



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:55 AM UTC

PDB ID : 5LFR / pdb_00005lfr
Title : Crystal structure of glycosylated Myelin-associated glycoprotein (MAG) Ig1-3
Authors : Pronker, M.F.; Janssen, B.J.C.
Deposited on : 2016-07-04
Resolution : 2.12 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

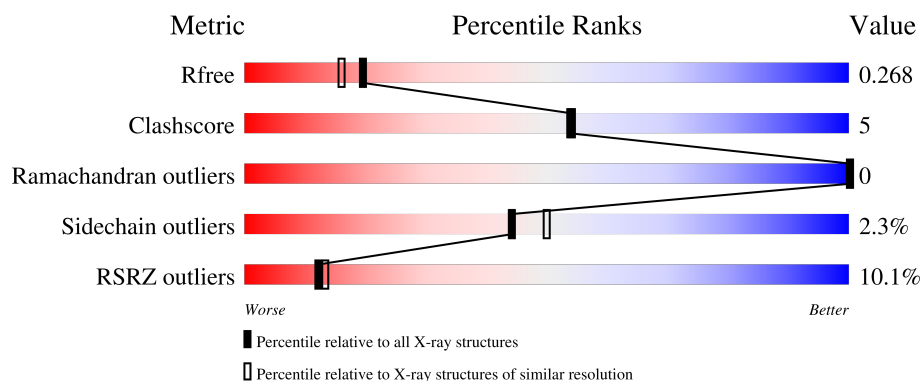
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	317	6% 87% 9% ..
1	B	317	14% 84% 14% ..
2	C	5	20% 80%
3	D	4	25% 75%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5162 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 Myelin-associated glycoprotein.

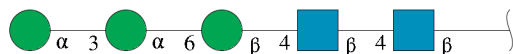
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2402	1524	407	457	14			
1	B	312	Total	C	N	O	S	0	2	0
			2449	1558	416	461	14			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLY	-	expression tag	UNP P20917
A	19	SER	-	expression tag	UNP P20917
A	326	ALA	-	expression tag	UNP P20917
A	327	ALA	-	expression tag	UNP P20917
A	328	ALA	-	expression tag	UNP P20917
A	329	HIS	-	expression tag	UNP P20917
A	330	HIS	-	expression tag	UNP P20917
A	331	HIS	-	expression tag	UNP P20917
A	332	HIS	-	expression tag	UNP P20917
A	333	HIS	-	expression tag	UNP P20917
A	334	HIS	-	expression tag	UNP P20917
B	18	GLY	-	expression tag	UNP P20917
B	19	SER	-	expression tag	UNP P20917
B	326	ALA	-	expression tag	UNP P20917
B	327	ALA	-	expression tag	UNP P20917
B	328	ALA	-	expression tag	UNP P20917
B	329	HIS	-	expression tag	UNP P20917
B	330	HIS	-	expression tag	UNP P20917
B	331	HIS	-	expression tag	UNP P20917
B	332	HIS	-	expression tag	UNP P20917
B	333	HIS	-	expression tag	UNP P20917
B	334	HIS	-	expression tag	UNP P20917

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

cetamido-2-deoxy-beta-D-glucopyranose.



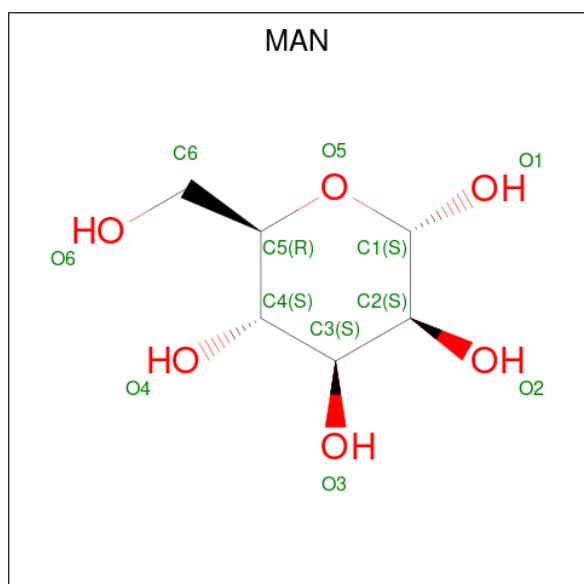
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 4 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).



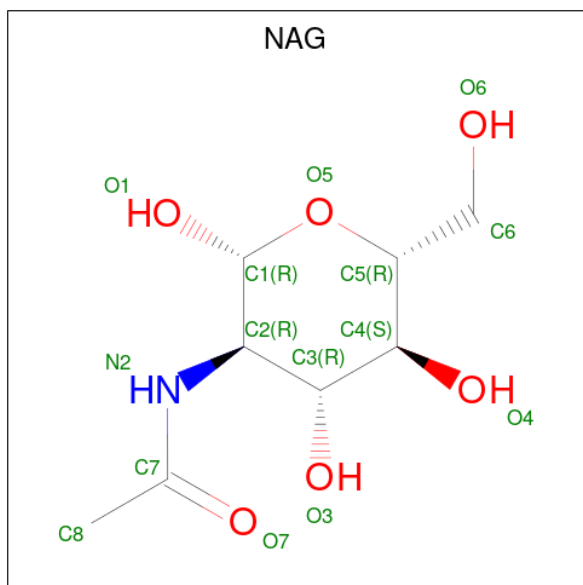
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		

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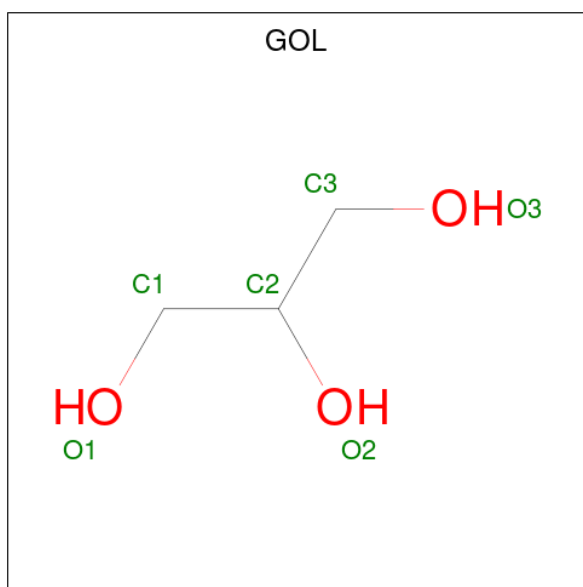
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



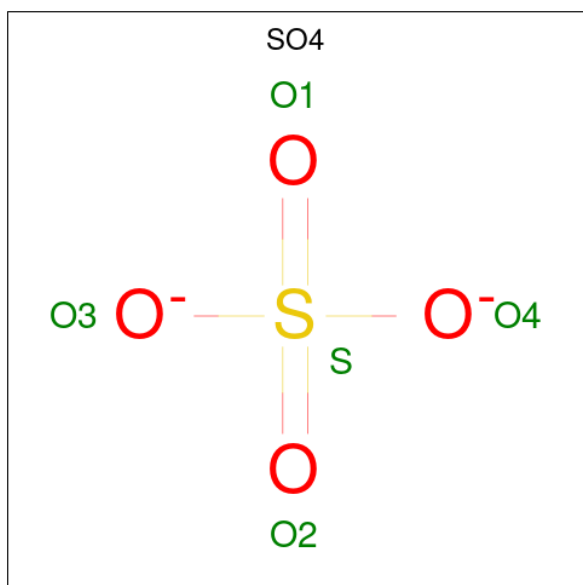
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

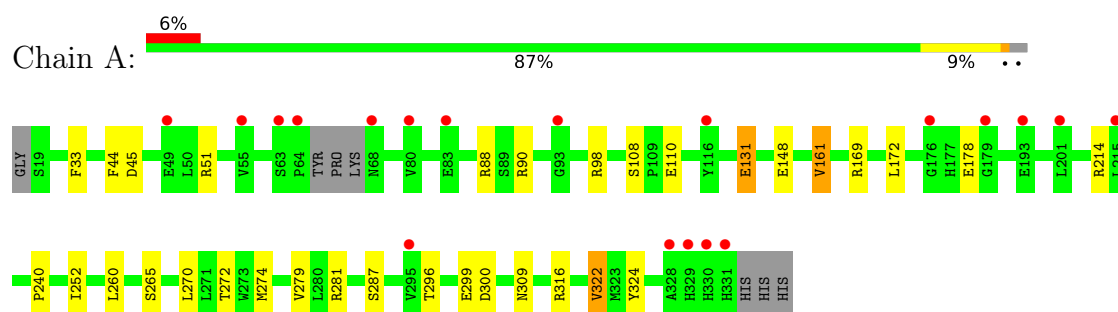
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	38	Total	O	0	0
			38	38		
8	B	16	Total	O	0	0
			16	16		

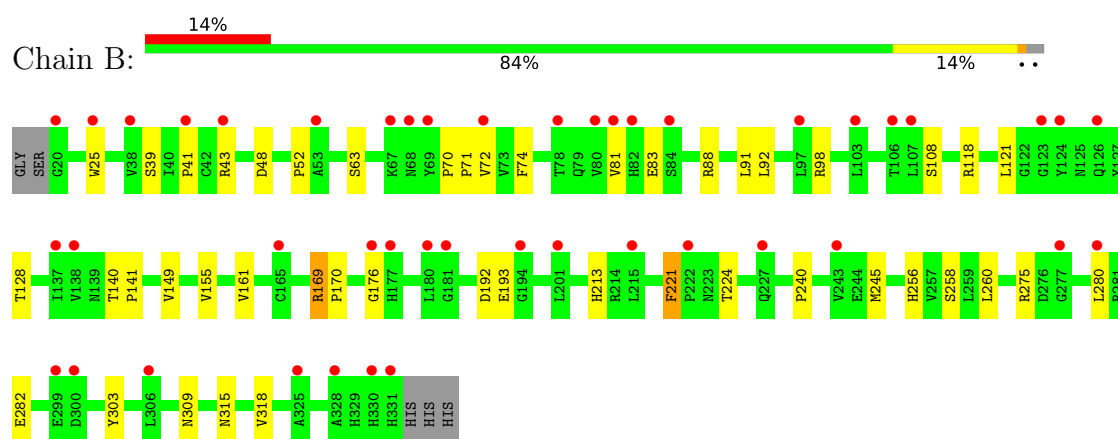
3 Residue-property plots [i](#)

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: Myelin-associated glycoprotein



- Molecule 1: Myelin-associated glycoprotein



- Molecule 2: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	43.06Å 60.40Å 79.22Å 72.70° 86.71° 83.01°	Depositor
Resolution (Å)	42.73 – 2.12 42.73 – 2.12	Depositor EDS
% Data completeness (in resolution range)	95.8 (42.73-2.12) 85.6 (42.73-2.12)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.85 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.224 , 0.262 0.236 , 0.268	Depositor DCC
R_{free} test set	2033 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5162	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.80% 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: NAG, SO4, BMA, MAN, GOL

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	0.28	0/2469	0.69	0/3374
1	B	0.27	0/2521	0.70	2/3447 (0.1%)
All	All	0.27	0/4990	0.69	2/6821 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	221	PHE	CA-C-N	5.43	126.63	119.84
1	B	221	PHE	C-N-CA	5.43	126.63	119.84

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	2402	0	2288	23	0
1	B	2449	0	2335	28	0
2	C	61	0	52	1	0
3	D	50	0	43	2	0
4	A	11	0	10	0	0
4	B	11	0	10	0	0
5	A	42	0	39	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	28	0	26	3	0
6	A	18	0	24	1	0
6	B	6	0	8	0	0
7	A	10	0	0	1	0
7	B	20	0	0	0	0
8	A	38	0	0	1	0
8	B	16	0	0	0	0
All	All	5162	0	4835	49	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 5.

All (49) 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:275:ARG:HG2	1:B:280:LEU:HD21	1.68	0.74
1:B:92:LEU:HB3	3:D:1:NAG:H62	1.69	0.74
1:A:45:ASP:OD1	1:A:98:ARG:NH1	2.28	0.66
1:B:63:SER:HB3	1:B:70:PRO:HB3	1.77	0.65
1:B:192:ASP:OD1	1:B:193:GLU:N	2.31	0.62
1:B:245:MET:HE3	1:B:318:VAL:HG13	1.84	0.58
1:A:148:GLU:OE2	1:B:43[A]:ARG:NH2	2.36	0.58
1:A:281:ARG:NH1	8:A:502:HOH:O	2.36	0.57
1:A:316:ARG:NH1	7:A:413:SO4:O4	2.37	0.57
1:A:309:ASN:O	1:B:98:ARG:NH1	2.40	0.55
1:B:176:GLY:O	1:B:213:HIS:NE2	2.31	0.55
1:A:33:PHE:HE2	1:A:161:VAL:HG13	1.73	0.54
1:B:52:PRO:HG3	1:B:121:LEU:HD23	1.89	0.54
1:A:270:LEU:HD22	1:B:48:ASP:HB3	1.91	0.53
6:A:412:GOL:H12	2:C:2:NAG:H3	1.90	0.53
1:B:39:SER:OG	3:D:2:NAG:H81	2.08	0.53
1:A:252:ILE:HA	1:A:324:TYR:HB2	1.90	0.53
1:A:88:ARG:NH2	1:A:108:SER:OG	2.34	0.52
1:B:88:ARG:NH2	1:B:108:SER:OG	2.42	0.51
5:B:407:NAG:O7	5:B:407:NAG:O3	2.20	0.51
1:B:118:ARG:NH2	1:B:128:THR:OG1	2.41	0.50
1:A:260:LEU:HD23	5:A:408:NAG:H62	1.97	0.47
1:B:256:HIS:NE2	1:B:258:SER:OG	2.48	0.47
1:A:131:GLU:H	1:A:131:GLU:CD	2.24	0.46
1:A:260:LEU:HD11	1:A:287:SER:HB2	1.98	0.46
1:B:303:TYR:HB2	1:B:318:VAL:HG23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:VAL:HG13	1:B:155:VAL:HG21	1.99	0.45
1:B:169:ARG:HA	1:B:170:PRO:HD3	1.76	0.44
1:B:240:PRO:HD3	1:B:309:ASN:HB3	1.98	0.44
1:A:240:PRO:HA	1:A:265:SER:HB3	1.99	0.44
1:A:272:THR:HG22	1:A:274:MET:HG3	1.99	0.44
1:A:44:PHE:O	1:A:98:ARG:HB3	2.18	0.44
1:B:39:SER:O	1:B:41:PRO:HD3	2.18	0.43
1:B:140:THR:HA	1:B:141:PRO:HD3	1.89	0.43
1:A:274:MET:HG2	1:A:279:VAL:HA	2.01	0.43
1:A:148:GLU:OE1	1:B:43[B]:ARG:NH1	2.51	0.42
1:A:178:GLU:CD	1:A:178:GLU:H	2.28	0.42
1:A:296:THR:H	1:A:299:GLU:HG2	1.84	0.42
5:B:407:NAG:HO3	5:B:407:NAG:C7	2.26	0.42
1:A:51:ARG:HH22	1:B:282:GLU:CD	2.28	0.42
1:B:25[A]:TRP:HB2	1:B:43[A]:ARG:HG2	2.02	0.42
1:A:300:ASP:OD1	1:A:322:VAL:HG23	2.20	0.41
1:B:74:PHE:CE2	1:B:91:LEU:HD22	2.55	0.41
1:B:260:LEU:HD23	5:B:406:NAG:H62	2.03	0.41
1:A:172:LEU:HD12	1:A:172:LEU:HA	1.91	0.41
1:B:221:PHE:HB2	1:B:224:THR:OG1	2.21	0.41
1:B:240:PRO:HD3	1:B:309:ASN:CB	2.51	0.41
1:B:71:PRO:HB3	1:B:83:GLU:HB2	2.03	0.41
1:A:240:PRO:HD3	1:A:309:ASN:OD1	2.21	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	306/317 (96%)	298 (97%)	8 (3%)	0	100	100
1	B	312/317 (98%)	301 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	618/634 (98%)	599 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	264/270 (98%)	257 (97%)	7 (3%)	39	44
1	B	268/270 (99%)	263 (98%)	5 (2%)	50	57
All	All	532/540 (98%)	520 (98%)	12 (2%)	44	50

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	ARG
1	A	110	GLU
1	A	131	GLU
1	A	161	VAL
1	A	169	ARG
1	A	214	ARG
1	A	322	VAL
1	B	72	VAL
1	B	81	VAL
1	B	161	VAL
1	B	169	ARG
1	B	315	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	GLN
1	B	125	ASN
1	B	218	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 ⓘ

9 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	NAG	C	1	2,1	14,14,15	0.33	0	17,19,21	0.42	0
2	NAG	C	2	2	14,14,15	0.44	0	17,19,21	0.39	0
2	BMA	C	3	2	11,11,12	0.83	0	15,15,17	1.01	1 (6%)
2	MAN	C	4	2	11,11,12	1.55	2 (18%)	15,15,17	1.95	2 (13%)
2	MAN	C	5	2	11,11,12	1.13	1 (9%)	15,15,17	1.60	2 (13%)
3	NAG	D	1	1,3	14,14,15	0.24	0	17,19,21	0.41	0
3	NAG	D	2	3	14,14,15	0.33	0	17,19,21	0.48	0
3	BMA	D	3	3	11,11,12	0.75	0	15,15,17	0.81	0
3	MAN	D	4	3	11,11,12	0.82	0	15,15,17	0.96	1 (6%)

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	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	1/2/19/22	0/1/1/1
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	C	5	2	-	2/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	1/2/19/22	0/1/1/1
3	MAN	D	4	3	-	1/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4	MAN	C2-C3	3.26	1.57	1.52
2	C	4	MAN	O5-C5	3.20	1.49	1.43
2	C	5	MAN	C4-C5	2.85	1.59	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	MAN	C1-O5-C5	6.63	121.08	112.19
2	C	5	MAN	C1-O5-C5	4.24	117.87	112.19
2	C	3	BMA	C1-O5-C5	2.37	115.36	112.19
2	C	5	MAN	O5-C5-C6	-2.30	103.19	107.66
3	D	4	MAN	C1-O5-C5	2.11	115.01	112.19
2	C	4	MAN	O3-C3-C2	2.03	114.19	110.05

There are no chirality outliers.

All (9) torsion outliers are listed below:

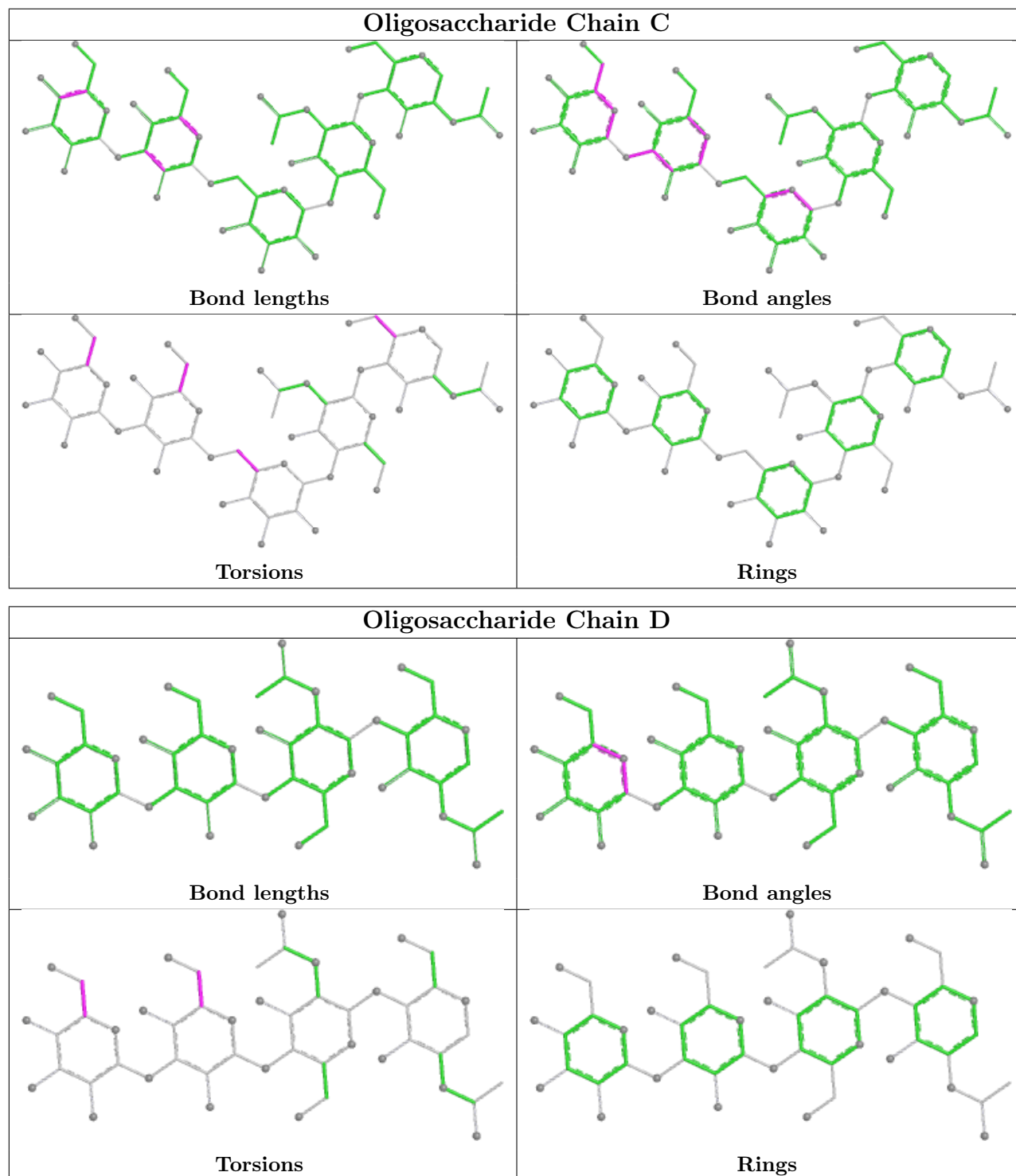
Mol	Chain	Res	Type	Atoms
2	C	5	MAN	O5-C5-C6-O6
2	C	5	MAN	C4-C5-C6-O6
2	C	4	MAN	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
2	C	4	MAN	C4-C5-C6-O6
3	D	4	MAN	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	1	0
3	D	2	NAG	1	0
2	C	2	NAG	1	0

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



5.6 Ligand geometry

17 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$
4	MAN	A	401	1	11,11,12	0.89	0	15,15,17	1.15	2 (13%)
6	GOL	A	410	-	5,5,5	0.38	0	5,5,5	0.31	0
7	SO4	A	413	-	4,4,4	0.24	0	6,6,6	0.07	0
5	NAG	B	406	1	14,14,15	0.21	0	17,19,21	0.42	0
7	SO4	A	414	-	4,4,4	0.23	0	6,6,6	0.07	0
7	SO4	B	411	-	4,4,4	0.23	0	6,6,6	0.07	0
5	NAG	A	409	1	14,14,15	0.19	0	17,19,21	0.41	0
7	SO4	B	412	-	4,4,4	0.23	0	6,6,6	0.12	0
6	GOL	B	408	-	5,5,5	0.37	0	5,5,5	0.32	0
7	SO4	B	410	-	4,4,4	0.23	0	6,6,6	0.08	0
6	GOL	A	411	-	5,5,5	0.37	0	5,5,5	0.31	0
5	NAG	A	407	1	14,14,15	0.32	0	17,19,21	0.52	0
6	GOL	A	412	-	5,5,5	0.36	0	5,5,5	0.36	0
4	MAN	B	401	1	11,11,12	0.91	0	15,15,17	1.26	2 (13%)
5	NAG	A	408	1	14,14,15	0.22	0	17,19,21	0.42	0
5	NAG	B	407	1	14,14,15	0.35	0	17,19,21	0.60	0
7	SO4	B	409	-	4,4,4	0.24	0	6,6,6	0.07	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	A	401	1	-	1/2/19/22	0/1/1/1
6	GOL	A	410	-	-	2/4/4/4	-
5	NAG	B	406	1	-	2/6/23/26	0/1/1/1
5	NAG	A	409	1	-	1/6/23/26	0/1/1/1
6	GOL	B	408	-	-	0/4/4/4	-
6	GOL	A	411	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	407	1	-	1/6/23/26	0/1/1/1
6	GOL	A	412	-	-	2/4/4/4	-
4	MAN	B	401	1	-	1/2/19/22	0/1/1/1
5	NAG	A	408	1	-	2/6/23/26	0/1/1/1
5	NAG	B	407	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	MAN	C1-O5-C5	3.07	116.30	112.19
4	A	401	MAN	C1-O5-C5	2.94	116.12	112.19
4	B	401	MAN	O2-C2-C3	-2.27	105.44	110.15
4	A	401	MAN	O2-C2-C3	-2.18	105.63	110.15

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	410	GOL	O1-C1-C2-C3
6	A	411	GOL	O1-C1-C2-C3
5	A	408	NAG	O5-C5-C6-O6
5	A	408	NAG	C4-C5-C6-O6
6	A	412	GOL	O1-C1-C2-C3
5	B	406	NAG	O5-C5-C6-O6
5	B	406	NAG	C4-C5-C6-O6
5	B	407	NAG	O5-C5-C6-O6
4	B	401	MAN	O5-C5-C6-O6
6	A	410	GOL	O1-C1-C2-O2
6	A	411	GOL	O1-C1-C2-O2
6	A	412	GOL	O1-C1-C2-O2
4	A	401	MAN	O5-C5-C6-O6
5	A	409	NAG	O5-C5-C6-O6
5	B	407	NAG	C3-C2-N2-C7
5	A	407	NAG	O5-C5-C6-O6
5	B	407	NAG	C1-C2-N2-C7
5	B	407	NAG	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	413	SO4	1	0
5	B	406	NAG	1	0
6	A	412	GOL	1	0
5	A	408	NAG	1	0
5	B	407	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

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	310/317 (97%)	0.72	19 (6%) 27 29	38, 60, 89, 129	0
1	B	312/317 (98%)	1.14	44 (14%) 6 7	32, 76, 107, 124	2 (0%)
All	All	622/634 (98%)	0.93	63 (10%) 12 13	32, 67, 98, 129	2 (0%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	25[A]	TRP	7.6
1	B	84	SER	4.6
1	B	194	GLY	4.5
1	B	80	VAL	4.2
1	B	78	THR	3.9
1	A	328	ALA	3.9
1	B	106	THR	3.7
1	B	53	ALA	3.7
1	A	64	PRO	3.6
1	B	20	GLY	3.5
1	B	43[A]	ARG	3.5
1	B	81	VAL	3.4
1	B	331	HIS	3.3
1	B	176	GLY	3.3
1	A	93	GLY	3.1
1	B	180	LEU	3.0
1	B	306	LEU	3.0
1	A	215	LEU	2.9
1	A	329	HIS	2.9
1	B	82	HIS	2.9
1	B	107	LEU	2.8
1	A	193	GLU	2.7
1	B	300	ASP	2.7
1	B	330	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	123	GLY	2.6
1	B	177	HIS	2.6
1	A	201	LEU	2.6
1	B	277	GLY	2.6
1	B	243	VAL	2.5
1	A	330	HIS	2.5
1	A	176	GLY	2.5
1	B	126	GLN	2.5
1	B	222	PRO	2.5
1	B	215	LEU	2.5
1	B	69	TYR	2.4
1	B	72	VAL	2.4
1	B	299	GLU	2.4
1	A	331	HIS	2.4
1	B	280	LEU	2.4
1	A	295	VAL	2.4
1	A	49	GLU	2.3
1	A	116	TYR	2.3
1	B	68	ASN	2.3
1	B	38	VAL	2.3
1	B	103	LEU	2.3
1	B	124	TYR	2.3
1	A	80	VAL	2.3
1	B	138	VAL	2.3
1	A	68	ASN	2.3
1	B	201	LEU	2.3
1	A	83	GLU	2.2
1	B	137	ILE	2.1
1	B	328	ALA	2.1
1	B	67	LYS	2.1
1	A	63	SER	2.1
1	B	165	CYS	2.1
1	A	179	GLY	2.1
1	A	55	VAL	2.1
1	B	97	LEU	2.1
1	B	325	ALA	2.1
1	B	227	GLN	2.0
1	B	181	GLY	2.0
1	B	41	PRO	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](#)

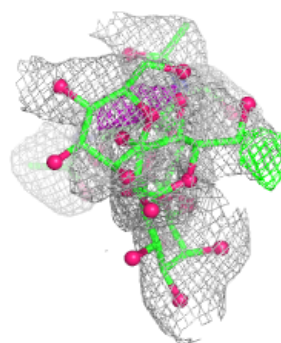
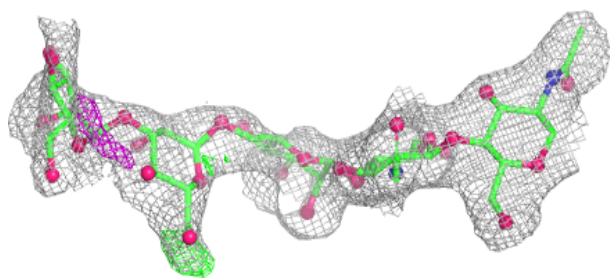
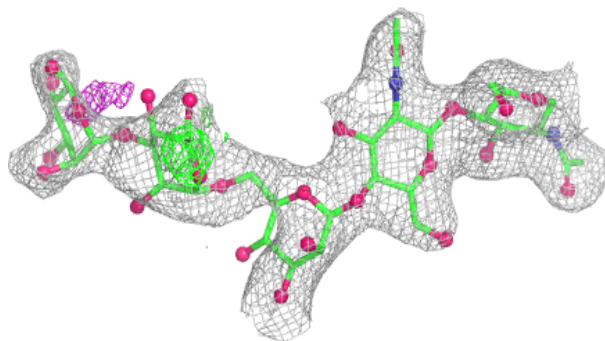
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MAN	C	4	11/12	0.45	0.18	109,116,120,122	0
3	BMA	D	3	11/12	0.49	0.13	103,112,117,121	0
2	MAN	C	5	11/12	0.64	0.15	112,118,123,125	0
3	MAN	D	4	11/12	0.72	0.15	130,132,134,136	0
2	BMA	C	3	11/12	0.73	0.11	97,107,112,113	0
3	NAG	D	2	14/15	0.85	0.13	75,80,87,99	0
3	NAG	D	1	14/15	0.86	0.12	55,64,75,77	0
2	NAG	C	2	14/15	0.86	0.10	56,85,99,104	0
2	NAG	C	1	14/15	0.91	0.11	42,61,71,72	0

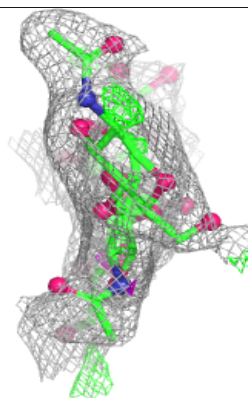
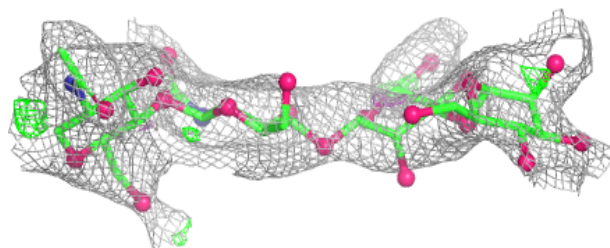
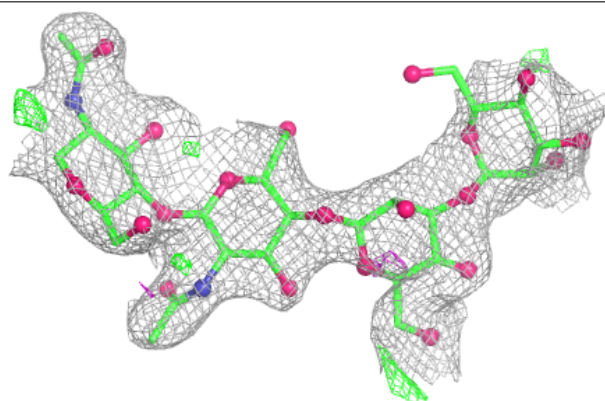
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

**Electron density around Chain D:**

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



6.4 Ligands [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
6	GOL	B	408	6/6	0.69	0.22	95,100,105,108	0
7	SO4	A	413	5/5	0.69	0.11	112,112,114,115	5
7	SO4	B	412	5/5	0.69	0.20	101,109,110,112	5
7	SO4	B	410	5/5	0.75	0.13	88,88,93,97	5
6	GOL	A	411	6/6	0.75	0.17	84,85,88,93	0
4	MAN	B	401	11/12	0.76	0.14	70,87,103,106	0
5	NAG	B	407	14/15	0.77	0.13	75,93,99,102	0
5	NAG	A	409	14/15	0.77	0.13	68,80,88,89	0
7	SO4	B	409	5/5	0.78	0.10	133,134,134,135	0
5	NAG	A	407	14/15	0.79	0.16	59,76,85,86	0
7	SO4	B	411	5/5	0.80	0.14	130,132,133,137	0
7	SO4	A	414	5/5	0.80	0.14	139,142,142,144	0
6	GOL	A	412	6/6	0.84	0.17	74,87,92,94	0
4	MAN	A	401	11/12	0.84	0.12	61,80,89,92	0
6	GOL	A	410	6/6	0.85	0.16	73,79,84,86	0
5	NAG	B	406	14/15	0.86	0.11	58,70,80,81	0
5	NAG	A	408	14/15	0.86	0.11	59,73,79,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.