Full wwPDB X-ray Structure Validation Report (i)

Sep 7, 2023 – 11:11 AM EDT

PDB ID	:	4GYJ
Title	:	Crystal structure of mutant (D318N) bacillus subtilis family 3 glycoside hydrolase (nagz) in complex with glcnac-murnac (space group P1)
Authors	:	Bacik, J.P.; Mark, B.L.
Deposited on	:	2012-09-05
Resolution	:	1.65 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 (i)) were used in the production of this report:

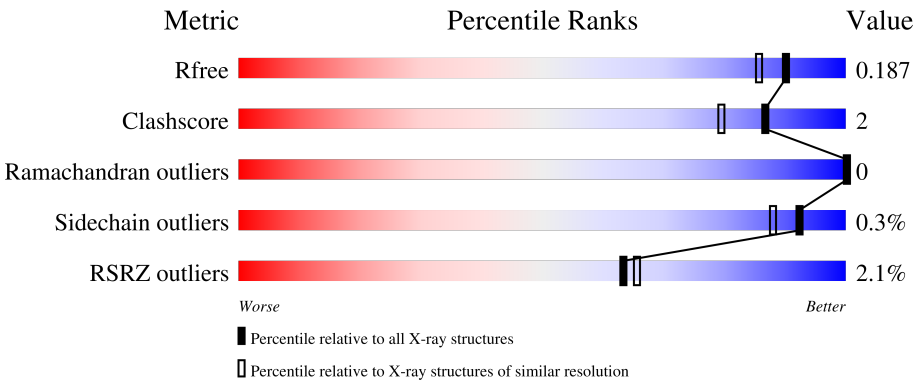
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	648	% 91% 5% 5%
1	B	648	3% 92% • 5%
2	C	2	50% 50%
2	D	2	50% 50%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10481 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 Uncharacterized lipoprotein ybbD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	618	4671	2955	802	894	20	0	2	0
1	B	617	4643	2937	797	890	19	0	2	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	MET	-	initiating methionine	UNP P40406
A	-2	GLY	-	expression tag	UNP P40406
A	-1	SER	-	expression tag	UNP P40406
A	0	SER	-	expression tag	UNP P40406
A	1	HIS	-	expression tag	UNP P40406
A	2	HIS	-	expression tag	UNP P40406
A	3	HIS	-	expression tag	UNP P40406
A	4	HIS	-	expression tag	UNP P40406
A	5	HIS	-	expression tag	UNP P40406
A	6	HIS	-	expression tag	UNP P40406
A	7	SER	-	expression tag	UNP P40406
A	8	SER	-	expression tag	UNP P40406
A	9	GLY	-	expression tag	UNP P40406
A	10	LEU	-	expression tag	UNP P40406
A	11	VAL	-	expression tag	UNP P40406
A	12	PRO	-	expression tag	UNP P40406
A	13	ARG	-	expression tag	UNP P40406
A	14	GLY	-	expression tag	UNP P40406
A	15	SER	-	expression tag	UNP P40406
A	16	HIS	-	expression tag	UNP P40406
A	17	MET	-	expression tag	UNP P40406
A	318	ASN	ASP	engineered mutation	UNP P40406
A	643	GLY	-	expression tag	UNP P40406
A	644	SER	-	expression tag	UNP P40406
B	-3	MET	-	initiating methionine	UNP P40406

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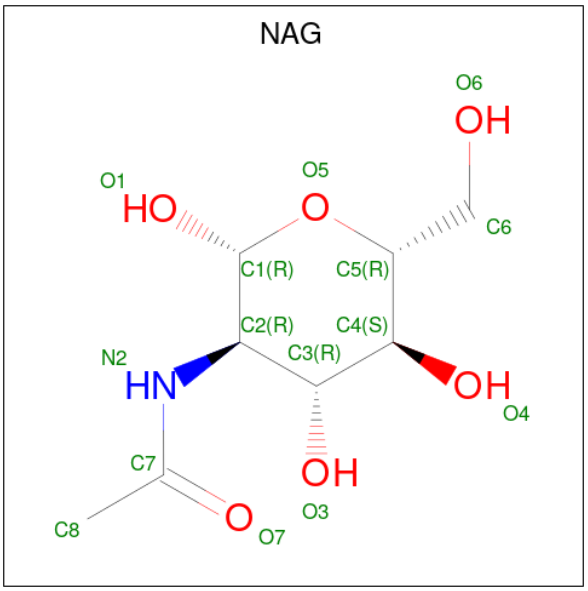
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP P40406
B	-1	SER	-	expression tag	UNP P40406
B	0	SER	-	expression tag	UNP P40406
B	1	HIS	-	expression tag	UNP P40406
B	2	HIS	-	expression tag	UNP P40406
B	3	HIS	-	expression tag	UNP P40406
B	4	HIS	-	expression tag	UNP P40406
B	5	HIS	-	expression tag	UNP P40406
B	6	HIS	-	expression tag	UNP P40406
B	7	SER	-	expression tag	UNP P40406
B	8	SER	-	expression tag	UNP P40406
B	9	GLY	-	expression tag	UNP P40406
B	10	LEU	-	expression tag	UNP P40406
B	11	VAL	-	expression tag	UNP P40406
B	12	PRO	-	expression tag	UNP P40406
B	13	ARG	-	expression tag	UNP P40406
B	14	GLY	-	expression tag	UNP P40406
B	15	SER	-	expression tag	UNP P40406
B	16	HIS	-	expression tag	UNP P40406
B	17	MET	-	expression tag	UNP P40406
B	318	ASN	ASP	engineered mutation	UNP P40406
B	643	GLY	-	expression tag	UNP P40406
B	644	SER	-	expression tag	UNP P40406

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-alpha-muramic acid.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	2	34	19	2	13	0	2	0
			Total	C	N	O			
2	D	2	34	19	2	13	0	2	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	15	8	1	6	0	1
			Total	C	N	O		
3	B	1	15	8	1	6	0	1

- Molecule 4 is water.

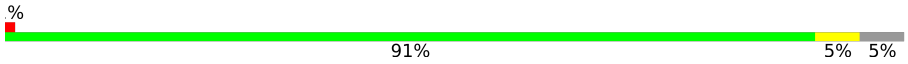
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	584	584	584	0	0
			Total	O		
4	B	485	485	485	0	0

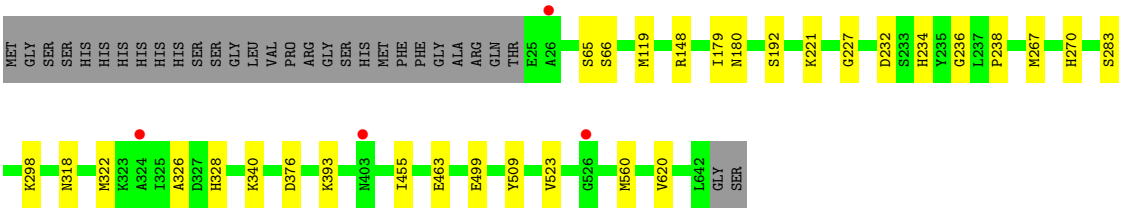
3 Residue-property plots (i)

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: Uncharacterized lipoprotein ybbD

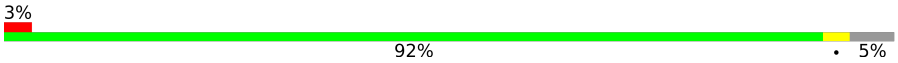
Chain A:

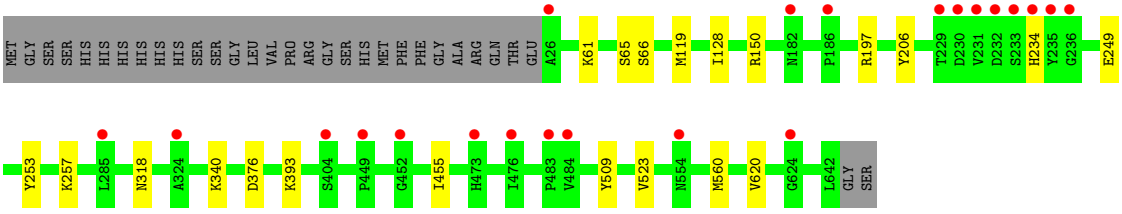




• Molecule 1: Uncharacterized lipoprotein ybbD

Chain B:





• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-alpha-muramic acid

Chain C:

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-alpha-muramic acid

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	58.45Å 73.39Å 83.43Å 98.65° 110.14° 92.43°	Depositor
Resolution (Å)	38.61 – 1.65 38.61 – 1.65	Depositor EDS
% Data completeness (in resolution range)	95.8 (38.61-1.65) 92.6 (38.61-1.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 1.65Å)	Xtriage
Refinement program	PHENIX 1.7.2_869	Depositor
R, R_{free}	0.163 , 0.190 0.161 , 0.187	Depositor DCC
R_{free} test set	7479 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	19.6	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 54.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	10481	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MUB, NAG

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	0.45	0/4758	0.56	0/6453
1	B	0.42	0/4733	0.55	0/6424
All	All	0.44	0/9491	0.55	0/12877

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	4671	0	4647	23	0
1	B	4643	0	4597	14	0
2	C	34	0	25	4	0
2	D	34	0	25	5	0
3	A	15	0	10	2	0
3	B	15	0	11	2	0
4	A	584	0	0	4	0
4	B	485	0	0	3	0
All	All	10481	0	9315	39	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 2.

All (39) 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:65:SER:HB3	2:C:1[A]:MUB:H81	1.38	1.05
1:A:65:SER:HB3	2:D:1[A]:MUB:H81	1.41	0.99
1:A:148:ARG:HH11	1:A:148:ARG:HG2	1.56	0.69
4:B:1264:HOH:O	2:D:1[A]:MUB:H82	1.94	0.67
1:A:66:SER:HB3	2:D:1[A]:MUB:H83	1.80	0.62
1:B:66:SER:HB3	2:C:1[A]:MUB:H83	1.82	0.61
1:A:455:ILE:HD13	1:A:509:TYR:HB2	1.85	0.59
1:B:455:ILE:HD13	1:B:509:TYR:HB2	1.85	0.59
1:B:234:HIS:NE2	3:B:702[B]:NAG:O1	2.35	0.58
4:A:815:HOH:O	2:C:1[A]:MUB:H82	2.04	0.58
1:A:119:MET:HG3	1:A:393:LYS:HE2	1.86	0.58
1:B:119:MET:HG3	1:B:393:LYS:HE2	1.85	0.56
1:A:65:SER:CB	2:D:1[A]:MUB:H81	2.27	0.55
1:B:150:ARG:HD3	1:B:206:TYR:CE2	2.43	0.53
1:A:234:HIS:HA	1:A:322[B]:MET:HG2	1.90	0.52
1:B:523:VAL:HG21	1:B:620:VAL:HG13	1.92	0.50
1:B:197:ARG:NH1	1:B:249:GLU:O	2.42	0.49
1:A:298:LYS:HE3	4:A:1165:HOH:O	2.13	0.49
1:B:318:ASN:HD21	3:B:702[B]:NAG:HN2	1.60	0.48
1:A:318:ASN:OD1	3:A:702[B]:NAG:H1	2.14	0.48
1:A:232:ASP:OD1	1:A:234:HIS:ND1	2.37	0.47
1:A:463:GLU:OE1	4:A:1315:HOH:O	2.20	0.47
1:A:326:ALA:O	4:A:1346:HOH:O	2.21	0.45
1:B:65:SER:CB	2:C:1[A]:MUB:H81	2.27	0.45
1:A:66:SER:CB	2:D:1[A]:MUB:H83	2.44	0.45
1:A:523:VAL:HG21	1:A:620:VAL:HG13	1.98	0.44
1:A:180:ASN:HB2	1:A:192:SER:HB3	2.01	0.43
1:A:234:HIS:NE2	3:A:702[B]:NAG:O1	2.52	0.43
1:A:270:HIS:CE1	1:A:318:ASN:HB3	2.53	0.42
1:A:340:LYS:HE2	1:A:376:ASP:HB3	2.00	0.42
1:B:128:ILE:HG23	4:B:1086:HOH:O	2.19	0.42
1:A:283:SER:OG	1:A:328:HIS:ND1	2.49	0.42
1:B:340:LYS:HE2	1:B:376:ASP:HB3	2.01	0.42
1:A:236:GLY:O	1:A:238:PRO:HD3	2.20	0.42
1:A:179:ILE:O	1:A:227:GLY:HA3	2.20	0.41
1:B:61:LYS:HD2	4:B:1172:HOH:O	2.20	0.41
1:A:221:LYS:HB3	1:A:267:MET:HB3	2.04	0.40
1:B:253:TYR:CZ	1:B:257:LYS:HE3	2.56	0.40
1:A:322[B]:MET:HB2	1:A:322[B]:MET:HE3	1.77	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	618/648 (95%)	602 (97%)	16 (3%)	0	100	100
1	B	617/648 (95%)	601 (97%)	16 (3%)	0	100	100
All	All	1235/1296 (95%)	1203 (97%)	32 (3%)	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	495/544 (91%)	493 (100%)	2 (0%)	91	85
1	B	489/544 (90%)	488 (100%)	1 (0%)	93	89
All	All	984/1088 (90%)	981 (100%)	3 (0%)	92	88

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	499	GLU
1	A	560	MET
1	B	560	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

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	MUB	C	1[A]	2	20,20,20	2.39	4 (20%)	24,28,28	1.47	4 (16%)
2	NAG	C	2[A]	2	14,14,15	1.88	3 (21%)	17,19,21	2.27	4 (23%)
2	MUB	D	1[A]	2	20,20,20	2.38	4 (20%)	24,28,28	1.34	3 (12%)
2	NAG	D	2[A]	2	14,14,15	1.83	3 (21%)	17,19,21	2.28	4 (23%)

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	MUB	C	1[A]	2	-	4/14/34/34	0/1/1/1
2	NAG	C	2[A]	2	-	0/6/23/26	0/1/1/1
2	MUB	D	1[A]	2	-	3/14/34/34	0/1/1/1
2	NAG	D	2[A]	2	-	0/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1[A]	MUB	C3-C2	-8.63	1.38	1.53
2	D	1[A]	MUB	C3-C2	-8.54	1.39	1.53
2	C	2[A]	NAG	C4-C3	-4.04	1.42	1.52
2	D	2[A]	NAG	C4-C3	-3.77	1.42	1.52
2	D	2[A]	NAG	O5-C5	3.58	1.50	1.43
2	C	2[A]	NAG	C7-N2	3.30	1.45	1.34
2	C	2[A]	NAG	O5-C5	3.18	1.49	1.43
2	D	2[A]	NAG	C7-N2	3.17	1.45	1.34
2	C	1[A]	MUB	C7-N2	3.16	1.45	1.34
2	D	1[A]	MUB	C2-N2	3.06	1.50	1.45
2	D	1[A]	MUB	C7-N2	3.03	1.44	1.34
2	C	1[A]	MUB	C2-N2	3.00	1.50	1.45
2	C	1[A]	MUB	O3-C3	2.04	1.49	1.43
2	D	1[A]	MUB	O3-C3	2.04	1.49	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2[A]	NAG	C1-O5-C5	6.72	121.30	112.19
2	C	2[A]	NAG	C1-O5-C5	6.72	121.30	112.19
2	D	1[A]	MUB	C1-C2-N2	-4.45	105.58	110.73
2	C	2[A]	NAG	O5-C1-C2	4.03	117.65	111.29
2	D	2[A]	NAG	O5-C1-C2	3.92	117.48	111.29
2	C	1[A]	MUB	C1-C2-N2	-3.69	106.45	110.73
2	D	2[A]	NAG	C2-N2-C7	-3.39	118.08	122.90
2	C	2[A]	NAG	C2-N2-C7	-3.38	118.09	122.90
2	C	1[A]	MUB	O11-C10-O10	-2.63	118.11	124.09
2	C	1[A]	MUB	C2-N2-C7	-2.50	117.09	123.18
2	D	1[A]	MUB	O11-C10-C9	2.24	122.08	113.89
2	D	1[A]	MUB	O11-C10-O10	-2.21	119.07	124.09
2	C	2[A]	NAG	C8-C7-N2	2.21	119.83	116.10
2	D	2[A]	NAG	C8-C7-N2	2.03	119.54	116.10
2	C	1[A]	MUB	O5-C1-C2	-2.03	107.48	109.52

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1[A]	MUB	O5-C5-C6-O6
2	D	1[A]	MUB	O5-C5-C6-O6
2	D	1[A]	MUB	C4-C5-C6-O6
2	C	1[A]	MUB	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	C	1[A]	MUB	O11-C10-C9-O3
2	D	1[A]	MUB	C3-C2-N2-C7
2	C	1[A]	MUB	O10-C10-C9-O3

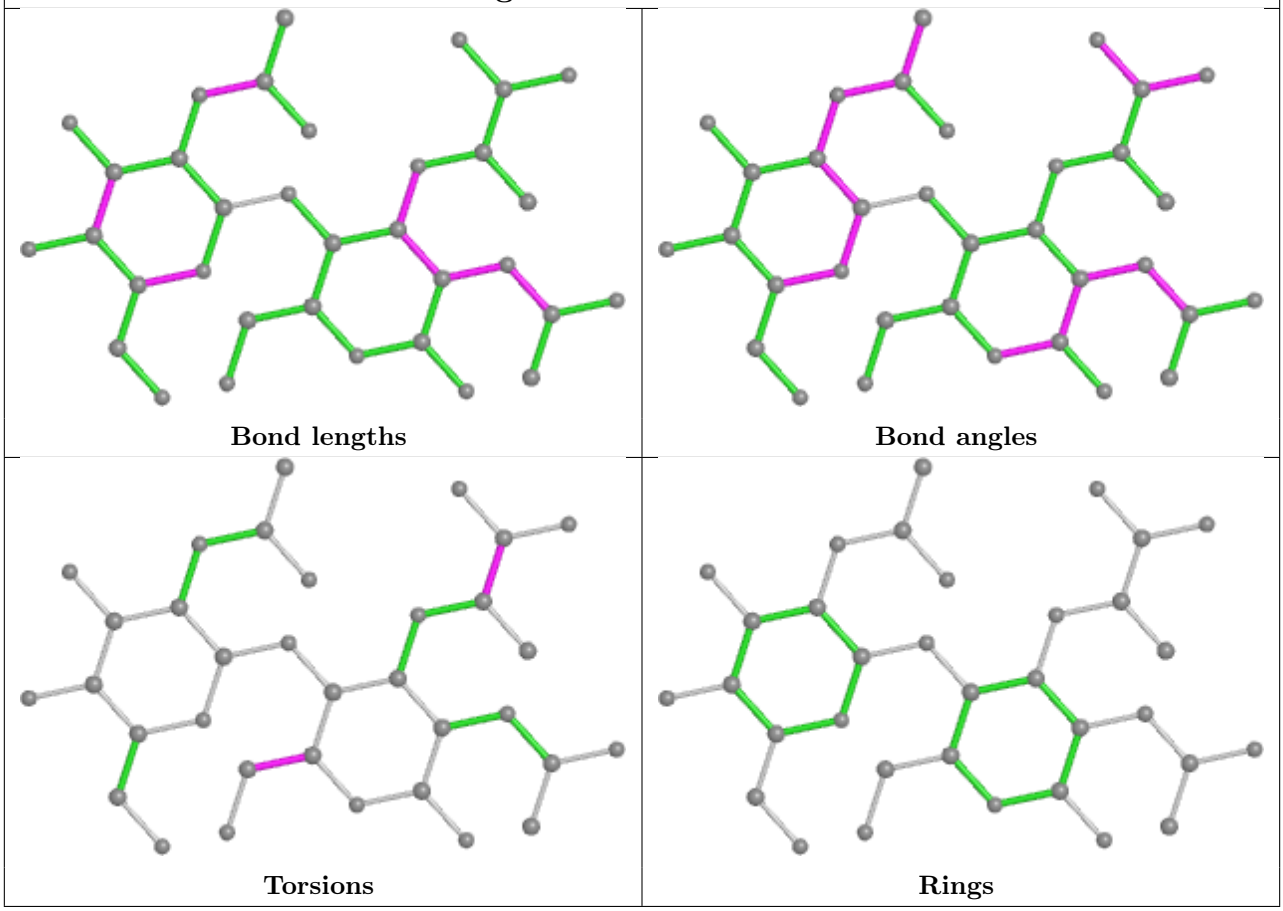
There are no ring outliers.

2 monomers are involved in 9 short contacts:

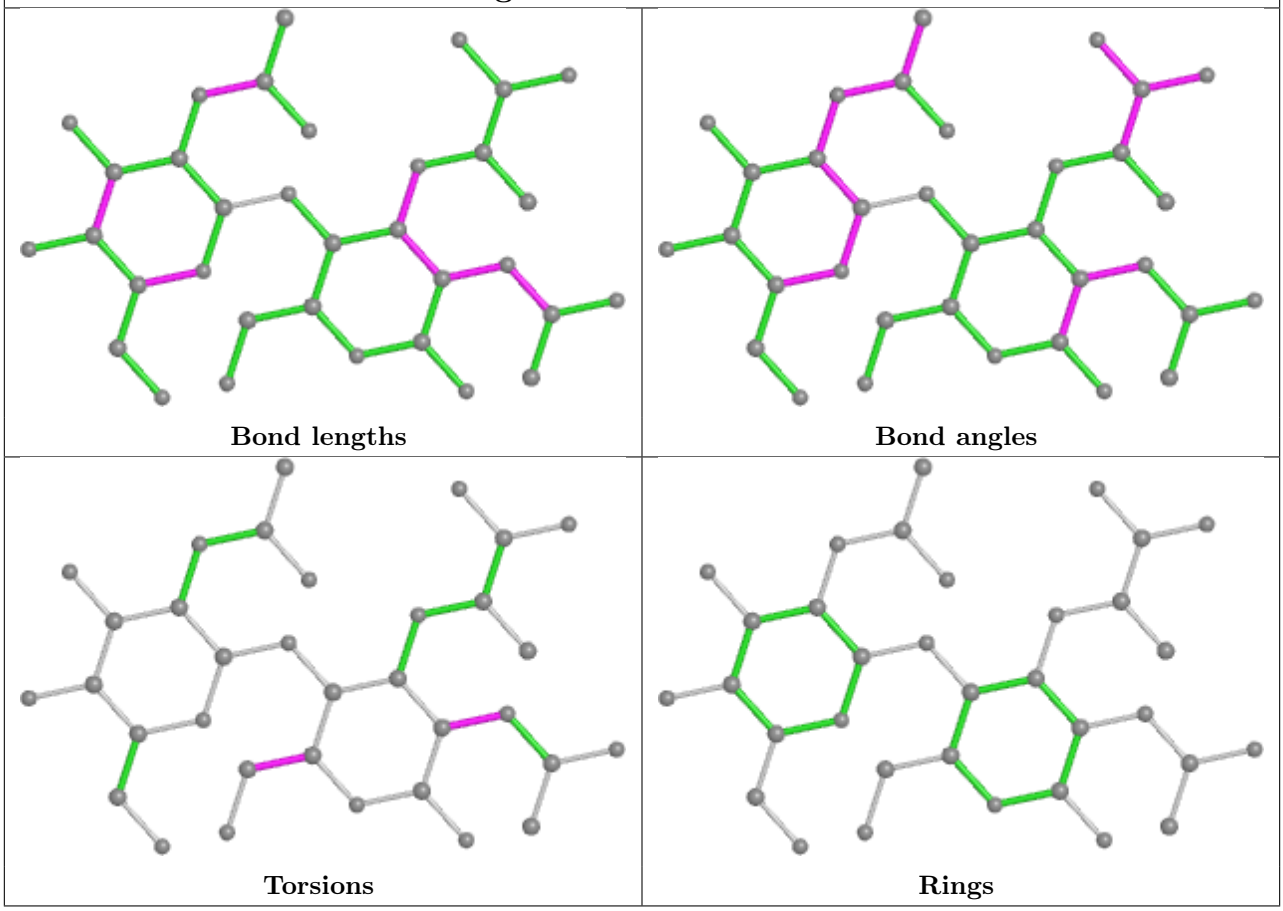
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1[A]	MUB	4	0
2	D	1[A]	MUB	5	0

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 C



Oligosaccharide Chain D



5.6 Ligand geometry (i)

2 ligands 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	$\#\|Z\| > 2$
3	NAG	B	702[B]	-	15,15,15	1.73	4 (26%)	21,21,21	1.72	4 (19%)
3	NAG	A	702[B]	-	15,15,15	1.74	4 (26%)	21,21,21	1.60	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
3	NAG	B	702[B]	-	-	0/6/26/26	0/1/1/1
3	NAG	A	702[B]	-	-	0/6/26/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702[B]	NAG	C4-C3	-3.72	1.42	1.52
3	B	702[B]	NAG	C4-C3	-3.62	1.43	1.52
3	A	702[B]	NAG	C7-N2	3.33	1.45	1.34
3	B	702[B]	NAG	C7-N2	3.15	1.45	1.34
3	B	702[B]	NAG	O5-C5	2.60	1.50	1.44
3	A	702[B]	NAG	O5-C5	2.29	1.49	1.44
3	A	702[B]	NAG	C1-C2	-2.11	1.50	1.52
3	B	702[B]	NAG	C1-C2	-2.03	1.50	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	702[B]	NAG	C1-C2-N2	-4.63	105.37	110.73
3	A	702[B]	NAG	C1-C2-N2	-4.58	105.42	110.73
3	A	702[B]	NAG	O5-C1-C2	3.22	112.75	109.52
3	B	702[B]	NAG	O5-C1-C2	3.04	112.57	109.52
3	B	702[B]	NAG	C1-C2-C3	2.45	113.89	110.54
3	B	702[B]	NAG	C4-C3-C2	2.32	113.74	110.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702[B]	NAG	2	0
3	A	702[B]	NAG	2	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	618/648 (95%)	-0.36	4 (0%)	89	90	13, 24, 48, 65	0
1	B	617/648 (95%)	-0.18	22 (3%)	42	43	15, 28, 50, 66	0
All	All	1235/1296 (95%)	-0.27	26 (2%)	63	65	13, 26, 50, 66	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	324	ALA	6.3
1	B	236	GLY	5.1
1	B	233	SER	4.4
1	A	324	ALA	4.0
1	B	404	SER	4.0
1	B	232	ASP	3.7
1	B	231	VAL	3.5
1	B	483	PRO	3.4
1	B	235	TYR	3.3
1	B	26	ALA	3.2
1	B	624	GLY	3.2
1	A	26	ALA	3.0
1	B	476	ILE	2.6
1	B	285	LEU	2.6
1	B	230	ASP	2.5
1	B	182	ASN	2.4
1	B	234	HIS	2.4
1	B	452	GLY	2.3
1	A	403	ASN	2.2
1	A	526	GLY	2.1
1	B	186	PRO	2.1
1	B	484	VAL	2.1
1	B	449	PRO	2.0
1	B	473	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	554	ASN	2.0
1	B	229	THR	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)

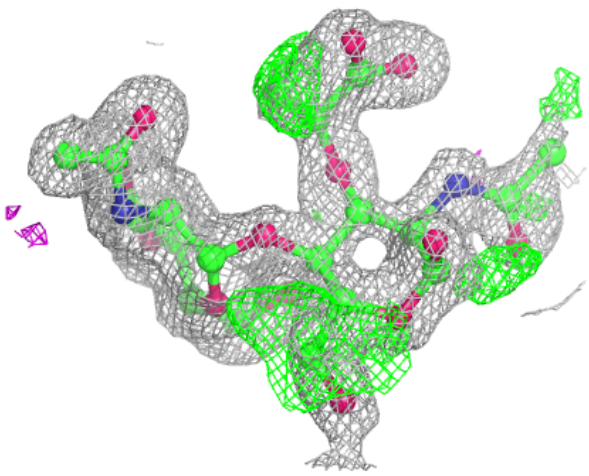
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

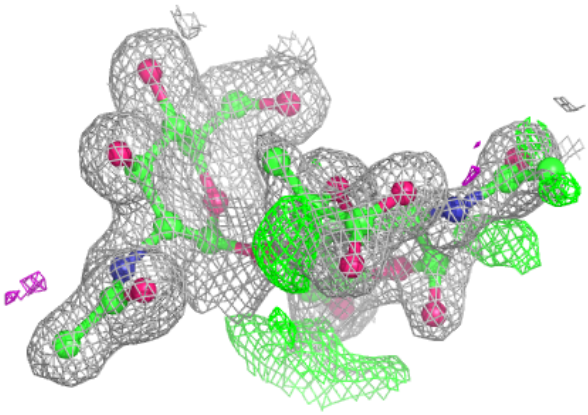
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MUB	D	1[A]	20/20	0.81	0.24	15,34,40,42	20
2	MUB	C	1[A]	20/20	0.86	0.18	18,30,36,42	20
2	NAG	D	2[A]	14/15	0.95	0.06	18,24,27,28	14
2	NAG	C	2[A]	14/15	0.97	0.07	16,21,24,25	14

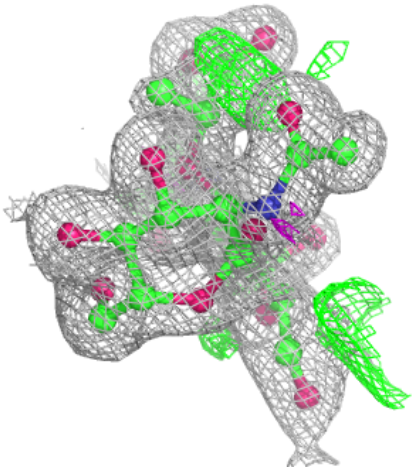
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

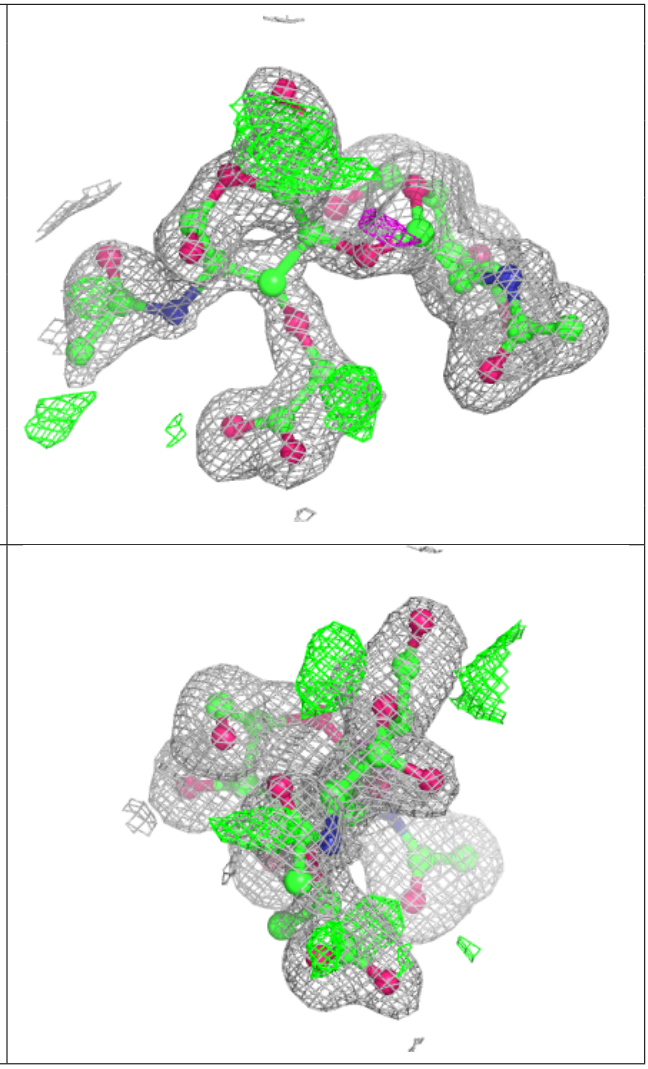






Electron density around Chain D:

$2mF_o$-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
3	NAG	B	702[B]	15/15	0.95	0.07	16,23,25,26	15
3	NAG	A	702[B]	15/15	0.97	0.07	13,20,24,25	15

6.5 Other polymers (i)

There are no such residues in this entry.