



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2020 – 12:39 PM EDT

PDB ID : 4YEE
Title : beta2 carbohydrate binding module (CBM) of AMP-activated protein kinase (AMPK) in complex with glucosyl-beta-cyclodextrin
Authors : Mobbs, J.; Gorman, M.A.; Parker, M.W.; Gooley, P.R.; Griffin, M.
Deposited on : 2015-02-24
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
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) : 2.14.6

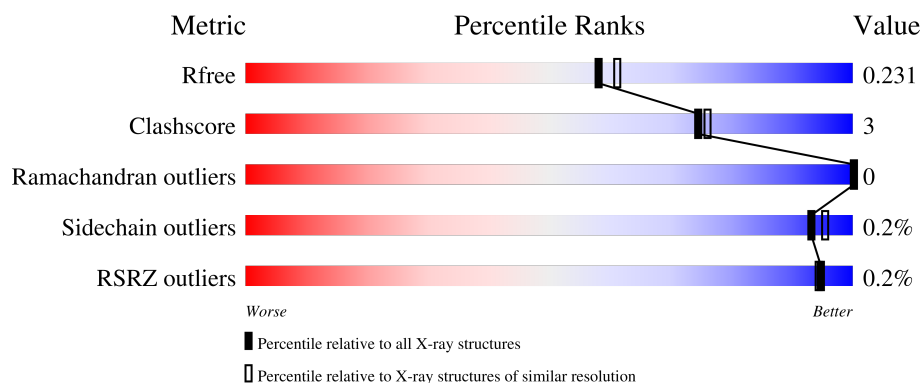
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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.






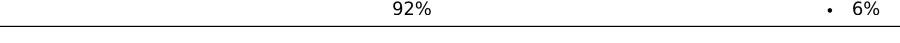
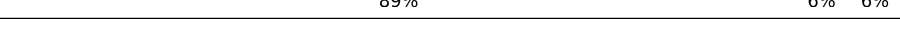
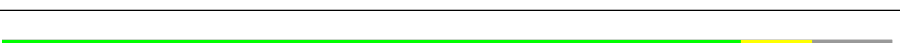
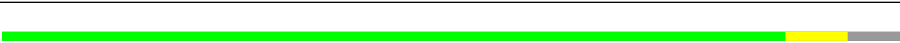




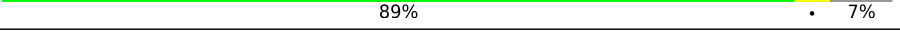
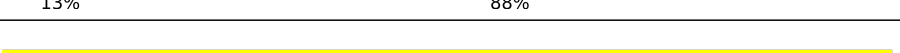
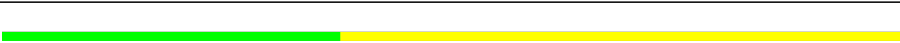
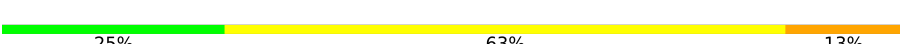
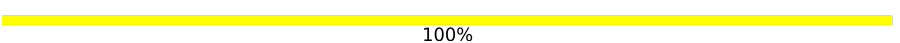
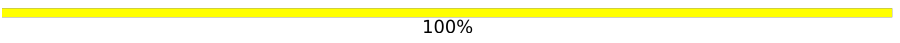




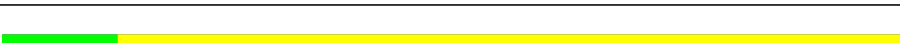



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	90	
1	B	90	
1	C	90	
1	D	90	
1	E	90	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	90	% 
1	G	90	
1	H	90	
1	I	90	
1	J	90	
1	K	90	
1	L	90	
1	M	90	
1	N	90	
1	O	90	
1	P	90	
1	Q	90	
1	R	90	% 
2	S	8	
2	T	8	
2	U	8	
2	V	8	
2	W	8	
2	X	8	
2	Y	8	
2	Z	8	
2	a	8	
2	b	8	
2	c	8	
2	d	8	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	e	8	<div><div></div><div>13%88%</div></div>
2	f	8	<div><div></div><div>100%</div></div>
2	g	8	<div><div></div><div>25%75%</div></div>
2	h	8	<div><div></div><div>38%63%</div></div>
2	i	8	<div><div></div><div>13%88%</div></div>
2	j	8	<div><div></div><div>25%75%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15355 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 5'-AMP-activated protein kinase subunit beta-2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	82	Total	C	N	O	0	0	0
			652	421	110	121			
1	B	83	Total	C	N	O	0	0	0
			667	429	114	124			
1	C	83	Total	C	N	O	0	1	0
			662	428	111	123			
1	D	79	Total	C	N	O	0	0	0
			630	408	104	118			
1	E	85	Total	C	N	O	0	1	0
			685	440	118	127			
1	F	85	Total	C	N	O	0	0	0
			682	438	117	127			
1	G	83	Total	C	N	O	0	1	0
			666	429	113	124			
1	H	85	Total	C	N	O	0	0	0
			675	434	114	127			
1	I	85	Total	C	N	O	0	0	0
			666	429	113	124			
1	J	85	Total	C	N	O	0	0	0
			671	431	114	126			
1	K	82	Total	C	N	O	0	0	0
			639	414	103	122			
1	L	82	Total	C	N	O	0	0	0
			654	422	111	121			
1	M	85	Total	C	N	O	0	0	0
			679	437	116	126			
1	N	84	Total	C	N	O	0	0	0
			672	432	115	125			
1	O	84	Total	C	N	O	0	0	0
			675	433	116	126			
1	P	85	Total	C	N	O	0	0	0
			678	435	116	127			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	Q	84	Total	C	N	O	0	0	0
			665	427	113	125			
1	R	84	Total	C	N	O	0	0	0
			662	425	111	126			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	GLY	-	expression tag	UNP Q9QZH4
A	68	PRO	-	expression tag	UNP Q9QZH4
A	69	LEU	-	expression tag	UNP Q9QZH4
A	70	GLY	-	expression tag	UNP Q9QZH4
A	71	SER	-	expression tag	UNP Q9QZH4
A	72	PRO	-	expression tag	UNP Q9QZH4
A	73	ASN	-	expression tag	UNP Q9QZH4
A	74	SER	-	expression tag	UNP Q9QZH4
B	67	GLY	-	expression tag	UNP Q9QZH4
B	68	PRO	-	expression tag	UNP Q9QZH4
B	69	LEU	-	expression tag	UNP Q9QZH4
B	70	GLY	-	expression tag	UNP Q9QZH4
B	71	SER	-	expression tag	UNP Q9QZH4
B	72	PRO	-	expression tag	UNP Q9QZH4
B	73	ASN	-	expression tag	UNP Q9QZH4
B	74	SER	-	expression tag	UNP Q9QZH4
C	67	GLY	-	expression tag	UNP Q9QZH4
C	68	PRO	-	expression tag	UNP Q9QZH4
C	69	LEU	-	expression tag	UNP Q9QZH4
C	70	GLY	-	expression tag	UNP Q9QZH4
C	71	SER	-	expression tag	UNP Q9QZH4
C	72	PRO	-	expression tag	UNP Q9QZH4
C	73	ASN	-	expression tag	UNP Q9QZH4
C	74	SER	-	expression tag	UNP Q9QZH4
D	67	GLY	-	expression tag	UNP Q9QZH4
D	68	PRO	-	expression tag	UNP Q9QZH4
D	69	LEU	-	expression tag	UNP Q9QZH4
D	70	GLY	-	expression tag	UNP Q9QZH4
D	71	SER	-	expression tag	UNP Q9QZH4
D	72	PRO	-	expression tag	UNP Q9QZH4
D	73	ASN	-	expression tag	UNP Q9QZH4
D	74	SER	-	expression tag	UNP Q9QZH4
E	67	GLY	-	expression tag	UNP Q9QZH4
E	68	PRO	-	expression tag	UNP Q9QZH4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	69	LEU	-	expression tag	UNP Q9QZH4
E	70	GLY	-	expression tag	UNP Q9QZH4
E	71	SER	-	expression tag	UNP Q9QZH4
E	72	PRO	-	expression tag	UNP Q9QZH4
E	73	ASN	-	expression tag	UNP Q9QZH4
E	74	SER	-	expression tag	UNP Q9QZH4
F	67	GLY	-	expression tag	UNP Q9QZH4
F	68	PRO	-	expression tag	UNP Q9QZH4
F	69	LEU	-	expression tag	UNP Q9QZH4
F	70	GLY	-	expression tag	UNP Q9QZH4
F	71	SER	-	expression tag	UNP Q9QZH4
F	72	PRO	-	expression tag	UNP Q9QZH4
F	73	ASN	-	expression tag	UNP Q9QZH4
F	74	SER	-	expression tag	UNP Q9QZH4
G	67	GLY	-	expression tag	UNP Q9QZH4
G	68	PRO	-	expression tag	UNP Q9QZH4
G	69	LEU	-	expression tag	UNP Q9QZH4
G	70	GLY	-	expression tag	UNP Q9QZH4
G	71	SER	-	expression tag	UNP Q9QZH4
G	72	PRO	-	expression tag	UNP Q9QZH4
G	73	ASN	-	expression tag	UNP Q9QZH4
G	74	SER	-	expression tag	UNP Q9QZH4
H	67	GLY	-	expression tag	UNP Q9QZH4
H	68	PRO	-	expression tag	UNP Q9QZH4
H	69	LEU	-	expression tag	UNP Q9QZH4
H	70	GLY	-	expression tag	UNP Q9QZH4
H	71	SER	-	expression tag	UNP Q9QZH4
H	72	PRO	-	expression tag	UNP Q9QZH4
H	73	ASN	-	expression tag	UNP Q9QZH4
H	74	SER	-	expression tag	UNP Q9QZH4
I	67	GLY	-	expression tag	UNP Q9QZH4
I	68	PRO	-	expression tag	UNP Q9QZH4
I	69	LEU	-	expression tag	UNP Q9QZH4
I	70	GLY	-	expression tag	UNP Q9QZH4
I	71	SER	-	expression tag	UNP Q9QZH4
I	72	PRO	-	expression tag	UNP Q9QZH4
I	73	ASN	-	expression tag	UNP Q9QZH4
I	74	SER	-	expression tag	UNP Q9QZH4
J	67	GLY	-	expression tag	UNP Q9QZH4
J	68	PRO	-	expression tag	UNP Q9QZH4
J	69	LEU	-	expression tag	UNP Q9QZH4
J	70	GLY	-	expression tag	UNP Q9QZH4

Continued on next page...

Continued from previous page...

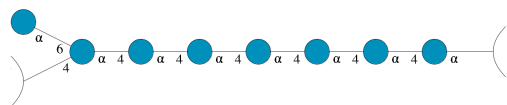
Chain	Residue	Modelled	Actual	Comment	Reference
J	71	SER	-	expression tag	UNP Q9QZH4
J	72	PRO	-	expression tag	UNP Q9QZH4
J	73	ASN	-	expression tag	UNP Q9QZH4
J	74	SER	-	expression tag	UNP Q9QZH4
K	67	GLY	-	expression tag	UNP Q9QZH4
K	68	PRO	-	expression tag	UNP Q9QZH4
K	69	LEU	-	expression tag	UNP Q9QZH4
K	70	GLY	-	expression tag	UNP Q9QZH4
K	71	SER	-	expression tag	UNP Q9QZH4
K	72	PRO	-	expression tag	UNP Q9QZH4
K	73	ASN	-	expression tag	UNP Q9QZH4
K	74	SER	-	expression tag	UNP Q9QZH4
L	67	GLY	-	expression tag	UNP Q9QZH4
L	68	PRO	-	expression tag	UNP Q9QZH4
L	69	LEU	-	expression tag	UNP Q9QZH4
L	70	GLY	-	expression tag	UNP Q9QZH4
L	71	SER	-	expression tag	UNP Q9QZH4
L	72	PRO	-	expression tag	UNP Q9QZH4
L	73	ASN	-	expression tag	UNP Q9QZH4
L	74	SER	-	expression tag	UNP Q9QZH4
M	67	GLY	-	expression tag	UNP Q9QZH4
M	68	PRO	-	expression tag	UNP Q9QZH4
M	69	LEU	-	expression tag	UNP Q9QZH4
M	70	GLY	-	expression tag	UNP Q9QZH4
M	71	SER	-	expression tag	UNP Q9QZH4
M	72	PRO	-	expression tag	UNP Q9QZH4
M	73	ASN	-	expression tag	UNP Q9QZH4
M	74	SER	-	expression tag	UNP Q9QZH4
N	67	GLY	-	expression tag	UNP Q9QZH4
N	68	PRO	-	expression tag	UNP Q9QZH4
N	69	LEU	-	expression tag	UNP Q9QZH4
N	70	GLY	-	expression tag	UNP Q9QZH4
N	71	SER	-	expression tag	UNP Q9QZH4
N	72	PRO	-	expression tag	UNP Q9QZH4
N	73	ASN	-	expression tag	UNP Q9QZH4
N	74	SER	-	expression tag	UNP Q9QZH4
O	67	GLY	-	expression tag	UNP Q9QZH4
O	68	PRO	-	expression tag	UNP Q9QZH4
O	69	LEU	-	expression tag	UNP Q9QZH4
O	70	GLY	-	expression tag	UNP Q9QZH4
O	71	SER	-	expression tag	UNP Q9QZH4
O	72	PRO	-	expression tag	UNP Q9QZH4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
O	73	ASN	-	expression tag	UNP Q9QZH4
O	74	SER	-	expression tag	UNP Q9QZH4
P	67	GLY	-	expression tag	UNP Q9QZH4
P	68	PRO	-	expression tag	UNP Q9QZH4
P	69	LEU	-	expression tag	UNP Q9QZH4
P	70	GLY	-	expression tag	UNP Q9QZH4
P	71	SER	-	expression tag	UNP Q9QZH4
P	72	PRO	-	expression tag	UNP Q9QZH4
P	73	ASN	-	expression tag	UNP Q9QZH4
P	74	SER	-	expression tag	UNP Q9QZH4
Q	67	GLY	-	expression tag	UNP Q9QZH4
Q	68	PRO	-	expression tag	UNP Q9QZH4
Q	69	LEU	-	expression tag	UNP Q9QZH4
Q	70	GLY	-	expression tag	UNP Q9QZH4
Q	71	SER	-	expression tag	UNP Q9QZH4
Q	72	PRO	-	expression tag	UNP Q9QZH4
Q	73	ASN	-	expression tag	UNP Q9QZH4
Q	74	SER	-	expression tag	UNP Q9QZH4
R	67	GLY	-	expression tag	UNP Q9QZH4
R	68	PRO	-	expression tag	UNP Q9QZH4
R	69	LEU	-	expression tag	UNP Q9QZH4
R	70	GLY	-	expression tag	UNP Q9QZH4
R	71	SER	-	expression tag	UNP Q9QZH4
R	72	PRO	-	expression tag	UNP Q9QZH4
R	73	ASN	-	expression tag	UNP Q9QZH4
R	74	SER	-	expression tag	UNP Q9QZH4

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



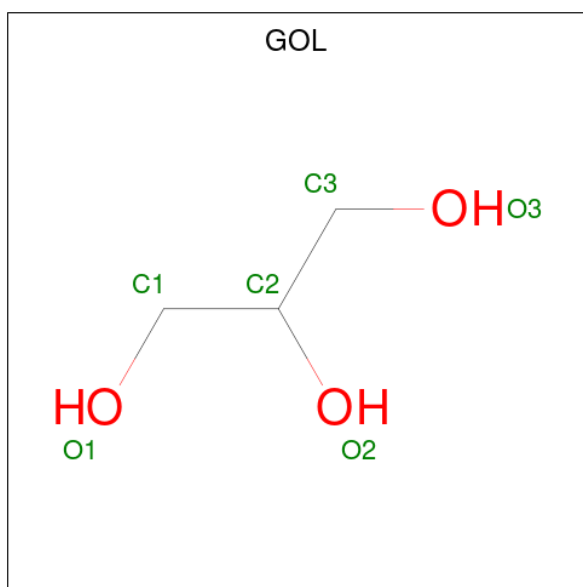
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	S	8	Total	C	O	0	0	0
			88	48	40			
2	T	8	Total	C	O	0	0	0
			88	48	40			
2	U	8	Total	C	O	0	0	0
			88	48	40			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	V	8	Total	C	O	0	0	0
			88	48	40			
2	W	8	Total	C	O	0	0	0
			88	48	40			
2	X	8	Total	C	O	0	0	0
			88	48	40			
2	Y	8	Total	C	O	0	0	0
			88	48	40			
2	Z	8	Total	C	O	0	0	0
			88	48	40			
2	a	8	Total	C	O	0	0	0
			88	48	40			
2	b	8	Total	C	O	0	0	0
			88	48	40			
2	c	8	Total	C	O	0	0	0
			88	48	40			
2	d	8	Total	C	O	0	0	0
			88	48	40			
2	e	8	Total	C	O	0	0	0
			88	48	40			
2	f	8	Total	C	O	0	0	0
			88	48	40			
2	g	8	Total	C	O	0	0	0
			88	48	40			
2	h	8	Total	C	O	0	0	0
			88	48	40			
2	i	8	Total	C	O	0	0	0
			88	48	40			
2	j	8	Total	C	O	0	0	0
			88	48	40			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	K	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	L	1	Total	C	O	0	0
			6	3	3		
3	M	1	Total	C	O	0	0
			6	3	3		
3	N	1	Total	C	O	0	0
			6	3	3		
3	N	1	Total	C	O	0	0
			6	3	3		
3	P	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	126	Total	O	0	0
			126	126		
4	B	110	Total	O	0	0
			110	110		
4	C	112	Total	O	0	0
			112	112		
4	D	107	Total	O	0	0
			107	107		
4	E	120	Total	O	0	0
			120	120		
4	F	101	Total	O	0	0
			101	101		
4	G	97	Total	O	0	0
			97	97		
4	H	86	Total	O	0	0
			86	86		
4	I	87	Total	O	0	0
			87	87		
4	J	84	Total	O	0	0
			84	84		
4	K	70	Total	O	0	0
			70	70		
4	L	79	Total	O	0	0
			79	79		
4	M	112	Total	O	0	0
			112	112		
4	N	75	Total	O	0	0
			75	75		

Continued on next page...


Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	94	Total 94	O 94	0	0
4	P	80	Total 80	O 80	0	0
4	Q	76	Total 76	O 76	0	0
4	R	61	Total 61	O 61	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.

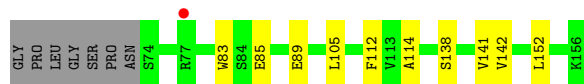
- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain A: 




- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain B: 




- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain C: 




- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain D: 




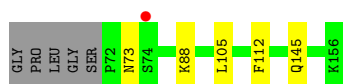
- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain E: 



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain F: 



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain G: 89% 8%



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain H: 86% 8% 6%



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain I: 92% 6%



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain J: 89% 6% 6%



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain K: 82% 9% 9%



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain L: 83% 8% 9%



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain M: 88% 7% 6%



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain N: 87% 7% 7%



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain O: 89% 7% 7%



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain P: 88% 7% 6%



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain Q: 89% 7% 7%



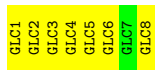
- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain R: 89% 7% 7%



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

Chain S: 13% 88% 7%



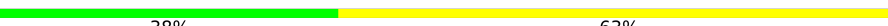
- Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose

4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose

Chain T:  100%

GLC1
GLC2
GLC3
GLC4
GLC5
GLC6
GLC7
GLC8

• Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose

Chain U:  38% 63%

GLC1
GLC2
GLC3
GLC4
GLC5
GLC6
GLC7
GLC8

• Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose

Chain V:  25% 63% 13%

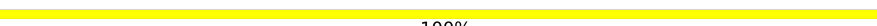
GLC1
GLC2
GLC3
GLC4
GLC5
GLC6
GLC7
GLC8

• Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose

Chain W:  100%

GLC1
GLC2
GLC3
GLC4
GLC5
GLC6
GLC7
GLC8

• Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose

Chain X:  100%

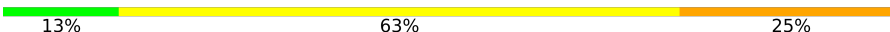
GLC1
GLC2
GLC3
GLC4
GLC5
GLC6
GLC7
GLC8

• Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose

Chain Y:  50% 50%

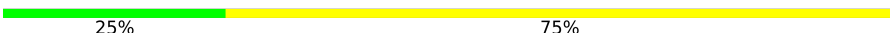
GLC1
GLC2
GLC3
GLC4
GLC5
GLC6
GLC7
GLC8

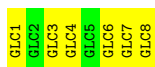
- Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose

Chain Z:  13% 63% 25%



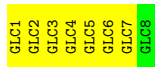
- Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose

Chain a:  25% 75%



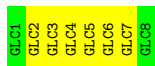
- Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose

Chain b:  13% 88%

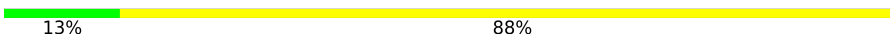


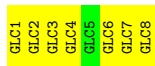
- Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose

Chain c:  25% 75%



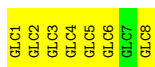
- Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose

Chain d:  13% 88%



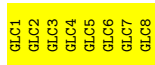
- Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose

Chain e:  13% 88%



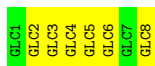
- Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose

Chain f: 100%



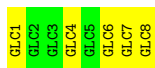
- Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose

Chain g: 25% 75%



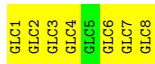
- Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose

Chain h: 38% 63%



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

Chain i: 13% 88%



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

Chain j: 25% 75%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	204.54Å 96.43Å 118.72Å 90.00° 125.46° 90.00°	Depositor
Resolution (Å)	43.38 – 2.00 48.38 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.38-2.00) 99.9 (48.38-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.169 , 0.225 0.177 , 0.231	Depositor DCC
R_{free} test set	6385 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.027 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15355	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.69	0/672	0.79	2/916 (0.2%)
1	B	0.72	0/687	0.77	0/934
1	C	0.76	1/685 (0.1%)	0.73	0/934
1	D	0.71	0/650	0.71	0/886
1	E	0.64	0/710	0.74	0/967
1	F	0.61	0/703	0.71	0/956
1	G	0.60	0/689	0.69	0/938
1	H	0.59	0/695	0.70	1/946 (0.1%)
1	I	0.60	0/687	0.71	0/938
1	J	0.60	0/692	0.68	0/944
1	K	0.59	0/658	0.70	0/899
1	L	0.66	0/674	0.77	1/918 (0.1%)
1	M	0.63	0/700	0.72	0/952
1	N	0.65	0/692	0.74	1/941 (0.1%)
1	O	0.63	0/695	0.69	0/945
1	P	0.60	0/699	0.73	0/952
1	Q	0.57	0/685	0.70	0/934
1	R	0.48	0/682	0.64	0/931
All	All	0.63	1/12355 (0.0%)	0.72	5/16831 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	93	SER	CB-OG	5.32	1.49	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	ASP	CB-CG-OD2	-7.14	111.88	118.30
1	N	111	ASP	CB-CG-OD1	5.70	123.43	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	ASP	CB-CG-OD1	5.67	123.41	118.30
1	L	111	ASP	CB-CG-OD1	5.45	123.21	118.30
1	H	146	LEU	CA-CB-CG	5.10	127.03	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	652	0	618	7	0
1	B	667	0	645	9	0
1	C	662	0	632	6	0
1	D	630	0	597	2	0
1	E	685	0	655	6	0
1	F	682	0	659	4	0
1	G	666	0	638	2	0
1	H	675	0	647	8	0
1	I	666	0	624	1	0
1	J	671	0	633	3	0
1	K	639	0	597	4	1
1	L	654	0	625	4	0
1	M	679	0	655	5	0
1	N	672	0	647	4	0
1	O	675	0	651	2	0
1	P	678	0	648	5	0
1	Q	665	0	627	2	0
1	R	662	0	620	2	0
2	S	88	0	72	0	0
2	T	88	0	72	0	0
2	U	88	0	72	0	0
2	V	88	0	72	1	0
2	W	88	0	72	0	0
2	X	88	0	72	0	0
2	Y	88	0	72	0	0
2	Z	88	0	72	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	a	88	0	72	0	0
2	b	88	0	72	0	0
2	c	88	0	72	0	0
2	d	88	0	72	0	0
2	e	88	0	72	0	0
2	f	88	0	72	0	0
2	g	88	0	72	0	0
2	h	88	0	72	0	0
2	i	88	0	72	0	0
2	j	88	0	72	0	0
3	A	12	0	16	1	0
3	B	12	0	16	2	0
3	C	12	0	16	2	0
3	D	6	0	8	0	0
3	E	6	0	8	0	0
3	F	6	0	8	0	0
3	H	12	0	16	2	0
3	I	12	0	16	0	0
3	K	6	0	8	1	0
3	L	6	0	8	0	0
3	M	6	0	8	0	0
3	N	12	0	16	0	0
3	P	6	0	8	2	0
4	A	126	0	0	1	0
4	B	110	0	0	1	0
4	C	112	0	0	0	0
4	D	107	0	0	1	0
4	E	120	0	0	0	0
4	F	101	0	0	3	0
4	G	97	0	0	1	0
4	H	86	0	0	2	0
4	I	87	0	0	0	0
4	J	84	0	0	1	0
4	K	70	0	0	1	0
4	L	79	0	0	1	1
4	M	112	0	0	3	0
4	N	75	0	0	1	0
4	O	94	0	0	0	1
4	P	80	0	0	0	1
4	Q	76	0	0	1	0
4	R	61	0	0	0	0
All	All	15355	0	12866	77	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (77) 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:J:139:GLU:OE1	4:J:370:HOH:O	1.95	0.82
2:Z:4:GLC:O3	2:Z:5:GLC:O2	2.02	0.73
1:B:142:VAL:HG11	1:B:152:LEU:HD22	1.71	0.71
1:H:148:THR:HG21	2:Z:6:GLC:H3	1.75	0.69
1:B:89:GLU:OE2	3:B:201:GOL:O2	2.14	0.66
1:F:145:GLN:NE2	4:F:301:HOH:O	2.28	0.65
1:I:122:GLU:OE2	1:I:154:HIS:NE2	2.32	0.61
1:C:107:LYS:HE2	1:C:109:HIS:O	2.02	0.59
1:E:122:GLU:CG	1:E:152:LEU:HD11	2.33	0.58
1:C:107:LYS:HD3	1:C:112:PHE:CZ	2.39	0.57
1:P:122:GLU:HG3	1:P:152:LEU:HD11	1.87	0.57
1:E:122:GLU:HG3	1:E:152:LEU:HD11	1.87	0.56
3:K:201:GOL:O1	4:K:343:HOH:O	2.18	0.56
1:P:122:GLU:CG	1:P:152:LEU:HD11	2.35	0.55
1:A:117:ASP:OD2	4:A:386:HOH:O	2.18	0.54
1:H:139:GLU:HG3	3:H:201:GOL:H12	1.89	0.53
2:Z:4:GLC:HO3	2:Z:5:GLC:HO2	1.26	0.52
1:M:120:GLU:HG2	4:M:366:HOH:O	2.09	0.52
1:E:97:ASN:ND2	1:E:101:THR:HG22	2.26	0.51
1:F:88:LYS:NZ	4:F:384:HOH:O	2.25	0.51
1:A:89:GLU:HG2	3:A:202:GOL:H11	1.91	0.51
1:H:122:GLU:HG2	1:H:154:HIS:CD2	2.47	0.50
1:B:105:LEU:HG	1:B:114:ALA:HB2	1.94	0.49
1:R:126:LYS:HE2	1:R:133:TRP:HB3	1.95	0.49
1:B:89:GLU:HB2	3:B:201:GOL:H12	1.93	0.49
1:H:139:GLU:HG3	3:H:201:GOL:C1	2.43	0.48
1:C:105:LEU:HB3	1:C:112:PHE:HB3	1.94	0.48
1:F:73:ASN:HB3	4:F:304:HOH:O	2.13	0.48
1:N:154:HIS:HB2	4:N:364:HOH:O	2.14	0.48
1:P:106:ILE:HD11	3:P:201:GOL:H12	1.94	0.48
1:R:105:LEU:HG	1:R:114:ALA:HB2	1.95	0.48
1:L:83:TRP:CZ2	1:L:85:GLU:HB2	2.49	0.47
1:G:78:PRO:HD2	4:G:339:HOH:O	2.15	0.47
1:P:106:ILE:HD11	3:P:201:GOL:C1	2.45	0.47
1:O:122:GLU:HG2	1:O:154:HIS:CD2	2.50	0.47
1:F:105:LEU:HB3	1:F:112:PHE:HB3	1.97	0.46
1:B:141:VAL:HG23	1:N:141:VAL:HG23	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:83:TRP:CZ2	1:K:85:GLU:HB2	2.51	0.46
1:H:134:VAL:CG2	4:H:308:HOH:O	2.63	0.46
1:E:107:LYS:HD3	1:E:112:PHE:CZ	2.50	0.46
1:J:105:LEU:HB3	1:J:112:PHE:HB3	1.97	0.45
1:D:105:LEU:HG	1:D:114:ALA:HB2	1.97	0.45
1:B:83:TRP:CZ2	1:B:85:GLU:HB2	2.52	0.45
1:G:83:TRP:CZ2	1:G:85:GLU:HB2	2.52	0.45
1:H:146:LEU:HD13	1:H:148:THR:HG23	1.97	0.45
1:J:122:GLU:HG3	1:J:152:LEU:HD11	1.99	0.45
1:C:114:ALA:HB1	3:C:202:GOL:H12	1.97	0.45
1:D:148:THR:HG21	2:V:6:GLC:H3	1.99	0.45
1:B:105:LEU:HB3	1:B:112:PHE:HB3	1.99	0.44
1:M:120:GLU:CG	4:M:366:HOH:O	2.65	0.44
1:E:81:ILE:HG21	1:E:92:ILE:HD12	1.97	0.44
1:L:105:LEU:HG	1:L:114:ALA:HB2	1.99	0.44
1:M:105:LEU:HB3	1:M:112:PHE:HB3	2.00	0.44
1:L:134:VAL:HG22	4:L:379:HOH:O	2.17	0.44
1:A:107:LYS:HD2	1:A:109:HIS:O	2.17	0.44
1:E:107:LYS:CD	1:E:112:PHE:CZ	3.01	0.43
1:H:83:TRP:CZ2	1:H:85:GLU:HB2	2.53	0.43
1:A:83:TRP:CZ2	1:A:85:GLU:HB2	2.53	0.43
1:A:115:ILE:HD12	3:C:202:GOL:O2	2.18	0.43
1:H:154:HIS:CD2	4:H:307:HOH:O	2.72	0.43
1:M:154:HIS:HB3	4:M:381:HOH:O	2.18	0.43
1:B:142:VAL:CG1	1:B:152:LEU:HD22	2.44	0.42
1:M:122:GLU:CG	1:M:152:LEU:HD11	2.49	0.42
1:O:105:LEU:HB3	1:O:112:PHE:HB3	2.02	0.42
1:Q:105:LEU:HB3	1:Q:112:PHE:HB3	2.02	0.42
1:K:94:GLY:HA2	1:K:99:TRP:CH2	2.55	0.42
1:Q:120:GLU:OE1	4:Q:301:HOH:O	2.22	0.42
1:L:105:LEU:HB3	1:L:112:PHE:HB3	2.01	0.42
1:B:138:SER:OG	4:B:375:HOH:O	2.22	0.41
1:C:105:LEU:HG	1:C:114:ALA:HB2	2.03	0.41
1:A:113:VAL:HG23	1:C:115:ILE:HD11	2.02	0.41
1:P:128:PHE:CZ	1:P:131:GLY:HA2	2.56	0.41
1:N:105:LEU:HB3	1:N:112:PHE:HB3	2.01	0.41
1:K:105:LEU:HB3	1:K:112:PHE:HB3	2.03	0.41
1:A:105:LEU:HB3	1:A:112:PHE:HB3	2.03	0.41
4:D:396:HOH:O	1:N:88:LYS:HE3	2.21	0.41
1:K:105:LEU:HG	1:K:114:ALA:HB2	2.02	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:110:ASN:OD1	1:K:110:ASN:OD1[2_656]	1.85	0.35
4:O:322:HOH:O	4:O:322:HOH:O[2_655]	2.08	0.12
4:L:302:HOH:O	4:P:311:HOH:O[2_655]	2.15	0.05

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	80/90 (89%)	79 (99%)	1 (1%)	0	100	100
1	B	81/90 (90%)	78 (96%)	3 (4%)	0	100	100
1	C	82/90 (91%)	80 (98%)	2 (2%)	0	100	100
1	D	77/90 (86%)	76 (99%)	1 (1%)	0	100	100
1	E	84/90 (93%)	83 (99%)	1 (1%)	0	100	100
1	F	83/90 (92%)	81 (98%)	2 (2%)	0	100	100
1	G	82/90 (91%)	81 (99%)	1 (1%)	0	100	100
1	H	83/90 (92%)	81 (98%)	2 (2%)	0	100	100
1	I	83/90 (92%)	81 (98%)	2 (2%)	0	100	100
1	J	83/90 (92%)	82 (99%)	1 (1%)	0	100	100
1	K	80/90 (89%)	79 (99%)	1 (1%)	0	100	100
1	L	80/90 (89%)	79 (99%)	1 (1%)	0	100	100
1	M	83/90 (92%)	82 (99%)	1 (1%)	0	100	100
1	N	82/90 (91%)	81 (99%)	1 (1%)	0	100	100
1	O	82/90 (91%)	81 (99%)	1 (1%)	0	100	100
1	P	83/90 (92%)	81 (98%)	2 (2%)	0	100	100
1	Q	82/90 (91%)	81 (99%)	1 (1%)	0	100	100
1	R	82/90 (91%)	81 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1472/1620 (91%)	1447 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	71/80 (89%)	71 (100%)	0	100	100
1	B	75/80 (94%)	75 (100%)	0	100	100
1	C	73/80 (91%)	73 (100%)	0	100	100
1	D	70/80 (88%)	70 (100%)	0	100	100
1	E	77/80 (96%)	77 (100%)	0	100	100
1	F	77/80 (96%)	77 (100%)	0	100	100
1	G	74/80 (92%)	74 (100%)	0	100	100
1	H	75/80 (94%)	75 (100%)	0	100	100
1	I	72/80 (90%)	72 (100%)	0	100	100
1	J	74/80 (92%)	74 (100%)	0	100	100
1	K	69/80 (86%)	69 (100%)	0	100	100
1	L	72/80 (90%)	72 (100%)	0	100	100
1	M	76/80 (95%)	76 (100%)	0	100	100
1	N	75/80 (94%)	75 (100%)	0	100	100
1	O	76/80 (95%)	76 (100%)	0	100	100
1	P	76/80 (95%)	75 (99%)	1 (1%)	69	74
1	Q	73/80 (91%)	72 (99%)	1 (1%)	67	72
1	R	73/80 (91%)	73 (100%)	0	100	100
All	All	1328/1440 (92%)	1326 (100%)	2 (0%)	93	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	89	GLU
1	Q	122	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	110	ASN
1	C	110	ASN
1	F	145	GLN
1	N	75	GLN
1	Q	73	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

144 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	S	1	2	11,11,12	0.57	0	15,15,17	1.19	1 (6%)
2	GLC	S	2	2	11,11,12	0.72	0	15,15,17	1.74	6 (40%)
2	GLC	S	3	2	11,11,12	0.46	0	15,15,17	1.21	2 (13%)
2	GLC	S	4	2	11,11,12	0.57	0	15,15,17	1.43	3 (20%)
2	GLC	S	5	2	11,11,12	0.57	0	15,15,17	1.31	2 (13%)
2	GLC	S	6	2	11,11,12	0.62	0	15,15,17	1.70	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	S	7	2	11,11,12	0.54	0	15,15,17	1.02	0
2	GLC	S	8	2	11,11,12	0.65	0	15,15,17	1.36	3 (20%)
2	GLC	T	1	2	11,11,12	0.80	0	15,15,17	1.45	2 (13%)
2	GLC	T	2	2	11,11,12	0.43	0	15,15,17	1.44	4 (26%)
2	GLC	T	3	2	11,11,12	0.49	0	15,15,17	1.24	2 (13%)
2	GLC	T	4	2	11,11,12	0.54	0	15,15,17	1.52	4 (26%)
2	GLC	T	5	2	11,11,12	0.85	0	15,15,17	1.21	2 (13%)
2	GLC	T	6	2	11,11,12	0.57	0	15,15,17	1.44	2 (13%)
2	GLC	T	7	2	11,11,12	0.68	0	15,15,17	1.01	1 (6%)
2	GLC	T	8	2	11,11,12	0.48	0	15,15,17	1.34	1 (6%)
2	GLC	U	1	2	11,11,12	0.72	0	15,15,17	1.59	3 (20%)
2	GLC	U	2	2	11,11,12	0.59	0	15,15,17	0.97	0
2	GLC	U	3	2	11,11,12	0.40	0	15,15,17	1.47	3 (20%)
2	GLC	U	4	2	11,11,12	0.76	0	15,15,17	1.92	1 (6%)
2	GLC	U	5	2	11,11,12	0.84	1 (9%)	15,15,17	1.34	1 (6%)
2	GLC	U	6	2	11,11,12	0.95	1 (9%)	15,15,17	1.63	3 (20%)
2	GLC	U	7	2	11,11,12	0.75	0	15,15,17	0.87	0
2	GLC	U	8	2	11,11,12	0.52	0	15,15,17	0.86	0
2	GLC	V	1	2	11,11,12	0.57	0	15,15,17	1.27	2 (13%)
2	GLC	V	2	2	11,11,12	0.63	0	15,15,17	1.70	4 (26%)
2	GLC	V	3	2	11,11,12	0.48	0	15,15,17	1.01	1 (6%)
2	GLC	V	4	2	11,11,12	0.38	0	15,15,17	1.12	0
2	GLC	V	5	2	11,11,12	0.39	0	15,15,17	1.03	1 (6%)
2	GLC	V	6	2	11,11,12	0.48	0	15,15,17	1.97	6 (40%)
2	GLC	V	7	2	11,11,12	0.63	0	15,15,17	0.76	0
2	GLC	V	8	2	11,11,12	0.50	0	15,15,17	1.17	2 (13%)
2	GLC	W	1	2	11,11,12	1.05	0	15,15,17	1.38	3 (20%)
2	GLC	W	2	2	11,11,12	0.62	0	15,15,17	1.08	1 (6%)
2	GLC	W	3	2	11,11,12	0.71	0	15,15,17	1.08	1 (6%)
2	GLC	W	4	2	11,11,12	0.60	0	15,15,17	1.59	2 (13%)
2	GLC	W	5	2	11,11,12	0.59	0	15,15,17	1.32	2 (13%)
2	GLC	W	6	2	11,11,12	0.46	0	15,15,17	1.52	4 (26%)
2	GLC	W	7	2	11,11,12	0.79	0	15,15,17	1.38	3 (20%)
2	GLC	W	8	2	11,11,12	0.43	0	15,15,17	1.60	2 (13%)
2	GLC	X	1	2	11,11,12	0.51	0	15,15,17	0.91	1 (6%)
2	GLC	X	2	2	11,11,12	0.52	0	15,15,17	0.88	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	X	3	2	11,11,12	0.71	0	15,15,17	1.44	4 (26%)
2	GLC	X	4	2	11,11,12	0.85	0	15,15,17	1.46	2 (13%)
2	GLC	X	5	2	11,11,12	0.91	0	15,15,17	1.81	5 (33%)
2	GLC	X	6	2	11,11,12	0.68	0	15,15,17	2.20	5 (33%)
2	GLC	X	7	2	11,11,12	0.68	0	15,15,17	1.18	2 (13%)
2	GLC	X	8	2	11,11,12	0.51	0	15,15,17	1.31	2 (13%)
2	GLC	Y	1	2	11,11,12	0.37	0	15,15,17	1.06	1 (6%)
2	GLC	Y	2	2	11,11,12	0.36	0	15,15,17	0.93	0
2	GLC	Y	3	2	11,11,12	0.39	0	15,15,17	1.12	0
2	GLC	Y	4	2	11,11,12	0.26	0	15,15,17	1.36	3 (20%)
2	GLC	Y	5	2	11,11,12	0.46	0	15,15,17	1.01	0
2	GLC	Y	6	2	11,11,12	0.78	0	15,15,17	1.78	5 (33%)
2	GLC	Y	7	2	11,11,12	0.33	0	15,15,17	0.80	0
2	GLC	Y	8	2	11,11,12	0.38	0	15,15,17	0.91	1 (6%)
2	GLC	Z	1	2	11,11,12	0.58	0	15,15,17	1.32	3 (20%)
2	GLC	Z	2	2	11,11,12	0.39	0	15,15,17	1.47	2 (13%)
2	GLC	Z	3	2	11,11,12	0.55	0	15,15,17	1.81	5 (33%)
2	GLC	Z	4	2	11,11,12	0.53	0	15,15,17	1.64	3 (20%)
2	GLC	Z	5	2	11,11,12	0.41	0	15,15,17	0.72	0
2	GLC	Z	6	2	11,11,12	0.38	0	15,15,17	1.60	3 (20%)
2	GLC	Z	7	2	11,11,12	0.57	0	15,15,17	0.85	0
2	GLC	Z	8	2	11,11,12	0.55	0	15,15,17	1.01	1 (6%)
2	GLC	a	1	2	11,11,12	0.47	0	15,15,17	1.32	2 (13%)
2	GLC	a	2	2	11,11,12	0.51	0	15,15,17	0.98	0
2	GLC	a	3	2	11,11,12	0.49	0	15,15,17	1.49	3 (20%)
2	GLC	a	4	2	11,11,12	0.58	0	15,15,17	1.35	1 (6%)
2	GLC	a	5	2	11,11,12	0.40	0	15,15,17	1.01	0
2	GLC	a	6	2	11,11,12	0.37	0	15,15,17	1.42	2 (13%)
2	GLC	a	7	2	11,11,12	0.78	0	15,15,17	1.70	5 (33%)
2	GLC	a	8	2	11,11,12	0.36	0	15,15,17	1.16	1 (6%)
2	GLC	b	1	2	11,11,12	0.41	0	15,15,17	1.28	2 (13%)
2	GLC	b	2	2	11,11,12	0.53	0	15,15,17	1.24	2 (13%)
2	GLC	b	3	2	11,11,12	0.44	0	15,15,17	1.01	1 (6%)
2	GLC	b	4	2	11,11,12	0.42	0	15,15,17	1.79	1 (6%)
2	GLC	b	5	2	11,11,12	0.47	0	15,15,17	0.98	1 (6%)
2	GLC	b	6	2	11,11,12	0.75	0	15,15,17	1.62	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	b	7	2	11,11,12	0.73	0	15,15,17	1.11	1 (6%)
2	GLC	b	8	2	11,11,12	0.53	0	15,15,17	0.90	0
2	GLC	c	1	2	11,11,12	0.52	0	15,15,17	0.88	0
2	GLC	c	2	2	11,11,12	0.42	0	15,15,17	1.05	1 (6%)
2	GLC	c	3	2	11,11,12	0.35	0	15,15,17	1.19	1 (6%)
2	GLC	c	4	2	11,11,12	0.44	0	15,15,17	1.81	3 (20%)
2	GLC	c	5	2	11,11,12	0.46	0	15,15,17	1.36	4 (26%)
2	GLC	c	6	2	11,11,12	0.47	0	15,15,17	1.63	3 (20%)
2	GLC	c	7	2	11,11,12	0.57	0	15,15,17	1.12	1 (6%)
2	GLC	c	8	2	11,11,12	0.51	0	15,15,17	0.83	0
2	GLC	d	1	2	11,11,12	0.59	0	15,15,17	1.06	1 (6%)
2	GLC	d	2	2	11,11,12	0.59	0	15,15,17	0.91	1 (6%)
2	GLC	d	3	2	11,11,12	0.60	0	15,15,17	1.26	1 (6%)
2	GLC	d	4	2	11,11,12	0.38	0	15,15,17	1.87	4 (26%)
2	GLC	d	5	2	11,11,12	0.72	0	15,15,17	1.03	0
2	GLC	d	6	2	11,11,12	0.70	0	15,15,17	2.00	5 (33%)
2	GLC	d	7	2	11,11,12	0.50	0	15,15,17	1.80	5 (33%)
2	GLC	d	8	2	11,11,12	0.69	0	15,15,17	1.05	2 (13%)
2	GLC	e	1	2	11,11,12	0.52	0	15,15,17	1.29	2 (13%)
2	GLC	e	2	2	11,11,12	0.34	0	15,15,17	1.34	1 (6%)
2	GLC	e	3	2	11,11,12	0.49	0	15,15,17	1.62	3 (20%)
2	GLC	e	4	2	11,11,12	0.50	0	15,15,17	1.50	2 (13%)
2	GLC	e	5	2	11,11,12	0.57	0	15,15,17	1.53	3 (20%)
2	GLC	e	6	2	11,11,12	0.61	0	15,15,17	1.63	3 (20%)
2	GLC	e	7	2	11,11,12	0.46	0	15,15,17	0.77	0
2	GLC	e	8	2	11,11,12	0.48	0	15,15,17	0.97	1 (6%)
2	GLC	f	1	2	11,11,12	0.87	1 (9%)	15,15,17	2.11	5 (33%)
2	GLC	f	2	2	11,11,12	0.71	0	15,15,17	1.62	3 (20%)
2	GLC	f	3	2	11,11,12	0.49	0	15,15,17	1.99	5 (33%)
2	GLC	f	4	2	11,11,12	0.88	1 (9%)	15,15,17	2.41	5 (33%)
2	GLC	f	5	2	11,11,12	0.60	0	15,15,17	1.51	1 (6%)
2	GLC	f	6	2	11,11,12	0.61	0	15,15,17	1.73	3 (20%)
2	GLC	f	7	2	11,11,12	0.59	0	15,15,17	1.32	3 (20%)
2	GLC	f	8	2	11,11,12	0.51	0	15,15,17	1.20	2 (13%)
2	GLC	g	1	2	11,11,12	0.55	0	15,15,17	0.92	0
2	GLC	g	2	2	11,11,12	0.49	0	15,15,17	1.39	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	g	3	2	11,11,12	0.54	0	15,15,17	1.03	1 (6%)
2	GLC	g	4	2	11,11,12	0.28	0	15,15,17	1.86	1 (6%)
2	GLC	g	5	2	11,11,12	0.58	0	15,15,17	1.28	2 (13%)
2	GLC	g	6	2	11,11,12	0.53	0	15,15,17	1.58	3 (20%)
2	GLC	g	7	2	11,11,12	0.43	0	15,15,17	1.06	0
2	GLC	g	8	2	11,11,12	0.68	0	15,15,17	1.06	1 (6%)
2	GLC	h	1	2	11,11,12	0.35	0	15,15,17	1.34	2 (13%)
2	GLC	h	2	2	11,11,12	0.23	0	15,15,17	0.74	0
2	GLC	h	3	2	11,11,12	0.24	0	15,15,17	0.79	0
2	GLC	h	4	2	11,11,12	0.26	0	15,15,17	1.73	3 (20%)
2	GLC	h	5	2	11,11,12	0.50	0	15,15,17	0.94	0
2	GLC	h	6	2	11,11,12	0.48	0	15,15,17	1.58	5 (33%)
2	GLC	h	7	2	11,11,12	0.54	0	15,15,17	1.22	1 (6%)
2	GLC	h	8	2	11,11,12	0.44	0	15,15,17	1.44	2 (13%)
2	GLC	i	1	2	11,11,12	0.57	0	15,15,17	1.31	1 (6%)
2	GLC	i	2	2	11,11,12	0.30	0	15,15,17	1.18	2 (13%)
2	GLC	i	3	2	11,11,12	0.43	0	15,15,17	1.44	3 (20%)
2	GLC	i	4	2	11,11,12	0.24	0	15,15,17	1.24	3 (20%)
2	GLC	i	5	2	11,11,12	0.46	0	15,15,17	0.89	0
2	GLC	i	6	2	11,11,12	0.64	0	15,15,17	1.49	4 (26%)
2	GLC	i	7	2	11,11,12	0.87	0	15,15,17	1.29	1 (6%)
2	GLC	i	8	2	11,11,12	0.46	0	15,15,17	1.20	1 (6%)
2	GLC	j	1	2	11,11,12	0.71	0	15,15,17	0.90	0
2	GLC	j	2	2	11,11,12	0.56	0	15,15,17	1.46	2 (13%)
2	GLC	j	3	2	11,11,12	0.37	0	15,15,17	1.60	4 (26%)
2	GLC	j	4	2	11,11,12	0.55	0	15,15,17	0.88	0
2	GLC	j	5	2	11,11,12	0.46	0	15,15,17	1.43	2 (13%)
2	GLC	j	6	2	11,11,12	0.41	0	15,15,17	2.22	6 (40%)
2	GLC	j	7	2	11,11,12	0.67	0	15,15,17	1.22	2 (13%)
2	GLC	j	8	2	11,11,12	0.41	0	15,15,17	1.74	3 (20%)

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	S	1	2	-	0/2/19/22	0/1/1/1
2	GLC	S	2	2	-	2/2/19/22	0/1/1/1
2	GLC	S	3	2	-	2/2/19/22	0/1/1/1
2	GLC	S	4	2	-	0/2/19/22	0/1/1/1
2	GLC	S	5	2	-	0/2/19/22	0/1/1/1
2	GLC	S	6	2	-	1/2/19/22	0/1/1/1
2	GLC	S	7	2	-	0/2/19/22	0/1/1/1
2	GLC	S	8	2	-	0/2/19/22	0/1/1/1
2	GLC	T	1	2	-	2/2/19/22	0/1/1/1
2	GLC	T	2	2	-	2/2/19/22	0/1/1/1
2	GLC	T	3	2	-	0/2/19/22	0/1/1/1
2	GLC	T	4	2	-	0/2/19/22	0/1/1/1
2	GLC	T	5	2	-	0/2/19/22	0/1/1/1
2	GLC	T	6	2	-	0/2/19/22	0/1/1/1
2	GLC	T	7	2	-	0/2/19/22	0/1/1/1
2	GLC	T	8	2	-	0/2/19/22	0/1/1/1
2	GLC	U	1	2	-	1/2/19/22	0/1/1/1
2	GLC	U	2	2	-	2/2/19/22	0/1/1/1
2	GLC	U	3	2	-	2/2/19/22	0/1/1/1
2	GLC	U	4	2	-	2/2/19/22	0/1/1/1
2	GLC	U	5	2	-	0/2/19/22	0/1/1/1
2	GLC	U	6	2	-	1/2/19/22	0/1/1/1
2	GLC	U	7	2	-	0/2/19/22	0/1/1/1
2	GLC	U	8	2	-	0/2/19/22	0/1/1/1
2	GLC	V	1	2	-	0/2/19/22	0/1/1/1
2	GLC	V	2	2	-	1/2/19/22	0/1/1/1
2	GLC	V	3	2	-	0/2/19/22	0/1/1/1
2	GLC	V	4	2	-	0/2/19/22	0/1/1/1
2	GLC	V	5	2	-	0/2/19/22	0/1/1/1
2	GLC	V	6	2	-	1/2/19/22	0/1/1/1
2	GLC	V	7	2	-	0/2/19/22	0/1/1/1
2	GLC	V	8	2	-	0/2/19/22	0/1/1/1
2	GLC	W	1	2	-	0/2/19/22	0/1/1/1
2	GLC	W	2	2	-	0/2/19/22	0/1/1/1
2	GLC	W	3	2	-	1/2/19/22	0/1/1/1
2	GLC	W	4	2	-	0/2/19/22	0/1/1/1
2	GLC	W	5	2	-	0/2/19/22	0/1/1/1
2	GLC	W	6	2	-	0/2/19/22	0/1/1/1
2	GLC	W	7	2	-	0/2/19/22	0/1/1/1
2	GLC	W	8	2	-	1/2/19/22	0/1/1/1
2	GLC	X	1	2	-	0/2/19/22	0/1/1/1
2	GLC	X	2	2	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	X	3	2	-	0/2/19/22	0/1/1/1
2	GLC	X	4	2	-	2/2/19/22	0/1/1/1
2	GLC	X	5	2	-	0/2/19/22	0/1/1/1
2	GLC	X	6	2	-	0/2/19/22	0/1/1/1
2	GLC	X	7	2	-	0/2/19/22	0/1/1/1
2	GLC	X	8	2	-	0/2/19/22	0/1/1/1
2	GLC	Y	1	2	-	0/2/19/22	0/1/1/1
2	GLC	Y	2	2	-	2/2/19/22	0/1/1/1
2	GLC	Y	3	2	-	0/2/19/22	0/1/1/1
2	GLC	Y	4	2	-	0/2/19/22	0/1/1/1
2	GLC	Y	5	2	-	0/2/19/22	0/1/1/1
2	GLC	Y	6	2	-	1/2/19/22	0/1/1/1
2	GLC	Y	7	2	-	0/2/19/22	0/1/1/1
2	GLC	Y	8	2	-	0/2/19/22	0/1/1/1
2	GLC	Z	1	2	-	2/2/19/22	0/1/1/1
2	GLC	Z	2	2	-	2/2/19/22	0/1/1/1
2	GLC	Z	3	2	-	2/2/19/22	0/1/1/1
2	GLC	Z	4	2	-	0/2/19/22	0/1/1/1
2	GLC	Z	5	2	-	0/2/19/22	0/1/1/1
2	GLC	Z	6	2	-	1/2/19/22	0/1/1/1
2	GLC	Z	7	2	-	0/2/19/22	0/1/1/1
2	GLC	Z	8	2	-	0/2/19/22	0/1/1/1
2	GLC	a	1	2	-	2/2/19/22	0/1/1/1
2	GLC	a	2	2	-	2/2/19/22	0/1/1/1
2	GLC	a	3	2	-	1/2/19/22	0/1/1/1
2	GLC	a	4	2	-	2/2/19/22	0/1/1/1
2	GLC	a	5	2	-	0/2/19/22	0/1/1/1
2	GLC	a	6	2	-	2/2/19/22	0/1/1/1
2	GLC	a	7	2	-	0/2/19/22	0/1/1/1
2	GLC	a	8	2	-	0/2/19/22	0/1/1/1
2	GLC	b	1	2	-	0/2/19/22	0/1/1/1
2	GLC	b	2	2	-	0/2/19/22	0/1/1/1
2	GLC	b	3	2	-	0/2/19/22	0/1/1/1
2	GLC	b	4	2	-	2/2/19/22	0/1/1/1
2	GLC	b	5	2	-	0/2/19/22	0/1/1/1
2	GLC	b	6	2	-	1/2/19/22	0/1/1/1
2	GLC	b	7	2	-	0/2/19/22	0/1/1/1
2	GLC	b	8	2	-	0/2/19/22	0/1/1/1
2	GLC	c	1	2	-	0/2/19/22	0/1/1/1
2	GLC	c	2	2	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	c	3	2	-	1/2/19/22	0/1/1/1
2	GLC	c	4	2	-	2/2/19/22	0/1/1/1
2	GLC	c	5	2	-	0/2/19/22	0/1/1/1
2	GLC	c	6	2	-	2/2/19/22	0/1/1/1
2	GLC	c	7	2	-	0/2/19/22	0/1/1/1
2	GLC	c	8	2	-	0/2/19/22	0/1/1/1
2	GLC	d	1	2	-	2/2/19/22	0/1/1/1
2	GLC	d	2	2	-	1/2/19/22	0/1/1/1
2	GLC	d	3	2	-	1/2/19/22	0/1/1/1
2	GLC	d	4	2	-	2/2/19/22	0/1/1/1
2	GLC	d	5	2	-	0/2/19/22	0/1/1/1
2	GLC	d	6	2	-	2/2/19/22	0/1/1/1
2	GLC	d	7	2	-	0/2/19/22	0/1/1/1
2	GLC	d	8	2	-	0/2/19/22	0/1/1/1
2	GLC	e	1	2	-	0/2/19/22	0/1/1/1
2	GLC	e	2	2	-	0/2/19/22	0/1/1/1
2	GLC	e	3	2	-	0/2/19/22	0/1/1/1
2	GLC	e	4	2	-	2/2/19/22	0/1/1/1
2	GLC	e	5	2	-	1/2/19/22	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	e	8	2	-	0/2/19/22	0/1/1/1
2	GLC	f	1	2	-	2/2/19/22	0/1/1/1
2	GLC	f	2	2	-	2/2/19/22	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	-	2/2/19/22	0/1/1/1
2	GLC	f	6	2	-	0/2/19/22	0/1/1/1
2	GLC	f	7	2	-	0/2/19/22	0/1/1/1
2	GLC	f	8	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	-	2/2/19/22	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	-	1/2/19/22	0/1/1/1
2	GLC	g	7	2	-	0/2/19/22	0/1/1/1
2	GLC	g	8	2	-	0/2/19/22	0/1/1/1
2	GLC	h	1	2	-	2/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	1/2/19/22	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	-	0/2/19/22	0/1/1/1
2	GLC	h	8	2	-	0/2/19/22	0/1/1/1
2	GLC	i	1	2	-	2/2/19/22	0/1/1/1
2	GLC	i	2	2	-	1/2/19/22	0/1/1/1
2	GLC	i	3	2	-	0/2/19/22	0/1/1/1
2	GLC	i	4	2	-	0/2/19/22	0/1/1/1
2	GLC	i	5	2	-	0/2/19/22	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	i	8	2	-	0/2/19/22	0/1/1/1
2	GLC	j	1	2	-	1/2/19/22	0/1/1/1
2	GLC	j	2	2	-	0/2/19/22	0/1/1/1
2	GLC	j	3	2	-	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	-	1/2/19/22	0/1/1/1
2	GLC	j	6	2	-	2/2/19/22	0/1/1/1
2	GLC	j	7	2	-	0/2/19/22	0/1/1/1
2	GLC	j	8	2	-	2/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	6	GLC	O5-C1	-2.65	1.39	1.43
2	f	1	GLC	C2-C3	2.29	1.55	1.52
2	f	4	GLC	C2-C3	2.28	1.55	1.52
2	U	5	GLC	O5-C1	-2.00	1.40	1.43

All (291) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	f	4	GLC	C1-C2-C3	6.88	118.12	109.67
2	U	4	GLC	C1-O5-C5	6.27	120.69	112.19
2	g	4	GLC	C1-O5-C5	6.08	120.43	112.19
2	f	1	GLC	C1-C2-C3	6.06	117.11	109.67
2	b	4	GLC	C1-O5-C5	5.84	120.11	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	j	8	GLC	C1-O5-C5	5.27	119.33	112.19
2	c	4	GLC	C1-O5-C5	5.21	119.25	112.19
2	X	6	GLC	C1-O5-C5	4.95	118.89	112.19
2	h	4	GLC	C1-O5-C5	4.77	118.66	112.19
2	j	6	GLC	O5-C1-C2	-4.74	103.46	110.77
2	d	4	GLC	C1-O5-C5	4.64	118.47	112.19
2	f	5	GLC	O5-C1-C2	-4.59	103.69	110.77
2	d	6	GLC	O4-C4-C3	-4.49	99.96	110.35
2	c	6	GLC	C1-O5-C5	4.48	118.27	112.19
2	f	2	GLC	O5-C1-C2	-4.40	103.97	110.77
2	V	6	GLC	O5-C5-C6	4.26	113.88	107.20
2	a	4	GLC	C1-O5-C5	4.20	117.88	112.19
2	W	8	GLC	O5-C5-C6	4.16	113.72	107.20
2	e	4	GLC	C1-O5-C5	4.14	117.80	112.19
2	U	6	GLC	O5-C5-C6	4.04	113.53	107.20
2	j	2	GLC	C1-C2-C3	4.00	114.58	109.67
2	X	4	GLC	C1-O5-C5	3.95	117.55	112.19
2	Y	6	GLC	O5-C5-C6	3.83	113.21	107.20
2	f	6	GLC	C6-C5-C4	3.80	121.91	113.00
2	Z	3	GLC	O3-C3-C2	3.75	117.17	109.99
2	h	8	GLC	C1-O5-C5	3.74	117.25	112.19
2	Z	2	GLC	O5-C1-C2	-3.57	105.26	110.77
2	e	5	GLC	C1-O5-C5	3.54	116.99	112.19
2	Z	6	GLC	O5-C5-C6	3.53	112.74	107.20
2	X	6	GLC	O5-C5-C6	3.52	112.72	107.20
2	f	6	GLC	O2-C2-C3	3.49	117.14	110.14
2	S	6	GLC	C3-C4-C5	3.49	116.46	110.24
2	T	6	GLC	O5-C5-C6	3.49	112.67	107.20
2	f	3	GLC	C1-C2-C3	3.45	113.91	109.67
2	e	2	GLC	C1-O5-C5	3.42	116.82	112.19
2	W	4	GLC	C1-O5-C5	3.39	116.79	112.19
2	X	5	GLC	O6-C6-C5	-3.39	99.65	111.29
2	V	2	GLC	C1-O5-C5	3.35	116.73	112.19
2	Z	4	GLC	C2-C3-C4	-3.33	105.14	110.89
2	Z	4	GLC	O5-C5-C6	3.31	112.39	107.20
2	T	8	GLC	C1-O5-C5	3.30	116.67	112.19
2	j	6	GLC	C1-O5-C5	3.29	116.66	112.19
2	f	6	GLC	O6-C6-C5	-3.28	100.03	111.29
2	g	6	GLC	C3-C4-C5	3.27	116.08	110.24
2	j	6	GLC	O5-C5-C6	3.25	112.30	107.20
2	S	6	GLC	C1-O5-C5	3.24	116.58	112.19
2	d	6	GLC	C3-C4-C5	3.23	116.00	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	5	GLC	C1-O5-C5	3.21	116.54	112.19
2	d	7	GLC	O2-C2-C3	3.20	116.55	110.14
2	S	4	GLC	C1-O5-C5	3.18	116.50	112.19
2	d	3	GLC	O5-C1-C2	-3.16	105.89	110.77
2	a	8	GLC	C1-O5-C5	3.16	116.48	112.19
2	T	4	GLC	C1-O5-C5	3.15	116.46	112.19
2	Z	2	GLC	C1-O5-C5	3.14	116.44	112.19
2	U	3	GLC	O5-C5-C6	3.13	112.11	107.20
2	f	3	GLC	C1-O5-C5	3.12	116.42	112.19
2	e	6	GLC	O5-C5-C6	3.11	112.09	107.20
2	h	4	GLC	O4-C4-C3	-3.11	103.15	110.35
2	T	1	GLC	C1-O5-C5	3.11	116.41	112.19
2	S	1	GLC	C1-O5-C5	3.10	116.40	112.19
2	W	8	GLC	C1-O5-C5	3.10	116.39	112.19
2	j	3	GLC	O5-C1-C2	-3.09	105.99	110.77
2	d	6	GLC	C6-C5-C4	3.09	120.24	113.00
2	f	4	GLC	C1-O5-C5	3.08	116.37	112.19
2	Z	6	GLC	C3-C4-C5	3.08	115.73	110.24
2	U	5	GLC	O2-C2-C3	-3.07	103.98	110.14
2	W	7	GLC	C3-C4-C5	3.07	115.72	110.24
2	e	3	GLC	O4-C4-C3	-3.07	103.25	110.35
2	U	3	GLC	C1-O5-C5	3.06	116.34	112.19
2	a	3	GLC	O4-C4-C3	-3.05	103.29	110.35
2	j	5	GLC	O3-C3-C4	-3.04	103.33	110.35
2	e	1	GLC	C1-O5-C5	3.03	116.30	112.19
2	e	6	GLC	O4-C4-C3	-3.03	103.35	110.35
2	U	1	GLC	O2-C2-C3	-3.01	104.10	110.14
2	W	4	GLC	O5-C1-C2	3.01	115.42	110.77
2	b	1	GLC	C1-O5-C5	2.99	116.25	112.19
2	h	6	GLC	C3-C4-C5	2.99	115.58	110.24
2	a	7	GLC	O3-C3-C2	2.99	115.72	109.99
2	i	2	GLC	O5-C1-C2	-2.99	106.15	110.77
2	T	3	GLC	C1-O5-C5	2.97	116.22	112.19
2	j	3	GLC	C1-C2-C3	2.96	113.30	109.67
2	g	2	GLC	O2-C2-C3	-2.94	104.24	110.14
2	i	1	GLC	C1-O5-C5	2.93	116.17	112.19
2	i	3	GLC	C1-O5-C5	2.92	116.15	112.19
2	g	2	GLC	O4-C4-C3	-2.91	103.62	110.35
2	T	2	GLC	O5-C5-C6	2.90	111.75	107.20
2	V	1	GLC	O6-C6-C5	-2.90	101.34	111.29
2	V	2	GLC	O4-C4-C3	-2.88	103.68	110.35
2	Z	3	GLC	O4-C4-C3	-2.88	103.68	110.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	6	GLC	C1-O5-C5	2.88	116.09	112.19
2	V	6	GLC	O3-C3-C2	2.84	115.44	109.99
2	g	6	GLC	C1-O5-C5	2.84	116.04	112.19
2	b	6	GLC	C3-C4-C5	2.82	115.27	110.24
2	e	6	GLC	C3-C4-C5	2.81	115.25	110.24
2	X	5	GLC	C2-C3-C4	2.81	115.76	110.89
2	f	4	GLC	O2-C2-C1	-2.81	103.41	109.15
2	b	6	GLC	C1-O5-C5	2.81	115.99	112.19
2	f	4	GLC	C2-C3-C4	2.80	115.74	110.89
2	e	3	GLC	C1-O5-C5	2.79	115.97	112.19
2	X	6	GLC	O3-C3-C4	-2.79	103.91	110.35
2	S	6	GLC	O5-C5-C6	2.78	111.56	107.20
2	i	7	GLC	O3-C3-C2	2.78	115.31	109.99
2	b	2	GLC	C1-O5-C5	2.76	115.93	112.19
2	i	8	GLC	O2-C2-C3	-2.76	104.62	110.14
2	f	2	GLC	C1-O5-C5	2.75	115.92	112.19
2	U	1	GLC	O6-C6-C5	-2.73	101.92	111.29
2	i	6	GLC	O4-C4-C3	-2.73	104.04	110.35
2	d	7	GLC	O3-C3-C4	-2.71	104.08	110.35
2	T	2	GLC	O2-C2-C3	-2.70	104.72	110.14
2	T	5	GLC	O6-C6-C5	-2.70	102.02	111.29
2	S	2	GLC	O5-C1-C2	-2.68	106.64	110.77
2	W	5	GLC	O5-C1-C2	-2.68	106.64	110.77
2	S	3	GLC	O5-C1-C2	-2.68	106.64	110.77
2	W	6	GLC	O5-C5-C6	2.67	111.38	107.20
2	d	4	GLC	C3-C4-C5	2.67	114.99	110.24
2	S	8	GLC	O5-C5-C6	2.66	111.38	107.20
2	f	1	GLC	C3-C4-C5	-2.66	105.49	110.24
2	W	6	GLC	C3-C4-C5	2.65	114.97	110.24
2	X	8	GLC	C1-O5-C5	2.65	115.79	112.19
2	j	5	GLC	C1-O5-C5	2.65	115.78	112.19
2	i	3	GLC	O2-C2-C3	-2.64	104.85	110.14
2	g	2	GLC	C1-O5-C5	2.64	115.77	112.19
2	S	8	GLC	C1-C2-C3	2.62	112.89	109.67
2	X	5	GLC	O4-C4-C3	-2.62	104.30	110.35
2	i	6	GLC	C6-C5-C4	2.62	119.14	113.00
2	i	4	GLC	C1-O5-C5	2.61	115.73	112.19
2	U	6	GLC	C3-C4-C5	2.60	114.88	110.24
2	Z	8	GLC	O3-C3-C2	-2.60	105.02	109.99
2	S	3	GLC	C1-O5-C5	2.60	115.71	112.19
2	U	3	GLC	O5-C1-C2	-2.60	106.76	110.77
2	Z	4	GLC	O5-C5-C4	-2.57	104.57	110.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	f	3	GLC	C6-C5-C4	-2.57	106.98	113.00
2	T	4	GLC	O4-C4-C3	-2.57	104.41	110.35
2	c	3	GLC	O4-C4-C3	-2.57	104.42	110.35
2	V	6	GLC	C3-C4-C5	2.56	114.81	110.24
2	X	6	GLC	O3-C3-C2	2.55	114.88	109.99
2	j	6	GLC	C1-C2-C3	-2.54	106.54	109.67
2	f	8	GLC	O4-C4-C3	-2.54	104.48	110.35
2	X	3	GLC	O2-C2-C1	-2.53	103.98	109.15
2	X	5	GLC	O5-C5-C4	-2.52	104.69	110.83
2	c	4	GLC	C1-C2-C3	2.51	112.76	109.67
2	T	2	GLC	O2-C2-C1	2.51	114.28	109.15
2	f	3	GLC	O3-C3-C2	2.50	114.79	109.99
2	b	1	GLC	O5-C1-C2	-2.50	106.92	110.77
2	S	2	GLC	O2-C2-C3	-2.49	105.14	110.14
2	j	3	GLC	O2-C2-C3	-2.49	105.15	110.14
2	a	3	GLC	O5-C1-C2	-2.49	106.92	110.77
2	T	4	GLC	O2-C2-C3	-2.48	105.18	110.14
2	X	7	GLC	C1-O5-C5	2.48	115.55	112.19
2	i	6	GLC	C1-O5-C5	2.47	115.54	112.19
2	c	5	GLC	C1-C2-C3	2.47	112.71	109.67
2	T	6	GLC	C3-C4-C5	2.47	114.65	110.24
2	e	5	GLC	O5-C1-C2	-2.47	106.97	110.77
2	f	7	GLC	O2-C2-C3	2.46	115.08	110.14
2	S	2	GLC	O4-C4-C3	-2.46	104.65	110.35
2	T	1	GLC	O5-C1-C2	-2.46	106.98	110.77
2	T	7	GLC	O2-C2-C3	2.44	115.03	110.14
2	g	6	GLC	C6-C5-C4	2.43	118.70	113.00
2	U	6	GLC	C1-O5-C5	2.42	115.47	112.19
2	d	7	GLC	O5-C5-C6	2.42	111.00	107.20
2	h	1	GLC	C1-O5-C5	2.41	115.46	112.19
2	V	2	GLC	O2-C2-C3	-2.41	105.31	110.14
2	V	1	GLC	O5-C5-C6	-2.41	103.43	107.20
2	f	4	GLC	O3-C3-C4	-2.40	104.79	110.35
2	S	2	GLC	O3-C3-C2	2.39	114.58	109.99
2	Y	1	GLC	C1-O5-C5	2.39	115.43	112.19
2	S	2	GLC	C3-C4-C5	-2.38	106.00	110.24
2	g	5	GLC	C1-O5-C5	2.38	115.41	112.19
2	b	6	GLC	C6-C5-C4	2.38	118.57	113.00
2	Y	6	GLC	O2-C2-C1	-2.37	104.29	109.15
2	d	6	GLC	O3-C3-C2	2.36	114.52	109.99
2	a	6	GLC	C6-C5-C4	2.36	118.53	113.00
2	i	4	GLC	O4-C4-C3	-2.36	104.90	110.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	e	1	GLC	O6-C6-C5	-2.36	103.21	111.29
2	S	5	GLC	O6-C6-C5	-2.35	103.23	111.29
2	X	3	GLC	O3-C3-C4	-2.35	104.92	110.35
2	X	1	GLC	O6-C6-C5	-2.35	103.24	111.29
2	Z	3	GLC	C1-O5-C5	2.34	115.37	112.19
2	a	3	GLC	O3-C3-C4	-2.34	104.94	110.35
2	c	6	GLC	C3-C4-C5	2.34	114.41	110.24
2	j	6	GLC	O2-C2-C1	2.34	113.93	109.15
2	Z	3	GLC	C1-C2-C3	2.33	112.53	109.67
2	f	7	GLC	C1-O5-C5	2.32	115.33	112.19
2	c	2	GLC	C1-O5-C5	2.31	115.33	112.19
2	c	7	GLC	O2-C2-C3	2.30	114.75	110.14
2	g	8	GLC	O4-C4-C3	-2.30	105.04	110.35
2	i	6	GLC	C3-C4-C5	2.29	114.33	110.24
2	V	6	GLC	O4-C4-C3	-2.29	105.06	110.35
2	W	6	GLC	C1-O5-C5	2.29	115.29	112.19
2	a	7	GLC	O2-C2-C3	2.28	114.71	110.14
2	f	8	GLC	O5-C5-C6	2.28	110.78	107.20
2	S	2	GLC	O5-C5-C6	2.28	110.78	107.20
2	j	7	GLC	O5-C5-C6	2.27	110.77	107.20
2	d	7	GLC	O3-C3-C2	2.27	114.34	109.99
2	Y	6	GLC	C6-C5-C4	2.26	118.31	113.00
2	h	6	GLC	C6-C5-C4	2.26	118.30	113.00
2	X	8	GLC	O3-C3-C2	-2.26	105.66	109.99
2	d	8	GLC	O2-C2-C1	2.26	113.78	109.15
2	e	4	GLC	O5-C5-C6	-2.26	103.67	107.20
2	b	7	GLC	C1-C2-C3	-2.26	106.89	109.67
2	X	3	GLC	O3-C3-C2	2.26	114.31	109.99
2	a	1	GLC	O3-C3-C4	-2.25	105.14	110.35
2	W	7	GLC	O3-C3-C2	2.25	114.30	109.99
2	Z	1	GLC	O3-C3-C4	-2.25	105.15	110.35
2	S	6	GLC	O5-C1-C2	2.25	114.24	110.77
2	Y	4	GLC	C1-C2-C3	2.25	112.43	109.67
2	W	1	GLC	C6-C5-C4	2.25	118.26	113.00
2	Y	6	GLC	O5-C1-C2	-2.24	107.31	110.77
2	j	7	GLC	O2-C2-C1	2.24	113.73	109.15
2	j	6	GLC	C6-C5-C4	2.24	118.25	113.00
2	U	1	GLC	C1-O5-C5	2.23	115.21	112.19
2	f	3	GLC	O5-C5-C4	2.23	116.24	110.83
2	Y	4	GLC	C1-O5-C5	2.23	115.21	112.19
2	c	5	GLC	O2-C2-C3	-2.22	105.68	110.14
2	Z	1	GLC	C1-C2-C3	2.22	112.40	109.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	6	GLC	C1-O5-C5	2.22	115.20	112.19
2	e	5	GLC	O3-C3-C4	-2.22	105.22	110.35
2	T	4	GLC	O4-C4-C5	2.22	114.80	109.30
2	W	2	GLC	C1-O5-C5	2.21	115.19	112.19
2	g	3	GLC	O5-C1-C2	-2.21	107.36	110.77
2	d	8	GLC	O3-C3-C2	-2.21	105.76	109.99
2	W	1	GLC	O2-C2-C1	-2.21	104.63	109.15
2	c	6	GLC	O5-C5-C6	2.21	110.67	107.20
2	c	5	GLC	C3-C4-C5	-2.21	106.30	110.24
2	Z	3	GLC	O5-C1-C2	-2.20	107.37	110.77
2	W	7	GLC	C2-C3-C4	-2.20	107.09	110.89
2	X	6	GLC	C6-C5-C4	2.20	118.16	113.00
2	c	4	GLC	O4-C4-C3	-2.20	105.27	110.35
2	j	3	GLC	O5-C5-C6	2.20	110.65	107.20
2	f	1	GLC	O2-C2-C1	-2.20	104.66	109.15
2	X	5	GLC	C3-C4-C5	-2.18	106.36	110.24
2	X	2	GLC	O4-C4-C3	-2.18	105.32	110.35
2	h	7	GLC	O5-C5-C6	2.17	110.61	107.20
2	W	3	GLC	O4-C4-C3	-2.17	105.33	110.35
2	T	2	GLC	O4-C4-C3	-2.16	105.35	110.35
2	a	1	GLC	C1-O5-C5	2.16	115.11	112.19
2	T	5	GLC	O4-C4-C3	-2.15	105.37	110.35
2	W	1	GLC	C3-C4-C5	-2.15	106.40	110.24
2	g	5	GLC	O4-C4-C3	-2.15	105.38	110.35
2	d	7	GLC	O5-C1-C2	2.15	114.09	110.77
2	j	8	GLC	C2-C3-C4	-2.15	107.18	110.89
2	Y	4	GLC	O4-C4-C3	-2.14	105.39	110.35
2	S	4	GLC	O4-C4-C3	-2.14	105.39	110.35
2	V	3	GLC	O5-C5-C6	2.13	110.55	107.20
2	f	1	GLC	O5-C5-C6	2.13	110.55	107.20
2	h	6	GLC	O6-C6-C5	-2.13	103.98	111.29
2	V	2	GLC	O5-C5-C6	-2.13	103.87	107.20
2	j	8	GLC	C6-C5-C4	-2.13	108.02	113.00
2	h	4	GLC	C1-C2-C3	2.13	112.28	109.67
2	f	7	GLC	O4-C4-C3	-2.12	105.44	110.35
2	h	6	GLC	C1-O5-C5	2.12	115.07	112.19
2	a	7	GLC	O5-C5-C4	-2.12	105.66	110.83
2	Y	8	GLC	O5-C5-C6	2.12	110.53	107.20
2	Z	1	GLC	C2-C3-C4	2.12	114.56	110.89
2	a	7	GLC	O2-C2-C1	-2.12	104.82	109.15
2	X	4	GLC	O2-C2-C3	-2.10	105.92	110.14
2	e	3	GLC	O2-C2-C3	-2.10	105.93	110.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	d	4	GLC	O4-C4-C3	-2.10	105.50	110.35
2	e	8	GLC	O5-C5-C6	2.10	110.49	107.20
2	X	7	GLC	O2-C2-C1	-2.10	104.86	109.15
2	j	2	GLC	C2-C3-C4	2.09	114.52	110.89
2	h	1	GLC	O6-C6-C5	-2.08	104.15	111.29
2	V	6	GLC	O5-C1-C2	-2.08	107.56	110.77
2	a	7	GLC	O5-C1-C2	-2.08	107.56	110.77
2	f	1	GLC	O5-C5-C4	-2.08	105.78	110.83
2	V	8	GLC	C1-O5-C5	2.07	115.00	112.19
2	V	8	GLC	O3-C3-C2	-2.07	106.03	109.99
2	V	5	GLC	C3-C4-C5	-2.07	106.55	110.24
2	Z	6	GLC	C1-O5-C5	2.06	114.98	112.19
2	i	4	GLC	O2-C2-C3	-2.06	106.01	110.14
2	b	2	GLC	O5-C1-C2	-2.06	107.59	110.77
2	d	4	GLC	O3-C3-C4	-2.06	105.59	110.35
2	h	8	GLC	C1-C2-C3	2.05	112.19	109.67
2	i	2	GLC	C1-O5-C5	2.05	114.97	112.19
2	i	3	GLC	O5-C1-C2	-2.05	107.61	110.77
2	d	2	GLC	O4-C4-C5	2.05	114.38	109.30
2	b	5	GLC	O4-C4-C5	2.04	114.36	109.30
2	h	6	GLC	O5-C5-C6	2.04	110.40	107.20
2	c	5	GLC	O5-C5-C6	2.03	110.39	107.20
2	W	6	GLC	O3-C3-C2	2.03	113.88	109.99
2	X	3	GLC	O5-C1-C2	-2.03	107.64	110.77
2	T	3	GLC	O5-C5-C6	2.02	110.38	107.20
2	b	6	GLC	O6-C6-C5	-2.02	104.35	111.29
2	S	4	GLC	O5-C5-C6	-2.02	104.05	107.20
2	d	6	GLC	O5-C5-C6	2.01	110.36	107.20
2	S	8	GLC	C2-C3-C4	-2.01	107.41	110.89
2	W	5	GLC	C3-C4-C5	-2.01	106.65	110.24
2	b	3	GLC	O2-C2-C1	-2.01	105.04	109.15
2	f	2	GLC	O5-C5-C4	2.01	115.71	110.83
2	a	6	GLC	O6-C6-C5	-2.00	104.42	111.29
2	d	1	GLC	C1-C2-C3	2.00	112.12	109.67

There are no chirality outliers.

All (99) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	U	2	GLC	O5-C5-C6-O6
2	Z	2	GLC	O5-C5-C6-O6
2	a	2	GLC	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	c	4	GLC	O5-C5-C6-O6
2	f	5	GLC	O5-C5-C6-O6
2	U	2	GLC	C4-C5-C6-O6
2	Z	2	GLC	C4-C5-C6-O6
2	U	3	GLC	O5-C5-C6-O6
2	Y	2	GLC	O5-C5-C6-O6
2	j	3	GLC	O5-C5-C6-O6
2	e	4	GLC	O5-C5-C6-O6
2	j	6	GLC	O5-C5-C6-O6
2	X	4	GLC	O5-C5-C6-O6
2	f	5	GLC	C4-C5-C6-O6
2	j	6	GLC	C4-C5-C6-O6
2	d	4	GLC	O5-C5-C6-O6
2	a	2	GLC	C4-C5-C6-O6
2	d	6	GLC	C4-C5-C6-O6
2	c	4	GLC	C4-C5-C6-O6
2	j	4	GLC	O5-C5-C6-O6
2	a	4	GLC	O5-C5-C6-O6
2	g	2	GLC	O5-C5-C6-O6
2	g	4	GLC	O5-C5-C6-O6
2	b	4	GLC	C4-C5-C6-O6
2	a	6	GLC	C4-C5-C6-O6
2	c	6	GLC	C4-C5-C6-O6
2	g	2	GLC	C4-C5-C6-O6
2	i	6	GLC	C4-C5-C6-O6
2	g	4	GLC	C4-C5-C6-O6
2	j	8	GLC	C4-C5-C6-O6
2	j	3	GLC	C4-C5-C6-O6
2	f	1	GLC	O5-C5-C6-O6
2	j	4	GLC	C4-C5-C6-O6
2	a	1	GLC	C4-C5-C6-O6
2	T	2	GLC	O5-C5-C6-O6
2	e	6	GLC	C4-C5-C6-O6
2	b	4	GLC	O5-C5-C6-O6
2	Z	3	GLC	O5-C5-C6-O6
2	f	1	GLC	C4-C5-C6-O6
2	S	3	GLC	O5-C5-C6-O6
2	f	2	GLC	O5-C5-C6-O6
2	a	4	GLC	C4-C5-C6-O6
2	Y	6	GLC	C4-C5-C6-O6
2	d	4	GLC	C4-C5-C6-O6
2	g	3	GLC	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	S	2	GLC	O5-C5-C6-O6
2	U	4	GLC	O5-C5-C6-O6
2	T	1	GLC	C4-C5-C6-O6
2	h	3	GLC	O5-C5-C6-O6
2	U	3	GLC	C4-C5-C6-O6
2	V	6	GLC	C4-C5-C6-O6
2	S	3	GLC	C4-C5-C6-O6
2	S	2	GLC	C4-C5-C6-O6
2	f	8	GLC	C4-C5-C6-O6
2	i	1	GLC	C4-C5-C6-O6
2	Z	6	GLC	C4-C5-C6-O6
2	a	1	GLC	O5-C5-C6-O6
2	f	8	GLC	O5-C5-C6-O6
2	d	2	GLC	O5-C5-C6-O6
2	j	8	GLC	O5-C5-C6-O6
2	a	6	GLC	O5-C5-C6-O6
2	T	1	GLC	O5-C5-C6-O6
2	g	6	GLC	C4-C5-C6-O6
2	d	6	GLC	O5-C5-C6-O6
2	h	1	GLC	C4-C5-C6-O6
2	Z	1	GLC	C4-C5-C6-O6
2	a	3	GLC	O5-C5-C6-O6
2	T	2	GLC	C4-C5-C6-O6
2	V	2	GLC	O5-C5-C6-O6
2	d	3	GLC	O5-C5-C6-O6
2	S	6	GLC	C4-C5-C6-O6
2	Z	3	GLC	C4-C5-C6-O6
2	i	2	GLC	O5-C5-C6-O6
2	f	3	GLC	O5-C5-C6-O6
2	c	3	GLC	O5-C5-C6-O6
2	Y	2	GLC	C4-C5-C6-O6
2	X	4	GLC	C4-C5-C6-O6
2	d	1	GLC	C4-C5-C6-O6
2	c	6	GLC	O5-C5-C6-O6
2	i	1	GLC	O5-C5-C6-O6
2	i	6	GLC	O5-C5-C6-O6
2	U	1	GLC	C4-C5-C6-O6
2	h	4	GLC	C4-C5-C6-O6
2	b	6	GLC	O5-C5-C6-O6
2	U	6	GLC	C4-C5-C6-O6
2	e	5	GLC	C4-C5-C6-O6
2	W	8	GLC	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	U	4	GLC	C4-C5-C6-O6
2	f	2	GLC	C4-C5-C6-O6
2	j	1	GLC	C4-C5-C6-O6
2	g	3	GLC	C4-C5-C6-O6
2	h	3	GLC	C4-C5-C6-O6
2	h	1	GLC	O5-C5-C6-O6
2	d	1	GLC	O5-C5-C6-O6
2	e	4	GLC	C4-C5-C6-O6
2	W	3	GLC	O5-C5-C6-O6
2	j	5	GLC	C4-C5-C6-O6
2	Z	1	GLC	O5-C5-C6-O6
2	e	6	GLC	O5-C5-C6-O6

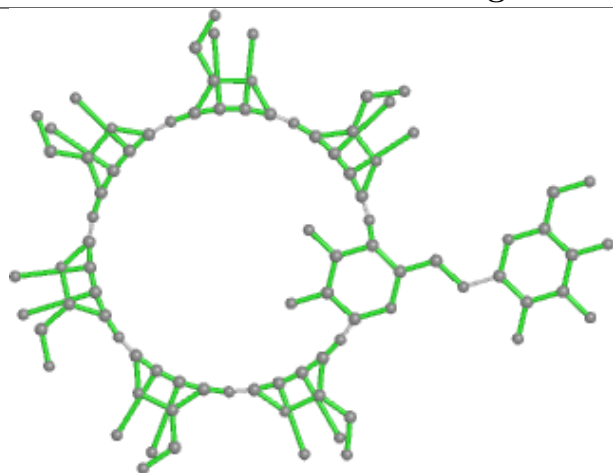
There are no ring outliers.

4 monomers are involved in 4 short contacts:

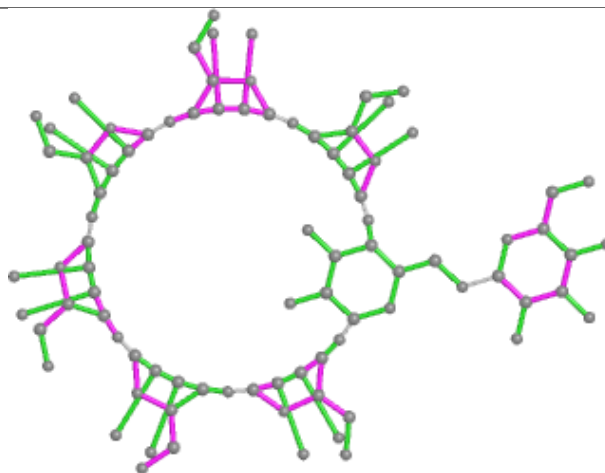
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	V	6	GLC	1	0
2	Z	4	GLC	2	0
2	Z	6	GLC	1	0
2	Z	5	GLC	2	0

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

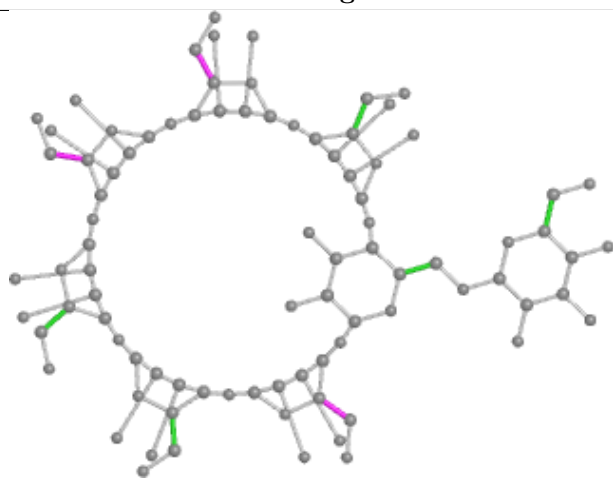
Oligosaccharide Chain S



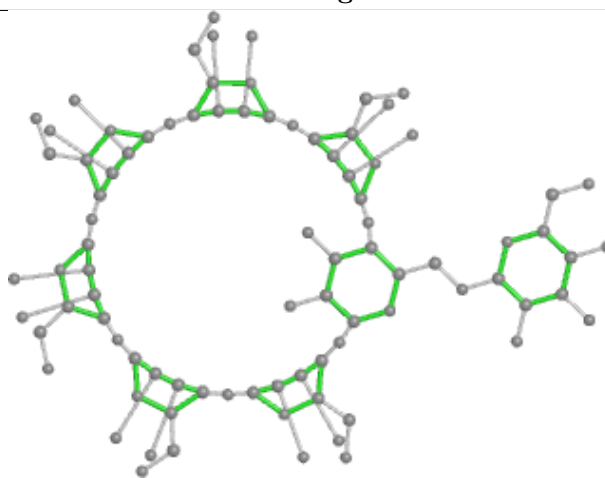
Bond lengths



Bond angles

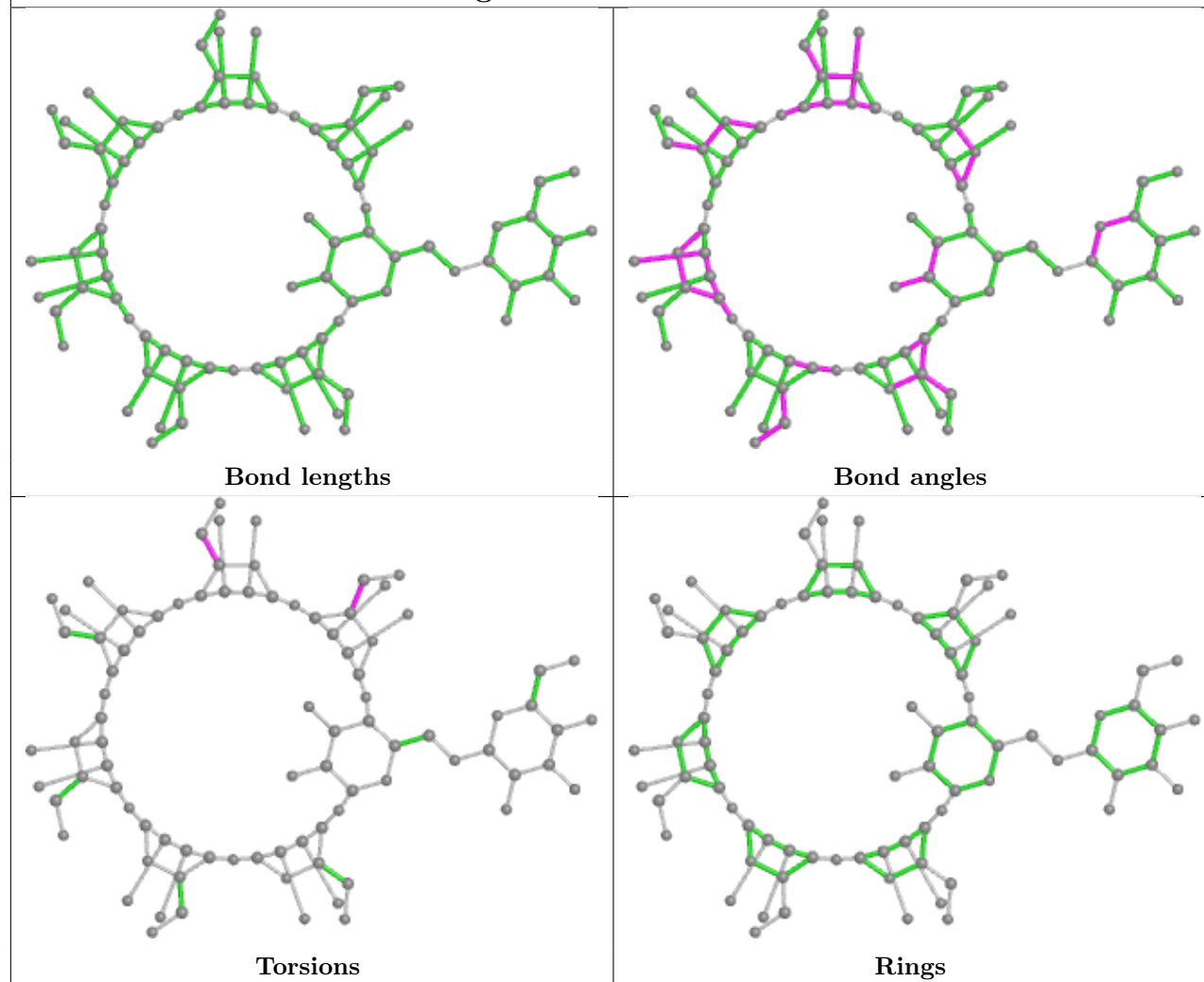


Torsions

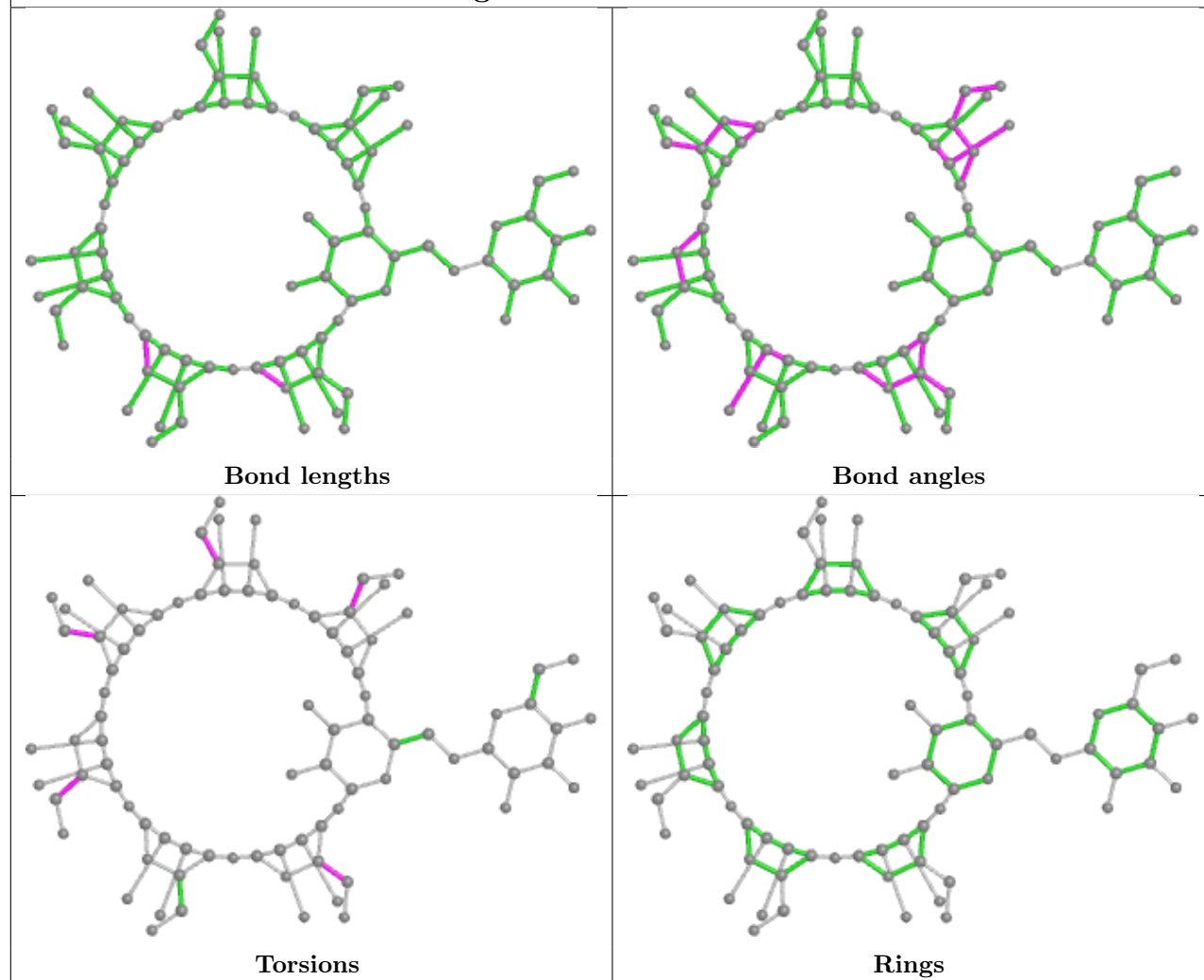


Rings

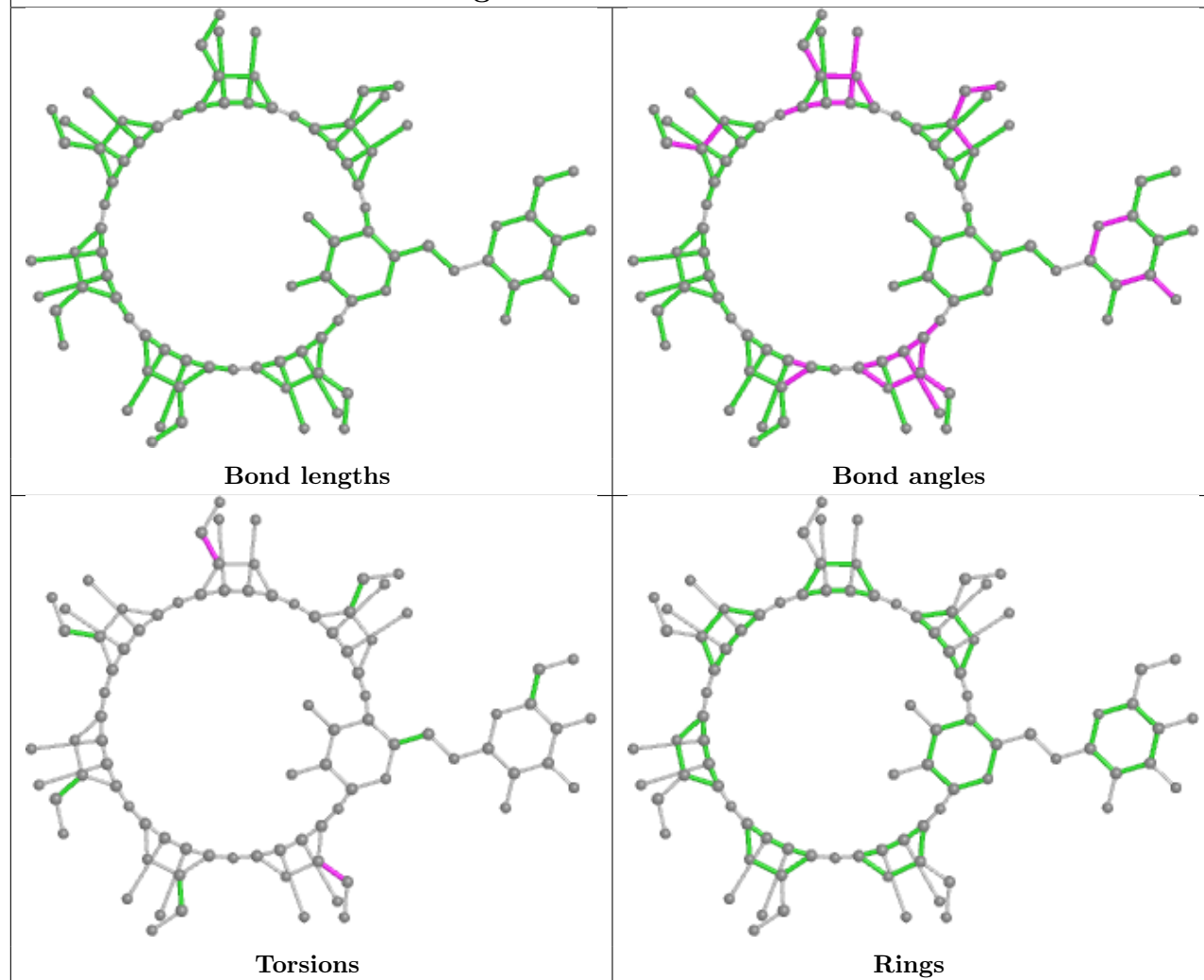
Oligosaccharide Chain T



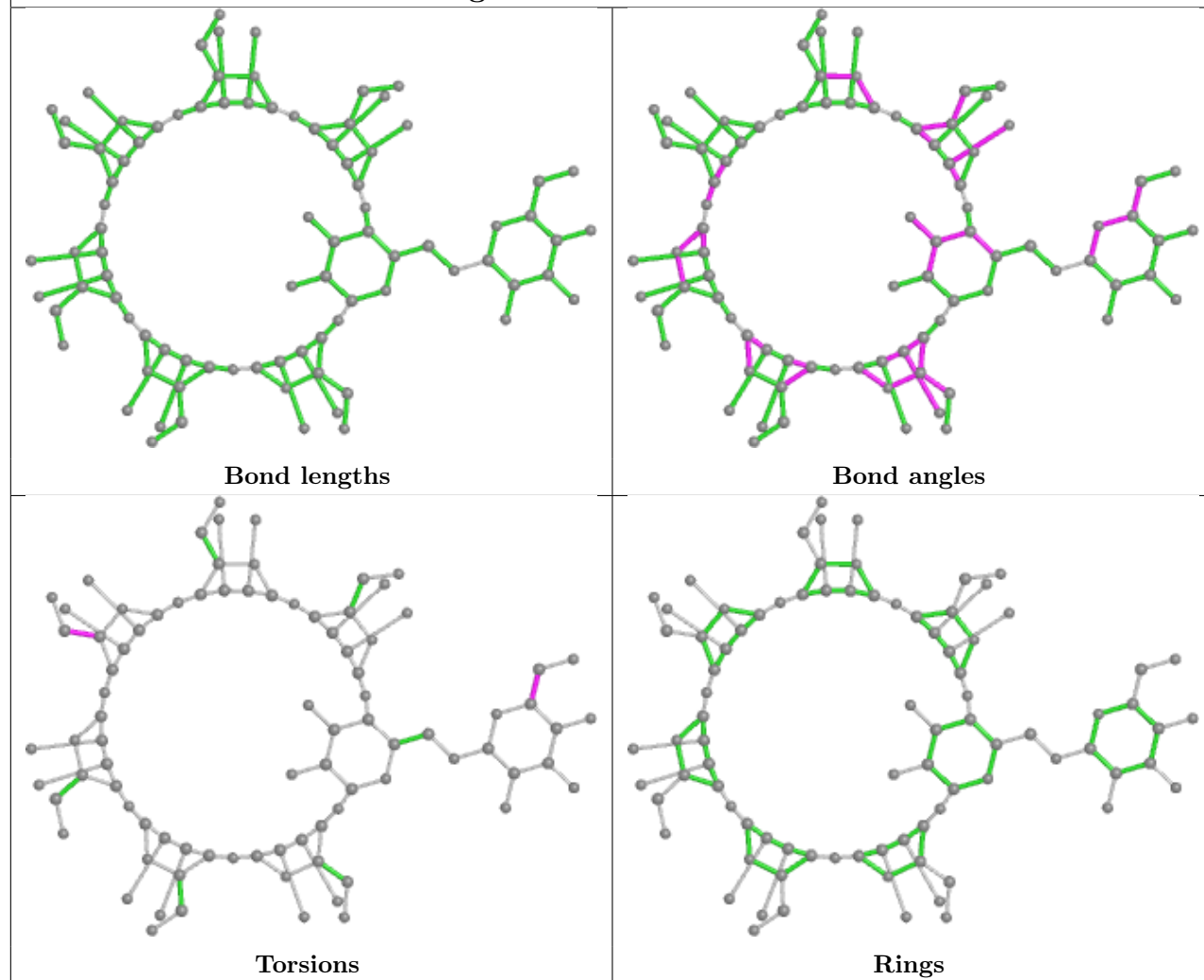
Oligosaccharide Chain U



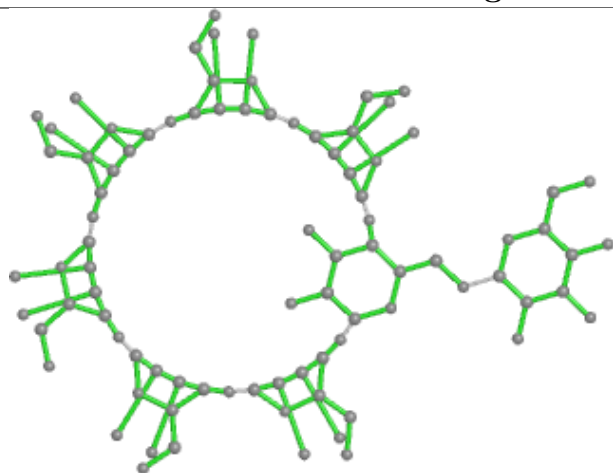
Oligosaccharide Chain V



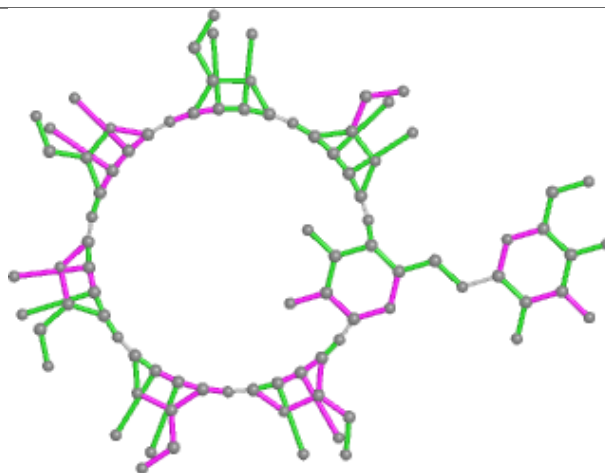
Oligosaccharide Chain W



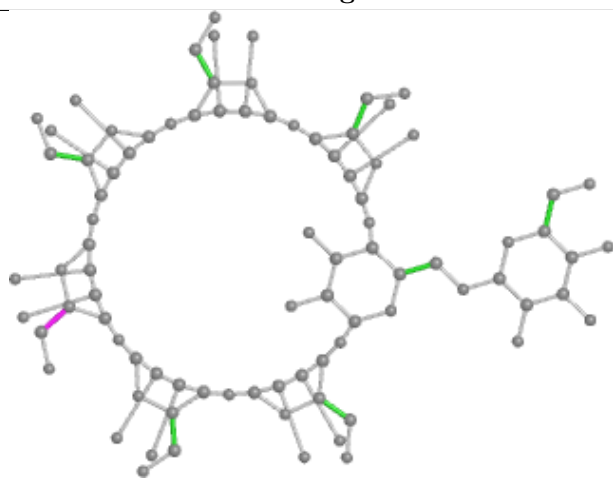
Oligosaccharide Chain X



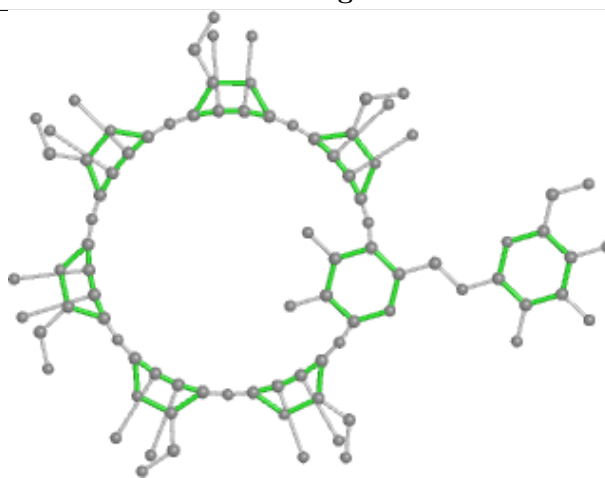
Bond lengths



Bond angles

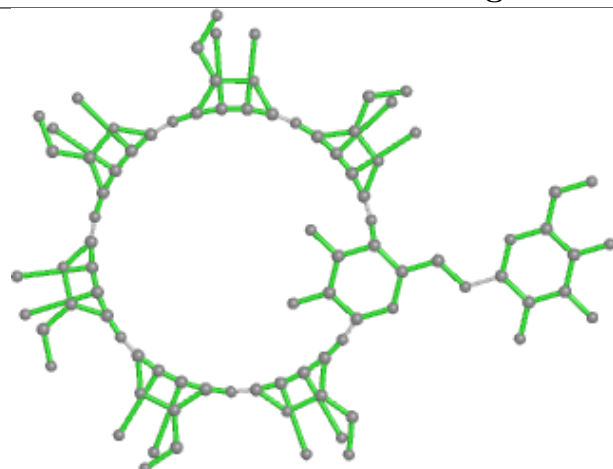


Torsions

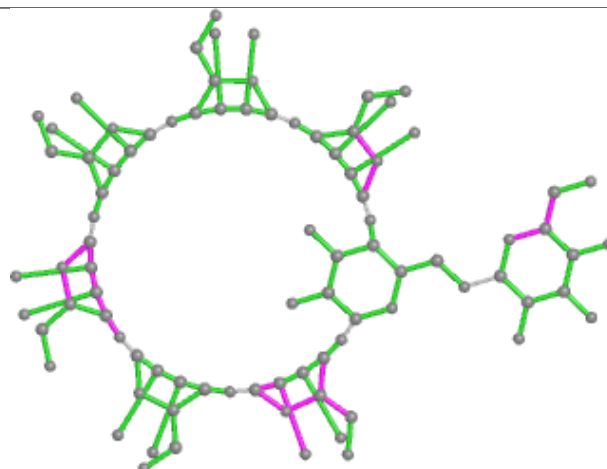


Rings

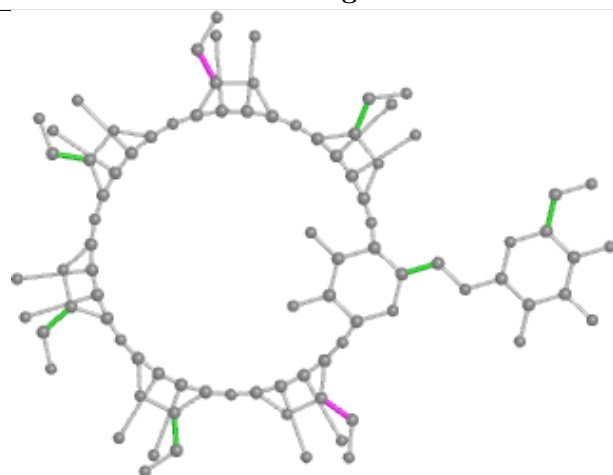
Oligosaccharide Chain Y



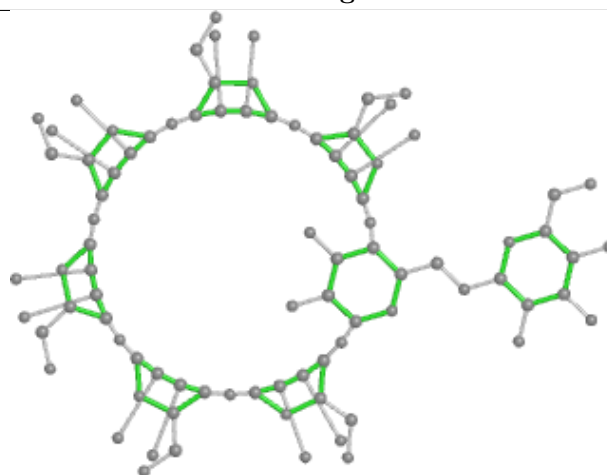
Bond lengths



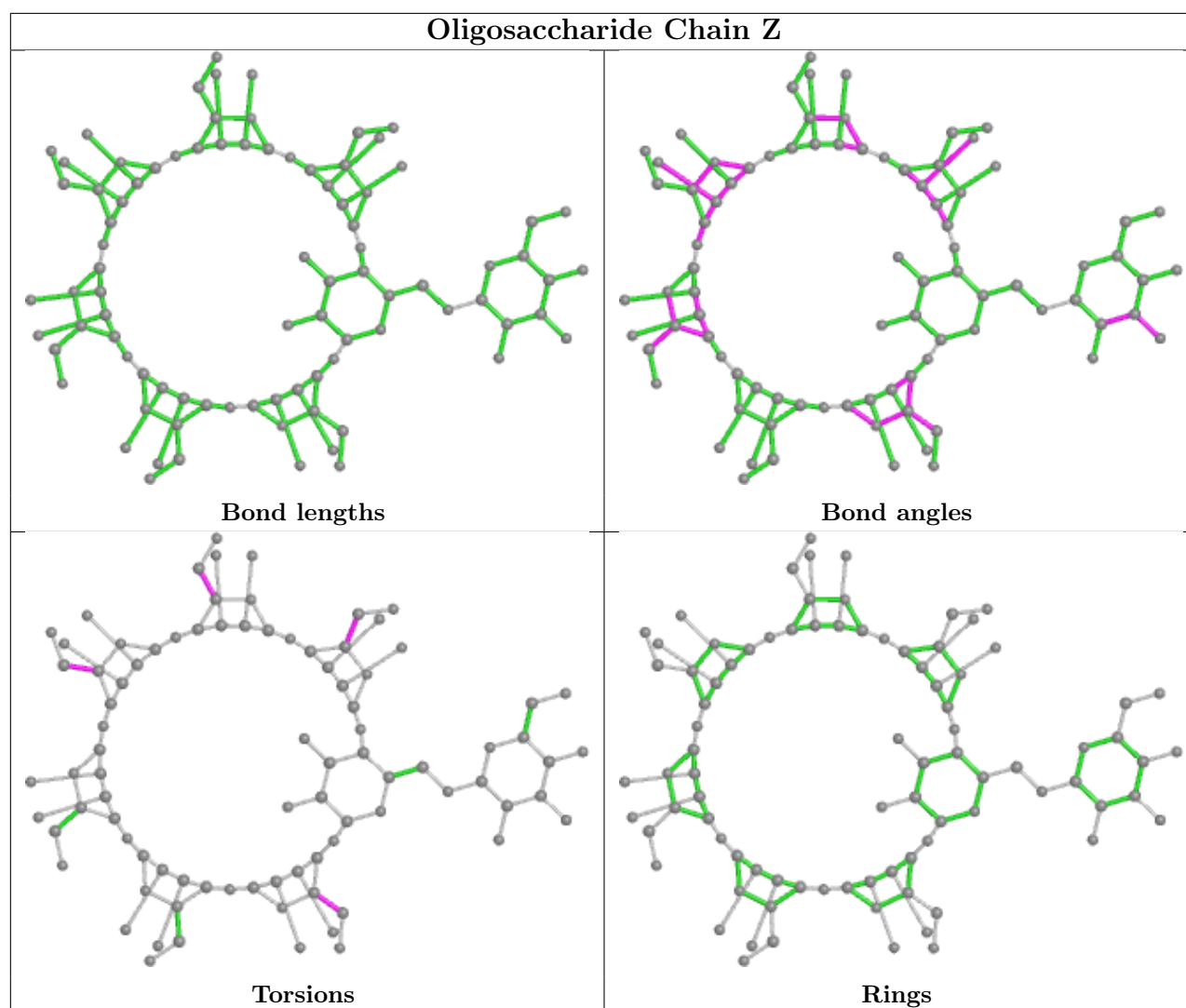
Bond angles



Torsions



Rings



5.6 Ligand geometry [i](#)

19 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	202	-	5,5,5	0.35	0	5,5,5	0.50	0
3	GOL	I	201	-	5,5,5	0.32	0	5,5,5	0.47	0
3	GOL	H	201	-	5,5,5	0.54	0	5,5,5	1.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	M	201	-	5,5,5	0.37	0	5,5,5	0.40	0
3	GOL	N	201	-	5,5,5	0.59	0	5,5,5	0.88	0
3	GOL	H	202	-	5,5,5	0.36	0	5,5,5	0.78	0
3	GOL	L	201	-	5,5,5	0.25	0	5,5,5	0.51	0
3	GOL	P	201	-	5,5,5	0.21	0	5,5,5	0.51	0
3	GOL	N	202	-	5,5,5	0.38	0	5,5,5	0.83	0
3	GOL	A	202	-	5,5,5	0.83	0	5,5,5	1.25	1 (20%)
3	GOL	C	202	-	5,5,5	0.36	0	5,5,5	0.59	0
3	GOL	C	201	-	5,5,5	0.36	0	5,5,5	0.18	0
3	GOL	I	202	-	5,5,5	0.74	0	5,5,5	0.81	0
3	GOL	A	201	-	5,5,5	0.48	0	5,5,5	0.46	0
3	GOL	B	201	-	5,5,5	0.62	0	5,5,5	0.89	0
3	GOL	E	201	-	5,5,5	0.31	0	5,5,5	0.43	0
3	GOL	F	201	-	5,5,5	0.39	0	5,5,5	0.75	0
3	GOL	K	201	-	5,5,5	0.27	0	5,5,5	0.78	0
3	GOL	D	201	-	5,5,5	0.30	0	5,5,5	0.91	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	202	-	-	1/4/4/4	-
3	GOL	I	201	-	-	0/4/4/4	-
3	GOL	H	201	-	-	4/4/4/4	-
3	GOL	M	201	-	-	4/4/4/4	-
3	GOL	N	201	-	-	3/4/4/4	-
3	GOL	H	202	-	-	2/4/4/4	-
3	GOL	L	201	-	-	2/4/4/4	-
3	GOL	P	201	-	-	2/4/4/4	-
3	GOL	N	202	-	-	0/4/4/4	-
3	GOL	A	202	-	-	2/4/4/4	-
3	GOL	C	202	-	-	2/4/4/4	-
3	GOL	C	201	-	-	0/4/4/4	-
3	GOL	I	202	-	-	2/4/4/4	-
3	GOL	A	201	-	-	2/4/4/4	-
3	GOL	B	201	-	-	4/4/4/4	-
3	GOL	E	201	-	-	0/4/4/4	-
3	GOL	F	201	-	-	3/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	K	201	-	-	2/4/4/4	-
3	GOL	D	201	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	202	GOL	O1-C1-C2	2.29	121.17	110.20

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	201	GOL	O1-C1-C2-C3
3	M	201	GOL	O1-C1-C2-C3
3	M	201	GOL	C1-C2-C3-O3
3	N	201	GOL	O1-C1-C2-C3
3	H	202	GOL	O1-C1-C2-O2
3	H	202	GOL	O1-C1-C2-C3
3	P	201	GOL	O1-C1-C2-C3
3	C	202	GOL	O1-C1-C2-C3
3	I	202	GOL	O1-C1-C2-O2
3	I	202	GOL	O1-C1-C2-C3
3	B	201	GOL	O1-C1-C2-C3
3	F	201	GOL	O1-C1-C2-C3
3	M	201	GOL	O2-C2-C3-O3
3	B	201	GOL	O1-C1-C2-O2
3	L	201	GOL	O1-C1-C2-C3
3	A	202	GOL	C1-C2-C3-O3
3	A	201	GOL	C1-C2-C3-O3
3	B	201	GOL	C1-C2-C3-O3
3	K	201	GOL	C1-C2-C3-O3
3	H	201	GOL	O1-C1-C2-O2
3	M	201	GOL	O1-C1-C2-O2
3	P	201	GOL	O1-C1-C2-O2
3	F	201	GOL	O1-C1-C2-O2
3	N	201	GOL	O1-C1-C2-O2
3	A	202	GOL	O2-C2-C3-O3
3	A	201	GOL	O2-C2-C3-O3
3	B	202	GOL	C1-C2-C3-O3
3	C	202	GOL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	K	201	GOL	O2-C2-C3-O3
3	N	201	GOL	O2-C2-C3-O3
3	B	201	GOL	O2-C2-C3-O3
3	F	201	GOL	O2-C2-C3-O3
3	H	201	GOL	O2-C2-C3-O3
3	H	201	GOL	C1-C2-C3-O3
3	L	201	GOL	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	201	GOL	2	0
3	P	201	GOL	2	0
3	A	202	GOL	1	0
3	C	202	GOL	2	0
3	B	201	GOL	2	0
3	K	201	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

6.1 Protein, DNA and RNA chains

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	82/90 (91%)	-0.67	0 100 100	15, 21, 39, 51	0
1	B	83/90 (92%)	-0.43	1 (1%) 79 78	15, 24, 49, 59	0
1	C	83/90 (92%)	-0.47	0 100 100	14, 20, 45, 60	0
1	D	79/90 (87%)	-0.68	0 100 100	16, 24, 40, 52	0
1	E	85/90 (94%)	-0.45	0 100 100	17, 25, 38, 57	0
1	F	85/90 (94%)	-0.43	1 (1%) 79 78	17, 29, 49, 79	0
1	G	83/90 (92%)	-0.61	0 100 100	21, 30, 48, 67	0
1	H	85/90 (94%)	-0.53	0 100 100	24, 34, 52, 61	0
1	I	85/90 (94%)	-0.50	0 100 100	23, 33, 48, 55	0
1	J	85/90 (94%)	-0.53	0 100 100	22, 31, 50, 59	0
1	K	82/90 (91%)	-0.46	0 100 100	24, 32, 52, 68	0
1	L	82/90 (91%)	-0.55	0 100 100	20, 31, 50, 70	0
1	M	85/90 (94%)	-0.57	0 100 100	20, 26, 47, 63	0
1	N	84/90 (93%)	-0.41	0 100 100	20, 32, 52, 67	0
1	O	84/90 (93%)	-0.67	0 100 100	20, 27, 41, 48	0
1	P	85/90 (94%)	-0.52	0 100 100	24, 33, 49, 58	0
1	Q	84/90 (93%)	-0.50	0 100 100	23, 36, 60, 73	0
1	R	84/90 (93%)	-0.24	1 (1%) 79 78	38, 49, 62, 79	0
All	All	1505/1620 (92%)	-0.51	3 (0%) 95 94	14, 30, 54, 79	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	154	HIS	2.3
1	F	74	SER	2.3
1	B	77	ARG	2.1

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

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

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	f	2	11/12	0.54	0.23	67,75,79,79	0
2	GLC	f	4	11/12	0.68	0.20	50,62,65,66	0
2	GLC	f	1	11/12	0.76	0.23	49,56,62,75	0
2	GLC	d	5	11/12	0.79	0.19	40,45,51,53	0
2	GLC	f	5	11/12	0.80	0.27	44,51,53,53	0
2	GLC	Z	3	11/12	0.83	0.12	48,56,61,62	0
2	GLC	i	4	11/12	0.83	0.15	53,62,64,65	0
2	GLC	Y	3	11/12	0.84	0.13	54,55,60,63	0
2	GLC	Z	4	11/12	0.84	0.17	59,60,63,65	0
2	GLC	Z	5	11/12	0.84	0.24	50,65,69,71	0
2	GLC	f	3	11/12	0.85	0.16	47,54,58,59	0
2	GLC	g	3	11/12	0.86	0.12	46,48,54,54	0
2	GLC	a	5	11/12	0.86	0.22	44,51,55,62	0
2	GLC	Z	8	11/12	0.86	0.13	38,47,52,56	0
2	GLC	g	4	11/12	0.86	0.11	44,51,55,58	0
2	GLC	j	5	11/12	0.87	0.14	46,51,60,61	0
2	GLC	Z	1	11/12	0.87	0.13	43,48,53,57	0
2	GLC	d	2	11/12	0.88	0.18	43,47,51,52	0
2	GLC	T	3	11/12	0.88	0.11	39,41,47,53	0
2	GLC	h	5	11/12	0.88	0.14	44,52,57,58	0
2	GLC	j	2	11/12	0.88	0.15	50,54,61,64	0
2	GLC	f	8	11/12	0.89	0.16	35,44,51,53	0
2	GLC	Y	2	11/12	0.89	0.15	42,48,55,58	0
2	GLC	j	4	11/12	0.89	0.14	49,53,58,61	0
2	GLC	h	3	11/12	0.89	0.09	52,60,62,63	0
2	GLC	i	1	11/12	0.90	0.12	31,36,42,43	0
2	GLC	j	6	11/12	0.90	0.10	41,46,47,50	0
2	GLC	e	3	11/12	0.90	0.11	45,48,53,53	0
2	GLC	b	3	11/12	0.90	0.12	45,46,49,53	0
2	GLC	j	8	11/12	0.90	0.14	40,45,51,54	0
2	GLC	j	3	11/12	0.90	0.13	38,47,51,54	0
2	GLC	h	4	11/12	0.90	0.17	58,61,67,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GLC	c	3	11/12	0.91	0.09	41,45,51,53	0
2	GLC	g	5	11/12	0.91	0.13	36,39,44,50	0
2	GLC	d	4	11/12	0.91	0.17	48,53,55,55	0
2	GLC	X	8	11/12	0.91	0.09	28,30,35,36	0
2	GLC	c	8	11/12	0.91	0.09	28,32,36,36	0
2	GLC	Z	2	11/12	0.91	0.16	61,67,74,74	0
2	GLC	d	1	11/12	0.91	0.10	33,36,39,43	0
2	GLC	i	2	11/12	0.92	0.12	45,48,57,64	0
2	GLC	f	6	11/12	0.92	0.14	40,42,47,51	0
2	GLC	d	3	11/12	0.92	0.12	42,45,51,59	0
2	GLC	g	8	11/12	0.92	0.11	30,37,39,41	0
2	GLC	g	2	11/12	0.92	0.13	40,46,50,53	0
2	GLC	Y	1	11/12	0.92	0.14	36,41,46,51	0
2	GLC	j	1	11/12	0.92	0.11	38,45,51,57	0
2	GLC	i	3	11/12	0.92	0.10	53,54,61,61	0
2	GLC	Z	6	11/12	0.92	0.15	47,49,53,53	0
2	GLC	a	3	11/12	0.92	0.13	46,50,53,57	0
2	GLC	a	2	11/12	0.93	0.16	42,45,47,48	0
2	GLC	b	4	11/12	0.93	0.09	44,50,56,57	0
2	GLC	W	4	11/12	0.93	0.12	26,35,40,51	0
2	GLC	S	2	11/12	0.93	0.11	30,33,38,43	0
2	GLC	Y	8	11/12	0.93	0.10	34,41,46,47	0
2	GLC	h	8	11/12	0.93	0.10	35,39,42,42	0
2	GLC	c	4	11/12	0.93	0.11	47,51,53,54	0
2	GLC	e	4	11/12	0.93	0.10	39,44,52,54	0
2	GLC	W	5	11/12	0.94	0.10	23,27,30,35	0
2	GLC	d	6	11/12	0.94	0.09	30,32,35,37	0
2	GLC	c	2	11/12	0.94	0.08	41,44,47,49	0
2	GLC	S	3	11/12	0.94	0.12	34,37,42,49	0
2	GLC	j	7	11/12	0.94	0.10	35,38,45,47	0
2	GLC	b	5	11/12	0.94	0.09	38,40,43,47	0
2	GLC	Y	6	11/12	0.94	0.09	31,33,36,37	0
2	GLC	X	5	11/12	0.94	0.09	21,24,27,34	0
2	GLC	U	3	11/12	0.94	0.09	34,36,38,47	0
2	GLC	b	8	11/12	0.94	0.14	29,36,38,42	0
2	GLC	S	4	11/12	0.94	0.09	30,34,39,40	0
2	GLC	a	4	11/12	0.94	0.13	50,55,62,63	0
2	GLC	e	2	11/12	0.94	0.09	36,40,48,49	0
2	GLC	Y	5	11/12	0.94	0.13	36,43,48,48	0
2	GLC	h	1	11/12	0.94	0.08	33,36,45,46	0
2	GLC	V	4	11/12	0.94	0.11	38,40,43,47	0
2	GLC	Y	4	11/12	0.94	0.11	48,58,60,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GLC	i	7	11/12	0.94	0.08	25,28,31,32	0
2	GLC	b	2	11/12	0.94	0.14	38,40,43,45	0
2	GLC	U	4	11/12	0.94	0.12	33,39,45,52	0
2	GLC	g	1	11/12	0.94	0.11	29,37,44,47	0
2	GLC	a	1	11/12	0.94	0.12	35,38,42,47	0
2	GLC	d	7	11/12	0.94	0.09	26,30,32,32	0
2	GLC	Z	7	11/12	0.94	0.09	39,40,43,44	0
2	GLC	a	8	11/12	0.94	0.13	31,38,43,44	0
2	GLC	g	7	11/12	0.95	0.08	27,31,34,34	0
2	GLC	g	6	11/12	0.95	0.07	28,32,35,36	0
2	GLC	X	4	11/12	0.95	0.09	23,26,31,39	0
2	GLC	d	8	11/12	0.95	0.12	23,27,32,38	0
2	GLC	c	5	11/12	0.95	0.11	32,41,45,48	0
2	GLC	b	6	11/12	0.95	0.09	26,30,35,36	0
2	GLC	e	1	11/12	0.95	0.08	24,30,36,45	0
2	GLC	T	2	11/12	0.95	0.09	28,37,40,46	0
2	GLC	T	5	11/12	0.95	0.10	24,28,30,36	0
2	GLC	V	6	11/12	0.95	0.08	25,26,29,31	0
2	GLC	T	6	11/12	0.95	0.07	18,20,21,21	0
2	GLC	T	4	11/12	0.95	0.11	32,39,45,48	0
2	GLC	e	6	11/12	0.95	0.09	28,29,33,37	0
2	GLC	i	5	11/12	0.95	0.11	35,50,52,57	0
2	GLC	a	7	11/12	0.95	0.09	26,31,33,34	0
2	GLC	c	7	11/12	0.95	0.09	28,31,33,33	0
2	GLC	W	1	11/12	0.95	0.09	22,25,29,32	0
2	GLC	f	7	11/12	0.95	0.10	35,39,41,42	0
2	GLC	i	6	11/12	0.95	0.09	28,34,39,39	0
2	GLC	a	6	11/12	0.95	0.09	32,39,43,43	0
2	GLC	e	5	11/12	0.95	0.09	34,38,44,47	0
2	GLC	X	1	11/12	0.95	0.09	19,21,23,29	0
2	GLC	S	5	11/12	0.95	0.08	24,25,29,33	0
2	GLC	V	5	11/12	0.95	0.10	31,34,37,41	0
2	GLC	W	8	11/12	0.95	0.08	23,27,31,33	0
2	GLC	V	3	11/12	0.95	0.08	35,39,45,51	0
2	GLC	b	1	11/12	0.95	0.09	29,31,35,36	0
2	GLC	h	7	11/12	0.95	0.09	27,31,34,36	0
2	GLC	c	6	11/12	0.96	0.08	31,33,35,35	0
2	GLC	h	6	11/12	0.96	0.10	32,38,42,43	0
2	GLC	V	7	11/12	0.96	0.09	22,23,25,25	0
2	GLC	V	1	11/12	0.96	0.07	23,27,33,34	0
2	GLC	U	5	11/12	0.96	0.09	20,23,27,29	0
2	GLC	Y	7	11/12	0.96	0.07	30,32,36,42	0

Continued on next page...

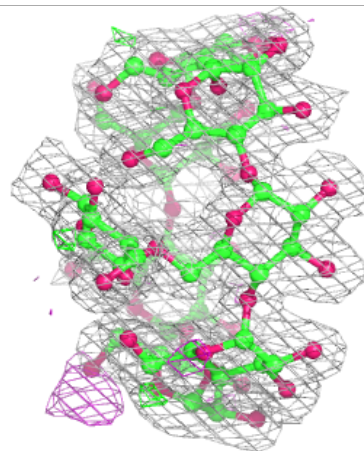
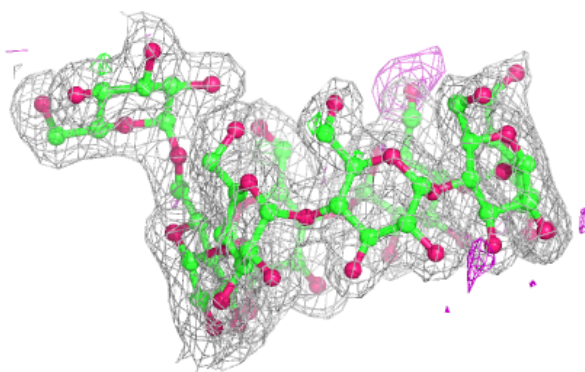
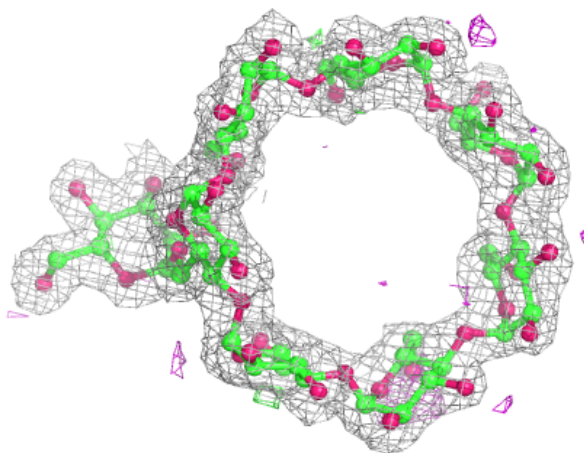
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GLC	W	2	11/12	0.96	0.08	27,28,33,35	0
2	GLC	i	8	11/12	0.96	0.11	33,36,42,43	0
2	GLC	U	2	11/12	0.96	0.10	25,29,35,43	0
2	GLC	h	2	11/12	0.96	0.11	44,50,61,69	0
2	GLC	V	2	11/12	0.96	0.10	32,34,44,50	0
2	GLC	W	3	11/12	0.96	0.08	27,30,36,38	0
2	GLC	X	3	11/12	0.96	0.08	21,22,28,29	0
2	GLC	X	6	11/12	0.97	0.08	19,22,24,25	0
2	GLC	T	8	11/12	0.97	0.08	15,18,21,21	0
2	GLC	e	8	11/12	0.97	0.08	31,34,35,37	0
2	GLC	c	1	11/12	0.97	0.08	33,38,41,43	0
2	GLC	U	1	11/12	0.97	0.07	20,22,25,30	0
2	GLC	T	1	11/12	0.97	0.09	21,25,31,37	0
2	GLC	b	7	11/12	0.97	0.06	23,26,28,32	0
2	GLC	X	2	11/12	0.97	0.08	21,24,26,27	0
2	GLC	S	1	11/12	0.97	0.09	19,23,29,34	0
2	GLC	X	7	11/12	0.97	0.08	18,19,21,22	0
2	GLC	S	8	11/12	0.97	0.08	17,18,21,25	0
2	GLC	e	7	11/12	0.98	0.08	22,25,27,30	0
2	GLC	V	8	11/12	0.98	0.07	21,23,24,28	0
2	GLC	S	6	11/12	0.98	0.07	19,20,22,23	0
2	GLC	U	8	11/12	0.98	0.08	16,18,20,22	0
2	GLC	U	6	11/12	0.98	0.09	17,18,20,20	0
2	GLC	W	6	11/12	0.98	0.09	20,23,25,25	0
2	GLC	W	7	11/12	0.98	0.08	20,20,22,23	0
2	GLC	T	7	11/12	0.98	0.10	18,19,21,22	0
2	GLC	S	7	11/12	0.98	0.08	17,18,19,20	0
2	GLC	U	7	11/12	0.98	0.09	14,17,18,20	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.

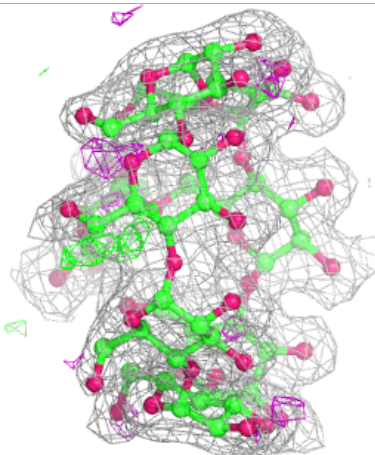
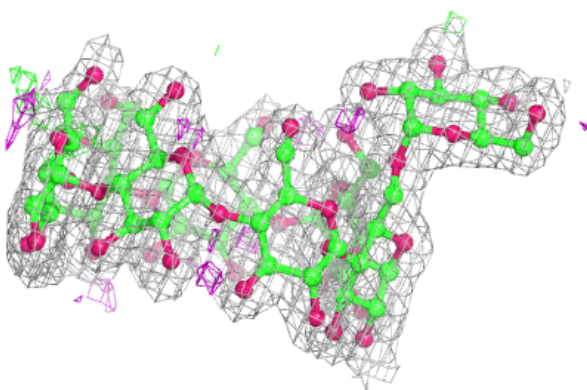
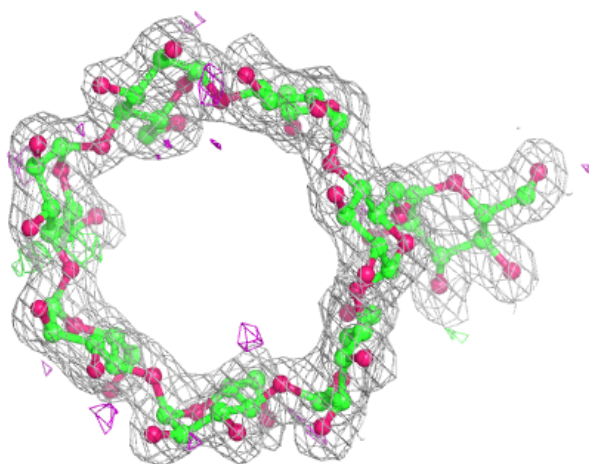
Electron density around Chain S:

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



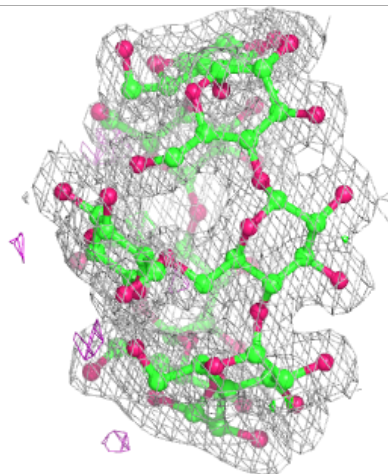
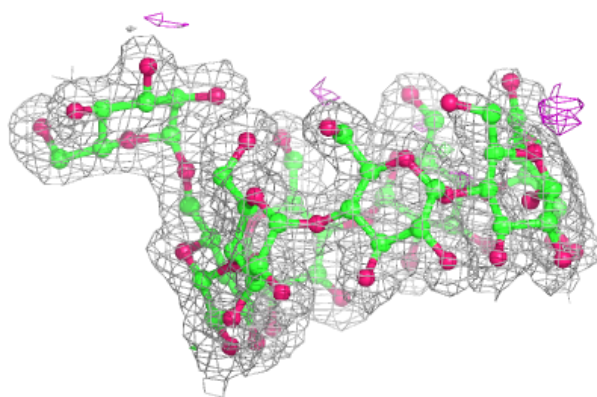
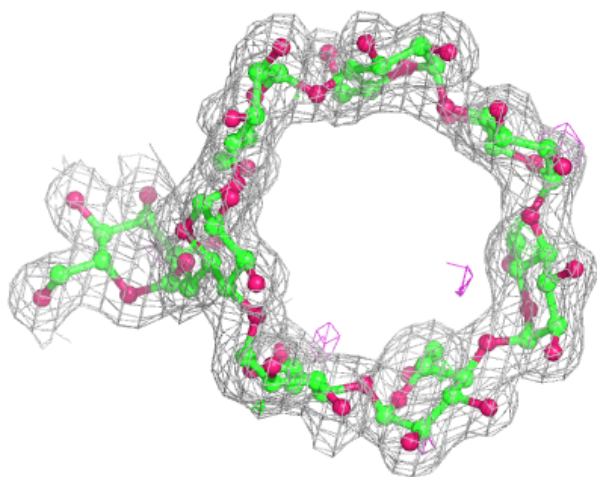
Electron density around Chain T:

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



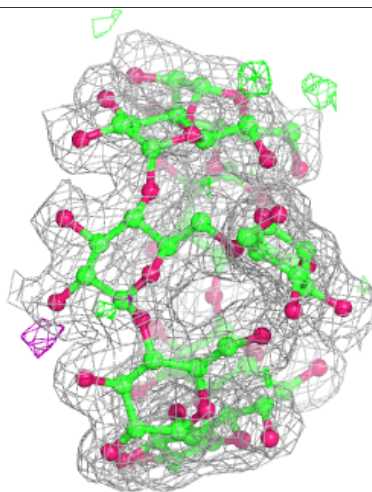
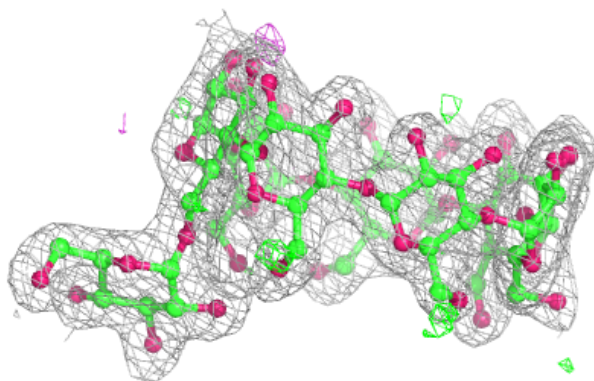
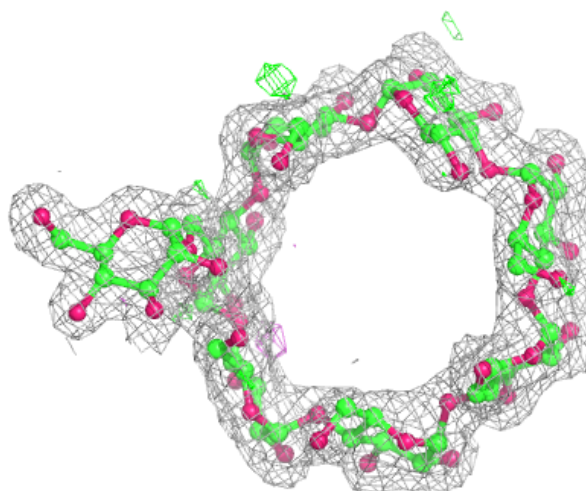
Electron density around Chain U:

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



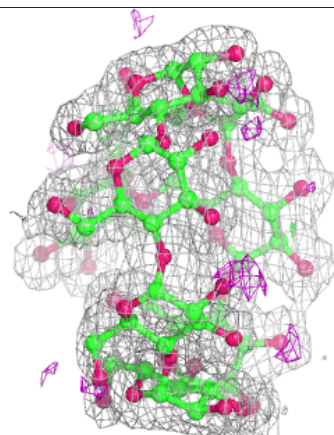
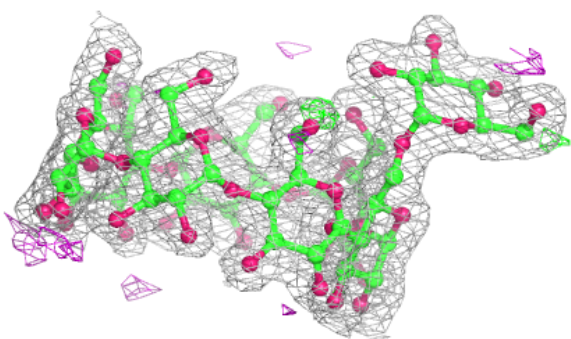
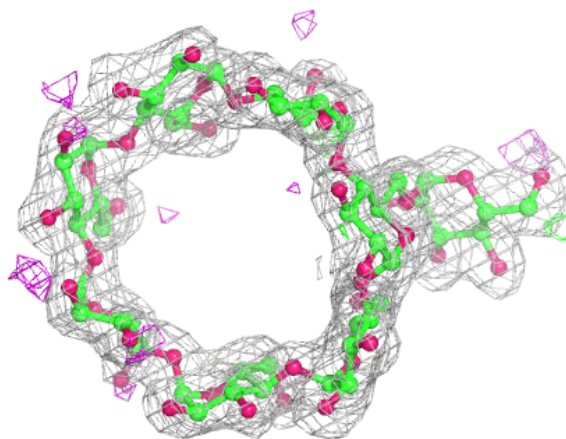
Electron density around Chain V:

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



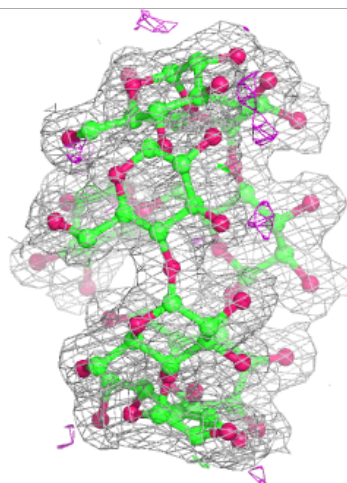
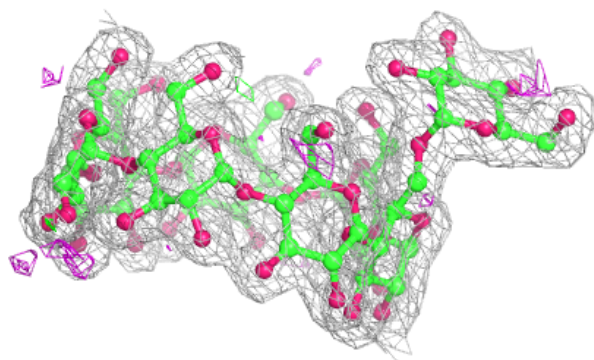
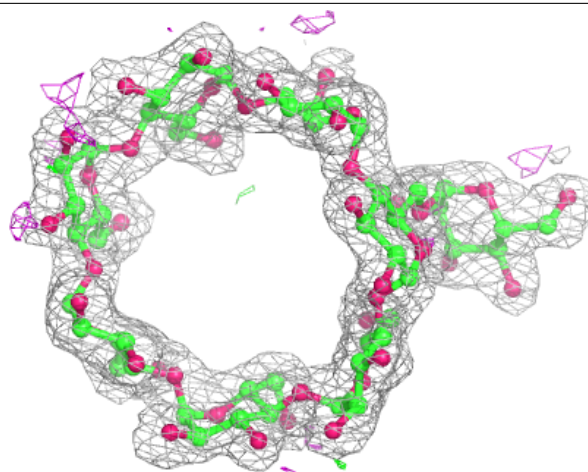
Electron density around Chain W:

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



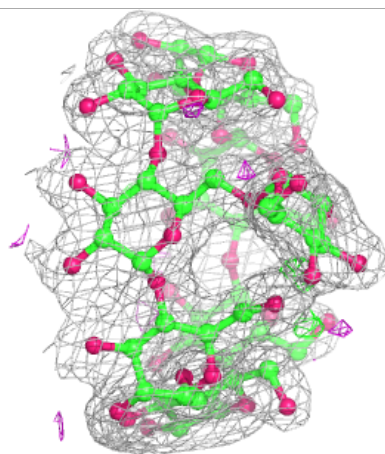
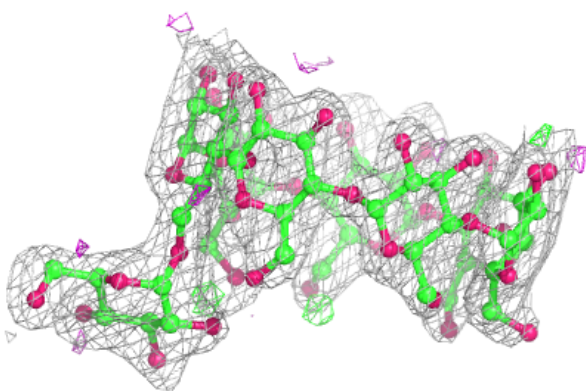
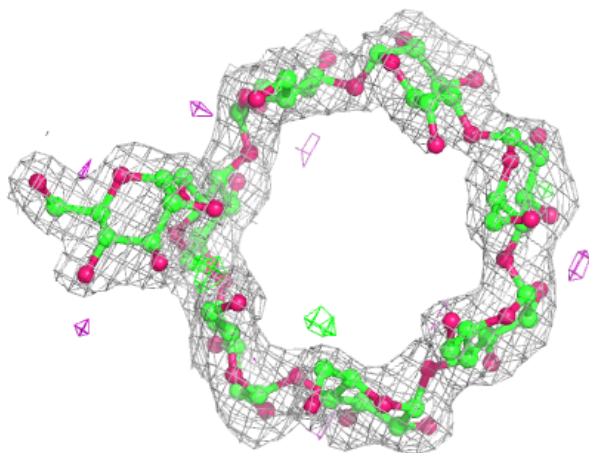
Electron density around Chain X:

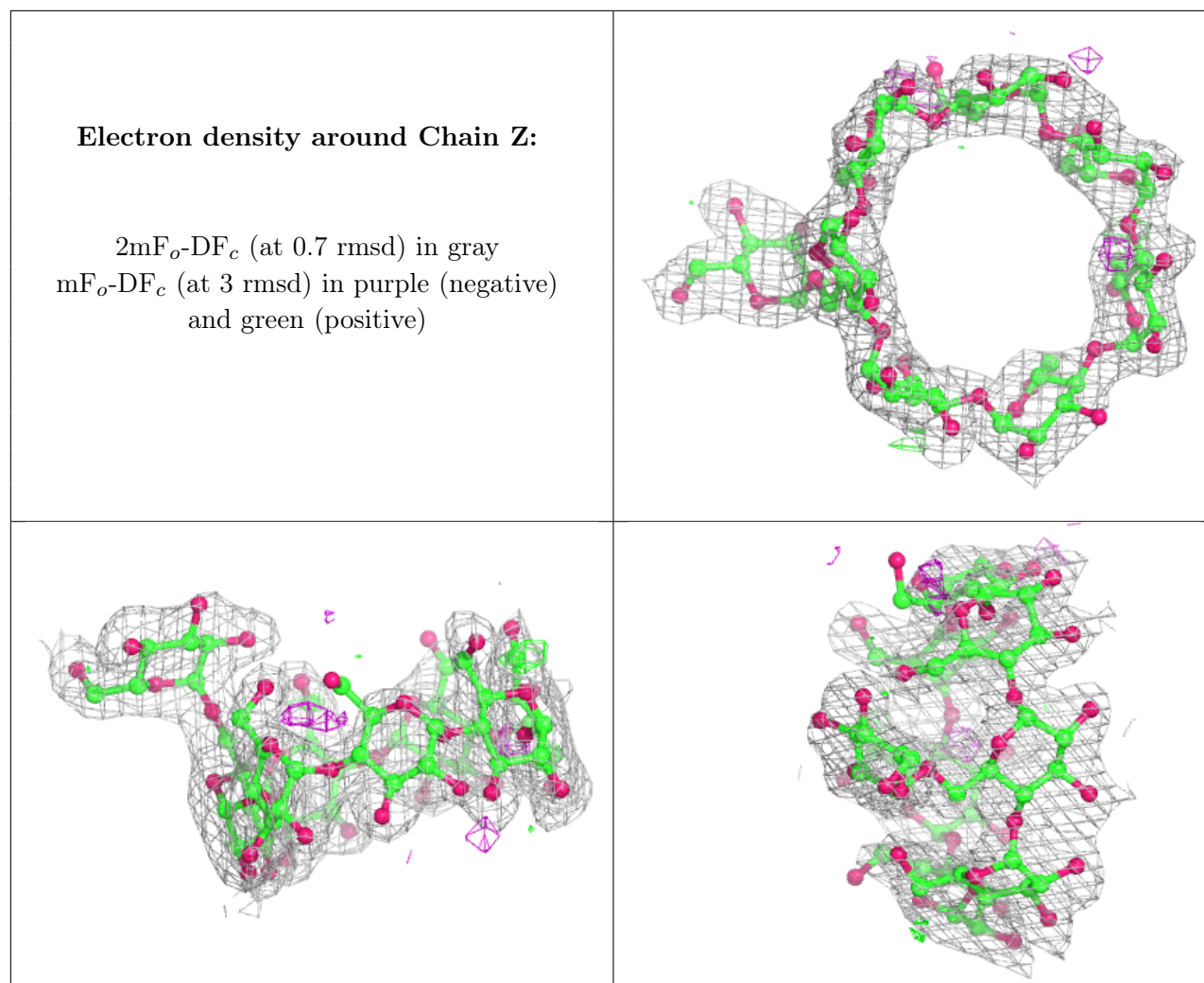
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain Y:

$2mF_o-DF_c$ (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(\AA^2)	Q<0.9
3	GOL	H	201	6/6	0.86	0.22	28,41,47,47	0
3	GOL	I	202	6/6	0.88	0.18	32,40,44,44	0
3	GOL	N	202	6/6	0.89	0.12	34,44,48,48	0
3	GOL	C	201	6/6	0.89	0.20	34,53,60,66	0
3	GOL	M	201	6/6	0.89	0.13	33,37,41,41	0
3	GOL	K	201	6/6	0.89	0.21	30,45,48,58	0
3	GOL	B	201	6/6	0.90	0.17	27,30,31,40	0
3	GOL	F	201	6/6	0.90	0.13	41,42,47,52	0
3	GOL	H	202	6/6	0.90	0.36	46,48,52,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	I	201	6/6	0.91	0.11	40,47,47,55	0
3	GOL	E	201	6/6	0.91	0.14	30,34,38,45	0
3	GOL	P	201	6/6	0.94	0.18	38,48,51,55	0
3	GOL	A	202	6/6	0.94	0.15	21,31,38,39	0
3	GOL	C	202	6/6	0.95	0.10	28,30,31,33	0
3	GOL	A	201	6/6	0.95	0.13	32,34,36,37	0
3	GOL	N	201	6/6	0.96	0.09	27,31,32,35	0
3	GOL	L	201	6/6	0.97	0.11	22,26,29,31	0
3	GOL	B	202	6/6	0.97	0.10	20,26,27,32	0
3	GOL	D	201	6/6	0.97	0.12	25,28,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.