



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:30 PM UTC

PDB ID : 5LF5 / pdb_00005lf5
Title : Myelin-associated glycoprotein (MAG) deglycosylated full extracellular domain with co-purified ligand
Authors : Pronker, M.F.; Janssen, B.J.C.
Deposited on : 2016-06-30
Resolution : 3.80 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

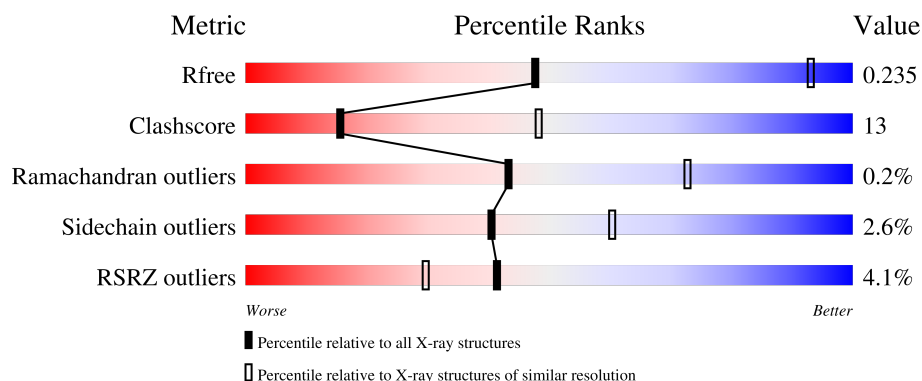
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	4% 68% 25% ••
2	B	2	50% 50%
3	C	3	100%

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
2	NAG	B	1	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3887 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	484	3750	2382	623	725	20	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

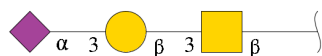
Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLY	-	expression tag	UNP P20917
A	19	SER	-	expression tag	UNP P20917
A	509	ALA	-	expression tag	UNP P20917
A	510	ALA	-	expression tag	UNP P20917
A	511	ALA	-	expression tag	UNP P20917
A	512	HIS	-	expression tag	UNP P20917
A	513	HIS	-	expression tag	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-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



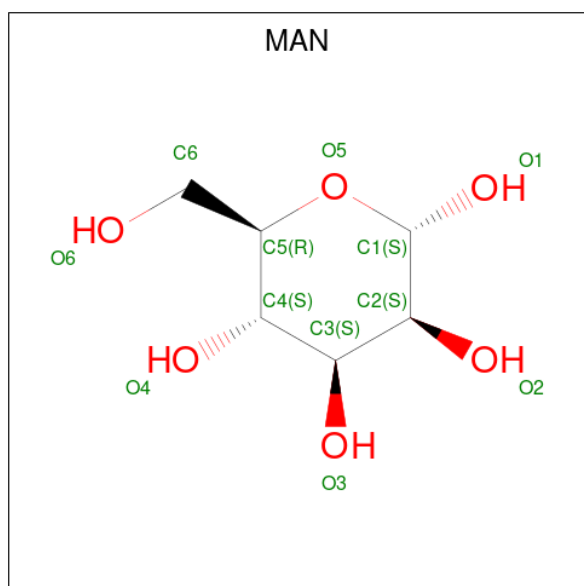
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	2	24	14	1	9	0	0	0

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			46	25	2	19			

- 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		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

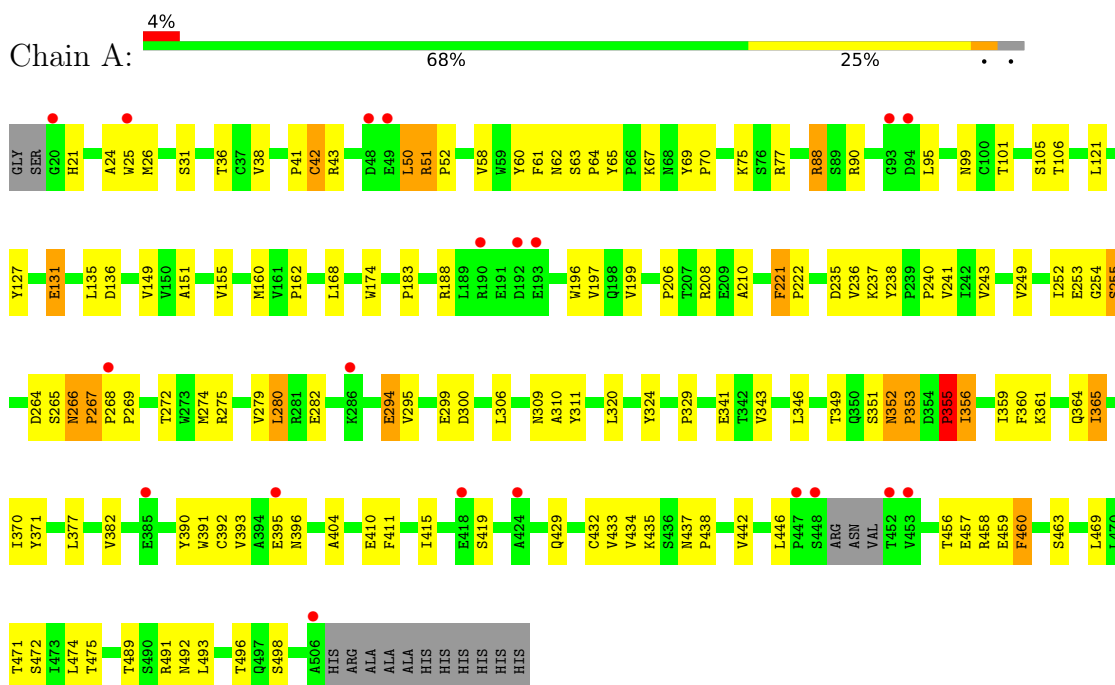


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

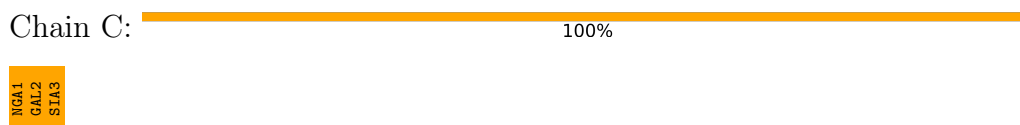
• Molecule 1: Myelin-associated glycoprotein



• Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	278.87Å 278.87Å 62.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	52.70 – 3.80 52.70 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (52.70-3.80) 92.7 (52.70-3.80)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.67 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.199 , 0.228 0.213 , 0.235	Depositor DCC
R_{free} test set	1767 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	95.0	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 101.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.059 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3887	wwPDB-VP
Average B, all atoms (Å ²)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NGA, GAL, SIA, FUC, NAG, MAN

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	0.42	1/3845 (0.0%)	0.98	17/5259 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	268	PRO	CA-C	5.63	1.57	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	PRO	CA-C-N	-11.60	108.01	120.66
1	A	268	PRO	C-N-CA	-11.60	108.01	120.66
1	A	266	ASN	CA-C-N	-10.64	109.42	120.38
1	A	266	ASN	C-N-CA	-10.64	109.42	120.38
1	A	279	VAL	N-CA-C	10.56	120.46	110.53
1	A	267	PRO	CA-C-N	-8.54	111.58	120.38
1	A	267	PRO	C-N-CA	-8.54	111.58	120.38
1	A	221	PHE	CA-C-N	6.62	128.12	119.84
1	A	221	PHE	C-N-CA	6.62	128.12	119.84
1	A	294	GLU	CA-C-N	6.00	128.62	120.63
1	A	294	GLU	C-N-CA	6.00	128.62	120.63
1	A	280	LEU	CB-CA-C	-5.88	109.24	117.23
1	A	355	PRO	CA-N-CD	-5.34	104.52	112.00
1	A	255	SER	N-CA-C	-5.20	103.17	110.35
1	A	51	ARG	CA-C-N	-5.09	114.56	119.90
1	A	51	ARG	C-N-CA	-5.09	114.56	119.90
1	A	353	PRO	N-CA-C	-5.03	102.11	112.47

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	3750	0	3628	100	0
2	B	24	0	22	0	0
3	C	46	0	40	5	0
4	A	11	0	10	1	0
5	A	56	0	52	0	0
All	All	3887	0	3752	102	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 13.

All (102) 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:267:PRO:CG	1:A:309:ASN:HD21	1.73	1.01
1:A:267:PRO:HG2	1:A:309:ASN:ND2	1.82	0.95
1:A:253:GLU:HB3	1:A:324:TYR:HD2	1.33	0.93
1:A:253:GLU:HB3	1:A:324:TYR:CD2	2.11	0.85
1:A:267:PRO:HG2	1:A:309:ASN:HD21	1.39	0.84
1:A:267:PRO:HG3	1:A:309:ASN:HD21	1.40	0.82
1:A:67:LYS:HB2	3:C:2:GAL:H61	1.69	0.74
1:A:63:SER:HB2	1:A:70:PRO:HB3	1.72	0.70
1:A:267:PRO:CG	1:A:309:ASN:ND2	2.45	0.70
1:A:456:THR:HB	1:A:458:ARG:HB2	1.73	0.69
1:A:346:LEU:HD12	1:A:346:LEU:C	2.17	0.69
3:C:1:NGA:N2	3:C:2:GAL:O2	2.26	0.68
1:A:254:GLY:HA2	1:A:294:GLU:HA	1.75	0.68
1:A:31:SER:HB3	1:A:136:ASP:HB3	1.75	0.67
1:A:309:ASN:OD1	1:A:310:ALA:N	2.31	0.62
1:A:50:LEU:HB2	1:A:52:PRO:HD3	1.83	0.61
1:A:238:TYR:CE1	1:A:266:ASN:HB2	2.35	0.61
1:A:346:LEU:HD12	1:A:346:LEU:O	2.00	0.60
1:A:274:MET:HA	1:A:280:LEU:HD13	1.82	0.60
1:A:433:VAL:HG12	1:A:471:THR:HA	1.83	0.60
1:A:131:GLU:N	1:A:131:GLU:OE2	2.36	0.59
1:A:41:PRO:HA	1:A:101:THR:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:LYS:HB3	1:A:390:TYR:CE1	2.40	0.57
1:A:38:VAL:HG11	1:A:135:LEU:HD11	1.87	0.56
1:A:351:SER:OG	1:A:353:PRO:O	2.20	0.56
1:A:249:VAL:HG23	1:A:320:LEU:HA	1.87	0.56
1:A:253:GLU:HG3	1:A:295:VAL:O	2.06	0.55
1:A:265:SER:OG	1:A:269:PRO:HB3	2.05	0.55
1:A:491:ARG:HG2	1:A:496:THR:HB	1.86	0.55
1:A:272:THR:HG22	1:A:282:GLU:HG3	1.87	0.55
1:A:149:VAL:O	1:A:236:VAL:HG23	2.06	0.54
1:A:65:TYR:OH	3:C:3:SIA:O9	2.24	0.54
1:A:208:ARG:HG2	1:A:238:TYR:HB2	1.90	0.54
1:A:352:ASN:HB2	1:A:353:PRO:HD3	1.91	0.53
1:A:95:LEU:H	1:A:95:LEU:HD12	1.74	0.53
3:C:2:GAL:H4	3:C:3:SIA:C1	2.39	0.53
1:A:356:ILE:HG13	1:A:370:ILE:HA	1.91	0.53
1:A:160:MET:HG2	1:A:199:VAL:HG22	1.91	0.53
1:A:42:CYS:H	1:A:101:THR:HG22	1.74	0.52
1:A:355:PRO:HB3	1:A:396:ASN:HD22	1.74	0.52
1:A:429:GLN:HB2	1:A:475:THR:HG22	1.92	0.51
1:A:415:ILE:HA	1:A:434:VAL:HG12	1.92	0.51
1:A:359:ILE:HD11	1:A:377:LEU:HB2	1.92	0.50
1:A:411:PHE:O	1:A:492:ASN:ND2	2.45	0.50
1:A:58:VAL:HG11	1:A:75:LYS:HE2	1.94	0.50
1:A:88:ARG:HD2	1:A:106:THR:O	2.11	0.49
1:A:456:THR:HA	1:A:457:GLU:C	2.36	0.49
1:A:370:ILE:HG22	1:A:371:TYR:CD2	2.48	0.49
1:A:235:ASP:O	1:A:237:LYS:NZ	2.35	0.49
1:A:360:PHE:HB2	1:A:365:ILE:HA	1.95	0.48
1:A:149:VAL:HG13	1:A:155:VAL:HG11	1.94	0.48
1:A:52:PRO:HG2	1:A:121:LEU:HD13	1.97	0.47
1:A:458:ARG:O	1:A:460:PHE:HD1	1.97	0.47
1:A:309:ASN:C	1:A:311:TYR:H	2.23	0.47
1:A:442:VAL:HG21	1:A:472:SER:OG	2.15	0.47
1:A:162:PRO:HA	1:A:197:VAL:HG22	1.97	0.47
1:A:459:GLU:HB2	1:A:474:LEU:HD11	1.97	0.47
1:A:24:ALA:O	1:A:131:GLU:HG3	2.16	0.46
1:A:64:PRO:HG2	1:A:65:TYR:CD1	2.50	0.46
1:A:393:VAL:HG22	1:A:395:GLU:HG3	1.97	0.46
1:A:460:PHE:CD1	1:A:460:PHE:N	2.83	0.46
1:A:346:LEU:C	1:A:346:LEU:CD1	2.86	0.46
1:A:42:CYS:SG	1:A:43:ARG:N	2.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ASN:OD1	1:A:101:THR:HG23	2.17	0.45
1:A:299:GLU:HA	1:A:299:GLU:OE1	2.17	0.45
1:A:36:THR:HG22	1:A:168:LEU:HD12	1.98	0.45
1:A:391:TRP:CZ3	1:A:404:ALA:HB2	2.52	0.45
1:A:127:TYR:CE1	3:C:3:SIA:H91	2.52	0.45
1:A:240:PRO:HA	1:A:264:ASP:O	2.17	0.44
1:A:51:ARG:N	1:A:52:PRO:HD3	2.33	0.44
1:A:275:ARG:NH1	1:A:300:ASP:O	2.51	0.44
1:A:410:GLU:HA	1:A:437:ASN:HB3	1.99	0.44
1:A:151:ALA:HA	1:A:206:PRO:HG2	2.00	0.43
1:A:272:THR:OG1	1:A:306:LEU:HB3	2.18	0.43
1:A:364:GLN:HG2	1:A:365:ILE:N	2.33	0.43
1:A:210:ALA:HB3	1:A:236:VAL:HG11	1.99	0.43
1:A:241:VAL:O	1:A:243:VAL:HG23	2.19	0.43
1:A:435:LYS:HB3	1:A:469:LEU:HD23	2.00	0.43
1:A:21:HIS:HB3	4:A:601:MAN:O3	2.19	0.42
1:A:61:PHE:CD1	1:A:62:ASN:HB2	2.55	0.42
1:A:174:TRP:CD1	1:A:183:PRO:HB3	2.54	0.42
1:A:25:TRP:HD1	1:A:26:MET:N	2.18	0.42
1:A:64:PRO:HG2	1:A:65:TYR:HD1	1.84	0.42
1:A:252:ILE:HB	1:A:255:SER:OG	2.20	0.42
1:A:343:VAL:HG23	1:A:382:VAL:HG21	2.02	0.42
1:A:88:ARG:HG3	1:A:105:SER:O	2.19	0.42
1:A:221:PHE:HA	1:A:222:PRO:HD3	1.93	0.42
1:A:341:GLU:O	1:A:382:VAL:HG23	2.20	0.41
1:A:160:MET:HB3	1:A:197:VAL:HG11	2.02	0.41
1:A:50:LEU:C	1:A:52:PRO:HD3	2.46	0.41
1:A:419:SER:CB	1:A:432:CYS:HA	2.49	0.41
1:A:60:TYR:CG	1:A:70:PRO:HG2	2.55	0.41
1:A:309:ASN:C	1:A:311:TYR:N	2.79	0.41
1:A:329:PRO:HA	1:A:349:THR:OG1	2.21	0.41
1:A:493:LEU:H	1:A:493:LEU:HD12	1.86	0.41
1:A:188:ARG:HD3	1:A:196:TRP:CE3	2.56	0.41
1:A:25:TRP:CD1	1:A:25:TRP:C	2.99	0.41
1:A:489:THR:HG22	1:A:498:SER:CB	2.51	0.40
1:A:463:SER:HB3	1:A:472:SER:HB3	2.02	0.40
1:A:69:TYR:HA	1:A:70:PRO:HD3	1.91	0.40
1:A:437:ASN:HB3	1:A:438:PRO:HD3	2.04	0.40
1:A:359:ILE:HG22	1:A:392:CYS:HA	2.02	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	480/500 (96%)	447 (93%)	32 (7%)	1 (0%)	43 73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	355	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	419/431 (97%)	408 (97%)	11 (3%)	40 60

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	CYS
1	A	50	LEU
1	A	77	ARG
1	A	88	ARG
1	A	90	ARG
1	A	131	GLU
1	A	352	ASN
1	A	356	ILE
1	A	365	ILE
1	A	446	LEU

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Mol	Chain	Res	Type
1	A	460	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	211	ASN
1	A	429	GLN
1	A	437	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

5 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	2,1	14,14,15	2.47	1 (7%)	17,19,21	2.47	7 (41%)
2	FUC	B	2	2	10,10,11	0.44	0	14,14,16	0.81	0
3	NGA	C	1	3	15,15,15	0.61	0	21,21,21	1.38	4 (19%)
3	GAL	C	2	3	11,11,12	1.10	2 (18%)	15,15,17	1.13	1 (6%)
3	SIA	C	3	3	20,20,21	1.56	2 (10%)	21,28,31	2.20	7 (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
2	NAG	B	1	2,1	1/1/5/7	5/6/23/26	0/1/1/1
2	FUC	B	2	2	-	-	0/1/1/1
3	NGA	C	1	3	-	4/6/26/26	0/1/1/1
3	GAL	C	2	3	-	1/2/19/22	0/1/1/1
3	SIA	C	3	3	-	4/18/34/38	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	C1-C2	9.05	1.64	1.52
3	C	3	SIA	C2-C1	4.96	1.58	1.52
3	C	2	GAL	O2-C2	-2.14	1.38	1.43
3	C	2	GAL	O3-C3	2.10	1.48	1.43
3	C	3	SIA	O6-C2	2.06	1.47	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	O5-C1-C2	-7.04	100.39	111.29
3	C	3	SIA	C4-C5-N5	5.96	122.17	110.44
2	B	1	NAG	C4-C3-C2	-4.26	104.78	111.02
3	C	3	SIA	O1A-C1-C2	-4.20	113.78	122.85
2	B	1	NAG	O5-C5-C6	3.24	113.96	107.66
3	C	3	SIA	O1B-C1-O1A	3.00	130.88	124.08
2	B	1	NAG	C6-C5-C4	-2.77	106.23	113.02
2	B	1	NAG	C2-N2-C7	-2.73	119.24	122.90
3	C	3	SIA	O10-C10-N5	2.69	126.74	121.98
3	C	1	NGA	O5-C1-C2	2.69	112.22	109.52
3	C	3	SIA	C11-C10-N5	-2.44	112.07	116.12
3	C	1	NGA	O3-C3-C2	2.37	114.31	109.58
3	C	2	GAL	O3-C3-C2	2.34	114.83	110.05
3	C	1	NGA	C1-C2-C3	-2.33	107.37	110.54
3	C	3	SIA	O7-C7-C8	2.21	113.96	108.93
3	C	1	NGA	O7-C7-C8	-2.15	118.23	122.05
2	B	1	NAG	C1-O5-C5	2.08	114.97	112.19
2	B	1	NAG	C3-C4-C5	-2.02	106.57	110.23
3	C	3	SIA	O4-C4-C3	2.01	114.86	109.86

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1	NAG	C1

All (14) torsion outliers are listed below:

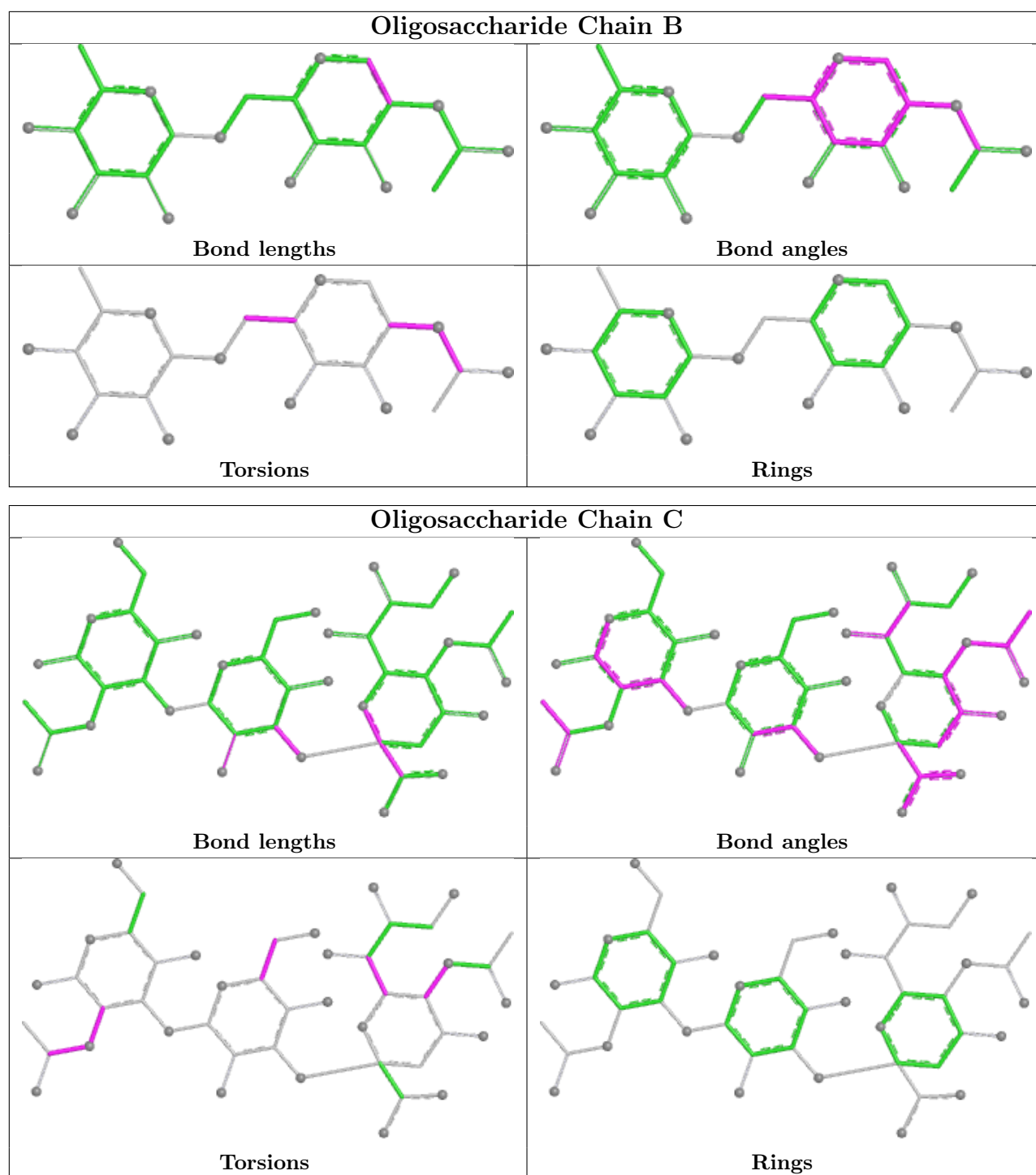
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C1-C2-N2-C7
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
3	C	1	NGA	O7-C7-N2-C2
3	C	3	SIA	C4-C5-N5-C10
3	C	3	SIA	O6-C6-C7-O7
3	C	1	NGA	C8-C7-N2-C2
2	B	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
3	C	1	NGA	C3-C2-N2-C7
3	C	2	GAL	O5-C5-C6-O6
3	C	3	SIA	C5-C6-C7-O7
3	C	1	NGA	C1-C2-N2-C7
3	C	3	SIA	O6-C6-C7-C8

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3	SIA	3	0
3	C	1	NGA	1	0
3	C	2	GAL	3	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 [i](#)

5 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
5	NAG	A	603	1	14,14,15	0.36	0	17,19,21	0.42	0
5	NAG	A	602	1	14,14,15	0.30	0	17,19,21	0.54	0
4	MAN	A	601	1	11,11,12	0.96	1 (9%)	15,15,17	0.92	1 (6%)
5	NAG	A	607	1	14,14,15	0.27	0	17,19,21	0.40	0
5	NAG	A	604	1	14,14,15	0.23	0	17,19,21	0.44	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
5	NAG	A	603	1	-	0/6/23/26	0/1/1/1
5	NAG	A	602	1	-	2/6/23/26	0/1/1/1
4	MAN	A	601	1	-	2/2/19/22	0/1/1/1
5	NAG	A	607	1	-	2/6/23/26	0/1/1/1
5	NAG	A	604	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	MAN	O5-C1	-2.25	1.39	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	MAN	O2-C2-C3	-2.01	105.98	110.15

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	MAN	O5-C5-C6-O6
5	A	602	NAG	C8-C7-N2-C2
5	A	602	NAG	O7-C7-N2-C2
5	A	607	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	601	MAN	C4-C5-C6-O6
5	A	607	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	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 [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	484/500 (96%)	0.18	20 (4%)	41 30	78, 142, 206, 265	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	506	ALA	5.0
1	A	190	ARG	3.6
1	A	448	SER	3.6
1	A	49	GLU	3.4
1	A	94	ASP	3.1
1	A	286	LYS	2.9
1	A	268	PRO	2.8
1	A	447	PRO	2.7
1	A	20	GLY	2.6
1	A	453	VAL	2.5
1	A	48	ASP	2.5
1	A	193	GLU	2.4
1	A	395	GLU	2.3
1	A	385	GLU	2.3
1	A	418	GLU	2.2
1	A	93	GLY	2.2
1	A	25	TRP	2.1
1	A	424	ALA	2.1
1	A	452	THR	2.0
1	A	192	ASP	2.0

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

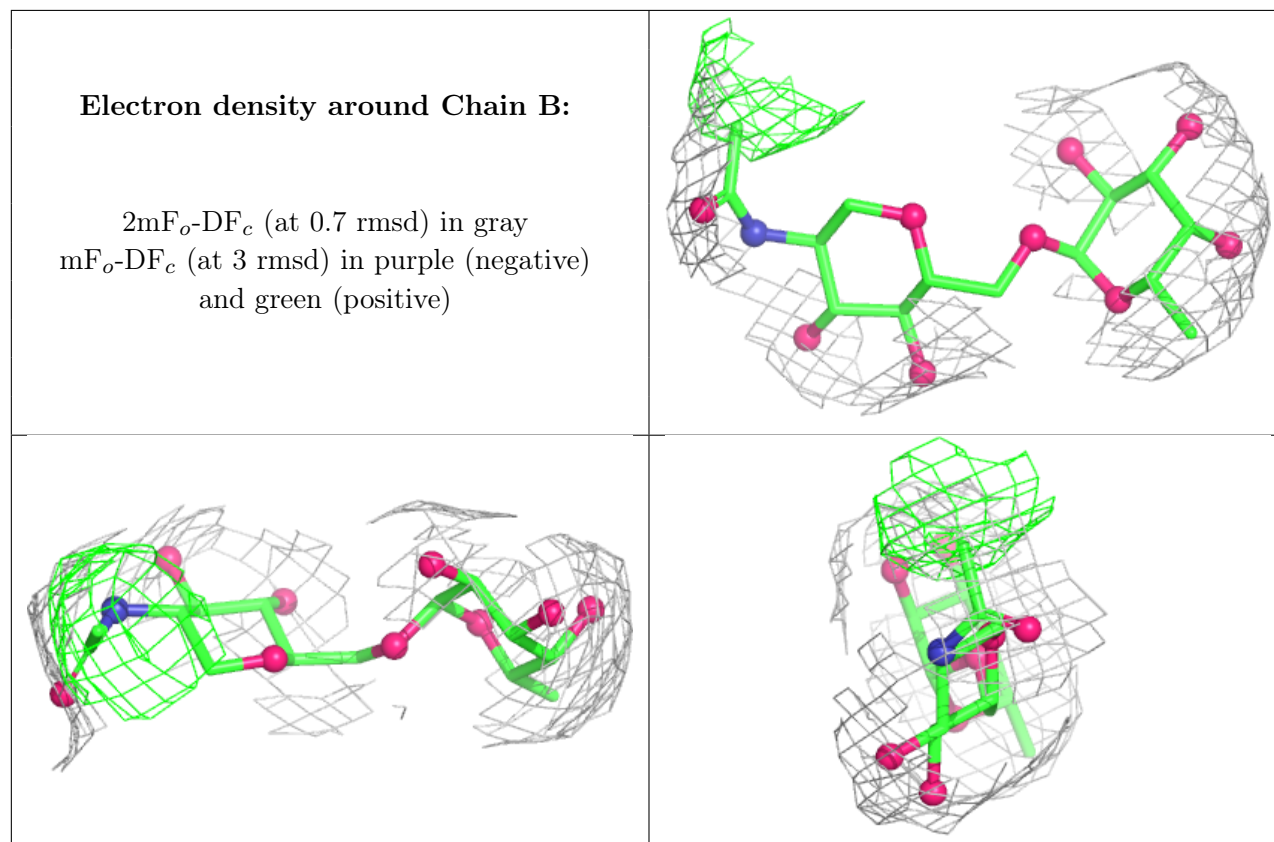
There are no non-standard protein/DNA/RNA residues in this entry.

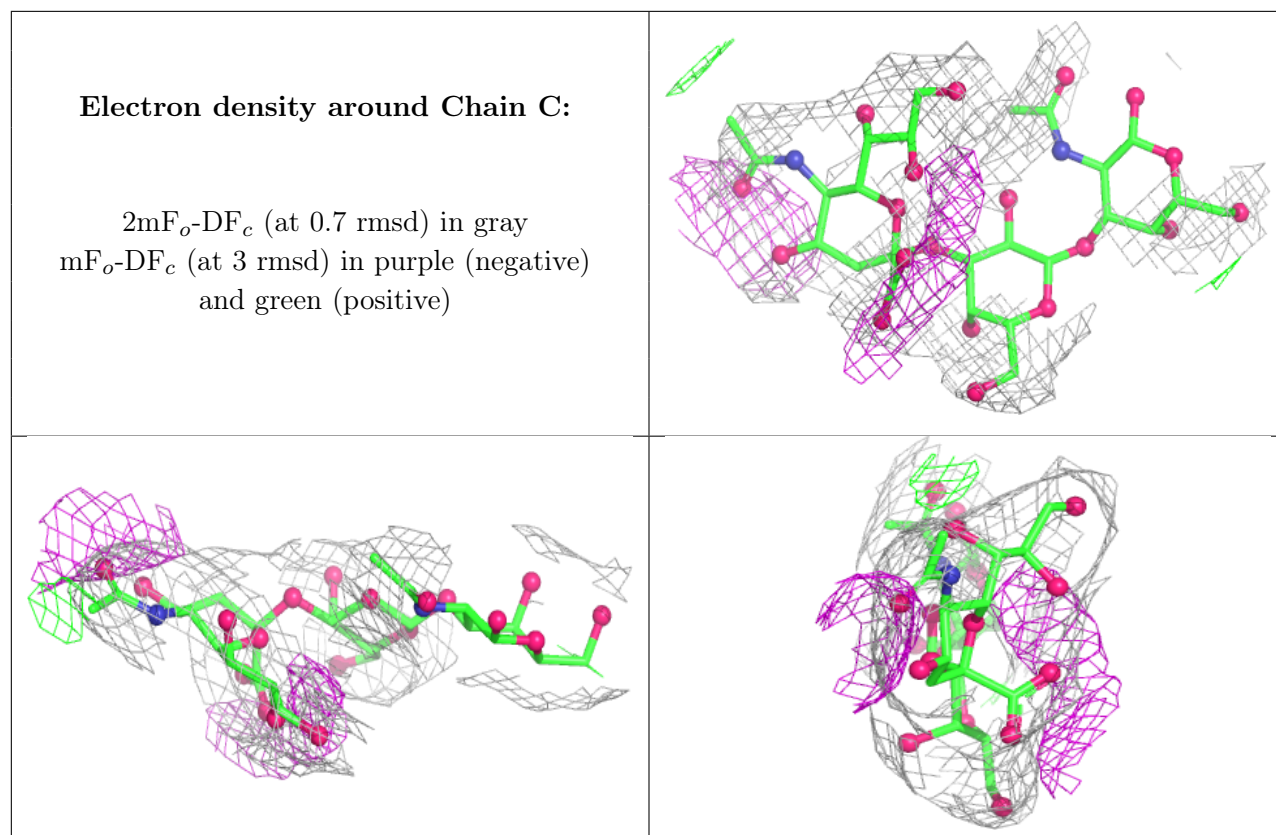
6.3 Carbohydrates ⓘ

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	NAG	B	1	14/15	0.49	0.13	147,187,207,215	0
3	NGA	C	1	15/15	0.78	0.13	143,160,186,190	0
2	FUC	B	2	10/11	0.81	0.11	143,175,217,227	0
3	SIA	C	3	20/21	0.90	0.12	86,111,141,156	0
3	GAL	C	2	11/12	0.93	0.09	96,115,135,148	0

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	A	604	14/15	0.69	0.16	177,217,238,240	0
5	NAG	A	603	14/15	0.78	0.17	185,228,240,242	0
5	NAG	A	607	14/15	0.85	0.12	115,156,177,178	0
5	NAG	A	602	14/15	0.90	0.23	77,129,156,189	0
4	MAN	A	601	11/12	0.92	0.11	81,149,205,212	0

6.5 Other polymers [i](#)

There are no such residues in this entry.