Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2026 – 04:15 PM JST

PDB ID	:	9XKN / pdb_00009xkn
Title	:	Tepidibacillus decaturensis alpha-glucan 4(6)-alpha-glucosyltransferase E666Q in complex with acarbose
Authors	:	Qin, T.; Saburi, W.; Takei, S.; Tagami, T.; Ota, T.; Kanai, K.; Ose, T.; Svensson, B.; Mori, H.
Deposited on	:	2025-11-06
Resolution	:	2.14 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:

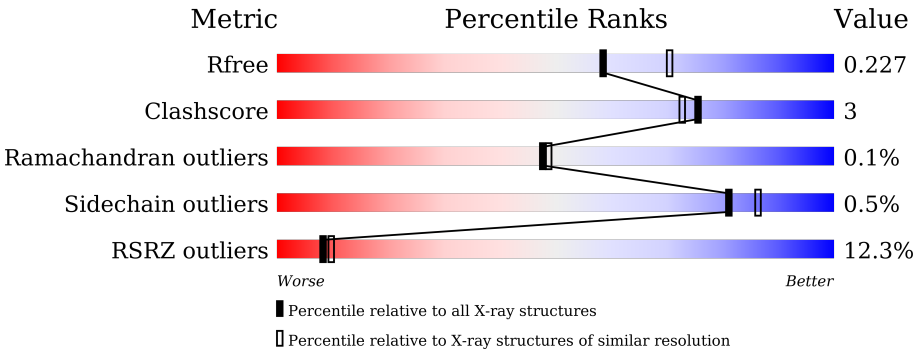
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.14 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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

Mol	Chain	Length	Quality of chain
1	A	887	% 94% 6%
1	B	887	24% 89% 11%
2	D	3	100%
2	E	3	100%
2	F	3	67% 33%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14909 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 GH15-like domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	887	Total	C	N	O	S	0	0	0
			7016	4414	1168	1418	16			
1	B	887	Total	C	N	O	S	0	0	0
			7016	4414	1168	1418	16			

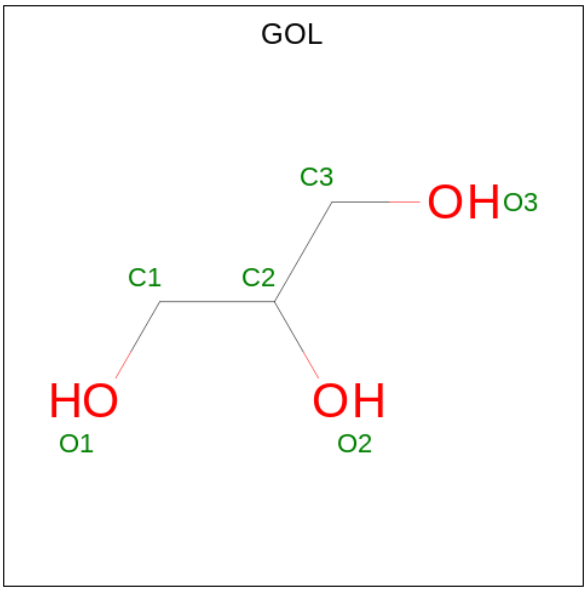
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	666	GLN	GLU	engineered mutation	UNP A0A135L1V7
B	666	GLN	GLU	engineered mutation	UNP A0A135L1V7

- Molecule 2 is an oligosaccharide called 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	3	Total	C	N	O	0	0	0
			33	18	1	14			
2	D	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	E	3	Total	C	N	O	0	0	0
			44	25	1	18			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total Ca 5 5	0	0
4	B	5	Total Ca 5 5	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	425	Total O 425 425	0	0
5	B	273	Total O 273 273	0	0

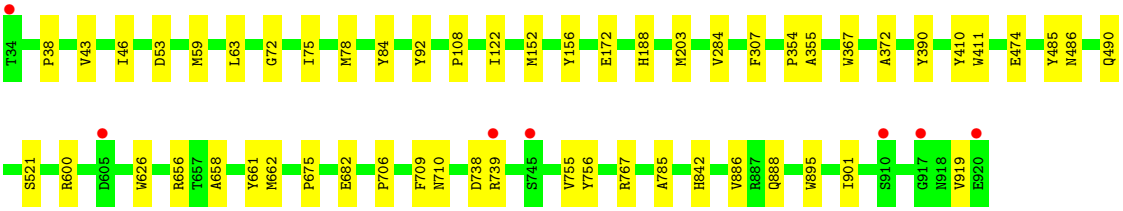
3 Residue-property plots (i)

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: GH15-like domain-containing protein

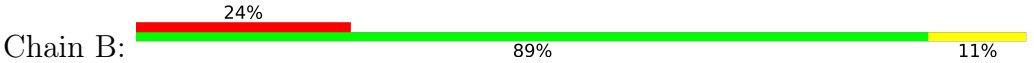
Chain A:

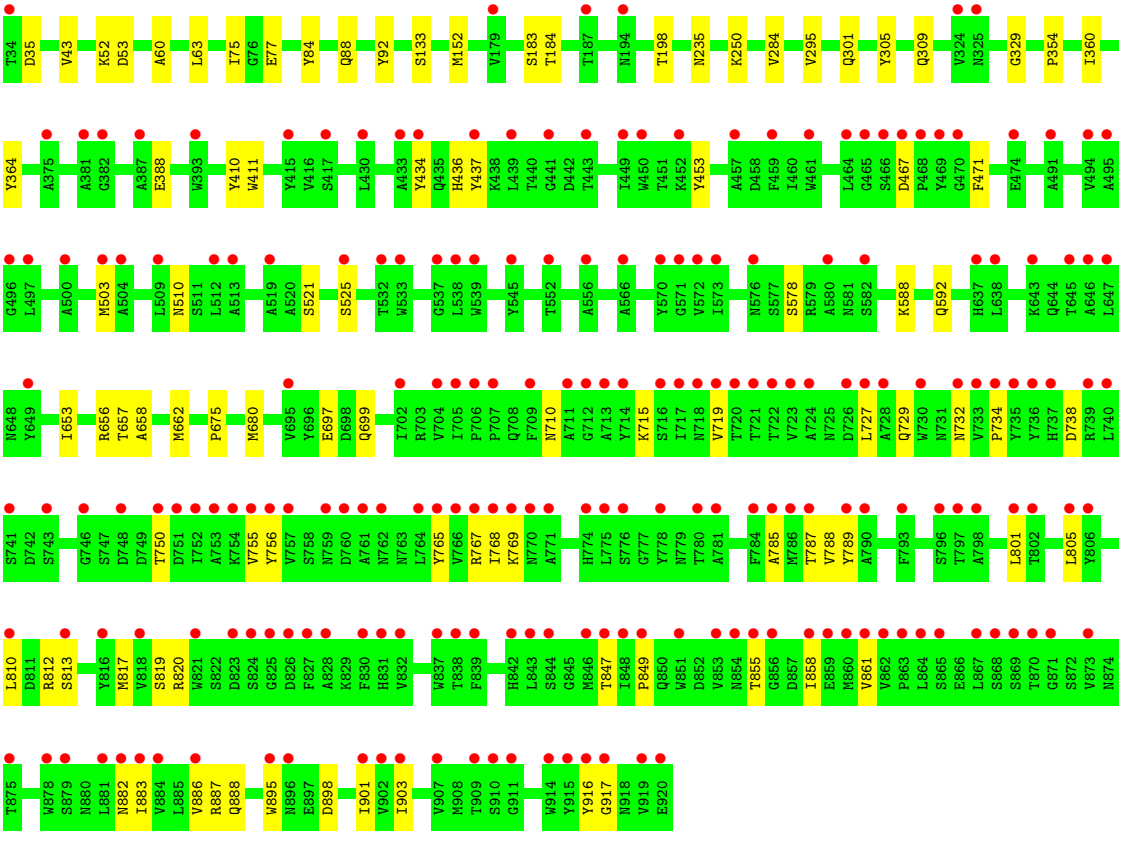




• Molecule 1: GH15-like domain-containing protein

Chain B:





• Molecule 2: 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain F:





• Molecule 2: 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain D:





• Molecule 2: 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain E:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	112.92Å 112.92Å 391.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.93 – 2.14 48.93 – 2.14	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.93-2.14) 100.0 (48.93-2.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 2.01Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.206 , 0.227 0.205 , 0.227	Depositor DCC
R_{free} test set	2000 reflections (1.20%)	wwPDB-VP
Wilson B-factor (Å^2)	34.7	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 37.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14909	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, GLC, GOL, AC1

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	0.09	0/7200	0.28	0/9839
1	B	0.09	0/7200	0.28	0/9839
All	All	0.09	0/14400	0.28	0/19678

There are no bond length outliers.

There are no bond angle outliers.

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	7016	0	6505	28	0
1	B	7016	0	6505	55	0
2	D	44	0	30	0	0
2	E	44	0	30	0	0
2	F	33	0	21	1	0
3	A	30	0	40	1	0
3	B	18	0	24	1	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	425	0	0	1	0
5	B	273	0	0	2	0
All	All	14909	0	13155	83	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 (83) 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:434:TYR:HA	1:B:503:MET:HE3	1.57	0.84
1:B:437:TYR:HB3	1:B:503:MET:HE1	1.73	0.70
1:B:788:VAL:HG22	1:B:883:ILE:HG13	1.74	0.69
1:B:235:ASN:HA	1:B:250:LYS:HD2	1.76	0.66
1:B:588:LYS:HE3	1:B:592:GLN:HE22	1.60	0.65
1:A:53:ASP:OD2	3:A:1004:GOL:O3	2.16	0.62
1:B:768:ILE:HB	1:B:858:ILE:HB	1.81	0.61
1:B:738:ASP:HB2	1:B:901:ILE:HD12	1.83	0.60
1:B:810:LEU:HB3	1:B:882:ASN:HD22	1.67	0.59
1:A:72:GLY:HA3	1:A:108:PRO:HB2	1.86	0.58
1:A:75:ILE:HB	1:A:92:TYR:HB3	1.85	0.58
1:A:785:ALA:HB3	1:A:886:VAL:HB	1.87	0.56
1:A:842:HIS:NE2	2:F:1:GLC:O3	2.30	0.55
1:B:755:VAL:HG11	1:B:903:ILE:HD11	1.89	0.54
1:A:43:VAL:HG21	1:A:46:ILE:HD11	1.90	0.54
1:B:75:ILE:HG13	1:B:152:MET:HE1	1.90	0.53
1:B:715:LYS:NZ	1:B:729:GLN:O	2.41	0.53
1:B:789:TYR:HB2	1:B:882:ASN:HB2	1.92	0.52
1:B:756:TYR:HB2	1:B:767:ARG:HB3	1.91	0.52
1:A:739:ARG:NH2	5:A:1102:HOH:O	2.31	0.52
1:A:156:TYR:OH	1:A:172:GLU:OE1	2.26	0.51
1:B:35:ASP:OD1	1:B:329:GLY:N	2.39	0.50
1:B:715:LYS:HZ2	1:B:732:ASN:HD21	1.60	0.50
1:A:738:ASP:HB2	1:A:901:ILE:HD12	1.93	0.50
1:B:183:SER:OG	1:B:184:THR:N	2.45	0.50
1:B:787:THR:HG23	1:B:819:SER:HB2	1.94	0.50
1:A:59:MET:HG2	1:A:63:LEU:HD21	1.93	0.49
1:A:658:ALA:HB3	1:A:662:MET:HB2	1.94	0.49
1:B:715:LYS:NZ	1:B:732:ASN:HD21	2.10	0.49
1:B:765:TYR:CD1	1:B:861:VAL:HG22	2.47	0.49
1:B:658:ALA:HB3	1:B:662:MET:HB2	1.94	0.49
1:B:75:ILE:HB	1:B:92:TYR:HB3	1.94	0.49
1:B:88:GLN:HG3	1:B:284:VAL:HG11	1.95	0.49
1:B:750:THR:HG21	1:B:887:ARG:HB2	1.96	0.48
1:B:785:ALA:HB3	1:B:886:VAL:HB	1.96	0.47
1:A:756:TYR:HB2	1:A:767:ARG:HB3	1.96	0.47
1:A:354:PRO:HD3	1:A:410:TYR:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ALA:HB1	3:B:1001:GOL:H11	1.96	0.47
1:B:467:ASP:OD2	1:B:471:PHE:N	2.37	0.46
1:B:453:TYR:CZ	1:B:503:MET:HG3	2.50	0.46
1:B:812:ARG:HG2	1:B:813:SER:H	1.81	0.46
1:B:719:VAL:HG13	1:B:847:THR:HB	1.97	0.46
1:B:77:GLU:OE2	1:B:364:TYR:OH	2.31	0.46
1:B:769:LYS:HA	1:B:769:LYS:HD2	1.67	0.45
1:A:78:MET:HE2	1:A:284:VAL:HG23	1.98	0.45
1:A:656:ARG:O	1:A:675:PRO:HG3	2.17	0.44
1:B:521:SER:CB	1:B:710:ASN:HB2	2.48	0.44
1:B:888:GLN:HB2	1:B:895:TRP:CD2	2.52	0.44
1:B:732:ASN:H	1:B:732:ASN:HD22	1.65	0.44
1:A:888:GLN:HB2	1:A:895:TRP:CD2	2.53	0.43
1:B:734:PRO:HB3	1:B:917:GLY:H	1.83	0.43
1:B:769:LYS:HE2	1:B:855:THR:O	2.17	0.43
1:B:63:LEU:HB2	1:B:360:ILE:HD12	2.00	0.43
1:B:301:GLN:HG2	1:B:305:TYR:CG	2.54	0.43
1:B:765:TYR:HD1	1:B:861:VAL:HG22	1.84	0.43
1:A:122:ILE:HD12	1:A:307:PHE:HD2	1.84	0.42
1:A:372:ALA:HA	1:A:390:TYR:CE2	2.54	0.42
1:B:656:ARG:O	1:B:675:PRO:HG3	2.19	0.42
1:A:600:ARG:HD3	1:A:626:TRP:CZ2	2.55	0.42
1:B:805:LEU:HD22	1:B:817:MET:HE1	2.01	0.42
1:A:474:GLU:HG3	1:A:485:TYR:CZ	2.54	0.42
1:B:388:GLU:HB2	1:B:436:HIS:NE2	2.34	0.42
1:B:84:TYR:HB3	1:B:411:TRP:HB3	2.00	0.42
1:B:43:VAL:HA	1:B:680:MET:HE3	2.02	0.42
1:B:801:LEU:HD23	1:B:801:LEU:HA	1.95	0.41
1:B:354:PRO:HD3	1:B:410:TYR:CE1	2.55	0.41
1:A:84:TYR:HB3	1:A:411:TRP:HB3	2.02	0.41
1:A:188:HIS:CE1	1:A:203:MET:HB3	2.56	0.41
1:B:52:LYS:HB3	1:B:52:LYS:HE3	1.86	0.41
1:B:697:GLU:OE1	1:B:699:GLN:NE2	2.53	0.41
1:B:820:ARG:NH1	1:B:849:PRO:O	2.54	0.41
1:B:198:THR:HG21	1:B:295:VAL:HG21	2.03	0.41
1:B:309:GLN:NE2	5:B:1112:HOH:O	2.53	0.41
1:A:706:PRO:HG2	1:A:709:PHE:CE2	2.56	0.40
1:A:75:ILE:HG13	1:A:152:MET:HE1	2.02	0.40
1:A:38:PRO:HD3	1:A:661:TYR:CZ	2.56	0.40
1:A:486:ASN:O	1:A:490:GLN:HG2	2.21	0.40
1:B:510:ASN:ND2	5:B:1104:HOH:O	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:732:ASN:H	1:B:732:ASN:ND2	2.18	0.40
1:B:525:SER:HA	1:B:916:TYR:HB2	2.03	0.40
1:B:653:ILE:O	1:B:657:THR:HG23	2.21	0.40
1:A:355:ALA:HB2	1:A:367:TRP:CE3	2.56	0.40
1:A:521:SER:CB	1:A:710:ASN:HB2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	885/887 (100%)	862 (97%)	23 (3%)	0	100	100
1	B	885/887 (100%)	857 (97%)	27 (3%)	1 (0%)	48	49
All	All	1770/1774 (100%)	1719 (97%)	50 (3%)	1 (0%)	48	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	53	ASP

5.3.2 Protein sidechains (i)

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	754/754 (100%)	751 (100%)	3 (0%)	84 88
1	B	754/754 (100%)	750 (100%)	4 (0%)	81 86
All	All	1508/1508 (100%)	1501 (100%)	7 (0%)	81 86

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	682	GLU
1	A	755	VAL
1	A	919	VAL
1	B	133	SER
1	B	578	SER
1	B	727	LEU
1	B	898	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	173	GLN
1	A	398	GLN
1	A	543	ASN
1	A	592	GLN
1	A	644	GLN
1	A	699	GLN
1	A	718	ASN
1	B	41	GLN
1	B	110	ASN
1	B	162	ASN
1	B	235	ASN
1	B	245	ASN
1	B	435	GLN
1	B	592	GLN
1	B	732	ASN
1	B	763	ASN
1	B	815	GLN
1	B	880	ASN
1	B	882	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

9 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	D	1	2	12,12,12	0.21	0	17,17,17	0.26	0
2	GLC	D	2	2	11,11,12	0.38	0	15,15,17	0.64	0
2	AC1	D	3	2	21,22,23	0.40	0	22,32,34	0.42	0
2	GLC	E	1	2	12,12,12	0.18	0	17,17,17	0.26	0
2	GLC	E	2	2	11,11,12	0.40	0	15,15,17	0.68	0
2	AC1	E	3	2	21,22,23	0.40	0	22,32,34	0.44	0
2	GLC	F	1	2	12,12,12	0.17	0	17,17,17	0.37	0
2	GLC	F	2	2	11,11,12	0.42	0	15,15,17	0.38	0
2	AC1	F	3	2	9,10,23	0.46	0	14,14,34	0.53	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
2	GLC	D	1	2	-	2/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	AC1	D	3	2	-	2/6/43/46	0/2/2/2
2	GLC	E	1	2	-	0/2/22/22	0/1/1/1
2	GLC	E	2	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AC1	E	3	2	-	2/6/43/46	0/2/2/2
2	GLC	F	1	2	-	2/2/22/22	0/1/1/1
2	GLC	F	2	2	-	0/2/19/22	0/1/1/1
2	AC1	F	3	2	-	-	0/1/1/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3	AC1	C5-C4-N4A-C1B
2	E	3	AC1	C5-C4-N4A-C1B
2	D	1	GLC	O5-C5-C6-O6
2	D	1	GLC	C4-C5-C6-O6
2	F	1	GLC	C4-C5-C6-O6
2	F	1	GLC	O5-C5-C6-O6
2	E	2	GLC	C4-C5-C6-O6
2	D	3	AC1	C3-C4-N4A-C1B
2	E	3	AC1	C3-C4-N4A-C1B
2	E	2	GLC	O5-C5-C6-O6

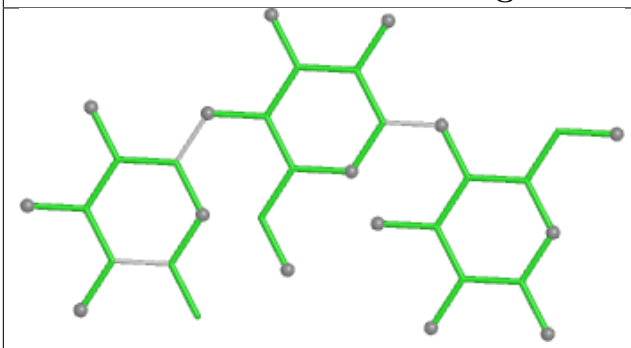
There are no ring outliers.

1 monomer is involved in 1 short contact:

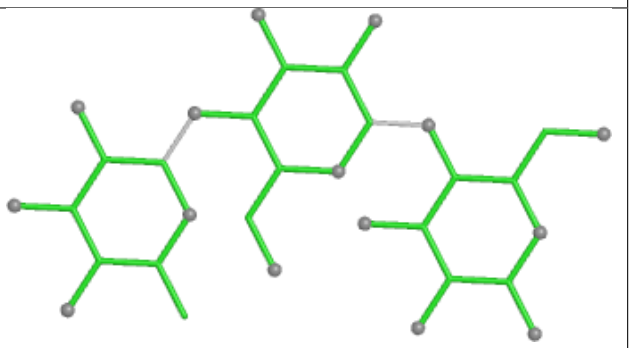
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	GLC	1	0

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

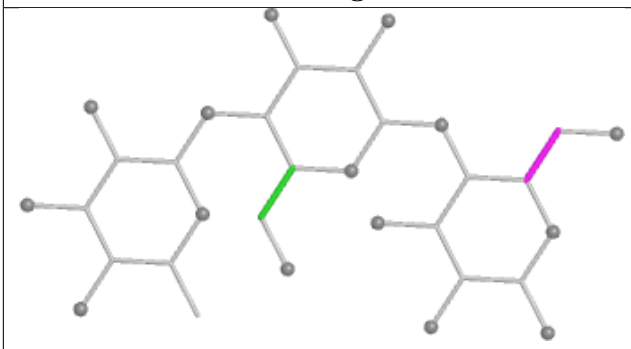
Oligosaccharide Chain F



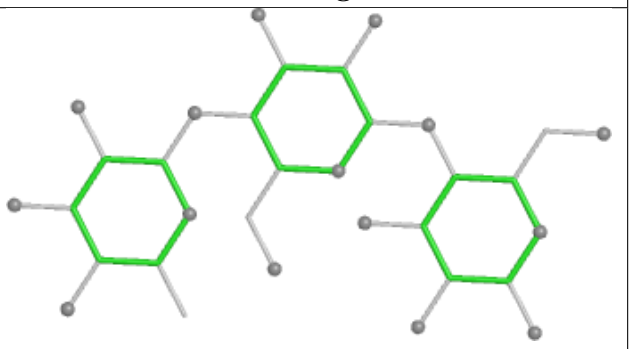
Bond lengths



Bond angles

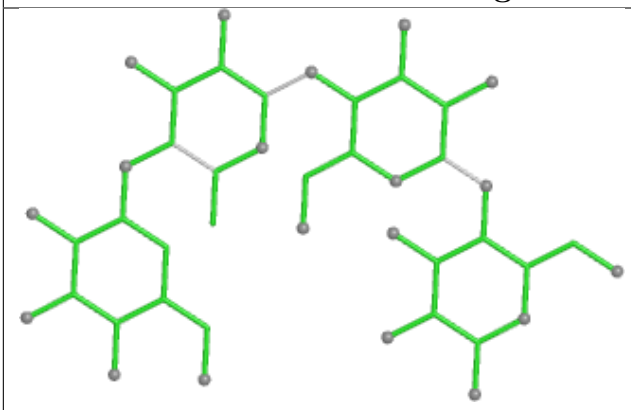


Torsions

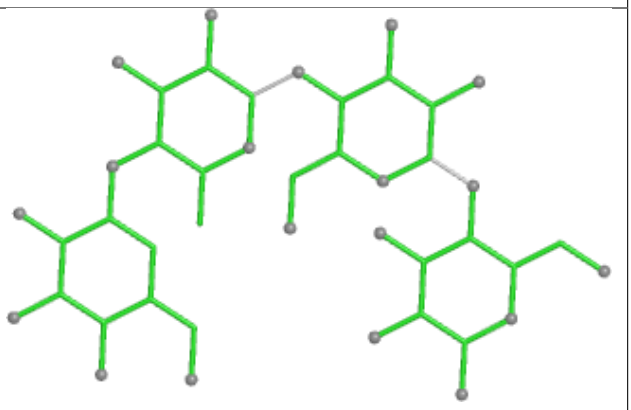


Rings

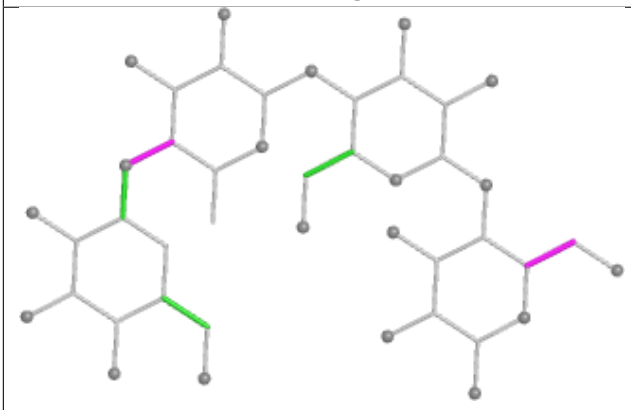
Oligosaccharide Chain D



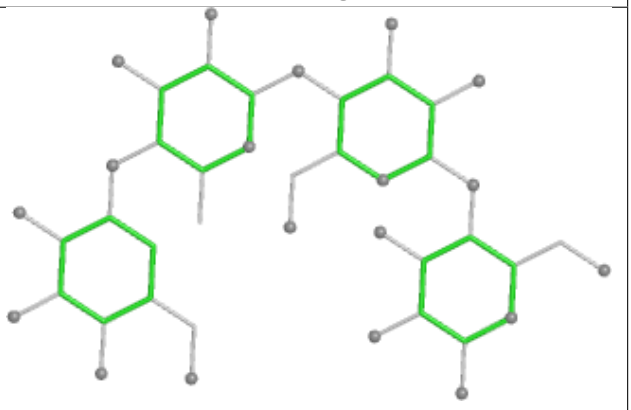
Bond lengths



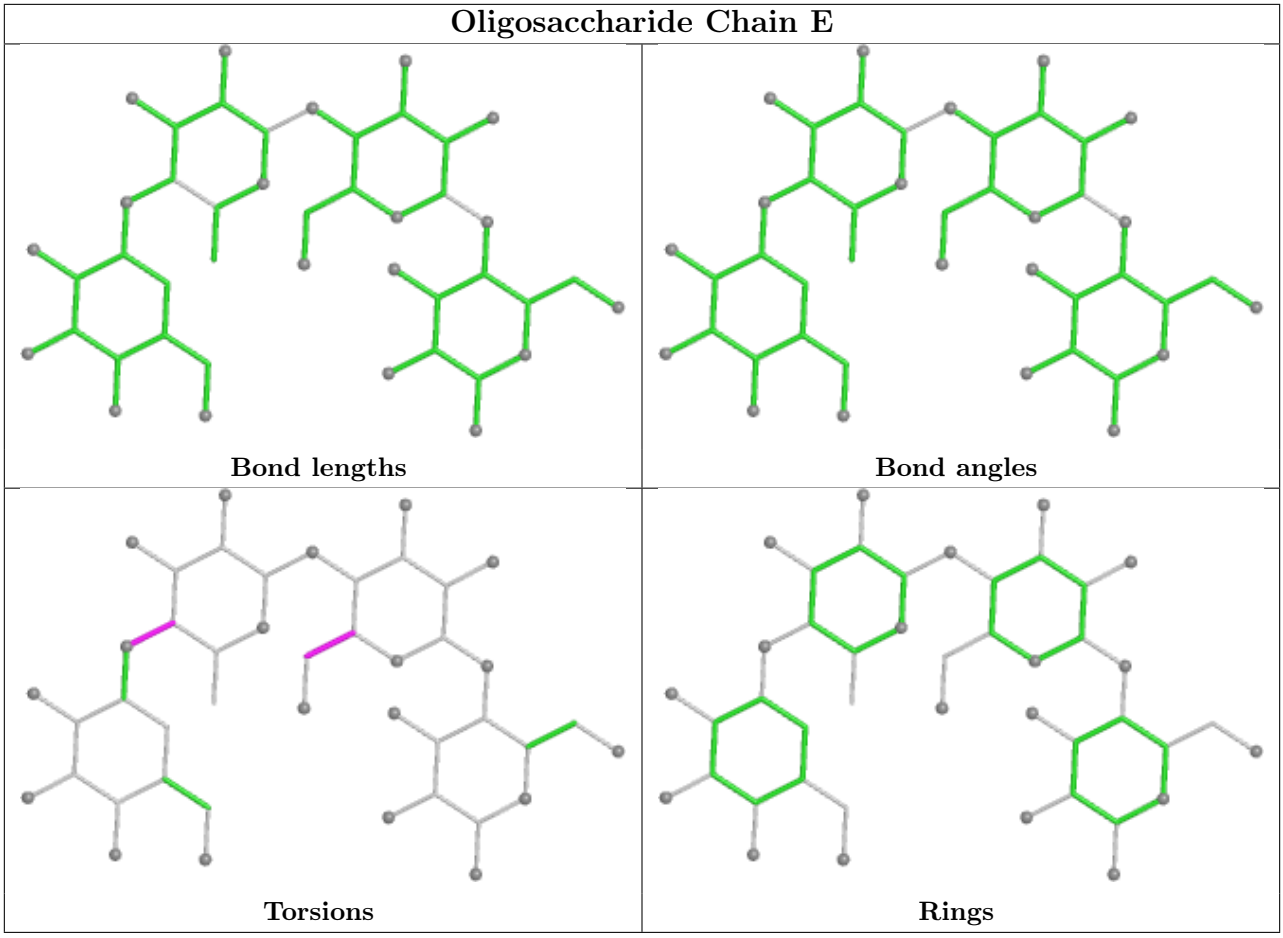
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 10 are monoatomic - leaving 8 for Mogul analysis.

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	1002	-	5,5,5	0.82	0	5,5,5	1.02	0
3	GOL	A	1003	-	5,5,5	0.91	0	5,5,5	0.99	0
3	GOL	B	1003	-	5,5,5	0.92	0	5,5,5	0.98	0
3	GOL	A	1001	-	5,5,5	0.92	0	5,5,5	0.99	0
3	GOL	A	1005	-	5,5,5	0.92	0	5,5,5	1.00	0
3	GOL	B	1001	-	5,5,5	0.87	0	5,5,5	1.01	0
3	GOL	A	1004	-	5,5,5	0.83	0	5,5,5	1.09	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	A	1002	-	5,5,5	0.90	0	5,5,5	1.00	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	1002	-	-	2/4/4/4	-
3	GOL	A	1003	-	-	1/4/4/4	-
3	GOL	B	1003	-	-	2/4/4/4	-
3	GOL	A	1001	-	-	2/4/4/4	-
3	GOL	A	1005	-	-	0/4/4/4	-
3	GOL	B	1001	-	-	0/4/4/4	-
3	GOL	A	1004	-	-	4/4/4/4	-
3	GOL	A	1002	-	-	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(^{o})	Ideal(^{o})
3	A	1004	GOL	C3-C2-C1	-2.01	103.87	111.70

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	GOL	O1-C1-C2-C3
3	A	1004	GOL	O1-C1-C2-C3
3	B	1002	GOL	C1-C2-C3-O3
3	A	1004	GOL	O1-C1-C2-O2
3	A	1004	GOL	C1-C2-C3-O3
3	B	1003	GOL	C1-C2-C3-O3
3	A	1001	GOL	O1-C1-C2-O2
3	B	1003	GOL	O2-C2-C3-O3
3	A	1004	GOL	O2-C2-C3-O3
3	B	1002	GOL	O2-C2-C3-O3
3	A	1003	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1001	GOL	1	0
3	A	1004	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, 95^{th} 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	887/887 (100%)	-0.02	7 (0%) 82 85	23, 30, 43, 64	0
1	B	887/887 (100%)	1.16	212 (23%) 2 2	22, 41, 68, 85	0
All	All	1774/1774 (100%)	0.57	219 (12%) 8 10	22, 34, 61, 85	0

All (219) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	755	VAL	5.7
1	B	465	GLY	5.6
1	B	719	VAL	5.2
1	B	764	LEU	4.8
1	B	853	VAL	4.8
1	B	798	ALA	4.8
1	B	713	ALA	4.6
1	B	705	ILE	4.6
1	B	903	ILE	4.6
1	B	848	ILE	4.5
1	B	768	ILE	4.4
1	B	722	THR	4.4
1	B	787	THR	4.3
1	B	863	PRO	4.3
1	B	415	TYR	4.3
1	B	766	VAL	4.2
1	B	753	ALA	4.2
1	B	861	VAL	4.2
1	B	730	TRP	4.2
1	B	702	ILE	4.2
1	B	916	TYR	4.2
1	B	500	ALA	4.1
1	B	858	ILE	4.1
1	B	843	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	917	GLY	4.1
1	B	865	SER	3.9
1	B	464	LEU	3.9
1	B	645	THR	3.8
1	B	727	LEU	3.8
1	B	793	PHE	3.8
1	B	721	THR	3.8
1	B	867	LEU	3.8
1	B	724	ALA	3.7
1	B	34	THR	3.7
1	B	726	ASP	3.7
1	B	851	TRP	3.7
1	B	733	VAL	3.7
1	B	879	SER	3.6
1	B	552	THR	3.6
1	B	449	ILE	3.6
1	B	780	THR	3.6
1	B	868	SER	3.6
1	B	847	THR	3.6
1	B	873	VAL	3.5
1	B	765	TYR	3.5
1	B	707	PRO	3.5
1	B	919	VAL	3.5
1	B	837	TRP	3.4
1	B	920	GLU	3.4
1	B	778	TYR	3.4
1	A	34	THR	3.3
1	B	870	THR	3.3
1	B	886	VAL	3.3
1	B	720	THR	3.3
1	B	750	THR	3.3
1	B	736	TYR	3.3
1	B	771	ALA	3.2
1	B	775	LEU	3.2
1	B	875	THR	3.2
1	A	917	GLY	3.2
1	B	862	VAL	3.2
1	B	790	ALA	3.2
1	B	909	THR	3.2
1	B	821	TRP	3.2
1	B	839	PHE	3.2
1	B	854	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	757	VAL	3.1
1	B	902	VAL	3.1
1	B	805	LEU	3.1
1	B	437	TYR	3.1
1	B	789	TYR	3.1
1	B	761	ALA	3.1
1	B	796	SER	3.1
1	B	580	ALA	3.1
1	B	762	ASN	3.1
1	B	826	ASP	3.1
1	B	774	HIS	3.1
1	B	883	ILE	3.1
1	A	605	ASP	3.0
1	B	760	ASP	3.0
1	B	827	PHE	3.0
1	B	869	SER	3.0
1	B	430	LEU	3.0
1	B	864	LEU	3.0
1	B	474	GLU	3.0
1	B	901	ILE	3.0
1	B	704	VAL	2.9
1	B	797	THR	2.9
1	B	638	LEU	2.9
1	B	712	GLY	2.9
1	B	907	VAL	2.9
1	B	573	ILE	2.9
1	B	752	ILE	2.9
1	B	469	TYR	2.9
1	B	466	SER	2.9
1	B	828	ALA	2.9
1	B	801	LEU	2.8
1	B	525	SER	2.8
1	B	716	SER	2.8
1	B	882	ASN	2.8
1	B	504	ALA	2.8
1	B	571	GLY	2.8
1	B	718	ASN	2.8
1	B	767	ARG	2.8
1	B	737	HIS	2.8
1	B	467	ASP	2.8
1	B	709	PHE	2.8
1	B	496	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	519	ALA	2.8
1	B	785	ALA	2.8
1	B	855	THR	2.8
1	B	831	HIS	2.8
1	B	823	ASP	2.8
1	B	728	ALA	2.8
1	B	512	LEU	2.8
1	B	734	PRO	2.8
1	B	706	PRO	2.7
1	B	582	SER	2.7
1	B	786	MET	2.7
1	B	830	PHE	2.7
1	B	832	VAL	2.7
1	B	914	TRP	2.7
1	B	825	GLY	2.7
1	B	740	LEU	2.7
1	B	810	LEU	2.7
1	B	818	VAL	2.7
1	B	751	ASP	2.7
1	B	754	LYS	2.6
1	A	920	GLU	2.6
1	B	393	TRP	2.6
1	B	748	ASP	2.6
1	B	570	TYR	2.6
1	B	382	GLY	2.6
1	B	187	THR	2.6
1	B	450	TRP	2.6
1	B	878	TRP	2.6
1	B	849	PRO	2.6
1	B	459	PHE	2.6
1	B	714	TYR	2.6
1	B	723	VAL	2.6
1	B	756	TYR	2.6
1	B	434	TYR	2.5
1	B	813	SER	2.5
1	B	860	MET	2.5
1	B	884	VAL	2.5
1	B	417	SER	2.5
1	B	513	ALA	2.5
1	B	439	LEU	2.5
1	B	770	ASN	2.5
1	B	461	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	806	TYR	2.4
1	B	443	THR	2.4
1	B	509	LEU	2.4
1	B	816	TYR	2.4
1	B	915	TYR	2.4
1	B	375	ALA	2.4
1	B	711	ALA	2.4
1	B	776	SER	2.4
1	B	802	THR	2.4
1	A	910	SER	2.4
1	B	746	GLY	2.3
1	B	457	ALA	2.3
1	B	545	TYR	2.3
1	B	735	TYR	2.3
1	B	824	SER	2.3
1	B	842	HIS	2.3
1	B	179	VAL	2.3
1	B	572	VAL	2.3
1	B	838	THR	2.3
1	B	495	ALA	2.3
1	B	533	TRP	2.3
1	B	576	ASN	2.3
1	B	381	ALA	2.3
1	B	452	LYS	2.3
1	B	646	ALA	2.3
1	B	769	LYS	2.3
1	B	781	ALA	2.3
1	A	745	SER	2.2
1	B	910	SER	2.2
1	B	324	VAL	2.2
1	A	739	ARG	2.2
1	B	643	LYS	2.2
1	B	566	ALA	2.2
1	B	846	MET	2.2
1	B	739	ARG	2.2
1	B	194	ASN	2.2
1	B	759	ASN	2.2
1	B	503	MET	2.2
1	B	433	ALA	2.2
1	B	859	GLU	2.2
1	B	647	LEU	2.2
1	B	637	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	741	SER	2.2
1	B	717	ILE	2.2
1	B	871	GLY	2.2
1	B	911	GLY	2.2
1	B	649	TYR	2.2
1	B	325	ASN	2.2
1	B	468	PRO	2.1
1	B	556	ALA	2.1
1	B	844	SER	2.1
1	B	856	GLY	2.1
1	B	491	ALA	2.1
1	B	743	SER	2.1
1	B	881	LEU	2.1
1	B	470	GLY	2.1
1	B	537	GLY	2.1
1	B	539	TRP	2.1
1	B	494	VAL	2.1
1	B	387	ALA	2.1
1	B	497	LEU	2.1
1	B	532	THR	2.1
1	B	441	GLY	2.1
1	B	784	PHE	2.1
1	B	895	TRP	2.1
1	B	538	LEU	2.0
1	B	732	ASN	2.0
1	B	896	ASN	2.0
1	B	695	VAL	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, 95^{th} 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	1	12/12	-	-	49,55,64,65	0

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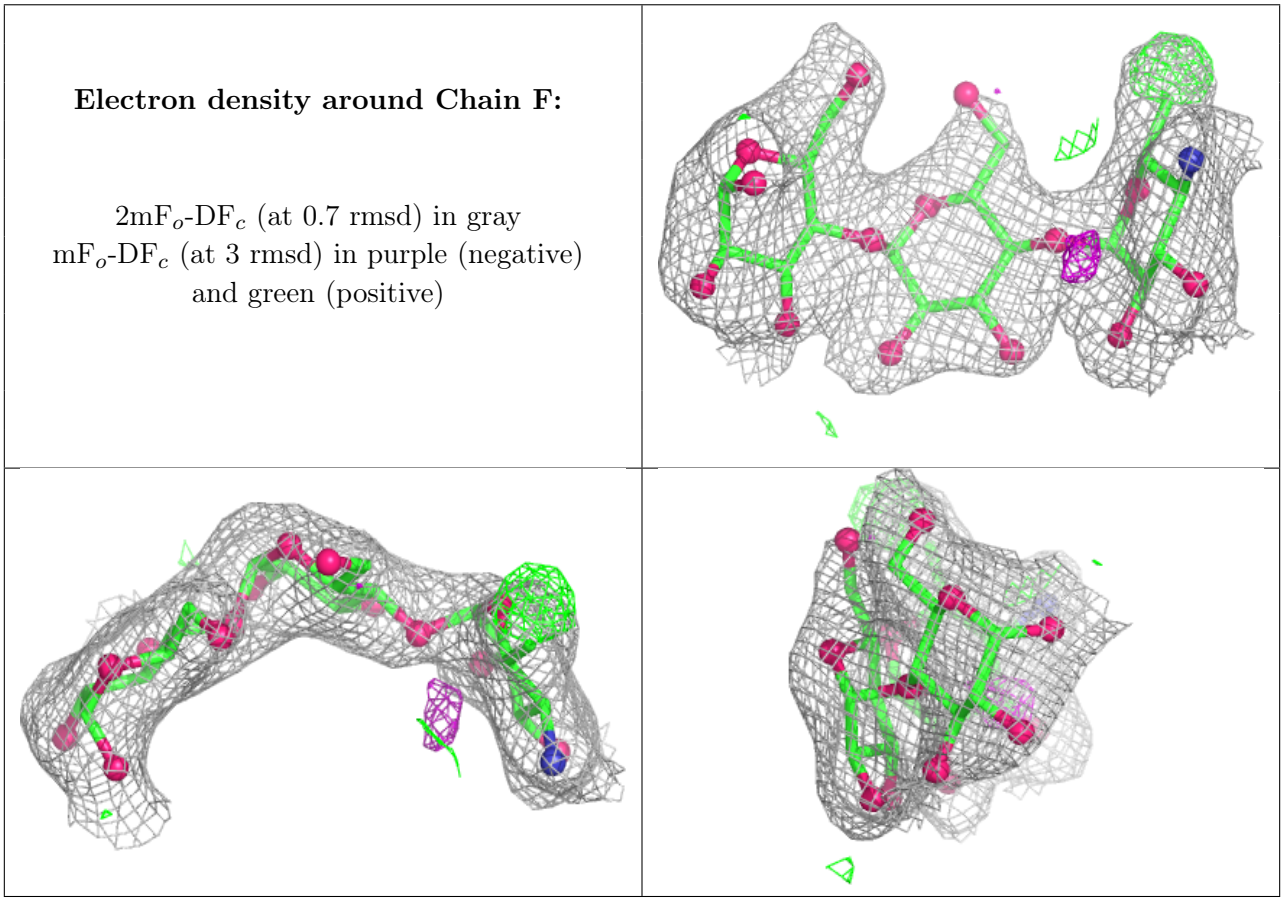
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	F	2	11/12	-	-	47,49,52,61	0
2	AC1	F	3	10/22	-	-	38,45,50,50	0
2	GLC	D	1	12/12	0.86	0.12	33,36,44,51	0
2	GLC	E	2	11/12	0.89	0.10	36,38,44,47	0
2	GLC	E	1	12/12	0.91	0.09	37,42,45,49	0
2	AC1	E	3	21/22	0.92	0.09	31,34,37,37	0
2	GLC	D	2	11/12	0.94	0.08	27,30,37,40	0
2	AC1	D	3	21/22	0.95	0.07	22,27,30,31	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.

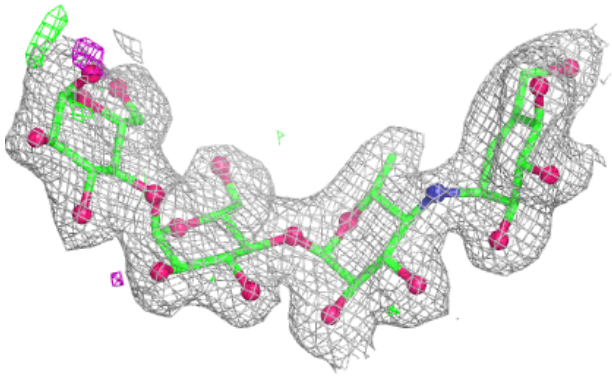
Electron density around Chain F:

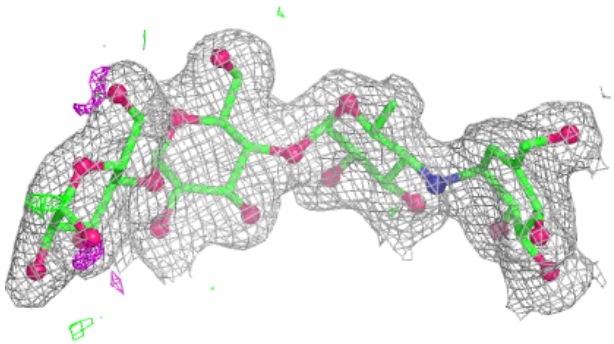
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

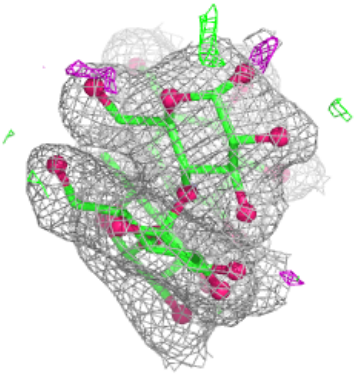


Electron density around Chain D:

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

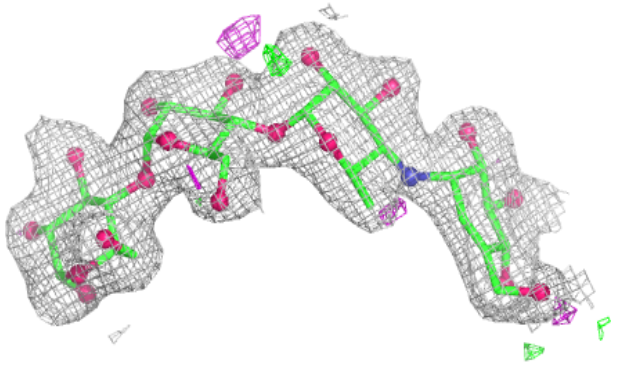


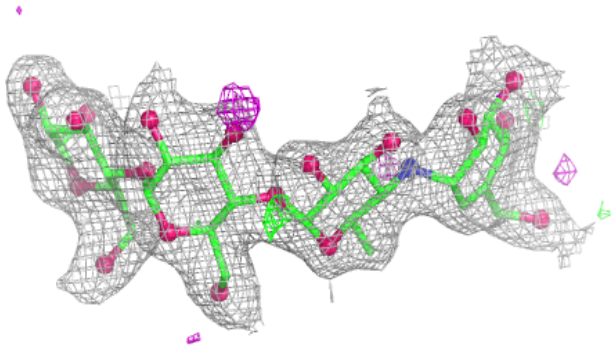


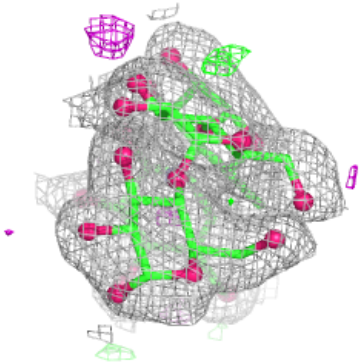


Electron density around Chain E:

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







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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	B	1002	6/6	0.68	0.22	38,44,50,54	0
3	GOL	A	1004	6/6	0.79	0.22	26,43,50,58	0
3	GOL	B	1001	6/6	0.82	0.21	38,41,43,48	0
4	CA	A	1008	1/1	0.82	0.14	60,60,60,60	0
3	GOL	A	1003	6/6	0.84	0.16	37,47,52,53	0
3	GOL	B	1003	6/6	0.88	0.15	31,34,39,48	0
3	GOL	A	1001	6/6	0.89	0.17	35,35,41,41	0
4	CA	A	1009	1/1	0.92	0.11	60,60,60,60	0
3	GOL	A	1005	6/6	0.94	0.08	33,35,36,43	0
3	GOL	A	1002	6/6	0.94	0.12	36,37,41,41	0
4	CA	B	1004	1/1	0.96	0.05	39,39,39,39	0
4	CA	B	1008	1/1	0.97	0.04	36,36,36,36	0
4	CA	B	1006	1/1	0.98	0.04	52,52,52,52	0
4	CA	B	1007	1/1	0.98	0.04	45,45,45,45	0
4	CA	A	1007	1/1	0.98	0.03	34,34,34,34	0
4	CA	A	1010	1/1	0.99	0.04	30,30,30,30	0
4	CA	A	1006	1/1	0.99	0.02	32,32,32,32	0
4	CA	B	1005	1/1	0.99	0.06	46,46,46,46	0

6.5 Other polymers (i)

There are no such residues in this entry.