



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:33 PM UTC

PDB ID : 7P39 / pdb_00007p39
Title : 4,6-alpha-glucanotransferase GtfB from *Limosilactobacillus reuteri* NCC 2613
complexed with acarbose
Authors : Pijning, T.; te Poele, E.; Gangoit, J.; Boerner, T.; Dijkhuizen, L.
Deposited on : 2021-07-07
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 ⓘ 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

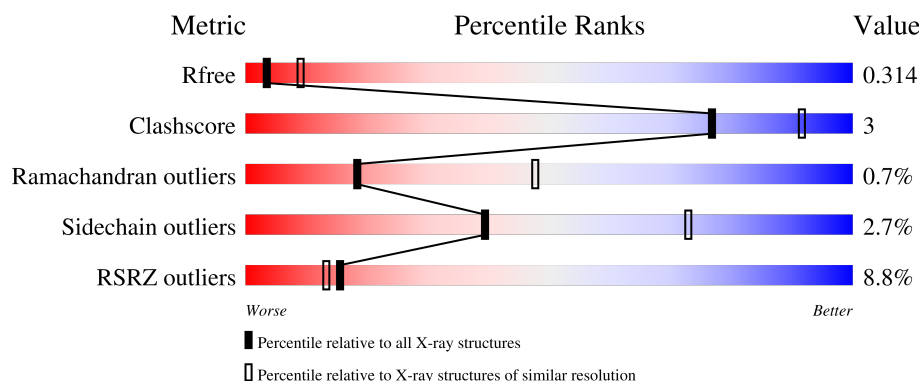
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 $\leq 5\%$. 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	881	 9% 85% 9% • 6%
1	B	881	 7% 86% 7% • 6%
2	D	3	 33% 67%
2	G	3	 33% 67%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13136 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	832	Total	C	N	O	S	0	0	0
			6511	4054	1101	1334	22			
1	B	832	Total	C	N	O	S	0	0	0
			6511	4054	1101	1334	22			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	397	MET	-	initiating methionine	UNP A0A1Z2RUH3
A	398	ALA	-	expression tag	UNP A0A1Z2RUH3
A	399	HIS	-	expression tag	UNP A0A1Z2RUH3
A	400	HIS	-	expression tag	UNP A0A1Z2RUH3
A	401	HIS	-	expression tag	UNP A0A1Z2RUH3
A	402	HIS	-	expression tag	UNP A0A1Z2RUH3
A	403	HIS	-	expression tag	UNP A0A1Z2RUH3
A	404	HIS	-	expression tag	UNP A0A1Z2RUH3
A	405	SER	-	expression tag	UNP A0A1Z2RUH3
A	406	ALA	-	expression tag	UNP A0A1Z2RUH3
A	407	ALA	-	expression tag	UNP A0A1Z2RUH3
A	408	LEU	-	expression tag	UNP A0A1Z2RUH3
A	409	GLU	-	expression tag	UNP A0A1Z2RUH3
A	410	VAL	-	expression tag	UNP A0A1Z2RUH3
A	411	LEU	-	expression tag	UNP A0A1Z2RUH3
A	412	PHE	-	expression tag	UNP A0A1Z2RUH3
A	413	GLN	-	expression tag	UNP A0A1Z2RUH3
A	414	GLY	-	expression tag	UNP A0A1Z2RUH3
A	415	PRO	-	expression tag	UNP A0A1Z2RUH3
A	416	GLY	-	expression tag	UNP A0A1Z2RUH3
B	397	MET	-	initiating methionine	UNP A0A1Z2RUH3
B	398	ALA	-	expression tag	UNP A0A1Z2RUH3
B	399	HIS	-	expression tag	UNP A0A1Z2RUH3
B	400	HIS	-	expression tag	UNP A0A1Z2RUH3
B	401	HIS	-	expression tag	UNP A0A1Z2RUH3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	402	HIS	-	expression tag	UNP A0A1Z2RUH3
B	403	HIS	-	expression tag	UNP A0A1Z2RUH3
B	404	HIS	-	expression tag	UNP A0A1Z2RUH3
B	405	SER	-	expression tag	UNP A0A1Z2RUH3
B	406	ALA	-	expression tag	UNP A0A1Z2RUH3
B	407	ALA	-	expression tag	UNP A0A1Z2RUH3
B	408	LEU	-	expression tag	UNP A0A1Z2RUH3
B	409	GLU	-	expression tag	UNP A0A1Z2RUH3
B	410	VAL	-	expression tag	UNP A0A1Z2RUH3
B	411	LEU	-	expression tag	UNP A0A1Z2RUH3
B	412	PHE	-	expression tag	UNP A0A1Z2RUH3
B	413	GLN	-	expression tag	UNP A0A1Z2RUH3
B	414	GLY	-	expression tag	UNP A0A1Z2RUH3
B	415	PRO	-	expression tag	UNP A0A1Z2RUH3
B	416	GLY	-	expression tag	UNP A0A1Z2RUH3

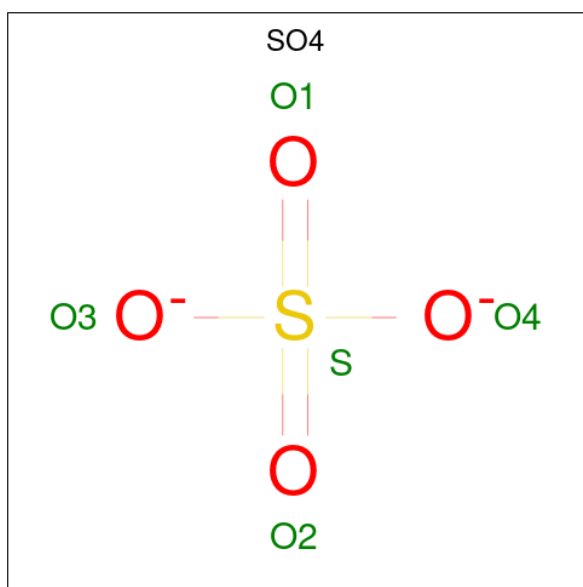
- Molecule 2 is an oligosaccharide called 4,6-dideoxy-4-[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	G	3	Total	C	N	O	0	0	0
			44	25	1	18			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

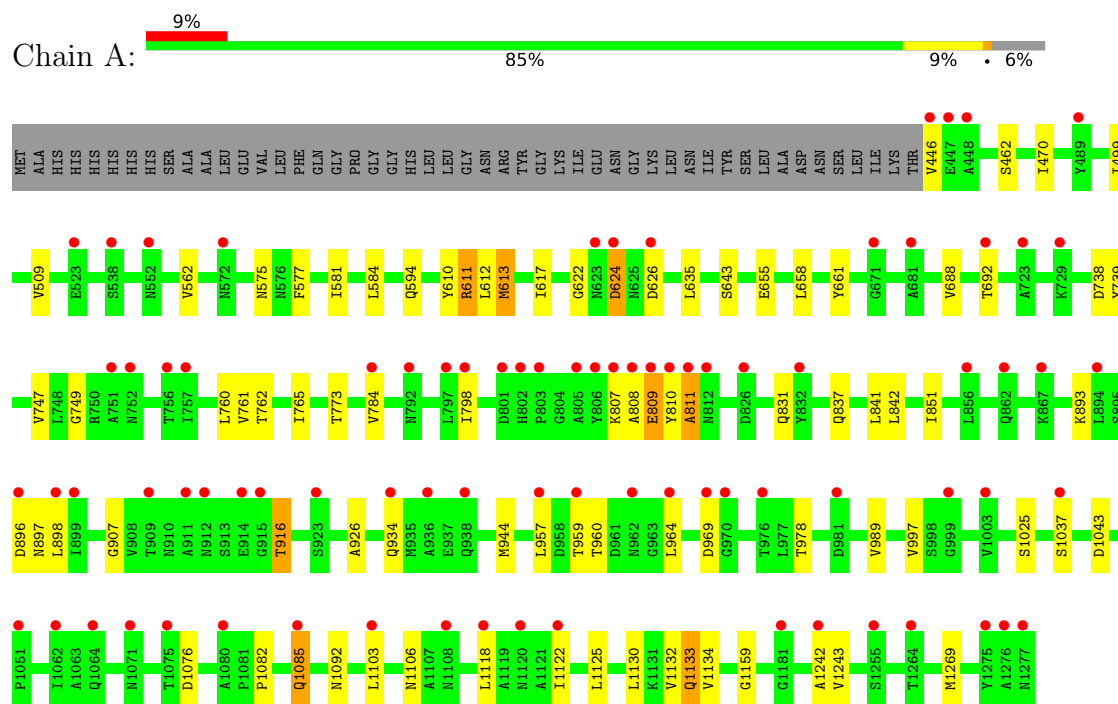
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total	O	0	0
			10	10		
5	B	9	Total	O	0	0
			9	9		

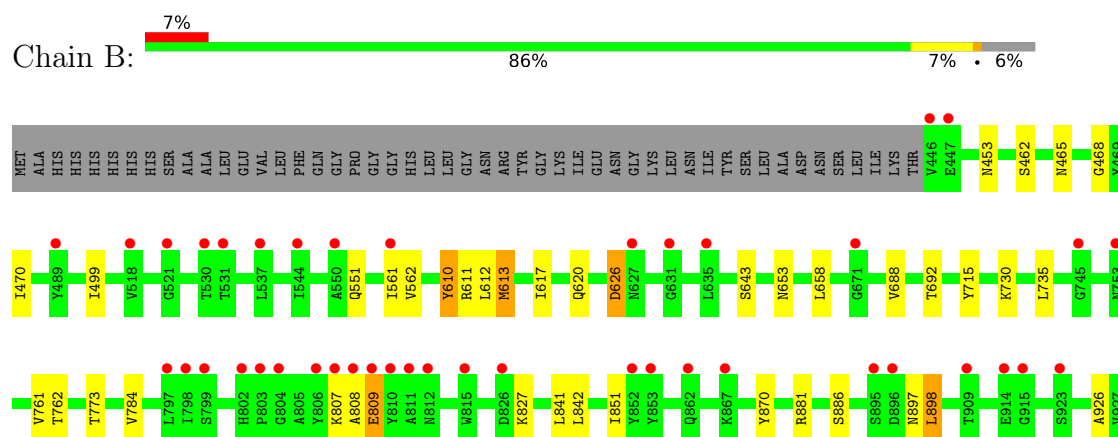
3 Residue-property plots

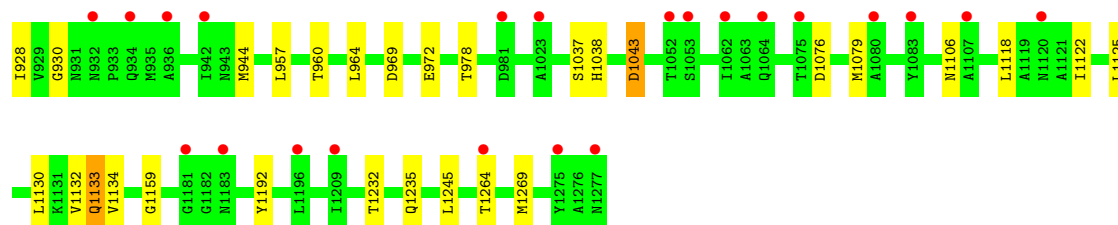
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Dextranucrase



• Molecule 1: Dextranucrase





- 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)-beta-D-glucopyranose

Chain D: 33% 67%



- 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)-beta-D-glucopyranose

Chain G: 33% 67%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.22Å 133.81Å 147.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.29 – 2.90 49.29 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.8 (49.29-2.90) 97.8 (49.29-2.90)	Depositor EDS
R_{merge}	0.43	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.91Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.293 , 0.315 0.295 , 0.314	Depositor DCC
R_{free} test set	2254 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	35.0	Xtrriage
Anisotropy	0.619	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 26.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	13136	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.53 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1296e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, AC1, SO4, CA, BGC

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	0.54	0/6653	0.79	5/9063 (0.1%)
1	B	0.54	0/6653	0.77	2/9063 (0.0%)
All	All	0.54	0/13306	0.78	7/18126 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1242	ALA	N-CA-C	8.58	123.39	113.19
1	A	897	ASN	N-CA-C	-7.42	98.65	110.14
1	B	610	TYR	N-CA-C	6.33	121.79	113.30
1	A	969	ASP	N-CA-C	5.90	117.52	111.14
1	B	626	ASP	N-CA-C	5.53	119.89	113.20
1	A	626	ASP	N-CA-C	-5.45	101.09	109.76
1	A	622	GLY	N-CA-C	-5.02	103.14	112.37

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	6511	0	6129	44	0
1	B	6511	0	6129	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	44	0	30	0	0
2	G	44	0	30	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	0	0
5	A	10	0	0	0	0
5	B	9	0	0	0	0
All	All	13136	0	12318	73	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 (73) 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:1122:ILE:HG23	1:A:1132:VAL:HG11	1.61	0.83
1:B:1122:ILE:HG23	1:B:1132:VAL:HG11	1.61	0.82
1:A:577:PHE:CZ	1:A:581:ILE:HD11	2.15	0.82
1:B:1076:ASP:HB3	1:B:1133:GLN:HE22	1.52	0.74
1:A:1076:ASP:HB3	1:A:1133:GLN:HE22	1.51	0.73
1:A:661:TYR:CE1	1:A:1103:LEU:HD23	2.28	0.69
1:A:581:ILE:HD12	1:A:584:LEU:HD12	1.75	0.67
1:B:1043:ASP:OD2	1:B:1079:MET:HA	1.95	0.67
1:B:1232:THR:HG21	1:B:1235:GLN:HE21	1.61	0.66
1:B:653:ASN:HD21	1:B:1192:TYR:H	1.43	0.65
1:B:784:VAL:HG23	1:B:841:LEU:HD22	1.80	0.63
1:A:898:LEU:HD21	1:A:989:VAL:HG21	1.81	0.62
1:B:1122:ILE:HG23	1:B:1132:VAL:CG1	2.29	0.62
1:A:784:VAL:HG23	1:A:841:LEU:HD22	1.80	0.61
1:A:1122:ILE:HG23	1:A:1132:VAL:CG1	2.29	0.61
1:B:761:VAL:HG23	1:B:762:THR:HG23	1.83	0.61
1:B:827:LYS:NZ	1:B:870:TYR:OH	2.35	0.59
1:A:761:VAL:HG23	1:A:762:THR:HG23	1.83	0.59
1:A:1085:GLN:NE2	1:A:1092:ASN:OD1	2.35	0.59
1:B:453:ASN:HD21	1:B:551:GLN:HE22	1.51	0.58
1:A:957:LEU:HD21	1:A:964:LEU:HD22	1.86	0.57
1:B:620:GLN:HE22	1:B:730:LYS:NZ	2.03	0.57
1:A:747:VAL:HG11	1:A:760:LEU:CD1	2.35	0.56
1:A:747:VAL:HG11	1:A:760:LEU:HD11	1.88	0.56
1:B:620:GLN:HE22	1:B:730:LYS:HZ1	1.52	0.55
1:A:658:LEU:HD13	1:A:1134:VAL:HG11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:TYR:O	1:A:612:LEU:HD12	2.08	0.53
1:B:610:TYR:O	1:B:612:LEU:N	2.42	0.53
1:A:499:ILE:HG23	1:A:1269:MET:HE1	1.92	0.52
1:B:658:LEU:HD13	1:B:1134:VAL:HG11	1.90	0.52
1:B:499:ILE:HG23	1:B:1269:MET:HE1	1.93	0.50
1:A:738:ASP:OD2	1:A:765:ILE:HG22	2.11	0.50
1:A:807:LYS:O	1:A:809:GLU:N	2.44	0.49
1:A:624:ASP:OD1	1:A:624:ASP:N	2.45	0.49
1:A:959:THR:CG2	1:A:997:VAL:HG21	2.43	0.49
1:A:926:ALA:HB2	1:A:944:MET:HE1	1.95	0.49
1:A:907:GLY:O	1:A:916:THR:HG23	2.13	0.48
1:A:831:GLN:HE21	1:A:837:GLN:HE22	1.61	0.48
1:B:926:ALA:HB2	1:B:944:MET:HE1	1.95	0.48
1:B:807:LYS:O	1:B:809:GLU:N	2.46	0.48
1:A:688:VAL:O	1:A:692:THR:HG23	2.14	0.47
1:A:842:LEU:HD21	1:A:851:ILE:HD11	1.97	0.47
1:B:1043:ASP:OD1	1:B:1043:ASP:C	2.57	0.47
1:B:688:VAL:O	1:B:692:THR:HG23	2.14	0.47
1:B:898:LEU:HD11	1:B:928:ILE:HG23	1.95	0.47
1:B:842:LEU:HD21	1:B:851:ILE:HD11	1.97	0.47
1:A:1082:PRO:HG2	1:A:1103:LEU:HD12	1.98	0.46
1:B:715:TYR:HB3	1:B:735:LEU:HB2	1.99	0.45
1:A:798:ILE:HD12	1:A:811:ALA:HB1	1.98	0.45
1:B:465:ASN:HD22	1:B:468:GLY:HA2	1.82	0.45
1:B:957:LEU:HD11	1:B:964:LEU:HB3	1.98	0.45
1:A:893:LYS:HE3	1:A:896:ASP:HA	1.99	0.45
1:A:661:TYR:HE1	1:A:1103:LEU:HD23	1.78	0.44
1:B:613:MET:HG2	1:B:1159:GLY:HA3	1.98	0.44
1:A:577:PHE:CE2	1:A:581:ILE:HD11	2.51	0.44
1:A:509:VAL:HG13	1:A:581:ILE:HD13	2.00	0.44
1:A:446:VAL:O	1:A:446:VAL:HG13	2.19	0.43
1:A:613:MET:HG2	1:A:1159:GLY:HA3	2.01	0.43
1:A:959:THR:HG21	1:A:997:VAL:HG11	2.01	0.42
1:A:959:THR:HG22	1:A:997:VAL:HG21	2.00	0.42
1:A:749:GLY:HA3	1:A:831:GLN:NE2	2.34	0.42
1:B:470:ILE:HD12	1:B:470:ILE:N	2.35	0.42
1:A:1125:LEU:HD12	1:A:1130:LEU:HD22	2.02	0.42
1:A:470:ILE:N	1:A:470:ILE:HD12	2.34	0.41
1:A:749:GLY:HA3	1:A:831:GLN:HE22	1.85	0.41
1:B:897:ASN:O	1:B:930:GLY:HA2	2.20	0.41
1:A:810:TYR:CG	1:A:811:ALA:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1125:LEU:HD12	1:B:1130:LEU:HD22	2.03	0.41
1:A:738:ASP:OD1	1:A:739:TYR:N	2.54	0.41
1:A:655:GLU:CD	1:A:692:THR:HG22	2.46	0.40
1:A:810:TYR:O	1:A:811:ALA:CB	2.68	0.40
1:B:881:ARG:NH2	1:B:1038:HIS:O	2.53	0.40
1:A:611:ARG:O	1:A:613:MET:HE3	2.22	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	830/881 (94%)	793 (96%)	30 (4%)	7 (1%)	16	44
1	B	830/881 (94%)	791 (95%)	34 (4%)	5 (1%)	21	51
All	All	1660/1762 (94%)	1584 (95%)	64 (4%)	12 (1%)	18	48

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	808	ALA
1	A	809	GLU
1	A	811	ALA
1	A	1243	VAL
1	B	808	ALA
1	A	611	ARG
1	B	809	GLU
1	A	617	ILE
1	B	617	ILE
1	A	1025	SER
1	B	611	ARG
1	B	886	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	702/741 (95%)	683 (97%)	19 (3%)	39	73
1	B	702/741 (95%)	683 (97%)	19 (3%)	39	73
All	All	1404/1482 (95%)	1366 (97%)	38 (3%)	39	73

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	462	SER
1	A	562	VAL
1	A	575	ASN
1	A	594	GLN
1	A	613	MET
1	A	624	ASP
1	A	635	LEU
1	A	643	SER
1	A	773	THR
1	A	916	THR
1	A	934	GLN
1	A	960	THR
1	A	978	THR
1	A	1037	SER
1	A	1043	ASP
1	A	1085	GLN
1	A	1106	ASN
1	A	1118	LEU
1	A	1133	GLN
1	B	462	SER
1	B	561	ILE
1	B	562	VAL
1	B	613	MET
1	B	626	ASP
1	B	643	SER
1	B	773	THR
1	B	898	LEU

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Mol	Chain	Res	Type
1	B	960	THR
1	B	969	ASP
1	B	972	GLU
1	B	978	THR
1	B	1037	SER
1	B	1043	ASP
1	B	1106	ASN
1	B	1118	LEU
1	B	1133	GLN
1	B	1245	LEU
1	B	1264	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	465	ASN
1	A	524	ASN
1	A	575	ASN
1	A	594	GLN
1	A	599	ASN
1	A	602	ASN
1	A	623	ASN
1	A	642	ASN
1	A	691	GLN
1	A	705	ASN
1	A	710	ASN
1	A	711	ASN
1	A	753	ASN
1	A	767	ASN
1	A	770	ASN
1	A	831	GLN
1	A	865	GLN
1	A	897	ASN
1	A	912	ASN
1	A	934	GLN
1	A	950	ASN
1	A	967	ASN
1	A	982	ASN
1	A	1056	ASN
1	A	1065	ASN
1	A	1108	ASN
1	A	1133	GLN

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Mol	Chain	Res	Type
1	A	1172	GLN
1	B	453	ASN
1	B	620	GLN
1	B	642	ASN
1	B	653	ASN
1	B	691	GLN
1	B	705	ASN
1	B	710	ASN
1	B	752	ASN
1	B	759	ASN
1	B	770	ASN
1	B	792	ASN
1	B	813	GLN
1	B	862	GLN
1	B	897	ASN
1	B	912	ASN
1	B	948	HIS
1	B	973	ASN
1	B	982	ASN
1	B	1012	GLN
1	B	1056	ASN
1	B	1065	ASN
1	B	1071	ASN
1	B	1085	GLN
1	B	1133	GLN
1	B	1258	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 ⓘ

6 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	BGC	D	1	2	12,12,12	0.52	0	17,17,17	0.73	0
2	GLC	D	2	2	11,11,12	0.31	0	15,15,17	0.96	1 (6%)
2	AC1	D	3	2	21,22,23	0.63	0	22,32,34	1.07	2 (9%)
2	BGC	G	1	2	12,12,12	0.49	0	17,17,17	0.64	0
2	GLC	G	2	2	11,11,12	0.30	0	15,15,17	0.96	1 (6%)
2	AC1	G	3	2	21,22,23	0.56	0	22,32,34	1.23	2 (9%)

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	BGC	D	1	2	-	0/2/22/22	0/1/1/1
2	GLC	D	2	2	-	2/2/19/22	0/1/1/1
2	AC1	D	3	2	-	2/6/43/46	0/2/2/2
2	BGC	G	1	2	-	0/2/22/22	0/1/1/1
2	GLC	G	2	2	-	2/2/19/22	0/1/1/1
2	AC1	G	3	2	-	3/6/43/46	0/2/2/2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	AC1	C7B-C1B-N4A	3.63	116.02	110.68
2	G	3	AC1	C1-C2-C3	3.57	114.85	109.64
2	G	3	AC1	C7B-C1B-N4A	3.03	115.14	110.68
2	D	2	GLC	C1-O5-C5	3.03	116.24	112.19
2	G	2	GLC	C1-O5-C5	2.94	116.12	112.19
2	D	3	AC1	C1-C2-C3	2.39	113.12	109.64

There are no chirality outliers.

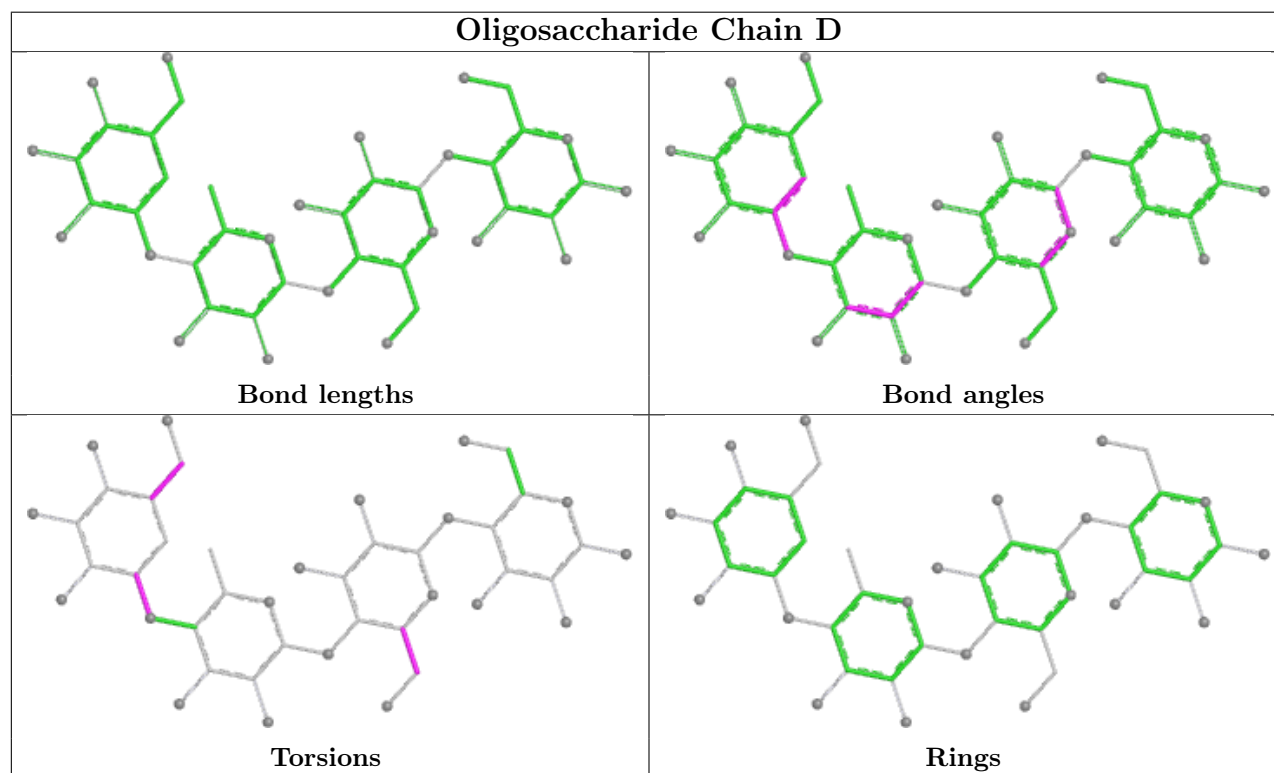
All (9) torsion outliers are listed below:

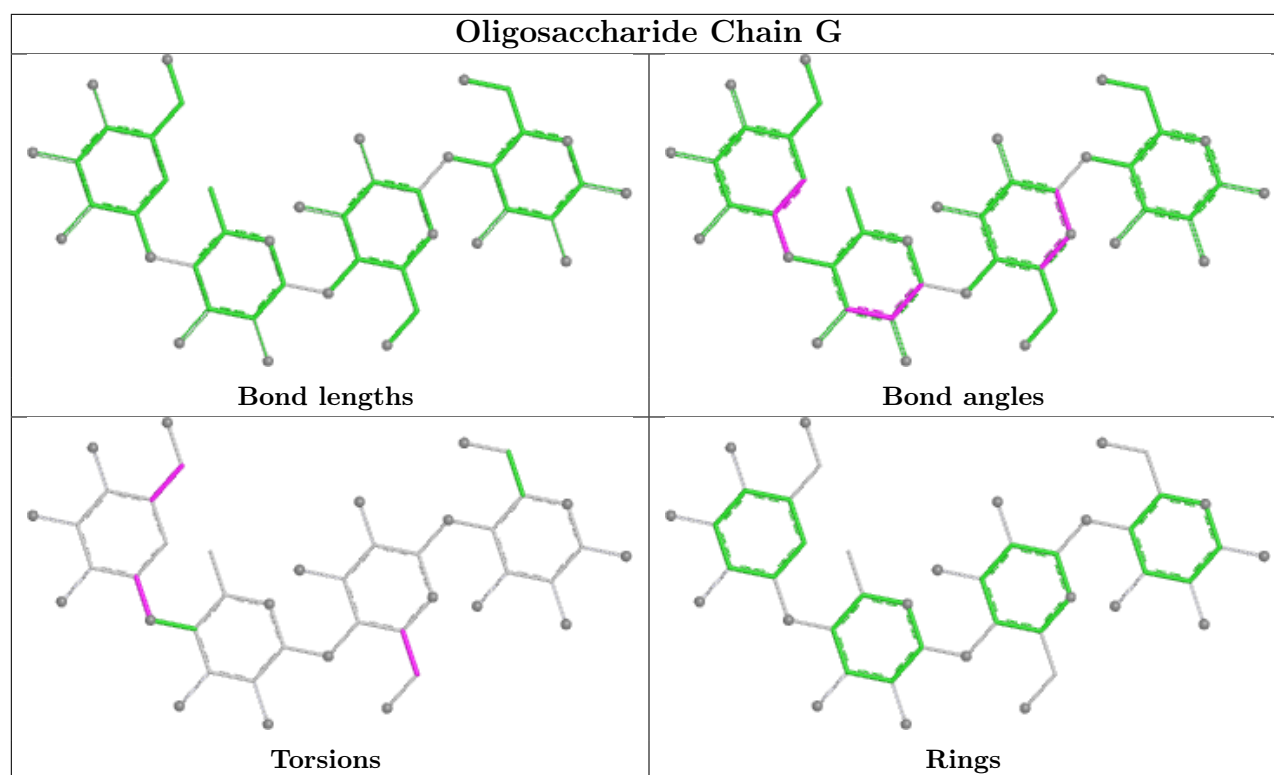
Mol	Chain	Res	Type	Atoms
2	D	3	AC1	C7B-C1B-N4A-C4
2	D	3	AC1	C7B-C5B-C6B-O6B
2	G	3	AC1	C7B-C1B-N4A-C4
2	G	3	AC1	C7B-C5B-C6B-O6B
2	D	2	GLC	O5-C5-C6-O6
2	G	2	GLC	O5-C5-C6-O6
2	D	2	GLC	C4-C5-C6-O6
2	G	2	GLC	C4-C5-C6-O6
2	G	3	AC1	C4A-C5B-C6B-O6B

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.





5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	SO4	A	1302	-	4,4,4	0.43	0	6,6,6	0.07	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	832/881 (94%)	1.04	83 (9%) 12 10	30, 41, 66, 102	0
1	B	832/881 (94%)	0.97	64 (7%) 19 16	29, 41, 56, 96	0
All	All	1664/1762 (94%)	1.01	147 (8%) 15 13	29, 41, 62, 102	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	808	ALA	6.2
1	B	808	ALA	5.7
1	B	811	ALA	4.9
1	A	1275	TYR	4.8
1	A	811	ALA	4.8
1	A	806	TYR	4.4
1	A	624	ASP	4.3
1	A	1075	THR	4.3
1	B	810	TYR	4.2
1	A	810	TYR	4.1
1	A	1085	GLN	4.0
1	B	803	PRO	3.9
1	A	626	ASP	3.9
1	B	896	ASP	3.7
1	A	489	TYR	3.7
1	B	671	GLY	3.7
1	A	803	PRO	3.6
1	B	807	LYS	3.6
1	B	1120	ASN	3.6
1	B	550	ALA	3.4
1	B	981	ASP	3.4
1	B	806	TYR	3.3
1	A	538	SER	3.3
1	A	915	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	826	ASP	3.2
1	B	895	SER	3.2
1	A	981	ASP	3.2
1	A	623	ASN	3.2
1	B	531	THR	3.2
1	B	1075	THR	3.1
1	A	807	LYS	3.1
1	B	802	HIS	3.1
1	B	753	ASN	3.1
1	B	489	TYR	3.0
1	B	1275	TYR	3.0
1	A	752	ASN	3.0
1	A	1120	ASN	3.0
1	A	970	GLY	3.0
1	A	681	ALA	3.0
1	A	1080	ALA	3.0
1	A	446	VAL	3.0
1	B	1023	ALA	2.9
1	B	631	GLY	2.9
1	A	969	ASP	2.9
1	B	934	GLN	2.9
1	A	923	SER	2.9
1	B	561	ILE	2.9
1	B	1062	ILE	2.9
1	A	797	LEU	2.9
1	A	914	GLU	2.8
1	A	1062	ILE	2.8
1	B	1052	THR	2.8
1	B	447	GLU	2.7
1	A	911	ALA	2.7
1	A	938	GLN	2.7
1	A	1108	ASN	2.7
1	B	812	ASN	2.7
1	B	932	ASN	2.7
1	A	1122	ILE	2.7
1	A	802	HIS	2.7
1	A	909	THR	2.6
1	B	936	ALA	2.6
1	B	797	LEU	2.6
1	B	530	THR	2.6
1	A	448	ALA	2.6
1	A	896	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1255	SER	2.6
1	A	805	ALA	2.6
1	A	1037	SER	2.5
1	B	815	TRP	2.5
1	B	1277	ASN	2.5
1	A	671	GLY	2.5
1	B	914	GLU	2.5
1	A	936	ALA	2.5
1	B	1053	SER	2.5
1	B	809	GLU	2.5
1	A	801	ASP	2.4
1	B	798	ILE	2.4
1	B	1264	THR	2.4
1	A	962	ASN	2.4
1	A	1277	ASN	2.4
1	B	627	ASN	2.4
1	A	809	GLU	2.4
1	A	751	ALA	2.4
1	A	957	LEU	2.4
1	A	572	ASN	2.4
1	B	1181	GLY	2.4
1	B	1080	ALA	2.4
1	A	756	THR	2.4
1	B	745	GLY	2.3
1	A	1242	ALA	2.3
1	A	934	GLN	2.3
1	B	862	GLN	2.3
1	B	909	THR	2.3
1	A	867	LYS	2.3
1	B	853	TYR	2.3
1	A	784	VAL	2.3
1	A	1051	PRO	2.3
1	A	798	ILE	2.2
1	B	942	ILE	2.2
1	A	959	THR	2.2
1	B	799	SER	2.2
1	A	757	ILE	2.2
1	B	446	VAL	2.2
1	A	552	ASN	2.2
1	A	1264	THR	2.2
1	B	1083	TYR	2.2
1	A	894	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	447	GLU	2.2
1	A	523	GLU	2.2
1	A	1064	GLN	2.2
1	A	999	GLY	2.2
1	B	804	GLY	2.2
1	B	923	SER	2.2
1	A	1118	LEU	2.1
1	A	899	ILE	2.1
1	A	862	GLN	2.1
1	A	912	ASN	2.1
1	A	1071	ASN	2.1
1	B	518	VAL	2.1
1	A	856	LEU	2.1
1	B	1107	ALA	2.1
1	B	1209	ILE	2.1
1	A	792	ASN	2.1
1	A	812	ASN	2.1
1	A	898	LEU	2.1
1	B	915	GLY	2.1
1	B	544	ILE	2.1
1	B	867	LYS	2.1
1	A	1103	LEU	2.1
1	A	1181	GLY	2.1
1	A	1276	ALA	2.1
1	B	852	TYR	2.1
1	B	635	LEU	2.0
1	B	1196	LEU	2.0
1	A	692	THR	2.0
1	A	976	THR	2.0
1	B	1064	GLN	2.0
1	A	964	LEU	2.0
1	B	537	LEU	2.0
1	B	1183	ASN	2.0
1	B	521	GLY	2.0
1	A	723	ALA	2.0
1	A	826	ASP	2.0
1	A	729	LYS	2.0
1	A	832	TYR	2.0
1	A	1003	VAL	2.0

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

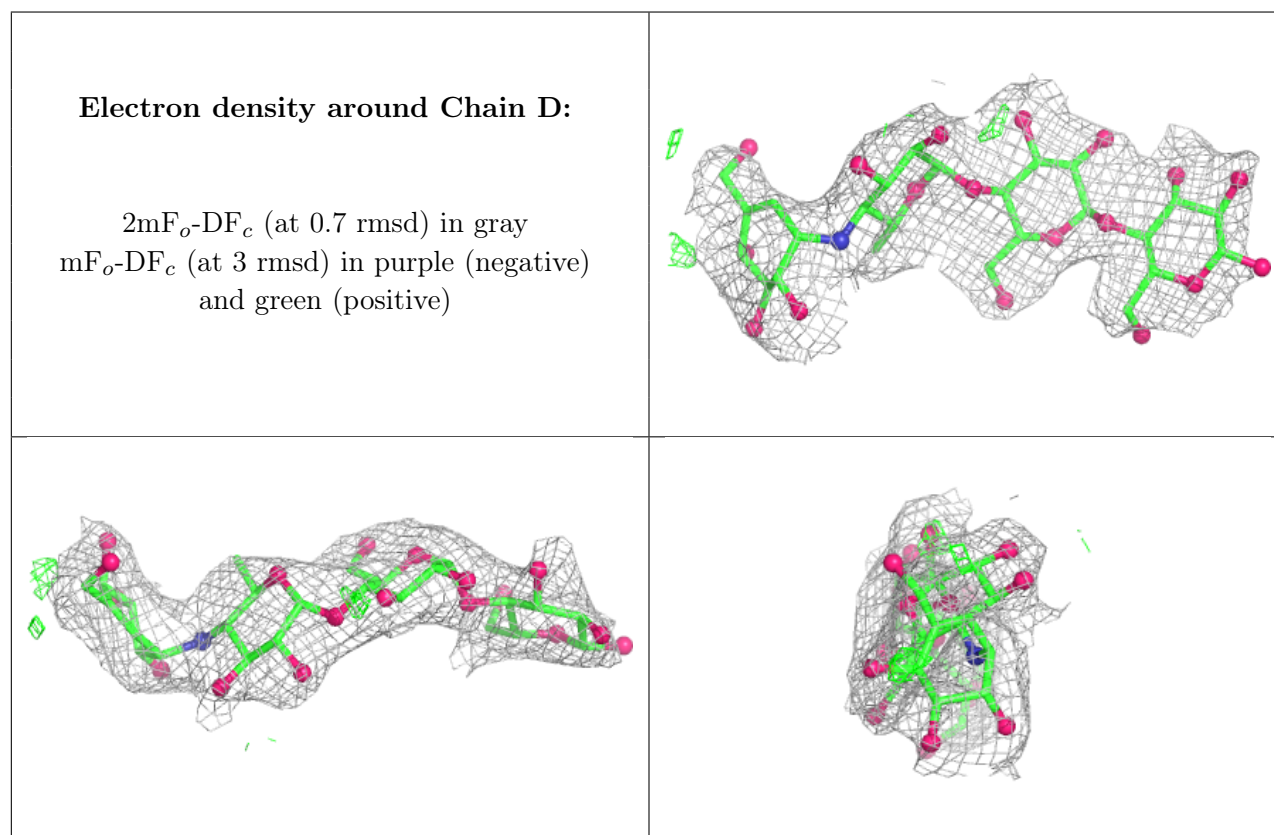
There are no non-standard protein/DNA/RNA residues in this entry.

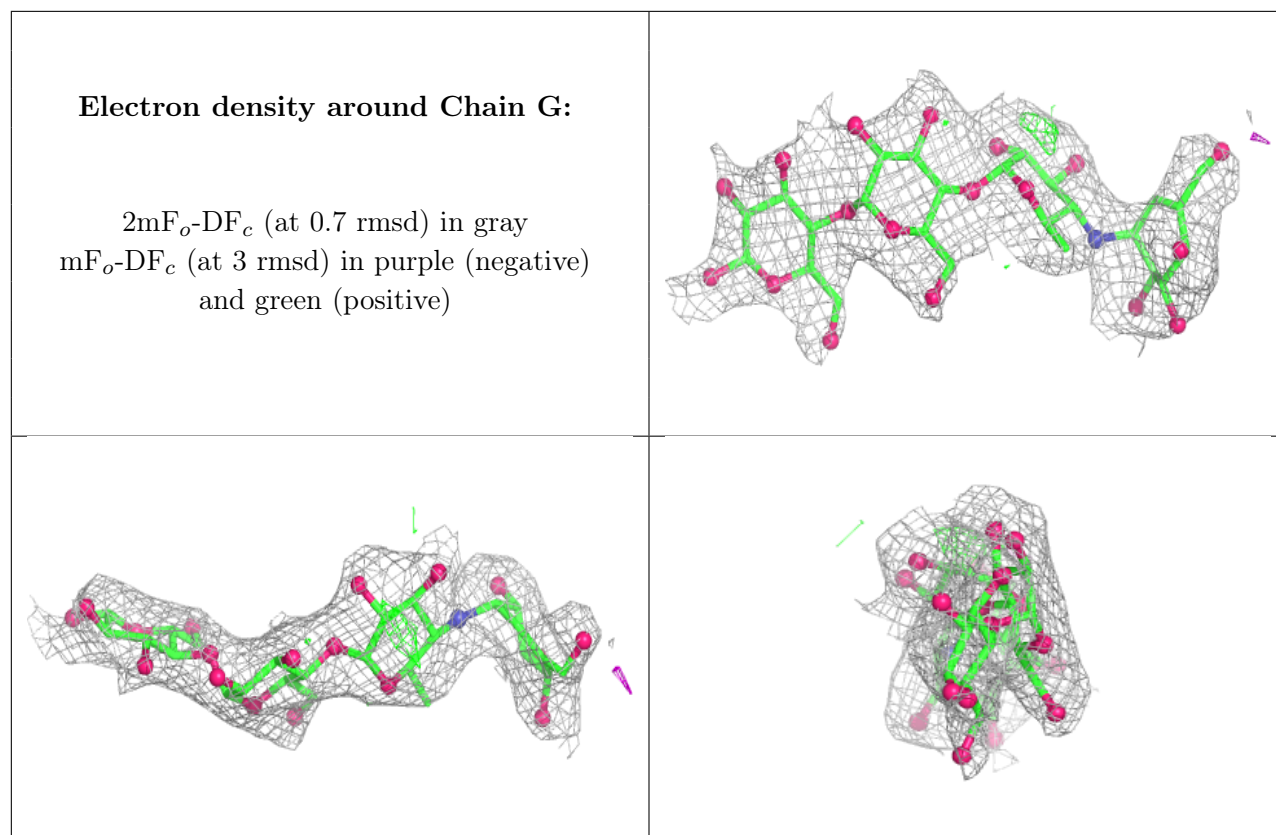
6.3 Carbohydrates [i](#)

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, 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
2	AC1	D	3	21/22	0.83	0.15	45,46,47,47	0
2	GLC	D	2	11/12	0.84	0.12	47,49,49,49	0
2	BGC	D	1	12/12	0.85	0.13	51,53,53,54	0
2	BGC	G	1	12/12	-	-	46,47,47,47	0
2	GLC	G	2	11/12	-	-	43,45,45,45	0
2	AC1	G	3	21/22	-	-	45,45,46,46	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.





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	SO4	A	1302	5/5	0.72	0.17	72,73,73,73	0
3	CA	A	1301	1/1	0.90	0.06	29,29,29,29	0
3	CA	B	1301	1/1	0.91	0.07	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.