



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 12:05 PM BST

PDB ID : 3RSZ
Title : Maltodextran bound basal state conformation of yeast glycogen synthase isoform 2
Authors : Baskaran, S.; Hurley, T.D.
Deposited on : 2011-05-02
Resolution : 3.01 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

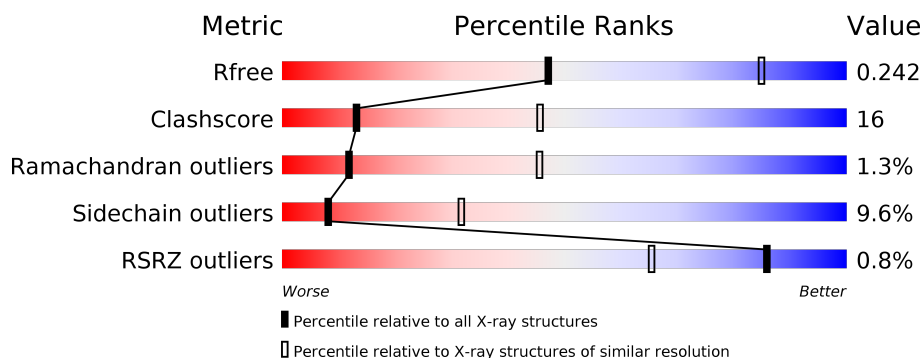
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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.





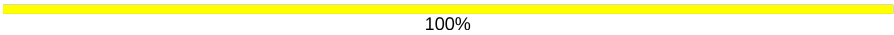

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	725	<div> <div>%</div> <div> <div></div> <div>54%</div> <div>25%</div> <div>5%</div> <div>16%</div> </div> </div>
1	B	725	<div> <div>%</div> <div> <div></div> <div>54%</div> <div>26%</div> <div>•</div> <div>16%</div> </div> </div>
1	C	725	<div> <div></div> <div> <div>53%</div> <div>27%</div> <div>5%</div> <div>15%</div> </div> </div>
1	D	725	<div> <div></div> <div> <div>54%</div> <div>26%</div> <div>•</div> <div>15%</div> </div> </div>
2	E	5	<div> <div></div> <div> <div>40%</div> <div>60%</div> </div> </div>
2	F	5	<div> <div></div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	4	
3	H	4	
3	I	4	
3	J	4	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GLC	J	1	-	-	-	X
3	GLC	J	4	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20011 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 Glycogen [starch] synthase isoform 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	611	Total	C	N	O	S	0	0	0
			4923	3148	857	899	19			
1	B	611	Total	C	N	O	S	0	0	0
			4923	3148	857	899	19			
1	C	613	Total	C	N	O	S	0	0	0
			4935	3154	860	902	19			
1	D	613	Total	C	N	O	S	0	0	0
			4935	3154	860	902	19			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P27472
A	-18	GLY	-	expression tag	UNP P27472
A	-17	SER	-	expression tag	UNP P27472
A	-16	SER	-	expression tag	UNP P27472
A	-15	HIS	-	expression tag	UNP P27472
A	-14	HIS	-	expression tag	UNP P27472
A	-13	HIS	-	expression tag	UNP P27472
A	-12	HIS	-	expression tag	UNP P27472
A	-11	HIS	-	expression tag	UNP P27472
A	-10	HIS	-	expression tag	UNP P27472
A	-9	SER	-	expression tag	UNP P27472
A	-8	SER	-	expression tag	UNP P27472
A	-7	GLY	-	expression tag	UNP P27472
A	-6	LEU	-	expression tag	UNP P27472
A	-5	VAL	-	expression tag	UNP P27472
A	-4	PRO	-	expression tag	UNP P27472
A	-3	ARG	-	expression tag	UNP P27472
A	-2	GLY	-	expression tag	UNP P27472
A	-1	SER	-	expression tag	UNP P27472
A	0	HIS	-	expression tag	UNP P27472
A	535	SER	ALA	SEE REMARK 999	UNP P27472

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Chain	Residue	Modelled	Actual	Comment	Reference
A	580	ALA	ARG	engineered mutation	UNP P27472
A	581	ALA	ARG	engineered mutation	UNP P27472
A	583	ALA	ARG	engineered mutation	UNP P27472
B	-19	MET	-	expression tag	UNP P27472
B	-18	GLY	-	expression tag	UNP P27472
B	-17	SER	-	expression tag	UNP P27472
B	-16	SER	-	expression tag	UNP P27472
B	-15	HIS	-	expression tag	UNP P27472
B	-14	HIS	-	expression tag	UNP P27472
B	-13	HIS	-	expression tag	UNP P27472
B	-12	HIS	-	expression tag	UNP P27472
B	-11	HIS	-	expression tag	UNP P27472
B	-10	HIS	-	expression tag	UNP P27472
B	-9	SER	-	expression tag	UNP P27472
B	-8	SER	-	expression tag	UNP P27472
B	-7	GLY	-	expression tag	UNP P27472
B	-6	LEU	-	expression tag	UNP P27472
B	-5	VAL	-	expression tag	UNP P27472
B	-4	PRO	-	expression tag	UNP P27472
B	-3	ARG	-	expression tag	UNP P27472
B	-2	GLY	-	expression tag	UNP P27472
B	-1	SER	-	expression tag	UNP P27472
B	0	HIS	-	expression tag	UNP P27472
B	535	SER	ALA	SEE REMARK 999	UNP P27472
B	580	ALA	ARG	engineered mutation	UNP P27472
B	581	ALA	ARG	engineered mutation	UNP P27472
B	583	ALA	ARG	engineered mutation	UNP P27472
C	-19	MET	-	expression tag	UNP P27472
C	-18	GLY	-	expression tag	UNP P27472
C	-17	SER	-	expression tag	UNP P27472
C	-16	SER	-	expression tag	UNP P27472
C	-15	HIS	-	expression tag	UNP P27472
C	-14	HIS	-	expression tag	UNP P27472
C	-13	HIS	-	expression tag	UNP P27472
C	-12	HIS	-	expression tag	UNP P27472
C	-11	HIS	-	expression tag	UNP P27472
C	-10	HIS	-	expression tag	UNP P27472
C	-9	SER	-	expression tag	UNP P27472
C	-8	SER	-	expression tag	UNP P27472
C	-7	GLY	-	expression tag	UNP P27472
C	-6	LEU	-	expression tag	UNP P27472
C	-5	VAL	-	expression tag	UNP P27472

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP P27472
C	-3	ARG	-	expression tag	UNP P27472
C	-2	GLY	-	expression tag	UNP P27472
C	-1	SER	-	expression tag	UNP P27472
C	0	HIS	-	expression tag	UNP P27472
C	535	SER	ALA	SEE REMARK 999	UNP P27472
C	580	ALA	ARG	engineered mutation	UNP P27472
C	581	ALA	ARG	engineered mutation	UNP P27472
C	583	ALA	ARG	engineered mutation	UNP P27472
D	-19	MET	-	expression tag	UNP P27472
D	-18	GLY	-	expression tag	UNP P27472
D	-17	SER	-	expression tag	UNP P27472
D	-16	SER	-	expression tag	UNP P27472
D	-15	HIS	-	expression tag	UNP P27472
D	-14	HIS	-	expression tag	UNP P27472
D	-13	HIS	-	expression tag	UNP P27472
D	-12	HIS	-	expression tag	UNP P27472
D	-11	HIS	-	expression tag	UNP P27472
D	-10	HIS	-	expression tag	UNP P27472
D	-9	SER	-	expression tag	UNP P27472
D	-8	SER	-	expression tag	UNP P27472
D	-7	GLY	-	expression tag	UNP P27472
D	-6	LEU	-	expression tag	UNP P27472
D	-5	VAL	-	expression tag	UNP P27472
D	-4	PRO	-	expression tag	UNP P27472
D	-3	ARG	-	expression tag	UNP P27472
D	-2	GLY	-	expression tag	UNP P27472
D	-1	SER	-	expression tag	UNP P27472
D	0	HIS	-	expression tag	UNP P27472
D	535	SER	ALA	SEE REMARK 999	UNP P27472
D	580	ALA	ARG	engineered mutation	UNP P27472
D	581	ALA	ARG	engineered mutation	UNP P27472
D	583	ALA	ARG	engineered mutation	UNP P27472

- Molecule 2 is a protein called Glycogen [starch] synthase isoform 2.

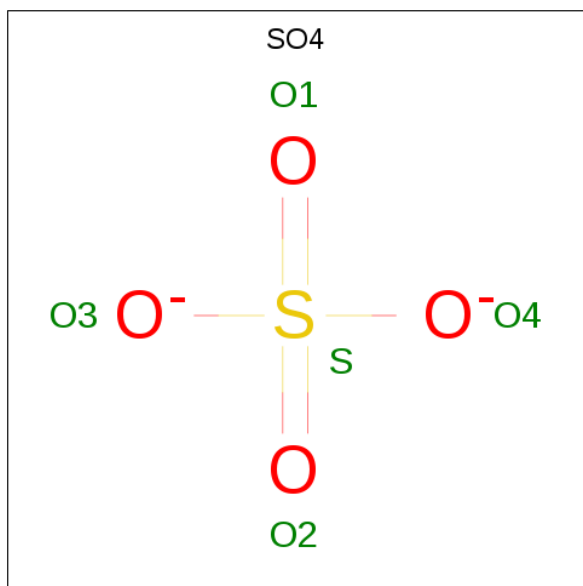
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	1	0	0
			10	6	2	2			
2	F	5	Total	C	N	O	1	0	0
			25	15	5	5			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	G	4	Total	C	O	0	0	0
			45	24	21			
3	H	4	Total	C	O	0	0	0
			45	24	21			
3	I	4	Total	C	O	0	0	0
			45	24	21			
3	J	4	Total	C	O	0	0	0
			45	24	21			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

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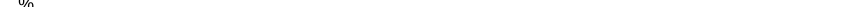
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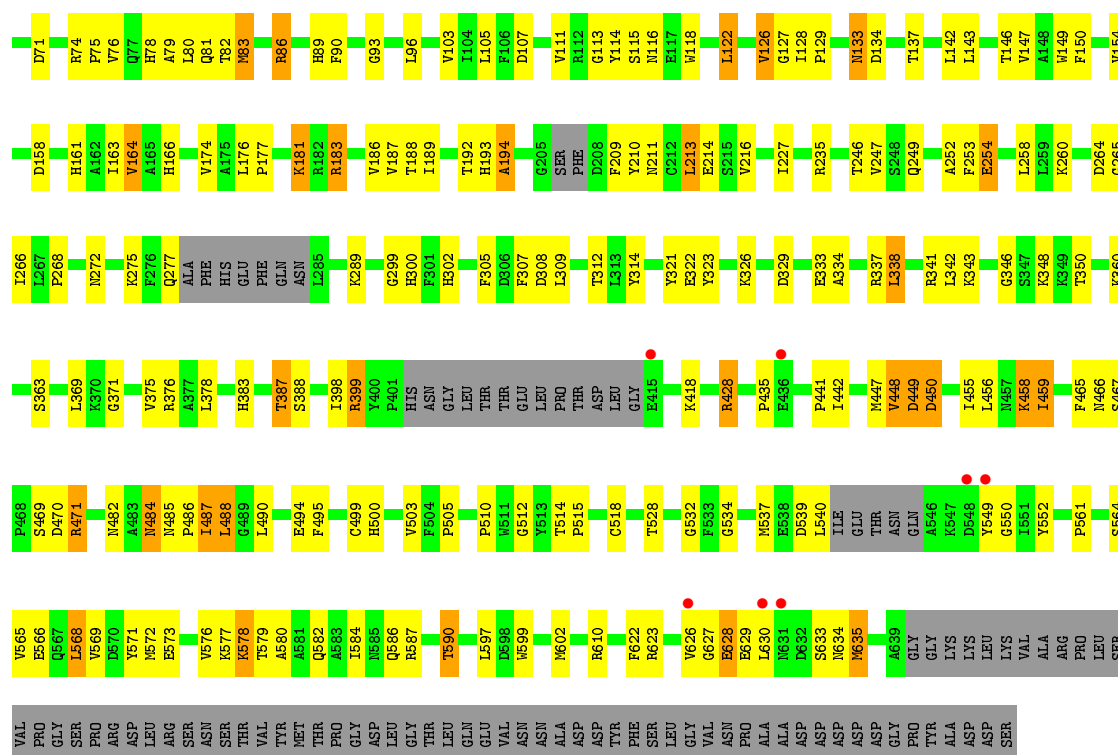
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

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.

- Chain A:

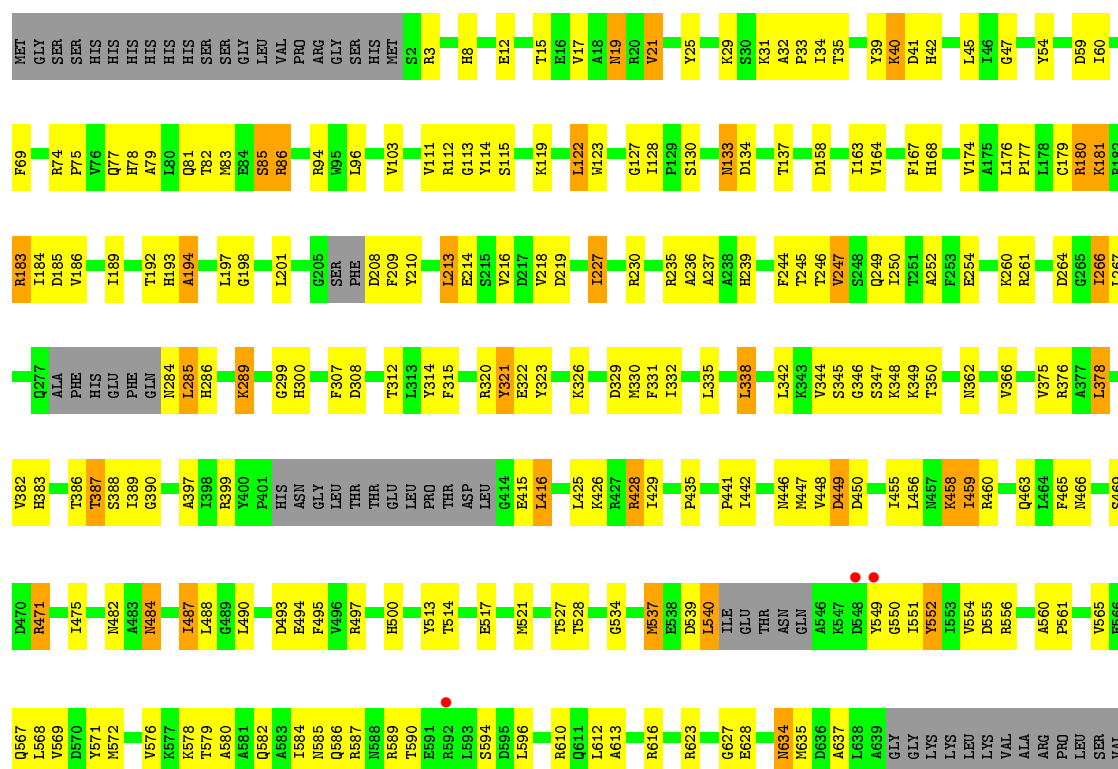
Residue	State	Residue	State	Residue	State	Residue	State	Residue	State
1 MET	Grey	51 SER	Green	101 VAL	Green	151 ARG	Green	201 VAL	Green
2 GLY	Green	52 SER	Green	102 LEU	Green	152 LEU	Green	202 LEU	Green
3 SER	Green	53 MET	Grey	103 GLN	Green	153 ASP	Green	203 ASP	Green
4 SER	Green	54 HIS	Green	104 LEU	Green	154 ASP	Green	204 ASP	Green
5 HIS	Green	55 HIS	Green	105 LEU	Green	155 ASP	Green	205 ASP	Green
6 HIS	Green	56 HIS	Green	106 VAL	Green	156 ASP	Green	206 ASP	Green
7 HIS	Green	57 HIS	Green	107 VAL	Green	157 ASP	Green	207 ASP	Green
8 HIS	Green	58 HIS	Green	108 VAL	Green	158 ASP	Green	208 ASP	Green
9 HIS	Green	59 HIS	Green	109 VAL	Green	159 ASP	Green	209 ASP	Green
10 HIS	Green	60 HIS	Green	110 VAL	Green	160 ASP	Green	210 ASP	Green
11 HIS	Green	61 HIS	Green	111 VAL	Green	161 ASP	Green	211 ASP	Green
12 HIS	Green	62 HIS	Green	112 VAL	Green	162 ASP	Green	212 ASP	Green
13 HIS	Green	63 HIS	Green	113 VAL	Green	163 ASP	Green	213 ASP	Green
14 HIS	Green	64 HIS	Green	114 VAL	Green	164 ASP	Green	214 ASP	Green
15 HIS	Green	65 HIS	Green	115 VAL	Green	165 ASP	Green	215 ASP	Green
16 HIS	Green	66 HIS	Green	116 VAL	Green	166 ASP	Green	216 ASP	Green
17 HIS	Green	67 HIS	Green	117 VAL	Green	167 ASP	Green	217 ASP	Green
18 HIS	Green	68 HIS	Green	118 VAL	Green	168 ASP	Green	218 ASP	Green
19 HIS	Green	69 HIS	Green	119 VAL	Green	169 ASP	Green	219 ASP	Green
20 HIS	Green	70 HIS	Green	120 VAL	Green	170 ASP	Green	220 ASP	Green
21 HIS	Green	71 HIS	Green	121 VAL	Green	171 ASP	Green	221 ASP	Green
22 HIS	Green	72 HIS	Green	122 VAL	Green	172 ASP	Green	222 ASP	Green
23 HIS	Green	73 HIS	Green	123 VAL	Green	173 ASP	Green	223 ASP	Green
24 HIS	Green	74 HIS	Green	124 VAL	Green	174 ASP	Green	224 ASP	Green
25 HIS	Green	75 HIS	Green	125 VAL	Green	175 ASP	Green	225 ASP	Green
26 HIS	Green	76 HIS	Green	126 VAL	Green	176 ASP	Green	226 ASP	Green
27 HIS	Green	77 HIS	Green	127 VAL	Green	177 ASP	Green	227 ASP	Green
28 HIS	Green	78 HIS	Green	128 VAL	Green	178 ASP	Green	228 ASP	Green
29 HIS	Green	79 HIS	Green	129 VAL	Green	179 ASP	Green	229 ASP	Green
30 HIS	Green	80 HIS	Green	130 VAL	Green	180 ASP	Green	230 ASP	Green
31 HIS	Green	81 HIS	Green	131 VAL	Green	181 ASP	Green	231 ASP	Green
32 HIS	Green	82 HIS	Green	132 VAL	Green	182 ASP	Green	232 ASP	Green
33 HIS	Green	83 HIS	Green	133 VAL	Green	183 ASP	Green	233 ASP	Green
34 HIS	Green	84 HIS	Green	134 VAL	Green	184 ASP	Green	234 ASP	Green
35 HIS	Green	85 HIS	Green	135 VAL	Green	185 ASP	Green	235 ASP	Green
36 HIS	Green	86 HIS	Green	136 VAL	Green	186 ASP	Green	236 ASP	Green
37 HIS	Green	87 HIS	Green	137 VAL	Green	187 ASP	Green	237 ASP	Green
38 HIS	Green	88 HIS	Green	138 VAL	Green	188 ASP	Green	238 ASP	Green
39 HIS	Green	89 HIS	Green	139 VAL	Green	189 ASP	Green	239 ASP	Green
40 HIS	Green	90 HIS	Green	140 VAL	Green	190 ASP	Green	240 ASP	Green
41 HIS	Green	91 HIS	Green	141 VAL	Green	191 ASP	Green	241 ASP	Green
42 HIS	Green	92 HIS	Green	142 VAL	Green	192 ASP	Green	242 ASP	Green
43 HIS	Green	93 HIS	Green	143 VAL	Green	193 ASP	Green	243 ASP	Green
44 HIS	Green	94 HIS	Green	144 VAL	Green	194 ASP	Green	244 ASP	Green
45 HIS	Green	95 HIS	Green	145 VAL	Green	195 ASP	Green	245 ASP	Green
46 HIS	Green	96 HIS	Green	146 VAL	Green	196 ASP	Green	246 ASP	Green
47 HIS	Green	97 HIS	Green	147 VAL	Green	197 ASP	Green	247 ASP	Green
48 HIS	Green	98 HIS	Green	148 VAL	Green	198 ASP	Green	248 ASP	Green
49 HIS	Green	99 HIS	Green	149 VAL	Green	199 ASP	Green	2	

- Chain B: 



• Molecule 1: Glycogen [starch] synthase isoform 2

Chain C: 53% 27% 5% 15%



PRO	GLY	SER	PRO	ARG	ASP	LEU	ARG	SER	ASN	THR	VAL	TYR	MET	THR	PRO	GLY	ASP	ASP	LEU	GLY	THR	LEU	GLN	GLU	VAL	ASN	ASN	ALA	ASP	ASP	TYR	PHE	SER	LEU	GLY	VAL	ASN	ASN	PRO	ALA	ALA	ASP	ASP	ASP	ASP	GLY	PRO	TYR	ALA	ASP	SER
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• Molecule 1: Glycogen [starch] synthase isoform 2

Chain D:  54% 26% 15%

THR	VAL	TYR	VAL	TYR	MET	THR	PRO	GLY	ASP	LEU	GLY	THR	THR	LEU	GLN	GLU	VAL	ASN	ASN	ALA	ASP	ASP	TYR	PHE	SER	LEU	VAL	ASN	PRO	ALA	ALA	ASP	ASP	ASP	ASP	ASP	GLY	PRO	TYR	ALA	LYS	LYS	LEU	LYS	VAL	ALA	ARG	PRO	LEU	SER	VAL	GLY	SER	PRO	ARG	ASP	LEU	ARG	SER	ASN	ASP	SER																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
F575	V576	K577	K578	T579	A580	A581	Q582	A583	I584	N585	Q586	R587	H588	R589	T590	S594	D595	L596	R610	G611	L612	R616	R623	M634	K635	D636	A637	L638	A639	GLY	GLY	LYS	LEU	LYS	VAL	ALA	ARG	PRO	LEU	SER	VAL	PRO	PRO	SER	ARG	ASP	LEU	ARG	SER	ASN	ASP	SER	GLY	SER	GLY	VAL	PRO	ARG	GLY	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER	GLY	VAL	PRO	ARG	GLY	SER

• Molecule 2: Glycogen [starch] synthase isoform 2

Chain E:  40% 60%

X3	X4	UNK	UNK	UNK
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• Molecule 2: Glycogen [starch] synthase isoform 2

Chain F:  100%


There are no outlier residues recorded for this chain.

• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain G:  50% 50%



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain H:  75% 25%



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain I:  100%



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain J:  25% 75%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.56Å 166.73Å 121.14Å 90.00° 103.25° 90.00°	Depositor
Resolution (Å)	47.56 – 3.01 47.56 – 3.01	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.56-3.01) 98.9 (47.56-3.01)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.207 , 0.244 0.200 , 0.242	Depositor DCC
R_{free} test set	3673 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	83.5	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20011	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, SO4

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	0.39	0/5038	0.54	0/6819
1	B	0.39	0/5038	0.54	0/6819
1	C	0.40	0/5050	0.56	0/6835
1	D	0.39	0/5050	0.55	1/6835 (0.0%)
All	All	0.39	0/20176	0.55	1/27308 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	540	LEU	CA-CB-CG	5.14	127.12	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4923	0	4850	165	0
1	B	4923	0	4850	156	0
1	C	4935	0	4859	169	0
1	D	4935	0	4859	168	0
2	E	10	0	4	0	0
2	F	25	0	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	45	0	39	1	0
3	H	45	0	39	2	0
3	I	45	0	39	0	0
3	J	45	0	39	2	0
4	A	20	0	0	1	0
4	B	20	0	0	0	0
4	C	20	0	0	1	0
4	D	20	0	0	1	0
All	All	20011	0	19585	644	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

The worst 5 of 644 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:539:ASP:O	1:C:540:LEU:HD23	1.57	1.02
1:C:314:TYR:H	1:C:500:HIS:HD2	1.10	0.95
1:D:314:TYR:H	1:D:500:HIS:HD2	1.07	0.93
1:B:235:ARG:HH21	1:B:260:LYS:HG3	1.35	0.91
1:A:235:ARG:HH21	1:A:260:LYS:HG3	1.34	0.90

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	601/725 (83%)	535 (89%)	56 (9%)	10 (2%)	9	39
1	B	601/725 (83%)	542 (90%)	49 (8%)	10 (2%)	9	39
1	C	603/725 (83%)	550 (91%)	46 (8%)	7 (1%)	13	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	603/725 (83%)	548 (91%)	50 (8%)	5 (1%)	19	57
All	All	2408/2900 (83%)	2175 (90%)	201 (8%)	32 (1%)	12	45

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	TYR
1	A	449	ASP
1	B	114	TYR
1	B	449	ASP
1	C	285	LEU

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	526/622 (85%)	478 (91%)	48 (9%)	9	34
1	B	526/622 (85%)	477 (91%)	49 (9%)	9	33
1	C	527/622 (85%)	474 (90%)	53 (10%)	7	29
1	D	527/622 (85%)	475 (90%)	52 (10%)	8	30
All	All	2106/2488 (85%)	1904 (90%)	202 (10%)	8	32

5 of 202 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	488	LEU
1	C	183	ARG
1	D	458	LYS
1	B	633	SER
1	C	86	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	500	HIS
1	C	8	HIS
1	D	300	HIS
1	B	567	GLN
1	B	634	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 ⓘ

16 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	$\# Z > 2$
3	GLC	G	1	3	12,12,12	0.79	0	17,17,17	1.06	1 (5%)
3	GLC	G	2	3	11,11,12	0.84	0	15,15,17	1.84	5 (33%)
3	GLC	G	3	3	11,11,12	1.38	1 (9%)	15,15,17	2.67	6 (40%)
3	GLC	G	4	3	11,11,12	1.21	1 (9%)	15,15,17	2.09	5 (33%)
3	GLC	H	1	3	12,12,12	1.11	1 (8%)	17,17,17	1.64	3 (17%)
3	GLC	H	2	3	11,11,12	0.80	0	15,15,17	2.02	6 (40%)
3	GLC	H	3	3	11,11,12	0.93	0	15,15,17	1.88	3 (20%)
3	GLC	H	4	3	11,11,12	0.84	0	15,15,17	1.72	4 (26%)
3	GLC	I	1	3	12,12,12	0.78	0	17,17,17	1.17	1 (5%)
3	GLC	I	2	3	11,11,12	0.81	0	15,15,17	1.50	3 (20%)
3	GLC	I	3	3	11,11,12	0.82	0	15,15,17	2.26	5 (33%)
3	GLC	I	4	3	11,11,12	0.92	0	15,15,17	1.83	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GLC	J	1	3	12,12,12	0.85	0	17,17,17	1.33	1 (5%)
3	GLC	J	2	3	11,11,12	0.91	0	15,15,17	1.60	4 (26%)
3	GLC	J	3	3	11,11,12	1.18	1 (9%)	15,15,17	2.17	5 (33%)
3	GLC	J	4	3	11,11,12	0.83	0	15,15,17	1.91	6 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	4	GLC	O5-C1	3.09	1.48	1.43
3	G	3	GLC	C4-C5	3.00	1.59	1.53
3	H	1	GLC	O4-C4	2.53	1.48	1.43
3	J	3	GLC	O5-C1	2.18	1.47	1.43

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	3	GLC	O4-C4-C5	6.21	124.71	109.30
3	I	3	GLC	O4-C4-C5	5.02	121.75	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	3	GLC	O5-C5-C6	4.90	114.89	107.20
3	G	4	GLC	C6-C5-C4	-4.65	102.12	113.00
3	J	3	GLC	C1-C2-C3	4.29	114.94	109.67

There are no chirality outliers.

All (3) torsion outliers are listed below:

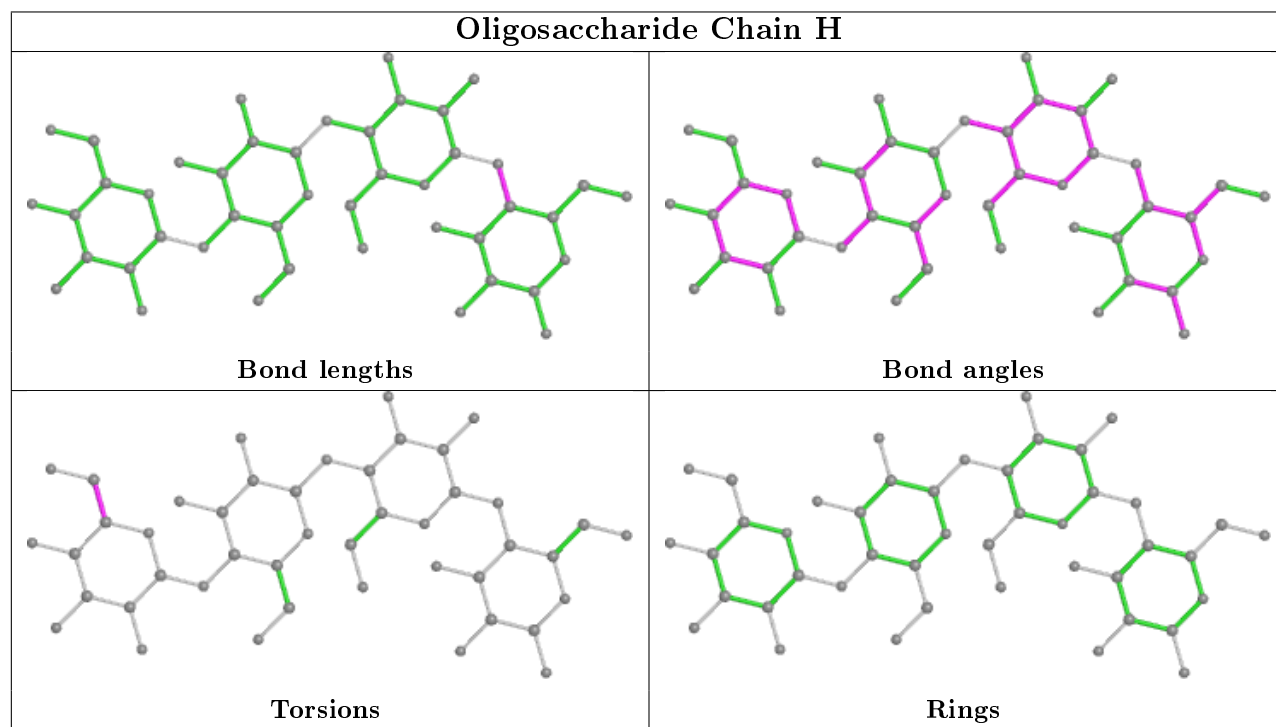
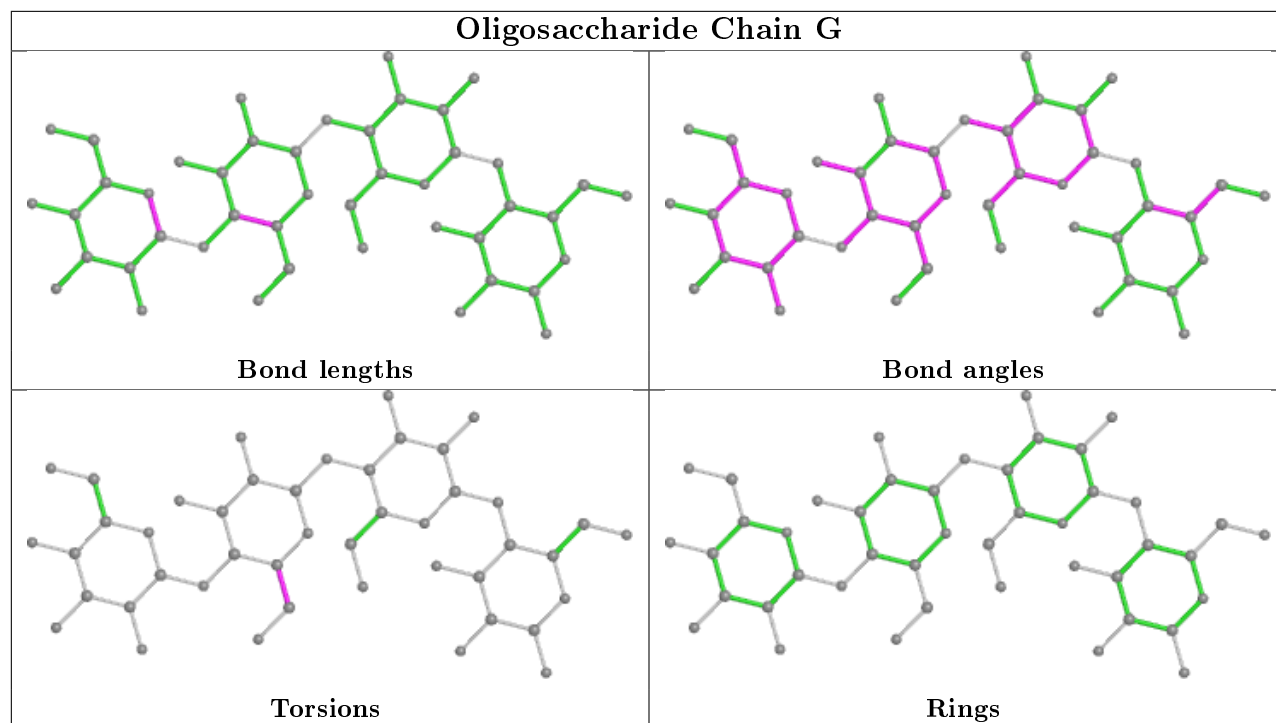
Mol	Chain	Res	Type	Atoms
3	H	4	GLC	O5-C5-C6-O6
3	G	3	GLC	O5-C5-C6-O6
3	H	4	GLC	C4-C5-C6-O6

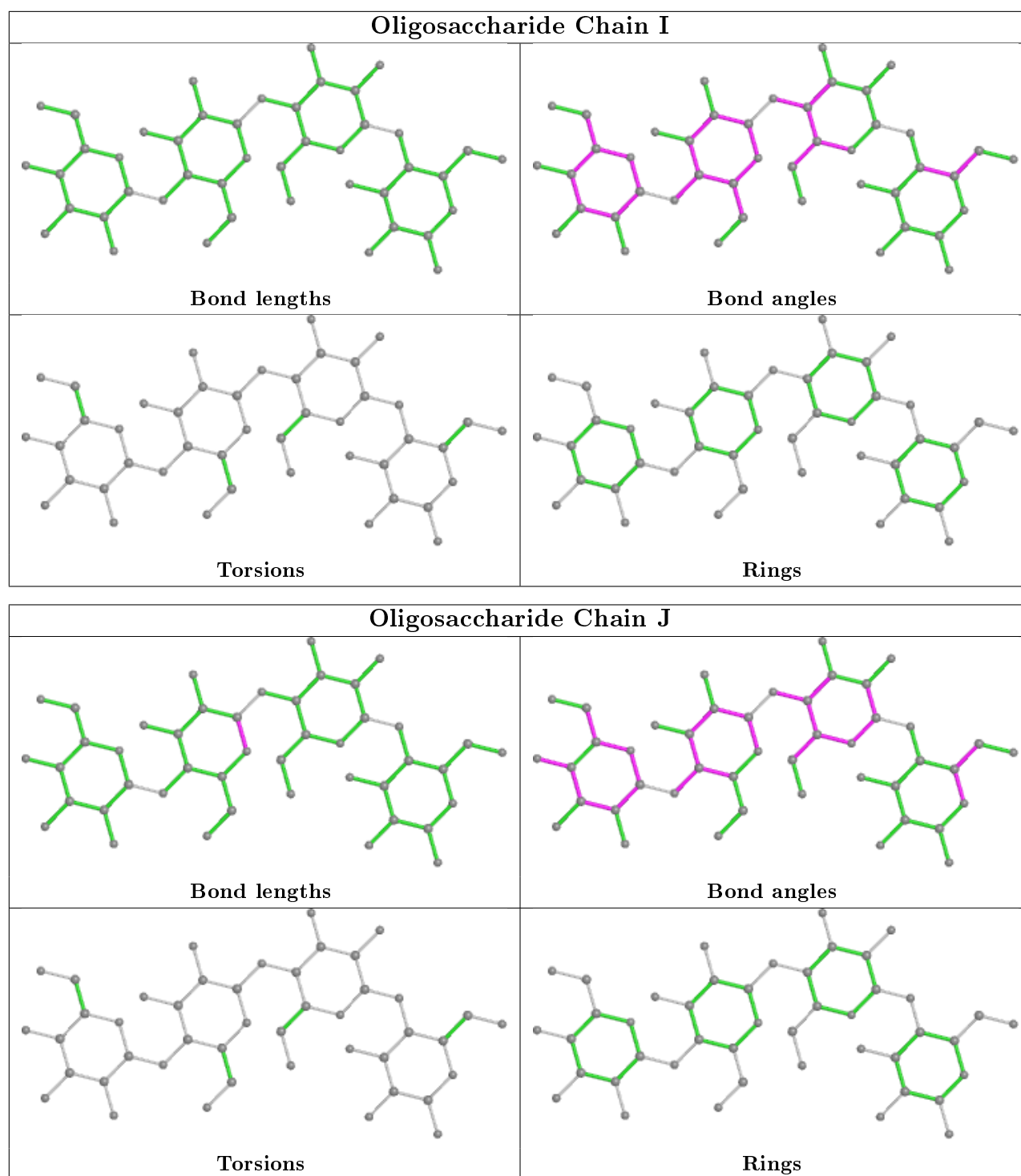
There are no ring outliers.

6 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	4	GLC	1	0
3	G	2	GLC	1	0
3	H	3	GLC	2	0
3	J	3	GLC	1	0
3	G	1	GLC	1	0
3	J	2	GLC	1	0

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





5.6 Ligand geometry [i](#)

16 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	$\# Z > 2$
4	SO4	D	801	-	4,4,4	0.33	0	6,6,6	0.41	0
4	SO4	B	801	-	4,4,4	0.16	0	6,6,6	0.26	0
4	SO4	C	706	-	4,4,4	0.18	0	6,6,6	0.27	0
4	SO4	C	804	-	4,4,4	0.13	0	6,6,6	0.20	0
4	SO4	D	804	-	4,4,4	0.13	0	6,6,6	0.24	0
4	SO4	A	804	-	4,4,4	0.15	0	6,6,6	0.20	0
4	SO4	B	804	-	4,4,4	0.12	0	6,6,6	0.11	0
4	SO4	D	803	-	4,4,4	0.16	0	6,6,6	0.18	0
4	SO4	A	801	-	4,4,4	0.15	0	6,6,6	0.13	0
4	SO4	B	706	-	4,4,4	0.20	0	6,6,6	0.22	0
4	SO4	C	801	-	4,4,4	0.19	0	6,6,6	0.08	0
4	SO4	B	802	-	4,4,4	0.34	0	6,6,6	0.29	0
4	SO4	A	803	-	4,4,4	0.19	0	6,6,6	0.21	0
4	SO4	D	802	-	4,4,4	0.15	0	6,6,6	0.21	0
4	SO4	A	802	-	4,4,4	0.23	0	6,6,6	0.41	0
4	SO4	C	803	-	4,4,4	0.18	0	6,6,6	0.16	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	801	SO4	1	0
4	C	801	SO4	1	0
4	D	802	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	611/725 (84%)	-0.18	7 (1%) 80 56	56, 79, 114, 153	0
1	B	611/725 (84%)	-0.20	7 (1%) 80 56	57, 80, 114, 154	0
1	C	613/725 (84%)	-0.31	3 (0%) 91 75	50, 78, 106, 133	0
1	D	613/725 (84%)	-0.27	2 (0%) 94 84	50, 77, 106, 133	0
2	E	0/5	-	-	-	-
2	F	0/5	-	-	-	-
All	All	2448/2910 (84%)	-0.24	19 (0%) 86 65	50, 78, 111, 154	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	631	ASN	4.3
1	A	549	TYR	4.1
1	B	630	LEU	3.5
1	A	548	ASP	3.4
1	B	549	TYR	3.0

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

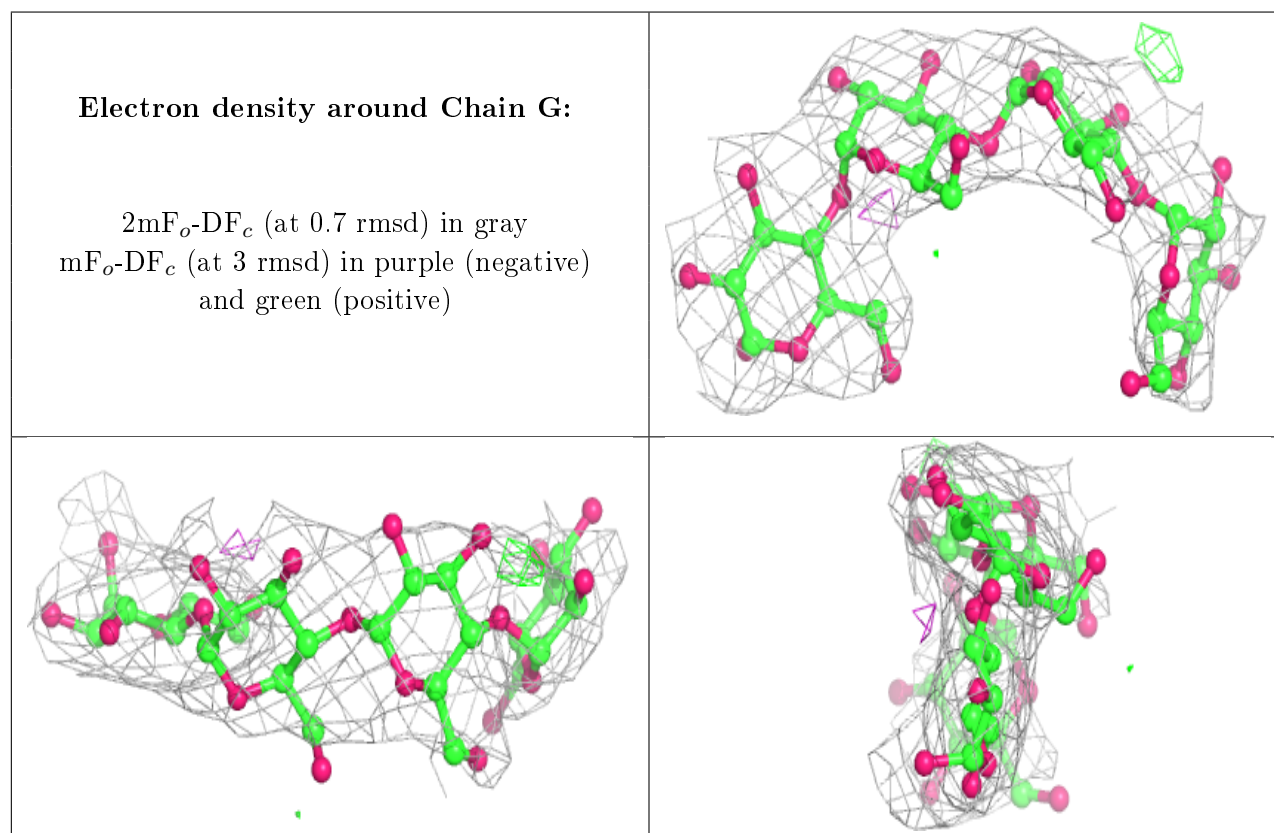
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

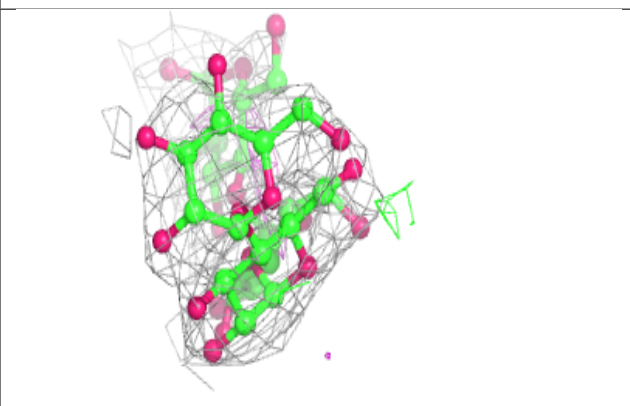
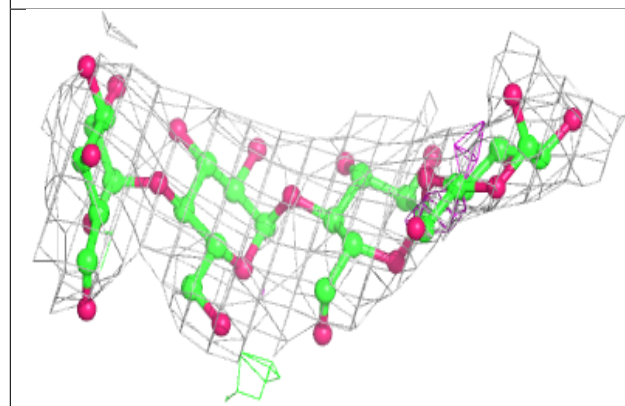
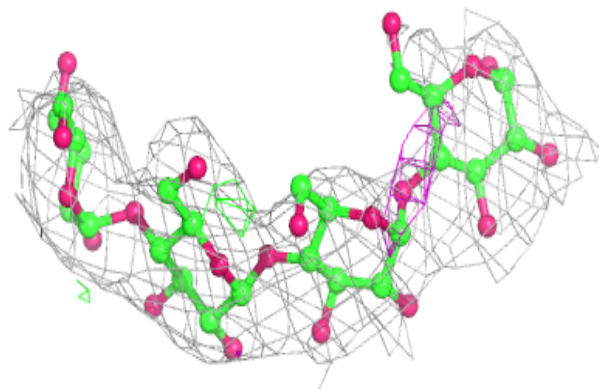
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GLC	J	4	11/12	0.69	0.45	123,130,136,140	0
3	GLC	G	4	11/12	0.76	0.33	127,138,144,144	0
3	GLC	J	1	12/12	0.79	0.52	91,108,114,118	0
3	GLC	H	1	12/12	0.82	0.25	82,95,103,106	0
3	GLC	J	3	11/12	0.85	0.27	99,114,129,131	0
3	GLC	H	4	11/12	0.86	0.24	98,110,116,123	0
3	GLC	I	4	11/12	0.87	0.27	119,124,127,131	0
3	GLC	J	2	11/12	0.87	0.36	90,93,105,112	0
3	GLC	G	1	12/12	0.89	0.16	89,95,100,100	0
3	GLC	I	1	12/12	0.89	0.20	92,95,100,110	0
3	GLC	G	3	11/12	0.91	0.15	105,117,130,131	0
3	GLC	G	2	11/12	0.92	0.19	95,100,108,112	0
3	GLC	H	3	11/12	0.92	0.19	84,89,108,112	0
3	GLC	I	2	11/12	0.93	0.21	89,96,104,112	0
3	GLC	I	3	11/12	0.94	0.14	96,106,116,117	0
3	GLC	H	2	11/12	0.95	0.27	80,86,92,92	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.

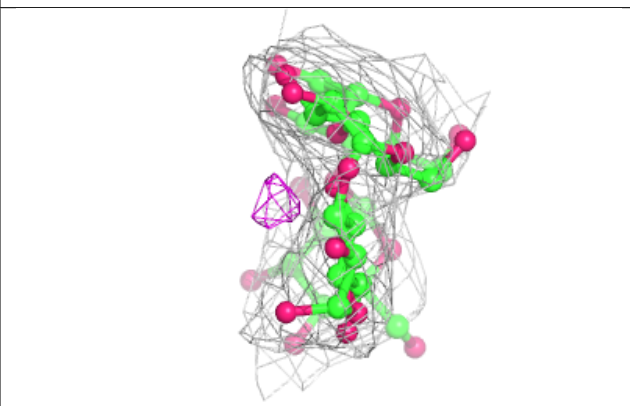
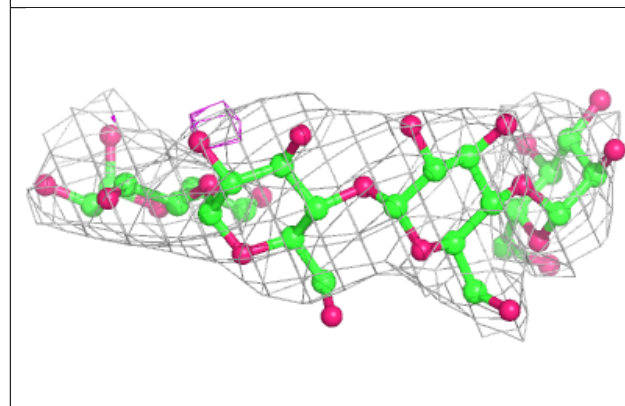
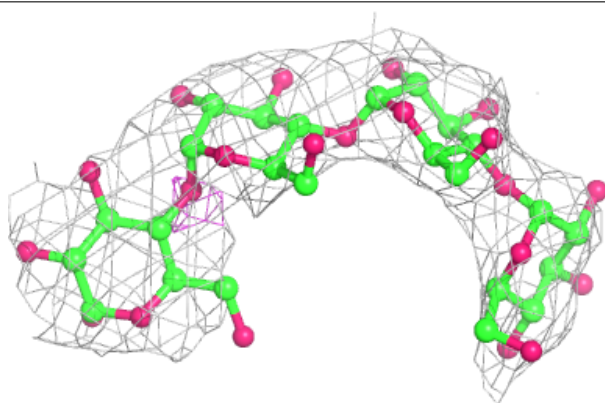


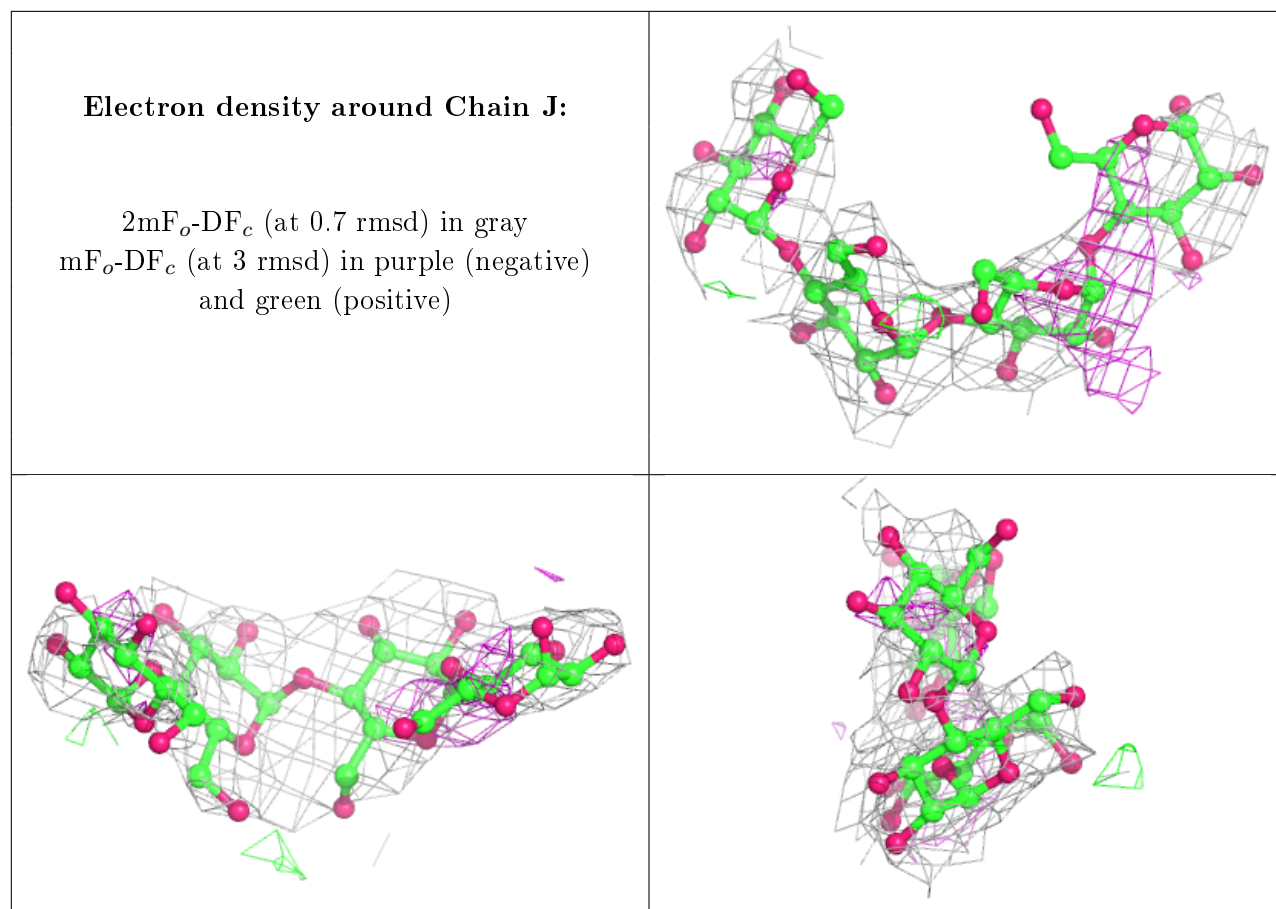
Electron density around Chain H:

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

**Electron density around Chain I:**

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





6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	D	801	5/5	0.47	0.30	95,97,124,140	0
4	SO4	D	803	5/5	0.83	0.20	109,116,122,132	0
4	SO4	C	803	5/5	0.83	0.26	105,118,128,139	0
4	SO4	B	802	5/5	0.88	0.29	84,95,108,127	0
4	SO4	D	804	5/5	0.88	0.27	121,122,126,138	0
4	SO4	A	804	5/5	0.89	0.19	122,133,134,143	0
4	SO4	C	706	5/5	0.90	0.20	103,106,122,136	0
4	SO4	A	803	5/5	0.90	0.18	93,99,118,120	0
4	SO4	B	804	5/5	0.90	0.21	129,130,133,146	0
4	SO4	B	801	5/5	0.91	0.22	87,89,108,114	0
4	SO4	B	706	5/5	0.91	0.17	96,107,112,125	0
4	SO4	A	802	5/5	0.92	0.26	77,83,98,116	0
4	SO4	C	804	5/5	0.94	0.28	126,128,131,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	A	801	5/5	0.95	0.15	83,90,100,102	0
4	SO4	D	802	5/5	0.95	0.16	89,93,109,112	0
4	SO4	C	801	5/5	0.96	0.12	90,90,110,114	0

6.5 Other polymers [i](#)

There are no such residues in this entry.