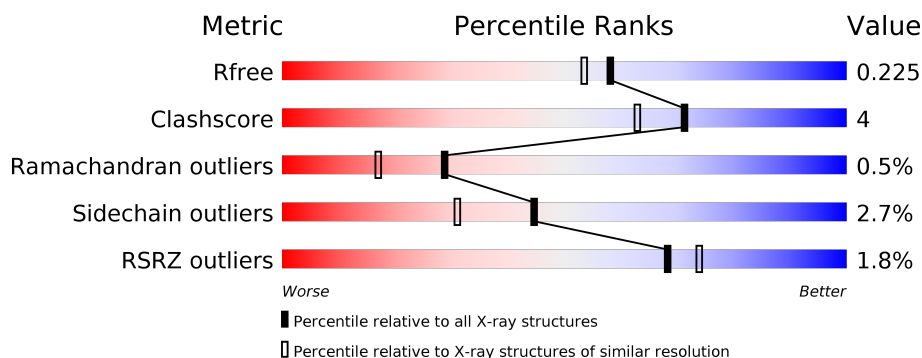
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.94 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	471	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div>•</div> </div> </div>
1	B	471	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>• 6%</div> </div> </div>
2	C	3	<div> <div></div> <div>67%</div> <div>33%</div> </div>
2	E	3	<div> <div></div> <div>67%</div> <div>33%</div> </div>
3	D	3	<div> <div></div> <div>67%</div> <div>33%</div> </div>
3	F	3	<div> <div></div> <div>100%</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7443 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 Cyclic maltosyl-maltose hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	442	Total	C	N	O	S	0	0	0
			3441	2180	600	650	11			
1	A	450	Total	C	N	O	S	0	0	0
			3487	2207	608	661	11			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	expression tag	UNP D2YYE1
B	-19	GLY	-	expression tag	UNP D2YYE1
B	-18	SER	-	expression tag	UNP D2YYE1
B	-17	SER	-	expression tag	UNP D2YYE1
B	-16	HIS	-	expression tag	UNP D2YYE1
B	-15	HIS	-	expression tag	UNP D2YYE1
B	-14	HIS	-	expression tag	UNP D2YYE1
B	-13	HIS	-	expression tag	UNP D2YYE1
B	-12	HIS	-	expression tag	UNP D2YYE1
B	-11	HIS	-	expression tag	UNP D2YYE1
B	-10	SER	-	expression tag	UNP D2YYE1
B	-9	SER	-	expression tag	UNP D2YYE1
B	-8	GLY	-	expression tag	UNP D2YYE1
B	-7	LEU	-	expression tag	UNP D2YYE1
B	-6	VAL	-	expression tag	UNP D2YYE1
B	-5	PRO	-	expression tag	UNP D2YYE1
B	-4	ARG	-	expression tag	UNP D2YYE1
B	-3	GLY	-	expression tag	UNP D2YYE1
B	-2	SER	-	expression tag	UNP D2YYE1
B	-1	HIS	-	expression tag	UNP D2YYE1
B	0	MET	-	expression tag	UNP D2YYE1
B	1	VAL	-	expression tag	UNP D2YYE1
A	-20	MET	-	expression tag	UNP D2YYE1
A	-19	GLY	-	expression tag	UNP D2YYE1
A	-18	SER	-	expression tag	UNP D2YYE1

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	SER	-	expression tag	UNP D2YYE1
A	-16	HIS	-	expression tag	UNP D2YYE1
A	-15	HIS	-	expression tag	UNP D2YYE1
A	-14	HIS	-	expression tag	UNP D2YYE1
A	-13	HIS	-	expression tag	UNP D2YYE1
A	-12	HIS	-	expression tag	UNP D2YYE1
A	-11	HIS	-	expression tag	UNP D2YYE1
A	-10	SER	-	expression tag	UNP D2YYE1
A	-9	SER	-	expression tag	UNP D2YYE1
A	-8	GLY	-	expression tag	UNP D2YYE1
A	-7	LEU	-	expression tag	UNP D2YYE1
A	-6	VAL	-	expression tag	UNP D2YYE1
A	-5	PRO	-	expression tag	UNP D2YYE1
A	-4	ARG	-	expression tag	UNP D2YYE1
A	-3	GLY	-	expression tag	UNP D2YYE1
A	-2	SER	-	expression tag	UNP D2YYE1
A	-1	HIS	-	expression tag	UNP D2YYE1
A	0	MET	-	expression tag	UNP D2YYE1
A	1	VAL	-	expression tag	UNP D2YYE1

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	3	Total	C	O	0	0	0
			34	18	16			
2	E	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	3	Total	C	O	0	0	0
			34	18	16			
3	F	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		

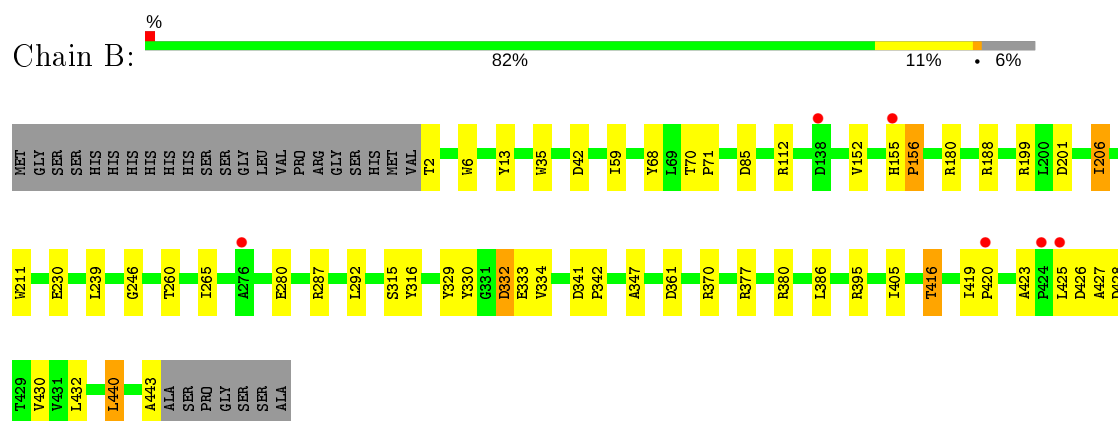
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	189	Total	O	0	0
			189	189		
5	A	189	Total	O	0	0
			189	189		

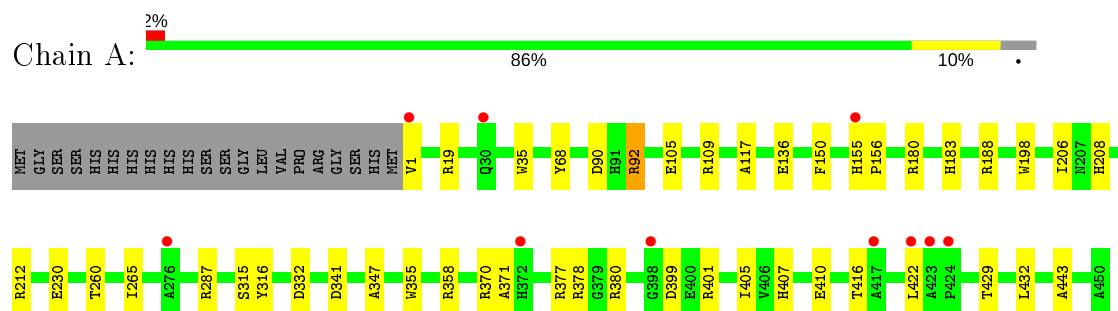
### 3 Residue-property plots [i](#)

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.

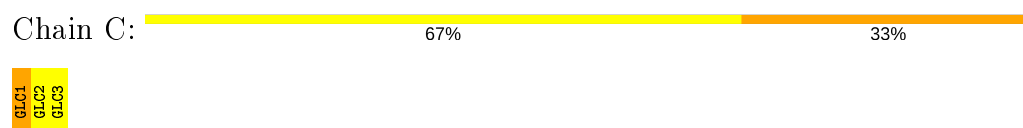
- Molecule 1: Cyclic maltosyl-maltose hydrolase



- Molecule 1: Cyclic maltosyl-maltose hydrolase



- Molecule 2: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 2: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose





- Molecule 3: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranos  
e



- Molecule 3: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranos  
e



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.29Å 180.22Å 62.93Å 90.00° 111.60° 90.00°	Depositor
Resolution (Å)	90.10 – 1.94 44.90 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.5 (90.10-1.94) 99.6 (44.90-1.94)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.188 , 0.223 0.197 , 0.225	Depositor DCC
$R_{free}$ test set	3718 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.8	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 50.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.098 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7443	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, CA, 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	1.02	1/3587 (0.0%)	1.03	15/4907 (0.3%)
1	B	1.08	0/3540	1.03	10/4842 (0.2%)
All	All	1.05	1/7127 (0.0%)	1.03	25/9749 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	92	ARG	CD-NE	-5.38	1.37	1.46

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	287	ARG	NE-CZ-NH2	-11.95	114.32	120.30
1	B	377	ARG	NE-CZ-NH1	-11.08	114.76	120.30
1	B	377	ARG	NE-CZ-NH2	10.72	125.66	120.30
1	B	287	ARG	NE-CZ-NH1	10.61	125.60	120.30
1	A	92	ARG	NE-CZ-NH2	-9.85	115.38	120.30
1	A	188	ARG	NE-CZ-NH2	-9.43	115.58	120.30
1	A	358	ARG	NE-CZ-NH1	8.91	124.76	120.30
1	B	332	ASP	CB-CG-OD1	8.02	125.52	118.30
1	A	401	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	B	85	ASP	CB-CG-OD1	7.31	124.88	118.30
1	A	287	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	A	109	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	A	92	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	A	188	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	A	287	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	A	180	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	A	19	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	401	ARG	NE-CZ-NH2	-5.77	117.41	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	188	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	A	341	ASP	CB-CG-OD1	5.58	123.32	118.30
1	B	332	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	B	199	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	370	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	180	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	B	370	ARG	NE-CZ-NH2	-5.17	117.72	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3487	0	3288	18	0
1	B	3441	0	3241	31	0
2	C	34	0	30	3	0
2	E	34	0	29	1	0
3	D	34	0	30	1	0
3	F	34	0	29	0	0
4	B	1	0	0	0	0
5	A	189	0	0	2	0
5	B	189	0	0	4	0
All	All	7443	0	6647	48	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 4.

All (48) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:HIS:ND1	1:A:155:HIS:O	2.07	0.86
1:B:416:THR:HB	1:B:428:ASP:O	1.88	0.73
1:B:112:ARG:NH1	5:B:601:HOH:O	2.22	0.70
1:B:180:ARG:NH2	5:B:603:HOH:O	2.27	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:TRP:HB3	5:A:778:HOH:O	1.95	0.67
2:C:1:GLC:O1	3:D:3:GLC:O6	2.16	0.63
1:B:230:GLU:OE1	2:C:1:GLC:H1	1.99	0.62
1:B:155:HIS:HB3	1:B:156:PRO:HD3	1.82	0.61
1:A:371:ALA:O	1:A:377:ARG:NH1	2.39	0.56
1:A:407:HIS:HB2	1:A:432:LEU:HD13	1.87	0.55
1:B:386:LEU:HD21	1:B:419:ILE:HG12	1.89	0.55
1:B:430:VAL:HG21	1:B:440:LEU:HD21	1.89	0.53
1:B:239:LEU:HD21	1:B:246:GLY:HA2	1.91	0.53
1:B:427:ALA:O	1:A:443:ALA:HB2	2.09	0.52
1:B:361:ASP:OD2	1:A:410:GLU:OE1	2.27	0.52
1:B:180:ARG:NH2	5:B:606:HOH:O	2.43	0.52
1:B:425:LEU:HD22	1:B:443:ALA:O	2.11	0.51
1:B:416:THR:HG21	1:B:426:ASP:CG	2.32	0.50
1:B:13:TYR:CD2	1:B:59:ILE:HD12	2.47	0.49
1:A:230:GLU:OE1	2:E:1:GLC:H1	2.13	0.48
1:A:35:TRP:CE2	1:A:347:ALA:HB1	2.49	0.48
1:B:180:ARG:NH1	5:B:613:HOH:O	2.47	0.46
1:A:378:ARG:HG3	5:A:626:HOH:O	2.15	0.46
1:A:260:THR:OG1	1:A:315:SER:OG	2.33	0.45
1:B:35:TRP:CE2	1:B:347:ALA:HB1	2.51	0.45
1:A:316:TYR:OH	1:A:332:ASP:HB3	2.17	0.45
1:B:420:PRO:HA	1:B:423:ALA:HB3	1.99	0.45
1:B:206:ILE:HD12	1:B:211:TRP:CZ2	2.52	0.45
1:B:405:ILE:HG22	1:B:432:LEU:HD11	2.00	0.44
1:A:117:ALA:HB2	1:A:198:TRP:CE3	2.53	0.44
1:A:208:HIS:O	1:A:212:ARG:HG3	2.18	0.43
1:B:341:ASP:HA	1:B:342:PRO:HA	1.89	0.43
1:A:405:ILE:CG2	1:A:432:LEU:HD11	2.50	0.42
1:B:380:ARG:O	1:B:395:ARG:HA	2.20	0.42
1:B:333:GLU:HG2	1:B:334:VAL:HG13	2.01	0.42
1:B:260:THR:HG1	1:B:315:SER:HG	1.65	0.41
1:B:316:TYR:OH	1:B:332:ASP:HB3	2.20	0.41
1:A:155:HIS:C	1:A:155:HIS:ND1	2.74	0.41
1:B:6:TRP:CZ3	1:B:112:ARG:HD2	2.55	0.41
1:A:405:ILE:HG22	1:A:432:LEU:HD11	2.02	0.41
1:B:201:ASP:OD1	2:C:1:GLC:C1	2.68	0.41
1:B:70:THR:HB	1:B:71:PRO:CD	2.51	0.41
1:A:90:ASP:OD2	1:A:92:ARG:HD2	2.20	0.41
1:A:136:GLU:HA	1:A:150:PHE:CE1	2.56	0.41
1:B:329:TYR:O	1:B:330:TYR:C	2.59	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:TYR:CE2	1:B:59:ILE:CD1	3.04	0.40
1:B:425:LEU:HD23	1:B:425:LEU:O	2.22	0.40
1:B:13:TYR:CE2	1:B:59:ILE:HD11	2.57	0.40

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	448/471 (95%)	431 (96%)	15 (3%)	2 (0%)	34	24
1	B	440/471 (93%)	422 (96%)	16 (4%)	2 (0%)	29	17
All	All	888/942 (94%)	853 (96%)	31 (4%)	4 (0%)	29	17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	PRO
1	B	206	ILE
1	A	206	ILE
1	B	156	PRO

### 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	354/372 (95%)	344 (97%)	10 (3%)	43	29
1	B	349/372 (94%)	340 (97%)	9 (3%)	46	32
All	All	703/744 (94%)	684 (97%)	19 (3%)	44	31

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2	THR
1	B	42	ASP
1	B	68	TYR
1	B	152	VAL
1	B	265	ILE
1	B	280	GLU
1	B	292	LEU
1	B	416	THR
1	B	440	LEU
1	A	1	VAL
1	A	68	TYR
1	A	105	GLU
1	A	183	HIS
1	A	265	ILE
1	A	380	ARG
1	A	399	ASP
1	A	416	THR
1	A	422	LEU
1	A	429	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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	C	1	2	12,12,12	1.27	1 (8%)	17,17,17	2.20	8 (47%)
2	GLC	C	2	2	11,11,12	0.73	0	15,15,17	1.09	1 (6%)
2	GLC	C	3	2	11,11,12	0.84	0	15,15,17	1.33	3 (20%)
3	BGC	D	1	3	12,12,12	0.53	0	17,17,17	1.06	1 (5%)
3	GLC	D	2	3	11,11,12	0.75	0	15,15,17	1.24	1 (6%)
3	GLC	D	3	3	11,11,12	0.59	0	15,15,17	1.37	3 (20%)
2	GLC	E	1	2	12,12,12	0.64	0	17,17,17	1.90	6 (35%)
2	GLC	E	2	2	11,11,12	0.84	0	15,15,17	1.19	2 (13%)
2	GLC	E	3	2	11,11,12	0.83	0	15,15,17	1.48	3 (20%)
3	BGC	F	1	3	12,12,12	0.97	1 (8%)	17,17,17	1.77	4 (23%)
3	GLC	F	2	3	11,11,12	0.94	1 (9%)	15,15,17	1.27	2 (13%)
3	GLC	F	3	3	11,11,12	0.89	0	15,15,17	1.85	6 (40%)

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	C	1	2	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	2/2/19/22	0/1/1/1
2	GLC	C	3	2	-	0/2/19/22	0/1/1/1
3	BGC	D	1	3	-	0/2/22/22	0/1/1/1
3	GLC	D	2	3	-	0/2/19/22	0/1/1/1
3	GLC	D	3	3	-	0/2/19/22	0/1/1/1
2	GLC	E	1	2	-	0/2/22/22	0/1/1/1
2	GLC	E	2	2	-	2/2/19/22	0/1/1/1
2	GLC	E	3	2	-	2/2/19/22	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	F	1	3	-	0/2/22/22	0/1/1/1
3	GLC	F	2	3	-	0/2/19/22	0/1/1/1
3	GLC	F	3	3	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	BGC	O5-C1	2.34	1.48	1.42
3	F	2	GLC	O4-C4	2.14	1.48	1.43
2	C	1	GLC	O4-C4	2.01	1.47	1.43

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	BGC	C1-O5-C5	-4.56	105.06	113.66
2	C	1	GLC	O5-C1-C2	-3.62	103.83	110.28
3	F	3	GLC	O4-C4-C3	-3.56	102.12	110.35
2	E	1	GLC	C4-C3-C2	-3.51	104.70	110.82
2	C	1	GLC	O4-C4-C3	-3.42	102.44	110.35
3	F	1	BGC	C1-C2-C3	-3.22	103.63	110.31
2	E	1	GLC	O5-C5-C4	3.21	115.52	109.69
2	E	3	GLC	O5-C5-C6	3.20	112.22	107.20
2	E	2	GLC	O5-C1-C2	-3.15	105.91	110.77
2	C	1	GLC	C6-C5-C4	-3.10	105.73	113.00
2	C	1	GLC	O3-C3-C2	3.09	117.50	110.35
3	F	3	GLC	C6-C5-C4	2.83	119.62	113.00
2	C	1	GLC	O4-C4-C5	2.69	115.99	109.30
2	E	1	GLC	O2-C2-C1	2.55	115.07	109.16
3	F	1	BGC	C6-C5-C4	2.53	118.94	113.00
3	F	2	GLC	O5-C5-C4	2.53	116.99	110.83
2	C	3	GLC	C1-O5-C5	2.51	115.59	112.19
3	D	3	GLC	O6-C6-C5	-2.50	102.71	111.29
2	E	1	GLC	O1-C1-C2	2.49	116.04	109.03
2	E	3	GLC	C1-O5-C5	2.46	115.53	112.19
3	D	3	GLC	C2-C3-C4	-2.46	106.64	110.89
2	E	2	GLC	C1-C2-C3	2.44	112.67	109.67
3	F	3	GLC	C1-O5-C5	2.44	115.50	112.19
2	C	1	GLC	C1-O5-C5	2.43	118.25	113.66
3	F	3	GLC	O4-C4-C5	2.41	115.29	109.30
2	C	1	GLC	O2-C2-C1	2.38	114.69	109.16
2	C	1	GLC	O5-C5-C4	2.34	113.94	109.69
2	C	3	GLC	C3-C4-C5	-2.33	106.08	110.24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	GLC	O5-C1-C2	-2.33	106.13	110.28
3	D	2	GLC	O3-C3-C2	-2.32	105.54	109.99
3	F	2	GLC	O5-C5-C6	-2.26	103.67	107.20
3	F	3	GLC	O6-C6-C5	2.23	118.95	111.29
3	D	1	BGC	O1-C1-O5	-2.21	103.74	110.38
3	D	3	GLC	O2-C2-C3	-2.20	105.73	110.14
2	C	3	GLC	O4-C4-C3	2.18	115.39	110.35
2	E	3	GLC	O2-C2-C1	2.15	113.55	109.15
3	F	1	BGC	O5-C5-C6	2.11	111.69	106.44
2	C	2	GLC	O3-C3-C2	-2.08	106.00	109.99
3	F	3	GLC	O3-C3-C4	2.05	115.09	110.35
2	E	1	GLC	O2-C2-C3	2.04	115.07	110.35

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	GLC	O5-C5-C6-O6
2	E	2	GLC	O5-C5-C6-O6
2	C	2	GLC	C4-C5-C6-O6
2	E	2	GLC	C4-C5-C6-O6
2	E	3	GLC	C4-C5-C6-O6
2	E	3	GLC	O5-C5-C6-O6

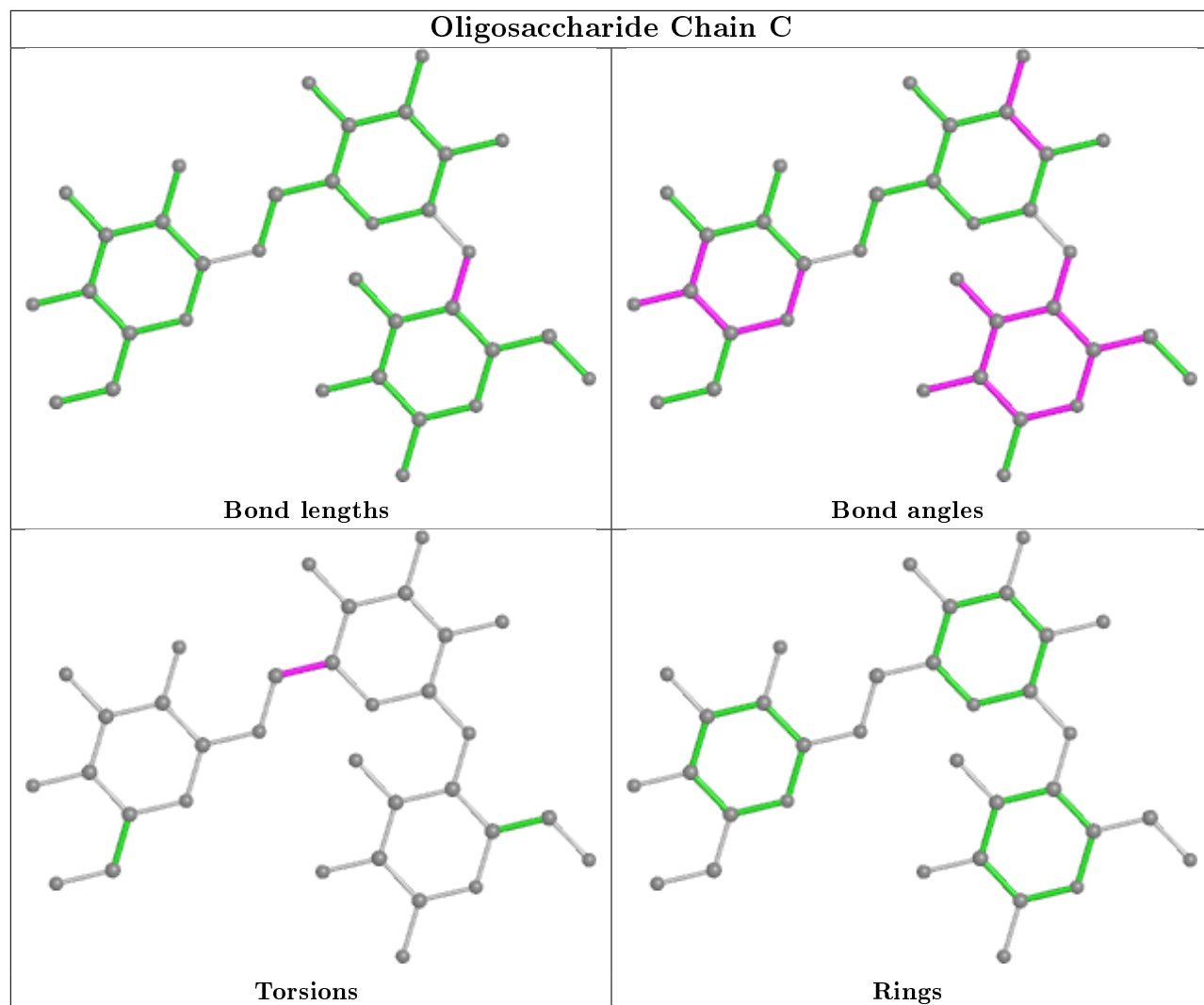
There are no ring outliers.

3 monomers are involved in 4 short contacts:

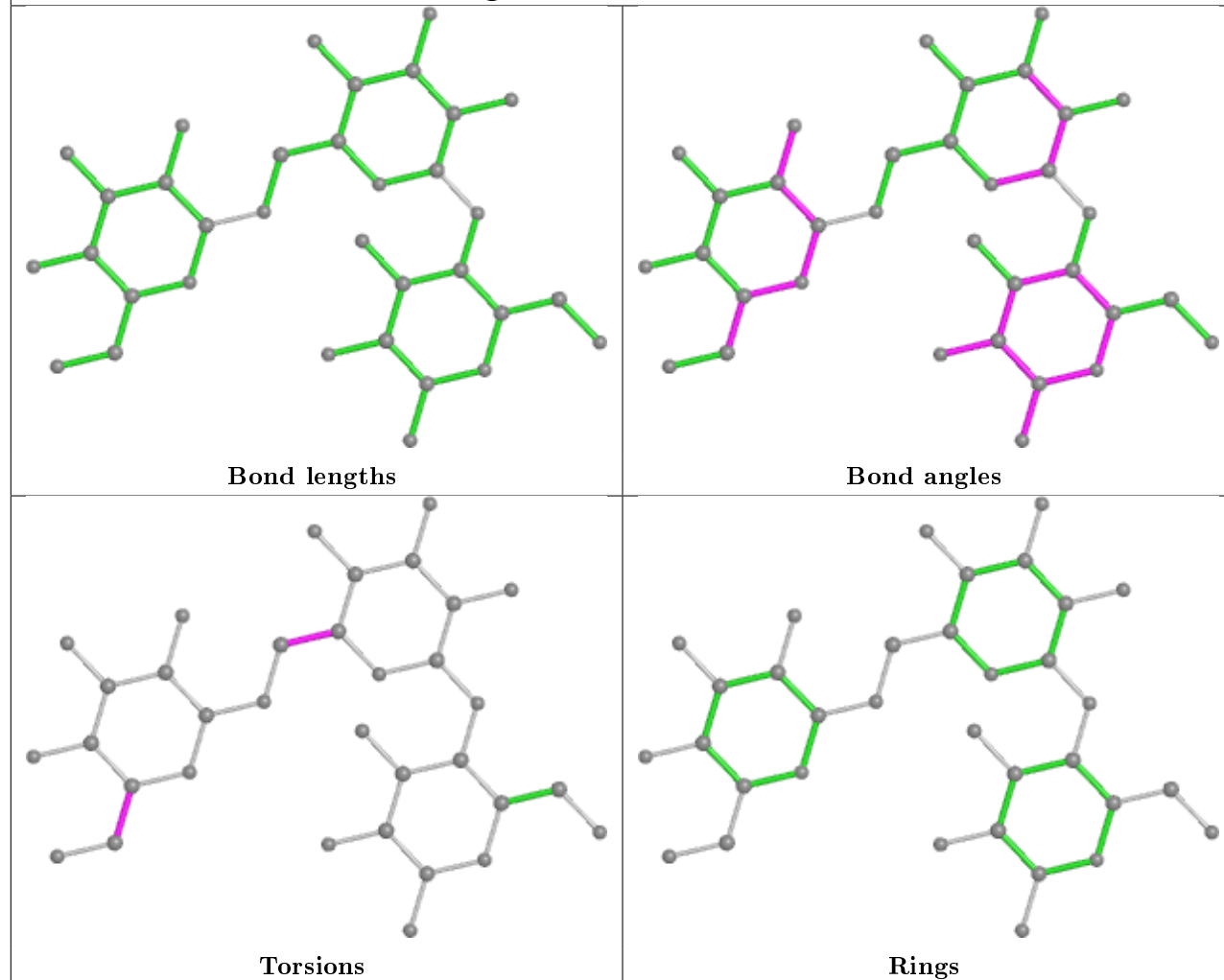
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	GLC	3	0
3	D	3	GLC	1	0
2	E	1	GLC	1	0

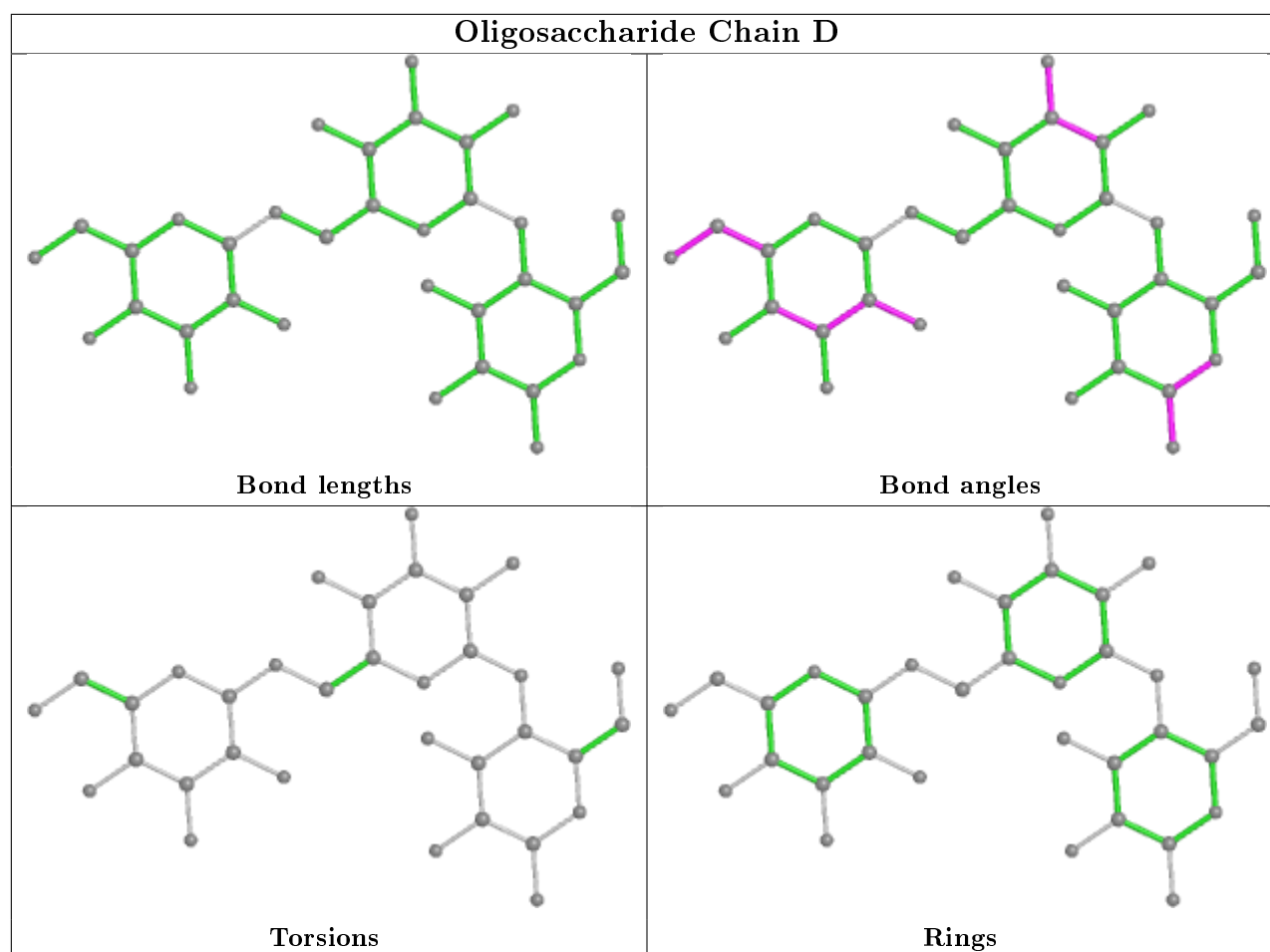
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

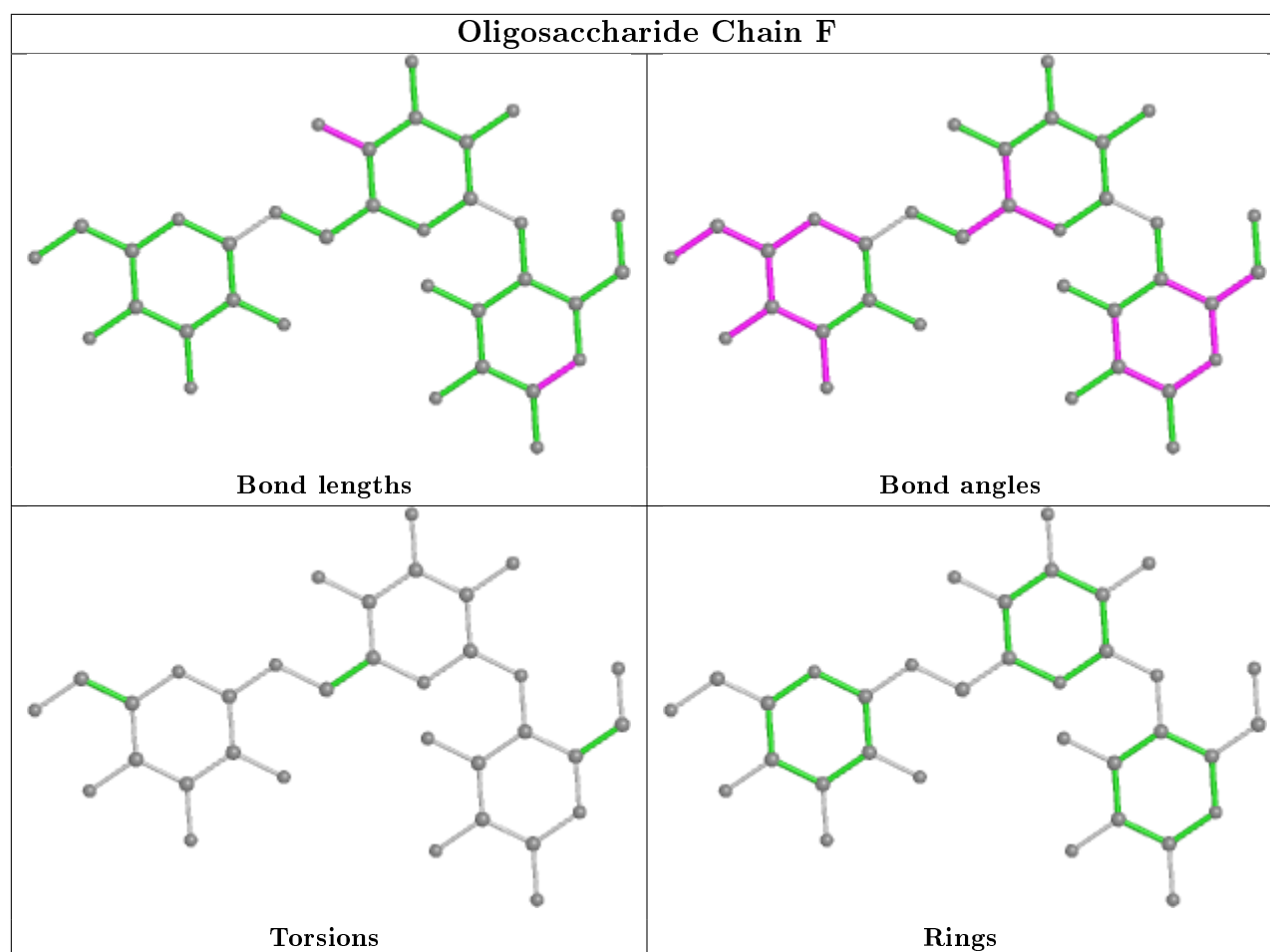




## Oligosaccharide Chain E







## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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 [i](#)

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	450/471 (95%)	0.01	10 (2%) 62 69	13, 21, 39, 68	0
1	B	442/471 (93%)	-0.03	6 (1%) 75 80	12, 20, 38, 66	0
All	All	892/942 (94%)	-0.01	16 (1%) 68 74	12, 21, 39, 68	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	425	LEU	5.7
1	B	420	PRO	5.0
1	A	155	HIS	3.9
1	A	424	PRO	3.3
1	A	276	ALA	3.3
1	B	155	HIS	3.2
1	A	417	ALA	3.2
1	A	398	GLY	2.6
1	B	138	ASP	2.4
1	A	372	HIS	2.4
1	B	424	PRO	2.3
1	A	1	VAL	2.2
1	B	276	ALA	2.2
1	A	422	LEU	2.1
1	A	30	GLN	2.1
1	A	423	ALA	2.0

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

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

## 6.3 Carbohydrates

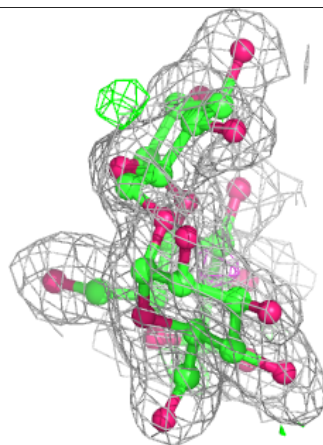
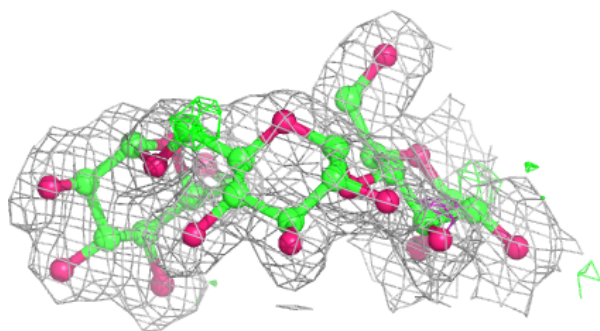
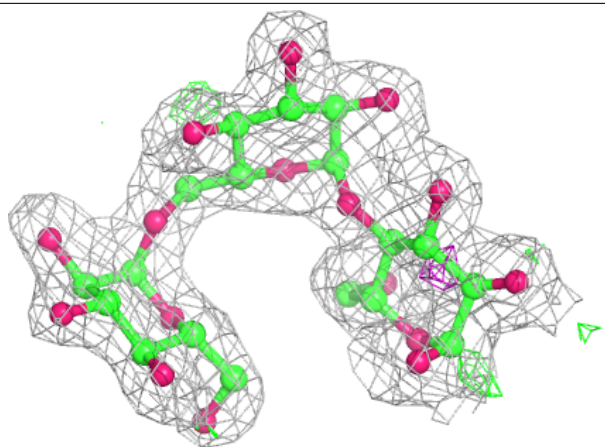
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GLC	D	3	11/12	0.76	0.15	34,36,40,42	0
3	BGC	F	1	12/12	0.81	0.23	23,29,32,38	0
3	GLC	F	2	11/12	0.84	0.18	30,33,35,35	0
3	GLC	F	3	11/12	0.85	0.32	23,25,26,29	11
2	GLC	E	3	11/12	0.86	0.16	32,34,36,39	0
3	GLC	D	2	11/12	0.89	0.14	27,30,33,34	0
2	GLC	C	1	12/12	0.89	0.13	18,20,23,24	0
2	GLC	E	1	12/12	0.89	0.36	8,11,15,15	12
3	BGC	D	1	12/12	0.90	0.21	23,30,36,37	0
2	GLC	E	2	11/12	0.91	0.16	18,23,32,32	0
2	GLC	C	3	11/12	0.93	0.14	28,29,32,33	0
2	GLC	C	2	11/12	0.93	0.10	21,24,33,36	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 C:**

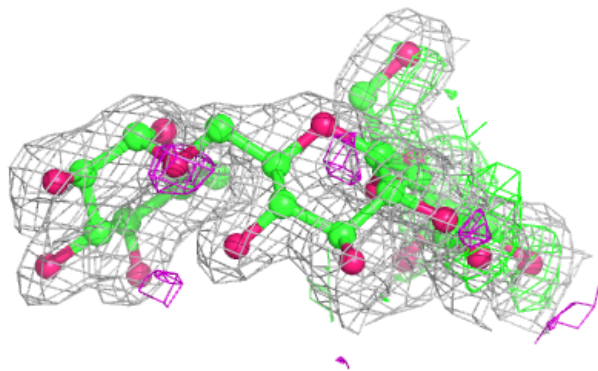
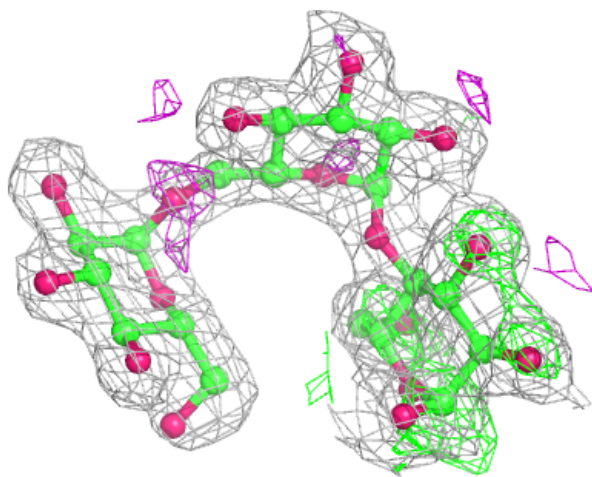
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





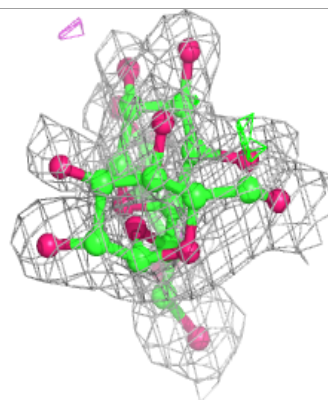
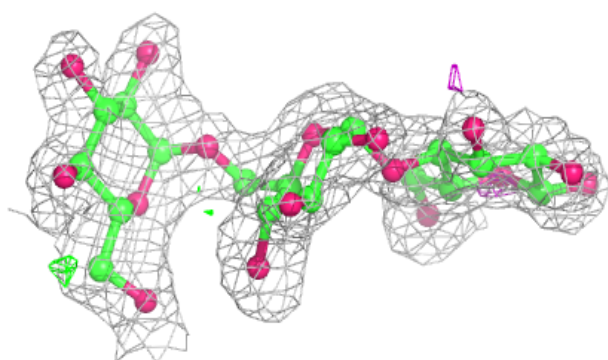
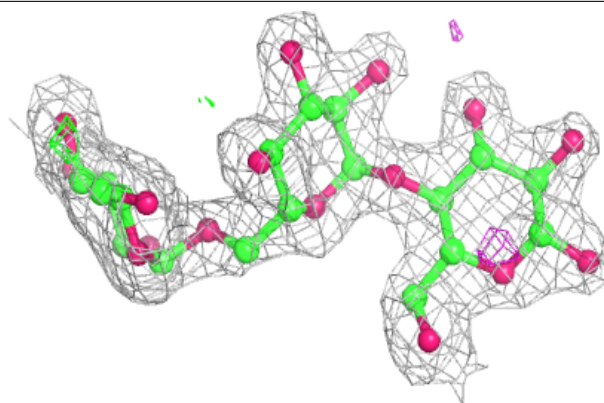
**Electron density around Chain E:**

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

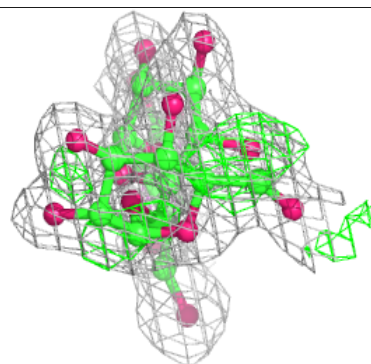
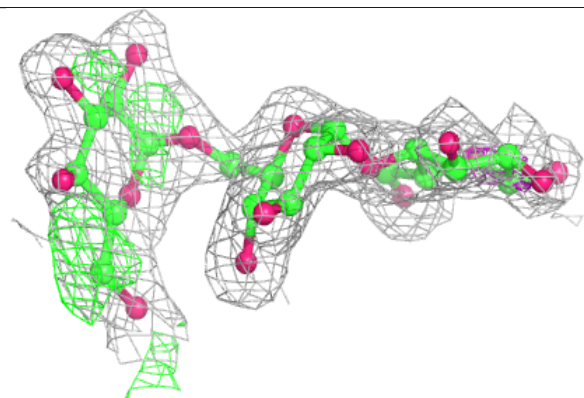
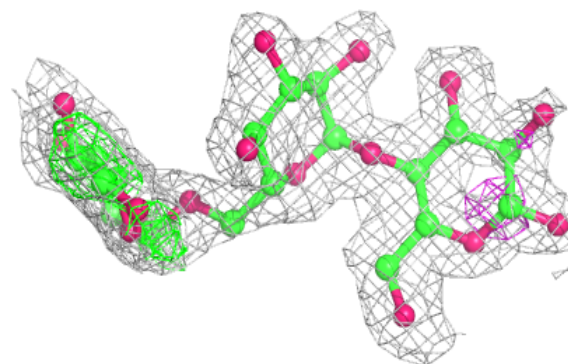


**Electron density around Chain D:**

$2mF_o-DF_c$  (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)



## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	CA	B	507	1/1	0.98	0.16	36,36,36,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.