



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2026 – 01:53 PM UTC

PDB ID : 4OKD / pdb_00004okd
Title : Crystal Structure of Chlamydomonas reinhardtii Isoamylase 1 (ISA1) in complex with maltoheptaose
Authors : Sim, L.; Palcic, M.
Deposited on : 2014-01-22
Resolution : 2.40 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

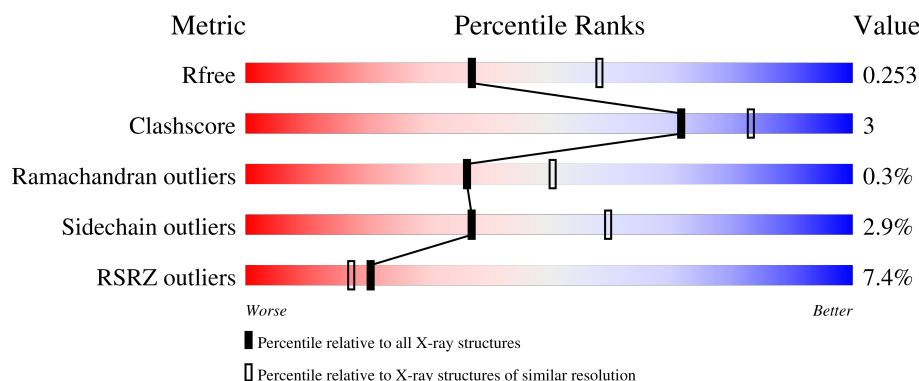
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

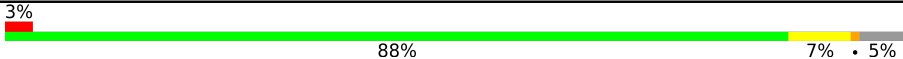
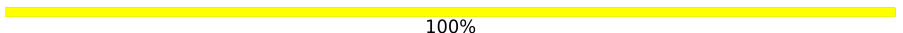
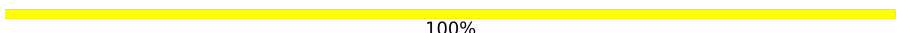
The reported resolution of this entry is 2.40 Å.

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.



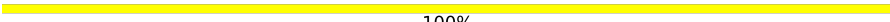
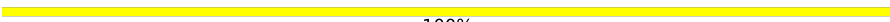
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	840	
1	B	840	
2	C	7	
2	F	7	
3	D	3	

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Mol	Chain	Length	Quality of chain
3	E	3	 100%
3	G	3	 100%

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
2	GLC	C	1	X	-	-	-
2	GLC	F	1	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13042 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 Isoamylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	801	Total	C	N	O	S	0	0	0
			6207	3919	1090	1168	30			
1	B	792	Total	C	N	O	S	0	1	0
			6134	3878	1077	1149	30			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	MET	-	expression tag	UNP Q7X8Q2
A	37	GLY	-	expression tag	UNP Q7X8Q2
A	38	SER	-	expression tag	UNP Q7X8Q2
A	39	SER	-	expression tag	UNP Q7X8Q2
A	40	HIS	-	expression tag	UNP Q7X8Q2
A	41	HIS	-	expression tag	UNP Q7X8Q2
A	42	HIS	-	expression tag	UNP Q7X8Q2
A	43	HIS	-	expression tag	UNP Q7X8Q2
A	44	HIS	-	expression tag	UNP Q7X8Q2
A	45	HIS	-	expression tag	UNP Q7X8Q2
A	46	SER	-	expression tag	UNP Q7X8Q2
A	47	SER	-	expression tag	UNP Q7X8Q2
A	48	GLY	-	expression tag	UNP Q7X8Q2
A	49	LEU	-	expression tag	UNP Q7X8Q2
A	50	VAL	-	expression tag	UNP Q7X8Q2
A	51	PRO	-	expression tag	UNP Q7X8Q2
A	52	ARG	-	expression tag	UNP Q7X8Q2
A	53	GLY	-	expression tag	UNP Q7X8Q2
A	54	SER	-	expression tag	UNP Q7X8Q2
A	55	HIS	-	expression tag	UNP Q7X8Q2
A	56	MET	-	expression tag	UNP Q7X8Q2
B	36	MET	-	expression tag	UNP Q7X8Q2
B	37	GLY	-	expression tag	UNP Q7X8Q2
B	38	SER	-	expression tag	UNP Q7X8Q2
B	39	SER	-	expression tag	UNP Q7X8Q2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	40	HIS	-	expression tag	UNP Q7X8Q2
B	41	HIS	-	expression tag	UNP Q7X8Q2
B	42	HIS	-	expression tag	UNP Q7X8Q2
B	43	HIS	-	expression tag	UNP Q7X8Q2
B	44	HIS	-	expression tag	UNP Q7X8Q2
B	45	HIS	-	expression tag	UNP Q7X8Q2
B	46	SER	-	expression tag	UNP Q7X8Q2
B	47	SER	-	expression tag	UNP Q7X8Q2
B	48	GLY	-	expression tag	UNP Q7X8Q2
B	49	LEU	-	expression tag	UNP Q7X8Q2
B	50	VAL	-	expression tag	UNP Q7X8Q2
B	51	PRO	-	expression tag	UNP Q7X8Q2
B	52	ARG	-	expression tag	UNP Q7X8Q2
B	53	GLY	-	expression tag	UNP Q7X8Q2
B	54	SER	-	expression tag	UNP Q7X8Q2
B	55	HIS	-	expression tag	UNP Q7X8Q2
B	56	MET	-	expression tag	UNP Q7X8Q2

- Molecule 2 is an oligosaccharide called 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.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	7	Total	C	O	0	0	0
			77	42	35			
2	F	7	Total	C	O	0	0	0
			77	42	35			

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



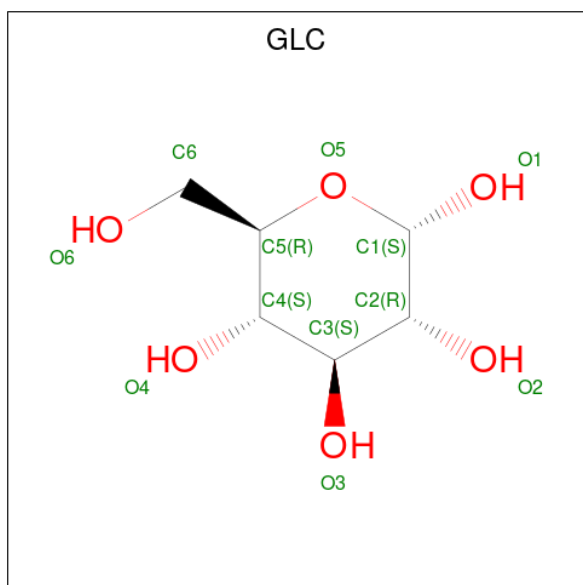
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	3	Total	C	O	0	0	0
			34	18	16			

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

- Molecule 4 is alpha-D-glucopyranose (CCD ID: GLC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	6	6		

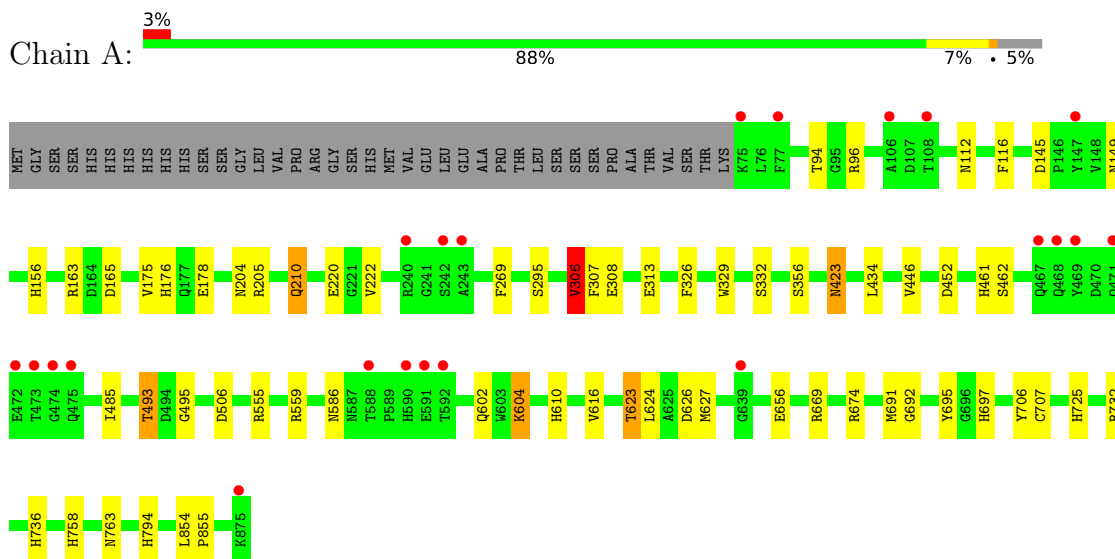
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	206	Total	O	0	0
			206	206		
5	B	227	Total	O	0	0
			227	227		

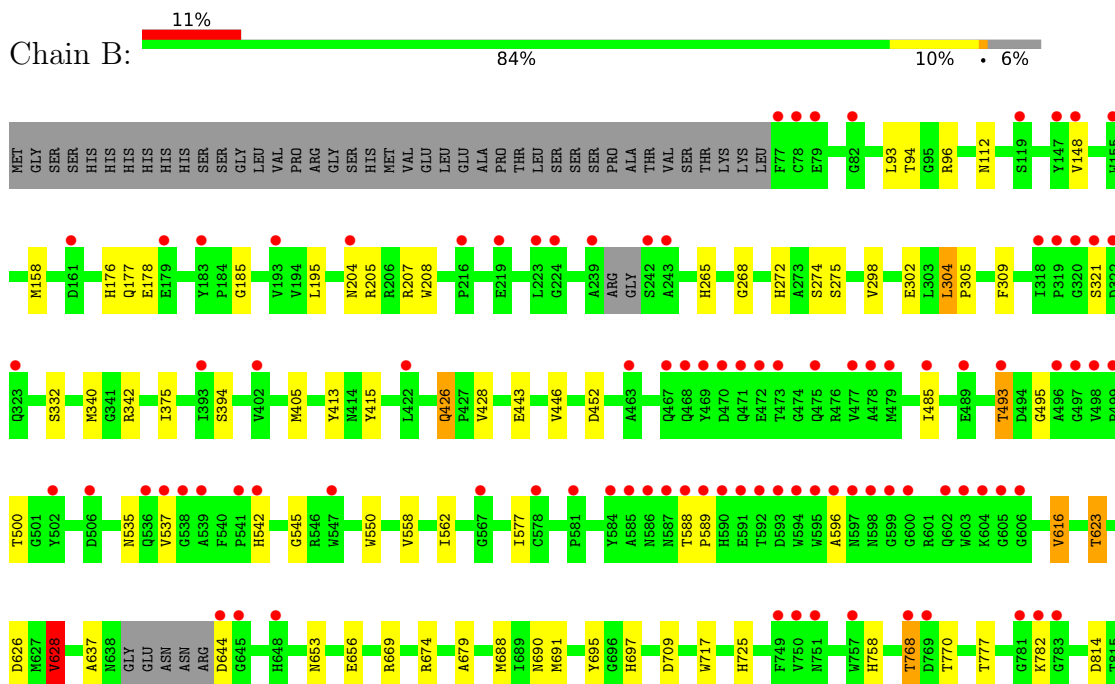
3 Residue-property plots [i](#)

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: Isoamylase



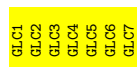
• Molecule 1: Isoamylase





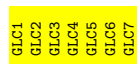
- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain C: 100%



- Molecule 2: 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

Chain F: 100%



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

Chain D: 33% 67%



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

Chain E: 100%



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

Chain G: 100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	102.75Å 102.75Å 487.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.95 – 2.40 45.95 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.2 (45.95-2.40) 97.2 (45.95-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.192 , 0.227 0.227 , 0.253	Depositor DCC
R_{free} test set	5040 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13042	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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

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	0.67	1/6390 (0.0%)	0.84	4/8723 (0.0%)
1	B	0.70	1/6319 (0.0%)	0.84	4/8629 (0.0%)
All	All	0.68	2/12709 (0.0%)	0.84	8/17352 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	452	ASP	CG-OD1	12.99	1.50	1.25
1	A	452	ASP	CG-OD1	12.96	1.50	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	616	VAL	N-CA-C	-6.74	106.22	112.96
1	A	306	VAL	N-CA-CB	-6.32	104.81	112.33
1	B	628	VAL	N-CA-C	-5.80	107.61	113.47
1	A	306	VAL	CB-CA-C	5.63	116.70	110.62
1	A	306	VAL	N-CA-C	-5.47	107.94	113.47
1	B	628	VAL	N-CA-CB	-5.37	105.94	112.33
1	A	604	LYS	N-CA-C	5.09	118.64	112.23
1	B	321	SER	N-CA-C	5.08	116.40	109.18

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	6207	0	5804	35	0
1	B	6134	0	5724	47	0
2	C	77	0	64	0	0
2	F	77	0	64	0	0
3	D	34	0	30	0	0
3	E	34	0	30	0	0
3	G	34	0	30	0	0
4	A	12	0	12	0	0
5	A	206	0	0	4	0
5	B	227	0	0	3	0
All	All	13042	0	11758	81	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 3.

All (81) 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:B:623:THR:HG21	1:B:697:HIS:O	1.74	0.86
1:B:443:GLU:HG2	5:B:1318:HOH:O	1.78	0.83
1:A:423:ASN:HD21	1:A:462:SER:H	1.39	0.70
1:B:405:MET:HE1	1:B:415:TYR:HE2	1.59	0.66
1:A:623:THR:HG21	1:A:697:HIS:O	2.00	0.62
1:B:542:HIS:HD2	1:B:545:GLY:H	1.49	0.61
1:A:96:ARG:H	1:A:112:ASN:HD21	1.47	0.60
1:A:623:THR:HG22	1:A:626:ASP:H	1.67	0.59
1:B:628:VAL:HG13	1:B:669:ARG:HG2	1.85	0.59
1:B:768:THR:HG23	1:B:770:THR:H	1.66	0.59
1:A:758:HIS:HD2	1:A:763:ASN:H	1.52	0.58
1:B:542:HIS:CD2	1:B:545:GLY:H	2.22	0.57
1:B:94:THR:HG22	1:B:148:VAL:HG12	1.87	0.57
1:B:176:HIS:HD2	1:B:178:GLU:H	1.55	0.55
1:B:265:HIS:HD2	1:B:268:GLY:H	1.55	0.55
1:B:96:ARG:H	1:B:112:ASN:HD21	1.55	0.54
1:A:176:HIS:HD2	1:A:178:GLU:H	1.55	0.53
1:A:493:THR:HG21	5:A:1181:HOH:O	2.08	0.53
1:A:758:HIS:CD2	1:A:763:ASN:H	2.27	0.52
1:B:674:ARG:HH12	1:B:725:HIS:CD2	2.28	0.52
1:B:623:THR:CG2	1:B:697:HIS:O	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:558:VAL:HG13	1:B:562:ILE:HD12	1.93	0.51
1:B:94:THR:HG22	1:B:148:VAL:CG1	2.39	0.51
1:B:674:ARG:HH12	1:B:725:HIS:HD2	1.58	0.50
1:B:204:ASN:OD1	1:B:205:ARG:N	2.39	0.50
1:A:555:ARG:O	1:A:559:ARG:HG3	2.12	0.50
1:B:405:MET:HE2	1:B:413:TYR:CG	2.46	0.50
1:B:550:TRP:CZ2	1:B:688:MET:HE1	2.48	0.49
1:A:307:PHE:O	1:A:308:GLU:C	2.56	0.49
1:B:309:PHE:CE1	1:B:340:MET:HE2	2.47	0.48
1:A:732:ARG:O	1:A:736:HIS:HD2	1.95	0.48
1:A:656:GLU:O	1:A:669:ARG:NH2	2.46	0.48
1:B:405:MET:HE3	1:B:500:THR:CG2	2.43	0.48
1:A:94:THR:O	1:A:156:HIS:HD2	1.96	0.48
1:B:426:GLN:OE1	1:B:428:VAL:N	2.42	0.48
1:B:272:HIS:HD2	1:B:274:SER:OG	1.97	0.48
1:B:588:THR:O	1:B:588:THR:HG23	2.14	0.48
1:A:485:ILE:O	1:A:493:THR:HB	2.14	0.47
1:B:485:ILE:O	1:B:493:THR:HB	2.14	0.47
1:B:814:ASP:HB3	1:B:817:LYS:HG2	1.96	0.47
1:A:692:GLY:HA2	1:A:695:TYR:CE2	2.50	0.46
1:B:709:ASP:N	5:B:1153:HOH:O	2.38	0.46
1:A:493:THR:HG22	1:A:495:GLY:H	1.81	0.46
1:A:116:PHE:CD1	1:A:116:PHE:C	2.95	0.45
1:A:758:HIS:HD2	1:A:763:ASN:N	2.13	0.45
1:B:207:ARG:C	1:B:342:ARG:HG2	2.41	0.45
1:B:304:LEU:HB3	1:B:305:PRO:HD2	1.99	0.45
1:B:93:LEU:HD12	1:B:158:MET:HE2	1.98	0.45
1:B:840:ARG:O	1:B:841:GLN:C	2.59	0.45
1:A:854:LEU:HD13	1:B:845:TRP:CD2	2.51	0.45
1:A:204:ASN:OD1	1:A:205:ARG:N	2.43	0.44
1:B:623:THR:HG23	5:B:1103:HOH:O	2.17	0.44
1:B:623:THR:HG22	1:B:626:ASP:H	1.83	0.44
1:A:674:ARG:NH2	1:A:725:HIS:HD2	2.15	0.43
1:B:208:TRP:N	1:B:342:ARG:HG2	2.34	0.43
1:A:306:VAL:HB	5:A:1122:HOH:O	2.18	0.43
1:B:816:SER:HB2	1:B:854:LEU:HD22	2.01	0.43
1:B:562:ILE:HD11	1:B:679:ALA:HB2	2.01	0.43
1:B:589:PRO:HB3	1:B:596:ALA:HB1	2.00	0.43
1:A:493:THR:CG2	5:A:1181:HOH:O	2.66	0.42
1:B:304:LEU:HB3	1:B:305:PRO:CD	2.50	0.42
1:B:653:ASN:HB2	1:B:656:GLU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:HIS:CD2	1:A:178:GLU:H	2.35	0.42
1:B:275:SER:HA	1:B:717:TRP:CD1	2.55	0.42
1:A:295:SER:HB2	5:A:1145:HOH:O	2.20	0.42
1:B:177:GLN:NE2	1:B:185:GLY:H	2.17	0.42
1:A:423:ASN:ND2	1:A:461:HIS:HB2	2.35	0.41
1:A:610:HIS:H	1:A:610:HIS:CD2	2.37	0.41
1:B:690:ASN:O	1:B:691:MET:C	2.62	0.41
1:A:165:ASP:OD1	1:A:165:ASP:C	2.64	0.41
1:A:329:TRP:CD2	1:A:706:TYR:HA	2.56	0.41
1:A:205:ARG:HD2	1:A:210:GLN:O	2.21	0.41
1:B:302:GLU:HA	1:B:375:ILE:O	2.21	0.41
1:B:758:HIS:CE1	1:B:777:THR:HG23	2.56	0.41
1:B:695:TYR:CE1	1:B:697:HIS:HB2	2.55	0.41
1:A:145:ASP:H	1:A:149:ASN:HD22	1.69	0.40
1:A:559:ARG:HG2	1:A:627:MET:HE3	2.02	0.40
1:A:794:HIS:C	1:A:855:PRO:HB3	2.46	0.40
1:A:326:PHE:O	1:A:707:CYS:HA	2.22	0.40
1:B:493:THR:CG2	1:B:495:GLY:H	2.33	0.40
1:A:269:PHE:HD1	1:A:691:MET:HE2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	799/840 (95%)	757 (95%)	41 (5%)	1 (0%)	48	64
1	B	787/840 (94%)	751 (95%)	33 (4%)	3 (0%)	30	43
All	All	1586/1680 (94%)	1508 (95%)	74 (5%)	4 (0%)	36	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	332	SER
1	B	394	SER
1	B	637	ALA
1	A	332	SER

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	636/686 (93%)	617 (97%)	19 (3%)	36	58
1	B	627/686 (91%)	610 (97%)	17 (3%)	39	62
All	All	1263/1372 (92%)	1227 (97%)	36 (3%)	37	60

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	ARG
1	A	175	VAL
1	A	210	GLN
1	A	220	GLU
1	A	222	VAL
1	A	306	VAL
1	A	313	GLU
1	A	356	SER
1	A	423	ASN
1	A	434	LEU
1	A	446	VAL
1	A	493	THR
1	A	506	ASP
1	A	586	ASN
1	A	602	GLN
1	A	604	LYS
1	A	616	VAL
1	A	623	THR
1	A	624	LEU
1	B	195	LEU

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Mol	Chain	Res	Type
1	B	298	VAL
1	B	304	LEU
1	B	426	GLN
1	B	446	VAL
1	B	493	THR
1	B	535	ASN
1	B	537	VAL
1	B	577	ILE
1	B	616	VAL
1	B	623	THR
1	B	628	VAL
1	B	644	ASP
1	B	768	THR
1	B	782	LYS
1	B	858	CYS
1	B	874	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	ASN
1	A	149	ASN
1	A	156	HIS
1	A	176	HIS
1	A	214	ASN
1	A	265	HIS
1	A	272	HIS
1	A	381	ASN
1	A	423	ASN
1	A	445	HIS
1	A	467	GLN
1	A	521	ASN
1	A	535	ASN
1	A	597	ASN
1	A	598	ASN
1	A	610	HIS
1	A	650	ASN
1	A	704	ASN
1	A	725	HIS
1	A	736	HIS
1	A	758	HIS
1	A	763	ASN

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Mol	Chain	Res	Type
1	A	800	GLN
1	A	849	HIS
1	B	112	ASN
1	B	176	HIS
1	B	177	GLN
1	B	265	HIS
1	B	272	HIS
1	B	317	GLN
1	B	362	GLN
1	B	381	ASN
1	B	400	ASN
1	B	461	HIS
1	B	542	HIS
1	B	638	ASN
1	B	649	ASN
1	B	650	ASN
1	B	690	ASN
1	B	758	HIS
1	B	763	ASN
1	B	849	HIS

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 ⓘ

23 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	C	1	2,1	11,11,12	0.62	0	15,15,17	3.02	3 (20%)
2	GLC	C	2	2	11,11,12	0.68	0	15,15,17	1.21	1 (6%)
2	GLC	C	3	2	11,11,12	0.68	0	15,15,17	1.40	1 (6%)
2	GLC	C	4	2	11,11,12	0.67	0	15,15,17	1.25	2 (13%)
2	GLC	C	5	2	11,11,12	0.56	0	15,15,17	1.23	1 (6%)
2	GLC	C	6	2	11,11,12	0.68	0	15,15,17	0.79	1 (6%)
2	GLC	C	7	2	11,11,12	0.49	0	15,15,17	1.06	1 (6%)
3	GLC	D	1	3	12,12,12	0.55	0	17,17,17	0.91	0
3	GLC	D	2	3	11,11,12	0.64	0	15,15,17	1.15	1 (6%)
3	GLC	D	3	3	11,11,12	0.64	0	15,15,17	1.39	2 (13%)
3	GLC	E	1	3	12,12,12	0.53	0	17,17,17	1.06	1 (5%)
3	GLC	E	2	3	11,11,12	0.61	0	15,15,17	0.84	1 (6%)
3	GLC	E	3	3	11,11,12	0.45	0	15,15,17	1.25	1 (6%)
2	GLC	F	1	2,1	11,11,12	0.82	0	15,15,17	2.39	6 (40%)
2	GLC	F	2	2	11,11,12	0.71	0	15,15,17	1.12	3 (20%)
2	GLC	F	3	2	11,11,12	0.68	0	15,15,17	1.15	2 (13%)
2	GLC	F	4	2	11,11,12	0.77	0	15,15,17	1.20	2 (13%)
2	GLC	F	5	2	11,11,12	0.87	0	15,15,17	1.20	3 (20%)
2	GLC	F	6	2	11,11,12	0.69	0	15,15,17	2.59	3 (20%)
2	GLC	F	7	2	11,11,12	0.55	0	15,15,17	1.49	3 (20%)
3	GLC	G	1	3	12,12,12	0.51	0	17,17,17	1.02	1 (5%)
3	GLC	G	2	3	11,11,12	0.65	0	15,15,17	1.20	2 (13%)
3	GLC	G	3	3	11,11,12	0.68	0	15,15,17	2.02	4 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	C	1	2,1	1/1/4/5	1/2/19/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	C	3	2	-	0/2/19/22	0/1/1/1
2	GLC	C	4	2	-	0/2/19/22	0/1/1/1
2	GLC	C	5	2	-	1/2/19/22	0/1/1/1
2	GLC	C	6	2	-	0/2/19/22	0/1/1/1
2	GLC	C	7	2	-	0/2/19/22	0/1/1/1

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

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	GLC	C1-O5-C5	10.51	126.27	112.19
2	F	6	GLC	C1-O5-C5	7.52	122.27	112.19
2	F	1	GLC	C1-O5-C5	6.40	120.76	112.19
2	F	6	GLC	O5-C5-C6	-5.02	97.90	107.66
3	G	3	GLC	C1-C2-C3	4.99	116.91	109.64
2	C	3	GLC	C1-O5-C5	4.49	118.21	112.19
3	E	3	GLC	C1-O5-C5	4.00	117.55	112.19
3	D	3	GLC	C1-O5-C5	3.97	117.51	112.19
2	C	1	GLC	C1-C2-C3	3.96	115.41	109.64
2	F	1	GLC	O5-C1-C2	3.63	119.45	110.79
3	G	2	GLC	C1-O5-C5	3.46	116.82	112.19
3	G	3	GLC	C2-C3-C4	3.38	116.81	110.86
3	G	3	GLC	C3-C4-C5	3.27	116.17	110.23
2	C	4	GLC	C1-O5-C5	3.14	116.39	112.19
2	F	7	GLC	O5-C5-C6	3.10	113.70	107.66
2	C	2	GLC	C1-C2-C3	2.93	113.91	109.64
3	G	3	GLC	C1-O5-C5	2.81	115.95	112.19
2	C	4	GLC	C1-C2-C3	2.68	113.55	109.64
2	F	4	GLC	C1-O5-C5	2.63	115.71	112.19
2	F	1	GLC	C1-C2-C3	2.62	113.46	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	GLC	O5-C5-C4	2.62	117.19	110.83
3	D	2	GLC	C1-O5-C5	2.59	115.66	112.19
2	F	3	GLC	C1-O5-C5	2.56	115.61	112.19
2	F	1	GLC	O5-C5-C6	2.52	112.57	107.66
2	F	3	GLC	O5-C5-C6	2.51	112.55	107.66
2	F	5	GLC	O2-C2-C3	2.51	115.34	110.15
2	F	6	GLC	O2-C2-C1	2.46	114.86	109.22
2	C	7	GLC	C1-O5-C5	2.44	115.45	112.19
2	F	7	GLC	C1-O5-C5	2.42	115.43	112.19
2	F	1	GLC	O4-C4-C5	-2.40	103.41	109.32
3	G	2	GLC	C1-C2-C3	2.39	113.12	109.64
2	C	6	GLC	C1-C2-C3	2.37	113.10	109.64
2	F	1	GLC	O5-C5-C4	2.32	116.46	110.83
2	F	7	GLC	O2-C2-C1	2.30	114.49	109.22
3	D	3	GLC	C3-C4-C5	-2.27	106.12	110.23
2	F	5	GLC	O5-C1-C2	-2.25	105.42	110.79
3	E	2	GLC	C1-O5-C5	2.23	115.17	112.19
3	G	1	GLC	O5-C5-C4	2.23	113.71	109.70
2	F	2	GLC	C1-O5-C5	2.20	115.14	112.19
2	F	5	GLC	O3-C3-C2	2.19	114.53	110.05
3	E	1	GLC	C1-O5-C5	2.11	117.74	113.65
2	C	5	GLC	C6-C5-C4	-2.08	107.92	113.02
2	F	4	GLC	C1-C2-C3	2.06	112.65	109.64
2	F	2	GLC	C1-C2-C3	2.06	112.64	109.64
2	F	2	GLC	O4-C4-C3	-2.02	105.62	110.38

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1	GLC	C1
2	F	1	GLC	C1

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	2	GLC	O5-C5-C6-O6
3	G	1	GLC	O5-C5-C6-O6
3	E	2	GLC	C4-C5-C6-O6
3	E	1	GLC	O5-C5-C6-O6
3	G	1	GLC	C4-C5-C6-O6
2	C	1	GLC	C4-C5-C6-O6
3	E	1	GLC	C4-C5-C6-O6

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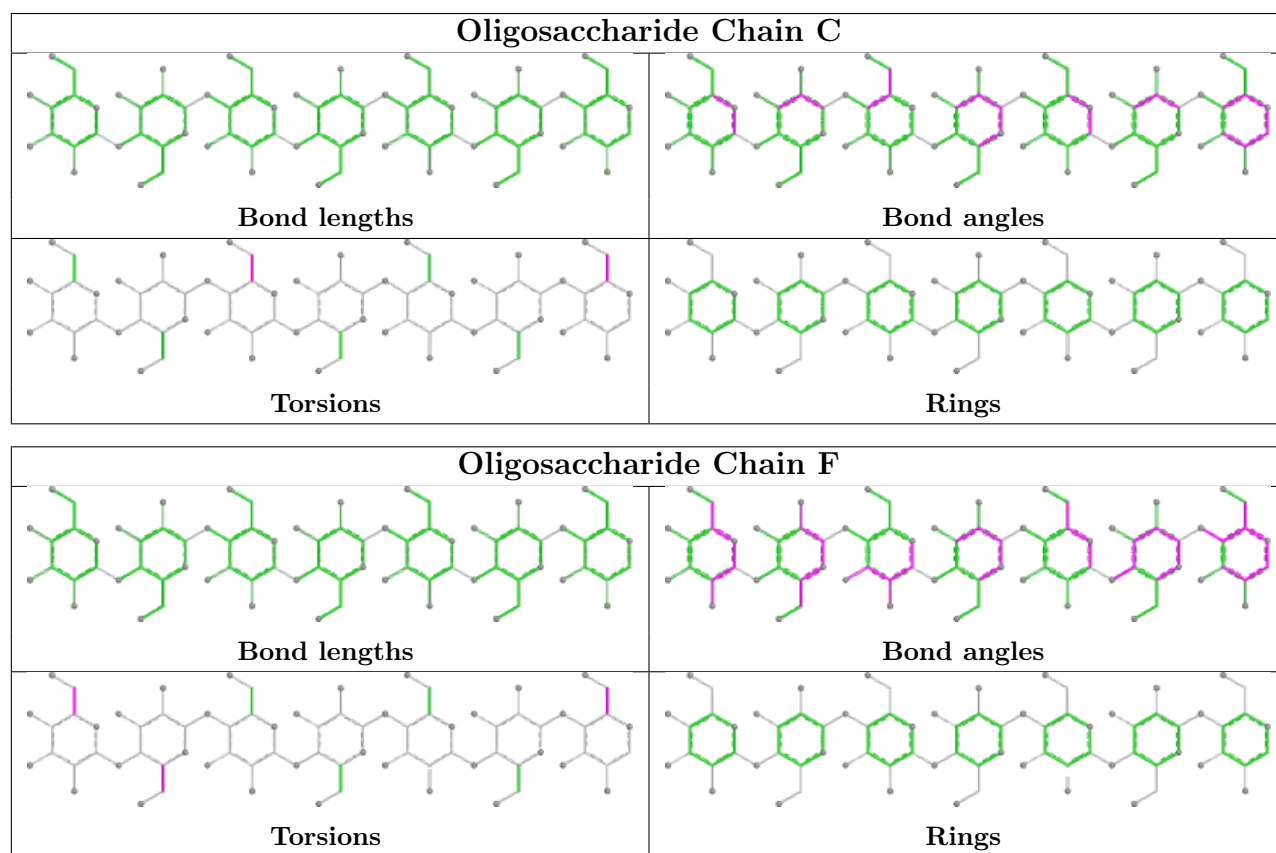
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Mol	Chain	Res	Type	Atoms
2	F	7	GLC	O5-C5-C6-O6
2	F	6	GLC	O5-C5-C6-O6
3	D	3	GLC	C4-C5-C6-O6
2	C	5	GLC	C4-C5-C6-O6
2	F	1	GLC	C4-C5-C6-O6
3	E	3	GLC	O5-C5-C6-O6
3	D	3	GLC	O5-C5-C6-O6

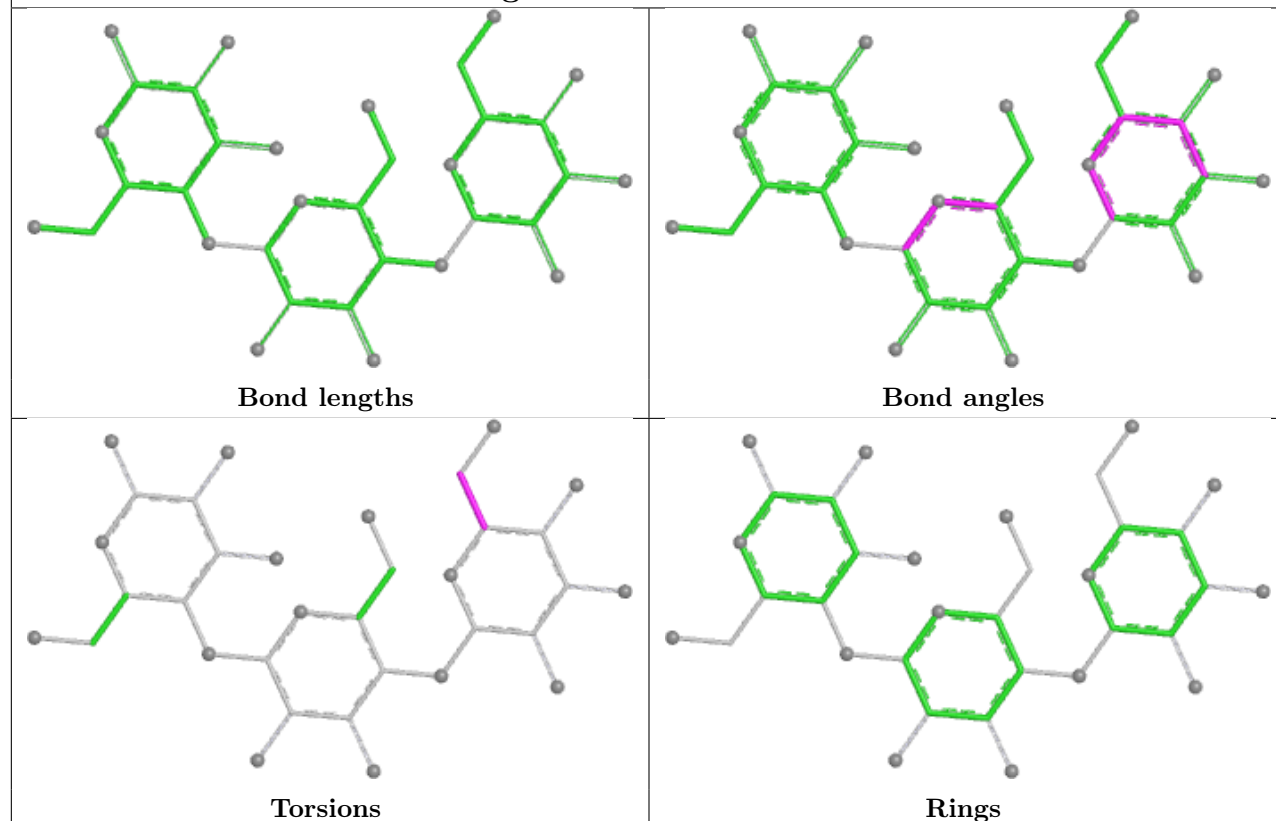
There are no ring outliers.

No monomer is involved in short contacts.

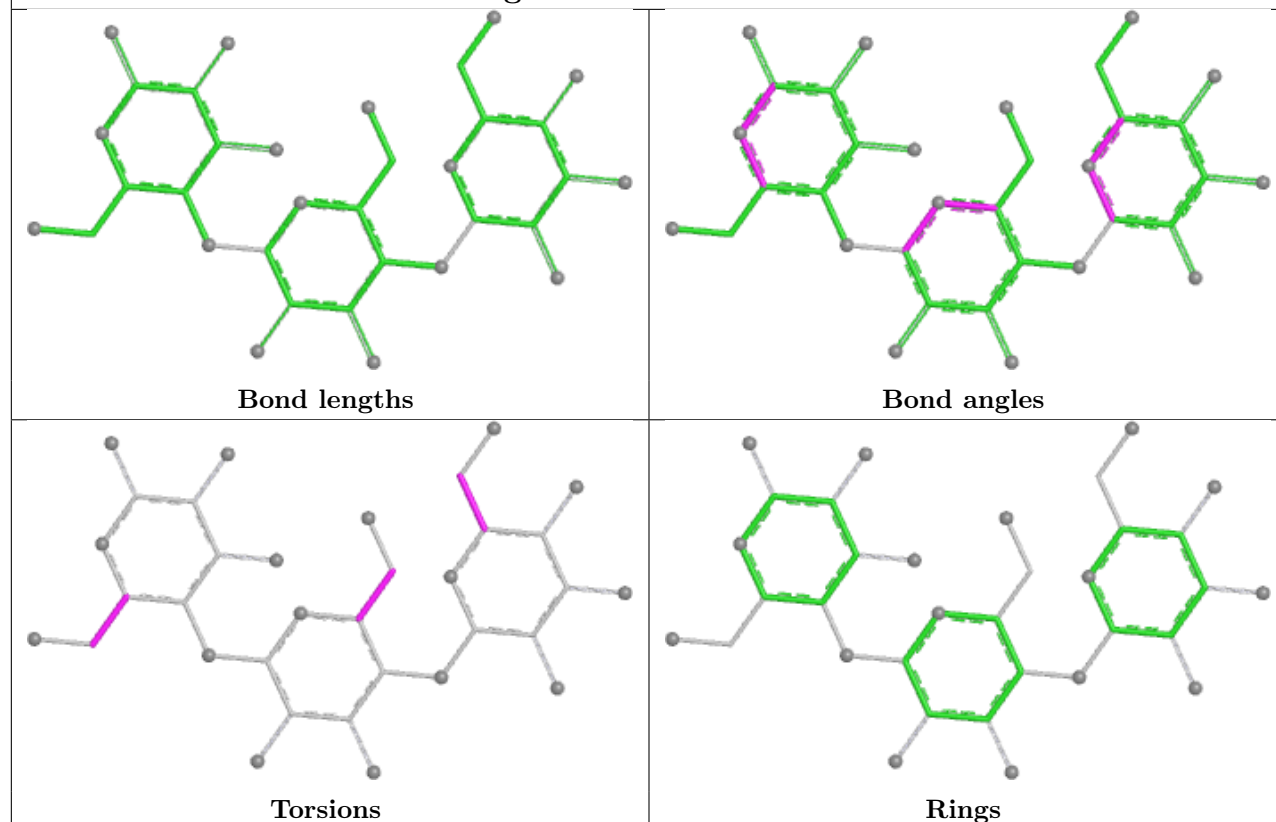
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

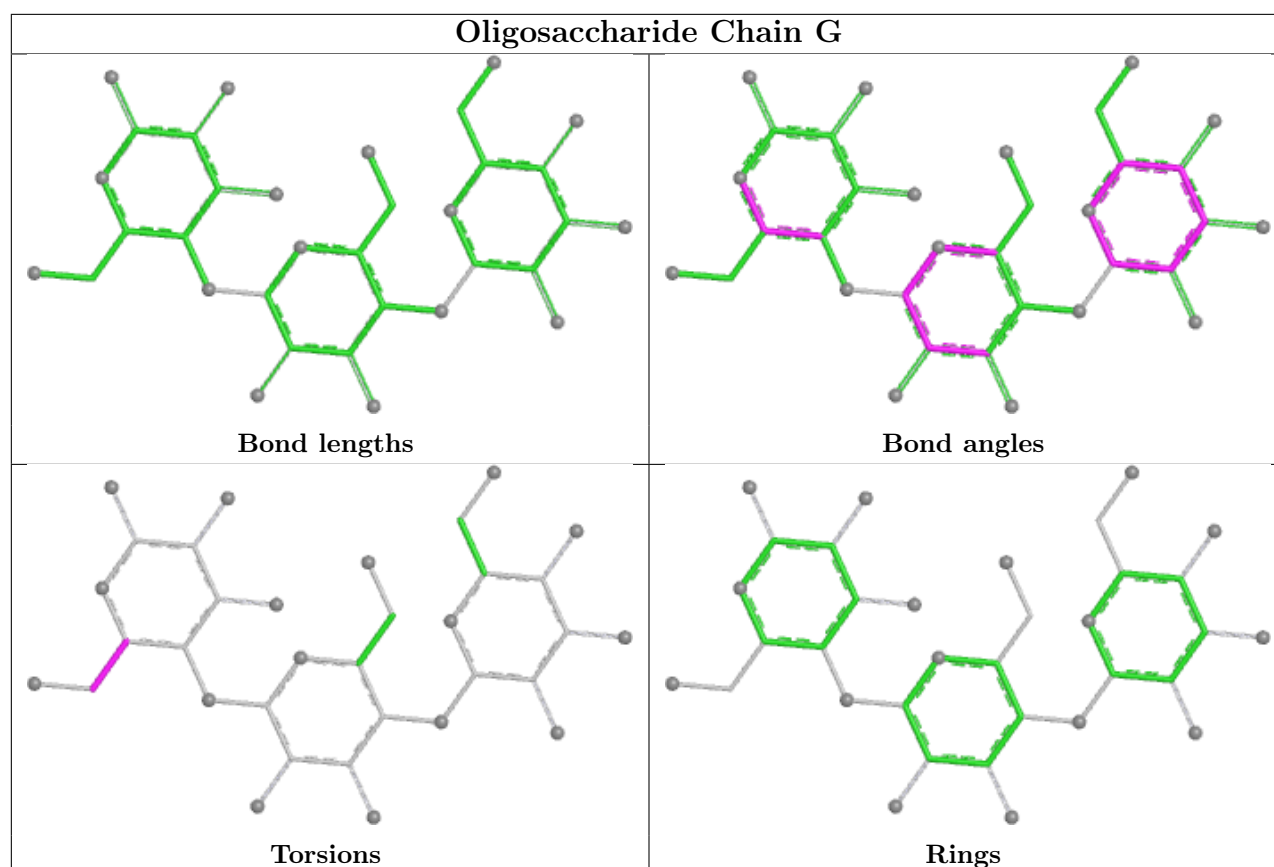


Oligosaccharide Chain D



Oligosaccharide Chain E





5.6 Ligand geometry [i](#)

1 ligand is 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	GLC	A	1008	-	12,12,12	0.61	0	17,17,17	1.69	5 (29%)

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
4	GLC	A	1008	-	-	2/2/22/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1008	GLC	O5-C1-C2	3.59	116.61	110.30
4	A	1008	GLC	C1-C2-C3	2.74	115.94	110.36
4	A	1008	GLC	C1-O5-C5	2.23	117.96	113.65
4	A	1008	GLC	C4-C3-C2	-2.17	107.02	110.83
4	A	1008	GLC	C3-C4-C5	-2.08	106.47	110.23

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1008	GLC	O5-C5-C6-O6
4	A	1008	GLC	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	801/840 (95%)	0.23	22 (2%) 56 52	37, 51, 87, 113	0
1	B	792/840 (94%)	0.92	96 (12%) 8 6	25, 48, 73, 115	1 (0%)
All	All	1593/1680 (94%)	0.57	118 (7%) 20 17	25, 50, 82, 115	1 (0%)

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	239	ALA	6.0
1	B	605	GLY	5.4
1	B	243	ALA	5.3
1	B	587	ASN	5.0
1	A	75	LYS	4.8
1	B	473	THR	4.8
1	B	322	ASP	4.7
1	B	470	ASP	4.6
1	A	475	GLN	4.0
1	B	471	GLN	4.0
1	B	757	TRP	3.9
1	B	644	ASP	3.9
1	B	79	GLU	3.8
1	B	588	THR	3.8
1	B	77	PHE	3.8
1	B	321	SER	3.6
1	B	584	TYR	3.5
1	B	750	VAL	3.5
1	A	471	GLN	3.5
1	B	595	TRP	3.5
1	B	603	TRP	3.5
1	A	472	GLU	3.4
1	B	323	GLN	3.3
1	B	749	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	473	THR	3.3
1	B	590	HIS	3.3
1	B	585	ALA	3.3
1	B	783	GLY	3.2
1	B	469	TYR	3.2
1	B	600	GLY	3.2
1	B	648	HIS	3.2
1	B	875	LYS	3.1
1	A	468	GLN	3.1
1	B	602	GLN	3.0
1	B	578	CYS	3.0
1	B	318	ILE	3.0
1	B	472	GLU	3.0
1	A	590	HIS	3.0
1	A	591	GLU	3.0
1	A	875	LYS	2.9
1	B	594	TRP	2.9
1	B	645	GLY	2.9
1	B	78	CYS	2.9
1	A	147	TYR	2.9
1	A	474	GLY	2.9
1	B	539	ALA	2.8
1	A	77	PHE	2.8
1	B	606	GLY	2.8
1	B	597	ASN	2.8
1	B	541	PRO	2.8
1	A	639	GLY	2.8
1	B	224	GLY	2.8
1	B	599	GLY	2.8
1	B	782	LYS	2.7
1	A	108	THR	2.7
1	B	768	THR	2.7
1	B	506	ASP	2.7
1	B	319	PRO	2.7
1	B	477	VAL	2.7
1	B	537	VAL	2.6
1	B	320	GLY	2.6
1	A	469	TYR	2.6
1	A	240	ARG	2.6
1	B	781	GLY	2.6
1	B	242	SER	2.6
1	B	216	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	874	ILE	2.5
1	A	592	THR	2.5
1	B	589	PRO	2.5
1	B	183	TYR	2.5
1	B	598	ASN	2.5
1	B	604	LYS	2.4
1	A	588	THR	2.4
1	B	497	GLY	2.4
1	B	475	GLN	2.4
1	B	147	TYR	2.4
1	B	478	ALA	2.4
1	B	179	GLU	2.4
1	B	204	ASN	2.3
1	B	591	GLU	2.3
1	A	242	SER	2.3
1	A	467	GLN	2.3
1	B	542	HIS	2.3
1	B	223	LEU	2.3
1	B	489	GLU	2.3
1	B	586	ASN	2.3
1	B	82	GLY	2.3
1	B	567	GLY	2.3
1	B	596	ALA	2.2
1	B	493	THR	2.2
1	B	536	GLN	2.2
1	B	547	TRP	2.2
1	B	498	VAL	2.2
1	B	581	PRO	2.2
1	B	496	ALA	2.2
1	B	499	PRO	2.2
1	B	463	ALA	2.2
1	B	751	ASN	2.2
1	B	467	GLN	2.2
1	B	592	THR	2.2
1	B	148	VAL	2.2
1	B	402	VAL	2.2
1	B	422	LEU	2.1
1	B	485	ILE	2.1
1	B	468	GLN	2.1
1	A	106	ALA	2.1
1	B	119	SER	2.1
1	B	593	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	769	ASP	2.1
1	B	538	GLY	2.1
1	B	219	GLU	2.1
1	B	193	VAL	2.1
1	A	243	ALA	2.1
1	B	479	MET	2.0
1	B	393	ILE	2.0
1	B	155	TRP	2.0
1	B	161	ASP	2.0
1	B	502	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

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

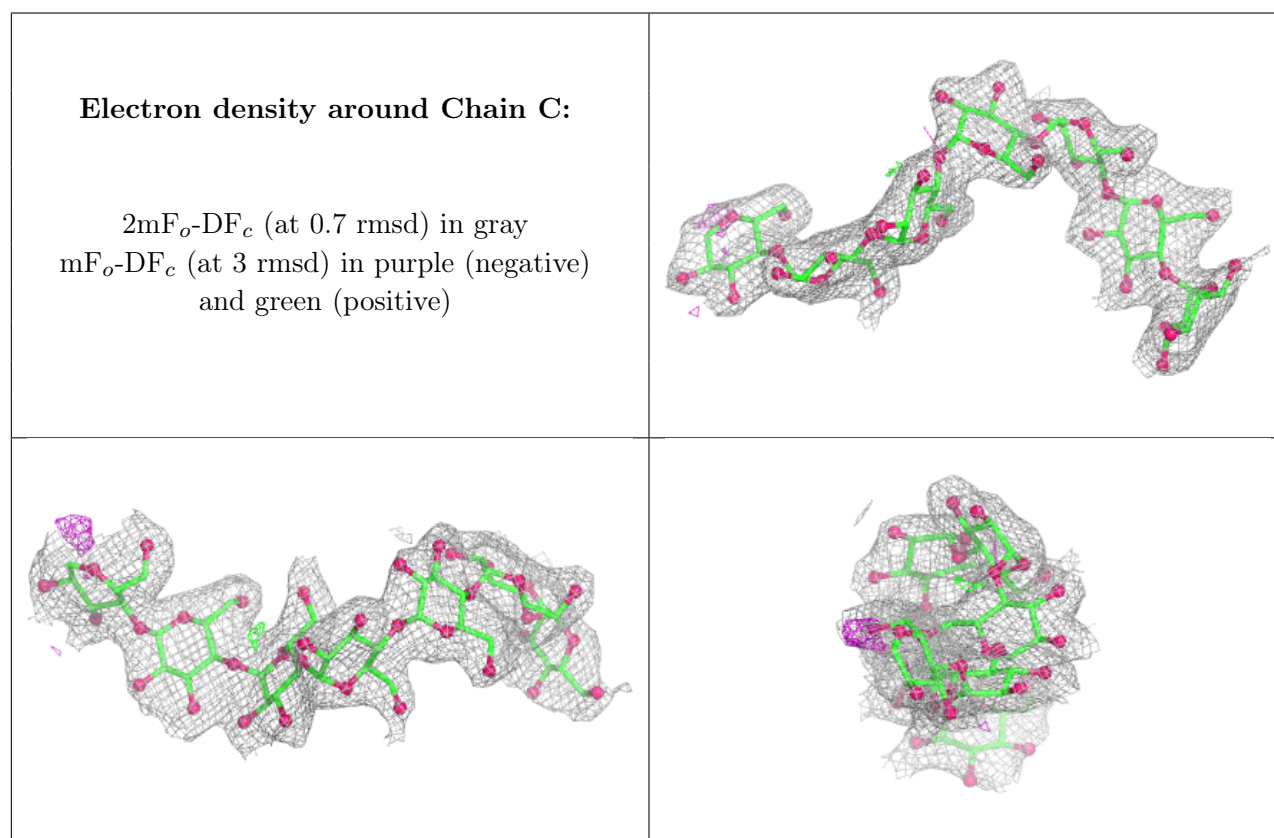
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GLC	G	1	12/12	0.80	0.14	75,81,83,83	0
3	GLC	G	3	11/12	0.80	0.17	74,76,77,78	0
2	GLC	F	7	11/12	0.81	0.16	59,65,69,71	0
3	GLC	E	1	12/12	0.82	0.12	78,84,88,90	0
2	GLC	F	3	11/12	0.83	0.14	55,58,63,63	0
3	GLC	G	2	11/12	0.83	0.15	70,72,74,75	0
2	GLC	F	6	11/12	0.83	0.12	51,56,61,63	0
2	GLC	F	4	11/12	0.85	0.14	50,56,59,61	0
3	GLC	E	3	11/12	0.86	0.13	79,84,87,88	0
2	GLC	F	1	11/12	0.86	0.13	55,56,58,59	0
2	GLC	C	7	11/12	0.88	0.12	76,81,84,85	0
3	GLC	D	1	12/12	0.89	0.10	69,76,78,79	0
2	GLC	C	4	11/12	0.89	0.11	54,59,64,66	0
2	GLC	F	5	11/12	0.89	0.12	52,55,56,58	0
2	GLC	F	2	11/12	0.90	0.11	52,55,56,56	0
2	GLC	C	5	11/12	0.90	0.09	57,60,63,63	0
2	GLC	C	3	11/12	0.91	0.10	53,57,58,60	0
3	GLC	D	3	11/12	0.91	0.11	65,67,69,70	0

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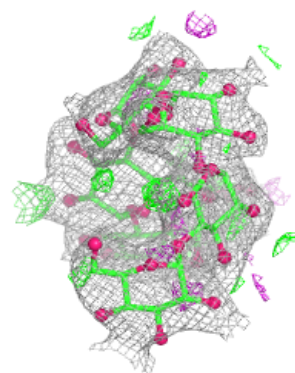
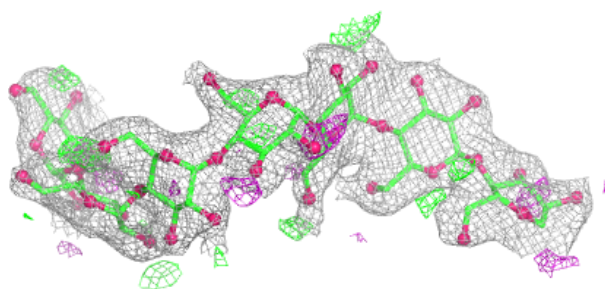
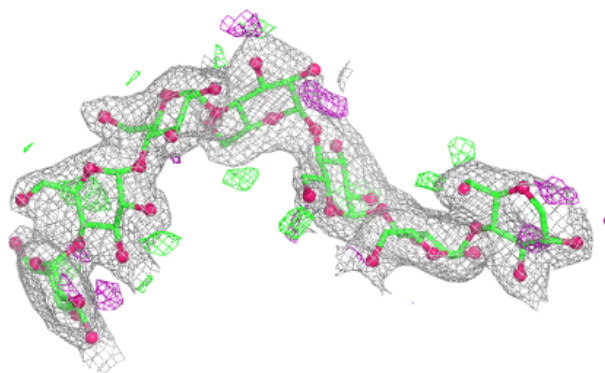
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	C	6	11/12	0.91	0.09	62,64,68,73	0
3	GLC	E	2	11/12	0.91	0.11	81,84,89,91	0
2	GLC	C	1	11/12	0.94	0.09	47,49,49,50	0
2	GLC	C	2	11/12	0.94	0.08	47,48,49,50	0
3	GLC	D	2	11/12	0.95	0.08	60,63,66,67	0

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.

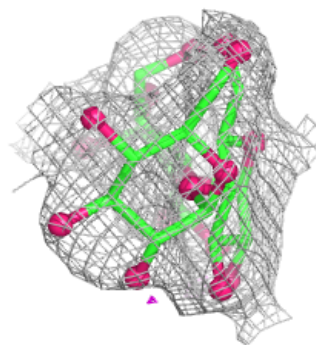
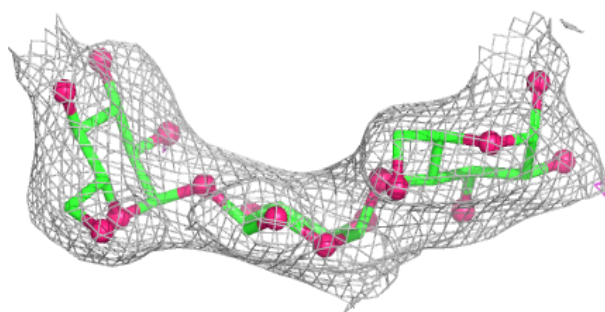
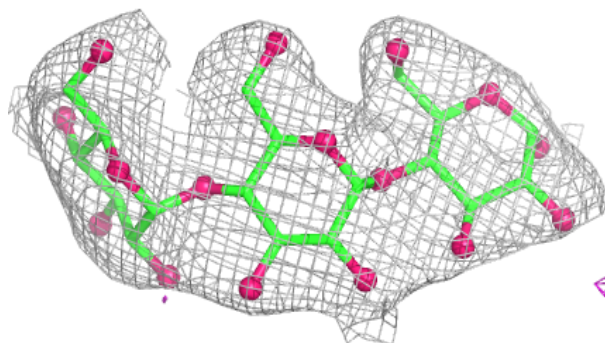


Electron density around Chain F:

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

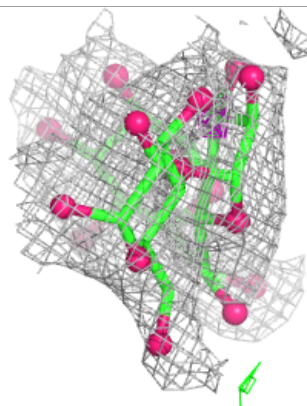
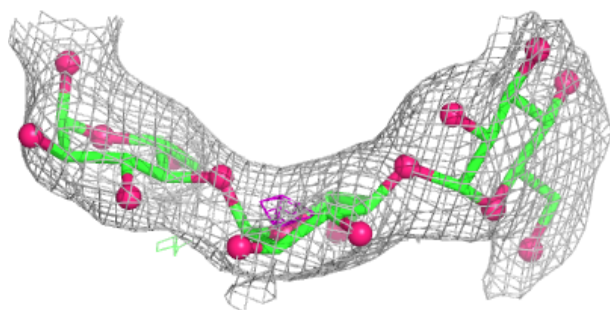
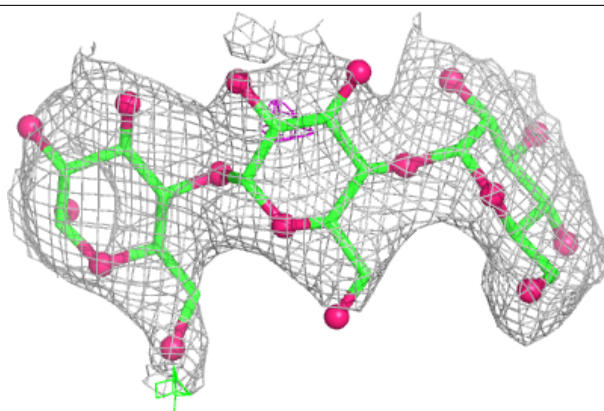
**Electron density around Chain D:**

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

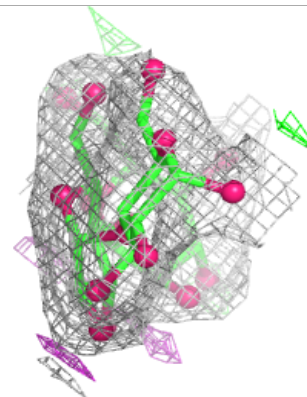
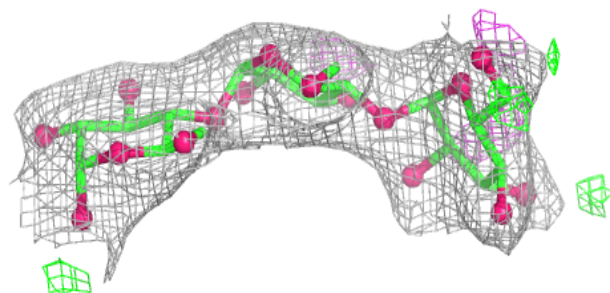
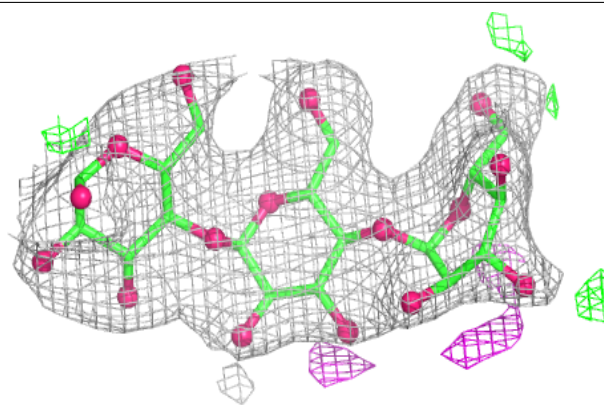


Electron density around Chain E:

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

**Electron density around Chain G:**

$2mF_o-DF_c$ (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($\text{\AA}^2$)	Q<0.9
4	GLC	A	1008	12/12	0.89	0.13	64,68,75,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.