Full wwPDB X-ray Structure Validation Report (i)

Sep 21, 2023 – 12:03 AM EDT

PDB ID	:	5E6Z
Title	:	Crystal structure of Ecoli Branching Enzyme with beta cyclodextrin
Authors	:	Feng, L.; Nosrati, M.; Geiger, J.H.
Deposited on	:	2015-10-11
Resolution	:	1.88 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 (i) 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 (i)) were used in the production of this report:

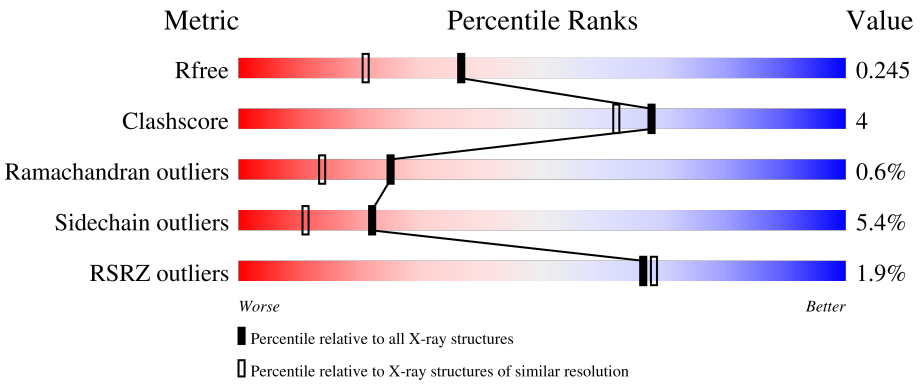
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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 <=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	612	4% 83% 11% • •
1	B	612	% 88% 8% • •
1	C	612	2% 81% 12% • 5%
1	D	612	% 85% 10% • •
2	E	7	14% 86%

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Mol	Chain	Length	Quality of chain
2	F	7	86% 14%
2	G	7	86% 14%
2	H	7	14% 86%
2	I	7	86% 14%
2	J	7	86% 14%

2 Entry composition (i)

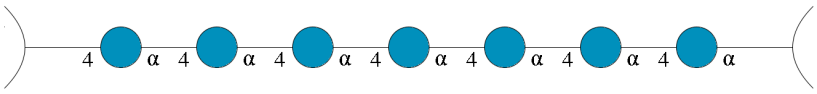
There are 4 unique types of molecules in this entry. The entry contains 21819 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 1,4-alpha-glucan branching enzyme GlgB.

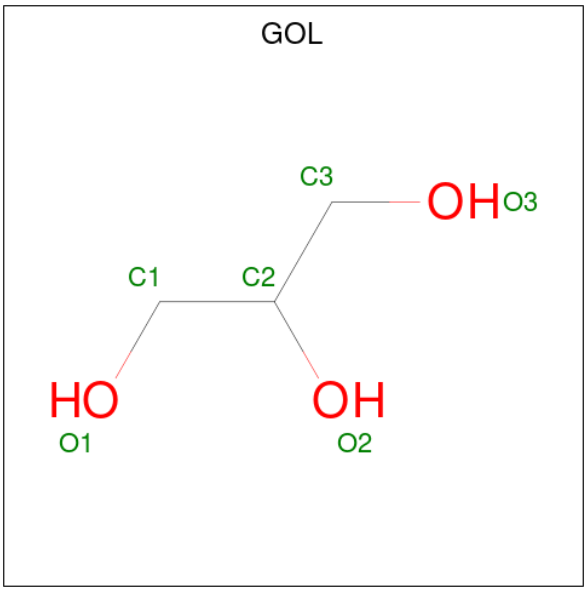
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	587	4866	3117	859	874	16	0	9	0
1	B	596	4953	3169	881	887	16	0	8	0
1	C	582	4810	3082	852	861	15	0	4	0
1	D	587	4849	3101	863	869	16	0	4	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	E	7	77	42	35	0	0	0
2	F	7	77	42	35	0	0	0
2	G	7	77	42	35	0	0	0
2	H	7	77	42	35	0	0	0
2	I	7	77	42	35	0	0	0
2	J	7	77	42	35	0	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

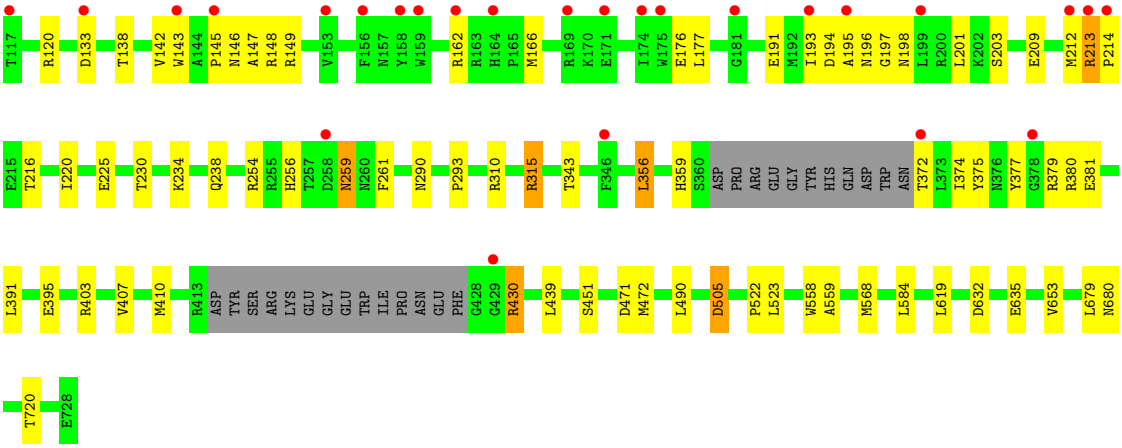
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	447	447	447	0	0
			Total	O		
4	B	615	615	615	0	0
			Total	O		
4	C	289	289	289	0	0
			Total	O		
4	D	486	486	486	0	0

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.

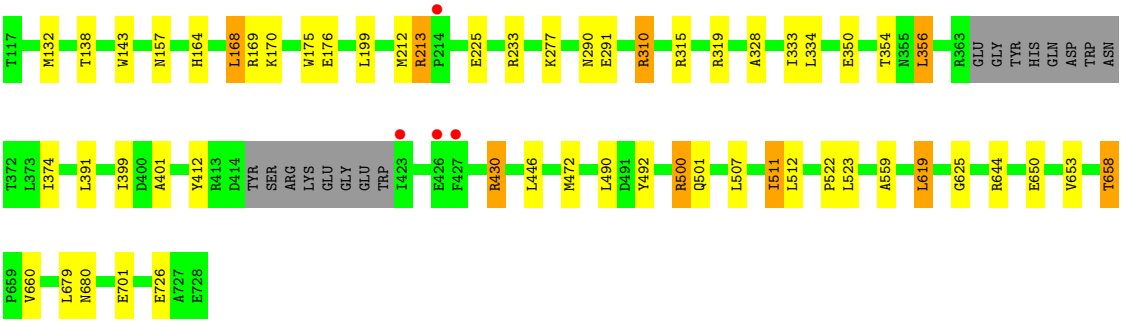
• Molecule 1: 1,4-alpha-glucan branching enzyme GlgB

Chain A:



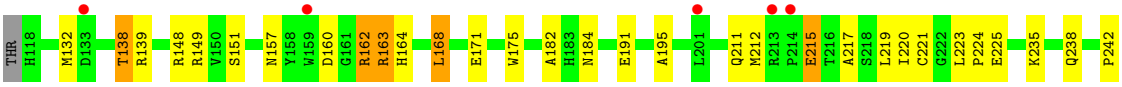
• Molecule 1: 1,4-alpha-glucan branching enzyme GlgB

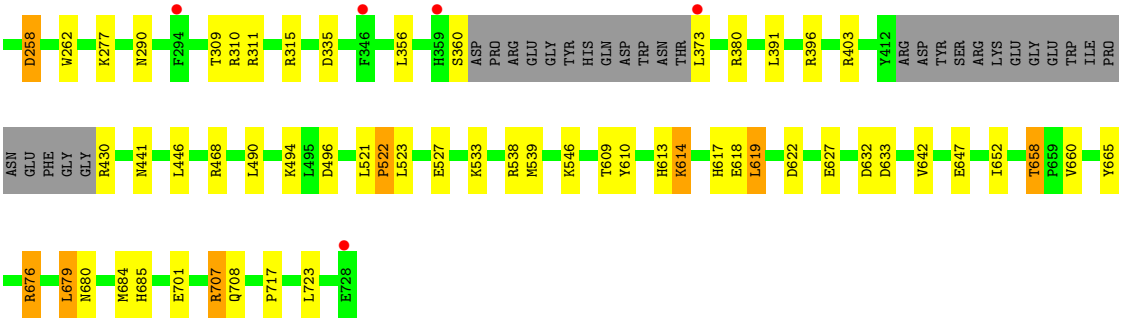
Chain B:



• Molecule 1: 1,4-alpha-glucan branching enzyme GlgB

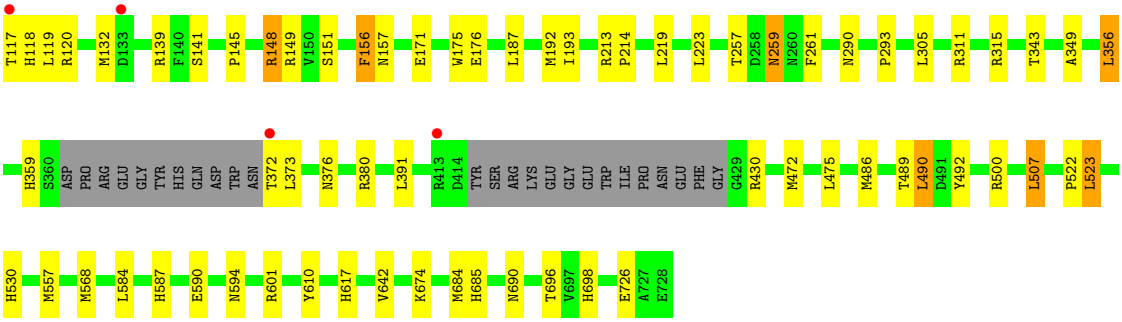
Chain C:





- Molecule 1: 1,4-alpha-glucan branching enzyme GlgB

Chain D:

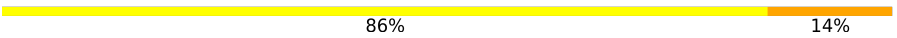


- Molecule 2: Cycloheptakis-(1-4)-(alpha-D-glucopyranose)

Chain E:

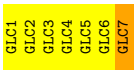
- Molecule 2: Cycloheptakis-(1-4)-(alpha-D-glucopyranose)

Chain F:



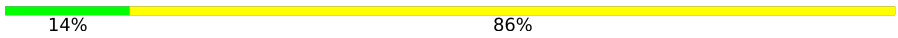
- Molecule 2: Cycloheptakis-(1-4)-(alpha-D-glucopyranose)

Chain G:



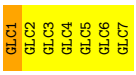
- Molecule 2: Cycloheptakis-(1-4)-(alpha-D-glucopyranose)

Chain H:



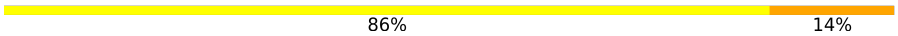
- Molecule 2: Cycloheptakis-(1-4)-(alpha-D-glucopyranose)

Chain I:



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

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	91.95Å 103.00Å 186.24Å 90.00° 91.57° 90.00°	Depositor
Resolution (Å)	44.93 – 1.88 44.93 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.4 (44.93-1.88) 99.4 (44.93-1.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 1.88Å)	Xtriage
Refinement program	PHENIX 1.7.2_869	Depositor
R, R_{free}	0.206 , 0.249 0.203 , 0.245	Depositor DCC
R_{free} test set	28010 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å^2)	24.9	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 35.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.067 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	21819	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, 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	0.38	0/5040	0.55	0/6845
1	B	0.44	0/5128	0.60	2/6962 (0.0%)
1	C	0.32	0/4973	0.49	0/6755
1	D	0.38	0/5014	0.55	0/6807
All	All	0.38	0/20155	0.55	2/27369 (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	D	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	500	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	B	500	ARG	NE-CZ-NH2	-6.26	117.17	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	156	PHE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4866	0	4604	39	0
1	B	4953	0	4700	28	0
1	C	4810	0	4547	49	0
1	D	4849	0	4597	35	0
2	E	77	0	63	0	0
2	F	77	0	63	1	0
2	G	77	0	63	1	0
2	H	77	0	63	0	0
2	I	77	0	63	1	0
2	J	77	0	63	1	0
3	A	12	0	16	0	0
3	B	12	0	16	0	0
3	C	6	0	8	0	0
3	D	12	0	16	0	0
4	A	447	0	0	9	1
4	B	615	0	0	7	1
4	C	289	0	0	9	0
4	D	486	0	0	7	1
All	All	21819	0	18882	149	2

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 (149) 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:403:ARG:NH1	4:A:902:HOH:O	2.11	0.84
1:B:658:THR:HG22	1:B:660:VAL:H	1.44	0.83
1:A:194:ASP:HB2	1:A:198:ASN:H	1.46	0.78
1:C:162[A]:ARG:NH1	4:C:902:HOH:O	2.16	0.78
1:D:151:SER:OG	4:D:901:HOH:O	2.02	0.76
1:A:149:ARG:HB3	1:A:193:ILE:HB	1.69	0.73
1:A:254:ARG:NH2	4:A:905:HOH:O	2.21	0.72
1:D:684:MET:H	1:D:690:ASN:HD22	1.35	0.72
1:D:132:MET:SD	1:D:139[A]:ARG:NH1	2.63	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:511:ILE:HB	4:B:1490:HOH:O	1.91	0.71
1:A:632[B]:ASP:OD1	4:A:901:HOH:O	2.08	0.70
1:C:162[B]:ARG:NH2	4:C:905:HOH:O	2.24	0.70
1:A:256:HIS:HB2	1:A:259:ASN:HD21	1.58	0.69
1:A:259:ASN:HD22	1:A:261:PHE:H	1.41	0.69
1:C:658:THR:HG22	1:C:660:VAL:H	1.58	0.68
1:C:162[A]:ARG:HH11	1:C:162[A]:ARG:HB2	1.58	0.68
1:B:169:ARG:NH1	1:B:176:GLU:OE2	2.27	0.68
1:B:213[A]:ARG:HD3	1:B:213[A]:ARG:H	1.60	0.66
1:A:194:ASP:HB3	1:A:196:ASN:H	1.60	0.65
1:A:213:ARG:NH1	1:A:293:PRO:O	2.28	0.65
1:A:632[B]:ASP:OD1	4:A:903:HOH:O	2.15	0.64
1:C:609:THR:O	4:C:901:HOH:O	2.15	0.64
1:C:494:LYS:HD3	1:C:538:ARG:HG2	1.80	0.64
1:A:471:ASP:OD1	4:A:904:HOH:O	2.15	0.62
1:A:212:MET:HG2	1:A:310:ARG:HG2	1.82	0.62
1:D:492:TYR:CZ	1:D:500:ARG:HG2	2.36	0.60
1:D:684:MET:H	1:D:690:ASN:ND2	1.99	0.60
1:C:527:GLU:O	1:C:538:ARG:NH1	2.26	0.60
1:D:139[A]:ARG:NH2	1:D:176:GLU:OE1	2.35	0.60
4:D:1071:HOH:O	2:J:2:GLC:H62	2.01	0.59
1:A:234:LYS:NZ	1:A:451:SER:O	2.30	0.58
1:C:163:ARG:NH1	4:C:913:HOH:O	2.36	0.58
1:B:701:GLU:OE2	4:B:901:HOH:O	2.17	0.58
1:D:259:ASN:HB3	1:D:261:PHE:H	1.69	0.57
1:C:242:PRO:HD3	1:C:617:HIS:CE1	2.39	0.57
1:D:349:ALA:O	4:D:902:HOH:O	2.18	0.57
1:B:233:ARG:NH1	4:B:915:HOH:O	2.38	0.56
1:B:492:TYR:CZ	1:B:500:ARG:HG2	2.41	0.56
1:D:696:THR:OG1	1:D:726:GLU:OE1	2.21	0.55
1:D:343:THR:HG22	1:D:373:LEU:HD12	1.87	0.55
1:C:162[B]:ARG:NH1	4:C:903:HOH:O	2.17	0.55
1:B:319:ARG:NH1	4:B:914:HOH:O	2.38	0.54
1:A:149:ARG:NH1	1:A:191:GLU:OE2	2.41	0.54
1:A:120:ARG:NH1	1:A:395:GLU:OE2	2.41	0.53
1:C:627:GLU:OE1	1:C:707:ARG:NH2	2.41	0.53
1:B:143:TRP:CH2	1:B:356:LEU:HD22	2.42	0.53
1:B:212:MET:HG3	1:B:310:ARG:HD3	1.91	0.53
1:D:486:MET:O	1:D:490:LEU:HB2	2.10	0.52
1:C:139:ARG:HD3	4:C:933:HOH:O	2.10	0.52
1:C:539:MET:O	1:C:546:LYS:NZ	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:ASN:OD1	1:C:164:HIS:ND1	2.42	0.51
1:A:635[A]:GLU:H	1:A:635[A]:GLU:CD	2.14	0.51
1:B:726:GLU:HG2	4:B:1293:HOH:O	2.10	0.51
1:C:224:PRO:HG2	1:C:396:ARG:HB3	1.92	0.51
1:B:644:ARG:CG	1:B:650:GLU:HG2	2.42	0.49
1:A:679:LEU:HG	1:A:680:ASN:N	2.27	0.49
1:C:262:TRP:CH2	1:C:311:ARG:HD3	2.47	0.49
1:B:658:THR:CG2	1:B:660:VAL:H	2.20	0.49
1:C:676[A]:ARG:NH2	4:C:912:HOH:O	2.36	0.48
1:D:594:ASN:HB2	4:D:1235:HOH:O	2.13	0.48
1:A:356:LEU:O	1:A:379:ARG:NH1	2.46	0.48
1:C:138:THR:HG23	1:C:182:ALA:HB3	1.95	0.47
1:C:309:THR:OG1	1:C:311:ARG:HG3	2.14	0.47
1:B:501:GLN:NE2	4:B:921:HOH:O	2.41	0.47
1:C:309:THR:OG1	4:C:904:HOH:O	2.20	0.47
1:D:120:ARG:NH2	4:D:918:HOH:O	2.37	0.47
1:C:652:ILE:HB	1:C:723:LEU:HB2	1.96	0.47
1:D:148:ARG:HG3	1:D:193:ILE:HG22	1.95	0.47
1:A:143:TRP:CH2	1:A:356:LEU:HD22	2.50	0.47
1:C:717:PRO:HG3	2:I:1:GLC:H62	1.97	0.47
1:D:530:HIS:HE1	4:D:1344:HOH:O	1.98	0.47
1:B:212:MET:HG2	1:B:213[A]:ARG:NH1	2.30	0.47
1:D:617:HIS:HE1	4:D:1335:HOH:O	1.97	0.46
1:C:138:THR:HG21	1:C:220:ILE:HD13	1.97	0.46
1:B:213[B]:ARG:NH2	1:B:291:GLU:OE1	2.38	0.46
1:B:679:LEU:HG	1:B:680:ASN:N	2.30	0.46
1:B:277[A]:LYS:HD2	1:B:328:ALA:HB1	1.96	0.46
1:A:559:ALA:HB1	1:A:653:VAL:HG21	1.98	0.46
1:B:619:LEU:HB3	1:B:625:GLY:HA3	1.97	0.46
1:D:213:ARG:NH2	1:D:293:PRO:O	2.49	0.46
1:D:587:HIS:O	1:D:590:GLU:HB2	2.16	0.46
1:A:238:GLN:HG2	4:A:1324:HOH:O	2.16	0.46
1:C:149:ARG:NH2	1:C:191:GLU:OE2	2.37	0.46
1:C:619:LEU:HG	1:C:622:ASP:HB3	1.99	0.45
1:D:145:PRO:HD2	1:D:356:LEU:HD11	1.98	0.45
1:A:148:ARG:HH12	1:A:197:GLY:HA2	1.80	0.45
1:A:148:ARG:NH2	1:A:195:ALA:O	2.49	0.45
1:A:407:VAL:HA	1:A:410:MET:HE2	1.99	0.45
1:A:138:THR:HG21	1:A:220:ILE:HG21	1.98	0.45
1:A:356:LEU:HD23	1:A:356:LEU:HA	1.77	0.45
1:C:149:ARG:NH1	1:C:151:SER:OG	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:685:HIS:CE1	1:D:685:HIS:HD2	2.35	0.45
1:A:430:ARG:H	1:A:430:ARG:HG2	1.49	0.45
1:D:359:HIS:CD2	1:D:376:ASN:HA	2.52	0.45
1:A:146:ASN:O	1:A:148:ARG:N	2.50	0.44
1:D:486:MET:HG2	1:D:490:LEU:HD22	1.98	0.44
1:A:261:PHE:CD2	2:F:6:GLC:H3	2.51	0.44
1:B:157:ASN:OD1	1:B:164:HIS:ND1	2.50	0.44
1:C:235:LYS:HA	1:C:238:GLN:HG3	1.98	0.44
1:C:258:ASP:OD1	1:C:258:ASP:N	2.43	0.44
1:C:335:ASP:OD1	1:C:403:ARG:HD3	2.18	0.44
1:D:213:ARG:HH22	1:D:311:ARG:NH1	2.16	0.44
1:C:168:LEU:HG	1:C:175:TRP:CE2	2.52	0.43
1:D:568:MET:HB2	1:D:584:LEU:HD11	1.99	0.43
1:C:633:ASP:OD2	1:C:665:TYR:OH	2.29	0.43
1:C:160:ASP:CG	1:C:162[A]:ARG:HG2	2.40	0.43
1:C:610:TYR:O	1:C:617:HIS:HD2	2.01	0.43
1:C:533:LYS:O	1:C:538:ARG:NH1	2.52	0.42
1:B:333:ILE:HG12	1:B:401:ALA:HB3	2.01	0.42
1:B:168:LEU:HG	1:B:175:TRP:CE2	2.54	0.42
1:C:211:GLN:HE21	1:C:217:ALA:H	1.65	0.42
1:C:613:HIS:HB2	4:C:901:HOH:O	2.19	0.42
1:C:614:LYS:O	1:C:618:GLU:HB2	2.19	0.42
1:C:685:HIS:NE2	1:D:685:HIS:HD2	2.18	0.42
1:D:489:THR:HG22	1:D:507:LEU:HD12	2.02	0.42
1:A:254:ARG:NE	4:A:952:HOH:O	2.53	0.42
1:B:334[B]:LEU:HG	1:B:399:ILE:HD12	2.00	0.42
1:C:521:LEU:HA	1:C:522:PRO:HD3	1.92	0.42
1:C:211:GLN:NE2	1:C:215:GLU:HB2	2.34	0.42
1:C:685:HIS:CD2	1:D:685:HIS:CD2	3.07	0.42
1:D:601:ARG:HD2	1:D:685:HIS:NE2	2.34	0.42
1:B:350:GLU:HA	1:B:354:THR:O	2.20	0.42
1:B:412:TYR:CE2	1:B:430:ARG:HD2	2.55	0.41
1:A:505:ASP:HB3	4:A:1284:HOH:O	2.19	0.41
1:A:230:THR:HB	4:A:1129:HOH:O	2.20	0.41
1:D:430:ARG:HB2	1:D:430:ARG:NH1	2.35	0.41
1:B:492:TYR:CE2	1:B:500:ARG:HG2	2.55	0.41
1:A:410:MET:HE1	1:A:439:LEU:HD21	2.02	0.41
1:C:685:HIS:CD2	1:D:685:HIS:HD2	2.39	0.41
1:A:145:PRO:HD2	1:A:356:LEU:HD21	2.03	0.41
1:A:568:MET:HB2	1:A:584:LEU:HD11	2.03	0.41
1:C:184:ASN:OD1	1:C:221:CYS:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:632:ASP:OD2	1:C:632:ASP:N	2.51	0.41
1:D:610:TYR:O	1:D:617:HIS:HD2	2.03	0.41
1:C:679:LEU:HG	1:C:680:ASN:N	2.35	0.41
1:C:701:GLU:OE2	1:C:708:GLN:NE2	2.54	0.41
1:A:166:MET:HA	1:A:177:LEU:HB2	2.03	0.41
1:A:209:GLU:HG3	1:A:315:ARG:HB3	2.02	0.41
4:B:1030:HOH:O	2:G:7:GLC:H62	2.21	0.41
1:C:148:ARG:NH2	1:C:195:ALA:O	2.54	0.41
1:C:468:ARG:HD3	1:C:468:ARG:HA	1.90	0.41
1:D:523:LEU:HD22	1:D:557:MET:SD	2.61	0.41
1:B:559:ALA:HB1	1:B:653:VAL:HG21	2.03	0.40
1:D:141:SER:HA	1:D:175:TRP:O	2.21	0.40
1:A:375:TYR:HB2	1:A:377:TYR:CZ	2.56	0.40
1:A:381:GLU:OE2	1:A:381:GLU:N	2.50	0.40
1:D:674:LYS:HG2	1:D:698:HIS:CD2	2.55	0.40
1:D:684:MET:HB3	1:D:684:MET:HE3	1.88	0.40

All (2) 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:D:1070:HOH:O	4:D:1328:HOH:O[2_655]	2.13	0.07
4:A:1291:HOH:O	4:B:1318:HOH:O[1_455]	2.17	0.03

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	589/612 (96%)	568 (96%)	16 (3%)	5 (1%)	19 9
1	B	598/612 (98%)	580 (97%)	17 (3%)	1 (0%)	47 37
1	C	580/612 (95%)	563 (97%)	15 (3%)	2 (0%)	41 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	585/612 (96%)	571 (98%)	9 (2%)	5 (1%)	17	7
All	All	2352/2448 (96%)	2282 (97%)	57 (2%)	13 (1%)	25	14

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	PRO
1	D	259	ASN
1	A	133	ASP
1	A	147	ALA
1	A	216	THR
1	C	212	MET
1	D	156	PHE
1	D	157	ASN
1	D	522	PRO
1	A	522	PRO
1	B	522	PRO
1	C	522	PRO
1	D	214	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	504/521 (97%)	479 (95%)	25 (5%)	24	13
1	B	514/521 (99%)	489 (95%)	25 (5%)	25	13
1	C	496/521 (95%)	458 (92%)	38 (8%)	13	4
1	D	502/521 (96%)	477 (95%)	25 (5%)	24	13
All	All	2016/2084 (97%)	1903 (94%)	113 (6%)	22	10

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	VAL

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Mol	Chain	Res	Type
1	A	162	ARG
1	A	176	GLU
1	A	201	LEU
1	A	203	SER
1	A	213	ARG
1	A	225	GLU
1	A	259	ASN
1	A	290	ASN
1	A	315	ARG
1	A	343	THR
1	A	356	LEU
1	A	359	HIS
1	A	372	THR
1	A	374	ILE
1	A	380	ARG
1	A	391	LEU
1	A	430	ARG
1	A	472	MET
1	A	490	LEU
1	A	505	ASP
1	A	523	LEU
1	A	558	TRP
1	A	619	LEU
1	A	720	THR
1	B	132	MET
1	B	138	THR
1	B	168	LEU
1	B	170	LYS
1	B	199	LEU
1	B	213[A]	ARG
1	B	213[B]	ARG
1	B	225	GLU
1	B	290	ASN
1	B	310	ARG
1	B	315	ARG
1	B	356	LEU
1	B	374	ILE
1	B	391	LEU
1	B	430	ARG
1	B	446	LEU
1	B	472	MET
1	B	490	LEU

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Mol	Chain	Res	Type
1	B	507	LEU
1	B	511	ILE
1	B	512[A]	LEU
1	B	512[B]	LEU
1	B	523	LEU
1	B	619	LEU
1	B	658	THR
1	C	132	MET
1	C	138	THR
1	C	162[A]	ARG
1	C	162[B]	ARG
1	C	163	ARG
1	C	168	LEU
1	C	171	GLU
1	C	215	GLU
1	C	219	LEU
1	C	223	LEU
1	C	225	GLU
1	C	258	ASP
1	C	277	LYS
1	C	290	ASN
1	C	310	ARG
1	C	315	ARG
1	C	356	LEU
1	C	360	SER
1	C	373	LEU
1	C	380	ARG
1	C	391	LEU
1	C	430	ARG
1	C	441	ASN
1	C	446	LEU
1	C	490	LEU
1	C	496	ASP
1	C	523	LEU
1	C	614	LYS
1	C	619	LEU
1	C	642[A]	VAL
1	C	642[B]	VAL
1	C	647	GLU
1	C	658	THR
1	C	676[A]	ARG
1	C	676[B]	ARG

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Mol	Chain	Res	Type
1	C	679	LEU
1	C	684	MET
1	C	707	ARG
1	D	117	THR
1	D	118	HIS
1	D	119	LEU
1	D	148	ARG
1	D	149	ARG
1	D	171	GLU
1	D	187	LEU
1	D	192	MET
1	D	219	LEU
1	D	223	LEU
1	D	257	THR
1	D	290	ASN
1	D	305	LEU
1	D	315	ARG
1	D	356	LEU
1	D	372	THR
1	D	380	ARG
1	D	391	LEU
1	D	472	MET
1	D	475	LEU
1	D	490	LEU
1	D	507	LEU
1	D	523	LEU
1	D	642[A]	VAL
1	D	642[B]	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	259	ASN
1	A	260	ASN
1	A	501	GLN
1	A	617	HIS
1	C	157	ASN
1	C	211	GLN
1	C	441	ASN
1	C	617	HIS
1	D	617	HIS
1	D	685	HIS

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Mol	Chain	Res	Type
1	D	690	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

42 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	2	11,11,12	1.54	2 (18%)	15,15,17	1.28	2 (13%)
2	GLC	E	2	2	11,11,12	1.60	2 (18%)	15,15,17	1.19	1 (6%)
2	GLC	E	3	2	11,11,12	1.37	1 (9%)	15,15,17	1.07	2 (13%)
2	GLC	E	4	2	11,11,12	1.96	2 (18%)	15,15,17	0.81	0
2	GLC	E	5	2	11,11,12	1.37	2 (18%)	15,15,17	1.02	1 (6%)
2	GLC	E	6	2	11,11,12	0.80	0	15,15,17	0.88	0
2	GLC	E	7	2	11,11,12	1.29	1 (9%)	15,15,17	1.14	1 (6%)
2	GLC	F	1	2	11,11,12	1.63	2 (18%)	15,15,17	1.34	2 (13%)
2	GLC	F	2	2	11,11,12	1.62	2 (18%)	15,15,17	0.83	1 (6%)
2	GLC	F	3	2	11,11,12	1.49	1 (9%)	15,15,17	1.27	2 (13%)
2	GLC	F	4	2	11,11,12	1.91	2 (18%)	15,15,17	0.98	0
2	GLC	F	5	2	11,11,12	1.38	2 (18%)	15,15,17	0.82	1 (6%)
2	GLC	F	6	2	11,11,12	1.04	1 (9%)	15,15,17	0.57	0
2	GLC	F	7	2	11,11,12	1.28	2 (18%)	15,15,17	1.06	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GLC	G	1	2	11,11,12	1.41	2 (18%)	15,15,17	1.84	3 (20%)
2	GLC	G	2	2	11,11,12	1.88	3 (27%)	15,15,17	0.67	0
2	GLC	G	3	2	11,11,12	1.48	1 (9%)	15,15,17	0.55	0
2	GLC	G	4	2	11,11,12	1.87	2 (18%)	15,15,17	1.12	0
2	GLC	G	5	2	11,11,12	1.39	1 (9%)	15,15,17	1.07	0
2	GLC	G	6	2	11,11,12	0.84	1 (9%)	15,15,17	1.26	2 (13%)
2	GLC	G	7	2	11,11,12	1.16	1 (9%)	15,15,17	1.44	2 (13%)
2	GLC	H	1	2	11,11,12	1.54	2 (18%)	15,15,17	1.47	2 (13%)
2	GLC	H	2	2	11,11,12	1.61	2 (18%)	15,15,17	1.02	1 (6%)
2	GLC	H	3	2	11,11,12	1.44	1 (9%)	15,15,17	0.91	0
2	GLC	H	4	2	11,11,12	1.85	2 (18%)	15,15,17	0.94	1 (6%)
2	GLC	H	5	2	11,11,12	1.39	3 (27%)	15,15,17	1.14	0
2	GLC	H	6	2	11,11,12	0.91	0	15,15,17	0.88	0
2	GLC	H	7	2	11,11,12	1.26	2 (18%)	15,15,17	1.11	2 (13%)
2	GLC	I	1	2	11,11,12	1.59	2 (18%)	15,15,17	1.36	2 (13%)
2	GLC	I	2	2	11,11,12	1.65	2 (18%)	15,15,17	1.10	1 (6%)
2	GLC	I	3	2	11,11,12	1.45	1 (9%)	15,15,17	0.96	0
2	GLC	I	4	2	11,11,12	1.88	2 (18%)	15,15,17	1.03	1 (6%)
2	GLC	I	5	2	11,11,12	1.42	3 (27%)	15,15,17	1.25	1 (6%)
2	GLC	I	6	2	11,11,12	0.90	0	15,15,17	1.15	1 (6%)
2	GLC	I	7	2	11,11,12	1.24	1 (9%)	15,15,17	1.07	0
2	GLC	J	1	2	11,11,12	1.57	2 (18%)	15,15,17	1.56	2 (13%)
2	GLC	J	2	2	11,11,12	1.66	2 (18%)	15,15,17	1.02	1 (6%)
2	GLC	J	3	2	11,11,12	1.35	1 (9%)	15,15,17	1.04	1 (6%)
2	GLC	J	4	2	11,11,12	1.88	2 (18%)	15,15,17	0.92	0
2	GLC	J	5	2	11,11,12	1.40	2 (18%)	15,15,17	1.18	1 (6%)
2	GLC	J	6	2	11,11,12	0.91	1 (9%)	15,15,17	1.44	3 (20%)
2	GLC	J	7	2	11,11,12	1.24	1 (9%)	15,15,17	1.06	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	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	E	2	2	-	0/2/19/22	0/1/1/1
2	GLC	E	3	2	-	0/2/19/22	0/1/1/1
2	GLC	E	4	2	-	0/2/19/22	0/1/1/1
2	GLC	E	5	2	-	0/2/19/22	0/1/1/1
2	GLC	E	6	2	-	2/2/19/22	0/1/1/1
2	GLC	E	7	2	-	0/2/19/22	0/1/1/1
2	GLC	F	1	2	-	0/2/19/22	0/1/1/1
2	GLC	F	2	2	-	0/2/19/22	0/1/1/1
2	GLC	F	3	2	-	2/2/19/22	0/1/1/1
2	GLC	F	4	2	-	2/2/19/22	0/1/1/1
2	GLC	F	5	2	-	0/2/19/22	0/1/1/1
2	GLC	F	6	2	-	1/2/19/22	0/1/1/1
2	GLC	F	7	2	-	2/2/19/22	0/1/1/1
2	GLC	G	1	2	-	0/2/19/22	0/1/1/1
2	GLC	G	2	2	-	2/2/19/22	0/1/1/1
2	GLC	G	3	2	-	0/2/19/22	0/1/1/1
2	GLC	G	4	2	-	2/2/19/22	0/1/1/1
2	GLC	G	5	2	-	0/2/19/22	0/1/1/1
2	GLC	G	6	2	-	0/2/19/22	0/1/1/1
2	GLC	G	7	2	-	0/2/19/22	0/1/1/1
2	GLC	H	1	2	-	2/2/19/22	0/1/1/1
2	GLC	H	2	2	-	0/2/19/22	0/1/1/1
2	GLC	H	3	2	-	2/2/19/22	0/1/1/1
2	GLC	H	4	2	-	2/2/19/22	0/1/1/1
2	GLC	H	5	2	-	0/2/19/22	0/1/1/1
2	GLC	H	6	2	-	0/2/19/22	0/1/1/1
2	GLC	H	7	2	-	2/2/19/22	0/1/1/1
2	GLC	I	1	2	-	2/2/19/22	0/1/1/1
2	GLC	I	2	2	-	2/2/19/22	0/1/1/1
2	GLC	I	3	2	-	2/2/19/22	0/1/1/1
2	GLC	I	4	2	-	2/2/19/22	0/1/1/1
2	GLC	I	5	2	-	2/2/19/22	0/1/1/1
2	GLC	I	6	2	-	2/2/19/22	0/1/1/1
2	GLC	I	7	2	-	0/2/19/22	0/1/1/1
2	GLC	J	1	2	-	0/2/19/22	0/1/1/1
2	GLC	J	2	2	-	0/2/19/22	0/1/1/1
2	GLC	J	3	2	-	0/2/19/22	0/1/1/1
2	GLC	J	4	2	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	J	5	2	-	0/2/19/22	0/1/1/1
2	GLC	J	6	2	-	0/2/19/22	0/1/1/1
2	GLC	J	7	2	-	2/2/19/22	0/1/1/1

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	4	GLC	O5-C1	5.23	1.52	1.43
2	J	4	GLC	O5-C1	5.13	1.51	1.43
2	F	4	GLC	O5-C1	5.13	1.51	1.43
2	I	4	GLC	O5-C1	4.97	1.51	1.43
2	G	4	GLC	O5-C1	4.90	1.51	1.43
2	H	4	GLC	O5-C1	4.84	1.51	1.43
2	G	2	GLC	O5-C1	-4.65	1.36	1.43
2	J	2	GLC	O5-C1	-4.10	1.37	1.43
2	F	3	GLC	O5-C1	-4.01	1.37	1.43
2	G	3	GLC	O5-C1	-4.00	1.37	1.43
2	H	3	GLC	O5-C1	-3.98	1.37	1.43
2	I	3	GLC	O5-C1	-3.93	1.37	1.43
2	E	2	GLC	O5-C1	-3.82	1.37	1.43
2	H	2	GLC	O5-C1	-3.79	1.37	1.43
2	I	2	GLC	O5-C1	-3.77	1.37	1.43
2	J	3	GLC	O5-C1	-3.76	1.37	1.43
2	F	2	GLC	O5-C1	-3.68	1.37	1.43
2	E	3	GLC	O5-C1	-3.64	1.37	1.43
2	I	1	GLC	O5-C1	-3.53	1.38	1.43
2	F	1	GLC	O5-C1	-3.47	1.38	1.43
2	E	1	GLC	O5-C1	-3.31	1.38	1.43
2	J	1	GLC	O5-C1	-3.17	1.38	1.43
2	H	1	GLC	O5-C1	-3.15	1.38	1.43
2	J	1	GLC	C2-C3	3.01	1.56	1.52
2	H	4	GLC	O4-C4	2.98	1.50	1.43
2	G	4	GLC	O4-C4	2.97	1.50	1.43
2	F	1	GLC	C2-C3	2.96	1.56	1.52
2	E	4	GLC	O4-C4	2.93	1.49	1.43
2	I	4	GLC	O4-C4	2.93	1.49	1.43
2	I	1	GLC	C2-C3	2.93	1.56	1.52
2	H	1	GLC	C2-C3	2.91	1.56	1.52
2	F	4	GLC	O4-C4	2.89	1.49	1.43
2	G	1	GLC	O5-C1	-2.89	1.39	1.43
2	J	4	GLC	O4-C4	2.85	1.49	1.43
2	E	1	GLC	C2-C3	2.73	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2	GLC	C2-C3	2.72	1.56	1.52
2	F	2	GLC	C2-C3	2.69	1.56	1.52
2	G	2	GLC	C2-C3	2.69	1.56	1.52
2	E	7	GLC	O5-C1	-2.66	1.39	1.43
2	I	7	GLC	O5-C1	-2.64	1.39	1.43
2	J	7	GLC	O5-C1	-2.55	1.39	1.43
2	J	2	GLC	C2-C3	2.53	1.56	1.52
2	H	2	GLC	C2-C3	2.53	1.56	1.52
2	H	7	GLC	O5-C1	-2.42	1.39	1.43
2	G	1	GLC	C2-C3	2.42	1.56	1.52
2	E	2	GLC	C2-C3	2.33	1.55	1.52
2	F	7	GLC	O5-C1	-2.32	1.40	1.43
2	J	5	GLC	C2-C3	2.31	1.55	1.52
2	G	7	GLC	O5-C1	-2.27	1.40	1.43
2	E	5	GLC	C2-C3	2.24	1.55	1.52
2	H	5	GLC	O4-C4	2.19	1.48	1.43
2	F	6	GLC	O5-C1	2.18	1.47	1.43
2	I	5	GLC	C2-C3	2.17	1.55	1.52
2	F	7	GLC	C2-C3	2.17	1.55	1.52
2	E	5	GLC	O4-C4	2.16	1.48	1.43
2	F	5	GLC	C2-C3	2.13	1.55	1.52
2	H	5	GLC	C2-C3	2.13	1.55	1.52
2	I	5	GLC	O4-C4	2.13	1.48	1.43
2	F	5	GLC	O4-C4	2.13	1.48	1.43
2	G	2	GLC	O4-C4	2.13	1.48	1.43
2	J	5	GLC	O2-C2	-2.09	1.38	1.43
2	H	7	GLC	C2-C3	2.05	1.55	1.52
2	J	6	GLC	O5-C1	2.04	1.47	1.43
2	I	5	GLC	O2-C2	-2.04	1.39	1.43
2	G	6	GLC	O5-C1	2.04	1.47	1.43
2	G	5	GLC	C2-C3	2.04	1.55	1.52
2	H	5	GLC	O2-C2	-2.00	1.39	1.43

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1	GLC	O5-C1-C2	5.69	119.56	110.77
2	H	1	GLC	O5-C1-C2	4.16	117.19	110.77
2	J	1	GLC	C1-C2-C3	4.16	114.78	109.67
2	J	1	GLC	O5-C1-C2	3.62	116.36	110.77
2	G	7	GLC	O5-C1-C2	3.40	116.02	110.77
2	I	1	GLC	O5-C1-C2	3.35	115.94	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1	GLC	C1-C2-C3	3.34	113.77	109.67
2	H	1	GLC	C1-C2-C3	3.19	113.59	109.67
2	E	1	GLC	C1-C2-C3	3.15	113.53	109.67
2	E	1	GLC	O5-C1-C2	2.98	115.37	110.77
2	F	1	GLC	O5-C1-C2	2.93	115.29	110.77
2	E	7	GLC	O5-C1-C2	2.77	115.05	110.77
2	J	6	GLC	C1-C2-C3	2.74	113.04	109.67
2	I	5	GLC	C1-C2-C3	2.69	112.97	109.67
2	G	6	GLC	C1-C2-C3	2.64	112.91	109.67
2	J	7	GLC	O5-C1-C2	2.63	114.84	110.77
2	E	2	GLC	C1-O5-C5	-2.60	108.67	112.19
2	E	5	GLC	C1-O5-C5	-2.59	108.69	112.19
2	H	7	GLC	O5-C1-C2	2.53	114.68	110.77
2	F	3	GLC	C1-C2-C3	2.40	112.62	109.67
2	I	6	GLC	C1-C2-C3	2.38	112.59	109.67
2	G	7	GLC	O5-C5-C6	2.38	110.93	107.20
2	J	6	GLC	C3-C4-C5	2.34	114.41	110.24
2	I	2	GLC	C1-C2-C3	2.30	112.49	109.67
2	H	7	GLC	C1-C2-C3	2.29	112.49	109.67
2	E	3	GLC	O4-C4-C3	-2.28	105.09	110.35
2	J	3	GLC	O5-C1-C2	2.26	114.26	110.77
2	F	3	GLC	C3-C4-C5	2.25	114.25	110.24
2	J	6	GLC	C2-C3-C4	2.24	114.77	110.89
2	J	5	GLC	C1-C2-C3	2.22	112.40	109.67
2	G	6	GLC	C1-O5-C5	-2.21	109.20	112.19
2	E	3	GLC	O5-C1-C2	2.19	114.16	110.77
2	H	2	GLC	C1-O5-C5	-2.19	109.23	112.19
2	H	4	GLC	C1-O5-C5	-2.14	109.29	112.19
2	F	5	GLC	C1-O5-C5	-2.09	109.36	112.19
2	F	7	GLC	O5-C1-C2	2.08	113.97	110.77
2	I	4	GLC	C1-O5-C5	-2.08	109.38	112.19
2	I	1	GLC	C1-O5-C5	2.07	114.99	112.19
2	F	2	GLC	O5-C5-C6	2.06	110.43	107.20
2	J	2	GLC	C1-O5-C5	-2.05	109.42	112.19
2	G	1	GLC	C6-C5-C4	-2.04	108.22	113.00
2	G	1	GLC	C1-C2-C3	2.03	112.16	109.67

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	7	GLC	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	H	3	GLC	O5-C5-C6-O6
2	H	7	GLC	C4-C5-C6-O6
2	I	4	GLC	O5-C5-C6-O6
2	I	5	GLC	C4-C5-C6-O6
2	J	7	GLC	C4-C5-C6-O6
2	I	6	GLC	O5-C5-C6-O6
2	J	7	GLC	O5-C5-C6-O6
2	F	7	GLC	C4-C5-C6-O6
2	H	3	GLC	C4-C5-C6-O6
2	F	3	GLC	O5-C5-C6-O6
2	I	1	GLC	O5-C5-C6-O6
2	I	5	GLC	O5-C5-C6-O6
2	F	3	GLC	C4-C5-C6-O6
2	F	4	GLC	C4-C5-C6-O6
2	I	1	GLC	C4-C5-C6-O6
2	H	7	GLC	O5-C5-C6-O6
2	I	6	GLC	C4-C5-C6-O6
2	E	6	GLC	O5-C5-C6-O6
2	I	4	GLC	C4-C5-C6-O6
2	E	6	GLC	C4-C5-C6-O6
2	G	4	GLC	C4-C5-C6-O6
2	I	3	GLC	O5-C5-C6-O6
2	I	3	GLC	C4-C5-C6-O6
2	F	4	GLC	O5-C5-C6-O6
2	G	2	GLC	C4-C5-C6-O6
2	E	1	GLC	C4-C5-C6-O6
2	H	1	GLC	C4-C5-C6-O6
2	H	1	GLC	O5-C5-C6-O6
2	G	2	GLC	O5-C5-C6-O6
2	H	4	GLC	C4-C5-C6-O6
2	I	2	GLC	C4-C5-C6-O6
2	E	1	GLC	O5-C5-C6-O6
2	G	4	GLC	O5-C5-C6-O6
2	I	2	GLC	O5-C5-C6-O6
2	F	6	GLC	O5-C5-C6-O6
2	H	4	GLC	O5-C5-C6-O6
2	J	4	GLC	C4-C5-C6-O6

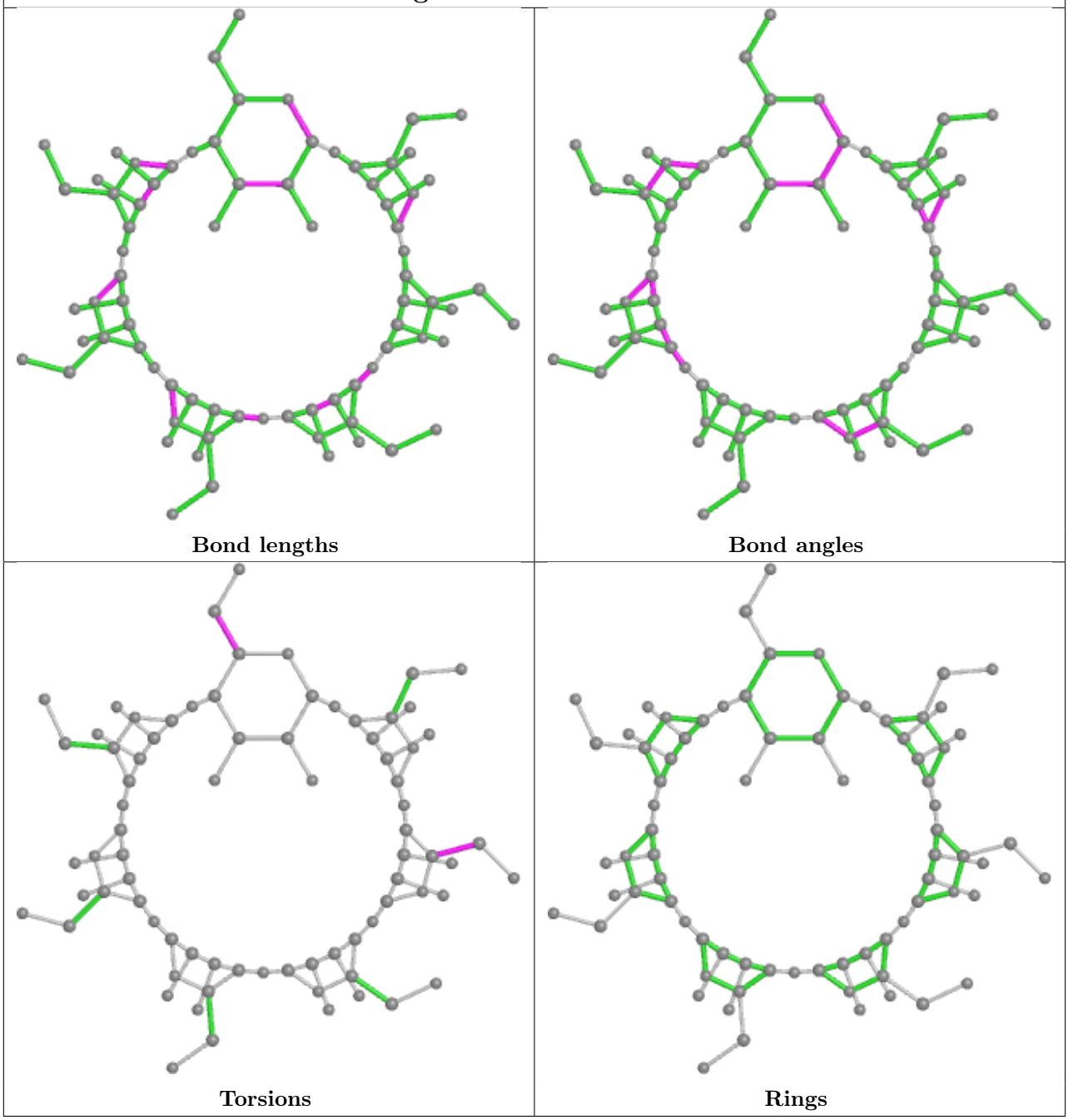
There are no ring outliers.

4 monomers are involved in 4 short contacts:

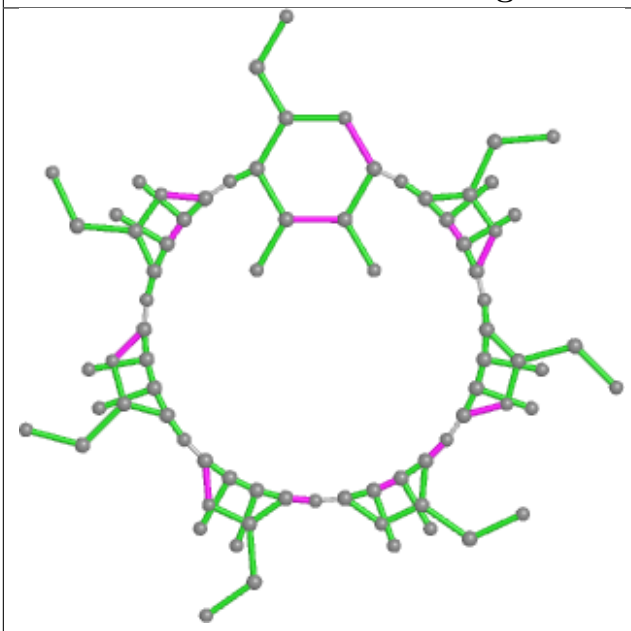
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	7	GLC	1	0
2	I	1	GLC	1	0
2	J	2	GLC	1	0
2	F	6	GLC	1	0

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

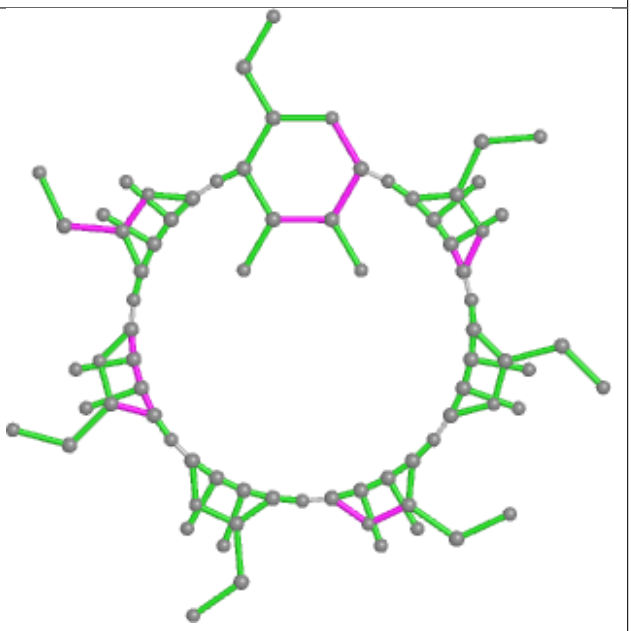
Oligosaccharide Chain E



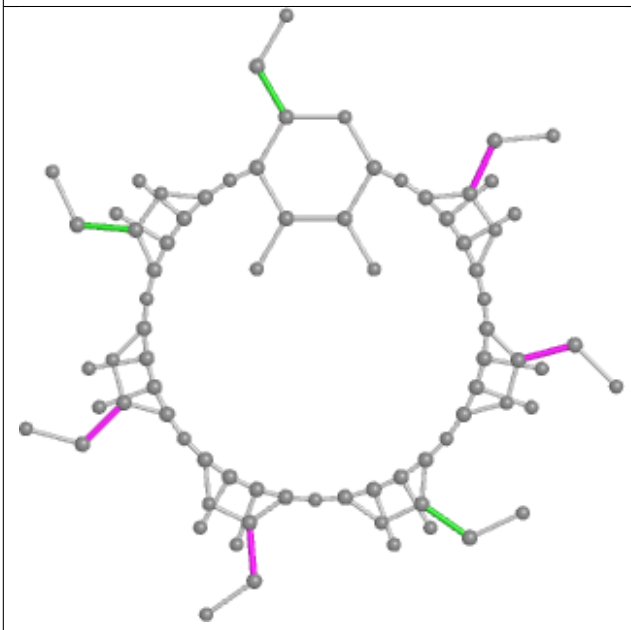
Oligosaccharide Chain F



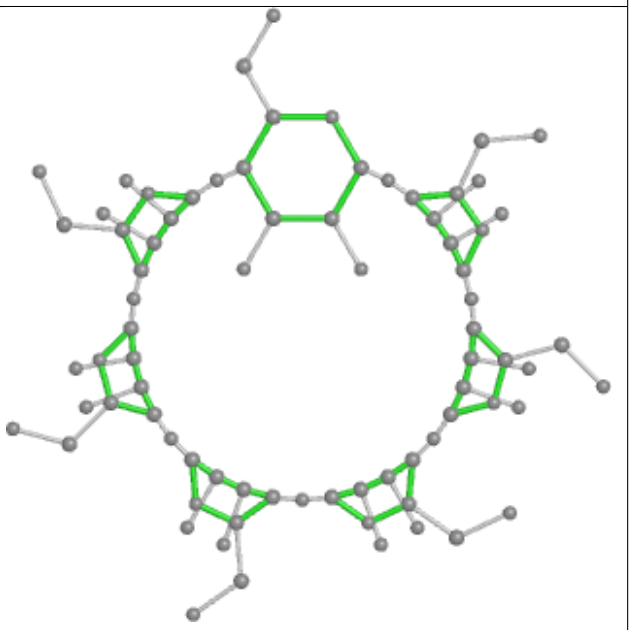
Bond lengths



Bond angles

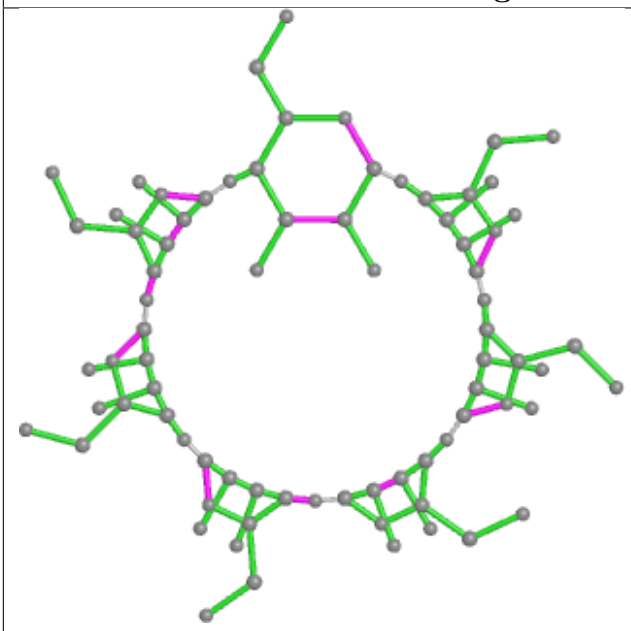


Torsions

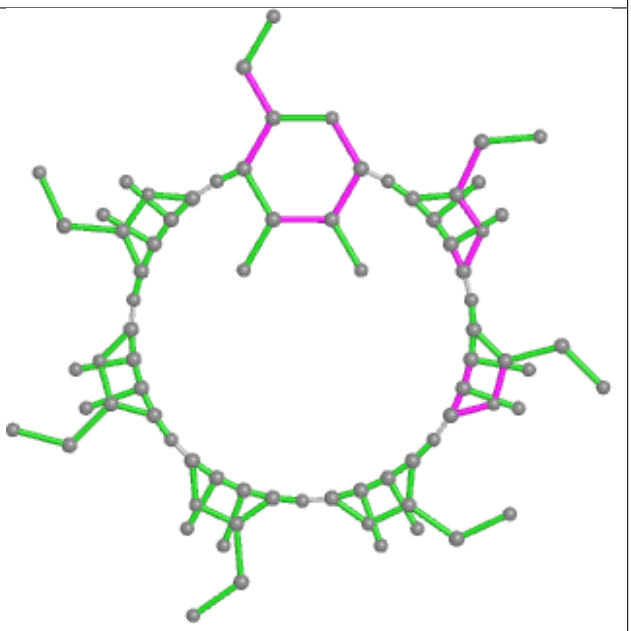


Rings

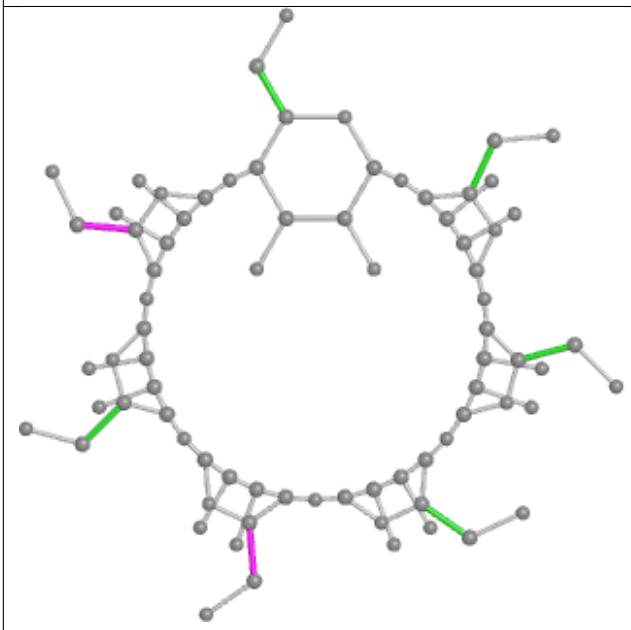
Oligosaccharide Chain G



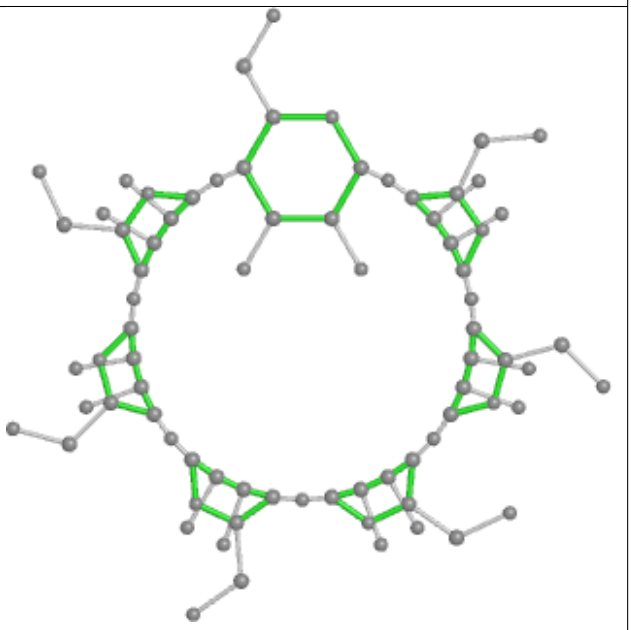
Bond lengths



Bond angles

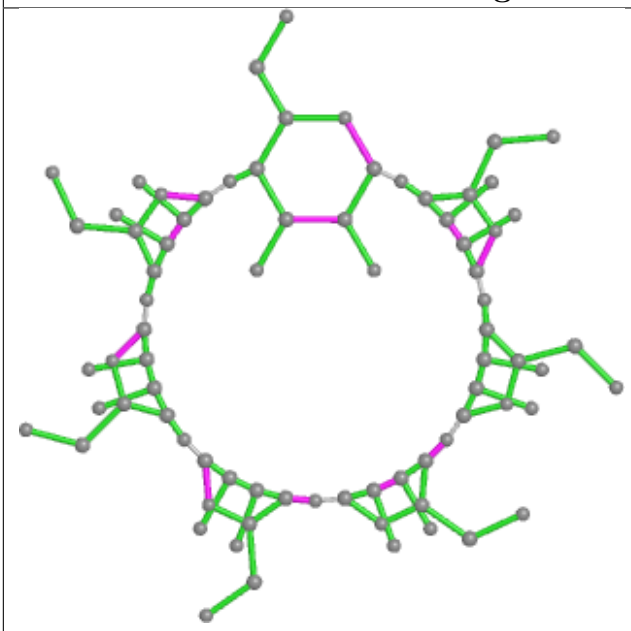


Torsions

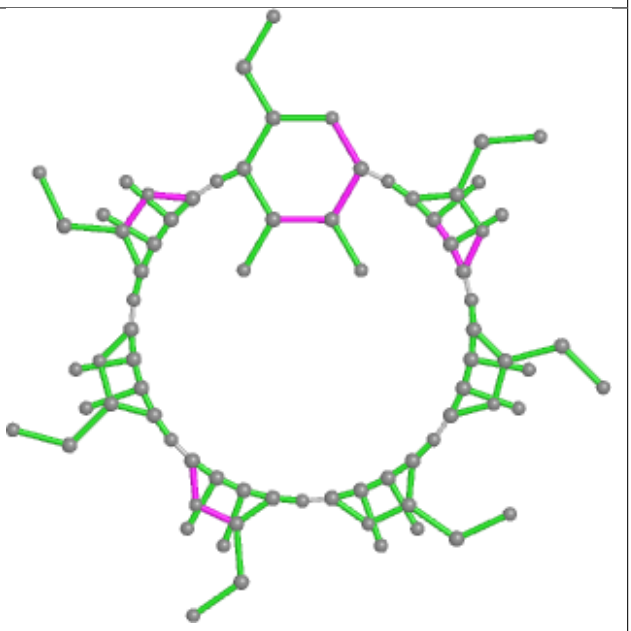


Rings

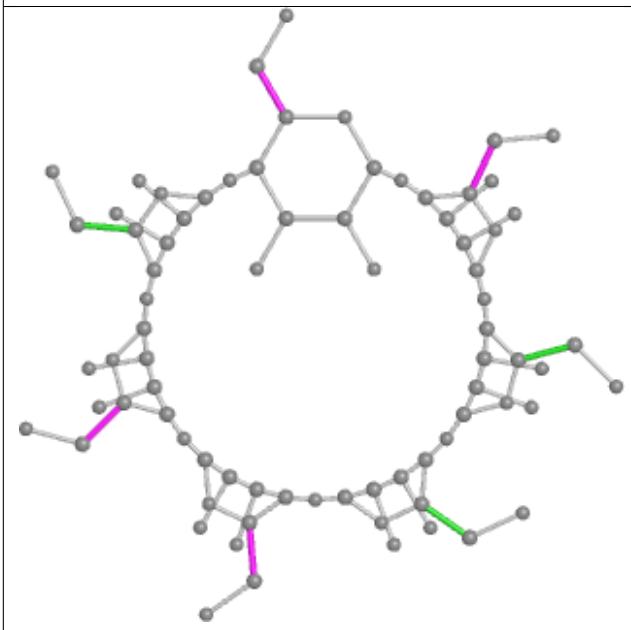
Oligosaccharide Chain H



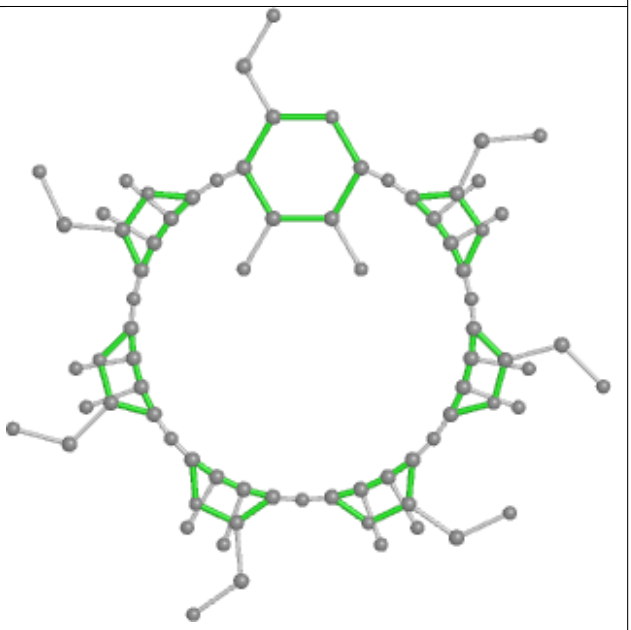
Bond lengths



Bond angles

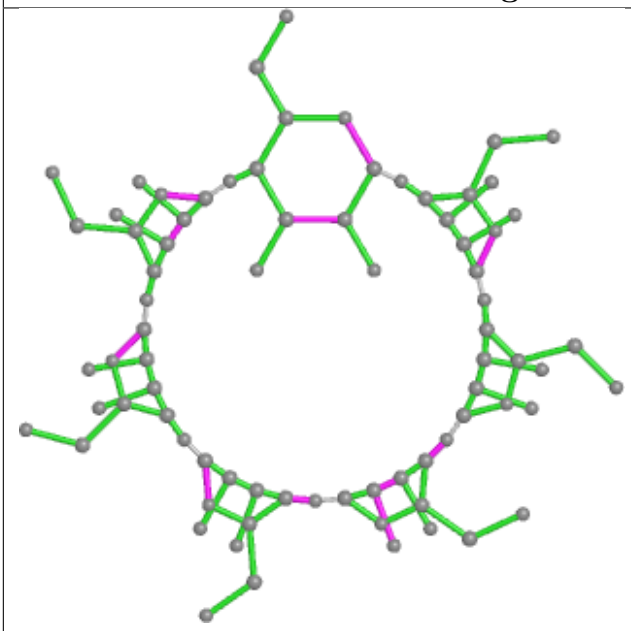


Torsions

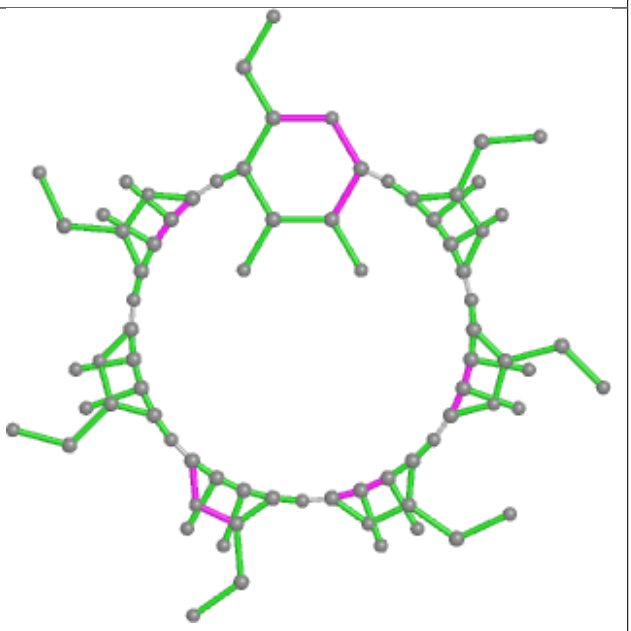


Rings

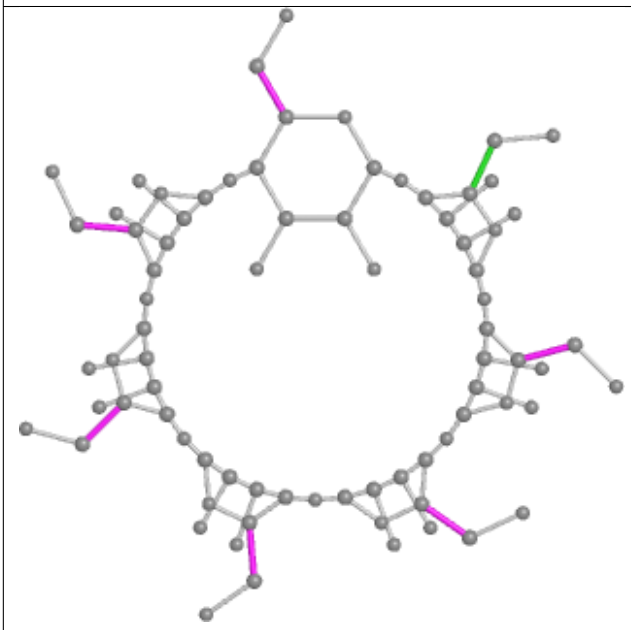
Oligosaccharide Chain I



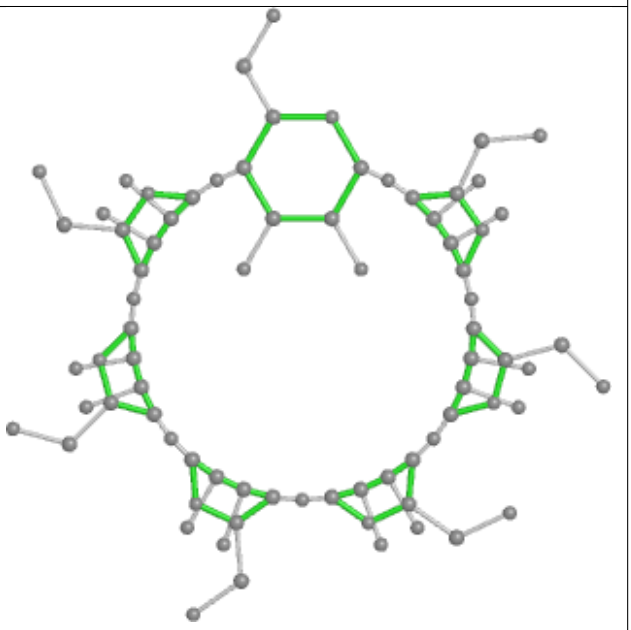
Bond lengths



Bond angles

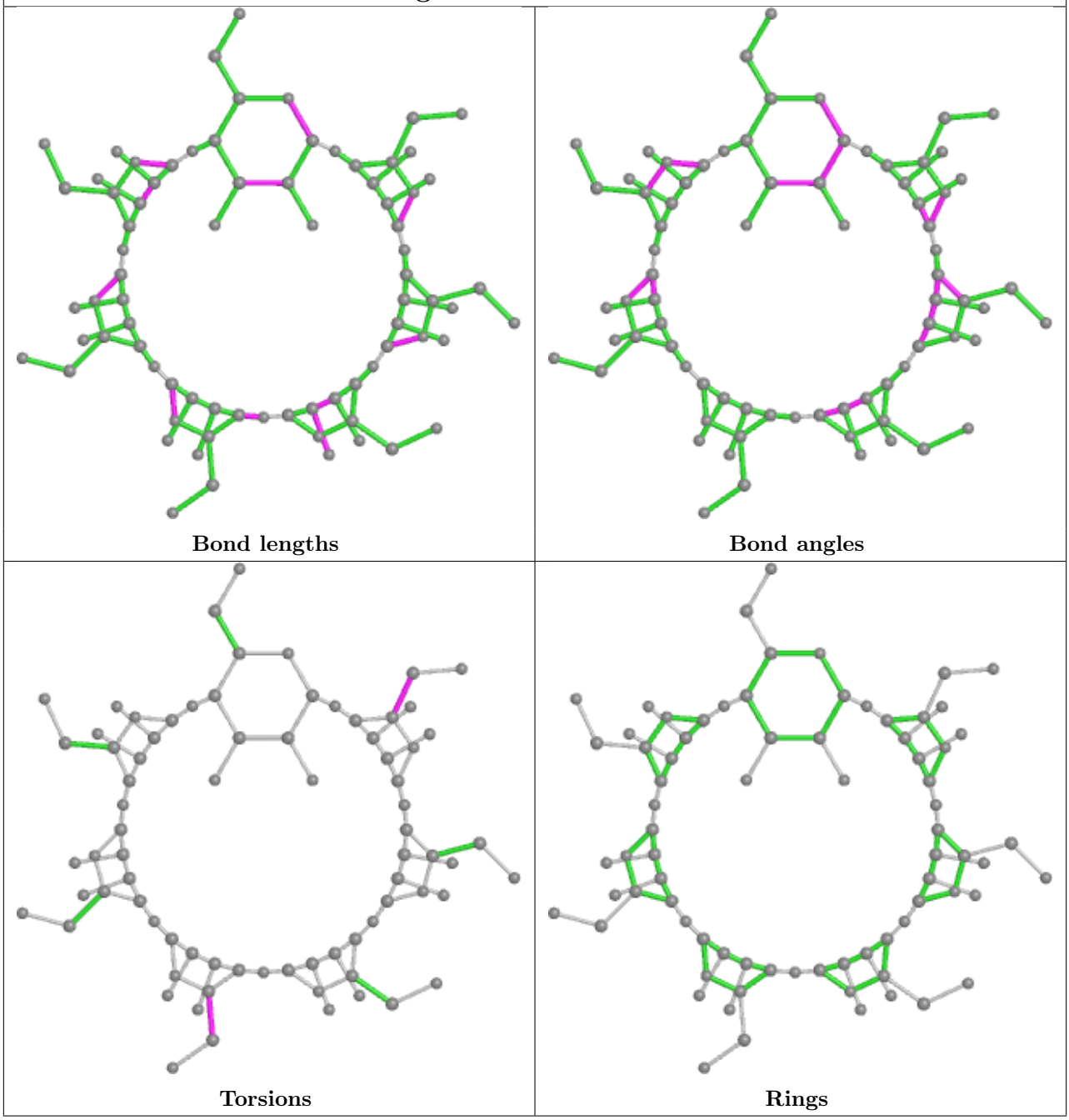


Torsions



Rings

Oligosaccharide Chain J



5.6 Ligand geometry (i)

7 ligands are modelled in this entry.

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

RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	B	802	-	5,5,5	0.37	0	5,5,5	0.39	0
3	GOL	A	804	-	5,5,5	0.30	0	5,5,5	0.37	0
3	GOL	B	803	-	5,5,5	0.35	0	5,5,5	0.21	0
3	GOL	D	802	-	5,5,5	0.38	0	5,5,5	0.32	0
3	GOL	A	803	-	5,5,5	0.31	0	5,5,5	0.48	0
3	GOL	C	803	-	5,5,5	0.37	0	5,5,5	0.39	0
3	GOL	D	803	-	5,5,5	0.33	0	5,5,5	0.38	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	GOL	B	802	-	-	0/4/4/4	-
3	GOL	A	804	-	-	1/4/4/4	-
3	GOL	B	803	-	-	4/4/4/4	-
3	GOL	D	802	-	-	0/4/4/4	-
3	GOL	A	803	-	-	2/4/4/4	-
3	GOL	C	803	-	-	4/4/4/4	-
3	GOL	D	803	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	803	GOL	C1-C2-C3-O3
3	B	803	GOL	O1-C1-C2-C3
3	B	803	GOL	C1-C2-C3-O3
3	C	803	GOL	O1-C1-C2-C3
3	D	803	GOL	O1-C1-C2-C3
3	A	803	GOL	O2-C2-C3-O3
3	B	803	GOL	O1-C1-C2-O2
3	B	803	GOL	O2-C2-C3-O3
3	C	803	GOL	O1-C1-C2-O2
3	D	803	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	C	803	GOL	O2-C2-C3-O3
3	C	803	GOL	C1-C2-C3-O3
3	A	804	GOL	O1-C1-C2-C3

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 (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	587/612 (95%)	0.10	26 (4%)	34	35	10, 27, 86, 112	3 (0%)
1	B	596/612 (97%)	-0.23	4 (0%)	87	88	9, 22, 39, 60	7 (1%)
1	C	582/612 (95%)	-0.02	10 (1%)	70	72	22, 36, 52, 71	2 (0%)
1	D	587/612 (95%)	-0.15	4 (0%)	87	88	15, 26, 46, 68	1 (0%)
All	All	2352/2448 (96%)	-0.08	44 (1%)	66	68	9, 28, 58, 112	13 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	429	GLY	4.9
1	A	117	THR	4.9
1	A	212	MET	4.9
1	D	117	THR	4.1
1	C	346	PHE	4.1
1	A	193	ILE	3.9
1	A	214	PRO	3.7
1	A	346	PHE	3.6
1	C	201	LEU	3.6
1	A	372	THR	3.3
1	A	378	GLY	3.3
1	A	175	TRP	3.1
1	A	195	ALA	3.1
1	C	359	HIS	3.0
1	A	156	PHE	2.9
1	B	423	ILE	2.9
1	A	153	VAL	2.8
1	C	294	PHE	2.8
1	A	133	ASP	2.8
1	C	213	ARG	2.8
1	A	171	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	214	PRO	2.6
1	C	133	ASP	2.6
1	C	373	LEU	2.6
1	B	427	PHE	2.6
1	A	143	TRP	2.6
1	C	728	GLU	2.5
1	A	181	GLY	2.5
1	A	174	ILE	2.5
1	A	145	PRO	2.5
1	A	164	HIS	2.4
1	A	213	ARG	2.4
1	A	159	TRP	2.4
1	A	169	ARG	2.3
1	A	199	LEU	2.3
1	B	426	GLU	2.3
1	A	258	ASP	2.3
1	A	158	TYR	2.2
1	C	159	TRP	2.2
1	D	413	ARG	2.2
1	A	162	ARG	2.1
1	D	133	ASP	2.1
1	B	214	PRO	2.0
1	D	372	THR	2.0

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	GLC	H	2	11/12	0.41	0.32	78,83,86,87	0
2	GLC	H	3	11/12	0.62	0.34	81,84,89,90	0
2	GLC	I	5	11/12	0.70	0.20	76,81,84,84	0
2	GLC	I	2	11/12	0.72	0.25	56,72,75,79	0
2	GLC	H	5	11/12	0.73	0.18	57,59,68,71	0

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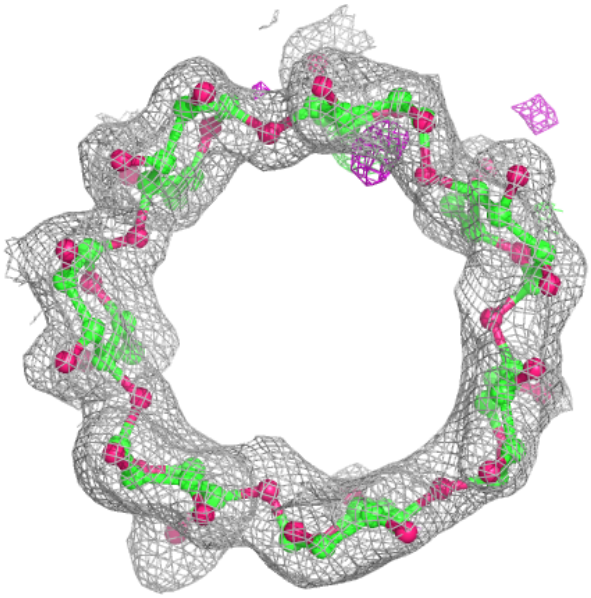
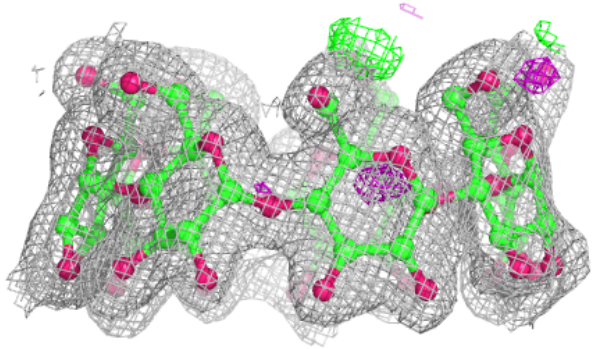
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	I	4	11/12	0.75	0.22	78,83,87,88	0
2	GLC	I	3	11/12	0.76	0.22	78,80,84,85	0
2	GLC	G	4	11/12	0.76	0.18	59,64,68,69	0
2	GLC	G	5	11/12	0.76	0.18	72,74,78,78	0
2	GLC	J	6	11/12	0.77	0.24	59,69,72,73	0
2	GLC	J	7	11/12	0.78	0.23	69,72,76,80	0
2	GLC	F	3	11/12	0.79	0.20	54,61,64,65	0
2	GLC	H	4	11/12	0.80	0.33	71,77,82,82	0
2	GLC	I	6	11/12	0.82	0.17	65,70,75,75	0
2	GLC	J	1	11/12	0.82	0.24	45,60,68,70	0
2	GLC	G	6	11/12	0.82	0.19	61,68,74,76	0
2	GLC	G	7	11/12	0.82	0.22	38,48,58,60	0
2	GLC	I	1	11/12	0.83	0.18	45,52,58,64	0
2	GLC	F	5	11/12	0.83	0.15	49,54,58,60	0
2	GLC	F	6	11/12	0.83	0.16	40,47,49,52	0
2	GLC	F	2	11/12	0.84	0.18	49,55,61,63	0
2	GLC	E	1	11/12	0.84	0.15	64,68,72,74	0
2	GLC	E	2	11/12	0.84	0.16	42,56,63,65	0
2	GLC	H	7	11/12	0.85	0.25	47,51,57,61	0
2	GLC	F	4	11/12	0.85	0.26	52,59,66,69	0
2	GLC	H	1	11/12	0.86	0.21	59,64,76,77	0
2	GLC	F	7	11/12	0.86	0.16	46,50,58,59	0
2	GLC	G	3	11/12	0.86	0.13	45,49,59,59	0
2	GLC	I	7	11/12	0.87	0.11	51,53,58,63	0
2	GLC	F	1	11/12	0.87	0.23	40,51,55,59	0
2	GLC	E	3	11/12	0.87	0.14	34,38,49,58	0
2	GLC	E	7	11/12	0.87	0.13	59,62,68,68	0
2	GLC	J	2	11/12	0.88	0.14	35,43,56,57	0
2	GLC	J	5	11/12	0.88	0.14	46,53,59,65	0
2	GLC	H	6	11/12	0.90	0.16	41,48,52,55	0
2	GLC	E	6	11/12	0.90	0.10	36,40,53,54	0
2	GLC	J	3	11/12	0.92	0.10	25,32,38,41	0
2	GLC	J	4	11/12	0.94	0.09	31,36,41,42	0
2	GLC	E	5	11/12	0.94	0.10	27,31,35,38	0
2	GLC	G	2	11/12	0.95	0.14	30,33,38,39	0
2	GLC	E	4	11/12	0.95	0.10	22,26,35,40	0
2	GLC	G	1	11/12	0.95	0.10	21,30,34,43	0

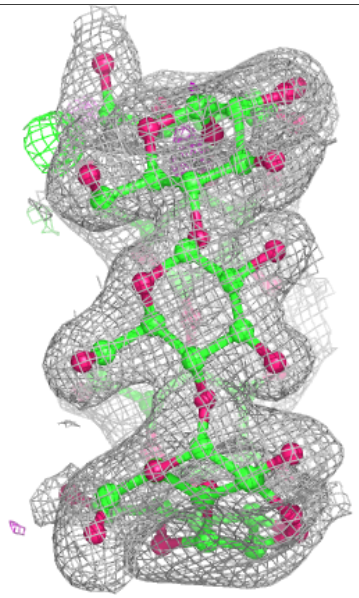
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

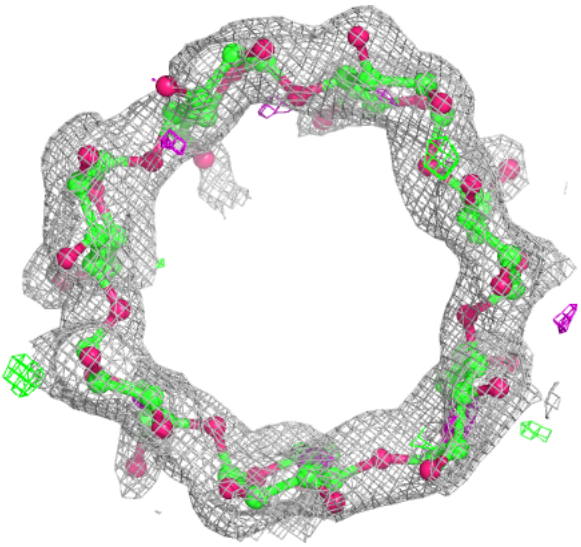


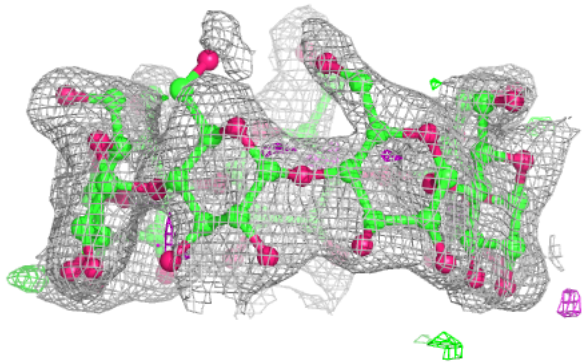


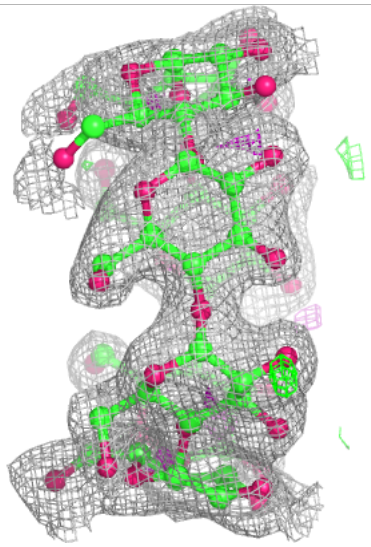


Electron density around Chain F:

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

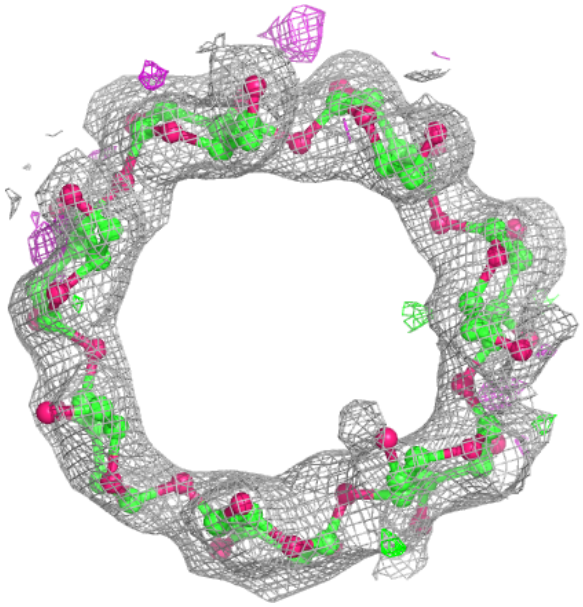


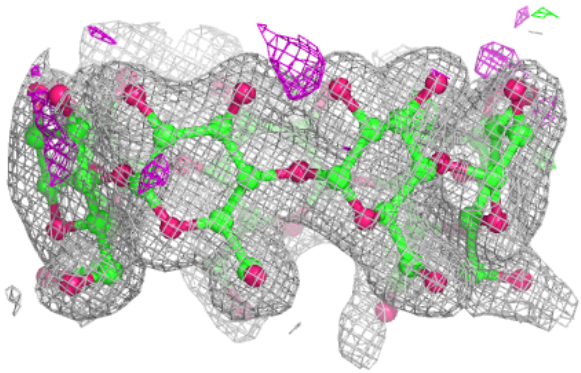


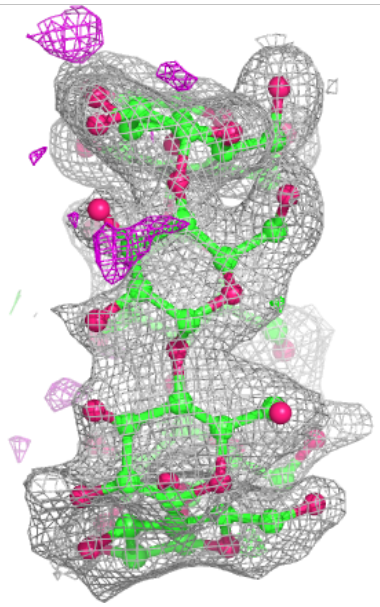


Electron density around Chain G:

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

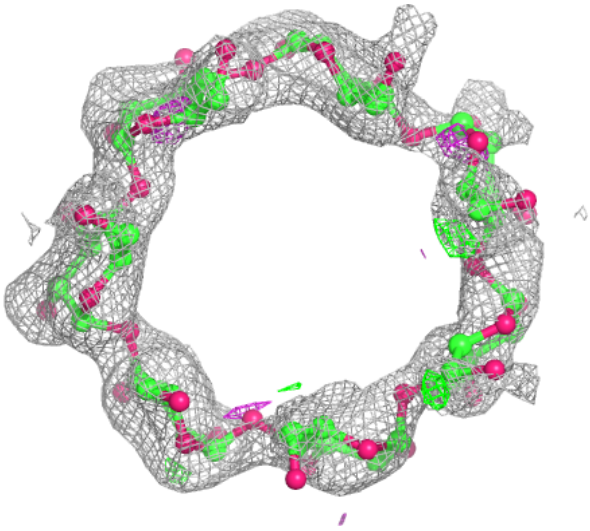


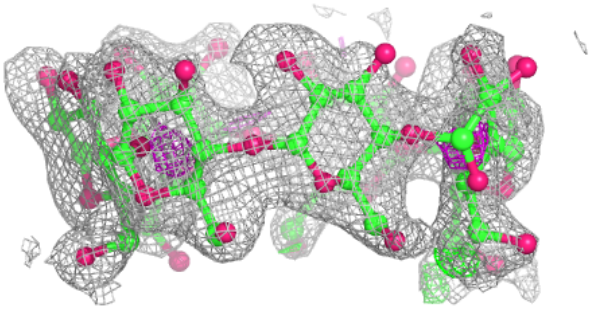


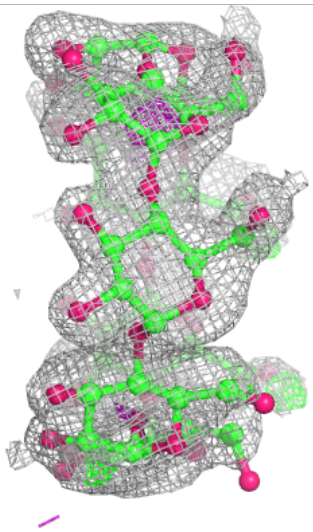


Electron density around Chain H:

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

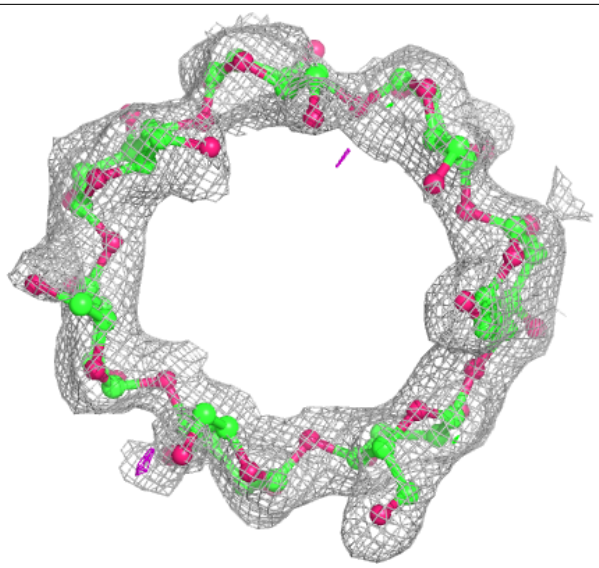


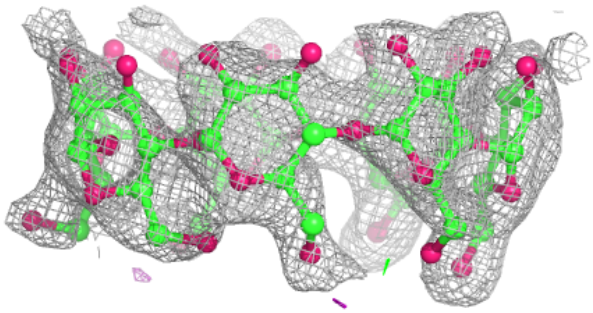


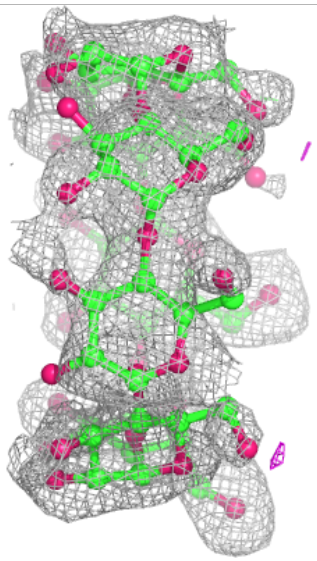


Electron density around Chain I:

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

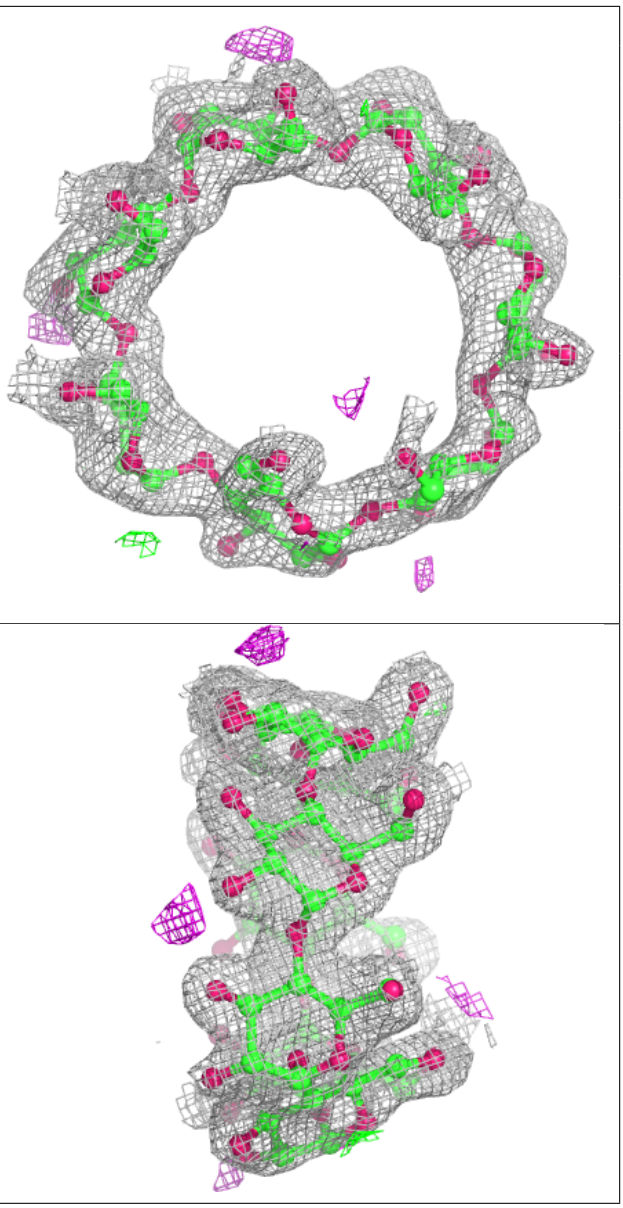






Electron density around Chain J:

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



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(Å^2)	Q<0.9
3	GOL	B	803	6/6	0.89	0.16	36,44,48,49	0
3	GOL	C	803	6/6	0.92	0.17	44,48,51,53	0
3	GOL	A	803	6/6	0.93	0.12	24,25,41,44	0
3	GOL	D	802	6/6	0.95	0.10	26,32,34,36	0
3	GOL	D	803	6/6	0.97	0.07	25,28,33,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	A	804	6/6	0.98	0.08	16,23,24,27	0
3	GOL	B	802	6/6	0.98	0.09	16,20,21,27	0

6.5 Other polymers (i)

There are no such residues in this entry.