Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2024 – 02:17 PM EST

PDB ID	:	3HZ3
Title	:	Lactobacillus reuteri N-terminally truncated glucansucrase GTF180(D1025N) -sucrose complex
Authors	:	Vujicic-Zagar, A.; Pijning, T.; Kralj, S.; Eeuwema, W.; Dijkhuizen, L.; Dijkstra, B.W.
Deposited on	:	2009-06-23
Resolution	:	2.22 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:

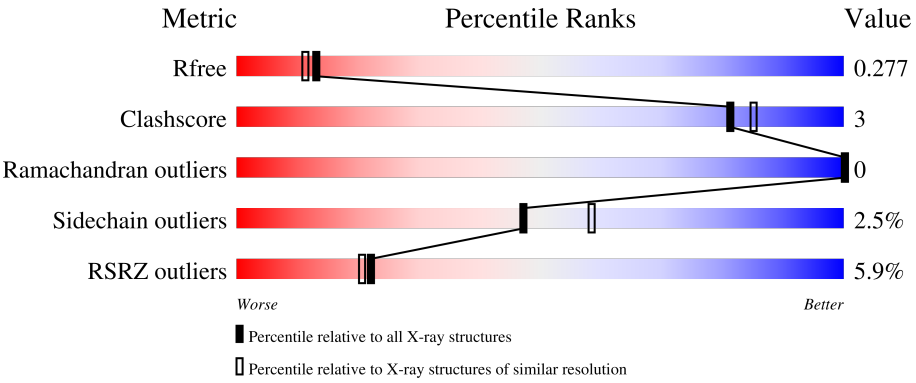
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.22 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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	1039	6% 88% 8% .
2	B	2	100%
2	C	2	50% 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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FRU	C	2	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8251 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.

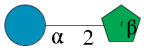
- Molecule 1 is a protein called Glucansucrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1003	Total	C	N	O	S	0	0	0
			7960	4979	1349	1611	21			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	740	MET	-	expression tag	UNP Q5SBN3
A	741	GLY	-	expression tag	UNP Q5SBN3
A	1025	ASN	ASP	engineered mutation	UNP Q5SBN3
A	1674	LEU	PHE	SEE REMARK 999	UNP Q5SBN3
A	1773	HIS	-	expression tag	UNP Q5SBN3
A	1774	HIS	-	expression tag	UNP Q5SBN3
A	1775	HIS	-	expression tag	UNP Q5SBN3
A	1776	HIS	-	expression tag	UNP Q5SBN3
A	1777	HIS	-	expression tag	UNP Q5SBN3
A	1778	HIS	-	expression tag	UNP Q5SBN3

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	O		0	0	0
			23	12	11				
2	C	2	Total	C	O		0	0	0
			23	12	11				

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0

- Molecule 4 is water.

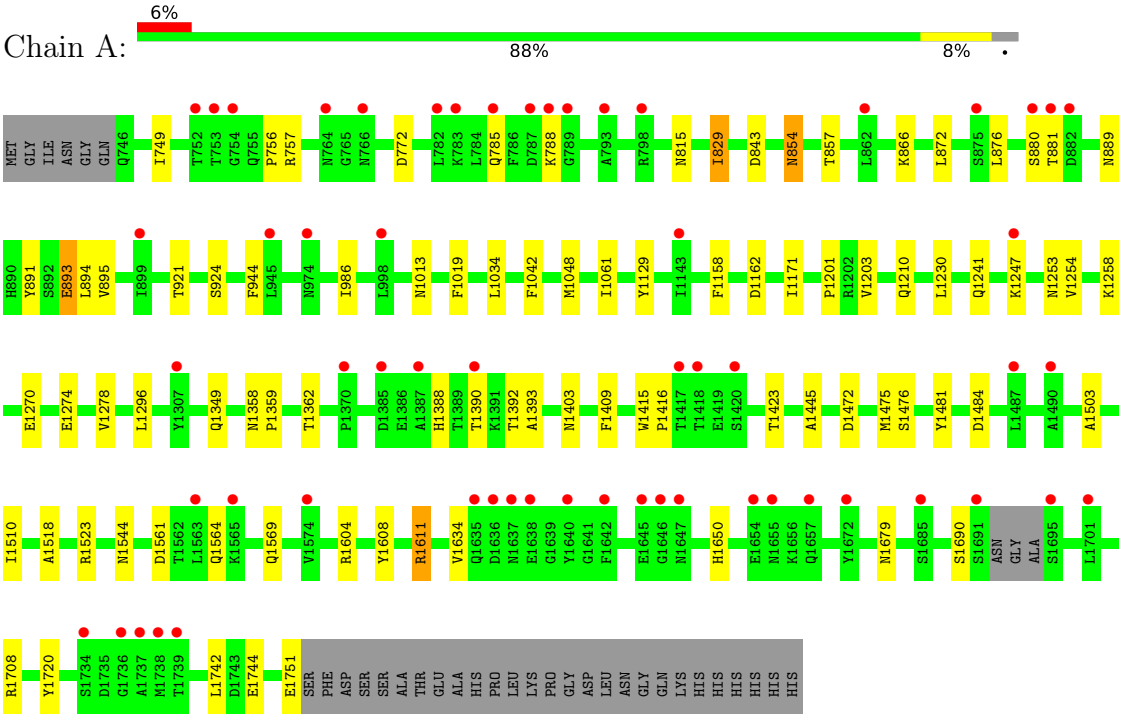
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	244	Total O 244 244	0	0

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.

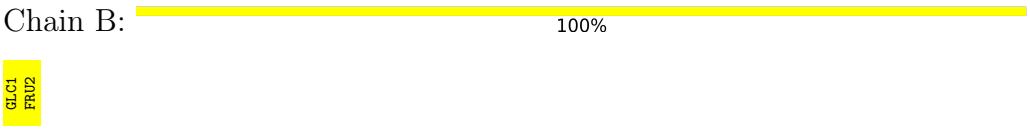
• Molecule 1: Glucansucrase

Chain A:



• Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain B:



• Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	57.78Å 66.23Å 82.72Å 107.13° 101.37° 85.40°	Depositor
Resolution (Å)	20.00 – 2.22 20.00 – 2.22	Depositor EDS
% Data completeness (in resolution range)	96.3 (20.00-2.22) 96.2 (20.00-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 2.21Å)	Xtriage
Refinement program	REFMAC 5.3.0011	Depositor
R, R_{free}	0.193 , 0.243 0.236 , 0.277	Depositor DCC
R_{free} test set	2723 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	31.4	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 44.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8251	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% 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: GLC, CA, FRU

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	0.66	0/8136	0.69	1/11066 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1296	LEU	CA-CB-CG	5.05	126.92	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7960	0	7511	40	0
2	B	23	0	21	0	0
2	C	23	0	21	1	0
3	A	1	0	0	0	0
4	A	244	0	0	2	0
All	All	8251	0	7553	41	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 (41) 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:A:1390:THR:HG23	1:A:1392:THR:HG22	1.78	0.66
1:A:1544:ASN:HD21	1:A:1604:ARG:HH22	1.42	0.65
1:A:815:ASN:HD22	1:A:1518:ALA:H	1.53	0.54
1:A:854:ASN:HD22	1:A:857:THR:H	1.58	0.52
1:A:866:LYS:HB2	1:A:872:LEU:HB2	1.92	0.52
1:A:1061:ILE:HB	1:A:1129:TYR:CE2	2.45	0.51
1:A:815:ASN:ND2	1:A:1518:ALA:H	2.08	0.50
1:A:749:ILE:HA	1:A:756:PRO:HA	1.94	0.50
1:A:866:LYS:HE3	1:A:876:LEU:O	2.12	0.49
1:A:1409:PHE:CG	1:A:1445:ALA:HB2	2.47	0.49
1:A:1158:PHE:HB2	1:A:1162:ASP:HB2	1.94	0.49
1:A:1475:MET:HG3	1:A:1484:ASP:HB3	1.95	0.49
1:A:1472:ASP:OD2	1:A:1476:SER:OG	2.22	0.48
1:A:1258:LYS:HD3	1:A:1270:GLU:OE1	2.13	0.48
1:A:1203:VAL:HG21	1:A:1230:LEU:HD21	1.97	0.47
1:A:1358:ASN:HB2	1:A:1359:PRO:CD	2.44	0.47
1:A:944:PHE:O	1:A:1523:ARG:HD2	2.15	0.46
1:A:986:ILE:HD11	1:A:1510:ILE:HG13	1.97	0.46
1:A:854:ASN:ND2	1:A:857:THR:H	2.15	0.45
1:A:894:LEU:HD12	1:A:894:LEU:HA	1.80	0.45
1:A:891:TYR:O	1:A:895:VAL:HG23	2.17	0.45
1:A:1247:LYS:HG2	4:A:182:HOH:O	2.16	0.44
1:A:1611:ARG:HD2	4:A:225:HOH:O	2.18	0.44
1:A:829:ILE:HD13	1:A:843:ASP:HB3	2.00	0.44
1:A:1171:ILE:HD12	1:A:1210:GLN:HG2	2.00	0.44
1:A:1388:HIS:HE1	1:A:1393:ALA:O	2.01	0.43
1:A:1423:THR:HB	1:A:1481:TYR:HB3	2.00	0.43
2:C:1:GLC:O6	2:C:1:GLC:O4	2.36	0.43
1:A:1604:ARG:HD3	1:A:1608:TYR:CE2	2.54	0.42
1:A:1720:TYR:HB3	1:A:1742:LEU:HD11	2.00	0.42
1:A:757:ARG:NH2	1:A:1751:GLU:OE2	2.53	0.42
1:A:889:ASN:O	1:A:893:GLU:HG3	2.20	0.42
1:A:1201:PRO:HD2	1:A:1403:ASN:O	2.20	0.41
1:A:1241:GLN:HA	1:A:1254:VAL:O	2.20	0.41
1:A:1019:PHE:CG	1:A:1503:ALA:HB2	2.55	0.41
1:A:1253:ASN:HB3	1:A:1278:VAL:HB	2.02	0.41
1:A:1034:LEU:HD23	1:A:1034:LEU:HA	1.86	0.41
1:A:1415:TRP:HA	1:A:1416:PRO:HD3	1.99	0.40
1:A:1650:HIS:HE1	1:A:1679:ASN:OD1	2.04	0.40
1:A:1270:GLU:O	1:A:1274:GLU:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1042:PHE:HB3	1:A:1048:MET:HG3	2.04	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	999/1039 (96%)	955 (96%)	44 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	855/883 (97%)	834 (98%)	21 (2%)	47	58

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	772	ASP
1	A	785	GLN
1	A	788	LYS
1	A	829	ILE
1	A	854	ASN

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Mol	Chain	Res	Type
1	A	880	SER
1	A	881	THR
1	A	893	GLU
1	A	921	THR
1	A	924	SER
1	A	1013	ASN
1	A	1349	GLN
1	A	1362	THR
1	A	1561	ASP
1	A	1564	GLN
1	A	1569	GLN
1	A	1611	ARG
1	A	1634	VAL
1	A	1690	SER
1	A	1708	ARG
1	A	1744	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	755	GLN
1	A	815	ASN
1	A	854	ASN
1	A	1013	ASN
1	A	1349	GLN
1	A	1544	ASN
1	A	1650	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

4 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	B	1	2	11,11,12	1.85	4 (36%)	15,15,17	1.96	4 (26%)
2	FRU	B	2	2	11,12,12	1.22	1 (9%)	10,18,18	1.16	2 (20%)
2	GLC	C	1	2	11,11,12	1.44	3 (27%)	15,15,17	2.80	6 (40%)
2	FRU	C	2	2	11,12,12	2.62	5 (45%)	10,18,18	1.72	2 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	B	1	2	-	2/2/19/22	0/1/1/1
2	FRU	B	2	2	-	0/5/24/24	0/1/1/1
2	GLC	C	1	2	-	1/2/19/22	0/1/1/1
2	FRU	C	2	2	-	3/5/24/24	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	FRU	O5-C2	5.13	1.51	1.43
2	C	2	FRU	O2-C2	4.86	1.49	1.40
2	B	1	GLC	O5-C1	3.97	1.50	1.43
2	B	2	FRU	O2-C2	2.87	1.45	1.40
2	B	1	GLC	O5-C5	2.82	1.49	1.43
2	C	1	GLC	O5-C1	2.69	1.48	1.43
2	C	2	FRU	C1-C2	2.60	1.56	1.52
2	C	2	FRU	O5-C5	2.47	1.49	1.43
2	C	2	FRU	O3-C3	2.42	1.47	1.42
2	B	1	GLC	C4-C3	2.19	1.57	1.52
2	C	1	GLC	C2-C3	2.14	1.55	1.52
2	C	1	GLC	C1-C2	2.06	1.56	1.52
2	B	1	GLC	C1-C2	2.05	1.56	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	GLC	C1-C2-C3	5.07	115.90	109.67
2	C	1	GLC	O5-C1-C2	5.07	118.60	110.77
2	C	1	GLC	C1-O5-C5	-4.94	105.50	112.19
2	C	1	GLC	O5-C5-C6	4.16	113.73	107.20
2	B	1	GLC	O5-C1-C2	-3.97	104.65	110.77
2	B	1	GLC	C1-O5-C5	3.90	117.48	112.19
2	C	2	FRU	O5-C5-C6	3.56	118.76	108.85
2	B	1	GLC	O5-C5-C6	-2.95	102.58	107.20
2	C	2	FRU	C6-C5-C4	-2.86	108.20	115.09
2	C	1	GLC	C3-C4-C5	-2.74	105.35	110.24
2	B	1	GLC	O2-C2-C1	2.69	114.66	109.15
2	C	1	GLC	C6-C5-C4	2.37	118.56	113.00
2	B	2	FRU	O4-C4-C3	-2.25	105.41	112.15
2	B	2	FRU	O5-C5-C6	-2.14	102.89	108.85

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	FRU	O1-C1-C2-C3
2	C	2	FRU	O1-C1-C2-O2
2	C	2	FRU	O1-C1-C2-O5
2	C	1	GLC	O5-C5-C6-O6
2	B	1	GLC	C4-C5-C6-O6
2	B	1	GLC	O5-C5-C6-O6

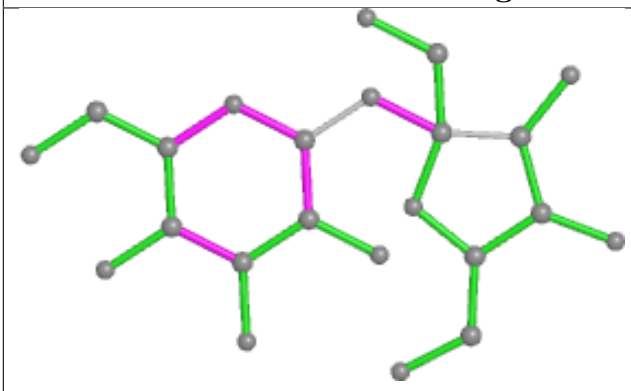
There are no ring outliers.

1 monomer is involved in 1 short contact:

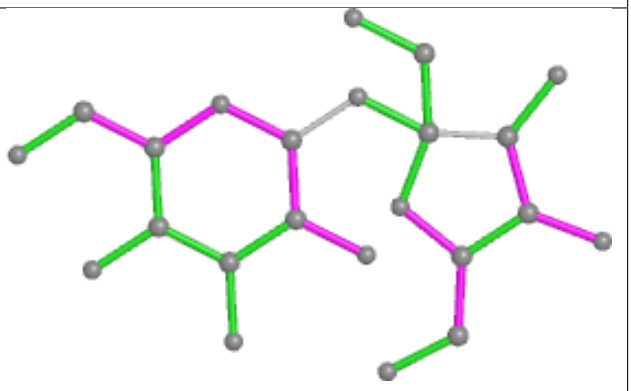
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	GLC	1	0

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

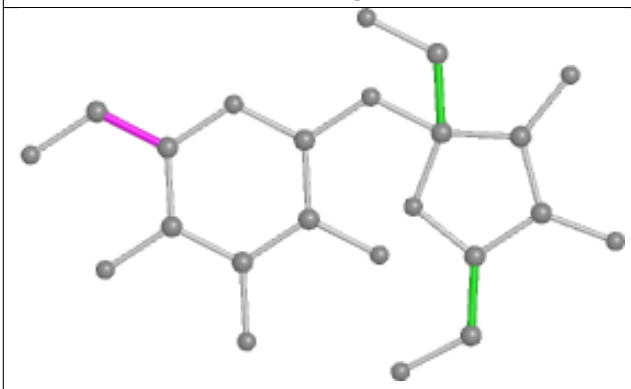
Oligosaccharide Chain B



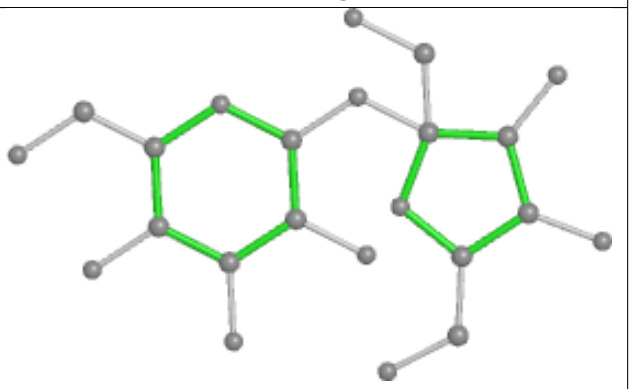
Bond lengths



Bond angles

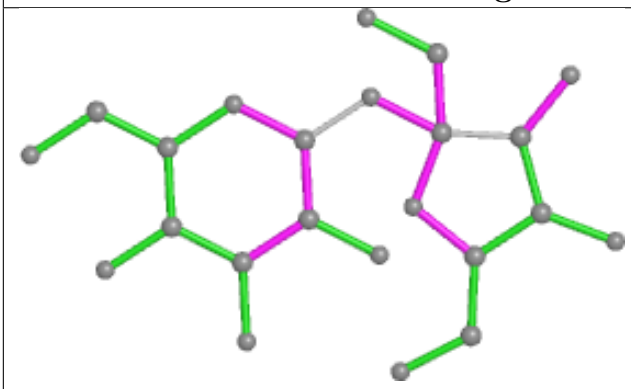


Torsions

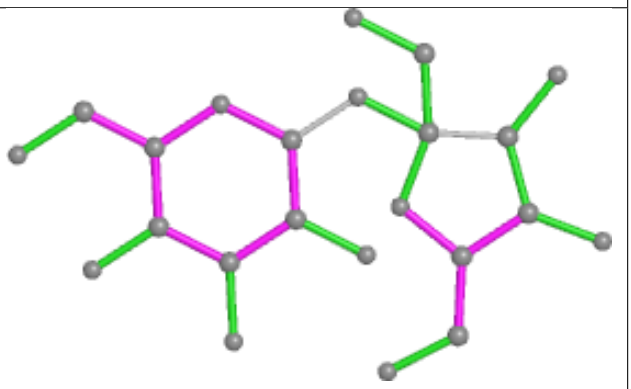


Rings

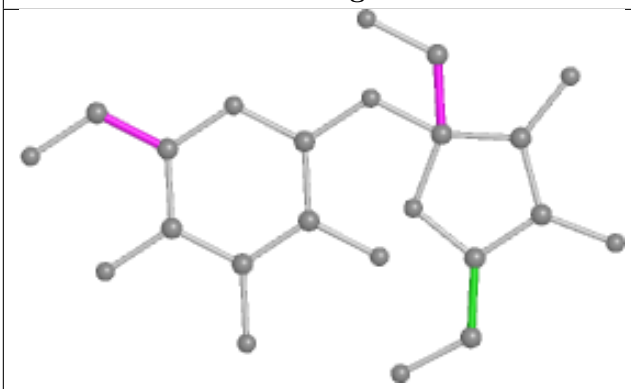
Oligosaccharide Chain C



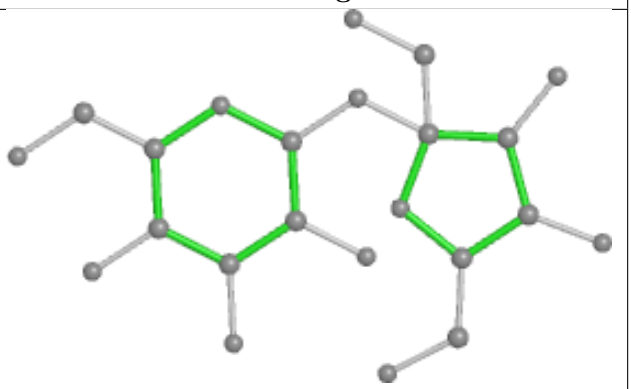
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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	1003/1039 (96%)	0.50	59 (5%)	22	21	35, 56, 84, 110	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1691	SER	5.0
1	A	766	ASN	4.8
1	A	881	THR	4.2
1	A	1636	ASP	4.1
1	A	882	ASP	4.1
1	A	1565	LYS	4.0
1	A	1387	ALA	3.9
1	A	752	THR	3.7
1	A	789	GLY	3.6
1	A	1647	ASN	3.4
1	A	1695	SER	3.2
1	A	1385	ASP	3.1
1	A	1637	ASN	3.1
1	A	1635	GLN	3.0
1	A	788	LYS	3.0
1	A	753	THR	2.9
1	A	1417	THR	2.9
1	A	783	LYS	2.9
1	A	862	LEU	2.9
1	A	1143	ILE	2.8
1	A	1638	GLU	2.8
1	A	785	GLN	2.8
1	A	782	LEU	2.7
1	A	1487	LEU	2.6
1	A	998	LEU	2.6
1	A	880	SER	2.6
1	A	1640	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1738	MET	2.6
1	A	764	ASN	2.6
1	A	754	GLY	2.6
1	A	1490	ALA	2.5
1	A	945	LEU	2.5
1	A	1734	SER	2.5
1	A	1642	PHE	2.5
1	A	1307	TYR	2.5
1	A	1739	THR	2.5
1	A	1655	ASN	2.5
1	A	875	SER	2.4
1	A	1657	GLN	2.4
1	A	1418	THR	2.4
1	A	1645	GLU	2.3
1	A	1737	ALA	2.3
1	A	1390	THR	2.3
1	A	1574	VAL	2.3
1	A	1420	SER	2.3
1	A	1654	GLU	2.3
1	A	1736	GLY	2.3
1	A	798	ARG	2.3
1	A	1247	LYS	2.2
1	A	1563	LEU	2.2
1	A	974	ASN	2.1
1	A	1646	GLY	2.1
1	A	787	ASP	2.1
1	A	1685	SER	2.1
1	A	1672	TYR	2.1
1	A	1701	LEU	2.0
1	A	1370	PRO	2.0
1	A	899	ILE	2.0
1	A	793	ALA	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,

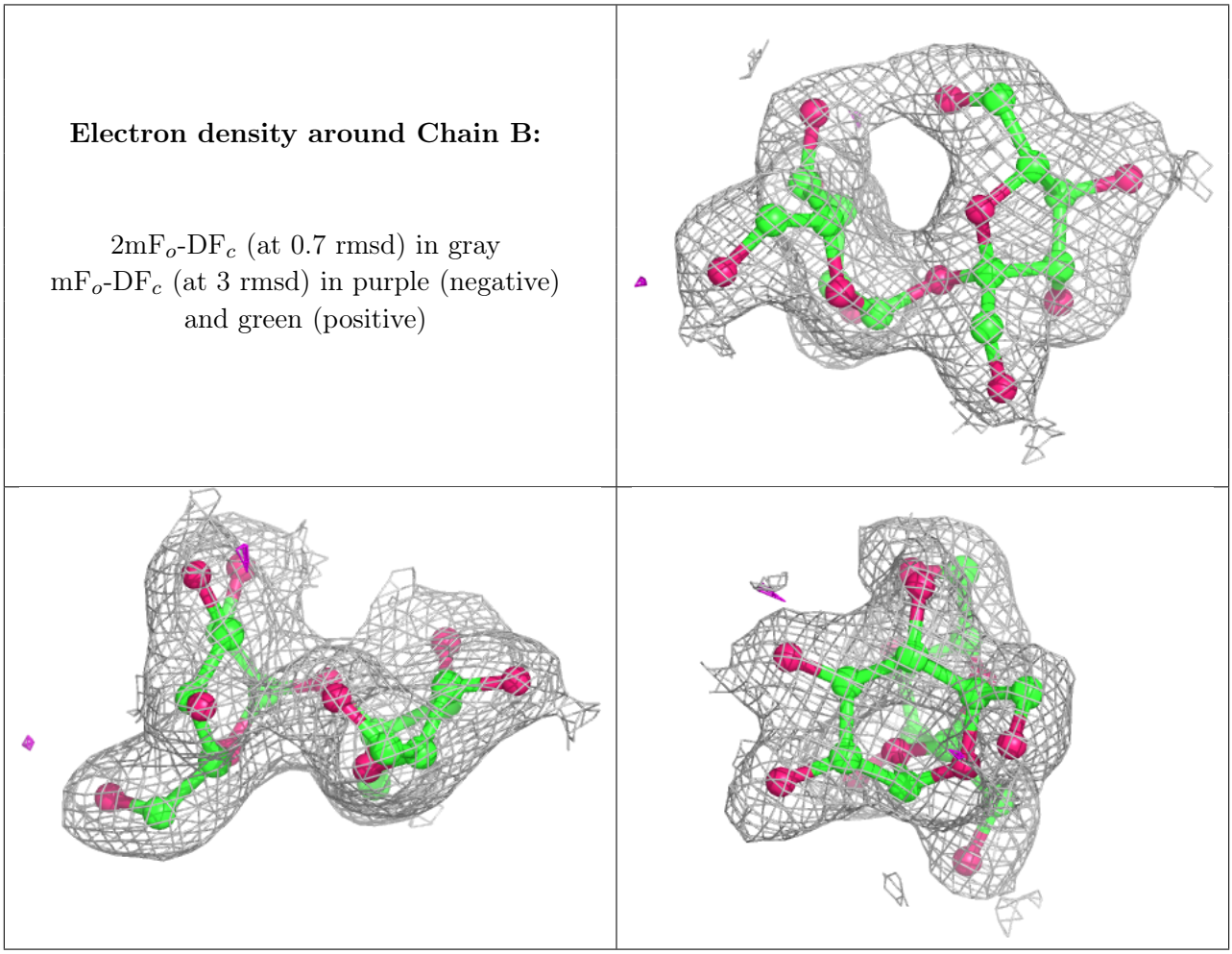
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FRU	C	2	12/12	0.53	0.50	59,67,71,72	0
2	GLC	C	1	11/12	0.74	0.21	49,54,64,67	0
2	GLC	B	1	11/12	0.92	0.12	37,39,43,44	0
2	FRU	B	2	12/12	0.95	0.12	36,40,43,43	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.

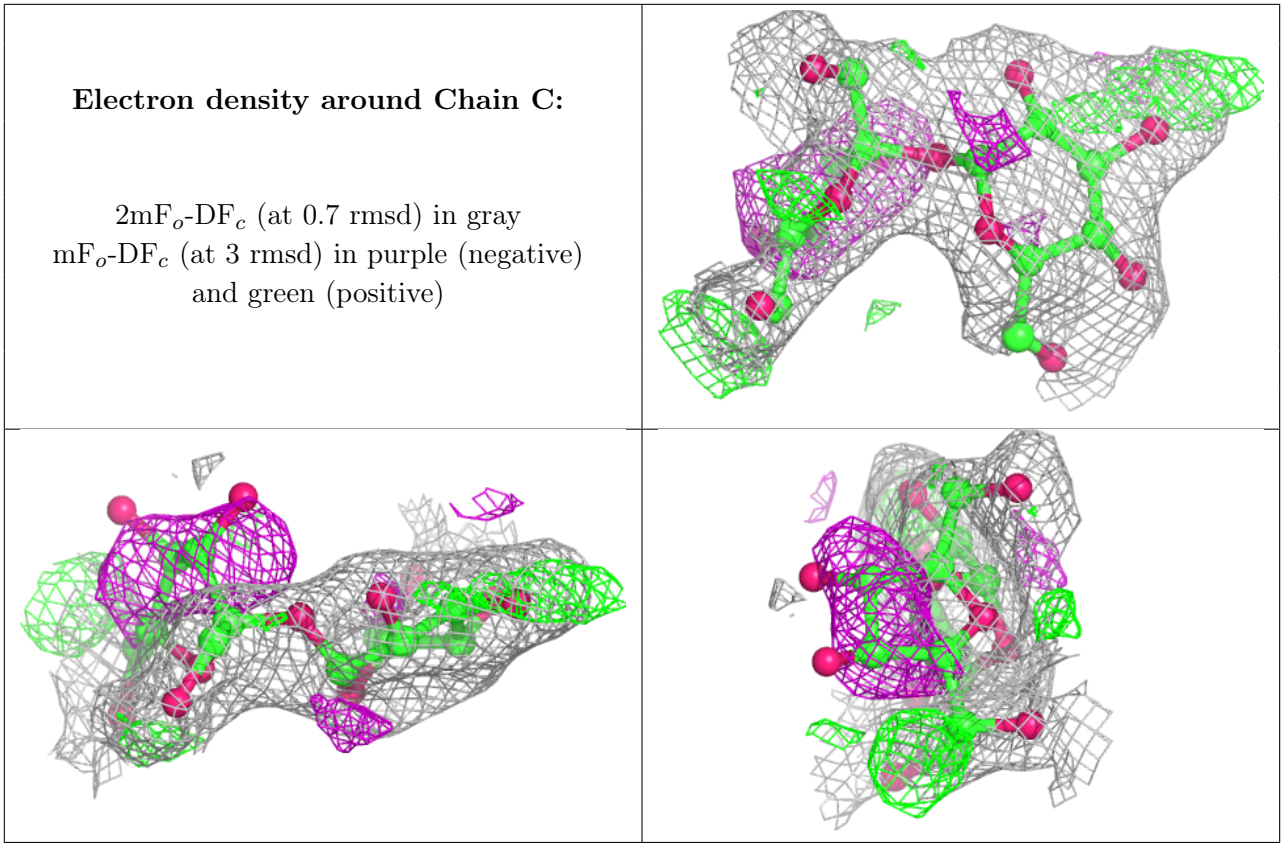
Electron density around Chain B:

$2mF_o$-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 C:

$2mF_o$-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
3	CA	A	1	1/1	0.98	0.10	36,36,36,36	0

6.5 Other polymers

There are no such residues in this entry.