



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:13 AM UTC

PDB ID : 5LFU / pdb_00005lfu
Title : Myelin-associated glycoprotein (MAG) glycosylated and lysine-methylated full extracellular domain
Authors : Pronker, M.F.; Janssen, B.J.C.
Deposited on : 2016-07-04
Resolution : 4.30 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

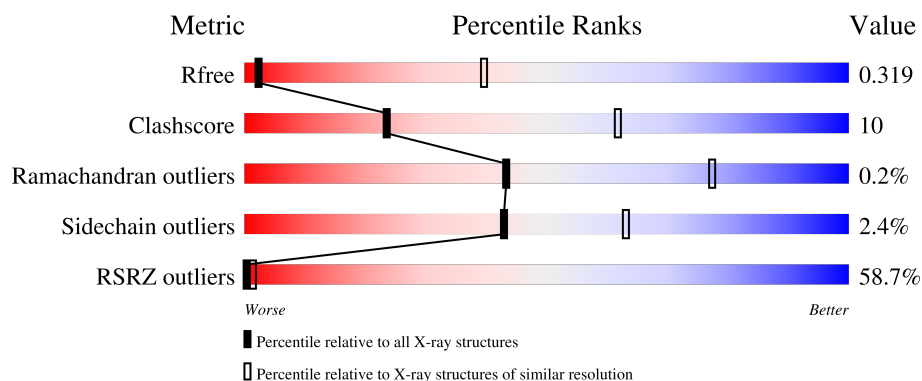
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.30 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	1052 (4.70-3.90)
Clashscore	190562	1097 (4.70-3.90)
Ramachandran outliers	187476	1001 (4.70-3.90)
Sidechain outliers	187428	1007 (4.72-3.88)
RSRZ outliers	180081	1049 (4.70-3.90)

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	500	
2	B	5	
3	C	2	
4	D	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	C	1	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3942 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.

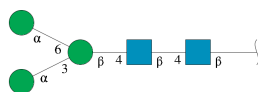
- Molecule 1 is a protein called Myelin-associated glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	487	3776	2397	630	729	20	0	0	0

There are 11 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	509	ALA	-	expression tag	UNP P20917
A	510	ALA	-	expression tag	UNP P20917
A	511	ALA	-	expression tag	UNP P20917
A	512	HIS	-	expression tag	UNP P20917
A	513	HIS	-	expression tag	UNP P20917
A	514	HIS	-	expression tag	UNP P20917
A	515	HIS	-	expression tag	UNP P20917
A	516	HIS	-	expression tag	UNP P20917
A	517	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-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



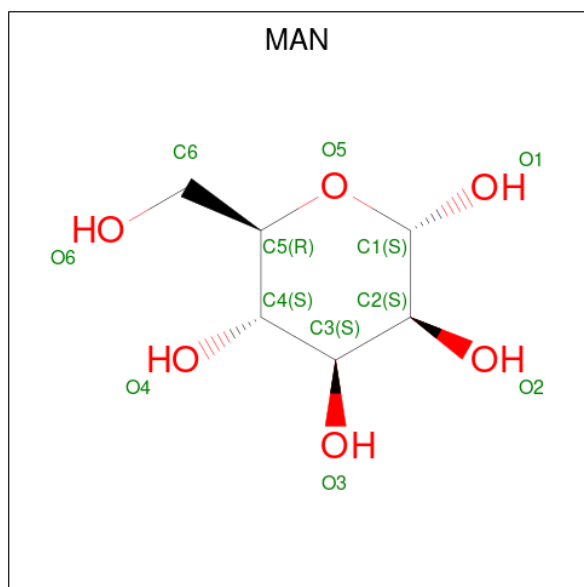
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).



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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

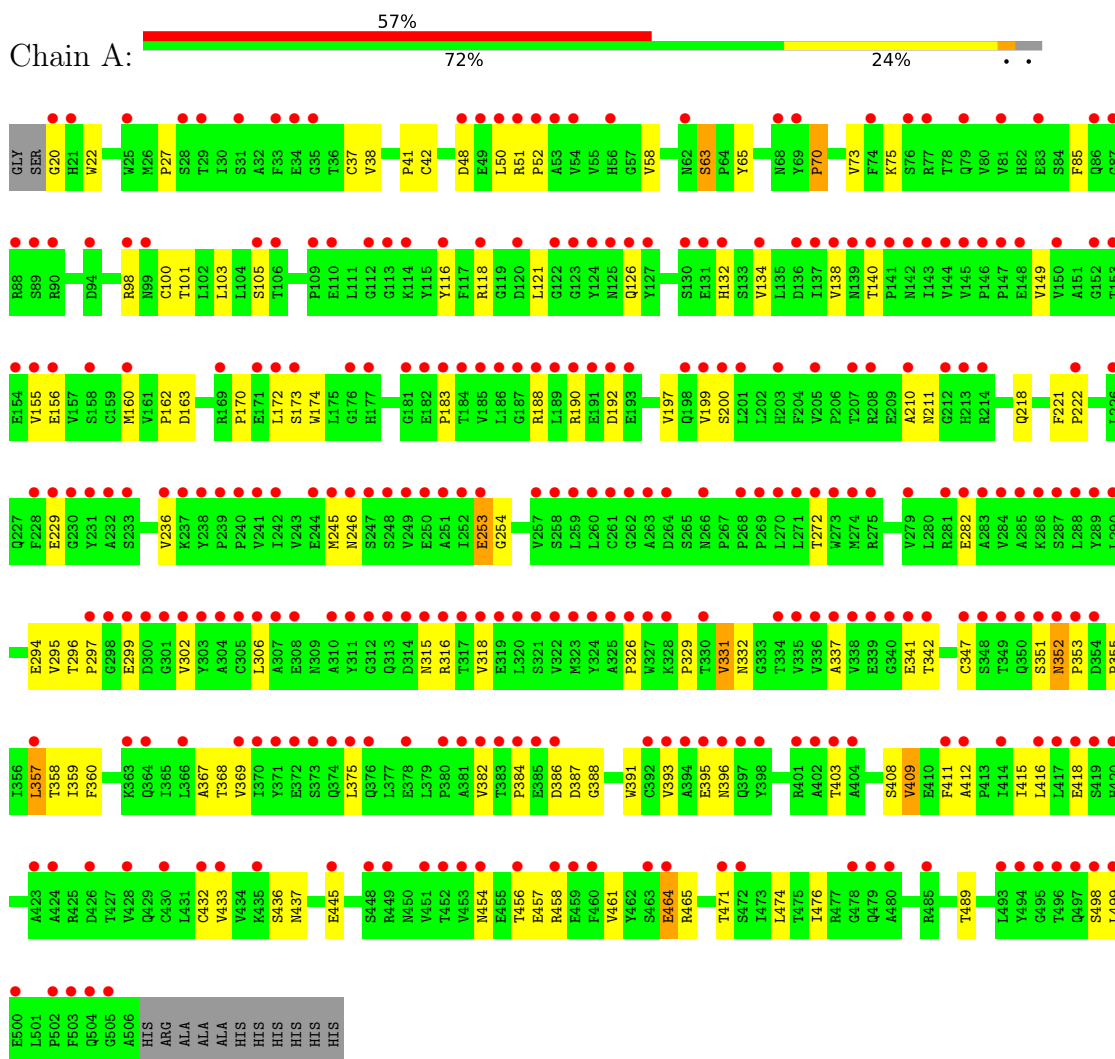


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

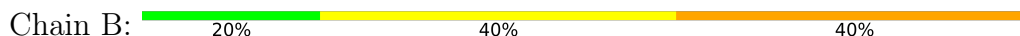
3 Residue-property plots [i](#)

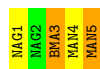
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 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: α -L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  50% 50%



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

Chain D:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	101.24Å 101.24Å 687.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	114.58 – 4.30 114.58 – 4.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (114.58-4.30) 91.0 (114.58-4.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.79 (at 4.30Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.285 , 0.295 0.307 , 0.319	Depositor DCC
R_{free} test set	769 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	240.5	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 579.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3942	wwPDB-VP
Average B, all atoms (Å ²)	420.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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: BMA, FUC, MAN, 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	0.51	0/3872	0.99	15/5297 (0.3%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	437	ASN	CA-C-N	-7.13	113.33	120.31
1	A	437	ASN	C-N-CA	-7.13	113.33	120.31
1	A	51	ARG	CA-C-N	-7.03	112.73	119.76
1	A	51	ARG	C-N-CA	-7.03	112.73	119.76
1	A	70	PRO	CA-C-N	6.00	126.31	119.83
1	A	70	PRO	C-N-CA	6.00	126.31	119.83
1	A	65	TYR	CA-C-N	5.73	125.35	119.56
1	A	65	TYR	C-N-CA	5.73	125.35	119.56
1	A	134	VAL	N-CA-C	5.72	116.34	107.99
1	A	63	SER	CA-C-N	5.38	126.57	119.84
1	A	63	SER	C-N-CA	5.38	126.57	119.84
1	A	192	ASP	CB-CA-C	-5.37	110.37	116.54
1	A	412	ALA	CA-C-N	5.15	126.28	119.84
1	A	412	ALA	C-N-CA	5.15	126.28	119.84
1	A	331	VAL	N-CA-C	5.13	115.30	108.11

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	3776	0	3655	78	1
2	B	61	0	52	1	0
3	C	24	0	22	3	0
4	D	28	0	25	0	0
5	A	11	0	10	1	0
6	A	42	0	39	0	0
All	All	3942	0	3803	79	1

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 10.

All (79) 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:63:SER:HB2	1:A:70:PRO:HB3	1.55	0.86
1:A:382:VAL:HG11	1:A:409:VAL:HG11	1.61	0.80
1:A:20:GLY:N	1:A:48:ASP:OD2	2.17	0.78
1:A:52:PRO:HG2	1:A:121:LEU:HB2	1.67	0.76
1:A:48:ASP:OD1	1:A:98:ARG:NH2	2.19	0.76
1:A:272:THR:HG22	1:A:282:GLU:HG3	1.71	0.73
1:A:436:SER:O	1:A:465:ARG:NH1	2.21	0.72
1:A:27:PRO:HG3	1:A:41:PRO:HG2	1.71	0.72
1:A:149:VAL:HG13	1:A:155:VAL:HG21	1.79	0.63
1:A:387:ASP:OD2	1:A:408:SER:HA	1.99	0.63
1:A:357:LEU:HD11	1:A:375:LEU:HB3	1.81	0.62
1:A:190:ARG:HD3	1:A:190:ARG:H	1.65	0.61
1:A:332:ASN:HB3	3:C:1:NAG:H82	1.83	0.59
1:A:352:ASN:OD1	1:A:352:ASN:N	2.35	0.59
1:A:163:ASP:OD2	1:A:188:ARG:NH2	2.33	0.59
1:A:162:PRO:HA	1:A:197:VAL:HG22	1.86	0.57
1:A:138:VAL:HG22	1:A:140:THR:H	1.70	0.56
1:A:329:PRO:HG2	1:A:403:THR:HB	1.88	0.56
1:A:461:VAL:HG12	1:A:474:LEU:HA	1.88	0.56
1:A:218:GLN:HG3	1:A:229:GLU:HG2	1.88	0.56
1:A:489:THR:HG22	1:A:498:SER:HB3	1.87	0.56
1:A:253:GLU:HA	1:A:295:VAL:HB	1.89	0.55
1:A:331:VAL:HG22	1:A:347:CYS:HA	1.89	0.55
1:A:306:LEU:HD13	1:A:315:ASN:HB3	1.90	0.52
1:A:210:ALA:HB3	1:A:236:VAL:HG11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:SER:HB3	1:A:355:PRO:HG3	1.92	0.52
1:A:369:VAL:HB	1:A:375:LEU:HD13	1.92	0.52
1:A:415:ILE:HD13	1:A:499:LEU:HB3	1.90	0.51
1:A:41:PRO:HA	1:A:101:THR:HG22	1.92	0.51
1:A:42:CYS:H	1:A:101:THR:HG22	1.74	0.51
1:A:174:TRP:CD1	1:A:183:PRO:HB3	2.46	0.51
1:A:116:TYR:CD1	1:A:132:HIS:HB3	2.46	0.50
1:A:245:MET:HE3	1:A:318:VAL:HG13	1.94	0.49
1:A:254:GLY:HA2	1:A:294:GLU:HA	1.94	0.49
1:A:170:PRO:HB3	1:A:221:PHE:CE2	2.48	0.49
1:A:358:THR:HG22	1:A:368:THR:HA	1.95	0.49
1:A:37:CYS:HA	1:A:105:SER:HA	1.95	0.49
1:A:149:VAL:HB	1:A:236:VAL:HA	1.94	0.49
1:A:357:LEU:HG	1:A:369:VAL:HG12	1.95	0.48
1:A:387:ASP:CG	1:A:408:SER:HA	2.38	0.48
1:A:456:THR:OG1	1:A:457:GLU:N	2.46	0.48
1:A:332:ASN:HB3	3:C:1:NAG:N2	2.28	0.48
1:A:387:ASP:OD1	1:A:388:GLY:N	2.47	0.48
1:A:384:PRO:HA	1:A:411:PHE:CE1	2.49	0.47
1:A:416:LEU:HB2	1:A:433:VAL:HG23	1.95	0.47
1:A:326:PRO:HB3	1:A:351:SER:HB2	1.96	0.47
1:A:353:PRO:HG2	1:A:396:ASN:HD21	1.79	0.47
1:A:73:VAL:HG22	1:A:85:PHE:CE2	2.50	0.47
1:A:50:LEU:HD13	1:A:121:LEU:HD13	1.97	0.47
1:A:170:PRO:HB3	1:A:221:PHE:HE2	1.81	0.46
1:A:454:ASN:H	1:A:458:ARG:HD2	1.81	0.46
1:A:353:PRO:HG2	1:A:396:ASN:ND2	2.31	0.46
1:A:433:VAL:HG12	1:A:471:THR:HA	1.96	0.46
1:A:173:SER:HB2	1:A:218:GLN:HB3	1.98	0.45
1:A:464:GLU:OE1	1:A:465:ARG:N	2.49	0.45
1:A:337:ALA:HB1	1:A:341:GLU:OE2	2.16	0.45
1:A:359:ILE:HG12	1:A:367:ALA:HB3	1.98	0.45
1:A:42:CYS:HB3	1:A:100:CYS:C	2.42	0.45
1:A:50:LEU:O	1:A:50:LEU:HD12	2.16	0.45
1:A:393:VAL:HG22	1:A:395:GLU:HG3	1.99	0.44
1:A:22:TRP:N	5:A:601:MAN:O2	2.50	0.43
1:A:245:MET:HB3	1:A:316:ARG:HH11	1.83	0.43
1:A:211:ASN:HB2	1:A:236:VAL:HG12	2.01	0.43
1:A:38:VAL:O	1:A:103:LEU:HA	2.18	0.43
2:B:3:BMA:H61	2:B:5:MAN:H2	1.44	0.43
1:A:297:PRO:HG3	1:A:352:ASN:HD21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ARG:NH1	1:A:126:GLN:HB2	2.34	0.42
1:A:382:VAL:HG13	1:A:386:ASP:HB2	2.01	0.42
1:A:172:LEU:HD13	1:A:200:SER:HB2	2.02	0.42
1:A:296:THR:OG1	1:A:299:GLU:HG2	2.19	0.42
1:A:58:VAL:HG11	1:A:75:LYS:HE2	2.02	0.42
1:A:489:THR:HG22	1:A:498:SER:CB	2.49	0.42
1:A:341:GLU:HG2	1:A:342:THR:H	1.85	0.41
1:A:160:MET:HG2	1:A:199:VAL:HG13	2.01	0.41
1:A:332:ASN:HB3	3:C:1:NAG:C8	2.50	0.41
1:A:454:ASN:N	1:A:458:ARG:HD2	2.36	0.40
1:A:156:GLU:O	1:A:156:GLU:HG3	2.21	0.40
1:A:218:GLN:HG3	1:A:229:GLU:CG	2.51	0.40
1:A:360:PHE:CE1	1:A:391:TRP:HB2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LYS:NZ	1:A:445:GLU:OE2[6_644]	2.08	0.12

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	485/500 (97%)	441 (91%)	43 (9%)	1 (0%)	43 77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	PRO

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	422/431 (98%)	412 (98%)	10 (2%)	43 63

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	246	ASN
1	A	253	GLU
1	A	302	VAL
1	A	352	ASN
1	A	357	LEU
1	A	409	VAL
1	A	418	GLU
1	A	432	CYS
1	A	464	GLU
1	A	476	ILE

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

Mol	Chain	Res	Type
1	A	203	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	B	1	1,2	14,14,15	0.66	1 (7%)	17,19,21	0.70	0
2	NAG	B	2	2	14,14,15	0.36	0	17,19,21	0.54	0
2	BMA	B	3	2	11,11,12	1.49	2 (18%)	15,15,17	1.47	3 (20%)
2	MAN	B	4	2	11,11,12	1.12	1 (9%)	15,15,17	0.97	1 (6%)
2	MAN	B	5	2	11,11,12	1.49	3 (27%)	15,15,17	1.46	1 (6%)
3	NAG	C	1	1,3	14,14,15	2.28	1 (7%)	17,19,21	1.92	1 (5%)
3	FUC	C	2	3	10,10,11	0.25	0	14,14,16	0.64	0
4	NAG	D	1	1,4	14,14,15	0.85	1 (7%)	17,19,21	1.11	2 (11%)
4	NAG	D	2	4	14,14,15	0.94	1 (7%)	17,19,21	0.78	1 (5%)

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	B	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	BMA	B	3	2	-	1/2/19/22	0/1/1/1
2	MAN	B	4	2	-	1/2/19/22	0/1/1/1
2	MAN	B	5	2	-	2/2/19/22	0/1/1/1
3	NAG	C	1	1,3	1/1/5/7	1/6/23/26	0/1/1/1
3	FUC	C	2	3	-	-	0/1/1/1
4	NAG	D	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	NAG	C1-C2	8.46	1.63	1.52
2	B	5	MAN	C2-C3	3.47	1.57	1.52
2	B	3	BMA	C4-C3	2.95	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2	NAG	C1-C2	2.89	1.56	1.52
2	B	3	BMA	C2-C3	2.67	1.56	1.52
4	D	1	NAG	O5-C1	2.57	1.48	1.43
2	B	5	MAN	C1-C2	2.23	1.57	1.52
2	B	1	NAG	O5-C1	-2.22	1.40	1.43
2	B	4	MAN	C4-C5	2.12	1.57	1.53
2	B	5	MAN	O5-C5	2.04	1.47	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	O5-C1-C2	-7.54	99.62	111.29
2	B	5	MAN	C1-O5-C5	4.72	118.51	112.19
2	B	3	BMA	C2-C3-C4	3.25	116.58	110.86
2	B	3	BMA	C3-C4-C5	3.12	115.89	110.23
4	D	1	NAG	O4-C4-C5	2.92	116.51	109.32
4	D	1	NAG	C1-O5-C5	2.77	115.90	112.19
4	D	2	NAG	C1-O5-C5	2.68	115.78	112.19
2	B	3	BMA	C1-C2-C3	2.57	113.39	109.64
2	B	4	MAN	C1-O5-C5	2.49	115.52	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	1	NAG	C1

All (11) torsion outliers are listed below:

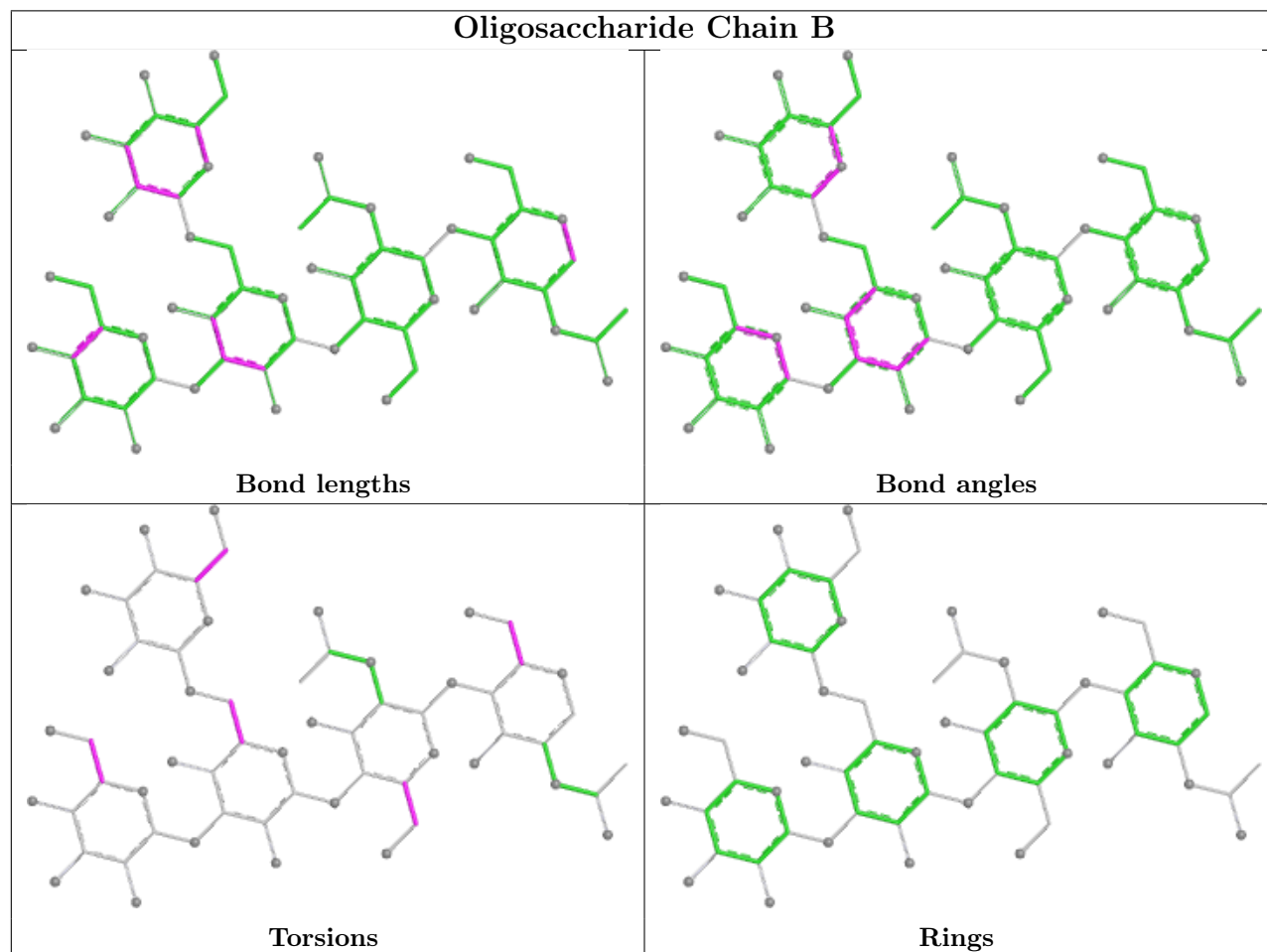
Mol	Chain	Res	Type	Atoms
4	D	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	5	MAN	O5-C5-C6-O6
2	B	5	MAN	C4-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
2	B	4	MAN	O5-C5-C6-O6
4	D	1	NAG	C1-C2-N2-C7
3	C	1	NAG	C8-C7-N2-C2

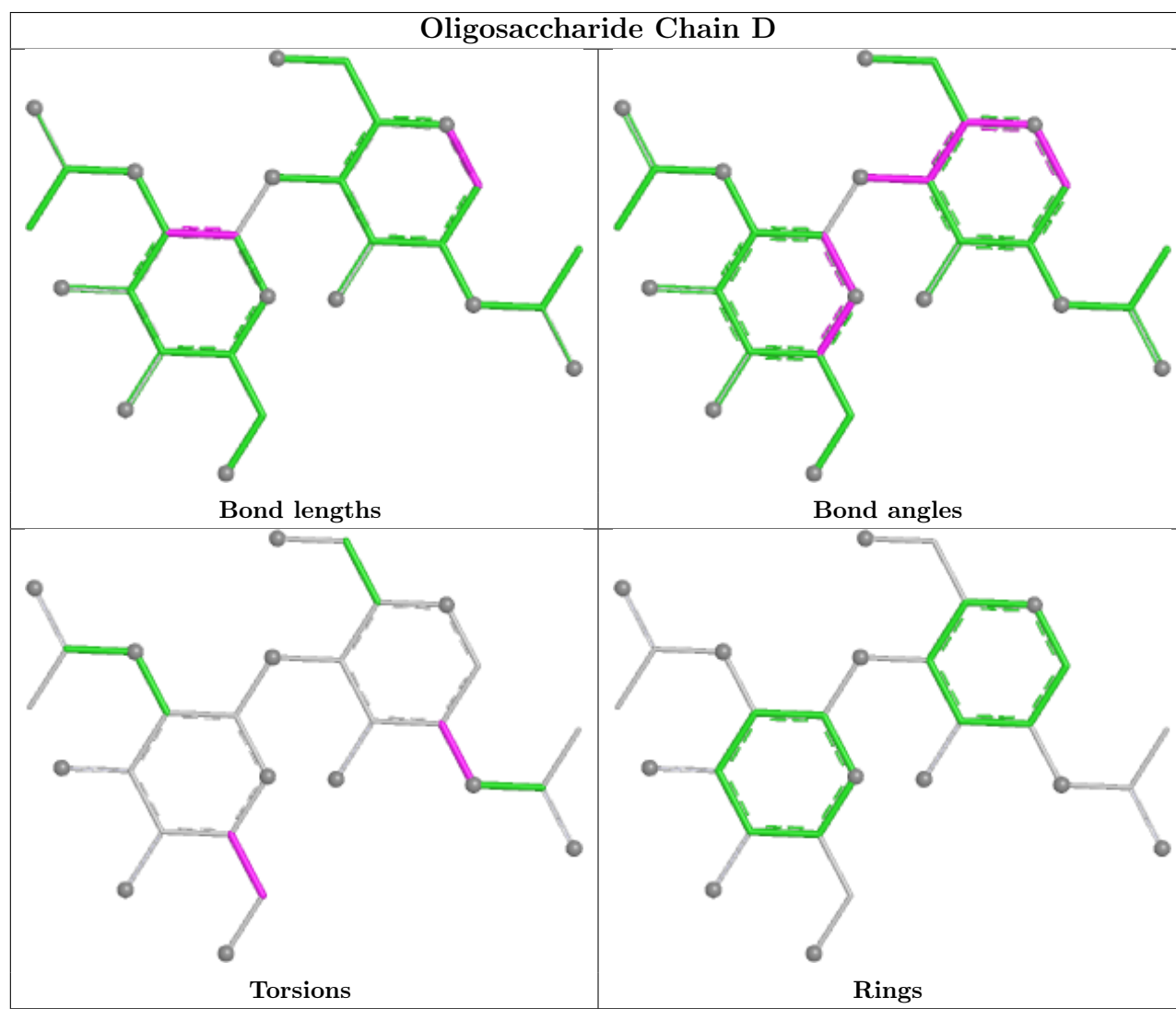
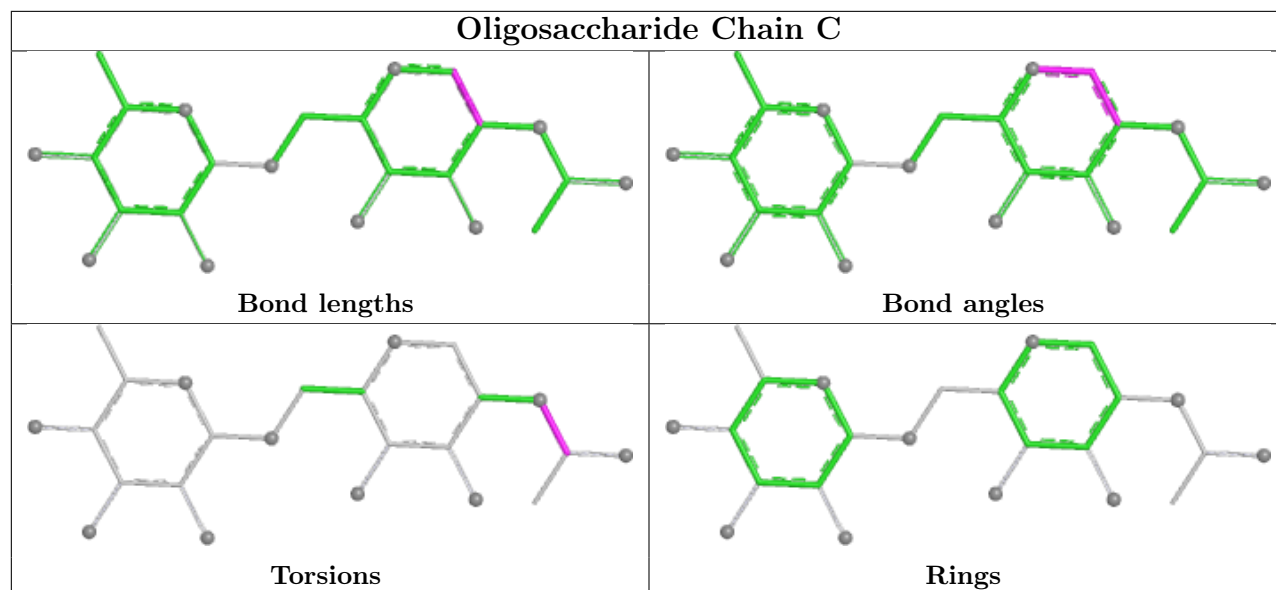
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	3	0
2	B	3	BMA	1	0
2	B	5	MAN	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

4 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$
6	NAG	A	609	1	14,14,15	0.56	0	17,19,21	0.48	0
6	NAG	A	608	1	14,14,15	0.81	1 (7%)	17,19,21	0.68	1 (5%)
6	NAG	A	607	1	14,14,15	0.82	1 (7%)	17,19,21	0.84	1 (5%)
5	MAN	A	601	1	11,11,12	1.63	2 (18%)	15,15,17	1.78	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
6	NAG	A	609	1	-	2/6/23/26	0/1/1/1
6	NAG	A	608	1	-	3/6/23/26	0/1/1/1
6	NAG	A	607	1	-	2/6/23/26	0/1/1/1
5	MAN	A	601	1	-	1/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	MAN	O5-C5	3.92	1.51	1.43
5	A	601	MAN	C4-C5	3.02	1.59	1.53
6	A	607	NAG	C1-C2	2.81	1.56	1.52
6	A	608	NAG	C1-C2	2.30	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	MAN	C1-O5-C5	5.80	119.96	112.19
6	A	607	NAG	C1-O5-C5	2.58	115.65	112.19
6	A	608	NAG	C1-O5-C5	2.25	115.20	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	609	NAG	O5-C5-C6-O6
6	A	609	NAG	C4-C5-C6-O6
6	A	608	NAG	C4-C5-C6-O6
6	A	608	NAG	O5-C5-C6-O6
6	A	607	NAG	C4-C5-C6-O6
6	A	607	NAG	O5-C5-C6-O6
5	A	601	MAN	O5-C5-C6-O6
6	A	608	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	MAN	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	487/500 (97%)	3.15	286 (58%) 0 1	347, 422, 477, 567	0

All (286) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	350	GLN	18.3
1	A	313	GLN	17.9
1	A	305	CYS	15.2
1	A	261	CYS	13.9
1	A	324	TYR	13.6
1	A	323	MET	11.4
1	A	321	SER	10.6
1	A	322	VAL	10.4
1	A	307	ALA	10.1
1	A	325	ALA	10.0
1	A	311	TYR	9.8
1	A	272	THR	9.8
1	A	314	ASP	9.5
1	A	189	LEU	9.3
1	A	308	GLU	9.2
1	A	186	LEU	8.9
1	A	122	GLY	8.8
1	A	287	SER	8.8
1	A	364	GLN	8.7
1	A	160	MET	8.1
1	A	317	THR	8.1
1	A	288	LEU	8.1
1	A	412	ALA	7.9
1	A	273	TRP	7.8
1	A	306	LEU	7.8
1	A	302	VAL	7.7
1	A	301	GLY	7.7

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Mol	Chain	Res	Type	RSRZ
1	A	156	GLU	7.6
1	A	187	GLY	7.6
1	A	62	ASN	7.5
1	A	418	GLU	7.5
1	A	184	THR	7.4
1	A	263	ALA	7.3
1	A	169	ARG	7.3
1	A	53	ALA	7.3
1	A	304	ALA	7.3
1	A	258	SER	7.2
1	A	237	LYS	7.2
1	A	154	GLU	7.1
1	A	352	ASN	7.0
1	A	136	ASP	7.0
1	A	203	HIS	6.9
1	A	300	ASP	6.9
1	A	262	GLY	6.8
1	A	29	THR	6.8
1	A	271	LEU	6.8
1	A	240	PRO	6.7
1	A	401	ARG	6.7
1	A	326	PRO	6.6
1	A	310	ALA	6.6
1	A	417	LEU	6.5
1	A	274	MET	6.4
1	A	140	THR	6.4
1	A	398	TYR	6.3
1	A	339	GLU	6.3
1	A	458	ARG	6.3
1	A	185	VAL	6.2
1	A	199	VAL	6.1
1	A	349	THR	6.0
1	A	496	THR	6.0
1	A	374	GLN	6.0
1	A	312	GLY	6.0
1	A	334	THR	6.0
1	A	342	THR	5.9
1	A	144	VAL	5.8
1	A	134	VAL	5.8
1	A	34	GLU	5.8
1	A	270	LEU	5.7
1	A	201	LEU	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	172	LEU	5.7
1	A	114	LYS	5.6
1	A	158	SER	5.6
1	A	303	TYR	5.6
1	A	250	GLU	5.6
1	A	112	GLY	5.5
1	A	86	GLN	5.5
1	A	269	PRO	5.4
1	A	493	LEU	5.4
1	A	383	THR	5.4
1	A	241	VAL	5.3
1	A	340	GLY	5.3
1	A	109	PRO	5.3
1	A	380	PRO	5.3
1	A	315	ASN	5.2
1	A	378	GLU	5.1
1	A	381	ALA	5.1
1	A	54	VAL	5.1
1	A	260	LEU	5.1
1	A	327	TRP	5.0
1	A	341	GLU	4.9
1	A	297	PRO	4.9
1	A	394	ALA	4.8
1	A	242	ILE	4.8
1	A	205	VAL	4.8
1	A	348	SER	4.8
1	A	318	VAL	4.8
1	A	376	GLN	4.7
1	A	497	GLN	4.7
1	A	190	ARG	4.7
1	A	363	LYS	4.7
1	A	173	SER	4.7
1	A	432	CYS	4.7
1	A	373	SER	4.7
1	A	251	ALA	4.7
1	A	123	GLY	4.6
1	A	419	SER	4.6
1	A	25	TRP	4.6
1	A	285	ALA	4.6
1	A	28	SER	4.6
1	A	351	SER	4.5
1	A	147	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	113	GLY	4.5
1	A	286	LYS	4.5
1	A	384	PRO	4.4
1	A	56	HIS	4.4
1	A	338	VAL	4.4
1	A	485	ARG	4.4
1	A	266	ASN	4.2
1	A	423	ALA	4.2
1	A	132	HIS	4.2
1	A	456	THR	4.2
1	A	478	GLY	4.2
1	A	500	GLU	4.1
1	A	494	TYR	4.1
1	A	192	ASP	4.1
1	A	385	GLU	4.1
1	A	76	SER	4.0
1	A	50	LEU	4.0
1	A	68	ASN	4.0
1	A	198	GLN	4.0
1	A	502	PRO	4.0
1	A	48	ASP	4.0
1	A	448	SER	4.0
1	A	424	ALA	4.0
1	A	289	TYR	4.0
1	A	471	THR	3.9
1	A	126	GLN	3.9
1	A	150	VAL	3.9
1	A	83	GLU	3.9
1	A	290	LEU	3.9
1	A	183	PRO	3.9
1	A	420	HIS	3.8
1	A	319	GLU	3.8
1	A	416	LEU	3.8
1	A	275	ARG	3.7
1	A	414	ILE	3.7
1	A	20	GLY	3.7
1	A	52	PRO	3.7
1	A	49	GLU	3.6
1	A	231	TYR	3.6
1	A	146	PRO	3.6
1	A	433	VAL	3.6
1	A	449	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	247	SER	3.5
1	A	98	ARG	3.5
1	A	106	THR	3.5
1	A	495	GLY	3.5
1	A	228	PHE	3.5
1	A	124	TYR	3.5
1	A	152	GLY	3.5
1	A	403	THR	3.5
1	A	245	MET	3.4
1	A	264	ASP	3.4
1	A	299	GLU	3.4
1	A	200	SER	3.4
1	A	87	GLY	3.4
1	A	411	PHE	3.3
1	A	282	GLU	3.3
1	A	354	ASP	3.3
1	A	397	GLN	3.3
1	A	139	ASN	3.3
1	A	232	ALA	3.2
1	A	143	ILE	3.2
1	A	253	GLU	3.2
1	A	279	VAL	3.2
1	A	404	ALA	3.2
1	A	213	HIS	3.2
1	A	89	SER	3.2
1	A	426	ASP	3.2
1	A	176	GLY	3.1
1	A	148	GLU	3.1
1	A	249	VAL	3.1
1	A	51	ARG	3.1
1	A	90	ARG	3.1
1	A	130	SER	3.1
1	A	504	GLN	3.1
1	A	370	ILE	3.1
1	A	238	TYR	3.0
1	A	207	THR	3.0
1	A	463	SER	3.0
1	A	451	VAL	3.0
1	A	337	ALA	3.0
1	A	252	ILE	3.0
1	A	375	LEU	3.0
1	A	330	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	171	GLU	3.0
1	A	283	ALA	3.0
1	A	153	THR	3.0
1	A	472	SER	2.9
1	A	233	SER	2.9
1	A	88	ARG	2.9
1	A	77	ARG	2.9
1	A	320	LEU	2.9
1	A	35	GLY	2.9
1	A	182	GLU	2.9
1	A	372	GLU	2.9
1	A	127	TYR	2.9
1	A	116	TYR	2.8
1	A	145	VAL	2.8
1	A	316	ARG	2.8
1	A	268	PRO	2.8
1	A	459	GLU	2.8
1	A	246	ASN	2.8
1	A	193	GLU	2.8
1	A	386	ASP	2.8
1	A	505	GLY	2.8
1	A	142	ASN	2.8
1	A	503	PHE	2.8
1	A	236	VAL	2.8
1	A	138	VAL	2.8
1	A	79	GLN	2.8
1	A	212	GLY	2.7
1	A	298	GLY	2.7
1	A	137	ILE	2.7
1	A	336	VAL	2.7
1	A	328	LYS	2.7
1	A	454	ASN	2.7
1	A	244	GLU	2.7
1	A	125	ASN	2.7
1	A	453	VAL	2.7
1	A	259	LEU	2.7
1	A	357	LEU	2.7
1	A	460	PHE	2.6
1	A	188	ARG	2.6
1	A	191	GLU	2.6
1	A	452	THR	2.6
1	A	131	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	21	HIS	2.5
1	A	181	GLY	2.5
1	A	94	ASP	2.5
1	A	369	VAL	2.5
1	A	402	ALA	2.5
1	A	395	GLU	2.5
1	A	464	GLU	2.5
1	A	208	ARG	2.4
1	A	239	PRO	2.4
1	A	335	VAL	2.4
1	A	33	PHE	2.4
1	A	81	VAL	2.4
1	A	284	VAL	2.4
1	A	120	ASP	2.4
1	A	382	VAL	2.4
1	A	105	SER	2.4
1	A	480	ALA	2.4
1	A	396	ASN	2.4
1	A	366	LEU	2.4
1	A	248	SER	2.4
1	A	392	CYS	2.4
1	A	141	PRO	2.3
1	A	347	CYS	2.3
1	A	428	VAL	2.3
1	A	498	SER	2.3
1	A	222	PRO	2.3
1	A	229	GLU	2.3
1	A	445	GLU	2.3
1	A	99	ASN	2.3
1	A	257	VAL	2.2
1	A	479	GLN	2.2
1	A	430	CYS	2.2
1	A	226	LEU	2.2
1	A	210	ALA	2.2
1	A	31	SER	2.2
1	A	155	VAL	2.2
1	A	214	ARG	2.2
1	A	69	TYR	2.1
1	A	110	GLU	2.1
1	A	435	LYS	2.1
1	A	118	ARG	2.1
1	A	371	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	74	PHE	2.1
1	A	230	GLY	2.1
1	A	353	PRO	2.1
1	A	281	ARG	2.1
1	A	499	LEU	2.0
1	A	177	HIS	2.0
1	A	393	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](#)

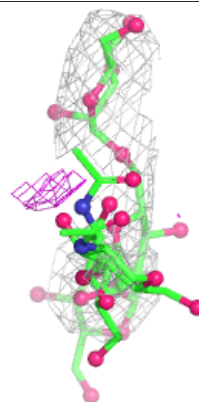
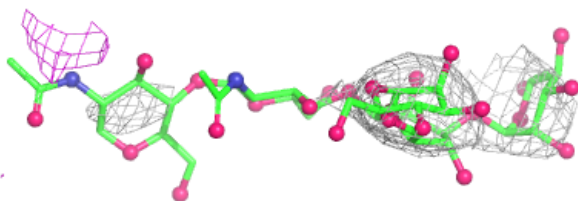
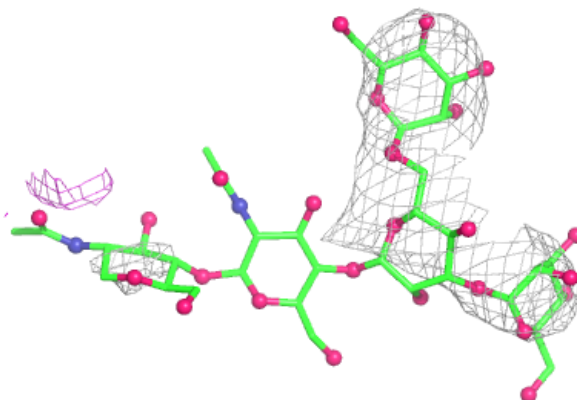
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	C	1	14/15	0.42	0.16	381,401,401,401	0
2	MAN	B	4	11/12	0.50	0.20	402,402,402,402	0
3	FUC	C	2	10/11	0.50	0.15	404,404,404,404	0
4	NAG	D	2	14/15	0.75	0.21	381,381,381,381	0
2	MAN	B	5	11/12	0.79	0.26	350,350,350,350	0
2	BMA	B	3	11/12	0.90	0.15	302,400,400,400	0
4	NAG	D	1	14/15	0.93	0.22	344,377,377,377	0
2	NAG	B	2	14/15	0.93	0.24	296,360,390,420	0
2	NAG	B	1	14/15	0.97	0.26	275,341,386,392	0

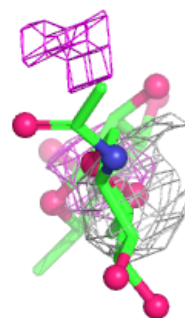
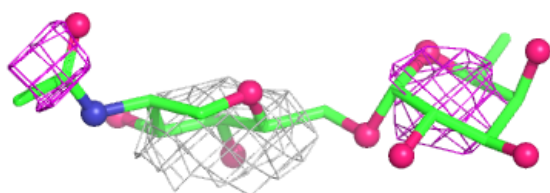
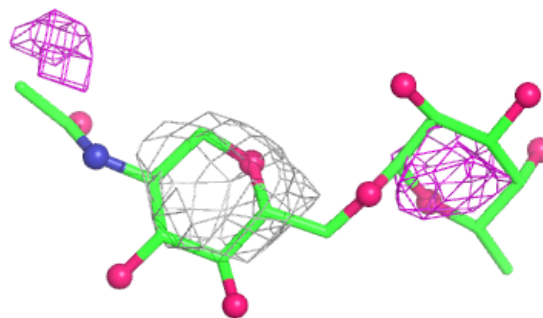
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

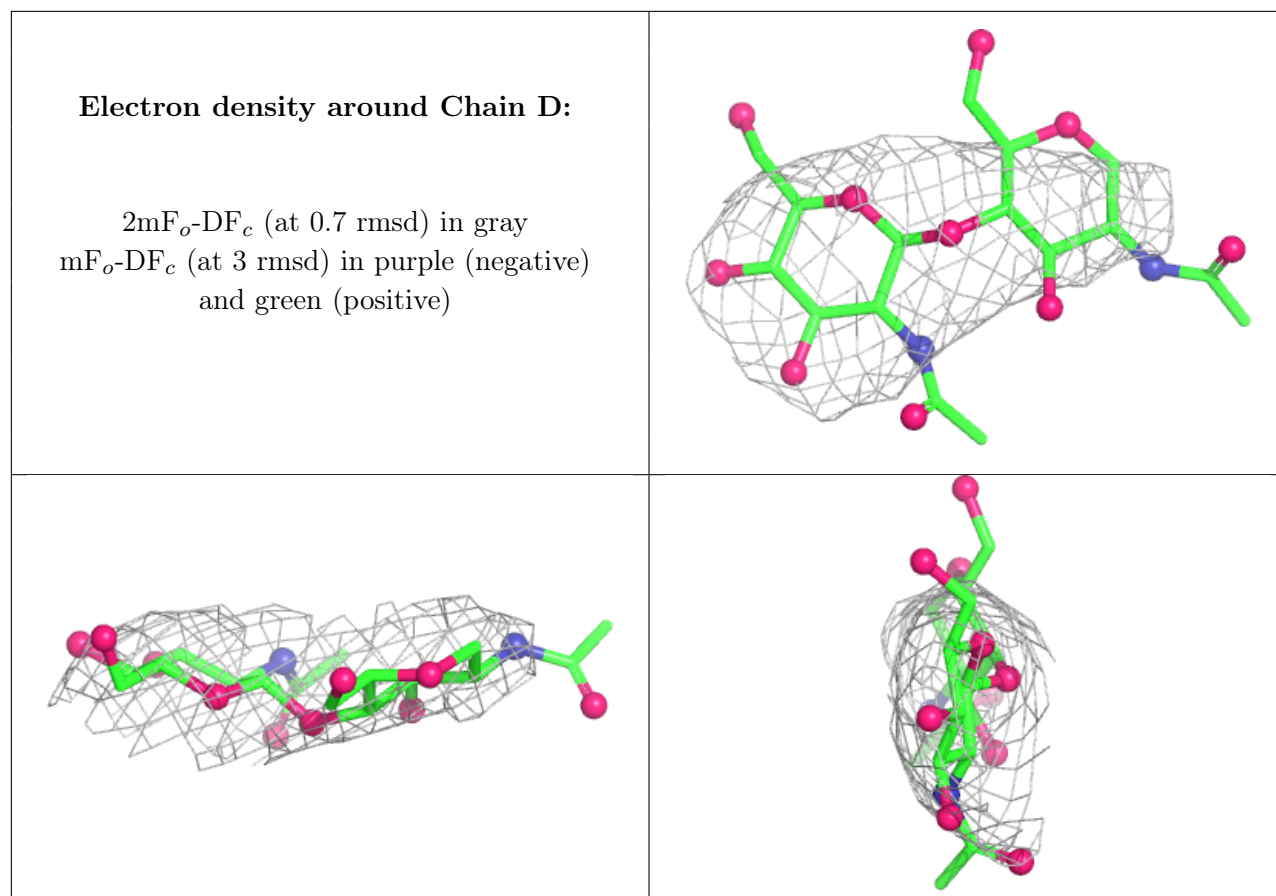
Electron density around Chain B:

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

**Electron density around Chain C:**

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





6.4 Ligands [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	NAG	A	608	14/15	0.34	0.27	363,399,399,399	0
6	NAG	A	607	14/15	0.36	0.19	413,413,413,413	0
5	MAN	A	601	11/12	0.58	0.15	366,373,385,386	0
6	NAG	A	609	14/15	0.71	0.19	306,361,361,361	0

6.5 Other polymers [i](#)

There are no such residues in this entry.