



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:49 AM UTC

PDB ID : 5N0C / pdb_00005n0c
Title : Crystal structure of the tetanus neurotoxin in complex with GM1a
Authors : Masuyer, G.; Conrad, J.; Stenmark, P.
Deposited on : 2017-02-02
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

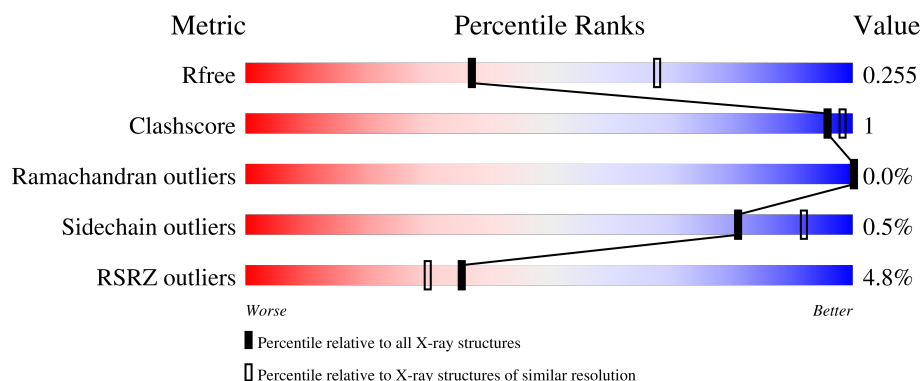
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	1335	4% 94% • •
1	B	1335	6% 94% • •
2	C	5	20% 80%
2	D	5	40% 60%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21439 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 Tetanus toxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1293	Total	C	N	O	S	0	0	0
			10444	6696	1704	2009	35			
1	B	1286	Total	C	N	O	S	0	0	0
			10398	6664	1697	2002	35			

There are 44 discrepancies between the modelled and reference sequences:

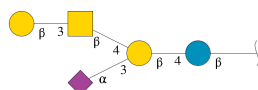
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P04958
A	-18	GLY	-	expression tag	UNP P04958
A	-17	SER	-	expression tag	UNP P04958
A	-16	SER	-	expression tag	UNP P04958
A	-15	HIS	-	expression tag	UNP P04958
A	-14	HIS	-	expression tag	UNP P04958
A	-13	HIS	-	expression tag	UNP P04958
A	-12	HIS	-	expression tag	UNP P04958
A	-11	HIS	-	expression tag	UNP P04958
A	-10	HIS	-	expression tag	UNP P04958
A	-9	SER	-	expression tag	UNP P04958
A	-8	SER	-	expression tag	UNP P04958
A	-7	GLY	-	expression tag	UNP P04958
A	-6	LEU	-	expression tag	UNP P04958
A	-5	VAL	-	expression tag	UNP P04958
A	-4	PRO	-	expression tag	UNP P04958
A	-3	ARG	-	expression tag	UNP P04958
A	-2	GLY	-	expression tag	UNP P04958
A	-1	SER	-	expression tag	UNP P04958
A	0	HIS	-	expression tag	UNP P04958
A	372	ALA	ARG	engineered mutation	UNP P04958
A	375	PHE	TYR	engineered mutation	UNP P04958
B	-19	MET	-	initiating methionine	UNP P04958
B	-18	GLY	-	expression tag	UNP P04958
B	-17	SER	-	expression tag	UNP P04958

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP P04958
B	-15	HIS	-	expression tag	UNP P04958
B	-14	HIS	-	expression tag	UNP P04958
B	-13	HIS	-	expression tag	UNP P04958
B	-12	HIS	-	expression tag	UNP P04958
B	-11	HIS	-	expression tag	UNP P04958
B	-10	HIS	-	expression tag	UNP P04958
B	-9	SER	-	expression tag	UNP P04958
B	-8	SER	-	expression tag	UNP P04958
B	-7	GLY	-	expression tag	UNP P04958
B	-6	LEU	-	expression tag	UNP P04958
B	-5	VAL	-	expression tag	UNP P04958
B	-4	PRO	-	expression tag	UNP P04958
B	-3	ARG	-	expression tag	UNP P04958
B	-2	GLY	-	expression tag	UNP P04958
B	-1	SER	-	expression tag	UNP P04958
B	0	HIS	-	expression tag	UNP P04958
B	372	ALA	ARG	engineered mutation	UNP P04958
B	375	PHE	TYR	engineered mutation	UNP P04958

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.

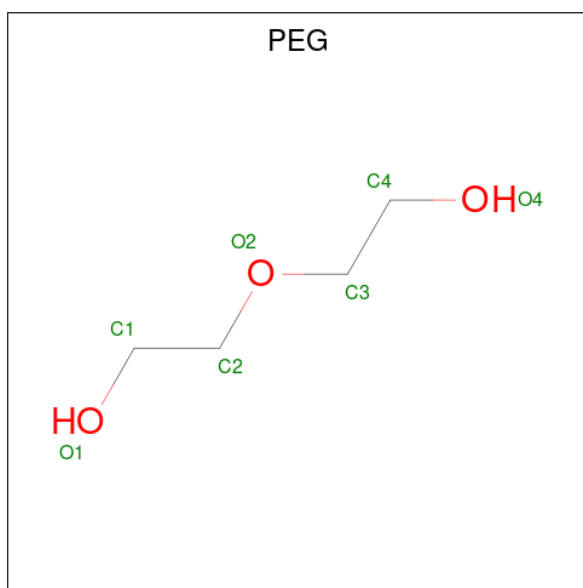


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	0	0	0
			68	37	2	29			
2	D	5	Total	C	N	O	0	0	0
			68	37	2	29			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	242	Total	O	0	0
			242	242		
5	B	210	Total	O	0	0
			210	210		

Chain C:  20% 80%

BGC1	GAL2	NGA3	GAL4	STAA5
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- Molecule 2: beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain D:  40% 60%

BGC1	GAL2	NGA3	GAL4	STAA5
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.23Å 137.45Å 152.40Å 90.00° 90.12° 90.00°	Depositor
Resolution (Å)	68.50 – 2.60 68.50 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (68.50-2.60) 99.8 (68.50-2.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.221 , 0.253 0.224 , 0.255	Depositor DCC
R_{free} test set	5742 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 35.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21439	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.92 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.3269e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: ZN, PEG, SIA, GAL, BGC, NGA

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	0.58	0/10667	0.77	0/14454
1	B	0.58	0/10619	0.77	0/14387
All	All	0.58	0/21286	0.77	0/28841

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

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	10444	0	10375	28	0
1	B	10398	0	10322	19	0
2	C	68	0	58	0	0
2	D	68	0	58	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	7	0	10	0	0
5	A	242	0	0	0	0
5	B	210	0	0	0	0
All	All	21439	0	20823	47	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 1.

All (47) 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:210:ILE:HD11	1:B:739:TYR:CE2	2.35	0.62
1:A:737:ARG:HB2	1:A:797:MET:HE2	1.82	0.62
1:A:737:ARG:CB	1:A:797:MET:HE2	2.33	0.59
1:B:726:TRP:HD1	1:B:809:MET:HE1	1.70	0.57
1:A:649:ALA:CB	1:A:741:MET:HE1	2.39	0.53
1:A:805:LEU:HA	1:A:809:MET:HE3	1.91	0.52
1:B:805:LEU:HA	1:B:809:MET:HE3	1.92	0.52
1:A:579:THR:HG21	1:A:591:LYS:HE2	1.91	0.51
1:B:1246:ARG:NH2	1:B:1296:ASP:O	2.43	0.51
1:A:1270:THR:HG22	1:A:1284:LEU:HD12	1.92	0.51
1:A:650:LEU:HG	1:A:741:MET:HE3	1.93	0.51
1:B:650:LEU:HG	1:B:741:MET:HE3	1.93	0.50
1:B:804:PHE:CD2	1:B:809:MET:HE2	2.47	0.50
1:A:210:ILE:HD11	1:A:739:TYR:CE2	2.47	0.49
1:B:726:TRP:CD1	1:B:809:MET:HE1	2.47	0.49
1:A:958:VAL:HG12	1:A:1084:VAL:HG12	1.95	0.49
1:A:741:MET:HE2	1:A:741:MET:HA	1.94	0.48
1:A:804:PHE:CD2	1:A:809:MET:HE2	2.48	0.48
1:B:788:LYS:HA	1:B:791:ILE:HD12	1.97	0.47
1:B:649:ALA:HB3	1:B:741:MET:HE1	1.96	0.47
1:B:39:ILE:CD1	1:B:92:VAL:HG22	2.45	0.46
1:B:649:ALA:CB	1:B:741:MET:HE1	2.45	0.46
1:A:734:PHE:HD1	1:A:797:MET:HE3	1.81	0.46
1:A:1246:ARG:NH2	1:A:1296:ASP:O	2.49	0.46
1:A:804:PHE:HD2	1:A:809:MET:HE2	1.80	0.45
1:A:177:ARG:NH1	1:A:182:ASN:OD1	2.50	0.45
1:B:646:ILE:HG22	1:B:741:MET:SD	2.57	0.45
1:A:909:TYR:CE1	1:A:934:ILE:HD12	2.52	0.45
1:A:726:TRP:CD1	1:A:809:MET:HE1	2.52	0.45
1:A:1285:ILE:C	1:A:1285:ILE:HD12	2.42	0.45
1:A:579:THR:HG21	1:A:591:LYS:CE	2.46	0.44
1:B:741:MET:HA	1:B:741:MET:HE2	1.98	0.44
1:A:726:TRP:HD1	1:A:809:MET:HE1	1.83	0.44
1:A:624:THR:HG23	1:A:785:LYS:HD2	2.00	0.42
1:B:596:PHE:CD1	1:B:626:GLU:HB3	2.55	0.42
1:A:222:LYS:CB	1:A:416:MET:HE3	2.50	0.41
1:B:848:GLU:HA	1:B:851:ILE:HG22	2.01	0.41
1:B:77:TYR:OH	1:B:201:GLU:OE1	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:PHE:O	1:A:89:GLN:NE2	2.46	0.41
1:A:487:GLU:N	1:A:488:PRO:CD	2.84	0.41
1:A:649:ALA:HB3	1:A:741:MET:HE1	2.02	0.41
1:B:210:ILE:HD11	1:B:739:TYR:CZ	2.55	0.41
1:A:101:ASN:HB3	1:A:367:PHE:CZ	2.56	0.41
1:A:596:PHE:CD1	1:A:626:GLU:HB3	2.56	0.41
1:B:695:THR:HG21	1:B:700:ILE:HD12	2.02	0.41
1:B:1114:LEU:CD1	1:B:1242:ALA:HB1	2.52	0.40
1:A:165:VAL:HG11	1:A:168:LYS:HG3	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	1287/1335 (96%)	1242 (96%)	45 (4%)	0	100	100
1	B	1280/1335 (96%)	1232 (96%)	47 (4%)	1 (0%)	48	70
All	All	2567/2670 (96%)	2474 (96%)	92 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	605	GLN

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	1178/1216 (97%)	1173 (100%)	5 (0%)	84	93
1	B	1173/1216 (96%)	1167 (100%)	6 (0%)	81	92
All	All	2351/2432 (97%)	2340 (100%)	11 (0%)	81	92

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

Mol	Chain	Res	Type
1	A	8	PHE
1	A	28	LYS
1	A	139	LEU
1	A	403	GLU
1	A	1262	ASN
1	B	8	PHE
1	B	210	ILE
1	B	289	ASN
1	B	866	ASN
1	B	874	GLU
1	B	994	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	169	ASN
1	A	208	ASN
1	A	339	GLN
1	A	348	GLN
1	A	368	ASN
1	A	401	ASN
1	A	526	ASN
1	A	625	ASN
1	A	780	ASN
1	A	807	ASN
1	A	816	GLN
1	A	893	ASN
1	A	903	ASN
1	A	972	ASN
1	A	998	ASN
1	A	1045	ASN

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Mol	Chain	Res	Type
1	A	1078	ASN
1	B	169	ASN
1	B	180	ASN
1	B	195	GLN
1	B	212	ASN
1	B	278	GLN
1	B	348	GLN
1	B	368	ASN
1	B	401	ASN
1	B	421	ASN
1	B	425	ASN
1	B	506	ASN
1	B	580	ASN
1	B	588	ASN
1	B	776	ASN
1	B	807	ASN
1	B	948	ASN
1	B	968	GLN
1	B	998	ASN
1	B	999	ASN
1	B	1068	ASN
1	B	1078	ASN
1	B	1080	ASN
1	B	1220	ASN
1	B	1288	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 ⓘ

10 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	BGC	C	1	2	12,12,12	0.77	0	17,17,17	1.38	4 (23%)
2	GAL	C	2	2	11,11,12	0.52	0	15,15,17	1.22	2 (13%)
2	NGA	C	3	2	14,14,15	0.41	0	17,19,21	0.89	0
2	GAL	C	4	2	11,11,12	0.32	0	15,15,17	0.90	1 (6%)
2	SIA	C	5	2	20,20,21	0.70	0	21,28,31	1.40	4 (19%)
2	BGC	D	1	2	12,12,12	0.75	0	17,17,17	1.37	4 (23%)
2	GAL	D	2	2	11,11,12	0.48	0	15,15,17	1.11	2 (13%)
2	NGA	D	3	2	14,14,15	0.33	0	17,19,21	0.97	0
2	GAL	D	4	2	11,11,12	0.32	0	15,15,17	0.62	0
2	SIA	D	5	2	20,20,21	0.67	0	21,28,31	1.32	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
2	BGC	C	1	2	-	0/2/22/22	0/1/1/1
2	GAL	C	2	2	-	2/2/19/22	0/1/1/1
2	NGA	C	3	2	-	1/6/23/26	0/1/1/1
2	GAL	C	4	2	-	2/2/19/22	0/1/1/1
2	SIA	C	5	2	-	4/18/34/38	0/1/1/1
2	BGC	D	1	2	-	0/2/22/22	0/1/1/1
2	GAL	D	2	2	-	2/2/19/22	0/1/1/1
2	NGA	D	3	2	-	2/6/23/26	0/1/1/1
2	GAL	D	4	2	-	2/2/19/22	0/1/1/1
2	SIA	D	5	2	-	5/18/34/38	0/1/1/1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	5	SIA	C11-C10-N5	3.49	121.90	116.12
2	C	1	BGC	C1-O5-C5	3.41	120.24	113.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	BGC	C1-O5-C5	2.92	119.30	113.65
2	C	2	GAL	C1-O5-C5	2.83	115.98	112.19
2	D	5	SIA	O1B-C1-C2	2.82	120.05	112.71
2	C	4	GAL	O5-C5-C6	2.73	112.97	107.66
2	D	5	SIA	C11-C10-N5	2.64	120.49	116.12
2	C	5	SIA	C5-N5-C10	2.45	128.84	123.11
2	D	2	GAL	C1-O5-C5	2.42	115.43	112.19
2	D	1	BGC	C1-C2-C3	2.37	115.18	110.36
2	C	5	SIA	O10-C10-C11	-2.35	117.86	122.05
2	D	1	BGC	O5-C1-C2	2.35	114.44	110.30
2	D	1	BGC	O4-C4-C3	2.32	115.85	110.38
2	C	5	SIA	O1B-C1-C2	2.27	118.62	112.71
2	C	1	BGC	O5-C5-C4	2.19	113.65	109.70
2	C	1	BGC	C1-C2-C3	2.12	114.68	110.36
2	C	2	GAL	O5-C5-C6	2.07	111.69	107.66
2	C	1	BGC	O4-C4-C5	2.03	114.33	109.32
2	D	2	GAL	C1-C2-C3	2.01	112.57	109.64

There are no chirality outliers.

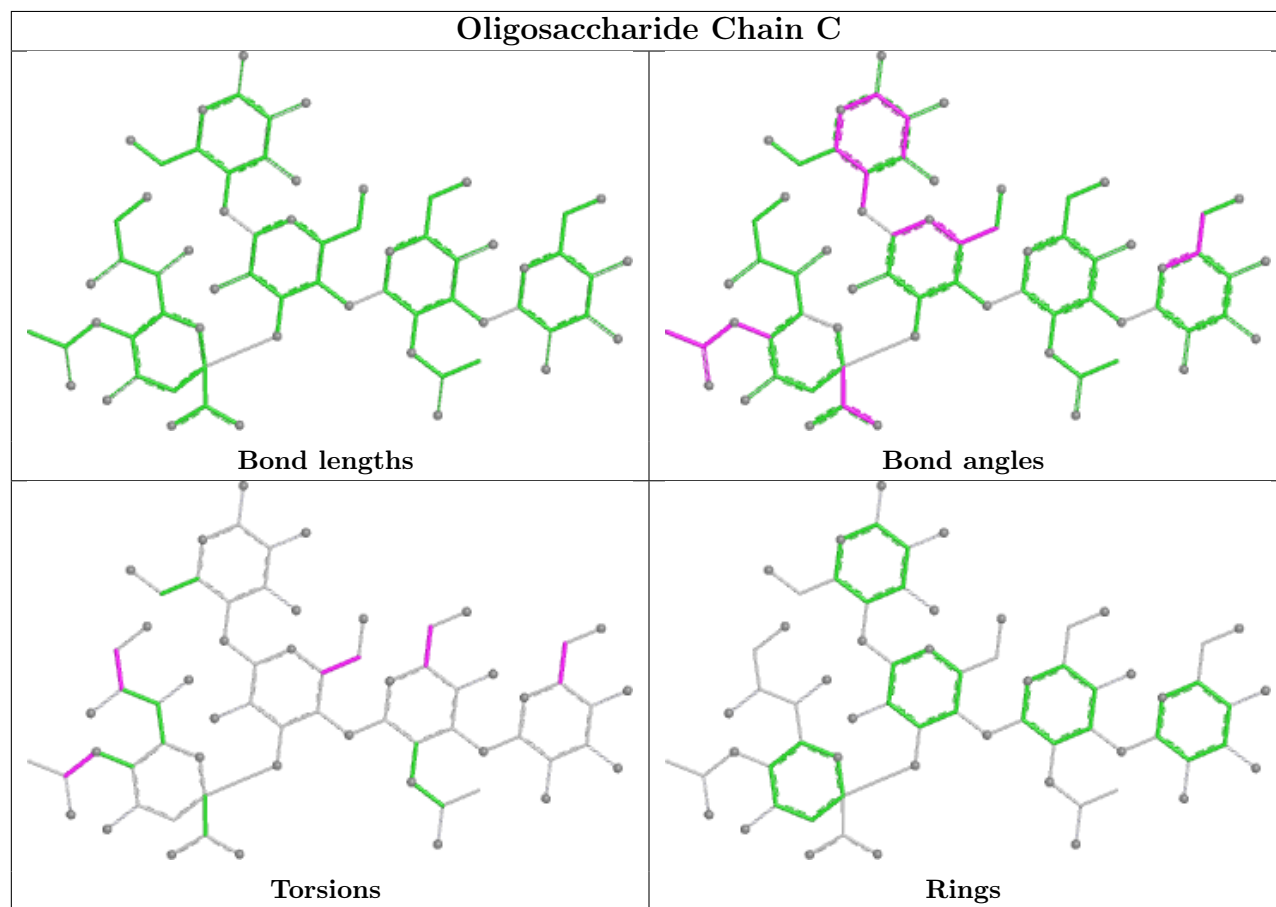
All (20) torsion outliers are listed below:

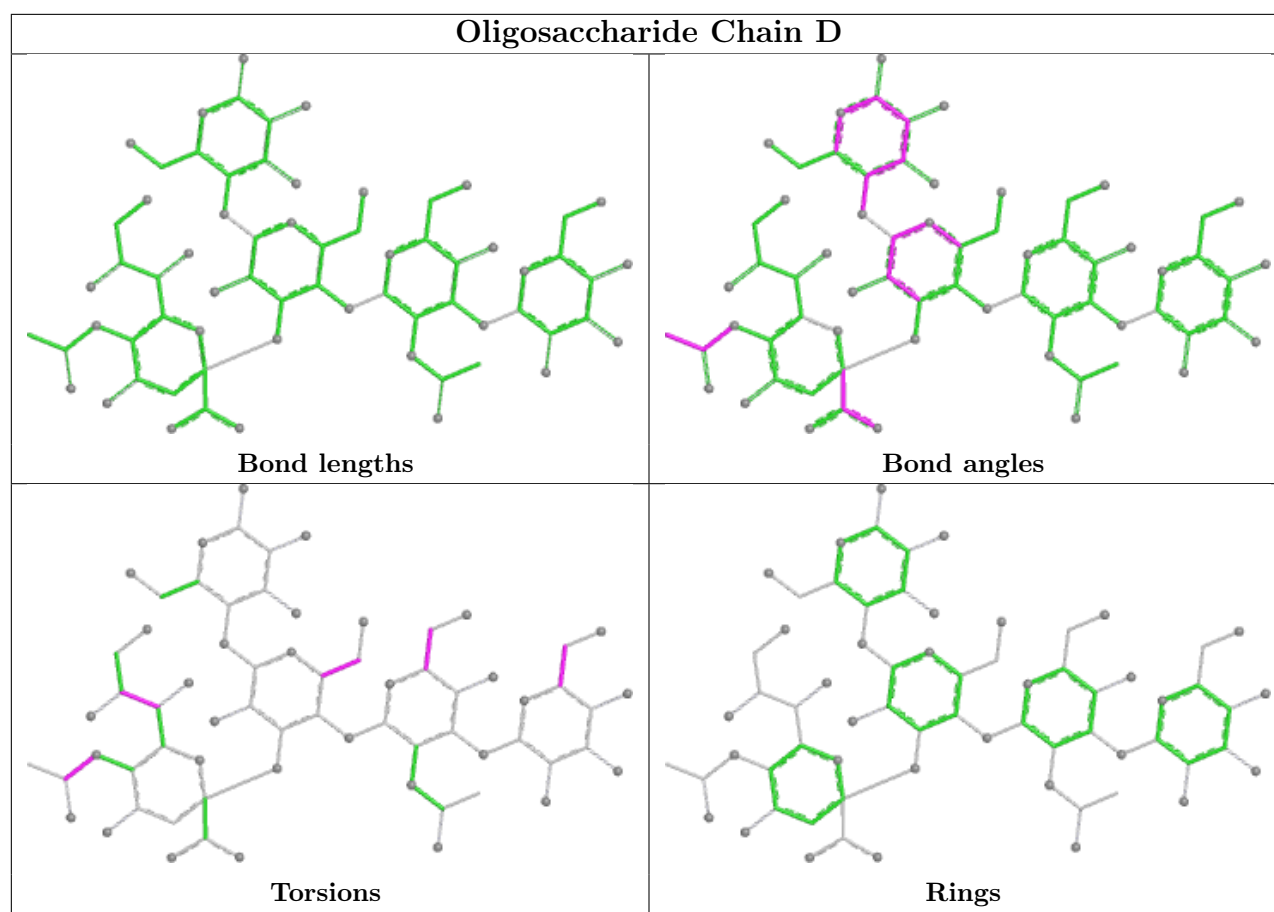
Mol	Chain	Res	Type	Atoms
2	C	5	SIA	O8-C8-C9-O9
2	C	4	GAL	O5-C5-C6-O6
2	C	5	SIA	C7-C8-C9-O9
2	C	2	GAL	O5-C5-C6-O6
2	C	4	GAL	C4-C5-C6-O6
2	D	3	NGA	O5-C5-C6-O6
2	D	2	GAL	C4-C5-C6-O6
2	C	2	GAL	C4-C5-C6-O6
2	C	5	SIA	C11-C10-N5-C5
2	C	5	SIA	O10-C10-N5-C5
2	D	5	SIA	C11-C10-N5-C5
2	D	5	SIA	O10-C10-N5-C5
2	D	2	GAL	O5-C5-C6-O6
2	D	4	GAL	C4-C5-C6-O6
2	D	4	GAL	O5-C5-C6-O6
2	D	3	NGA	C4-C5-C6-O6
2	C	3	NGA	O5-C5-C6-O6
2	D	5	SIA	C6-C7-C8-O8
2	D	5	SIA	O7-C7-C8-O8
2	D	5	SIA	O7-C7-C8-C9

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PEG	A	1407	-	6,6,6	0.45	0	5,5,5	0.32	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	PEG	A	1407	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	1293/1335 (96%)	0.13	50 (3%) 43 38	18, 41, 90, 138	0
1	B	1286/1335 (96%)	0.33	75 (5%) 29 23	16, 48, 103, 159	0
All	All	2579/2670 (96%)	0.23	125 (4%) 35 30	16, 44, 96, 159	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	987	ILE	7.0
1	A	841	ILE	6.3
1	A	522	ILE	4.8
1	B	847	LEU	4.8
1	B	844	LEU	4.6
1	A	839	ILE	4.4
1	B	858	PRO	4.4
1	B	841	ILE	4.3
1	B	522	ILE	4.3
1	B	610	ILE	4.3
1	A	842	THR	4.0
1	B	613	LEU	4.0
1	A	538	TYR	4.0
1	A	858	PRO	3.9
1	B	609	GLY	3.8
1	A	442	ILE	3.7
1	A	870	TRP	3.7
1	B	1186	ILE	3.7
1	B	611	LEU	3.5
1	A	1	MET	3.4
1	B	607	ALA	3.4
1	A	1186	ILE	3.4
1	B	870	TRP	3.4
1	B	848	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	445	PRO	3.3
1	B	658	GLU	3.3
1	B	503	LEU	3.3
1	B	851	ILE	3.3
1	B	498	THR	3.2
1	B	1202	TYR	3.2
1	B	1	MET	3.1
1	A	869	CYS	3.1
1	A	871	VAL	3.1
1	A	573	LEU	3.1
1	A	611	LEU	3.0
1	B	573	LEU	3.0
1	B	842	THR	3.0
1	B	501	LYS	3.0
1	A	610	ILE	3.0
1	B	657	TYR	3.0
1	B	697	LYS	2.9
1	B	659	GLY	2.9
1	B	838	PHE	2.9
1	B	857	THR	2.9
1	A	766	PRO	2.9
1	B	538	TYR	2.9
1	A	857	THR	2.9
1	B	1113	PHE	2.9
1	B	336	SER	2.8
1	B	612	PHE	2.8
1	A	655	GLN	2.8
1	B	1058	ILE	2.8
1	B	997	GLY	2.8
1	B	846	LYS	2.8
1	A	1111	ILE	2.8
1	A	945	ASP	2.8
1	B	499	LYS	2.7
1	B	502	PRO	2.7
1	A	498	THR	2.7
1	B	854	VAL	2.7
1	B	702	LYS	2.7
1	B	587	ILE	2.7
1	A	609	GLY	2.7
1	A	606	GLY	2.6
1	B	699	LYS	2.6
1	A	1260	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	463	GLY	2.6
1	A	855	PHE	2.6
1	B	603	VAL	2.6
1	B	1111	ILE	2.5
1	B	840	GLY	2.5
1	B	656	GLY	2.5
1	B	1044	ALA	2.5
1	B	981	LYS	2.5
1	B	521	LYS	2.5
1	A	613	LEU	2.5
1	A	844	LEU	2.4
1	B	1182	PRO	2.4
1	B	762	ILE	2.4
1	B	867	LEU	2.4
1	B	758	TYR	2.4
1	B	902	PHE	2.4
1	B	536	ILE	2.4
1	B	845	LYS	2.3
1	A	278	GLN	2.3
1	B	871	VAL	2.3
1	A	373	LEU	2.3
1	A	695	THR	2.3
1	B	1187	ASP	2.3
1	B	1056	ALA	2.3
1	B	698	GLU	2.3
1	A	443	ILE	2.3
1	B	839	ILE	2.3
1	B	831	TYR	2.3
1	A	656	GLY	2.3
1	A	988	GLY	2.3
1	A	771	ILE	2.2
1	A	847	LEU	2.2
1	A	875	GLU	2.2
1	A	944	ASN	2.2
1	A	464	GLY	2.2
1	B	764	SER	2.2
1	B	701	ILE	2.2
1	B	653	VAL	2.2
1	B	334	LYS	2.2
1	B	1059	THR	2.1
1	B	654	LYS	2.1
1	B	576	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	822	THR	2.1
1	B	608	GLN	2.1
1	B	655	GLN	2.1
1	A	854	VAL	2.1
1	A	760	TYR	2.1
1	B	1054	GLY	2.1
1	A	1056	ALA	2.1
1	A	523	THR	2.1
1	A	1017	ARG	2.0
1	A	521	LYS	2.0
1	A	840	GLY	2.0
1	A	440	LYS	2.0
1	A	981	LYS	2.0
1	B	789	ALA	2.0
1	B	837	LYS	2.0
1	B	696	GLN	2.0
1	B	496	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

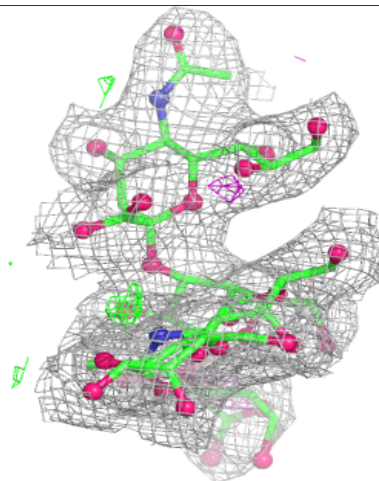
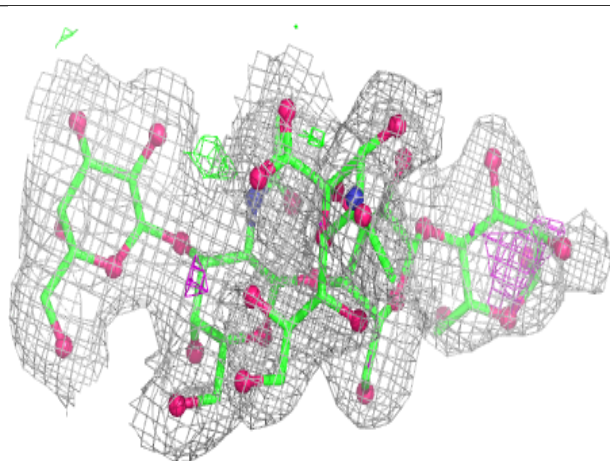
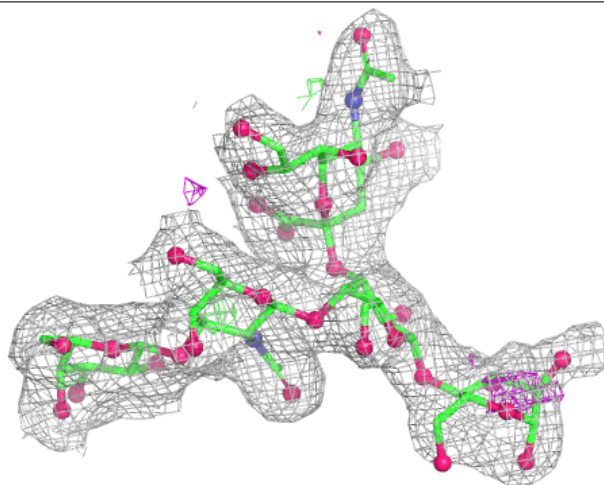
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

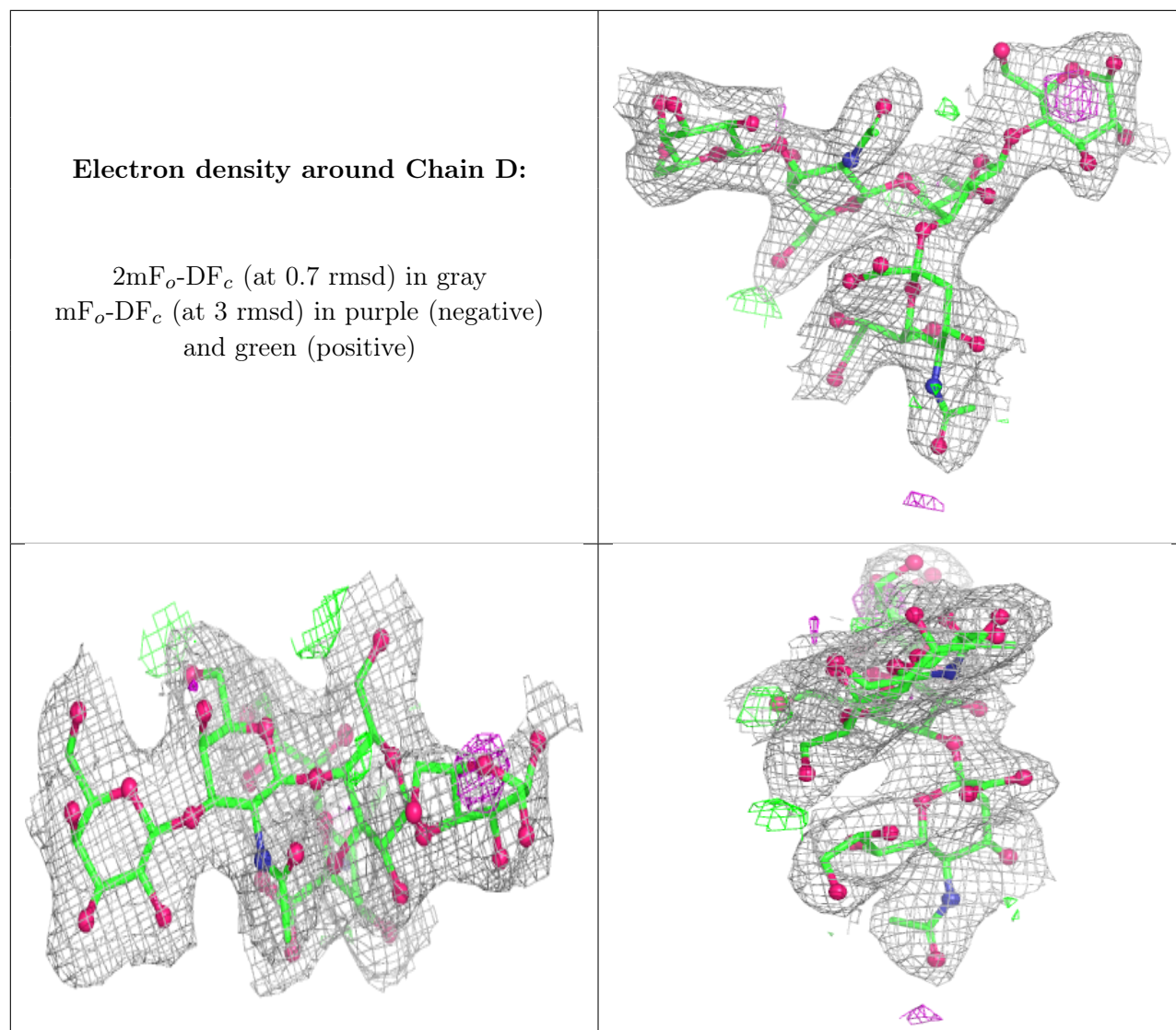
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BGC	D	1	12/12	0.75	0.14	60,68,70,72	0
2	BGC	C	1	12/12	0.77	0.14	57,68,70,70	0
2	GAL	D	2	11/12	0.86	0.11	46,49,52,54	0
2	SIA	D	5	20/21	0.91	0.08	40,43,46,47	0
2	NGA	D	3	14/15	0.92	0.08	40,41,42,43	0
2	SIA	C	5	20/21	0.92	0.09	41,43,44,44	0
2	GAL	C	2	11/12	0.93	0.07	40,44,47,49	0
2	NGA	C	3	14/15	0.94	0.07	32,35,36,37	0
2	GAL	D	4	11/12	0.96	0.05	37,38,38,39	0
2	GAL	C	4	11/12	0.96	0.08	32,32,32,33	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)





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PEG	A	1407	7/7	0.84	0.17	63,67,71,72	0
3	ZN	B	1406	1/1	0.99	0.02	52,52,52,52	0
3	ZN	A	1406	1/1	0.99	0.03	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.