Full wwPDB X-ray Structure Validation Report (i)

Mar 4, 2024 – 12:08 PM JST

PDB ID	:	8HWK
Title	:	Limosilactobacillus reuteri N1 GtfB-maltohexaose
Authors	:	Dong, J.J.; Bai, Y.X.
Deposited on	:	2022-12-30
Resolution	:	2.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

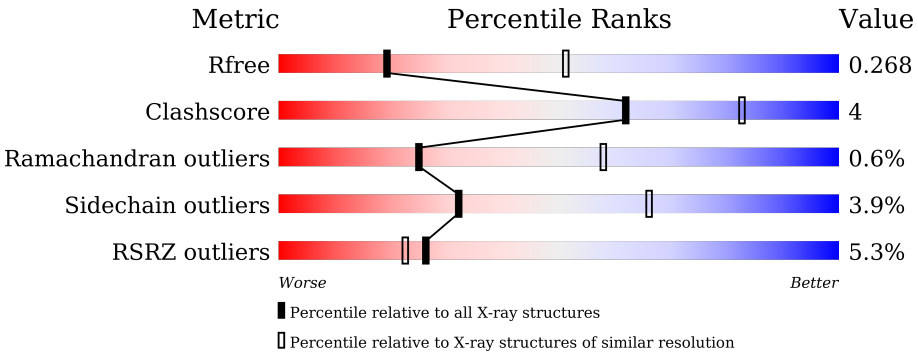
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	833	5% 85% 14% ••
1	B	833	6% 86% 13% ••
2	C	6	17% 33% 50%
2	D	6	17% 33% 50%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	C	1	-	-	-	X
2	GLC	C	2	-	-	-	X
2	GLC	C	3	-	-	-	X
2	GLC	D	1	-	-	-	X
2	GLC	D	3	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13187 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 dextransucrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	827	Total	C	N	O	S	0	0	0
			6457	4025	1095	1315	22			
1	B	827	Total	C	N	O	S	0	0	0
			6457	4025	1095	1315	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MET	-	initiating methionine	UNP A0A848PDI7
B	25	MET	-	initiating methionine	UNP A0A848PDI7

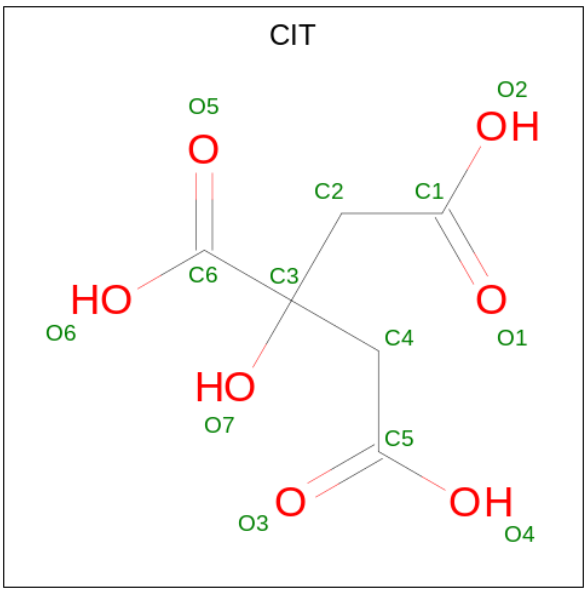
- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	6	Total	C	O		0	0	0
			67	36	31				
2	D	6	Total	C	O		0	0	0
			67	36	31				

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

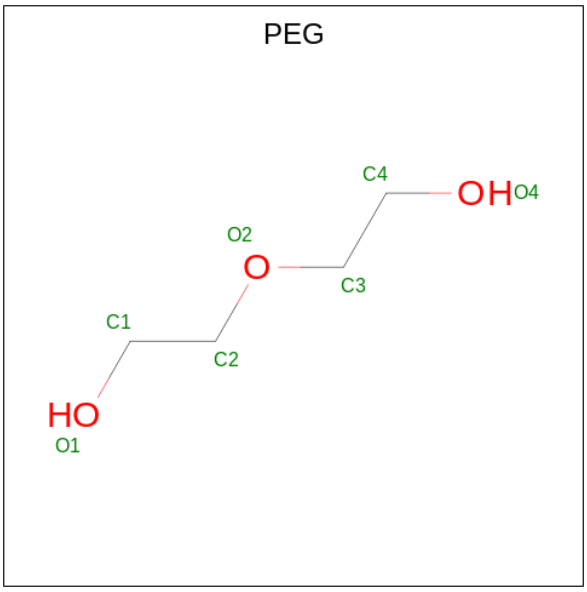
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 6 7	0	0
4	B	1	Total C O 13 6 7	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 7 4 3	0	0

- Molecule 6 is water.

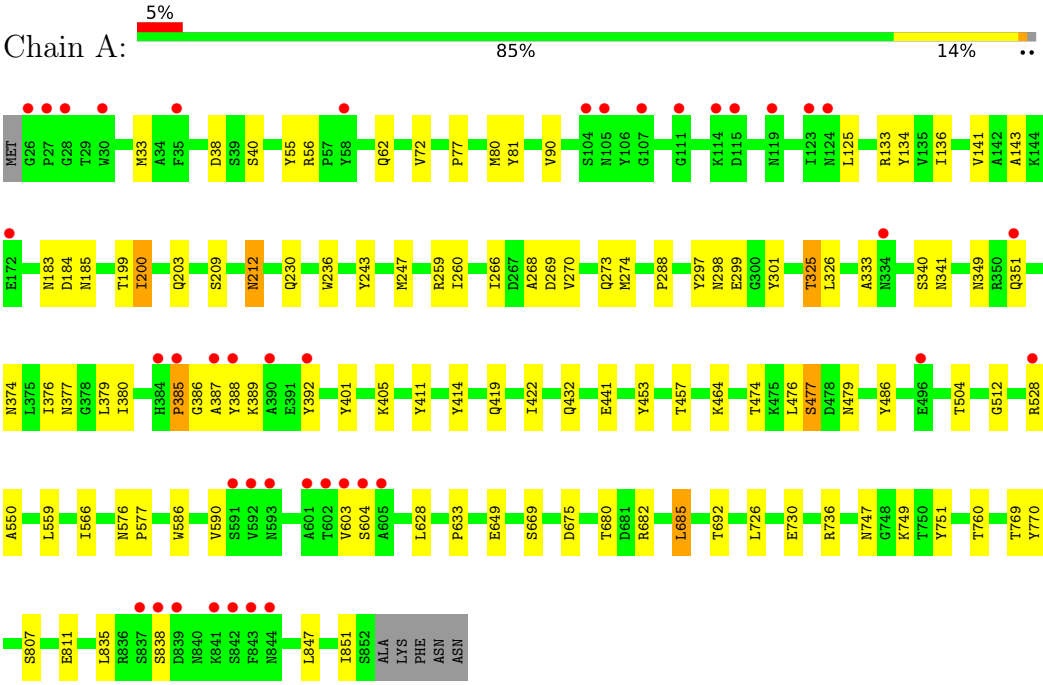
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	45	Total O 45 45	0	0
6	B	52	Total O 52 52	0	0

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.

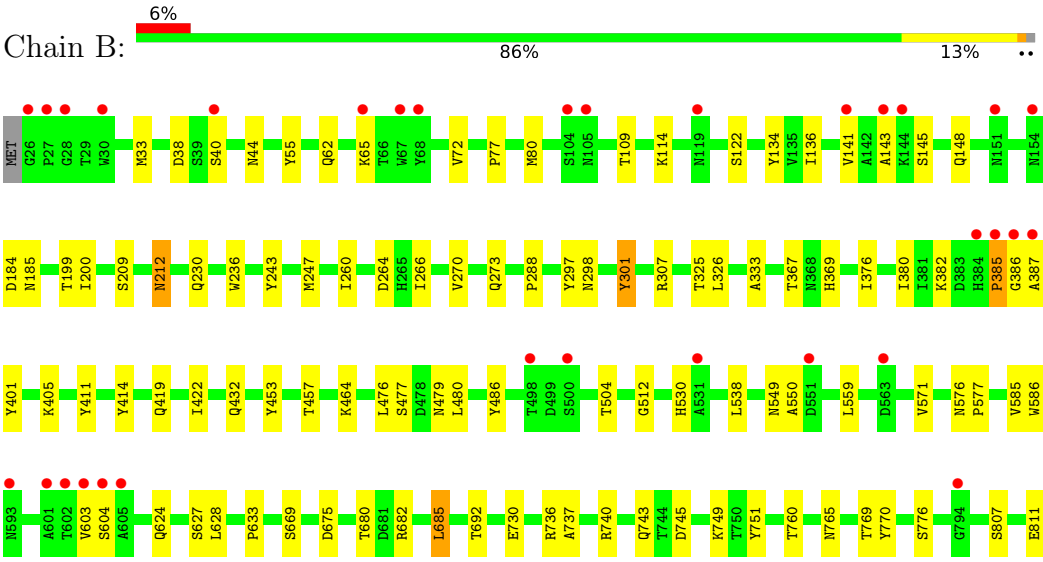
• Molecule 1: dextransucrase

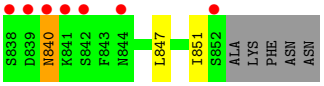
Chain A:



• Molecule 1: dextransucrase

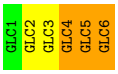
Chain B:





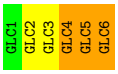
• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain C:



• 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 D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	206.15Å 101.19Å 106.79Å 90.00° 108.84° 90.00°	Depositor
Resolution (Å)	23.74 – 2.90 23.73 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (23.74-2.90) 99.7 (23.73-2.90)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.75 (at 2.89Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.215 , 0.261 0.223 , 0.268	Depositor DCC
R_{free} test set	2323 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	30.9	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	13187	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.70% 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: CIT, NA, PEG, 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	0.57	0/6597	0.72	0/8984
1	B	0.57	1/6597 (0.0%)	0.72	1/8984 (0.0%)
All	All	0.57	1/13194 (0.0%)	0.72	1/17968 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	745	ASP	CB-CG	5.16	1.62	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	307	ARG	NE-CZ-NH1	5.14	122.87	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6457	0	6094	57	0
1	B	6457	0	6094	53	0
2	C	67	0	57	4	0
2	D	67	0	57	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	13	0	5	0	0
4	B	13	0	5	1	0
5	A	7	0	10	0	0
5	B	7	0	10	1	0
6	A	45	0	0	0	0
6	B	52	0	0	0	0
All	All	13187	0	12332	111	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 4.

All (111) 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:633:PRO:HG2	2:D:6:GLC:O2	1.64	0.98
1:B:835:LEU:HD11	1:B:847:LEU:HD21	1.55	0.87
1:A:835:LEU:HD11	1:A:847:LEU:HD21	1.56	0.86
1:A:633:PRO:HG2	2:C:6:GLC:O2	1.83	0.78
1:A:374:ASN:O	1:A:377:ASN:O	2.02	0.78
1:B:692:THR:O	2:D:5:GLC:O3	2.05	0.73
1:A:200:ILE:HD12	1:A:212:ASN:O	1.91	0.70
2:C:4:GLC:O3	2:C:5:GLC:O5	2.12	0.68
1:A:266:ILE:HD12	1:A:270:VAL:HG21	1.76	0.67
2:D:4:GLC:O3	2:D:5:GLC:O5	2.12	0.67
1:B:266:ILE:HD12	1:B:270:VAL:HG21	1.82	0.62
1:B:260:ILE:HD13	1:B:298:ASN:OD1	2.00	0.61
1:A:260:ILE:HD12	1:A:298:ASN:OD1	2.02	0.60
1:A:236:TRP:CZ2	1:A:682:ARG:HG2	2.38	0.59
1:B:236:TRP:CZ2	1:B:682:ARG:HG2	2.37	0.59
1:B:243:TYR:CE1	1:B:685:LEU:HD22	2.39	0.58
1:A:692:THR:O	2:C:5:GLC:O3	2.20	0.58
1:A:243:TYR:CE1	1:A:685:LEU:HD22	2.40	0.57
1:A:835:LEU:CD1	1:A:847:LEU:HD21	2.31	0.56
1:B:835:LEU:CD1	1:B:847:LEU:HD21	2.32	0.55
1:B:376:ILE:O	1:B:380:ILE:HG12	2.07	0.55
1:B:212:ASN:O	1:B:740:ARG:NH2	2.40	0.54
1:A:376:ILE:O	1:A:380:ILE:HG12	2.08	0.54
1:A:77:PRO:HG2	1:A:80:MET:HG3	1.89	0.54
1:A:504:THR:HB	1:A:590:VAL:CG1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:LEU:HD22	1:A:675:ASP:OD2	2.08	0.53
1:B:628:LEU:HD22	1:B:675:ASP:OD2	2.09	0.53
1:B:77:PRO:HG2	1:B:80:MET:HG3	1.90	0.53
1:A:230:GLN:OE1	1:A:273:GLN:NE2	2.39	0.52
1:B:183:ASN:OD1	1:B:185:ASN:HB2	2.10	0.51
1:A:259:ARG:NH2	1:A:299:GLU:OE1	2.44	0.50
1:A:730:GLU:OE1	1:A:760:THR:OG1	2.23	0.50
1:B:326:LEU:HD21	1:B:422:ILE:HG21	1.94	0.50
1:A:326:LEU:HB3	1:A:419:GLN:HE21	1.77	0.50
1:A:747:ASN:HB2	1:B:382:LYS:O	2.11	0.50
1:A:183:ASN:OD1	1:A:185:ASN:HB2	2.11	0.50
1:B:576:ASN:HB2	1:B:577:PRO:CD	2.42	0.50
1:B:504:THR:HB	1:B:590:VAL:CG1	2.41	0.50
1:A:559:LEU:HD12	1:A:586:TRP:CH2	2.46	0.49
1:B:549:ASN:O	1:B:550:ALA:HB3	2.12	0.49
1:B:559:LEU:HD12	1:B:586:TRP:CH2	2.47	0.49
1:B:326:LEU:HB3	1:B:419:GLN:HE21	1.78	0.48
1:A:576:ASN:HB2	1:A:577:PRO:CD	2.44	0.48
1:B:453:TYR:CZ	1:B:457:THR:HG21	2.49	0.48
1:A:38:ASP:OD1	1:A:40:SER:OG	2.25	0.47
1:A:769:THR:HB	1:A:770:TYR:CD2	2.49	0.47
1:B:369:HIS:CD2	1:B:624:GLN:HE22	2.32	0.47
1:B:837:SER:HB2	1:B:840:ASN:HD22	1.79	0.47
1:A:453:TYR:CZ	1:A:457:THR:HG21	2.50	0.47
1:B:243:TYR:CE1	1:B:247:MET:HG3	2.50	0.47
1:B:730:GLU:OE1	1:B:760:THR:OG1	2.23	0.47
1:B:769:THR:HB	1:B:770:TYR:CD2	2.50	0.47
1:A:326:LEU:HD21	1:A:422:ILE:HG21	1.97	0.47
1:A:401:TYR:O	1:A:405:LYS:HG2	2.15	0.47
1:B:851:ILE:HG22	1:B:851:ILE:O	2.15	0.47
1:A:372:ARG:NH1	1:A:441:GLU:OE1	2.47	0.46
1:A:549:ASN:O	1:A:550:ALA:HB3	2.15	0.46
1:B:401:TYR:O	1:B:405:LYS:HG2	2.15	0.46
1:B:333:ALA:HB2	1:B:414:TYR:CE1	2.51	0.46
1:A:333:ALA:HB2	1:A:414:TYR:CE1	2.51	0.46
1:A:260:ILE:HD11	1:A:274:MET:SD	2.56	0.45
1:B:62:GLN:O	1:B:134:TYR:HB3	2.16	0.45
1:A:62:GLN:O	1:A:134:TYR:HB3	2.15	0.45
1:A:80:MET:SD	1:A:136:ILE:HG21	2.56	0.45
1:A:62:GLN:HE22	1:A:141:VAL:HG21	1.81	0.45
1:B:765:ASN:HB2	5:B:903:PEG:H41	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:LYS:O	1:A:389:LYS:HG3	2.17	0.45
1:A:851:ILE:O	1:A:851:ILE:HG22	2.16	0.44
1:A:243:TYR:CE1	1:A:247:MET:HG3	2.52	0.44
1:B:38:ASP:OD1	1:B:40:SER:OG	2.26	0.44
1:B:486:TYR:O	1:B:530:HIS:HE1	2.01	0.44
1:A:203:GLN:HG3	1:A:268:ALA:HB3	2.00	0.44
1:A:90:VAL:HG22	1:A:125:LEU:HD21	2.00	0.44
1:A:385:PRO:O	1:A:387:ALA:N	2.51	0.44
1:B:385:PRO:O	1:B:387:ALA:N	2.51	0.44
1:A:486:TYR:O	1:A:530:HIS:HE1	2.01	0.44
1:B:389:LYS:O	1:B:389:LYS:HG3	2.17	0.44
1:A:807:SER:O	1:A:811:GLU:HG3	2.18	0.43
1:A:325:THR:HG21	1:A:341:ASN:O	2.18	0.43
1:A:389:LYS:O	1:A:389:LYS:CG	2.67	0.43
1:B:62:GLN:HE22	1:B:141:VAL:HG21	1.84	0.43
1:B:538:LEU:HD23	1:B:585:VAL:HG11	2.01	0.43
1:A:288:PRO:HD3	1:A:604:SER:HB2	2.01	0.43
1:B:80:MET:SD	1:B:136:ILE:HG21	2.59	0.43
1:B:288:PRO:HD3	1:B:604:SER:HB2	2.01	0.43
1:A:747:ASN:CB	1:B:382:LYS:O	2.67	0.42
1:A:199:THR:OG1	1:A:212:ASN:HB2	2.18	0.42
1:B:389:LYS:O	1:B:389:LYS:CG	2.67	0.42
1:B:72:VAL:O	1:B:72:VAL:HG12	2.19	0.42
1:B:212:ASN:ND2	1:B:212:ASN:H	2.17	0.42
1:A:56:ARG:NH1	1:A:72:VAL:HG12	2.34	0.42
1:A:736:ARG:HB2	1:A:751:TYR:CZ	2.55	0.42
2:C:4:GLC:C3	2:C:5:GLC:O5	2.62	0.42
1:B:736:ARG:HB2	1:B:751:TYR:CZ	2.55	0.42
1:A:269:ASP:OD2	1:A:792:SER:OG	2.29	0.42
1:A:528:ARG:O	1:A:528:ARG:HG2	2.19	0.42
1:A:81:TYR:CE2	1:A:133:ARG:HD3	2.55	0.41
1:B:230:GLN:OE1	1:B:273:GLN:NE2	2.42	0.41
1:B:143:ALA:HB1	1:B:148:GLN:HE22	1.84	0.41
1:B:807:SER:O	1:B:811:GLU:HG3	2.21	0.41
1:A:479:ASN:O	1:A:512:GLY:HA2	2.21	0.41
1:B:199:THR:OG1	1:B:212:ASN:HB2	2.21	0.41
1:B:479:ASN:O	1:B:512:GLY:HA2	2.21	0.41
1:A:143:ALA:HB1	1:A:148:GLN:HE22	1.86	0.41
1:B:480:LEU:HD21	1:B:571:VAL:HG21	2.03	0.41
1:A:368:ASN:OD1	1:A:368:ASN:C	2.58	0.40
1:A:649:GLU:HA	1:A:649:GLU:OE2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:ASN:OD1	1:A:351:GLN:HB2	2.22	0.40
1:B:264:ASP:OD2	4:B:902:CIT:O6	2.40	0.40
1:B:737:ALA:HA	1:B:743:GLN:HA	2.04	0.40
1:B:301:TYR:C	1:B:301:TYR:CD1	2.95	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	825/833 (99%)	756 (92%)	63 (8%)	6 (1%)	22	54
1	B	825/833 (99%)	758 (92%)	63 (8%)	4 (0%)	29	61
All	All	1650/1666 (99%)	1514 (92%)	126 (8%)	10 (1%)	25	58

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	386	GLY
1	B	386	GLY
1	A	33	MET
1	A	200	ILE
1	A	477	SER
1	B	33	MET
1	B	200	ILE
1	A	838	SER
1	B	385	PRO
1	A	385	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	695/700 (99%)	669 (96%)	26 (4%)	34	68
1	B	695/700 (99%)	667 (96%)	28 (4%)	31	65
All	All	1390/1400 (99%)	1336 (96%)	54 (4%)	32	66

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	TYR
1	A	145	SER
1	A	184	ASP
1	A	209	SER
1	A	212	ASN
1	A	297	TYR
1	A	301	TYR
1	A	325	THR
1	A	340	SER
1	A	379	LEU
1	A	388	TYR
1	A	392	TYR
1	A	411	TYR
1	A	432	GLN
1	A	464	LYS
1	A	474	THR
1	A	476	LEU
1	A	477	SER
1	A	566	ILE
1	A	603	VAL
1	A	669	SER
1	A	680	THR
1	A	685	LEU
1	A	726	LEU
1	A	749	LYS
1	A	776	SER
1	B	44	ASN

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Mol	Chain	Res	Type
1	B	55	TYR
1	B	65	LYS
1	B	109	THR
1	B	114	LYS
1	B	122	SER
1	B	145	SER
1	B	172	GLU
1	B	184	ASP
1	B	209	SER
1	B	212	ASN
1	B	297	TYR
1	B	301	TYR
1	B	325	THR
1	B	367	THR
1	B	411	TYR
1	B	432	GLN
1	B	464	LYS
1	B	476	LEU
1	B	477	SER
1	B	603	VAL
1	B	627	SER
1	B	669	SER
1	B	680	THR
1	B	685	LEU
1	B	749	LYS
1	B	776	SER
1	B	840	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	62	GLN
1	A	151	ASN
1	A	177	GLN
1	A	201	ASN
1	A	334	ASN
1	A	335	ASN
1	A	410	GLN
1	A	413	GLN
1	A	419	GLN
1	A	638	ASN

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Mol	Chain	Res	Type
1	A	767	GLN
1	A	840	ASN
1	B	46	ASN
1	B	130	GLN
1	B	151	ASN
1	B	212	ASN
1	B	334	ASN
1	B	335	ASN
1	B	369	HIS
1	B	410	GLN
1	B	413	GLN
1	B	419	GLN
1	B	432	GLN
1	B	494	ASN
1	B	638	ASN
1	B	765	ASN
1	B	767	GLN
1	B	840	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

12 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	12,12,12	0.60	0	17,17,17	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GLC	C	2	2	11,11,12	0.69	0	15,15,17	3.99	8 (53%)
2	GLC	C	3	2	11,11,12	0.36	0	15,15,17	2.04	4 (26%)
2	GLC	C	4	2	11,11,12	0.47	0	15,15,17	1.40	2 (13%)
2	GLC	C	5	2	11,11,12	0.37	0	15,15,17	2.69	6 (40%)
2	GLC	C	6	2	11,11,12	0.36	0	15,15,17	2.11	5 (33%)
2	GLC	D	1	2	12,12,12	0.59	0	17,17,17	0.76	0
2	GLC	D	2	2	11,11,12	0.71	0	15,15,17	3.99	8 (53%)
2	GLC	D	3	2	11,11,12	0.35	0	15,15,17	2.03	5 (33%)
2	GLC	D	4	2	11,11,12	0.48	0	15,15,17	1.40	2 (13%)
2	GLC	D	5	2	11,11,12	0.37	0	15,15,17	2.69	6 (40%)
2	GLC	D	6	2	11,11,12	0.36	0	15,15,17	2.11	5 (33%)

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	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	C	3	2	-	1/2/19/22	0/1/1/1
2	GLC	C	4	2	-	0/2/19/22	0/1/1/1
2	GLC	C	5	2	-	0/2/19/22	0/1/1/1
2	GLC	C	6	2	-	0/2/19/22	0/1/1/1
2	GLC	D	1	2	-	0/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	GLC	D	3	2	-	1/2/19/22	0/1/1/1
2	GLC	D	4	2	-	0/2/19/22	0/1/1/1
2	GLC	D	5	2	-	0/2/19/22	0/1/1/1
2	GLC	D	6	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	GLC	C2-C3-C4	-8.27	96.58	110.89
2	D	2	GLC	C2-C3-C4	-8.26	96.60	110.89
2	C	2	GLC	O4-C4-C3	7.87	128.53	110.35
2	D	2	GLC	O4-C4-C3	7.86	128.53	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	GLC	C3-C4-C5	-6.10	99.36	110.24
2	D	2	GLC	C3-C4-C5	-6.10	99.36	110.24
2	D	5	GLC	O5-C1-C2	5.07	118.60	110.77
2	C	5	GLC	O5-C1-C2	5.04	118.55	110.77
2	C	3	GLC	C1-C2-C3	4.75	115.50	109.67
2	D	3	GLC	C1-C2-C3	4.70	115.44	109.67
2	D	2	GLC	O5-C5-C4	-4.46	99.97	110.83
2	C	2	GLC	O5-C5-C4	-4.46	99.99	110.83
2	D	6	GLC	C1-C2-C3	4.32	114.98	109.67
2	C	6	GLC	C1-C2-C3	4.32	114.97	109.67
2	C	5	GLC	C1-C2-C3	4.14	114.76	109.67
2	D	5	GLC	C1-C2-C3	4.12	114.74	109.67
2	C	5	GLC	C2-C3-C4	-4.07	103.85	110.89
2	D	5	GLC	C2-C3-C4	-4.05	103.88	110.89
2	D	6	GLC	O5-C1-C2	3.96	116.89	110.77
2	C	6	GLC	O5-C1-C2	3.95	116.87	110.77
2	C	2	GLC	O4-C4-C5	3.91	119.00	109.30
2	D	2	GLC	O4-C4-C5	3.91	119.00	109.30
2	C	5	GLC	C1-O5-C5	3.75	117.28	112.19
2	D	5	GLC	C1-O5-C5	3.73	117.24	112.19
2	D	3	GLC	C2-C3-C4	3.61	117.13	110.89
2	C	3	GLC	C2-C3-C4	3.57	117.07	110.89
2	D	4	GLC	C1-O5-C5	3.52	116.96	112.19
2	C	4	GLC	C1-O5-C5	3.50	116.93	112.19
2	D	5	GLC	C3-C4-C5	-3.43	104.12	110.24
2	C	5	GLC	C3-C4-C5	-3.40	104.17	110.24
2	C	2	GLC	C1-C2-C3	3.26	113.67	109.67
2	D	2	GLC	C1-C2-C3	3.22	113.63	109.67
2	C	2	GLC	O3-C3-C4	3.21	117.76	110.35
2	D	2	GLC	O3-C3-C4	3.19	117.73	110.35
2	D	5	GLC	O4-C4-C5	3.12	117.05	109.30
2	C	5	GLC	O4-C4-C5	3.10	116.99	109.30
2	C	6	GLC	C3-C4-C5	-2.81	105.22	110.24
2	D	6	GLC	C3-C4-C5	-2.81	105.22	110.24
2	C	6	GLC	C1-O5-C5	2.63	115.75	112.19
2	D	6	GLC	C1-O5-C5	2.60	115.72	112.19
2	D	6	GLC	O5-C5-C4	-2.58	104.56	110.83
2	C	6	GLC	O5-C5-C4	-2.57	104.57	110.83
2	D	2	GLC	C6-C5-C4	2.53	118.93	113.00
2	C	2	GLC	C6-C5-C4	2.52	118.91	113.00
2	D	3	GLC	O4-C4-C3	-2.51	104.54	110.35
2	C	3	GLC	O4-C4-C3	-2.51	104.56	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	4	GLC	O4-C4-C3	-2.04	105.63	110.35
2	D	4	GLC	O4-C4-C3	-2.04	105.64	110.35
2	C	3	GLC	O2-C2-C3	-2.03	106.07	110.14
2	D	3	GLC	O2-C2-C3	-2.03	106.07	110.14
2	D	3	GLC	O5-C1-C2	-2.03	107.64	110.77

There are no chirality outliers.

All (2) torsion outliers are listed below:

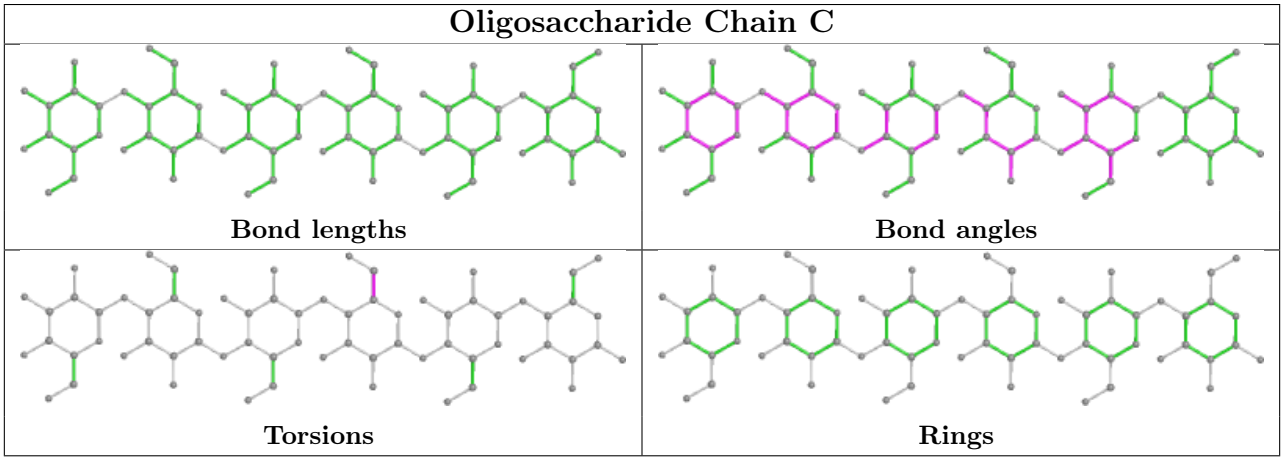
Mol	Chain	Res	Type	Atoms
2	C	3	GLC	C4-C5-C6-O6
2	D	3	GLC	C4-C5-C6-O6

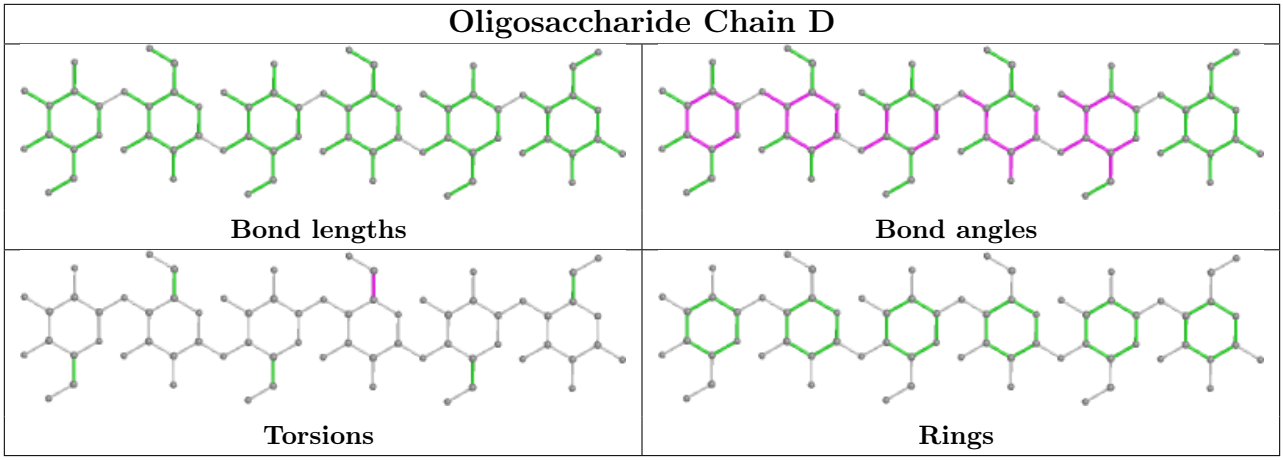
There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	4	GLC	1	0
2	C	5	GLC	3	0
2	D	6	GLC	1	0
2	D	5	GLC	2	0
2	C	4	GLC	2	0
2	C	6	GLC	1	0

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





5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
4	CIT	A	902	-	12,12,12	1.07	0	17,17,17	1.30	4 (23%)
4	CIT	B	902	-	12,12,12	1.07	0	17,17,17	1.58	4 (23%)
5	PEG	A	903	-	6,6,6	0.45	0	5,5,5	0.63	0
5	PEG	B	903	-	6,6,6	0.39	0	5,5,5	0.70	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
4	CIT	A	902	-	-	4/16/16/16	-
4	CIT	B	902	-	-	1/16/16/16	-
5	PEG	A	903	-	-	2/4/4/4	-
5	PEG	B	903	-	-	2/4/4/4	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	902	CIT	O7-C3-C6	-3.24	104.31	108.86
4	B	902	CIT	O6-C6-C3	2.70	117.74	113.05
4	A	902	CIT	O2-C1-C2	2.43	122.14	114.35
4	B	902	CIT	C3-C2-C1	-2.33	108.17	113.81
4	A	902	CIT	C3-C2-C1	2.29	119.35	113.81
4	B	902	CIT	O5-C6-C3	-2.23	119.09	122.25
4	A	902	CIT	O1-C1-C2	-2.20	116.51	122.94
4	A	902	CIT	O6-C6-C3	2.09	116.68	113.05

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	903	PEG	O1-C1-C2-O2
5	B	903	PEG	O1-C1-C2-O2
4	A	902	CIT	O1-C1-C2-C3
4	A	902	CIT	O2-C1-C2-C3
5	A	903	PEG	C1-C2-O2-C3
4	B	902	CIT	C6-C3-C4-C5
4	A	902	CIT	O7-C3-C4-C5
4	A	902	CIT	C6-C3-C4-C5
5	B	903	PEG	C1-C2-O2-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	902	CIT	1	0
5	B	903	PEG	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	827/833 (99%)	0.08	42 (5%)	28	24	12, 25, 62, 111	0
1	B	827/833 (99%)	0.09	46 (5%)	24	20	12, 25, 68, 103	0
All	All	1654/1666 (99%)	0.09	88 (5%)	26	22	12, 25, 67, 111	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	26	GLY	7.3
1	A	838	SER	7.1
1	A	603	VAL	6.7
1	B	27	PRO	6.7
1	B	388	TYR	6.7
1	B	838	SER	6.6
1	B	390	ALA	6.0
1	A	27	PRO	6.0
1	A	839	ASP	5.6
1	B	26	GLY	5.5
1	A	385	PRO	5.5
1	B	28	GLY	5.4
1	B	837	SER	5.4
1	A	837	SER	5.1
1	B	385	PRO	5.1
1	B	841	LYS	5.0
1	B	839	ASP	4.6
1	A	842	SER	4.6
1	A	388	TYR	4.5
1	A	28	GLY	4.4
1	B	65	LYS	4.2
1	B	603	VAL	4.0
1	B	602	THR	3.9
1	B	105	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	30	TRP	3.7
1	A	602	THR	3.5
1	A	390	ALA	3.2
1	A	392	TYR	3.2
1	B	119	ASN	3.1
1	B	842	SER	3.0
1	B	605	ALA	3.0
1	A	605	ALA	2.9
1	A	105	ASN	2.9
1	B	601	ALA	2.9
1	A	115	ASP	2.9
1	A	841	LYS	2.9
1	B	141	VAL	2.9
1	B	498	THR	2.8
1	B	604	SER	2.8
1	A	119	ASN	2.7
1	A	114	LYS	2.7
1	B	144	LYS	2.7
1	A	124	ASN	2.7
1	B	836	ARG	2.7
1	B	563	ASP	2.6
1	A	35	PHE	2.6
1	B	592	VAL	2.6
1	A	172	GLU	2.6
1	B	591	SER	2.6
1	A	387	ALA	2.6
1	A	843	PHE	2.6
1	B	67	TRP	2.6
1	A	30	TRP	2.6
1	A	593	ASN	2.6
1	A	111	GLY	2.5
1	B	500	SER	2.5
1	B	143	ALA	2.4
1	B	151	ASN	2.4
1	A	334	ASN	2.4
1	A	104	SER	2.4
1	B	386	GLY	2.4
1	A	351	GLN	2.4
1	A	604	SER	2.4
1	A	107	GLY	2.3
1	A	123	ILE	2.3
1	B	68	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	852	SER	2.3
1	A	592	VAL	2.3
1	A	496	GLU	2.3
1	B	389	LYS	2.3
1	B	840	ASN	2.2
1	A	384	HIS	2.2
1	B	531	ALA	2.2
1	B	387	ALA	2.2
1	B	40	SER	2.1
1	B	794	GLY	2.1
1	A	601	ALA	2.1
1	A	844	ASN	2.1
1	B	384	HIS	2.1
1	B	154	ASN	2.1
1	B	593	ASN	2.1
1	B	844	ASN	2.1
1	A	528	ARG	2.1
1	A	58	TYR	2.0
1	A	591	SER	2.0
1	A	145	SER	2.0
1	B	104	SER	2.0
1	B	551	ASP	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	D	1	12/12	0.44	0.74	78,94,103,103	0
2	GLC	C	1	12/12	0.47	0.74	78,94,103,103	0
2	GLC	C	3	11/12	0.62	0.44	57,63,66,69	0
2	GLC	D	2	11/12	0.63	0.38	53,65,73,73	0
2	GLC	D	3	11/12	0.66	0.44	57,63,66,69	0
2	GLC	C	2	11/12	0.67	0.43	53,65,73,73	0

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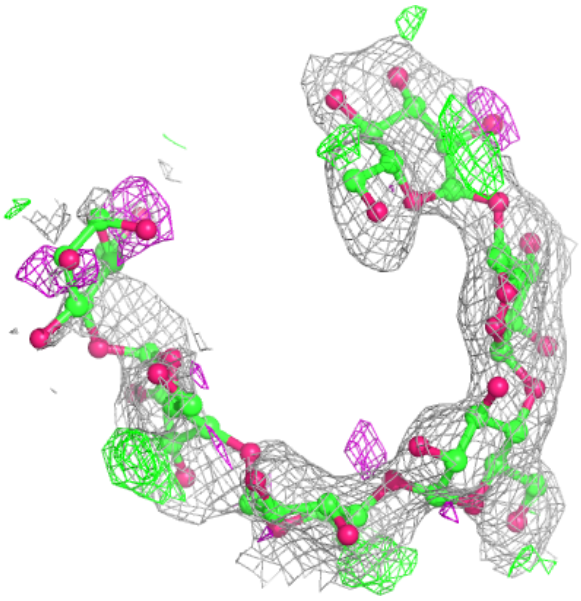
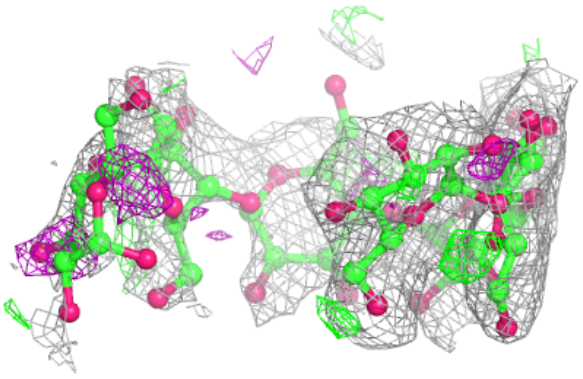
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	C	6	11/12	0.76	0.34	38,44,49,50	0
2	GLC	D	6	11/12	0.82	0.34	38,44,49,50	0
2	GLC	D	4	11/12	0.83	0.41	46,49,55,55	0
2	GLC	C	4	11/12	0.83	0.30	46,49,55,55	0
2	GLC	D	5	11/12	0.85	0.25	38,44,49,50	0
2	GLC	C	5	11/12	0.87	0.26	38,44,49,50	0

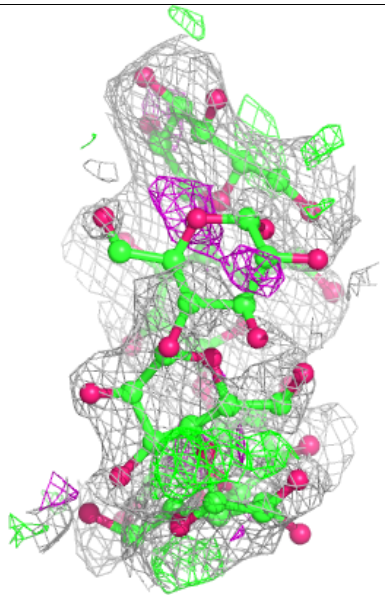
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

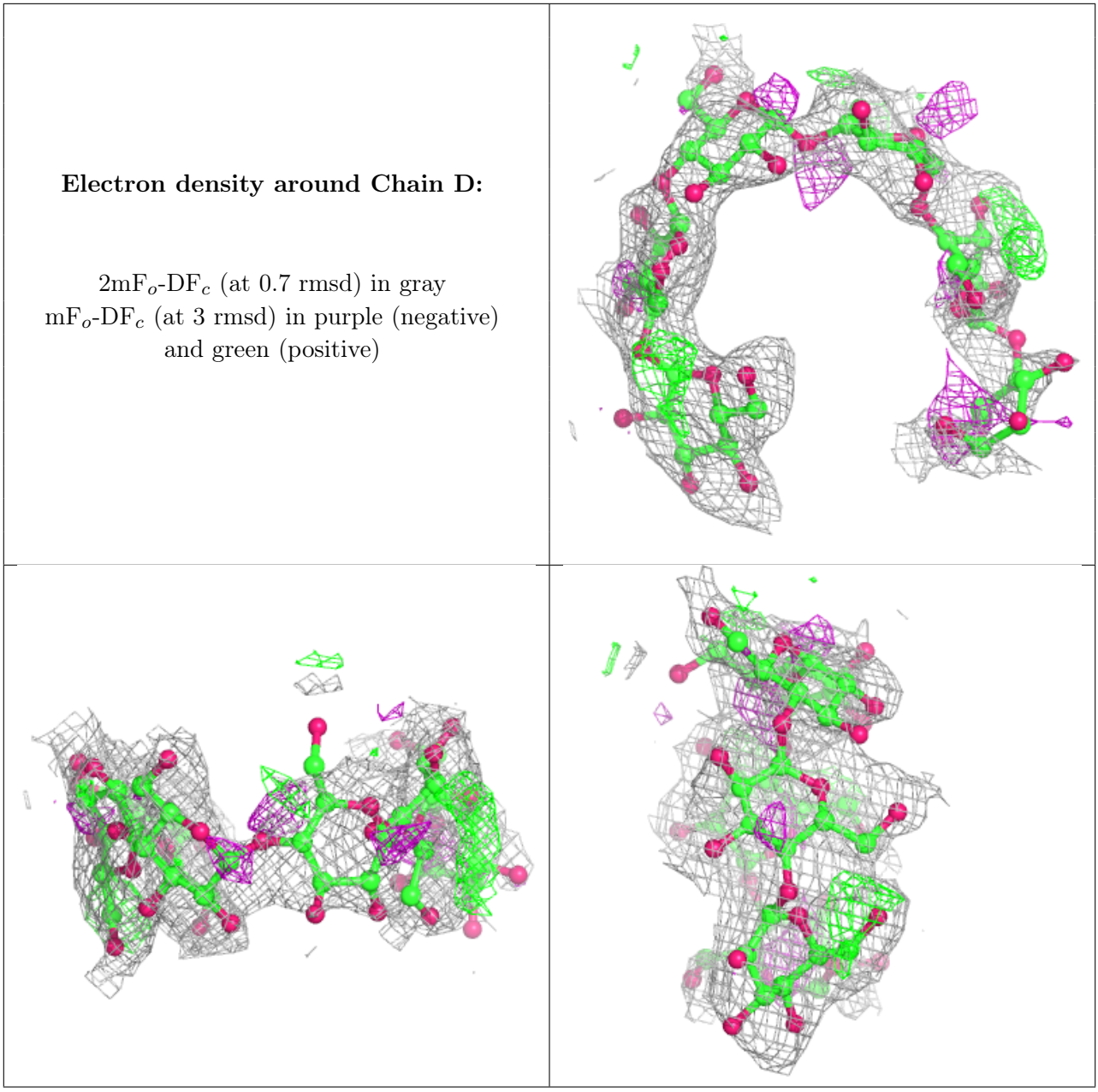






Electron density around Chain D:

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



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, 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
4	CIT	B	902	13/13	0.89	0.29	41,45,50,51	0
4	CIT	A	902	13/13	0.90	0.23	33,37,39,41	0
3	NA	A	901	1/1	0.91	0.10	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PEG	A	903	7/7	0.93	0.23	28,32,33,35	0
5	PEG	B	903	7/7	0.94	0.19	21,23,24,25	0
3	NA	B	901	1/1	0.99	0.07	15,15,15,15	0

6.5 Other polymers (i)

There are no such residues in this entry.