



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 06:11 AM BST

PDB ID : 4ZO9
Title : Crystal Structure of mutant (D270A) beta-glucosidase from *Listeria innocua* in complex with laminaribiose
Authors : Nakajima, M.; Yoshida, R.; Miyanaga, A.; Abe, K.; Takahashi, Y.; Sugimoto, N.; Toyozumi, H.; Nakai, H.; Kitaoka, M.; Taguchi, H.
Deposited on : 2015-05-06
Resolution : 1.99 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 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 : 2.13.1
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) : 2.13.1

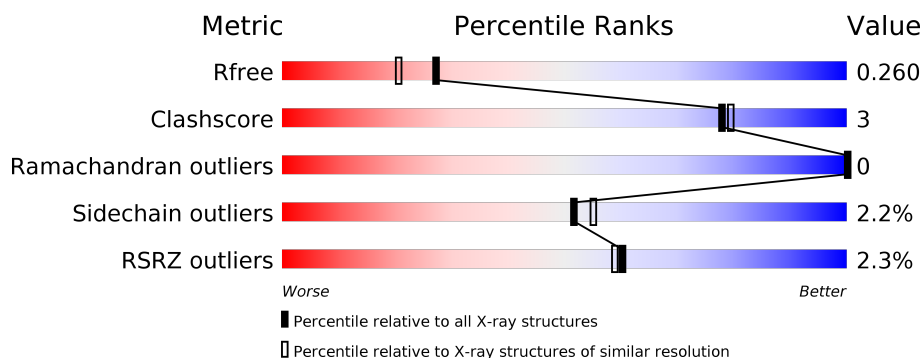
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on 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	731	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>7%</div> </div> <div>•</div> </div>
1	B	731	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>8%</div> </div> <div>••</div> </div>
2	C	2	<div> <div>100%</div> </div>
2	D	2	<div> <div>100%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11867 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 Lin1840 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	724	Total	C	N	O	S	0	3	0
			5612	3553	930	1103	26			
1	B	724	Total	C	N	O	S	0	1	0
			5597	3543	928	1101	25			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLU	LYS	engineered mutation	UNP Q92AS9
A	270	ALA	ASP	engineered mutation	UNP Q92AS9
A	724	LEU	-	expression tag	UNP Q92AS9
A	725	GLU	-	expression tag	UNP Q92AS9
A	726	HIS	-	expression tag	UNP Q92AS9
A	727	HIS	-	expression tag	UNP Q92AS9
A	728	HIS	-	expression tag	UNP Q92AS9
A	729	HIS	-	expression tag	UNP Q92AS9
A	730	HIS	-	expression tag	UNP Q92AS9
A	731	HIS	-	expression tag	UNP Q92AS9
B	2	GLU	LYS	engineered mutation	UNP Q92AS9
B	270	ALA	ASP	engineered mutation	UNP Q92AS9
B	724	LEU	-	expression tag	UNP Q92AS9
B	725	GLU	-	expression tag	UNP Q92AS9
B	726	HIS	-	expression tag	UNP Q92AS9
B	727	HIS	-	expression tag	UNP Q92AS9
B	728	HIS	-	expression tag	UNP Q92AS9
B	729	HIS	-	expression tag	UNP Q92AS9
B	730	HIS	-	expression tag	UNP Q92AS9
B	731	HIS	-	expression tag	UNP Q92AS9

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-3)-alpha-D-glucopyranose.

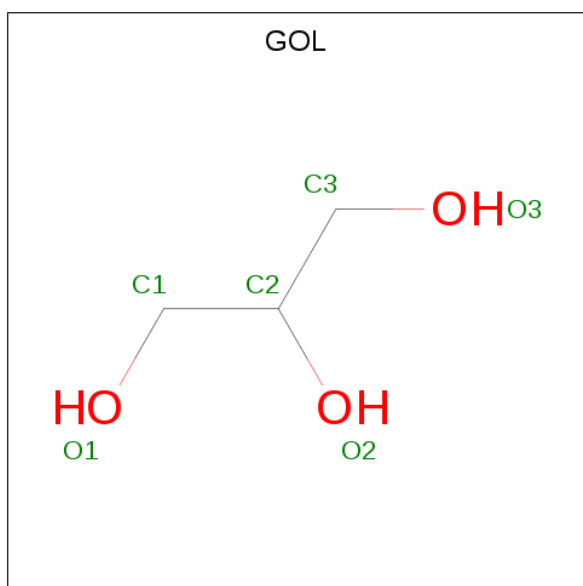


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	2	0
			23	12	11			
2	D	2	Total	C	O	0	2	0
			23	12	11			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			12	6	6		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is beta-D-glucopyranose (three-letter code: BGC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	1
			12	6	6		
5	A	1	Total	C	O	0	1
			11	6	5		
5	B	1	Total	C	O	0	1
			12	6	6		
5	B	1	Total	C	O	0	1
			11	6	5		

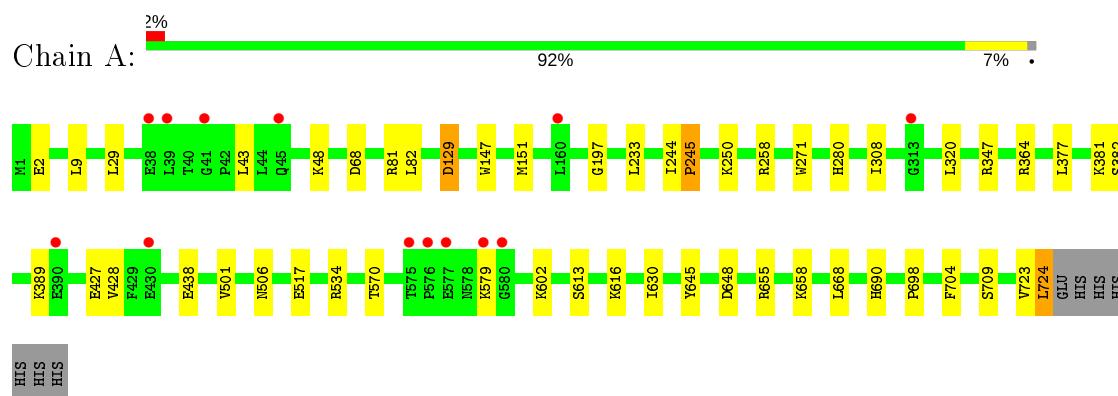
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	297	Total	O	0	0
			297	297		
6	B	249	Total	O	0	0
			249	249		

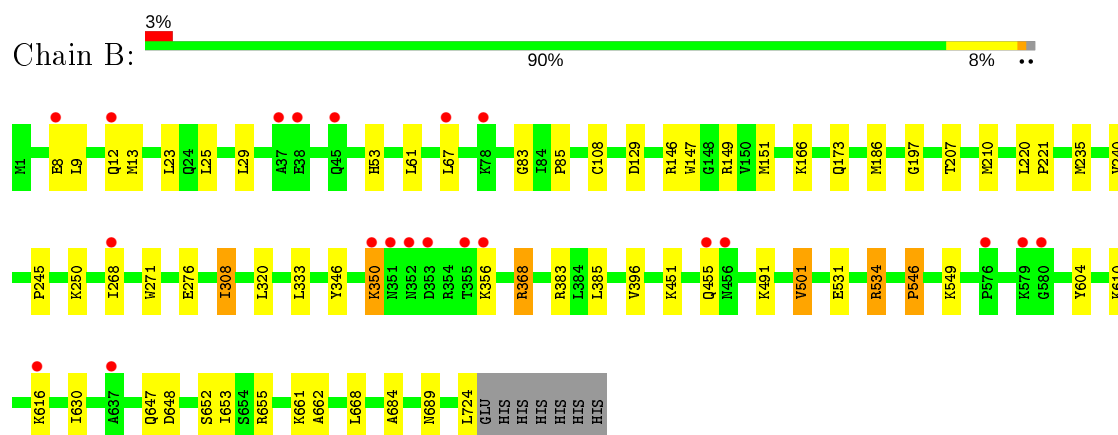
3 Residue-property plots [i](#)

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.

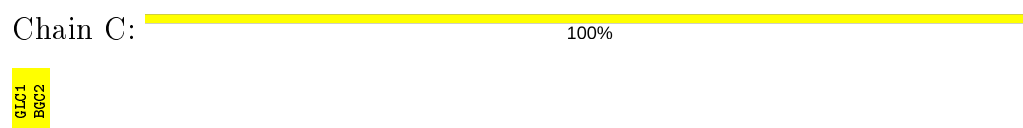
- Molecule 1: Lin1840 protein



- Molecule 1: Lin1840 protein



- Molecule 2: beta-D-glucopyranose-(1-3)-alpha-D-glucopyranose



- Molecule 2: beta-D-glucopyranose-(1-3)-alpha-D-glucopyranose



GLC1
BGC2

4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	89.49 Å 94.76 Å 215.23 Å 90.00° 96.32° 90.00°	Depositor
Resolution (Å)	36.91 – 1.99 36.92 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.6 (36.91-1.99) 99.6 (36.92-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 1.98 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.189 , 0.257 0.197 , 0.260	Depositor DCC
R_{free} test set	6130 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	15.0	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11867	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, GOL, MG, 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	0.85	0/5717	0.90	7/7747 (0.1%)
1	B	0.81	1/5702 (0.0%)	0.88	7/7727 (0.1%)
All	All	0.83	1/11419 (0.0%)	0.89	14/15474 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	276	GLU	CD-OE2	-6.22	1.18	1.25

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	655	ARG	NE-CZ-NH2	8.31	124.46	120.30
1	A	655	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	68	ASP	CB-CG-OD1	6.52	124.17	118.30
1	B	368	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	A	648	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	B	149	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	B	368	ARG	NE-CZ-NH1	-6.10	117.25	120.30
1	B	146	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	B	501	VAL	CB-CA-C	-5.62	100.72	111.40
1	A	129	ASP	CB-CG-OD1	5.48	123.23	118.30
1	B	534	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	A	501	VAL	CB-CA-C	-5.13	101.66	111.40
1	A	347	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	364	ARG	NE-CZ-NH2	-5.01	117.80	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	5612	0	5571	33	0
1	B	5597	0	5555	36	0
2	C	23	0	12	0	0
2	D	23	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	12	0	16	1	0
4	B	6	0	8	0	0
5	A	23	0	12	0	0
5	B	23	0	12	0	0
6	A	297	0	0	7	0
6	B	249	0	0	6	0
All	All	11867	0	11198	65	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 (65) 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:356:LYS:HG2	6:B:901:HOH:O	1.81	0.80
1:A:723:VAL:HG12	1:A:724:LEU:HD13	1.76	0.66
1:A:81:ARG:CZ	1:A:82:LEU:HD21	2.26	0.65
1:A:517:GLU:OE1	6:A:901:HOH:O	2.15	0.63
1:A:244:ILE:CD1	1:B:652:SER:O	2.49	0.60
1:A:244:ILE:HD11	1:B:652:SER:O	2.02	0.58
4:A:802[B]:GOL:H11	1:B:207:THR:HG21	1.86	0.58
1:A:690:HIS:HB2	6:B:1034:HOH:O	2.04	0.57
1:A:29:LEU:HD21	1:A:43:LEU:HD23	1.87	0.56
1:B:9:LEU:O	1:B:13:MET:HG3	2.06	0.56
1:A:271:TRP:CD1	1:A:271:TRP:C	2.80	0.55
1:A:250:LYS:HG2	6:A:944:HOH:O	2.05	0.55
1:A:244:ILE:HD11	1:B:653:ILE:HD13	1.90	0.54
1:B:53:HIS:CD2	1:B:308:ILE:HD12	2.43	0.53
1:B:724:LEU:N	1:B:724:LEU:HD12	2.24	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:ILE:HG23	1:A:668:LEU:HD11	1.91	0.51
1:A:658:LYS:HE2	1:A:709:SER:O	2.10	0.51
1:B:61:LEU:HD21	1:B:271:TRP:CZ3	2.46	0.51
1:B:630:ILE:HG23	1:B:668:LEU:HD11	1.93	0.50
1:B:385:LEU:HD21	1:B:501:VAL:HG21	1.93	0.50
1:A:2:GLU:OE1	1:A:2:GLU:HA	2.11	0.50
1:B:250:LYS:HG2	6:B:1084:HOH:O	2.12	0.50
1:A:381:LYS:O	1:A:382:SER:CB	2.58	0.49
1:A:81:ARG:NH2	1:A:82:LEU:HD21	2.28	0.49
1:B:25:LEU:HB3	1:B:29:LEU:HD12	1.95	0.49
1:A:381:LYS:O	1:A:382:SER:HB2	2.14	0.48
1:B:23:LEU:HD22	1:B:308:ILE:HG13	1.95	0.48
1:B:53:HIS:CD2	1:B:308:ILE:CD1	2.98	0.47
1:B:271:TRP:C	1:B:271:TRP:CD1	2.88	0.47
1:A:147:TRP:CZ3	1:A:197:GLY:HA2	2.51	0.46
1:A:258:ARG:HD3	6:A:1058:HOH:O	2.16	0.46
1:A:698:PRO:HD2	6:A:1187:HOH:O	2.14	0.46
1:A:506:ASN:OD1	1:A:506:ASN:N	2.49	0.46
1:A:81:ARG:CZ	1:A:82:LEU:CD2	2.93	0.45
1:A:724:LEU:HA	1:A:724:LEU:HD12	1.84	0.44
1:A:723:VAL:O	1:A:724:LEU:HB2	2.18	0.44
1:A:534:ARG:HG2	6:A:1094:HOH:O	2.18	0.44
1:A:389:LYS:CE	1:A:428:VAL:O	2.66	0.43
1:B:220:LEU:N	1:B:221:PRO:CD	2.81	0.43
1:B:240:VAL:HA	1:B:245:PRO:HA	2.01	0.43
1:B:235:MET:HA	1:B:268:ILE:O	2.19	0.43
1:B:546:PRO:HD2	1:B:604:TYR:CE2	2.53	0.43
1:B:662:ALA:HB2	6:B:1022:HOH:O	2.18	0.42
1:B:368:ARG:NH1	1:B:534:ARG:HD3	2.35	0.42
1:A:389:LYS:HE3	1:A:428:VAL:O	2.19	0.42
1:A:427:GLU:OE2	6:A:902:HOH:O	2.21	0.42
1:B:8:GLU:O	1:B:12:GLN:HG3	2.19	0.42
1:B:346:TYR:CD2	1:B:350:LYS:HG2	2.55	0.42
1:B:724:LEU:N	1:B:724:LEU:CD1	2.83	0.42
1:A:377:LEU:HD23	1:A:602:LYS:HB2	2.02	0.42
1:A:645:TYR:HB2	1:A:704:PHE:HB2	2.02	0.41
1:B:689:ASN:HB2	6:B:1055:HOH:O	2.19	0.41
1:A:245:PRO:HG3	1:A:280:HIS:CG	2.55	0.41
1:A:250:LYS:HG3	6:A:1163:HOH:O	2.19	0.41
1:A:233:LEU:HD12	1:A:233:LEU:N	2.36	0.41
1:A:244:ILE:CD1	1:B:653:ILE:HD13	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:531:GLU:OE1	1:B:534:ARG:HD2	2.21	0.41
1:B:147:TRP:CZ3	1:B:197:GLY:HA2	2.56	0.41
1:B:647:GLN:HG2	1:B:648:ASP:N	2.36	0.41
1:B:108:CYS:HA	1:B:549:LYS:O	2.21	0.41
1:B:83:GLY:O	1:B:85:PRO:HD3	2.21	0.41
1:B:451:LYS:HE3	1:B:455:GLN:NE2	2.35	0.40
1:B:173:GLN:HG2	1:B:186:MET:O	2.21	0.40
1:B:661:LYS:HE3	1:B:684:ALA:O	2.22	0.40
1:B:166:LYS:HD3	6:B:1052:HOH:O	2.20	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	725/731 (99%)	708 (98%)	17 (2%)	0	100	100
1	B	723/731 (99%)	707 (98%)	16 (2%)	0	100	100
All	All	1448/1462 (99%)	1415 (98%)	33 (2%)	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	607/611 (99%)	594 (98%)	13 (2%)	53	57
1	B	605/611 (99%)	590 (98%)	15 (2%)	47	49
All	All	1212/1222 (99%)	1184 (98%)	28 (2%)	52	53

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	48	LYS
1	A	129	ASP
1	A	151	MET
1	A	245	PRO
1	A	308	ILE
1	A	320	LEU
1	A	438	GLU
1	A	570	THR
1	A	579	LYS
1	A	613	SER
1	A	616	LYS
1	A	724	LEU
1	B	67	LEU
1	B	129	ASP
1	B	151	MET
1	B	210[A]	MET
1	B	210[B]	MET
1	B	308	ILE
1	B	320	LEU
1	B	333	LEU
1	B	350	LYS
1	B	383	ARG
1	B	396	VAL
1	B	491	LYS
1	B	546	PRO
1	B	610	LYS
1	B	616	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	574	GLN

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 ⓘ

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	C	1[B]	2	12,12,12	1.20	1 (8%)	17,17,17	1.62	3 (17%)
2	BGC	C	2[B]	2	11,11,12	1.40	1 (9%)	15,15,17	2.22	4 (26%)
2	GLC	D	1[B]	2	12,12,12	0.94	0	17,17,17	1.51	2 (11%)
2	BGC	D	2[B]	2	11,11,12	0.90	0	15,15,17	2.18	2 (13%)

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[B]	2	-	1/2/22/22	0/1/1/1
2	BGC	C	2[B]	2	-	0/2/19/22	0/1/1/1
2	GLC	D	1[B]	2	-	1/2/22/22	0/1/1/1
2	BGC	D	2[B]	2	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2[B]	BGC	O5-C5	3.42	1.50	1.43
2	C	1[B]	GLC	O5-C5	-2.02	1.39	1.44

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2[B]	BGC	C1-O5-C5	7.49	122.35	112.19
2	C	2[B]	BGC	C1-O5-C5	5.75	119.98	112.19
2	C	2[B]	BGC	O5-C5-C6	4.04	113.54	107.20
2	C	1[B]	GLC	O5-C5-C6	-3.68	97.28	106.44
2	D	1[B]	GLC	O6-C6-C5	-3.58	99.02	111.29
2	C	2[B]	BGC	O5-C1-C2	3.34	115.93	110.77
2	C	1[B]	GLC	C1-O5-C5	-2.67	108.63	113.66
2	D	2[B]	BGC	C2-C3-C4	-2.58	106.42	110.89
2	D	1[B]	GLC	O5-C5-C6	-2.54	100.12	106.44
2	C	2[B]	BGC	C2-C3-C4	-2.33	106.87	110.89
2	C	1[B]	GLC	O6-C6-C5	-2.27	103.49	111.29

There are no chirality outliers.

All (4) torsion outliers are listed below:

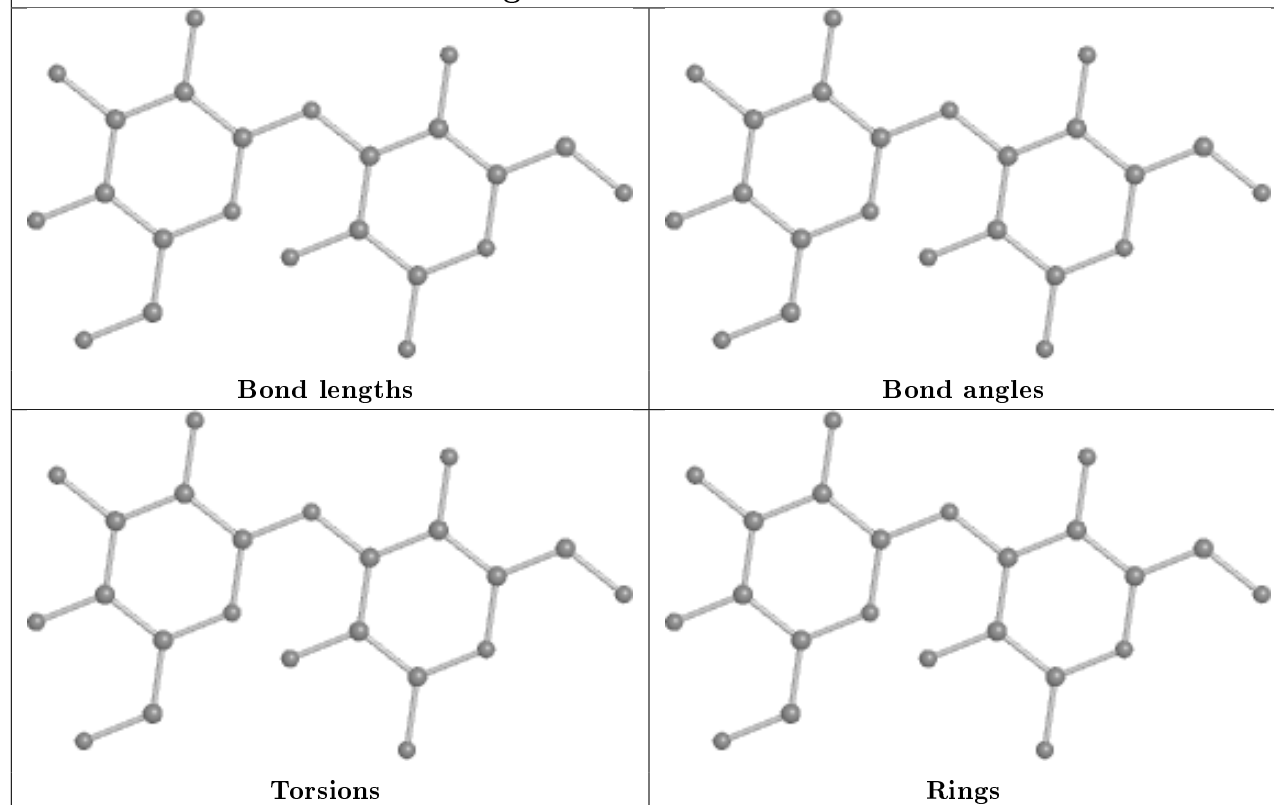
Mol	Chain	Res	Type	Atoms
2	D	1[B]	GLC	O5-C5-C6-O6
2	C	1[B]	GLC	O5-C5-C6-O6
2	D	2[B]	BGC	C4-C5-C6-O6
2	D	2[B]	BGC	O5-C5-C6-O6

There are no ring outliers.

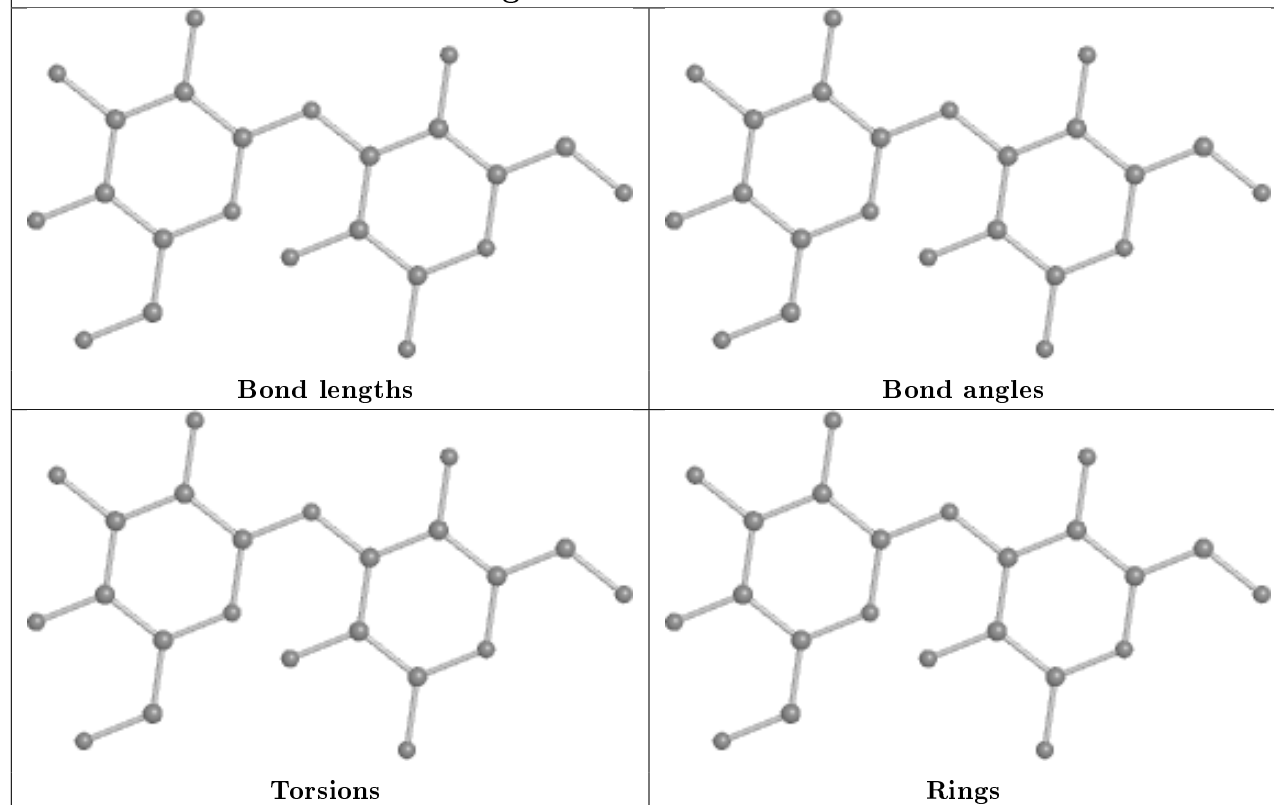
No monomer is involved in short contacts.

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

Oligosaccharide Chain C



Oligosaccharide Chain D



5.6 Ligand geometry

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	$\# Z > 2$
5	BGC	B	804[A]	5	12,12,12	0.53	0	17,17,17	1.17	2 (11%)
4	GOL	B	802	-	5,5,5	0.43	0	5,5,5	0.83	0
5	BGC	A	804[A]	5	12,12,12	0.57	0	17,17,17	1.14	1 (5%)
4	GOL	A	802[A]	-	5,5,5	0.30	0	5,5,5	0.50	0
4	GOL	A	802[B]	-	5,5,5	0.37	0	5,5,5	0.57	0
5	BGC	B	806[A]	5	11,11,12	0.42	0	15,15,17	2.31	2 (13%)
5	BGC	A	806[A]	5	11,11,12	0.56	0	15,15,17	2.23	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
5	BGC	B	804[A]	5	-	1/2/22/22	0/1/1/1
4	GOL	B	802	-	-	2/4/4/4	-
5	BGC	A	804[A]	5	-	1/2/22/22	0/1/1/1
4	GOL	A	802[A]	-	-	2/4/4/4	-
4	GOL	A	802[B]	-	-	2/4/4/4	-
5	BGC	B	806[A]	5	-	0/2/19/22	0/1/1/1
5	BGC	A	806[A]	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	806[A]	BGC	C1-O5-C5	7.66	122.57	112.19
5	A	806[A]	BGC	C1-O5-C5	6.75	121.33	112.19
5	A	804[A]	BGC	C3-C4-C5	2.97	115.54	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	804[A]	BGC	C3-C4-C5	2.85	115.32	110.24
5	B	806[A]	BGC	C2-C3-C4	-2.80	106.04	110.89
5	A	806[A]	BGC	C2-C3-C4	-2.51	106.54	110.89
5	B	804[A]	BGC	O5-C5-C4	2.50	114.23	109.69
5	A	806[A]	BGC	O5-C1-C2	2.33	114.37	110.77
5	A	806[A]	BGC	C1-C2-C3	2.09	112.24	109.67
5	A	806[A]	BGC	O5-C5-C6	2.04	110.40	107.20

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	802	GOL	O1-C1-C2-C3
4	A	802[B]	GOL	O1-C1-C2-C3
4	A	802[B]	GOL	O1-C1-C2-O2
5	B	804[A]	BGC	O5-C5-C6-O6
5	A	804[A]	BGC	O5-C5-C6-O6
4	B	802	GOL	O1-C1-C2-O2
4	A	802[A]	GOL	C1-C2-C3-O3
4	A	802[A]	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	802[B]	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, 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	724/731 (99%)	-0.01	13 (1%) 68 66	6, 14, 30, 45	0
1	B	724/731 (99%)	0.08	21 (2%) 51 50	6, 16, 33, 47	0
All	All	1448/1462 (99%)	0.03	34 (2%) 60 59	6, 15, 31, 47	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	351	ASN	4.7
1	B	580	GLY	4.3
1	A	576	PRO	4.1
1	B	576	PRO	4.0
1	A	39	LEU	3.8
1	B	579	LYS	3.8
1	A	579	LYS	3.7
1	A	580	GLY	3.6
1	B	37	ALA	3.6
1	B	353	ASP	3.2
1	B	350	LYS	3.1
1	B	352	ASN	2.8
1	A	38	GLU	2.8
1	A	430	GLU	2.8
1	B	356	LYS	2.8
1	B	78	LYS	2.8
1	B	8	GLU	2.7
1	A	577	GLU	2.6
1	B	616	LYS	2.5
1	B	268	ILE	2.4
1	A	45	GLN	2.3
1	A	575	THR	2.3
1	A	160	LEU	2.2
1	B	45	GLN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	41	GLY	2.2
1	B	12	GLN	2.2
1	B	355	THR	2.2
1	B	67	LEU	2.1
1	B	38	GLU	2.1
1	A	313	GLY	2.1
1	A	390	GLU	2.1
1	B	455	GLN	2.1
1	B	637	ALA	2.0
1	B	456	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

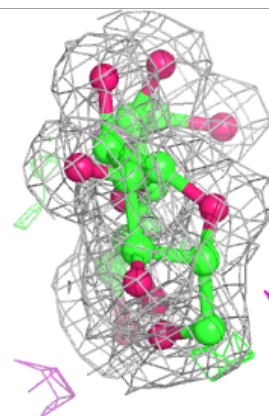
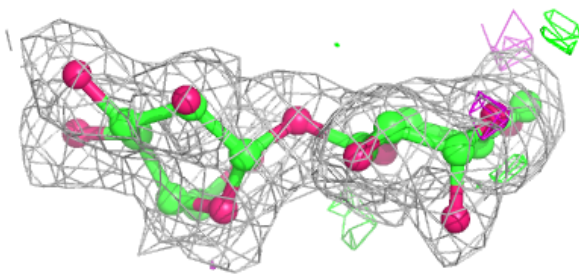
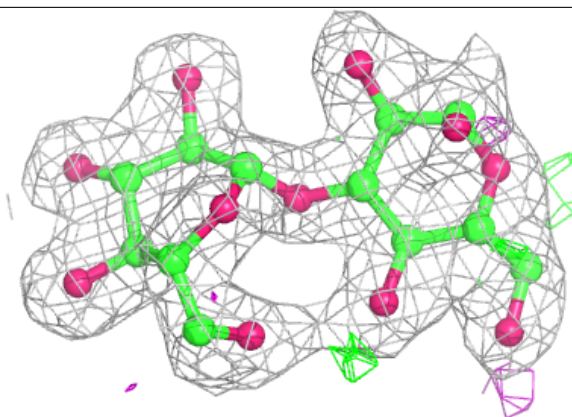
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	C	1[B]	12/12	0.94	0.08	8,10,12,14	12
2	GLC	D	1[B]	12/12	0.95	0.09	7,8,9,9	12
2	BGC	C	2[B]	11/12	0.97	0.11	5,8,9,10	11
2	BGC	D	2[B]	11/12	0.97	0.10	5,7,7,7	11

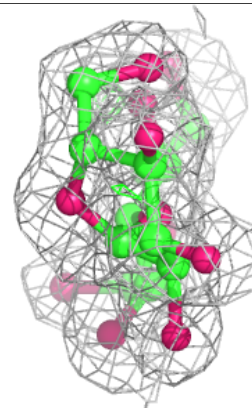
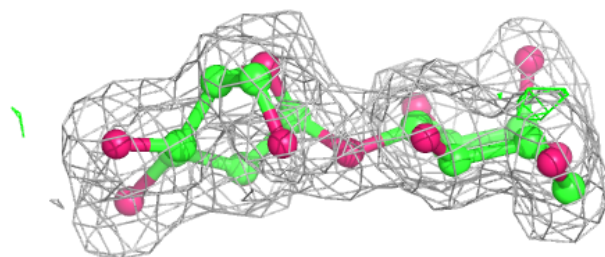
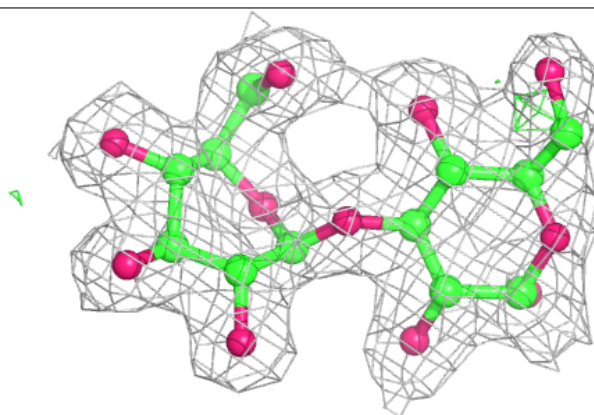
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	B	802	6/6	0.92	0.16	18,25,28,32	0
5	BGC	B	804[A]	12/12	0.95	0.10	16,23,27,27	12
5	BGC	A	804[A]	12/12	0.95	0.10	17,21,24,26	12
4	GOL	A	802[A]	6/6	0.95	0.18	20,26,28,32	6
4	GOL	A	802[B]	6/6	0.95	0.18	7,13,16,18	6
5	BGC	A	806[A]	11/12	0.96	0.11	8,15,17,19	11
3	MG	B	801	1/1	0.96	0.06	18,18,18,18	0
5	BGC	B	806[A]	11/12	0.97	0.10	12,20,24,27	11
3	MG	A	801	1/1	0.98	0.06	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.