Full wwPDB X-ray Structure Validation Report (i)

Sep 20, 2023 – 01:47 AM EDT

PDB ID	:	5E6Y
Title	:	Crystal structure of E.Coli branching enzyme in complex with alpha cyclodextrin
Authors	:	Feng, L.; Nosrati, M.; Geiger, J.H.
Deposited on	:	2015-10-11
Resolution	:	2.60 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 (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:

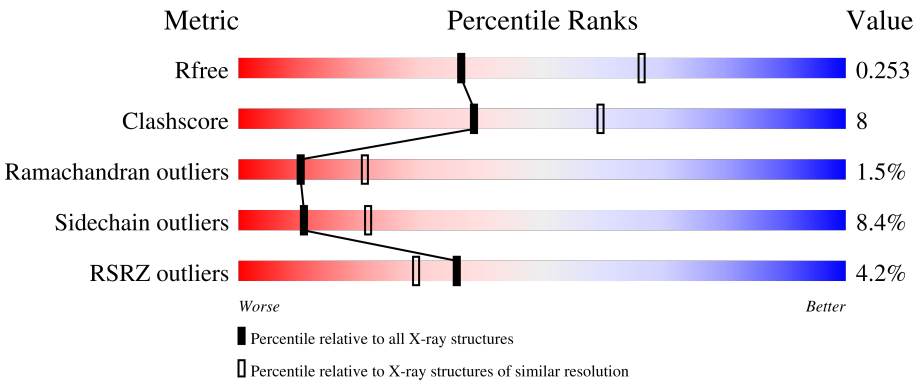
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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	13% 73% 20%
1	B	612	2% 73% 21%
1	C	612	% 75% 17% 5%
1	D	612	75% 18%
2	E	6	83% 17%

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Mol	Chain	Length	Quality of chain
2	F	6	17% 83%
2	G	6	17% 83%
2	H	6	33% 67%
2	I	6	17% 83%
2	J	6	67% 33%
2	K	6	83% 17%
2	L	6	17% 50% 33%
2	M	6	83% 17%

2 Entry composition (i)

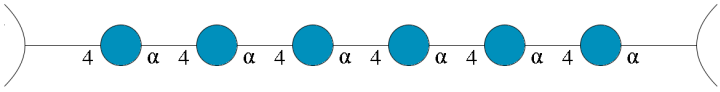
There are 4 unique types of molecules in this entry. The entry contains 20457 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	4729	3025	831	860	13	0	0	0
1	B	594	4873	3116	861	880	16	0	0	0
1	C	584	4814	3079	855	864	16	0	1	0
1	D	589	4836	3090	860	870	16	0	0	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	E	6	66	36	30	0	0	0
2	F	6	66	36	30	0	0	0
2	G	6	66	36	30	0	0	0
2	H	6	66	36	30	0	0	0
2	I	6	66	36	30	0	0	0
2	J	6	66	36	30	0	0	0
2	K	6	66	36	30	0	0	0
2	L	6	66	36	30	0	0	0

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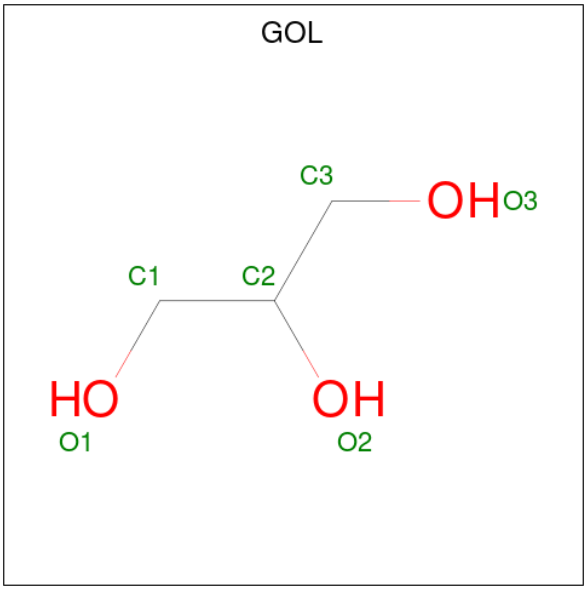
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	M	6	66	36	30	0	0	0

- 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	D	1	6	3	3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	128	128	128	0	0
			Total	O		
4	B	188	188	188	0	0
			Total	O		
4	C	72	72	72	0	0

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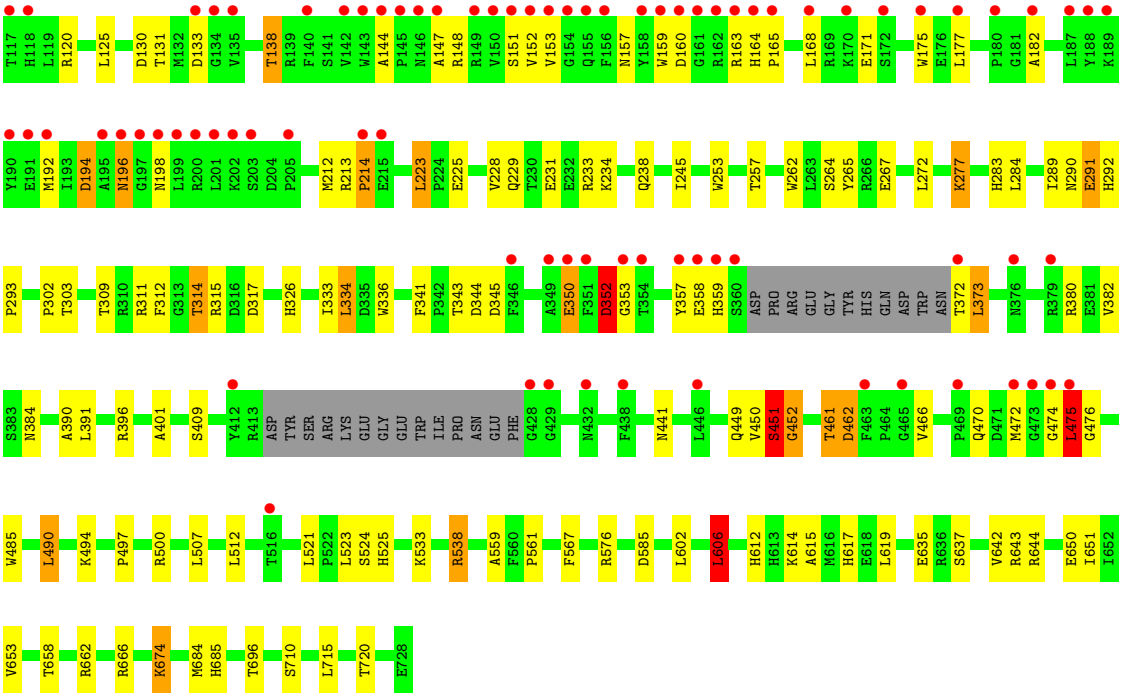
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	D	193	193	193	0	0

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.

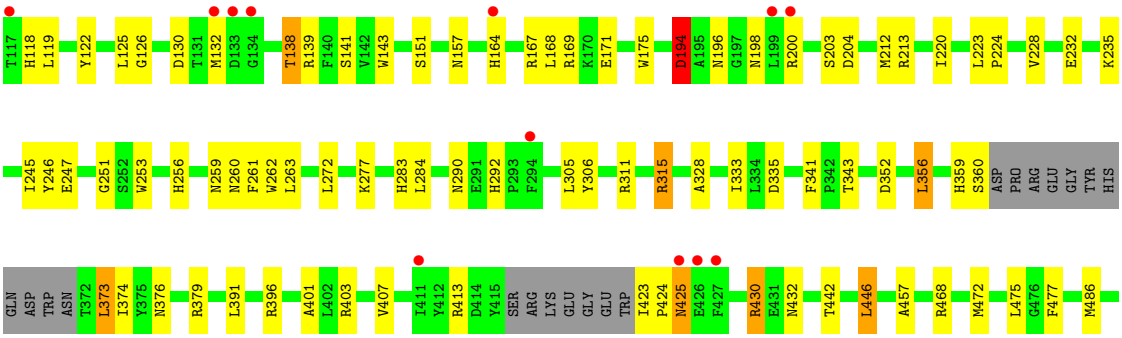
• Molecule 1: 1,4-alpha-glucan branching enzyme GlgB

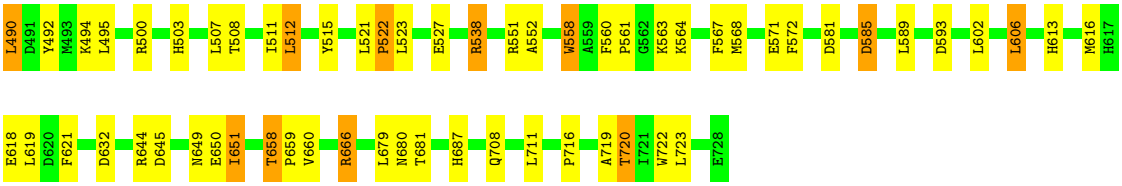
Chain A:



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

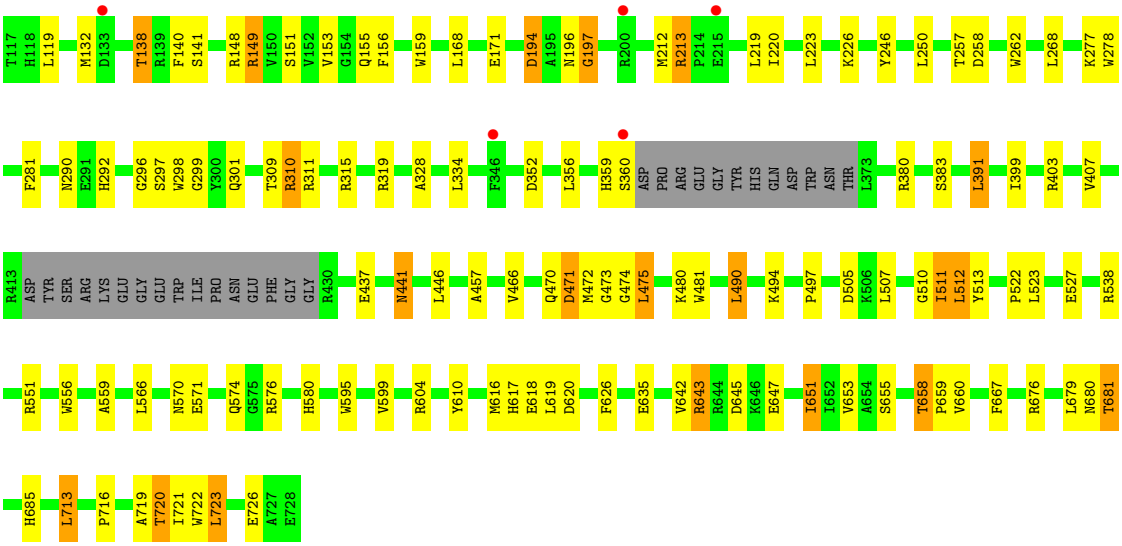
Chain B:





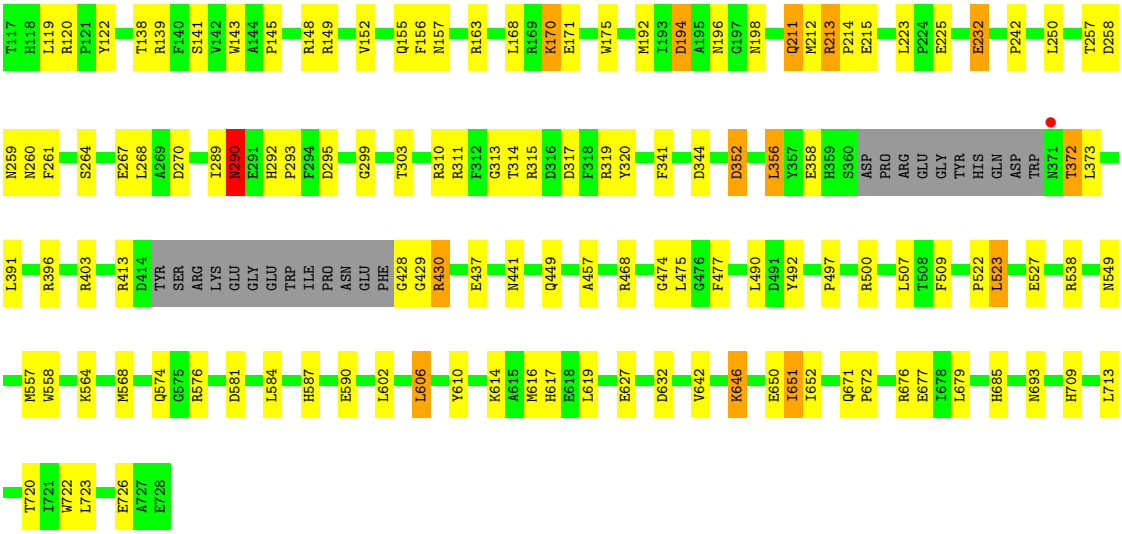
• Molecule 1: 1,4-alpha-glucan branching enzyme GlgB

Chain C:



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

Chain D:

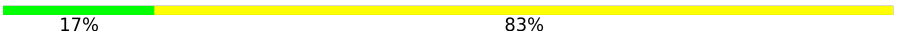


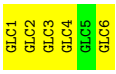
• Molecule 2: Cyclohexakis-(1-4)-(alpha-D-glucopyranose)

Chain E:

• Molecule 2: Cyclohexakis-(1-4)-(alpha-D-glucopyranose)

Chain F:



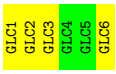


• Molecule 2: Cyclohexakis-(1-4)-(alpha-D-glucopyranose)

Chain G:

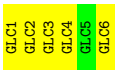
• Molecule 2: Cyclohexakis-(1-4)-(alpha-D-glucopyranose)

Chain H:



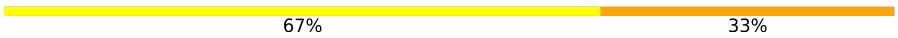
• Molecule 2: Cyclohexakis-(1-4)-(alpha-D-glucopyranose)

Chain I:



• Molecule 2: Cyclohexakis-(1-4)-(alpha-D-glucopyranose)

Chain J:

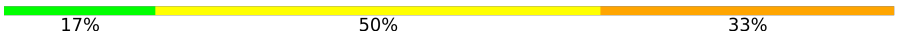


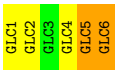
• Molecule 2: Cyclohexakis-(1-4)-(alpha-D-glucopyranose)

Chain K:

• Molecule 2: Cyclohexakis-(1-4)-(alpha-D-glucopyranose)

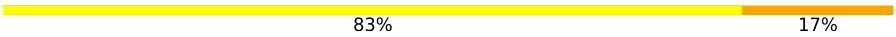
Chain L:





• Molecule 2: Cyclohexakis-(1-4)-(alpha-D-glucopyranose)

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.02Å 103.81Å 186.08Å 90.00° 91.97° 90.00°	Depositor
Resolution (Å)	42.43 – 2.60 45.32 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.2 (42.43-2.60) 95.2 (45.32-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.7.2_869	Depositor
R, R_{free}	0.190 , 0.256 0.188 , 0.253	Depositor DCC
R_{free} test set	10357 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å^2)	53.1	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.053 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	20457	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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	0.40	0/4882	0.56	1/6644 (0.0%)
1	B	0.48	0/5029	0.61	0/6832
1	C	0.43	0/4970	0.59	1/6748 (0.0%)
1	D	0.51	0/4989	0.67	0/6774
All	All	0.46	0/19870	0.61	2/26998 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
All	All	0	2

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	C	723	LEU	CA-CB-CG	5.43	127.78	115.30
1	A	606	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	473	GLY	Peptide
1	D	289	ILE	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	4729	0	4365	78	0
1	B	4873	0	4580	85	0
1	C	4814	0	4554	64	0
1	D	4836	0	4567	65	0
2	E	66	0	54	1	0
2	F	66	0	54	0	0
2	G	66	0	54	1	0
2	H	66	0	54	0	0
2	I	66	0	54	0	0
2	J	66	0	54	2	0
2	K	66	0	54	1	0
2	L	66	0	54	2	0
2	M	66	0	54	1	0
3	A	12	0	16	0	0
3	B	12	0	16	1	0
3	D	6	0	8	0	0
4	A	128	0	0	3	0
4	B	188	0	0	8	0
4	C	72	0	0	2	0
4	D	193	0	0	5	0
All	All	20457	0	18592	289	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 8.

All (289) 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:157:ASN:HD21	1:A:164:HIS:HB2	1.37	0.90
1:C:149:ARG:HH12	1:C:151:SER:HB2	1.38	0.88
1:C:470:GLN:HA	1:C:474:GLY:HA2	1.57	0.86
1:B:292:HIS:O	1:B:311:ARG:NH1	2.15	0.80
1:A:644:ARG:NH2	1:A:650:GLU:OE1	2.15	0.79
1:A:292:HIS:O	1:A:311:ARG:NH1	2.16	0.77
1:C:149:ARG:NH1	1:C:151:SER:HB2	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:ARG:HG3	1:C:310:ARG:HH11	1.52	0.75
1:B:277:LYS:HD2	1:B:328:ALA:HB1	1.70	0.74
1:B:194:ASP:HB3	1:B:196:ASN:H	1.51	0.73
1:C:658:THR:HG23	1:C:660:VAL:H	1.53	0.73
1:C:250:LEU:HD22	1:C:268:LEU:HD13	1.71	0.72
1:D:194:ASP:HB3	1:D:196:ASN:H	1.54	0.72
1:B:224:PRO:HG2	1:B:396:ARG:HB3	1.70	0.72
1:B:373:LEU:H	1:B:373:LEU:HD23	1.55	0.72
1:C:527:GLU:O	1:C:538:ARG:NH1	2.22	0.69
1:A:533:LYS:O	1:A:538:ARG:NH2	2.24	0.69
1:B:658:THR:HG22	1:B:660:VAL:H	1.58	0.69
1:D:492:TYR:CZ	1:D:500:ARG:HG2	2.28	0.68
1:C:292:HIS:CD2	1:C:311:ARG:HH11	2.11	0.68
1:D:527:GLU:O	1:D:538:ARG:NH2	2.27	0.68
1:D:250:LEU:HD22	1:D:268:LEU:HD13	1.76	0.67
1:A:262:TRP:CZ3	1:A:311:ARG:HG2	2.30	0.67
1:A:138:THR:OG1	1:A:182:ALA:O	2.12	0.66
1:B:262:TRP:CZ3	1:B:311:ARG:HG2	2.30	0.66
1:A:194:ASP:N	1:A:194:ASP:OD1	2.29	0.66
1:C:511:ILE:HG22	2:J:1:GLC:H62	1.77	0.65
1:A:160:ASP:HB3	1:A:163:ARG:HH12	1.62	0.65
1:D:602:LEU:HG	1:D:606:LEU:HD22	1.78	0.65
1:D:549:ASN:HA	4:D:1034:HOH:O	1.96	0.65
1:D:152:VAL:O	1:D:157:ASN:ND2	2.31	0.64
1:D:403:ARG:NH1	4:D:903:HOH:O	2.31	0.63
1:C:297:SER:HB2	1:C:301:GLN:HG3	1.81	0.62
1:A:194:ASP:HB2	1:A:353:GLY:HA3	1.80	0.62
1:A:262:TRP:CH2	1:A:311:ARG:HG2	2.34	0.62
1:B:157:ASN:HD21	1:B:164:HIS:HB2	1.64	0.61
1:B:492:TYR:CZ	1:B:500:ARG:HG2	2.35	0.61
1:A:662:ARG:HB2	1:A:715:LEU:HB2	1.82	0.61
1:D:292:HIS:O	1:D:311:ARG:NH1	2.34	0.60
1:A:291:GLU:HG2	1:A:309:THR:HA	1.82	0.59
1:B:138:THR:HG21	1:B:220:ILE:HD13	1.84	0.59
1:C:685:HIS:CE1	1:D:685:HIS:HD2	2.19	0.59
1:D:232:GLU:H	1:D:232:GLU:CD	2.05	0.59
1:B:130:ASP:OD2	1:B:139:ARG:NH1	2.30	0.59
1:C:403:ARG:NH1	4:C:902:HOH:O	2.32	0.59
1:B:247:GLU:HG2	1:B:567:PHE:HD1	1.68	0.58
1:C:262:TRP:CH2	1:C:311:ARG:HD3	2.38	0.58
1:A:153:VAL:HB	1:A:159:TRP:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:VAL:HG13	1:A:475:LEU:HD23	1.85	0.58
1:C:667:PHE:HE1	1:C:713:LEU:HD11	1.69	0.57
1:B:572:PHE:HB2	1:B:589:LEU:HD21	1.85	0.57
1:C:153:VAL:HB	1:C:159:TRP:HA	1.85	0.57
1:A:350:GLU:N	1:A:358:GLU:OE1	2.38	0.57
1:C:278:TRP:O	1:C:604:ARG:HD2	2.05	0.57
1:B:260:ASN:ND2	4:B:912:HOH:O	2.38	0.56
1:D:215:GLU:HB2	2:K:4:GLC:H5	1.86	0.56
1:A:576:ARG:NH2	4:A:902:HOH:O	2.26	0.56
1:A:196:ASN:OD1	1:A:196:ASN:N	2.38	0.56
1:A:130:ASP:OD1	1:A:131:THR:N	2.39	0.56
1:A:293:PRO:HD3	1:A:303:THR:HG23	1.87	0.56
1:B:651:ILE:CD1	1:B:722:TRP:HB3	2.36	0.56
1:B:512:LEU:HD13	2:G:5:GLC:H62	1.88	0.55
1:B:593:ASP:OD2	1:B:687:HIS:NE2	2.36	0.55
1:B:616:MET:SD	1:B:651:ILE:HG12	2.46	0.55
1:A:461:THR:OG1	1:A:462:ASP:N	2.35	0.55
1:B:413:ARG:HE	1:B:432:ASN:HA	1.72	0.55
1:C:651:ILE:CD1	1:C:722:TRP:HB3	2.37	0.55
1:D:145:PRO:HD2	1:D:356:LEU:HD11	1.89	0.55
1:A:290:ASN:O	1:A:292:HIS:ND1	2.39	0.54
1:A:585:ASP:OD1	4:A:901:HOH:O	2.18	0.54
1:C:194:ASP:HB3	1:C:197:GLY:H	1.72	0.54
1:B:527:GLU:O	1:B:538:ARG:NH2	2.37	0.54
1:A:152:VAL:O	1:A:157:ASN:ND2	2.39	0.54
1:A:615:ALA:HB3	1:A:651:ILE:HD12	1.89	0.54
1:A:497:PRO:HA	1:A:500:ARG:HD2	1.90	0.54
1:C:471:ASP:N	1:C:471:ASP:OD1	2.41	0.54
1:C:556:TRP:HE3	1:C:655:SER:HG	1.56	0.54
1:A:559:ALA:HB1	1:A:653:VAL:HG21	1.88	0.54
1:C:490:LEU:O	1:C:494:LYS:HG3	2.08	0.53
1:D:676:ARG:NE	1:D:726:GLU:OE1	2.23	0.53
1:B:232:GLU:OE1	1:B:232:GLU:N	2.35	0.53
1:B:256:HIS:NE2	1:B:263:LEU:HD23	2.23	0.53
1:D:319:ARG:NH2	1:D:396:ARG:O	2.42	0.53
1:B:552:ALA:HA	1:B:720:THR:HG23	1.91	0.53
1:B:494:LYS:HG2	1:B:538:ARG:HG2	1.91	0.52
1:D:120:ARG:NH2	1:D:449:GLN:OE1	2.41	0.52
1:A:151:SER:HB2	1:A:165:PRO:HA	1.90	0.52
1:B:315:ARG:HD3	4:B:915:HOH:O	2.08	0.52
1:C:551:ARG:NH1	1:C:681:THR:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ASN:ND2	1:A:164:HIS:HB2	2.16	0.52
1:C:309:THR:OG1	1:C:311:ARG:HG3	2.09	0.52
1:B:341:PHE:HD1	1:B:373:LEU:HD12	1.74	0.52
1:C:681:THR:HB	1:C:720:THR:H	1.74	0.52
1:B:138:THR:HG21	1:B:220:ILE:HG21	1.92	0.52
1:D:261:PHE:CD1	2:L:6:GLC:H3	2.45	0.51
1:B:335:ASP:OD1	1:B:403:ARG:HD3	2.11	0.51
1:A:602:LEU:HG	1:A:606:LEU:HD22	1.92	0.51
1:D:651:ILE:HD13	1:D:722:TRP:HB3	1.91	0.51
1:A:470:GLN:HA	1:A:474:GLY:HA2	1.91	0.51
1:A:685:HIS:HD2	4:A:1009:HOH:O	1.93	0.51
1:B:508:THR:O	1:B:511:ILE:HG22	2.10	0.51
1:C:296:GLY:HA2	1:C:580:HIS:CE1	2.45	0.51
1:A:635:GLU:H	1:A:635:GLU:CD	2.13	0.51
1:D:558:TRP:HA	1:D:564:LYS:HE3	1.92	0.50
1:B:376:ASN:OD1	1:B:379:ARG:HB2	2.11	0.50
1:D:509:PHE:HA	2:M:3:GLC:H62	1.94	0.50
1:A:168:LEU:HD13	1:A:175:TRP:CE2	2.45	0.50
1:A:168:LEU:HB2	1:A:175:TRP:CZ3	2.47	0.49
1:C:138:THR:HG21	1:C:220:ILE:HD13	1.93	0.49
1:C:470:GLN:OE1	1:C:470:GLN:N	2.38	0.49
1:B:430:ARG:CD	1:B:430:ARG:H	2.26	0.49
1:D:194:ASP:HB2	1:D:198:ASN:H	1.76	0.49
1:A:614:LYS:HA	1:A:617:HIS:NE2	2.28	0.49
1:B:486:MET:O	1:B:490:LEU:HB2	2.12	0.49
1:B:658:THR:CG2	1:B:660:VAL:H	2.24	0.49
1:C:407:VAL:HG21	1:C:457:ALA:HB1	1.94	0.49
1:C:651:ILE:HD13	1:C:722:TRP:HB3	1.94	0.49
1:A:314:THR:HG23	1:A:317:ASP:OD2	2.13	0.48
1:C:148:ARG:NH2	1:C:196:ASN:O	2.46	0.48
1:B:407:VAL:HG21	1:B:457:ALA:HB1	1.95	0.48
1:D:372:THR:O	1:D:372:THR:OG1	2.32	0.48
1:C:574:GLN:HG2	1:C:576:ARG:O	2.12	0.48
1:C:620:ASP:OD1	1:C:643:ARG:NH2	2.42	0.48
1:A:194:ASP:OD1	1:A:198:ASN:N	2.47	0.48
1:C:494:LYS:HD3	1:C:538:ARG:HG2	1.94	0.48
1:D:693:ASN:OD1	1:D:713:LEU:HB2	2.14	0.47
1:A:450:VAL:O	1:A:452:GLY:N	2.47	0.47
1:A:474:GLY:O	1:A:476:GLY:N	2.47	0.47
1:B:168:LEU:HB2	1:B:175:TRP:CH2	2.50	0.47
1:C:292:HIS:O	1:C:311:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:ARG:HG3	1:C:310:ARG:NH1	2.22	0.47
1:C:297:SER:C	1:C:299:GLY:H	2.18	0.47
1:B:585:ASP:OD2	4:B:901:HOH:O	2.20	0.47
1:C:685:HIS:NE2	1:D:685:HIS:HD2	2.13	0.47
1:D:497:PRO:HA	1:D:500:ARG:HD3	1.97	0.47
1:A:168:LEU:HB2	1:A:175:TRP:CE3	2.50	0.46
1:A:262:TRP:CZ3	2:E:3:GLC:H62	2.49	0.46
1:B:430:ARG:H	1:B:430:ARG:HD2	1.78	0.46
1:B:708:GLN:O	4:B:902:HOH:O	2.21	0.46
1:D:211:GLN:O	1:D:212:MET:HG2	2.14	0.46
1:D:492:TYR:CE2	1:D:500:ARG:HG2	2.51	0.46
1:D:652:ILE:HB	1:D:723:LEU:HB2	1.97	0.46
1:C:437:GLU:O	1:C:441:ASN:HB2	2.15	0.46
1:C:511:ILE:HG12	1:C:626:PHE:CE1	2.50	0.46
1:D:428:GLY:HA2	1:D:429:GLY:HA3	1.60	0.46
1:D:568:MET:HB2	1:D:584:LEU:HD11	1.98	0.46
1:A:277:LYS:HD3	4:B:1006:HOH:O	2.13	0.46
1:B:602:LEU:HG	1:B:606:LEU:HD22	1.97	0.46
1:C:559:ALA:HB1	1:C:653:VAL:HG21	1.98	0.46
1:C:610:TYR:O	1:C:617:HIS:HD2	1.99	0.46
1:D:139:ARG:HD2	4:D:1074:HOH:O	2.15	0.46
1:A:253:TRP:CH2	1:A:272:LEU:HA	2.50	0.46
1:B:126:GLY:HA2	1:B:204:ASP:OD2	2.16	0.46
1:C:680:ASN:HA	1:C:721:ILE:HG22	1.98	0.46
1:C:334:LEU:HB3	1:C:399:ILE:HD13	1.98	0.46
1:A:233:ARG:HD3	1:A:326:HIS:CD2	2.51	0.45
1:A:451:SER:O	1:A:451:SER:OG	2.31	0.45
1:B:679:LEU:HG	1:B:680:ASN:N	2.32	0.45
1:B:719:ALA:HB2	4:B:960:HOH:O	2.16	0.45
1:D:646:LYS:HB3	1:D:646:LYS:HE2	1.73	0.45
1:D:242:PRO:HD3	1:D:617:HIS:CE1	2.52	0.45
1:A:644:ARG:HD3	1:A:650:GLU:HG2	1.98	0.45
1:C:155:GLN:HB2	4:C:956:HOH:O	2.16	0.45
1:D:192:MET:SD	1:D:352:ASP:HA	2.56	0.45
1:A:380:ARG:O	1:A:384:ASN:ND2	2.34	0.45
1:B:490:LEU:HD12	1:B:490:LEU:HA	1.77	0.45
1:C:618:GLU:OE1	1:C:645:ASP:HB2	2.16	0.45
1:D:170:LYS:HE2	4:D:944:HOH:O	2.16	0.45
1:A:666:ARG:NH1	1:A:710:SER:OG	2.47	0.45
1:C:616:MET:SD	1:C:651:ILE:HG12	2.56	0.45
1:A:292:HIS:HB3	1:A:302:PRO:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:ILE:HG12	1:B:283:HIS:HB2	1.99	0.45
1:D:341:PHE:CZ	1:D:358:GLU:HB3	2.52	0.45
1:D:616:MET:SD	1:D:651:ILE:HG12	2.57	0.45
1:A:265:TYR:CE2	1:A:312:PHE:HB2	2.52	0.45
1:B:457:ALA:HB2	1:B:477:PHE:CE1	2.52	0.45
1:B:645:ASP:OD2	1:B:649:ASN:HB2	2.17	0.45
1:D:429:GLY:HA2	1:D:430:ARG:HA	1.56	0.45
1:A:264:SER:OG	1:A:267:GLU:HG3	2.17	0.44
1:B:359:HIS:CG	1:B:360:SER:N	2.85	0.44
1:B:551:ARG:HB3	1:B:681:THR:HB	1.99	0.44
1:C:298:TRP:HE1	1:C:580:HIS:CD2	2.35	0.44
1:B:122:TYR:HB3	1:B:306:TYR:CE2	2.53	0.44
1:B:343:THR:HG22	1:B:373:LEU:HD11	1.98	0.44
1:D:523:LEU:HD22	1:D:557:MET:SD	2.57	0.44
1:A:223:LEU:HB3	1:A:396:ARG:NH2	2.33	0.44
1:B:169:ARG:HD3	1:B:171:GLU:OE2	2.18	0.44
1:B:341:PHE:CD1	1:B:373:LEU:HD12	2.53	0.44
1:D:264:SER:HB2	4:D:937:HOH:O	2.18	0.44
1:D:437:GLU:O	1:D:441:ASN:HB2	2.17	0.44
1:B:558:TRP:HA	1:B:564:LYS:HE3	2.00	0.44
1:D:627:GLU:HB3	1:D:642:VAL:HG12	2.00	0.43
1:B:413:ARG:CZ	1:B:425:ASN:HB3	2.49	0.43
1:A:284:LEU:HD12	1:A:284:LEU:HA	1.88	0.43
1:A:333:ILE:HG12	1:A:401:ALA:HB3	2.01	0.43
1:A:637:SER:HB2	1:A:658:THR:HG23	2.00	0.43
1:B:143:TRP:CH2	1:B:356:LEU:HD22	2.53	0.43
1:B:373:LEU:H	1:B:373:LEU:CD2	2.30	0.43
1:B:568:MET:O	4:B:903:HOH:O	2.21	0.43
1:B:658:THR:HG23	1:B:659:PRO:HD2	1.99	0.43
1:A:485:TRP:CD2	1:A:521:LEU:HD22	2.54	0.43
1:B:560:PHE:CG	1:B:561:PRO:HD2	2.54	0.43
1:C:140:PHE:HZ	1:C:220:ILE:HD11	1.84	0.43
1:C:391:LEU:HD12	1:C:391:LEU:HA	1.91	0.43
1:B:442:THR:HG22	1:B:446:LEU:HD22	2.00	0.43
1:D:314:THR:O	1:D:317:ASP:HB2	2.18	0.43
1:A:336:TRP:CH2	1:A:390:ALA:HB2	2.54	0.42
1:B:251:GLY:N	4:B:917:HOH:O	2.45	0.42
1:C:512:LEU:HD13	2:J:4:GLC:H62	2.01	0.42
1:B:632:ASP:OD1	1:B:632:ASP:N	2.52	0.42
1:C:566:LEU:HG	1:C:570:ASN:HB2	2.00	0.42
1:D:290:ASN:HD22	1:D:290:ASN:HA	1.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:ASN:HB3	1:B:200:ARG:NH1	2.33	0.42
1:B:468:ARG:NH2	1:B:515:TYR:O	2.52	0.42
1:D:168:LEU:HB2	1:D:175:TRP:CE2	2.54	0.42
1:D:310:ARG:HD2	1:D:313:GLY:O	2.20	0.42
1:B:716:PRO:HB2	1:B:719:ALA:HB3	2.01	0.42
1:C:667:PHE:CE1	1:C:713:LEU:HD11	2.53	0.42
1:C:676:ARG:HD2	1:C:726:GLU:OE2	2.20	0.42
1:D:457:ALA:HB2	1:D:477:PHE:CD1	2.54	0.42
1:C:277:LYS:HD2	1:C:328:ALA:HB1	2.02	0.42
1:C:571:GLU:O	1:C:599:VAL:HG12	2.20	0.42
1:A:212:MET:C	1:A:214:PRO:HD2	2.39	0.42
1:B:253:TRP:CH2	1:B:272:LEU:HA	2.54	0.42
1:B:490:LEU:O	1:B:494:LYS:HG3	2.19	0.42
1:D:264:SER:OG	1:D:267:GLU:HG3	2.19	0.42
1:C:510:GLY:HA2	1:C:513:TYR:CE2	2.55	0.42
1:C:658:THR:HA	1:C:659:PRO:HD3	1.90	0.42
1:D:120:ARG:HG2	1:D:122:TYR:CZ	2.55	0.42
1:A:357:TYR:HD1	1:A:382:VAL:HG22	1.84	0.42
1:A:674:LYS:NZ	1:A:696:THR:HG21	2.34	0.42
1:B:141:SER:HA	1:B:175:TRP:O	2.20	0.42
1:B:284:LEU:HD12	1:B:284:LEU:HA	1.90	0.42
1:A:341:PHE:O	1:A:343:THR:HG23	2.19	0.41
1:B:157:ASN:OD1	1:B:164:HIS:CD2	2.73	0.41
1:B:644:ARG:HG2	1:B:650:GLU:HG2	2.02	0.41
1:D:292:HIS:CG	1:D:299:GLY:HA2	2.55	0.41
1:D:317:ASP:O	1:D:320:TYR:HB3	2.20	0.41
1:D:564:LYS:HE2	1:D:610:TYR:CE1	2.54	0.41
1:A:229:GLN:HG2	1:A:234:LYS:HG3	2.01	0.41
1:A:466:VAL:HG22	1:A:475:LEU:HD23	2.02	0.41
1:C:359:HIS:CG	1:C:360:SER:H	2.38	0.41
1:A:265:TYR:CZ	1:A:312:PHE:HB2	2.55	0.41
1:B:356:LEU:HD23	1:B:356:LEU:HA	1.92	0.41
1:B:521:LEU:HA	1:B:522:PRO:HD3	1.83	0.41
1:A:245:ILE:HG12	1:A:283:HIS:HB2	2.02	0.41
1:A:561:PRO:HA	1:A:643:ARG:NH2	2.34	0.41
1:B:651:ILE:HD13	1:B:722:TRP:HB3	2.03	0.41
1:D:143:TRP:CH2	1:D:356:LEU:HD22	2.55	0.41
1:D:523:LEU:HD12	1:D:523:LEU:HA	1.98	0.41
1:A:120:ARG:NH1	1:A:449:GLN:OE1	2.34	0.41
1:C:685:HIS:CD2	1:D:685:HIS:CD2	3.08	0.41
1:D:156:PHE:HD1	1:D:157:ASN:OD1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ASP:HB3	1:A:163:ARG:NH1	2.31	0.41
1:A:373:LEU:H	1:A:373:LEU:HG	1.65	0.41
1:C:643:ARG:HD2	1:C:643:ARG:HA	1.82	0.41
1:A:357:TYR:CD1	1:A:382:VAL:HG22	2.55	0.41
1:A:289:ILE:HG13	1:A:334:LEU:HD11	2.01	0.41
1:B:333:ILE:HG12	1:B:401:ALA:HB3	2.02	0.41
1:B:563:LYS:HE2	1:B:621:PHE:CZ	2.56	0.41
1:B:613:HIS:HB3	3:B:802:GOL:H32	2.01	0.41
1:B:666:ARG:HA	1:B:711:LEU:O	2.21	0.41
1:D:468:ARG:O	1:D:474:GLY:HA3	2.21	0.41
1:A:494:LYS:HD3	1:A:538:ARG:HG2	2.03	0.41
1:B:495:LEU:HD11	1:B:503:HIS:CD2	2.56	0.41
1:D:671:GLN:HA	1:D:672:PRO:HD2	1.98	0.41
1:D:677:GLU:HA	1:D:723:LEU:HD13	2.01	0.41
1:A:525:HIS:HB3	1:A:567:PHE:CE1	2.56	0.40
1:A:144:ALA:HB1	1:A:352:ASP:HB2	2.02	0.40
1:A:490:LEU:HD12	1:A:490:LEU:HA	1.83	0.40
1:B:125:LEU:HA	1:B:141:SER:HB2	2.03	0.40
1:B:246:TYR:OH	1:B:571:GLU:OE1	2.27	0.40
1:C:466:VAL:HG22	1:C:475:LEU:HD12	2.04	0.40
1:C:716:PRO:HB2	1:C:719:ALA:HB3	2.03	0.40
1:D:170:LYS:CD	1:D:170:LYS:H	2.33	0.40
1:D:642:VAL:CG2	1:D:650:GLU:HB3	2.51	0.40
1:A:192:MET:HE1	1:A:352:ASP:HA	2.02	0.40
1:B:168:LEU:HB2	1:B:175:TRP:CZ3	2.55	0.40
1:B:259:ASN:HB2	1:B:261:PHE:CE1	2.55	0.40
1:B:423:ILE:HA	1:B:424:PRO:HD2	1.96	0.40
1:B:606:LEU:HD12	1:B:606:LEU:HA	1.91	0.40
1:C:246:TYR:HB2	1:C:281:PHE:CG	2.57	0.40
1:D:293:PRO:HD3	1:D:303:THR:HG23	2.02	0.40
1:A:265:TYR:HB2	1:A:317:ASP:HB3	2.03	0.40
1:A:358:GLU:H	1:A:358:GLU:CD	2.20	0.40
1:C:480:LYS:HG2	1:C:481:TRP:O	2.20	0.40
1:D:260:ASN:HB3	2:L:5:GLC:O2	2.22	0.40
1:D:574:GLN:HG2	1:D:576:ARG:O	2.22	0.40
1:D:587:HIS:O	1:D:590:GLU:HB2	2.22	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	581/612 (95%)	506 (87%)	62 (11%)	13 (2%)	6 12
1	B	588/612 (96%)	546 (93%)	38 (6%)	4 (1%)	22 43
1	C	579/612 (95%)	532 (92%)	41 (7%)	6 (1%)	15 32
1	D	583/612 (95%)	543 (93%)	29 (5%)	11 (2%)	8 15
All	All	2331/2448 (95%)	2127 (91%)	170 (7%)	34 (2%)	10 21

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213	ARG
1	A	225	GLU
1	A	451	SER
1	B	194	ASP
1	B	212	MET
1	C	194	ASP
1	C	213	ARG
1	D	149	ARG
1	D	194	ASP
1	D	214	PRO
1	D	290	ASN
1	A	612	HIS
1	D	259	ASN
1	A	125	LEU
1	A	177	LEU
1	A	475	LEU
1	B	585	ASP
1	A	147	ALA
1	A	148	ARG
1	C	197	GLY
1	C	522	PRO
1	D	257	THR

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Mol	Chain	Res	Type
1	D	413	ARG
1	D	522	PRO
1	A	133	ASP
1	A	214	PRO
1	A	352	ASP
1	C	226	LYS
1	D	211	GLN
1	D	709	HIS
1	A	452	GLY
1	B	522	PRO
1	C	497	PRO
1	D	213	ARG

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	475/521 (91%)	434 (91%)	41 (9%)	10	20
1	B	502/521 (96%)	462 (92%)	40 (8%)	12	24
1	C	498/521 (96%)	451 (91%)	47 (9%)	8	17
1	D	499/521 (96%)	462 (93%)	37 (7%)	13	28
All	All	1974/2084 (95%)	1809 (92%)	165 (8%)	11	21

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	THR
1	A	171	GLU
1	A	194	ASP
1	A	196	ASN
1	A	223	LEU
1	A	228	VAL
1	A	231	GLU
1	A	238	GLN
1	A	257	THR

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Mol	Chain	Res	Type
1	A	277	LYS
1	A	291	GLU
1	A	314	THR
1	A	315	ARG
1	A	334	LEU
1	A	344	ASP
1	A	345	ASP
1	A	350	GLU
1	A	352	ASP
1	A	359	HIS
1	A	372	THR
1	A	373	LEU
1	A	391	LEU
1	A	409	SER
1	A	441	ASN
1	A	451	SER
1	A	461	THR
1	A	462	ASP
1	A	472	MET
1	A	475	LEU
1	A	490	LEU
1	A	507	LEU
1	A	512	LEU
1	A	523	LEU
1	A	524	SER
1	A	538	ARG
1	A	606	LEU
1	A	619	LEU
1	A	642	VAL
1	A	674	LYS
1	A	684	MET
1	A	720	THR
1	B	118	HIS
1	B	119	LEU
1	B	132	MET
1	B	138	THR
1	B	151	SER
1	B	167	ARG
1	B	194	ASP
1	B	203	SER
1	B	213	ARG
1	B	223	LEU

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Mol	Chain	Res	Type
1	B	228	VAL
1	B	235	LYS
1	B	290	ASN
1	B	305	LEU
1	B	315	ARG
1	B	352	ASP
1	B	356	LEU
1	B	373	LEU
1	B	374	ILE
1	B	391	LEU
1	B	425	ASN
1	B	430	ARG
1	B	446	LEU
1	B	472	MET
1	B	475	LEU
1	B	490	LEU
1	B	507	LEU
1	B	512	LEU
1	B	523	LEU
1	B	538	ARG
1	B	558	TRP
1	B	581	ASP
1	B	606	LEU
1	B	618	GLU
1	B	619	LEU
1	B	651	ILE
1	B	658	THR
1	B	666	ARG
1	B	720	THR
1	B	723	LEU
1	C	119	LEU
1	C	132	MET
1	C	138	THR
1	C	141	SER
1	C	149	ARG
1	C	156	PHE
1	C	168	LEU
1	C	171	GLU
1	C	212	MET
1	C	213	ARG
1	C	219	LEU
1	C	223	LEU

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Mol	Chain	Res	Type
1	C	257	THR
1	C	258	ASP
1	C	290	ASN
1	C	310	ARG
1	C	315	ARG
1	C	319	ARG
1	C	352	ASP
1	C	356	LEU
1	C	380	ARG
1	C	383	SER
1	C	391	LEU
1	C	441	ASN
1	C	446	LEU
1	C	471	ASP
1	C	472	MET
1	C	475	LEU
1	C	490	LEU
1	C	505	ASP
1	C	507	LEU
1	C	511	ILE
1	C	512	LEU
1	C	523	LEU
1	C	595	TRP
1	C	619	LEU
1	C	635	GLU
1	C	642	VAL
1	C	643	ARG
1	C	647	GLU
1	C	651	ILE
1	C	658	THR
1	C	679	LEU
1	C	681	THR
1	C	713	LEU
1	C	720	THR
1	C	723	LEU
1	D	119	LEU
1	D	138	THR
1	D	141	SER
1	D	148	ARG
1	D	155	GLN
1	D	163	ARG
1	D	170	LYS

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Mol	Chain	Res	Type
1	D	171	GLU
1	D	213	ARG
1	D	223	LEU
1	D	225	GLU
1	D	232	GLU
1	D	258	ASP
1	D	270	ASP
1	D	290	ASN
1	D	295	ASP
1	D	315	ARG
1	D	344	ASP
1	D	352	ASP
1	D	356	LEU
1	D	372	THR
1	D	373	LEU
1	D	391	LEU
1	D	430	ARG
1	D	475	LEU
1	D	490	LEU
1	D	507	LEU
1	D	523	LEU
1	D	581	ASP
1	D	606	LEU
1	D	614	LYS
1	D	619	LEU
1	D	632	ASP
1	D	646	LYS
1	D	651	ILE
1	D	679	LEU
1	D	720	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	ASN
1	A	164	HIS
1	B	157	ASN
1	B	164	HIS
1	B	425	ASN
1	B	525	HIS
1	C	580	HIS
1	C	617	HIS

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Mol	Chain	Res	Type
1	D	164	HIS
1	D	290	ASN
1	D	617	HIS
1	D	685	HIS

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)

54 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	1.01	1 (9%)	15,15,17	1.66	3 (20%)
2	GLC	E	2	2	11,11,12	2.57	1 (9%)	15,15,17	1.93	5 (33%)
2	GLC	E	3	2	11,11,12	0.89	0	15,15,17	2.21	4 (26%)
2	GLC	E	4	2	11,11,12	1.11	1 (9%)	15,15,17	2.04	3 (20%)
2	GLC	E	5	2	11,11,12	0.92	0	15,15,17	1.34	2 (13%)
2	GLC	E	6	2	11,11,12	0.92	0	15,15,17	1.22	2 (13%)
2	GLC	F	1	2	11,11,12	0.78	0	15,15,17	1.51	3 (20%)
2	GLC	F	2	2	11,11,12	2.76	1 (9%)	15,15,17	1.95	3 (20%)
2	GLC	F	3	2	11,11,12	1.14	0	15,15,17	1.90	3 (20%)
2	GLC	F	4	2	11,11,12	1.03	1 (9%)	15,15,17	0.93	0
2	GLC	F	5	2	11,11,12	0.94	0	15,15,17	0.88	0
2	GLC	F	6	2	11,11,12	0.95	0	15,15,17	1.30	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	0.79	0	15,15,17	0.94	0
2	GLC	G	2	2	11,11,12	2.40	1 (9%)	15,15,17	1.30	1 (6%)
2	GLC	G	3	2	11,11,12	1.06	1 (9%)	15,15,17	2.00	4 (26%)
2	GLC	G	4	2	11,11,12	0.89	0	15,15,17	1.39	4 (26%)
2	GLC	G	5	2	11,11,12	0.95	0	15,15,17	0.94	0
2	GLC	G	6	2	11,11,12	1.04	0	15,15,17	1.51	4 (26%)
2	GLC	H	1	2	11,11,12	0.92	1 (9%)	15,15,17	1.42	3 (20%)
2	GLC	H	2	2	11,11,12	2.36	1 (9%)	15,15,17	1.46	2 (13%)
2	GLC	H	3	2	11,11,12	0.95	1 (9%)	15,15,17	1.05	1 (6%)
2	GLC	H	4	2	11,11,12	0.88	0	15,15,17	0.85	0
2	GLC	H	5	2	11,11,12	0.84	0	15,15,17	0.92	0
2	GLC	H	6	2	11,11,12	0.89	0	15,15,17	1.10	1 (6%)
2	GLC	I	1	2	11,11,12	1.02	1 (9%)	15,15,17	1.59	3 (20%)
2	GLC	I	2	2	11,11,12	2.59	1 (9%)	15,15,17	1.50	4 (26%)
2	GLC	I	3	2	11,11,12	1.02	0	15,15,17	1.67	3 (20%)
2	GLC	I	4	2	11,11,12	0.92	0	15,15,17	1.25	1 (6%)
2	GLC	I	5	2	11,11,12	0.93	0	15,15,17	0.82	0
2	GLC	I	6	2	11,11,12	0.97	0	15,15,17	1.31	2 (13%)
2	GLC	J	1	2	11,11,12	0.80	0	15,15,17	1.22	1 (6%)
2	GLC	J	2	2	11,11,12	2.59	1 (9%)	15,15,17	1.28	1 (6%)
2	GLC	J	3	2	11,11,12	0.86	0	15,15,17	1.26	2 (13%)
2	GLC	J	4	2	11,11,12	0.89	0	15,15,17	1.42	2 (13%)
2	GLC	J	5	2	11,11,12	0.91	0	15,15,17	1.33	2 (13%)
2	GLC	J	6	2	11,11,12	0.82	0	15,15,17	1.22	1 (6%)
2	GLC	K	1	2	11,11,12	0.90	0	15,15,17	2.26	6 (40%)
2	GLC	K	2	2	11,11,12	2.67	1 (9%)	15,15,17	1.99	4 (26%)
2	GLC	K	3	2	11,11,12	1.13	1 (9%)	15,15,17	1.50	2 (13%)
2	GLC	K	4	2	11,11,12	0.98	1 (9%)	15,15,17	1.86	4 (26%)
2	GLC	K	5	2	11,11,12	1.04	1 (9%)	15,15,17	1.04	1 (6%)
2	GLC	K	6	2	11,11,12	0.95	0	15,15,17	1.24	2 (13%)
2	GLC	L	1	2	11,11,12	1.04	1 (9%)	15,15,17	1.45	3 (20%)
2	GLC	L	2	2	11,11,12	2.64	1 (9%)	15,15,17	1.49	4 (26%)
2	GLC	L	3	2	11,11,12	0.98	0	15,15,17	1.06	0
2	GLC	L	4	2	11,11,12	1.03	0	15,15,17	1.28	1 (6%)
2	GLC	L	5	2	11,11,12	1.20	1 (9%)	15,15,17	1.50	2 (13%)
2	GLC	L	6	2	11,11,12	0.84	0	15,15,17	1.18	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GLC	M	1	2	11,11,12	0.96	1 (9%)	15,15,17	1.07	1 (6%)
2	GLC	M	2	2	11,11,12	2.46	1 (9%)	15,15,17	1.26	1 (6%)
2	GLC	M	3	2	11,11,12	0.86	0	15,15,17	1.16	3 (20%)
2	GLC	M	4	2	11,11,12	0.99	1 (9%)	15,15,17	0.84	0
2	GLC	M	5	2	11,11,12	0.90	0	15,15,17	1.27	1 (6%)
2	GLC	M	6	2	11,11,12	0.84	0	15,15,17	1.20	2 (13%)

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
2	GLC	E	2	2	-	0/2/19/22	0/1/1/1
2	GLC	E	3	2	-	2/2/19/22	0/1/1/1
2	GLC	E	4	2	-	2/2/19/22	0/1/1/1
2	GLC	E	5	2	-	2/2/19/22	0/1/1/1
2	GLC	E	6	2	-	2/2/19/22	0/1/1/1
2	GLC	F	1	2	-	2/2/19/22	0/1/1/1
2	GLC	F	2	2	-	0/2/19/22	0/1/1/1
2	GLC	F	3	2	-	1/2/19/22	0/1/1/1
2	GLC	F	4	2	-	0/2/19/22	0/1/1/1
2	GLC	F	5	2	-	0/2/19/22	0/1/1/1
2	GLC	F	6	2	-	0/2/19/22	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	-	1/2/19/22	0/1/1/1
2	GLC	G	4	2	-	0/2/19/22	0/1/1/1
2	GLC	G	5	2	-	0/2/19/22	0/1/1/1
2	GLC	G	6	2	-	2/2/19/22	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	-	0/2/19/22	0/1/1/1
2	GLC	H	4	2	-	0/2/19/22	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	I	1	2	-	1/2/19/22	0/1/1/1
2	GLC	I	2	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	I	3	2	-	0/2/19/22	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	-	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	-	1/2/19/22	0/1/1/1
2	GLC	J	3	2	-	2/2/19/22	0/1/1/1
2	GLC	J	4	2	-	2/2/19/22	0/1/1/1
2	GLC	J	5	2	-	0/2/19/22	0/1/1/1
2	GLC	J	6	2	-	2/2/19/22	0/1/1/1
2	GLC	K	1	2	-	2/2/19/22	0/1/1/1
2	GLC	K	2	2	-	2/2/19/22	0/1/1/1
2	GLC	K	3	2	-	0/2/19/22	0/1/1/1
2	GLC	K	4	2	-	2/2/19/22	0/1/1/1
2	GLC	K	5	2	-	2/2/19/22	0/1/1/1
2	GLC	K	6	2	-	0/2/19/22	0/1/1/1
2	GLC	L	1	2	-	2/2/19/22	0/1/1/1
2	GLC	L	2	2	-	2/2/19/22	0/1/1/1
2	GLC	L	3	2	-	2/2/19/22	0/1/1/1
2	GLC	L	4	2	-	0/2/19/22	0/1/1/1
2	GLC	L	5	2	-	1/2/19/22	0/1/1/1
2	GLC	L	6	2	-	0/2/19/22	0/1/1/1
2	GLC	M	1	2	-	0/2/19/22	0/1/1/1
2	GLC	M	2	2	-	0/2/19/22	0/1/1/1
2	GLC	M	3	2	-	0/2/19/22	0/1/1/1
2	GLC	M	4	2	-	2/2/19/22	0/1/1/1
2	GLC	M	5	2	-	2/2/19/22	0/1/1/1
2	GLC	M	6	2	-	1/2/19/22	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2	GLC	O5-C1	8.59	1.57	1.43
2	K	2	GLC	O5-C1	8.45	1.57	1.43
2	L	2	GLC	O5-C1	8.29	1.57	1.43
2	I	2	GLC	O5-C1	8.29	1.57	1.43
2	J	2	GLC	O5-C1	8.11	1.56	1.43
2	E	2	GLC	O5-C1	8.08	1.56	1.43
2	M	2	GLC	O5-C1	7.83	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	2	GLC	O5-C1	7.61	1.55	1.43
2	H	2	GLC	O5-C1	7.45	1.55	1.43
2	L	5	GLC	C2-C3	3.01	1.57	1.52
2	I	1	GLC	C2-C3	2.49	1.56	1.52
2	E	1	GLC	C2-C3	2.35	1.56	1.52
2	L	1	GLC	C2-C3	2.30	1.55	1.52
2	K	3	GLC	C2-C3	2.27	1.55	1.52
2	E	4	GLC	C2-C3	2.25	1.55	1.52
2	M	4	GLC	C2-C3	2.15	1.55	1.52
2	M	1	GLC	C2-C3	2.10	1.55	1.52
2	K	4	GLC	C4-C5	2.06	1.57	1.53
2	K	5	GLC	C2-C3	2.04	1.55	1.52
2	H	3	GLC	C2-C3	2.03	1.55	1.52
2	G	3	GLC	O5-C1	2.03	1.47	1.43
2	H	1	GLC	C2-C3	2.03	1.55	1.52
2	F	4	GLC	C2-C3	2.01	1.55	1.52

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	4	GLC	C1-C2-C3	5.74	116.72	109.67
2	G	3	GLC	C1-O5-C5	5.35	119.44	112.19
2	E	3	GLC	C1-O5-C5	5.34	119.43	112.19
2	F	3	GLC	C1-C2-C3	5.26	116.13	109.67
2	K	4	GLC	C1-O5-C5	4.80	118.70	112.19
2	F	2	GLC	C1-C2-C3	4.66	115.39	109.67
2	E	1	GLC	C1-C2-C3	4.43	115.12	109.67
2	K	2	GLC	C1-C2-C3	4.42	115.10	109.67
2	E	2	GLC	C3-C4-C5	4.06	117.48	110.24
2	K	1	GLC	O5-C5-C4	4.05	120.68	110.83
2	K	1	GLC	C3-C4-C5	4.00	117.38	110.24
2	F	2	GLC	C2-C3-C4	3.98	117.79	110.89
2	I	3	GLC	C1-C2-C3	3.93	114.50	109.67
2	K	4	GLC	O5-C5-C4	3.90	120.32	110.83
2	K	1	GLC	C1-O5-C5	3.75	117.27	112.19
2	E	3	GLC	O5-C5-C4	3.72	119.89	110.83
2	K	3	GLC	C1-C2-C3	3.68	114.19	109.67
2	I	1	GLC	C1-C2-C3	3.64	114.14	109.67
2	K	2	GLC	C2-C3-C4	3.56	117.06	110.89
2	L	1	GLC	C1-C2-C3	3.48	113.94	109.67
2	I	6	GLC	C1-C2-C3	3.47	113.94	109.67
2	K	1	GLC	C1-C2-C3	3.41	113.86	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	4	GLC	C1-C2-C3	3.40	113.84	109.67
2	E	3	GLC	C1-C2-C3	-3.36	105.53	109.67
2	F	3	GLC	C2-C3-C4	3.35	116.69	110.89
2	G	3	GLC	O5-C5-C4	3.34	118.96	110.83
2	K	2	GLC	C3-C4-C5	3.34	116.19	110.24
2	E	2	GLC	C1-C2-C3	3.29	113.71	109.67
2	E	2	GLC	C2-C3-C4	3.29	116.59	110.89
2	E	5	GLC	C1-C2-C3	3.25	113.66	109.67
2	L	5	GLC	C1-C2-C3	3.21	113.62	109.67
2	H	1	GLC	C1-C2-C3	3.17	113.56	109.67
2	G	6	GLC	C3-C4-C5	3.13	115.83	110.24
2	E	4	GLC	C2-C3-C4	3.06	116.19	110.89
2	J	5	GLC	C1-C2-C3	3.05	113.42	109.67
2	I	1	GLC	C2-C3-C4	3.03	116.15	110.89
2	F	6	GLC	C1-C2-C3	3.02	113.38	109.67
2	H	2	GLC	C1-O5-C5	-3.02	108.10	112.19
2	J	4	GLC	C1-C2-C3	2.97	113.31	109.67
2	F	2	GLC	C3-C4-C5	2.96	115.51	110.24
2	L	5	GLC	C2-C3-C4	2.88	115.88	110.89
2	E	1	GLC	C2-C3-C4	2.87	115.87	110.89
2	I	3	GLC	C2-C3-C4	2.85	115.83	110.89
2	K	3	GLC	C2-C3-C4	2.82	115.77	110.89
2	G	4	GLC	C3-C4-C5	2.81	115.25	110.24
2	G	6	GLC	C1-C2-C3	2.77	113.07	109.67
2	K	1	GLC	C2-C3-C4	2.75	115.66	110.89
2	I	4	GLC	C1-O5-C5	-2.75	108.47	112.19
2	I	3	GLC	C1-O5-C5	-2.71	108.52	112.19
2	G	3	GLC	O5-C1-C2	2.68	114.90	110.77
2	I	2	GLC	O5-C5-C4	2.62	117.19	110.83
2	K	6	GLC	C1-C2-C3	2.61	112.88	109.67
2	H	6	GLC	C1-C2-C3	2.61	112.87	109.67
2	E	2	GLC	O4-C4-C3	-2.60	104.33	110.35
2	H	2	GLC	O5-C1-C2	-2.59	106.77	110.77
2	G	3	GLC	C3-C4-C5	2.56	114.81	110.24
2	K	5	GLC	C1-C2-C3	2.55	112.80	109.67
2	F	1	GLC	C2-C3-C4	2.54	115.30	110.89
2	L	1	GLC	C1-O5-C5	-2.54	108.75	112.19
2	K	2	GLC	O4-C4-C3	-2.53	104.49	110.35
2	K	1	GLC	C6-C5-C4	-2.52	107.09	113.00
2	J	6	GLC	C3-C4-C5	2.51	114.71	110.24
2	E	1	GLC	C1-O5-C5	-2.46	108.86	112.19
2	E	6	GLC	C1-O5-C5	-2.45	108.87	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	2	GLC	C1-O5-C5	-2.44	108.89	112.19
2	L	2	GLC	C1-C2-C3	2.43	112.65	109.67
2	M	3	GLC	O4-C4-C3	-2.42	104.75	110.35
2	H	3	GLC	O4-C4-C3	-2.41	104.78	110.35
2	E	3	GLC	O5-C1-C2	2.41	114.48	110.77
2	M	6	GLC	O5-C5-C4	2.40	116.67	110.83
2	I	2	GLC	C3-C4-C5	2.39	114.50	110.24
2	J	2	GLC	C2-C3-C4	2.38	115.02	110.89
2	E	4	GLC	C3-C4-C5	2.38	114.48	110.24
2	J	5	GLC	C6-C5-C4	-2.38	107.44	113.00
2	I	1	GLC	C1-O5-C5	-2.37	108.98	112.19
2	H	1	GLC	C2-C3-C4	2.36	114.98	110.89
2	L	1	GLC	C2-C3-C4	2.36	114.97	110.89
2	J	3	GLC	O5-C5-C4	2.35	116.55	110.83
2	M	2	GLC	O5-C1-C2	-2.34	107.16	110.77
2	F	1	GLC	C3-C4-C5	2.32	114.38	110.24
2	L	6	GLC	C6-C5-C4	-2.30	107.62	113.00
2	E	6	GLC	C1-C2-C3	2.29	112.48	109.67
2	K	6	GLC	C2-C3-C4	2.26	114.81	110.89
2	L	2	GLC	C3-C4-C5	2.26	114.28	110.24
2	E	2	GLC	O5-C5-C4	2.25	116.31	110.83
2	J	1	GLC	C6-C5-C4	-2.25	107.73	113.00
2	M	5	GLC	C2-C3-C4	2.25	114.78	110.89
2	K	4	GLC	O5-C1-C2	2.22	114.19	110.77
2	I	2	GLC	C1-C2-C3	-2.19	106.97	109.67
2	M	1	GLC	C1-C2-C3	2.18	112.34	109.67
2	J	4	GLC	C2-C3-C4	2.17	114.64	110.89
2	I	6	GLC	C1-O5-C5	-2.16	109.26	112.19
2	G	6	GLC	C6-C5-C4	-2.16	107.95	113.00
2	H	1	GLC	C1-O5-C5	-2.16	109.27	112.19
2	K	4	GLC	C3-C4-C5	2.16	114.08	110.24
2	F	1	GLC	C1-O5-C5	-2.14	109.29	112.19
2	E	5	GLC	C2-C3-C4	2.14	114.60	110.89
2	G	4	GLC	C6-C5-C4	-2.14	108.00	113.00
2	I	2	GLC	C1-O5-C5	2.12	115.07	112.19
2	J	3	GLC	C6-C5-C4	-2.10	108.09	113.00
2	G	4	GLC	O4-C4-C3	-2.10	105.50	110.35
2	L	6	GLC	O5-C5-C4	2.09	115.91	110.83
2	M	6	GLC	C6-C5-C4	-2.06	108.18	113.00
2	G	4	GLC	O5-C5-C4	2.05	115.83	110.83
2	M	3	GLC	C6-C5-C4	-2.04	108.23	113.00
2	F	3	GLC	O4-C4-C3	-2.04	105.64	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	3	GLC	O5-C5-C4	2.04	115.78	110.83
2	L	6	GLC	C1-O5-C5	2.03	114.94	112.19
2	L	2	GLC	O5-C5-C4	2.02	115.75	110.83
2	G	6	GLC	O5-C5-C4	2.01	115.73	110.83
2	L	2	GLC	C2-C3-C4	2.01	114.37	110.89

There are no chirality outliers.

All (54) torsion outliers are listed below:

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

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

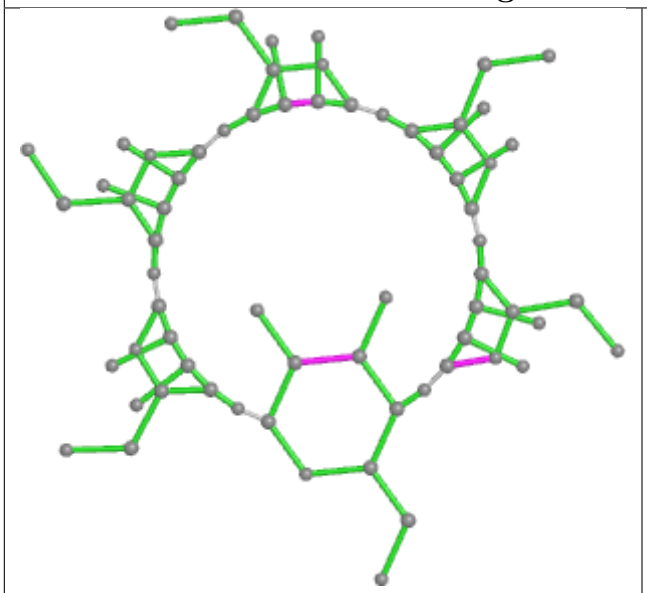
There are no ring outliers.

8 monomers are involved in 8 short contacts:

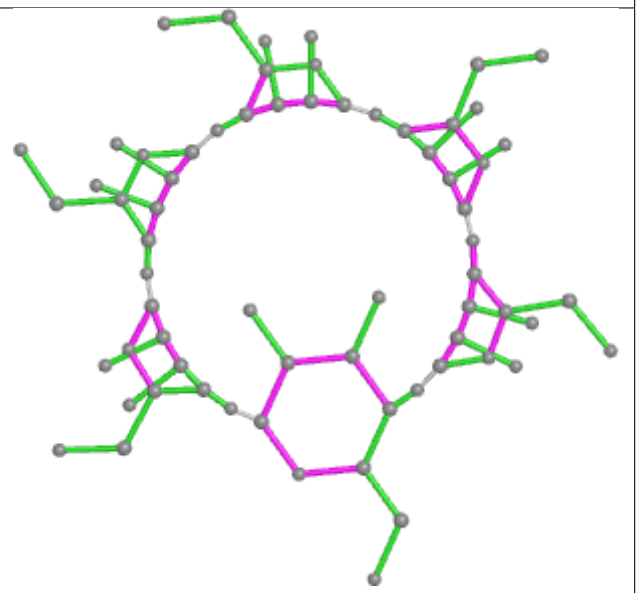
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	1	GLC	1	0
2	M	3	GLC	1	0
2	G	5	GLC	1	0
2	K	4	GLC	1	0
2	J	4	GLC	1	0
2	E	3	GLC	1	0
2	L	5	GLC	1	0
2	L	6	GLC	1	0

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

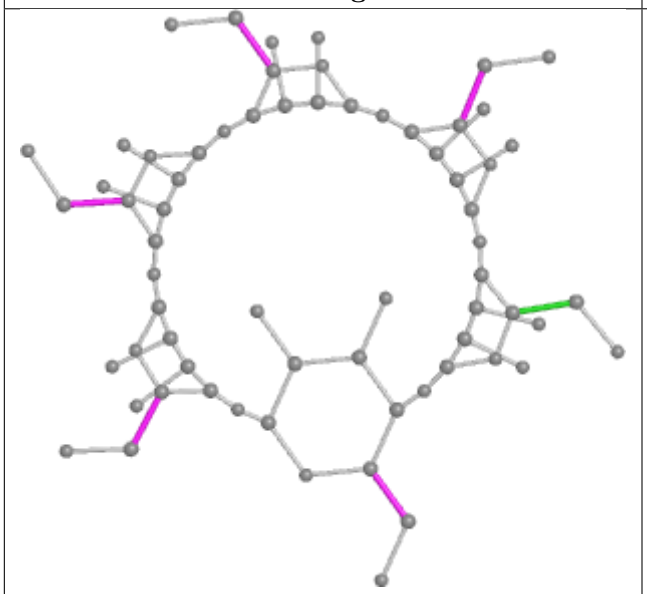
Oligosaccharide Chain E



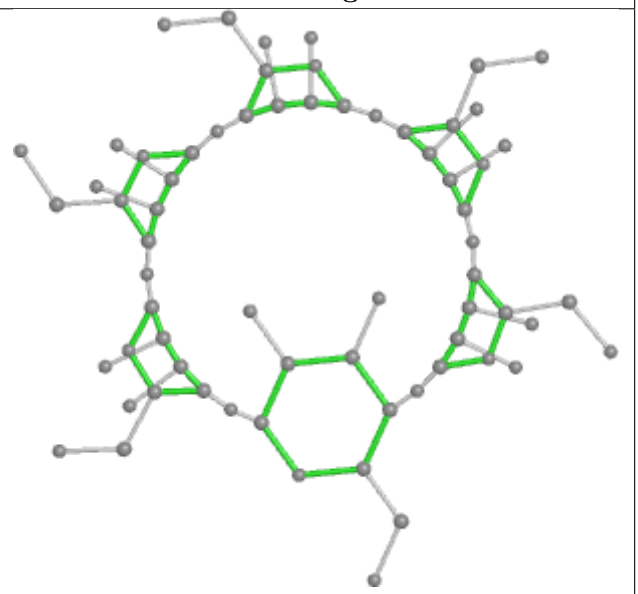
Bond lengths



Bond angles

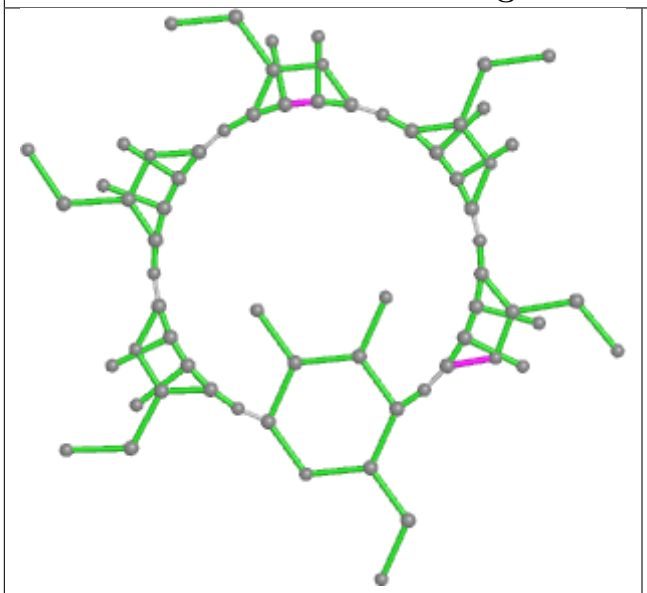


Torsions

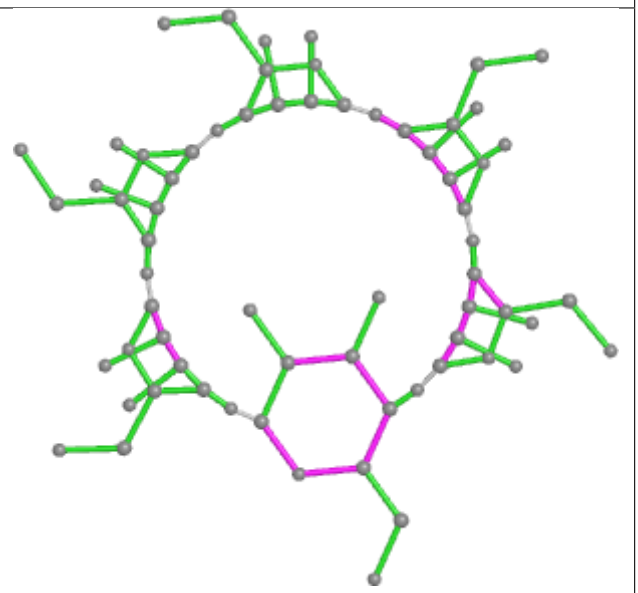


Rings

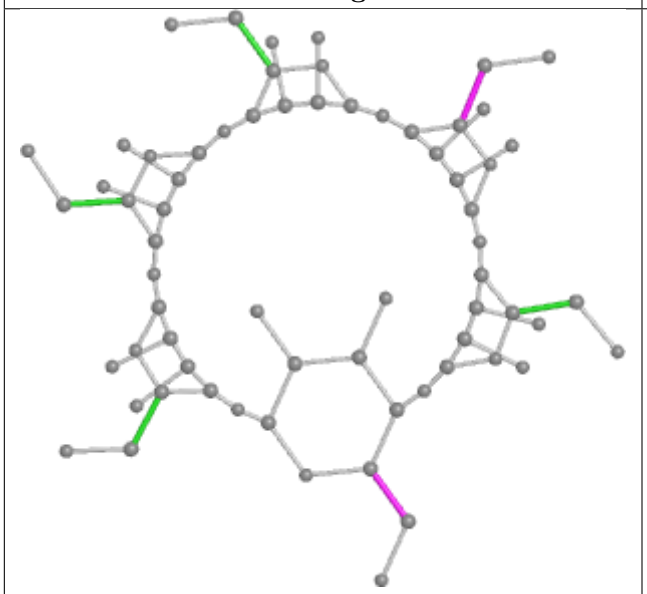
Oligosaccharide Chain F



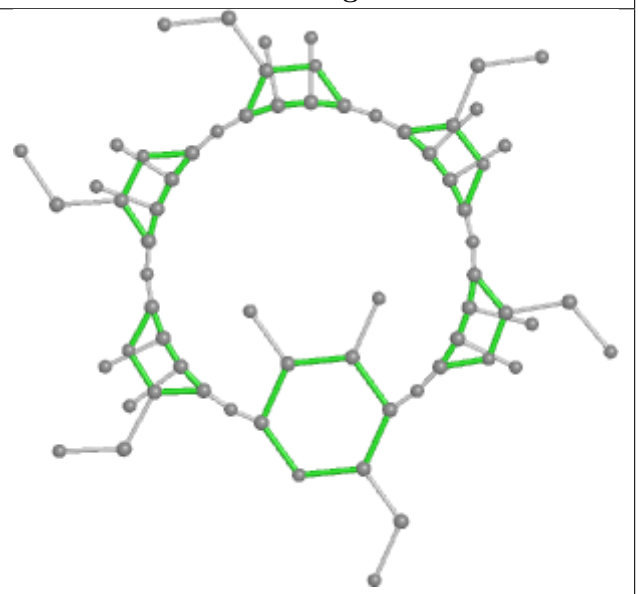
Bond lengths



Bond angles

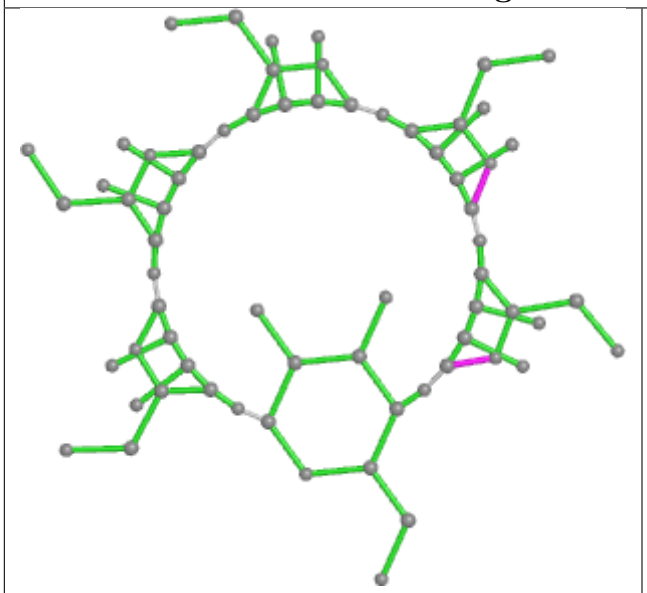


Torsions

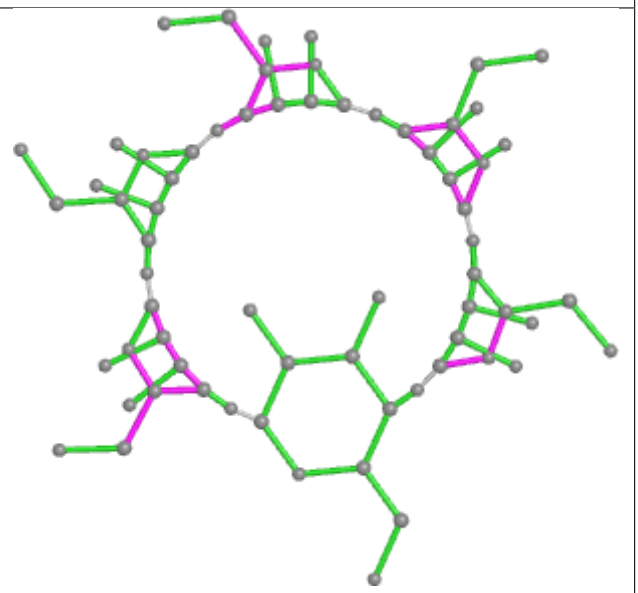


Rings

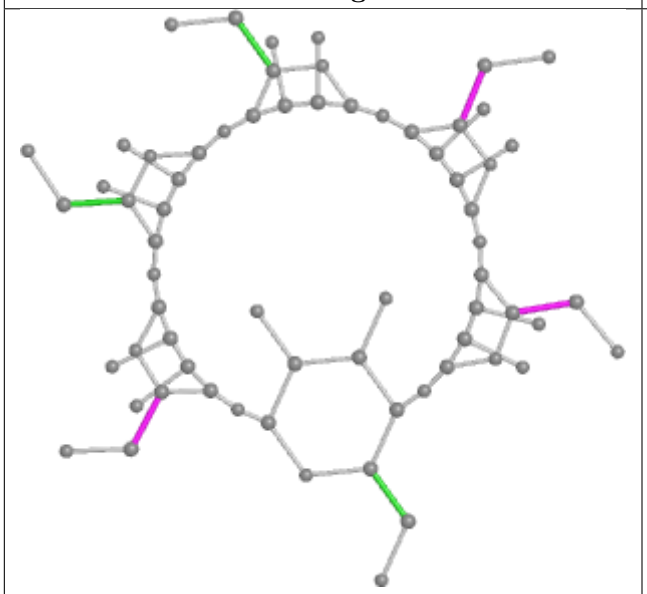
Oligosaccharide Chain G



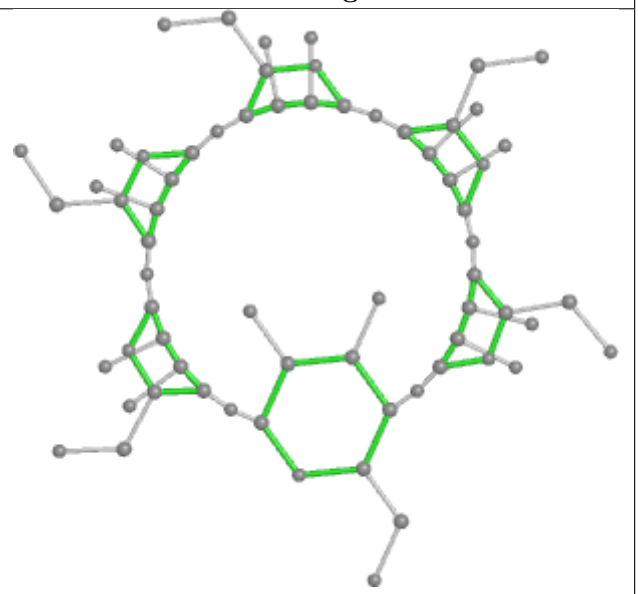
Bond lengths



Bond angles

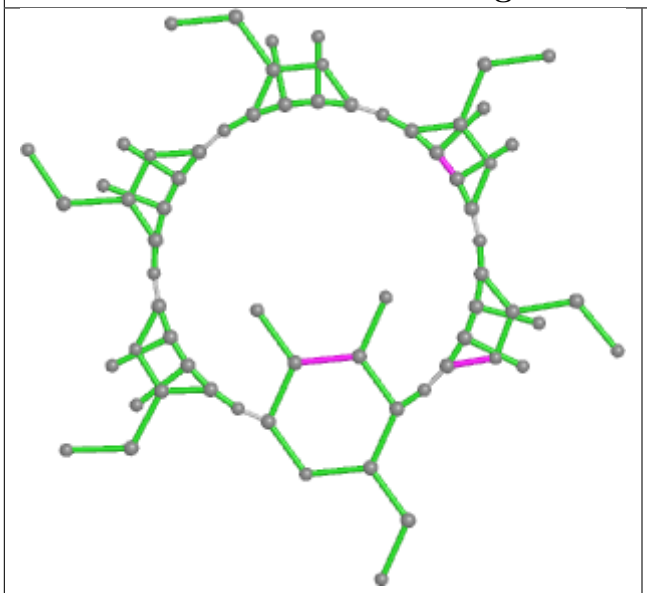


Torsions

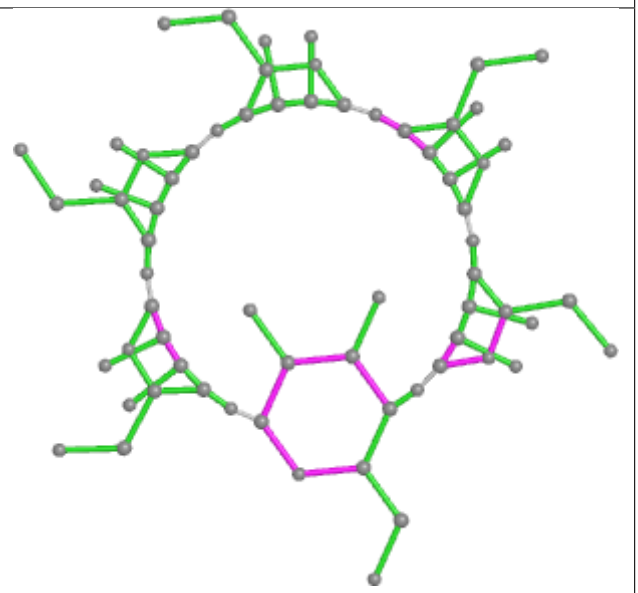


Rings

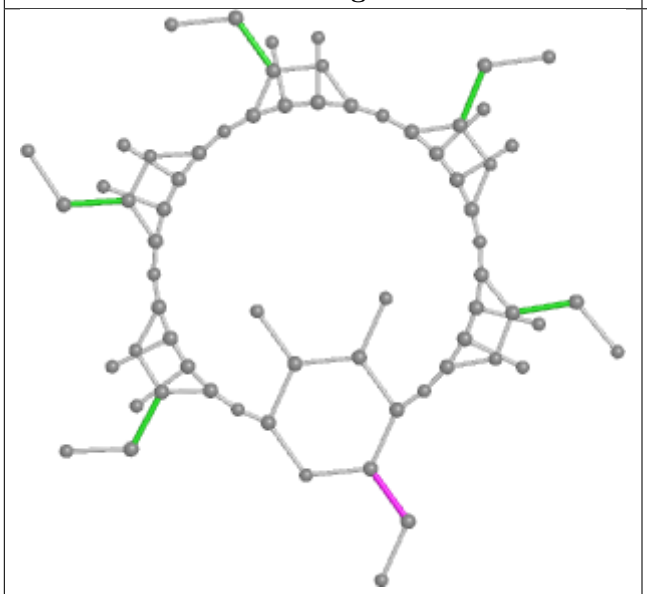
Oligosaccharide Chain H



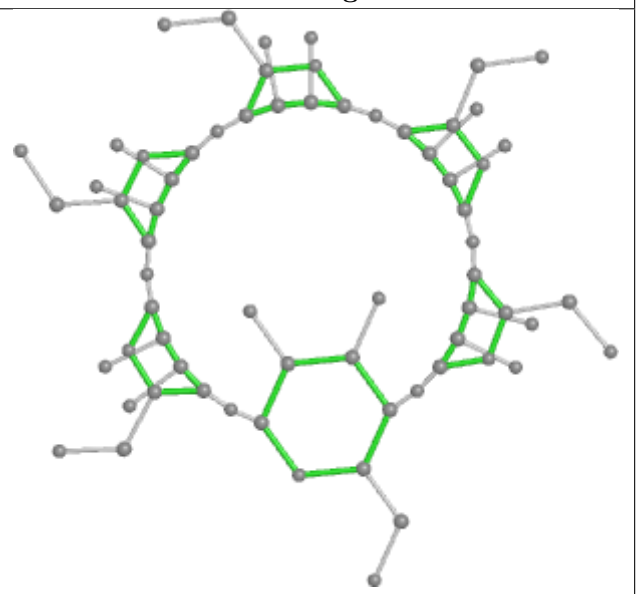
Bond lengths



Bond angles

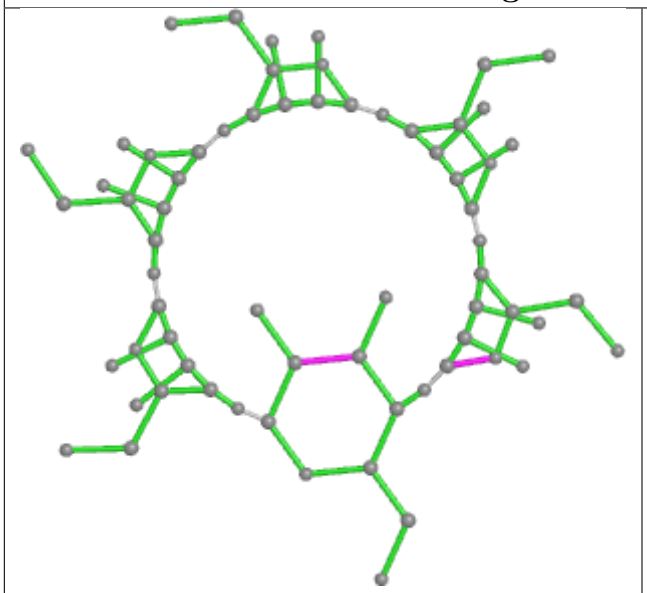


Torsions

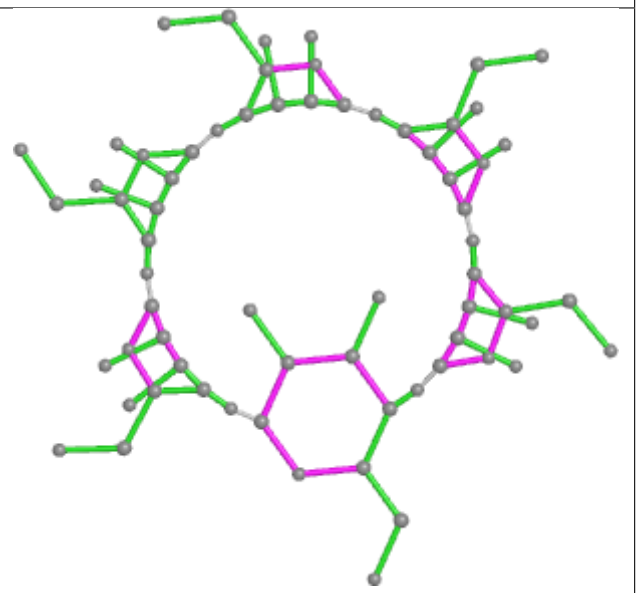


Rings

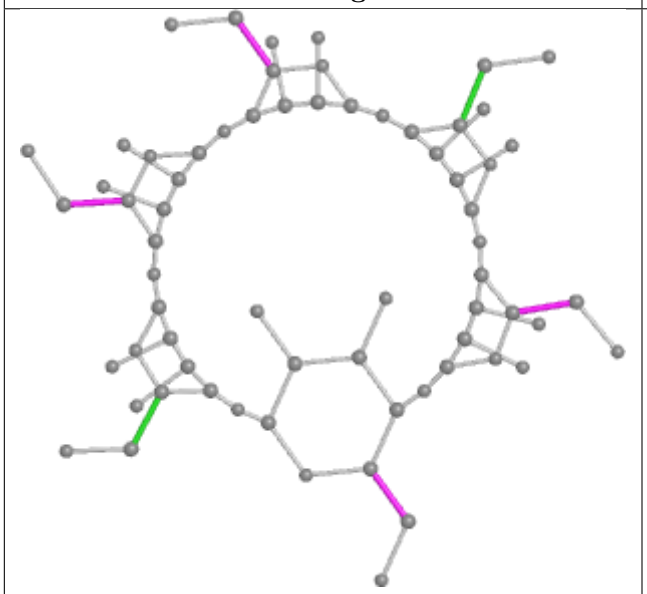
Oligosaccharide Chain I



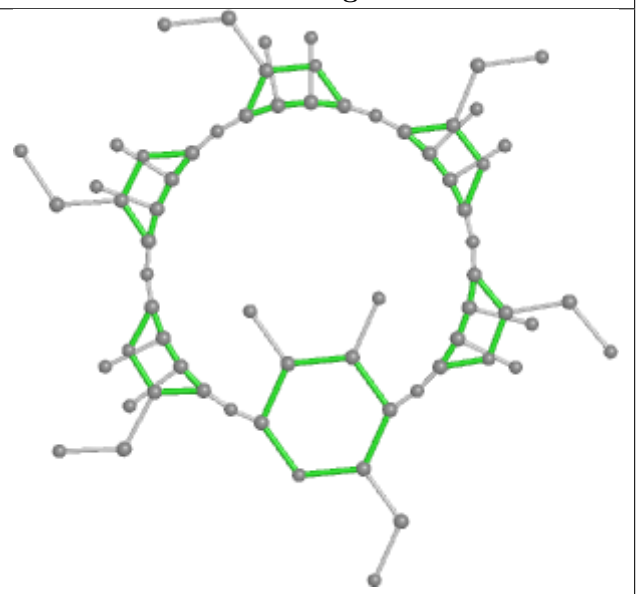
Bond lengths



Bond angles

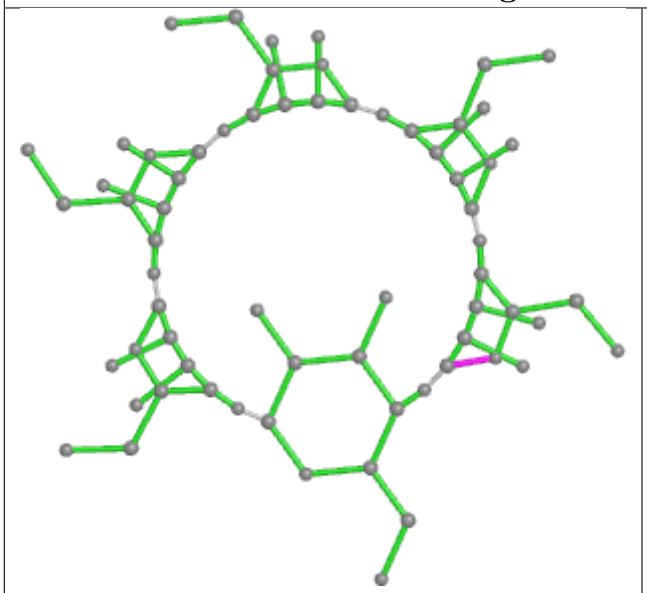


Torsions

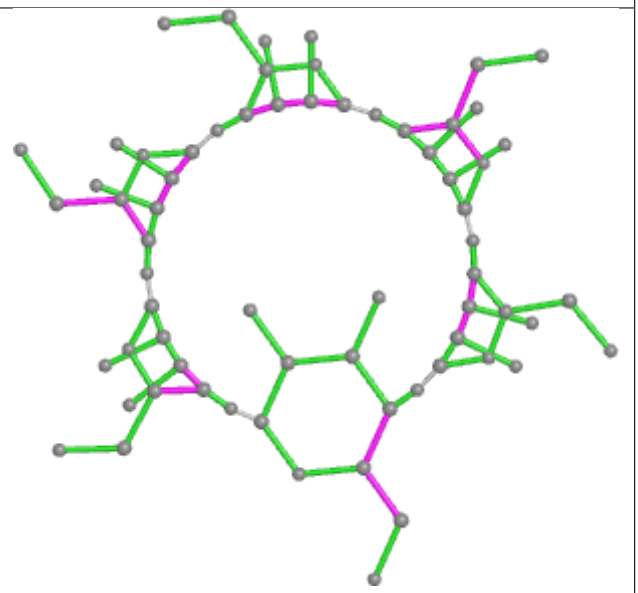


Rings

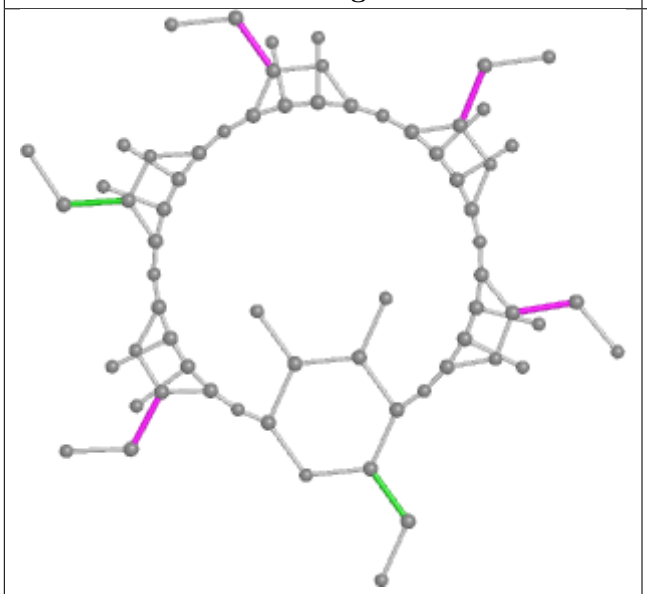
Oligosaccharide Chain J



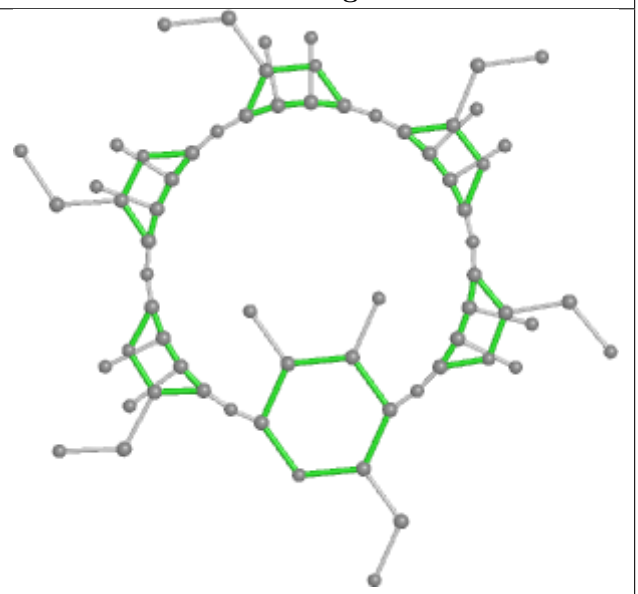
Bond lengths



Bond angles

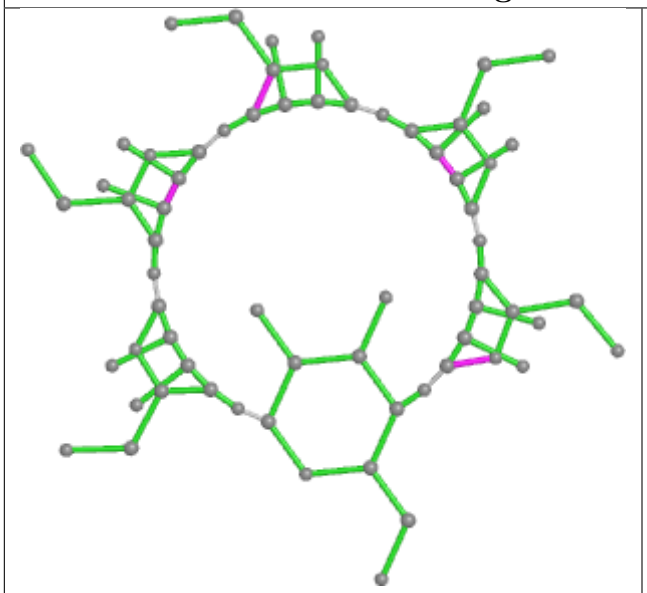


Torsions

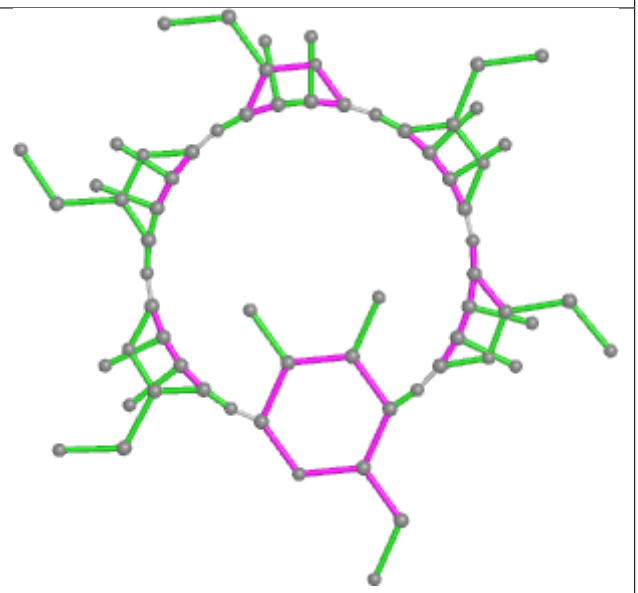


Rings

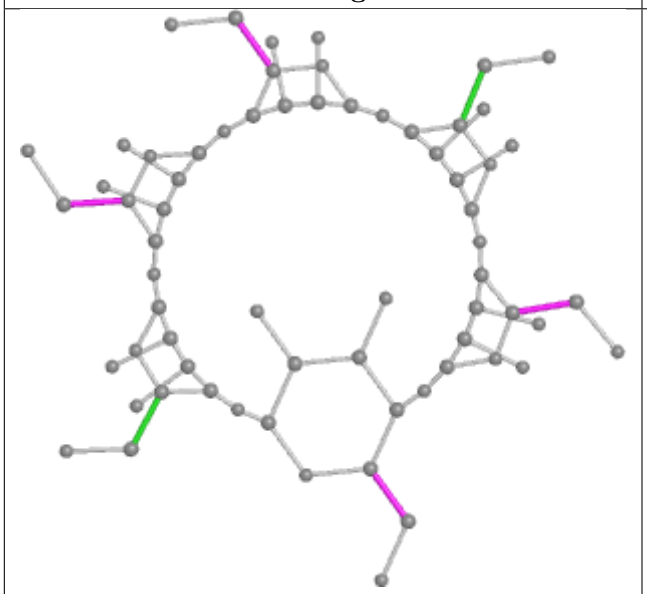
Oligosaccharide Chain K



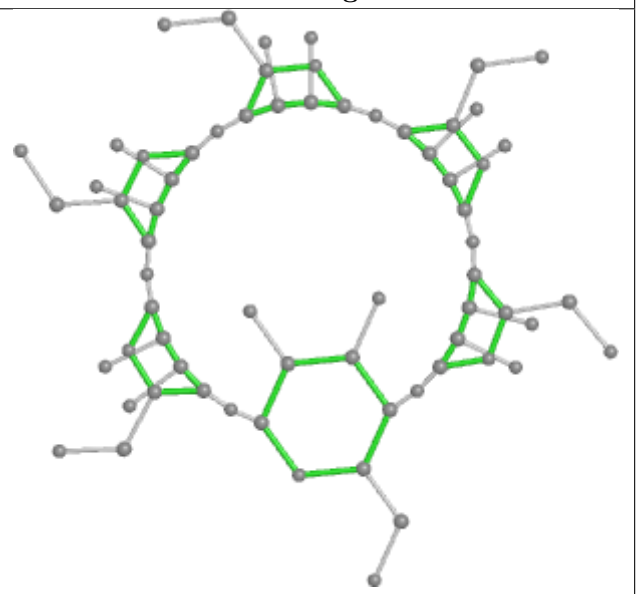
Bond lengths



Bond angles

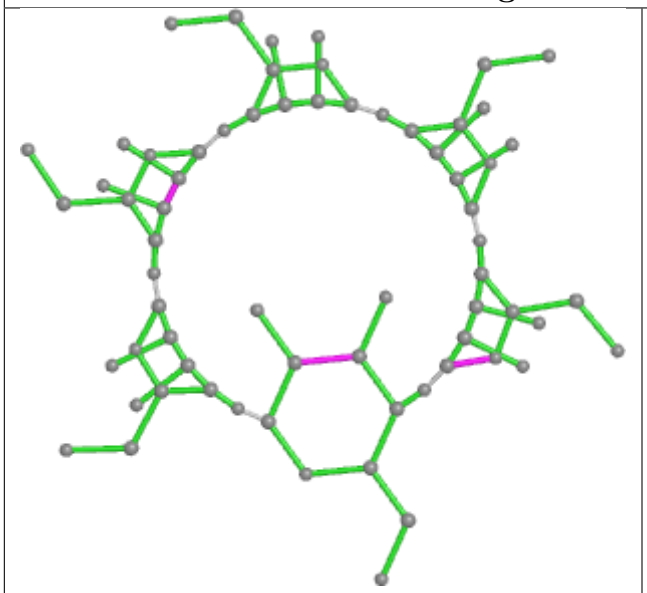


Torsions

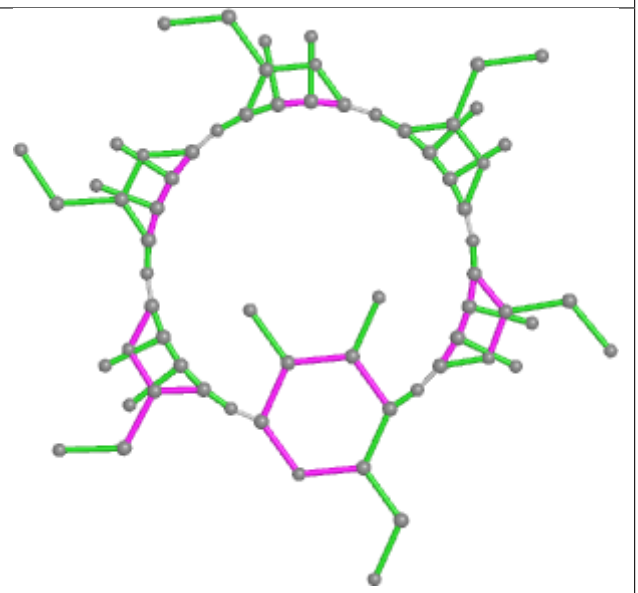


Rings

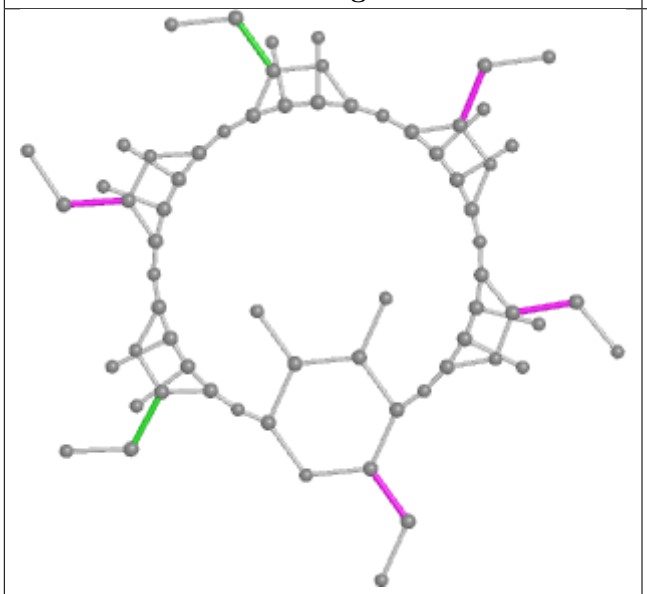
Oligosaccharide Chain L



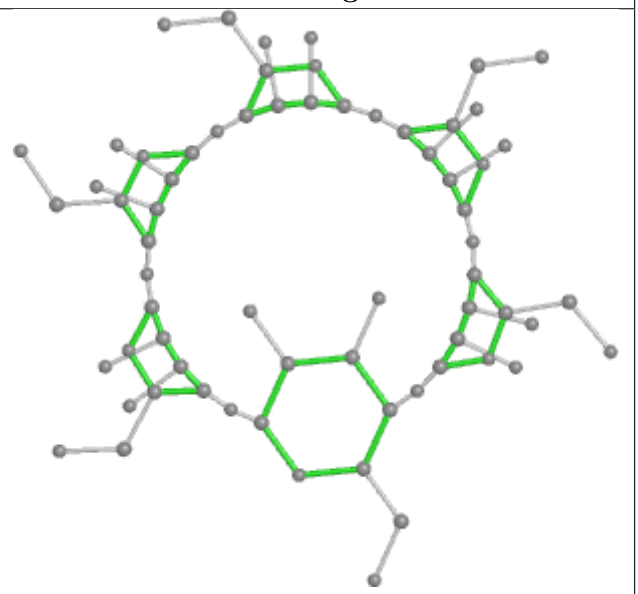
Bond lengths



Bond angles

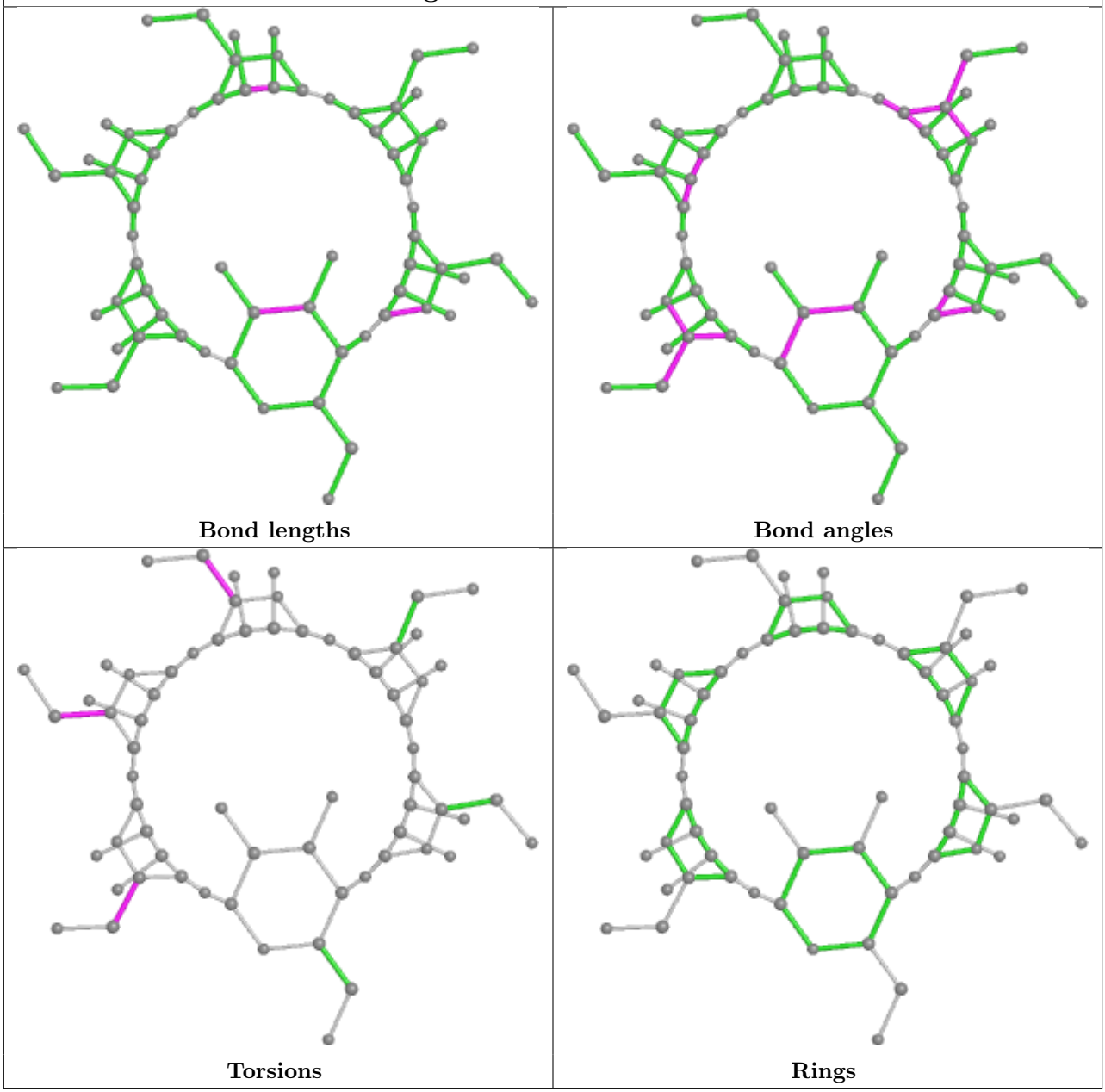


Torsions



Rings

Oligosaccharide Chain M



5.6 Ligand geometry (i)

5 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	0.42	0	5,5,5	0.22	0
3	GOL	D	804	-	5,5,5	0.27	0	5,5,5	0.44	0
3	GOL	A	804	-	5,5,5	0.38	0	5,5,5	0.21	0
3	GOL	B	803	-	5,5,5	0.38	0	5,5,5	0.31	0
3	GOL	A	803	-	5,5,5	0.41	0	5,5,5	0.30	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	-	-	2/4/4/4	-
3	GOL	D	804	-	-	4/4/4/4	-
3	GOL	A	804	-	-	0/4/4/4	-
3	GOL	B	803	-	-	4/4/4/4	-
3	GOL	A	803	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	802	GOL	O1-C1-C2-C3
3	B	803	GOL	O1-C1-C2-C3
3	D	804	GOL	C1-C2-C3-O3
3	B	803	GOL	C1-C2-C3-O3
3	D	804	GOL	O1-C1-C2-C3
3	B	802	GOL	O1-C1-C2-O2
3	B	803	GOL	O1-C1-C2-O2
3	B	803	GOL	O2-C2-C3-O3
3	D	804	GOL	O1-C1-C2-O2
3	D	804	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	802	GOL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	587/612 (95%)	0.35	80 (13%)	3	1	33, 64, 136, 151	2 (0%)
1	B	594/612 (97%)	-0.24	12 (2%)	65	60	34, 53, 84, 104	2 (0%)
1	C	584/612 (95%)	-0.26	5 (0%)	84	82	35, 55, 79, 96	0
1	D	589/612 (96%)	-0.39	1 (0%)	95	95	30, 43, 69, 97	3 (0%)
All	All	2354/2448 (96%)	-0.13	98 (4%)	36	29	30, 53, 106, 151	7 (0%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	190	TYR	6.3
1	A	159	TRP	6.2
1	A	201	LEU	6.2
1	A	475	LEU	6.1
1	B	133	ASP	5.4
1	A	187	LEU	5.3
1	A	145	PRO	4.9
1	A	349	ALA	4.8
1	A	214	PRO	4.8
1	A	146	ASN	4.7
1	A	359	HIS	4.6
1	A	134	GLY	4.5
1	A	153	VAL	4.5
1	A	429	GLY	4.5
1	A	175	TRP	4.5
1	A	158	TYR	4.4
1	A	165	PRO	4.4
1	A	428	GLY	4.3
1	A	473	GLY	4.3
1	A	192	MET	4.3
1	A	150	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	411	ILE	4.2
1	A	196	ASN	4.0
1	A	351	PHE	4.0
1	A	350	GLU	3.9
1	A	472	MET	3.9
1	A	202	LYS	3.8
1	A	144	ALA	3.8
1	B	427	PHE	3.8
1	A	160	ASP	3.7
1	A	346	PHE	3.7
1	A	180	PRO	3.7
1	A	162	ARG	3.6
1	A	118	HIS	3.6
1	A	353	GLY	3.4
1	A	188	TYR	3.4
1	B	199	LEU	3.4
1	A	215	GLU	3.4
1	A	172	SER	3.3
1	A	143	TRP	3.3
1	A	163	ARG	3.3
1	A	195	ALA	3.2
1	A	372	THR	3.2
1	A	140	PHE	3.2
1	A	438	PHE	3.1
1	A	147	ALA	3.1
1	A	197	GLY	3.1
1	A	117	THR	3.1
1	B	426	GLU	3.1
1	A	151	SER	3.0
1	A	474	GLY	3.0
1	A	164	HIS	3.0
1	A	191	GLU	2.9
1	A	465	GLY	2.9
1	A	142	VAL	2.9
1	A	168	LEU	2.9
1	A	152	VAL	2.9
1	A	360	SER	2.8
1	B	117	THR	2.7
1	A	155	GLN	2.6
1	A	200	ARG	2.6
1	C	360	SER	2.6
1	A	161	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	469	PRO	2.6
1	C	133	ASP	2.6
1	A	156	PHE	2.6
1	A	357	TYR	2.6
1	A	446	LEU	2.6
1	A	135	VAL	2.5
1	A	376	ASN	2.5
1	A	198	ASN	2.5
1	A	199	LEU	2.5
1	B	200	ARG	2.5
1	B	134	GLY	2.5
1	A	412	TYR	2.5
1	A	463	PHE	2.5
1	B	164	HIS	2.4
1	A	154	GLY	2.4
1	A	133	ASP	2.4
1	C	215	GLU	2.3
1	A	149	ARG	2.3
1	A	205	PRO	2.3
1	B	132	MET	2.2
1	C	200	ARG	2.2
1	D	371	ASN	2.2
1	A	182	ALA	2.2
1	A	170	LYS	2.2
1	B	294	PHE	2.2
1	A	189	LYS	2.2
1	A	177	LEU	2.2
1	A	354	THR	2.1
1	A	516	THR	2.1
1	A	379	ARG	2.1
1	B	425	ASN	2.1
1	C	346	PHE	2.1
1	A	432	ASN	2.1
1	A	203	SER	2.1
1	A	358	GLU	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	K	1	11/12	0.71	0.29	116,128,135,136	0
2	GLC	K	3	11/12	0.73	0.39	124,128,134,134	0
2	GLC	K	4	11/12	0.79	0.35	103,115,120,123	0
2	GLC	K	6	11/12	0.82	0.23	88,102,118,126	0
2	GLC	K	5	11/12	0.84	0.32	87,99,103,115	0
2	GLC	F	3	11/12	0.85	0.21	86,90,98,100	0
2	GLC	I	4	11/12	0.85	0.23	95,100,104,106	0
2	GLC	F	2	11/12	0.85	0.30	99,104,106,107	0
2	GLC	K	2	11/12	0.85	0.40	125,132,137,139	0
2	GLC	I	3	11/12	0.86	0.21	84,94,98,103	0
2	GLC	E	4	11/12	0.86	0.18	85,94,101,102	0
2	GLC	E	2	11/12	0.87	0.23	76,91,95,98	0
2	GLC	G	3	11/12	0.88	0.39	93,100,103,107	0
2	GLC	G	6	11/12	0.88	0.23	60,80,87,89	0
2	GLC	L	1	11/12	0.89	0.19	65,80,90,98	0
2	GLC	H	5	11/12	0.90	0.18	81,85,88,89	0
2	GLC	I	5	11/12	0.90	0.20	87,95,102,104	0
2	GLC	E	1	11/12	0.90	0.27	84,90,99,104	0
2	GLC	L	2	11/12	0.91	0.29	82,92,98,102	0
2	GLC	M	5	11/12	0.91	0.20	77,81,89,90	0
2	GLC	F	4	11/12	0.92	0.21	67,77,85,89	0
2	GLC	J	3	11/12	0.92	0.24	87,90,96,100	0
2	GLC	J	4	11/12	0.92	0.24	87,95,99,100	0
2	GLC	F	5	11/12	0.92	0.18	69,74,85,86	0
2	GLC	F	6	11/12	0.92	0.20	78,87,98,99	0
2	GLC	L	3	11/12	0.92	0.24	82,90,92,94	0
2	GLC	L	5	11/12	0.92	0.28	73,82,86,89	0
2	GLC	E	6	11/12	0.92	0.12	85,95,102,103	0
2	GLC	G	5	11/12	0.93	0.24	55,71,74,79	0
2	GLC	I	6	11/12	0.93	0.23	81,89,98,101	0
2	GLC	J	1	11/12	0.93	0.17	65,73,82,84	0
2	GLC	E	5	11/12	0.93	0.12	94,96,99,101	0
2	GLC	G	1	11/12	0.93	0.29	85,92,101,102	0
2	GLC	I	2	11/12	0.93	0.13	73,80,87,90	0
2	GLC	G	2	11/12	0.93	0.22	90,97,100,101	0
2	GLC	M	4	11/12	0.93	0.15	61,68,72,80	0
2	GLC	E	3	11/12	0.93	0.16	74,84,89,91	0

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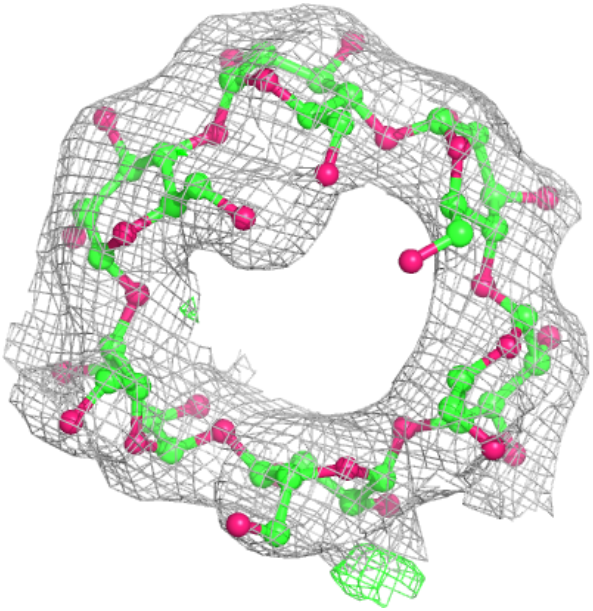
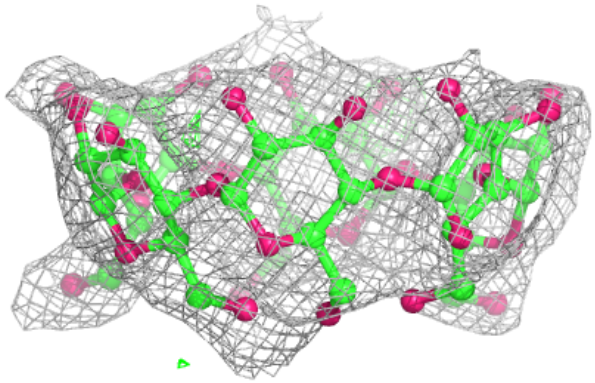
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	H	4	11/12	0.94	0.18	71,77,86,87	0
2	GLC	F	1	11/12	0.94	0.15	91,99,105,113	0
2	GLC	L	4	11/12	0.94	0.22	76,82,87,87	0
2	GLC	J	5	11/12	0.94	0.21	93,98,100,102	0
2	GLC	M	1	11/12	0.94	0.19	61,73,78,80	0
2	GLC	G	4	11/12	0.94	0.22	82,87,92,93	0
2	GLC	H	1	11/12	0.94	0.24	71,77,81,85	0
2	GLC	L	6	11/12	0.95	0.13	55,65,73,74	0
2	GLC	I	1	11/12	0.95	0.24	86,91,93,95	0
2	GLC	M	2	11/12	0.95	0.11	46,57,61,66	0
2	GLC	H	3	11/12	0.95	0.12	53,58,65,67	0
2	GLC	H	6	11/12	0.95	0.23	75,79,84,84	0
2	GLC	J	6	11/12	0.96	0.21	87,94,99,101	0
2	GLC	M	3	11/12	0.96	0.13	54,55,63,66	0
2	GLC	M	6	11/12	0.96	0.15	68,75,81,82	0
2	GLC	H	2	11/12	0.97	0.13	56,60,64,67	0
2	GLC	J	2	11/12	0.97	0.17	69,73,81,84	0

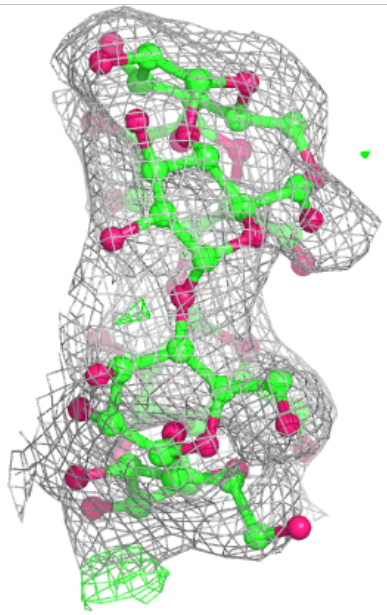
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

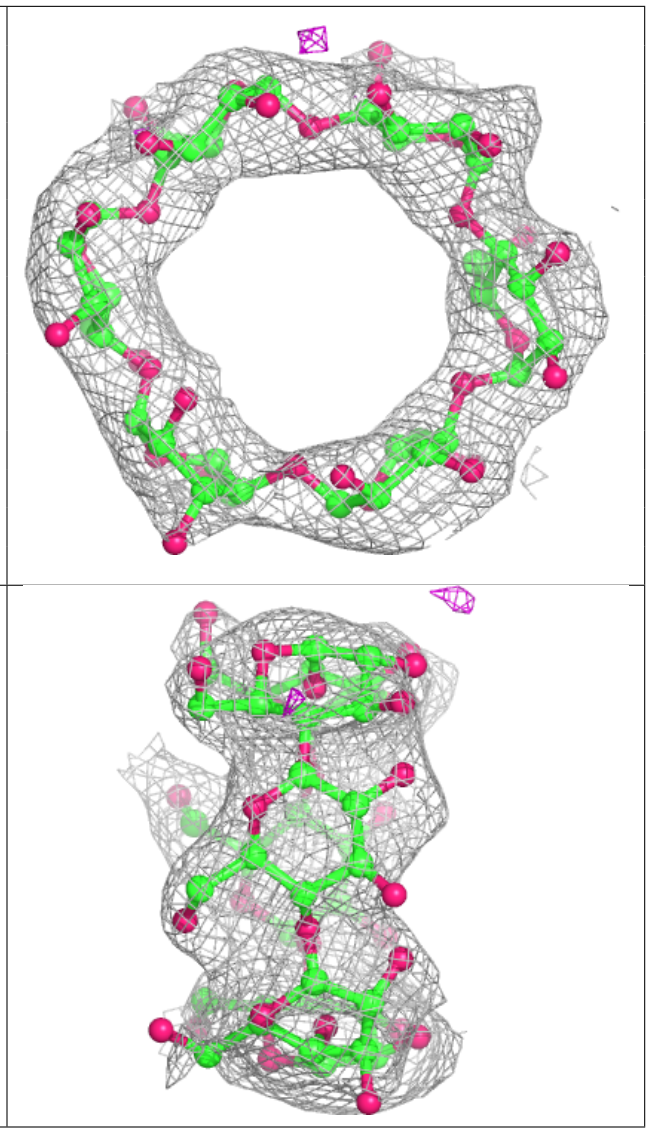






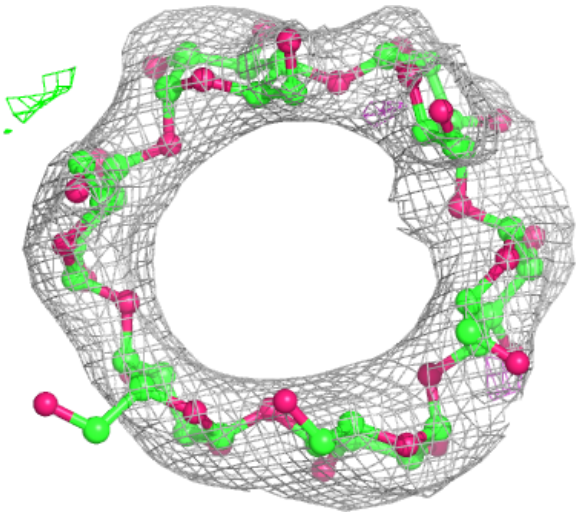
Electron density around Chain F:

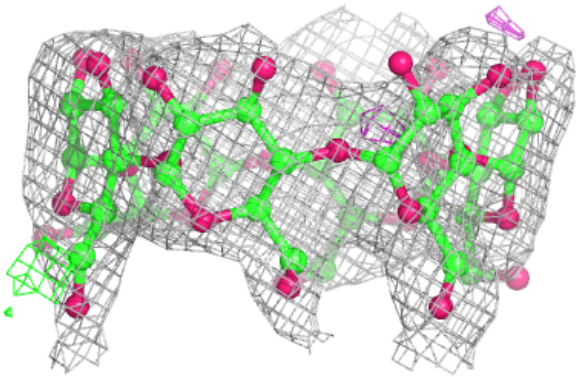
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

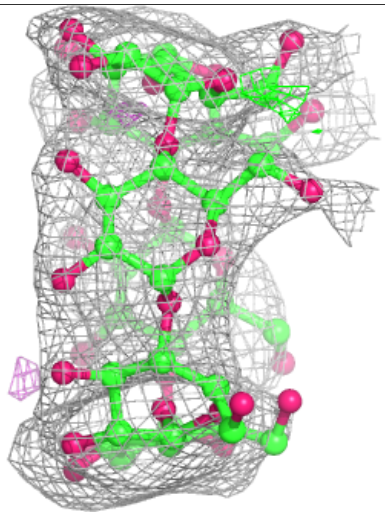


Electron density around Chain G:

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

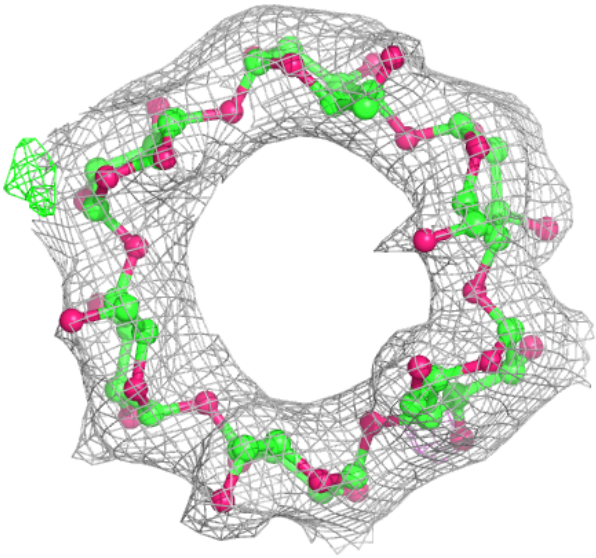


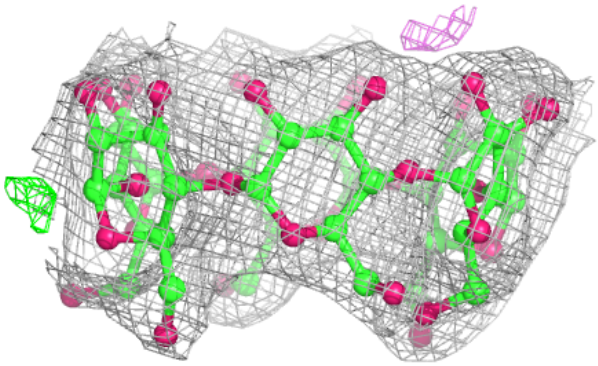


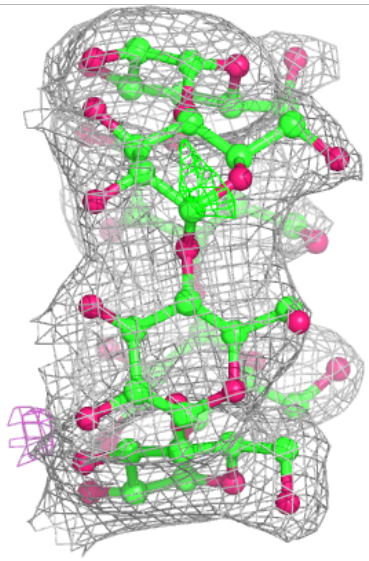


Electron density around Chain H:

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

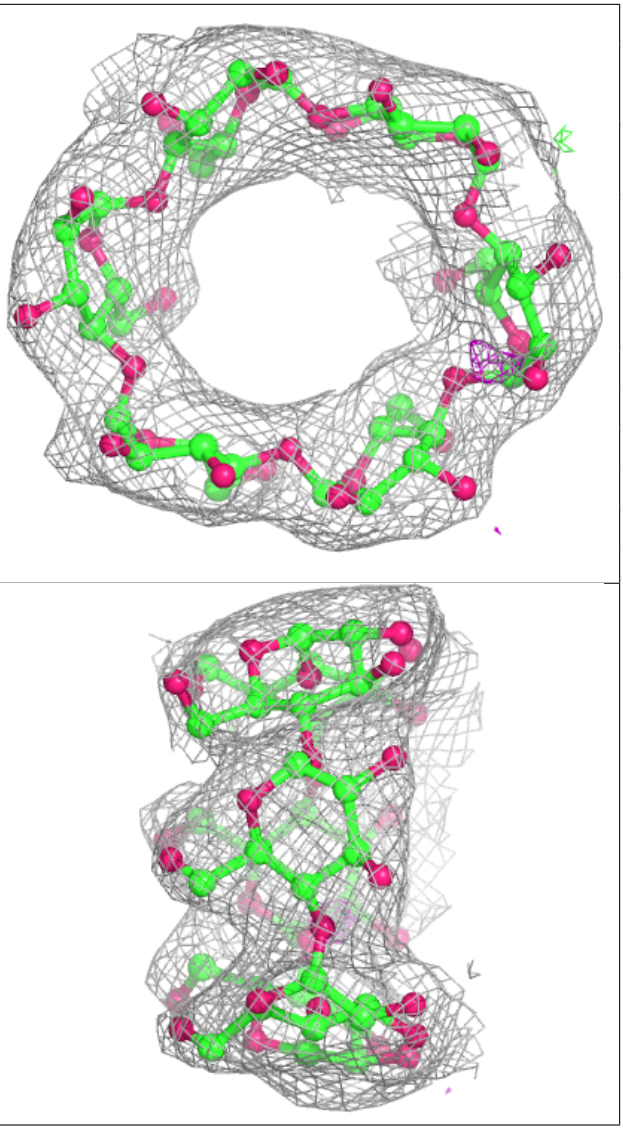






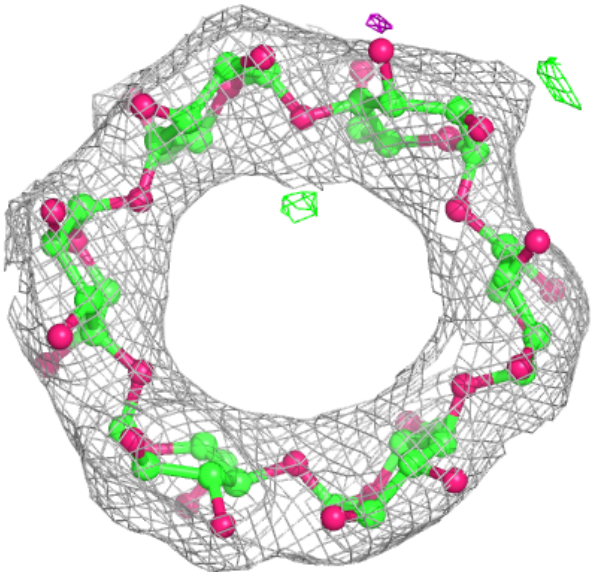
Electron density around Chain I:

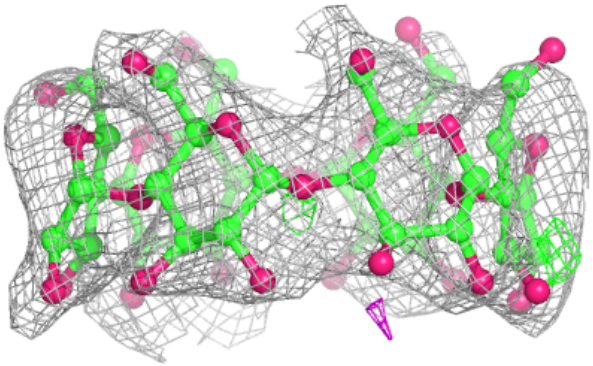
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

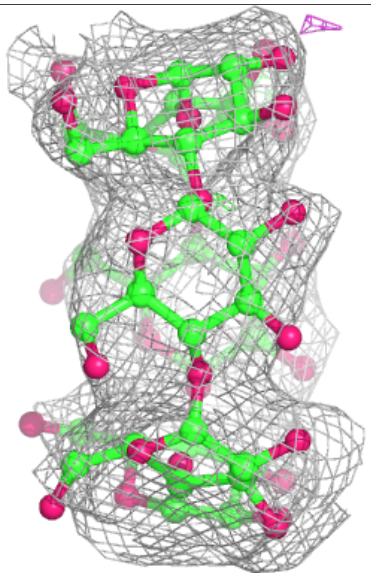


Electron density around Chain J:

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

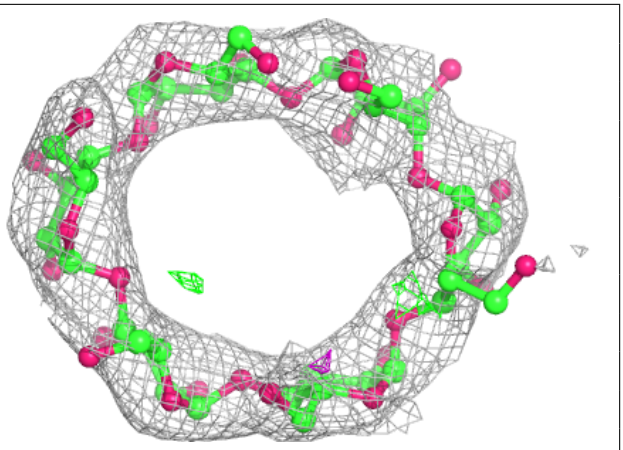


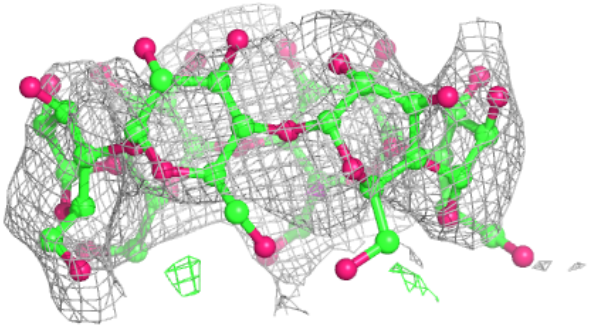


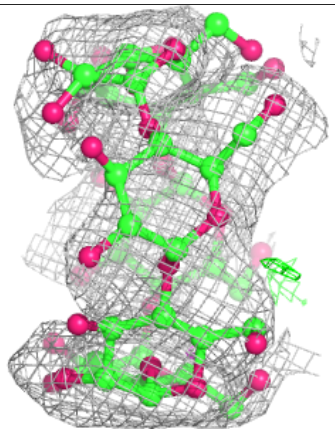


Electron density around Chain K:

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

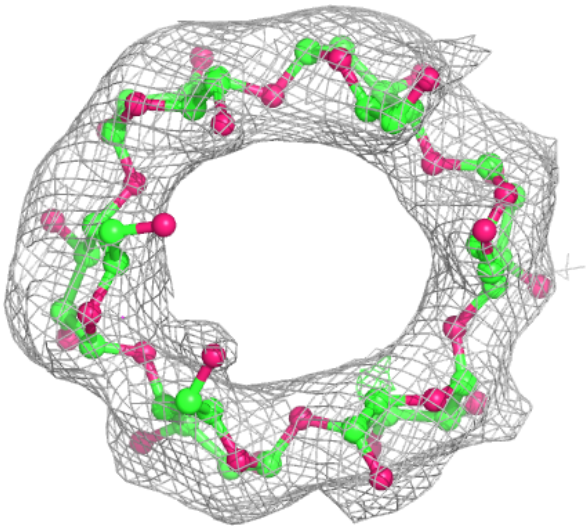


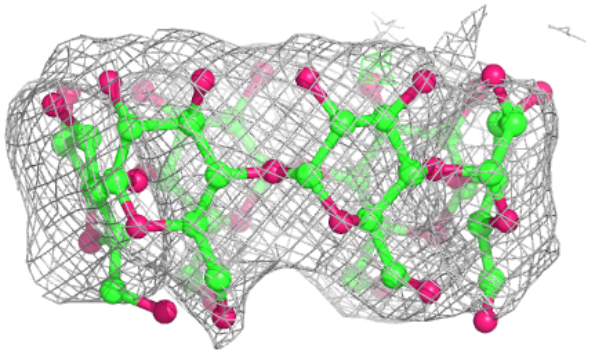


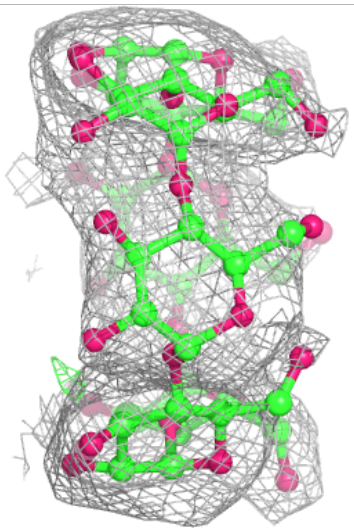


Electron density around Chain L:

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

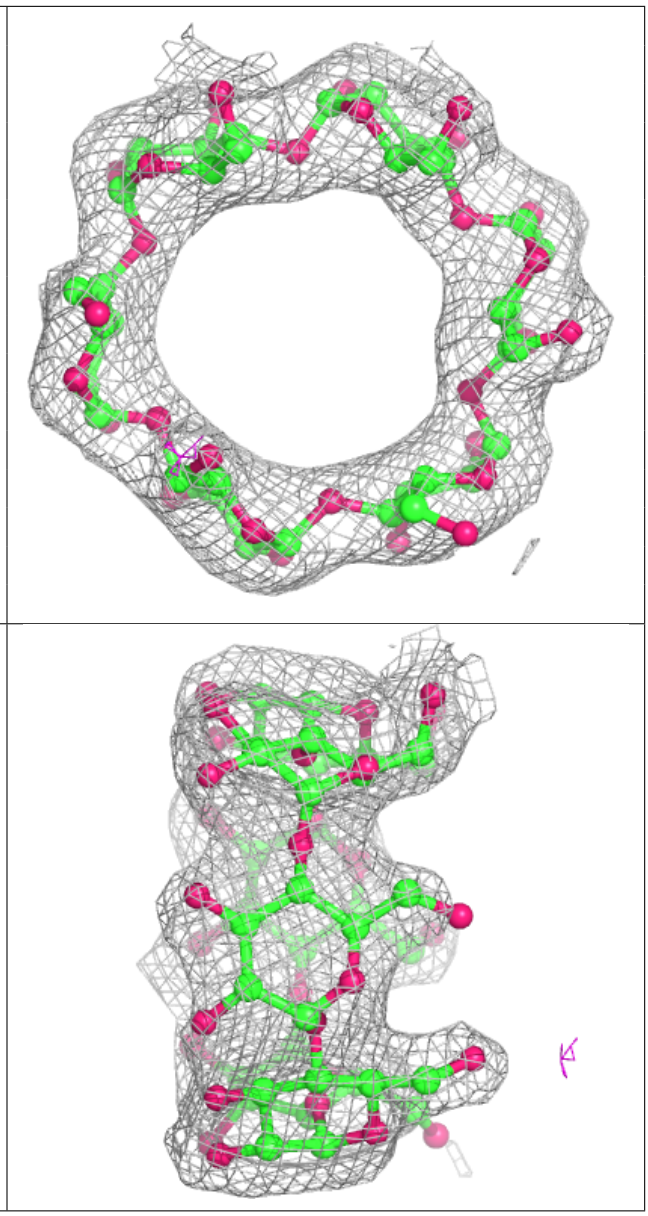






Electron density around Chain M:

$2mF_o$-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	0.79	0.17	70,74,75,76	0
3	GOL	A	803	6/6	0.92	0.34	58,59,64,66	0
3	GOL	D	804	6/6	0.96	0.14	48,51,53,57	0
3	GOL	A	804	6/6	0.97	0.13	44,47,52,58	0
3	GOL	B	802	6/6	0.97	0.18	45,51,58,62	0

6.5 Other polymers (i)

There are no such residues in this entry.