



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 05:30 AM UTC

PDB ID : 4JJJ / pdb_00004jjj
Title : The structure of T. fusca GH48 D224N mutant
Authors : Alahuhta, P.M.; Lunin, V.V.
Deposited on : 2013-03-07
Resolution : 1.60 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

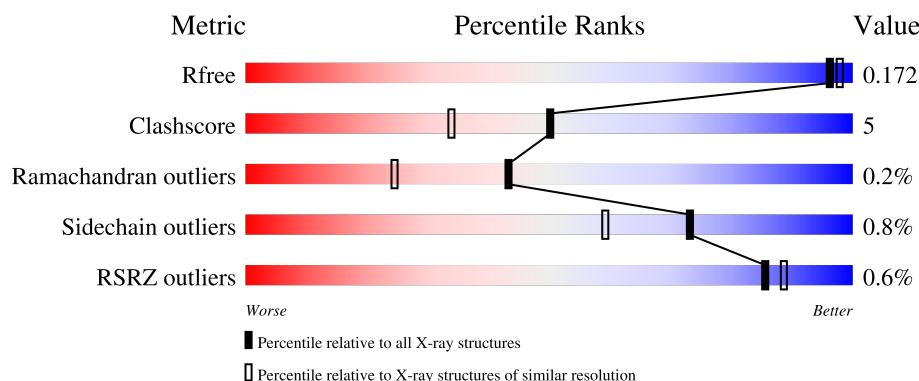
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	642	88% 10% ..
2	B	2	50% 50%
3	C	2	100%
4	D	6	83% 17%

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
9	ACT	A	737	-	X	-	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 6750 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 Cellulose 1,4-beta-cellobiosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	636	Total	C	N	O	S	0	43	0
			5415	3426	901	1066	22			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	224	ASN	ASP	engineered mutation	UNP Q47NH7

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	B	2	Total	C	O	0	2	0
			23	12	11			

- Molecule 3 is an oligosaccharide called beta-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	C	2	Total	C	O	0	2	0
			23	12	11			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	D	6	Total	C	O	0	1	0
			68	36	32			

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	Ca	0	0
			4	4		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	Na	0	0
			3	3		

- Molecule 7 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	4	Total	Fe	0	1
			5	5		

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	21	Total	Zn	0	1
			22	22		

- Molecule 9 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			4	2	2		

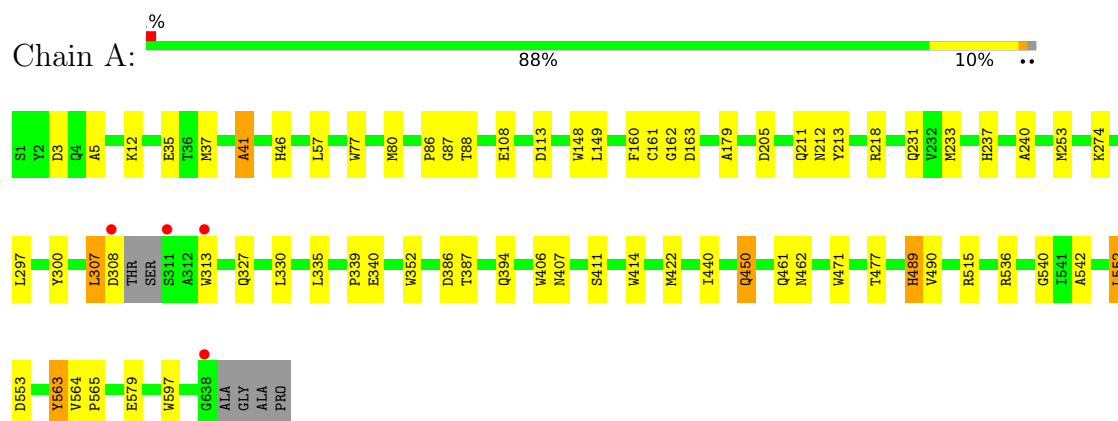
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1136	Total 1175	O 1175	0	39

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.

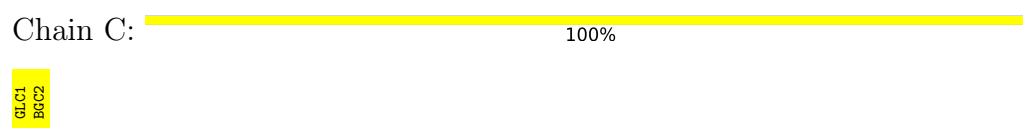
- Molecule 1: Cellulose 1,4-beta-cellobiosidase



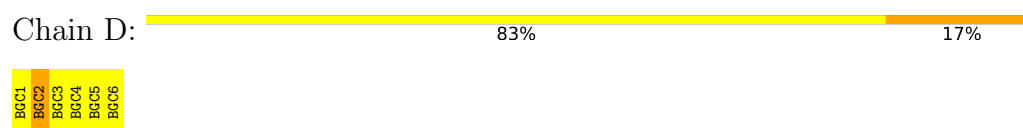
- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



- Molecule 3: beta-D-glucopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 4: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.46Å 88.49Å 66.75Å 90.00° 113.72° 90.00°	Depositor
Resolution (Å)	25.00 – 1.60 25.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (25.00-1.60) 99.3 (25.00-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.121 , 0.164 0.135 , 0.172	Depositor DCC
R_{free} test set	4003 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	9.5	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6750	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.16% 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: FE, ACT, GLC, CA, ZN, BGC, EDO, NA

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	1.39	16/5596 (0.3%)	1.21	7/7652 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	240	ALA	CA-CB	-5.81	1.44	1.53
1	A	542	ALA	CA-C	-5.80	1.45	1.52
1	A	536	ARG	CD-NE	-5.58	1.38	1.46
1	A	87	GLY	C-O	-5.55	1.18	1.23
1	A	564	VAL	CA-C	5.51	1.58	1.52
1	A	313	TRP	CA-C	5.48	1.59	1.52
1	A	563	TYR	C-N	5.43	1.39	1.33
1	A	233	MET	SD-CE	-5.34	1.66	1.79
1	A	12	LYS	C-O	-5.28	1.18	1.24
1	A	414	TRP	N-CA	5.28	1.52	1.46
1	A	489	HIS	C-O	-5.17	1.17	1.23
1	A	540	GLY	CA-C	-5.17	1.44	1.51
1	A	163	ASP	N-CA	5.13	1.53	1.46
1	A	339	PRO	N-CA	5.13	1.54	1.47
1	A	5	ALA	N-CA	5.09	1.52	1.46
1	A	565	PRO	C-O	-5.06	1.18	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	515	ARG	NE-CZ-NH2	-6.12	113.69	119.20
1	A	179	ALA	N-CA-C	5.88	119.56	112.38
1	A	564	VAL	O-C-N	5.21	127.04	121.10
1	A	407	ASN	CA-CB-CG	5.17	117.77	112.60
1	A	86	PRO	CA-C-N	-5.07	117.25	122.27
1	A	86	PRO	C-N-CA	-5.07	117.25	122.27
1	A	387	THR	CA-C-O	5.03	123.04	119.32

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	307	LEU	Peptide
1	A	41	ALA	Peptide
1	A	46	HIS	Peptide

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	5415	0	4888	55	0
2	B	23	0	12	1	0
3	C	23	0	12	0	0
4	D	68	0	54	1	0
5	A	4	0	0	0	0
6	A	3	0	0	0	0
7	A	5	0	0	0	0
8	A	22	0	0	0	0
9	A	8	0	6	0	0
10	A	4	0	6	0	0
11	A	1175	0	0	21	1
All	All	6750	0	4978	56	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 5.

All (56) 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:77[B]:TRP:CE3	1:A:80[B]:MET:CE	2.29	1.16
1:A:253[B]:MET:HE2	1:A:340[B]:GLU:HB3	1.26	1.10
1:A:77[B]:TRP:CZ3	1:A:80[B]:MET:HE1	1.87	1.09
1:A:77[B]:TRP:CZ3	1:A:80[B]:MET:CE	2.35	1.08
1:A:253[B]:MET:HE2	1:A:340[B]:GLU:CB	1.83	1.06
1:A:253[B]:MET:CE	1:A:340[B]:GLU:HB2	1.86	1.05
1:A:253[B]:MET:CE	1:A:340[B]:GLU:CB	2.39	1.00
11:A:1114[A]:HOH:O	2:B:1[A]:BGC:O1	1.84	0.96
1:A:253[B]:MET:HE1	1:A:340[B]:GLU:HB2	1.46	0.95
1:A:77[B]:TRP:CE3	1:A:80[B]:MET:HE3	2.04	0.92
1:A:57:LEU:HD11	1:A:80[A]:MET:HE1	1.51	0.92
1:A:77[B]:TRP:CZ3	1:A:80[B]:MET:HE3	2.09	0.86
1:A:450[B]:GLN:NE2	11:A:1076:HOH:O	2.17	0.77
1:A:297:LEU:H	1:A:327:GLN:HE22	1.31	0.73
1:A:77[B]:TRP:CH2	1:A:80[B]:MET:HE1	2.27	0.69
1:A:77[B]:TRP:CE3	1:A:80[B]:MET:HE1	2.16	0.67
1:A:88:THR:OG1	11:A:965[A]:HOH:O	2.13	0.67
1:A:212[B]:ASN:OD1	11:A:1803[B]:HOH:O	2.12	0.66
1:A:394:GLN:N	1:A:477[A]:THR:HG22	2.12	0.63
1:A:253[B]:MET:CE	1:A:340[B]:GLU:HB3	2.10	0.61
1:A:237[B]:HIS:HB2	1:A:253[B]:MET:SD	2.40	0.61
1:A:77[B]:TRP:CE3	1:A:80[B]:MET:HE2	2.31	0.59
1:A:462:ASN:ND2	11:A:1131:HOH:O	2.36	0.59
1:A:253[B]:MET:HE1	1:A:340[B]:GLU:CB	2.19	0.58
1:A:461:GLN:HG3	11:A:1326:HOH:O	2.03	0.58
1:A:35:GLU:HB2	11:A:1879:HOH:O	2.05	0.56
1:A:300:TYR:CE2	4:D:2[B]:BGC:H6C2	2.41	0.55
1:A:274:LYS:HE3	11:A:1903:HOH:O	2.07	0.55
1:A:308:ASP:HB2	11:A:1859:HOH:O	2.08	0.54
1:A:162:GLY:HA2	11:A:1294[B]:HOH:O	2.08	0.54
1:A:37[B]:MET:HE1	1:A:597:TRP:HE3	1.74	0.52
1:A:231:GLN:HG3	1:A:330:LEU:HD12	1.91	0.52
1:A:579:GLU:OE1	11:A:1744:HOH:O	2.19	0.51
1:A:489:HIS:CE1	11:A:1660:HOH:O	2.65	0.49
1:A:160:PHE:O	1:A:161[B]:CYS:C	2.54	0.49
1:A:205:ASP:HB3	1:A:213:TYR:CZ	2.49	0.48
1:A:422[B]:MET:HE1	1:A:440:ILE:HG22	1.96	0.48
1:A:212[B]:ASN:HA	11:A:1803[B]:HOH:O	2.14	0.47
1:A:57:LEU:CD1	1:A:80[A]:MET:HE1	2.33	0.47
1:A:422[B]:MET:HG2	11:A:1459:HOH:O	2.14	0.47
1:A:335:LEU:HD13	1:A:352:TRP:CE2	2.50	0.46
1:A:553:ASP:CG	11:A:988:HOH:O	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:TRP:HB2	1:A:411:SER:HB3	1.99	0.45
1:A:330:LEU:C	1:A:330:LEU:HD13	2.42	0.45
1:A:552[A]:LEU:C	1:A:552[A]:LEU:HD12	2.42	0.45
1:A:3:ASP:HB3	11:A:1049:HOH:O	2.17	0.44
1:A:3:ASP:CB	11:A:1049:HOH:O	2.66	0.43
1:A:386:ASP:CG	11:A:1927:HOH:O	2.62	0.42
1:A:108:GLU:OE1	11:A:1221:HOH:O	2.21	0.42
1:A:113:ASP:HA	1:A:563:TYR:CE2	2.54	0.42
1:A:148:TRP:CE2	1:A:149:LEU:HB2	2.55	0.42
1:A:308:ASP:N	11:A:1297:HOH:O	2.37	0.41
1:A:108:GLU:OE2	11:A:979[A]:HOH:O	2.21	0.41
1:A:471:TRP:CZ3	1:A:490:VAL:HB	2.56	0.41
1:A:307:LEU:O	1:A:308:ASP:HB2	2.21	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)
11:A:1470:HOH:O	11:A:1872:HOH:O[2_747]	2.12	0.08

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	677/642 (106%)	659 (97%)	17 (2%)	1 (0%)	48 27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	ALA

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	567/525 (108%)	561 (99%)	6 (1%)	65 46

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	211	GLN
1	A	218	ARG
1	A	450[A]	GLN
1	A	450[B]	GLN
1	A	552[A]	LEU
1	A	552[B]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	121	ASN
1	A	127	GLN
1	A	141	ASN
1	A	221	ASN
1	A	327	GLN
1	A	403	GLN
1	A	489	HIS
1	A	609	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 ⓘ

11 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	B	1[A]	2	12,12,12	0.98	1 (8%)	17,17,17	1.14	2 (11%)
2	BGC	B	2[A]	2	11,11,12	0.70	0	15,15,17	1.23	1 (6%)
3	GLC	C	1[B]	3	12,12,12	1.14	1 (8%)	17,17,17	1.20	3 (17%)
3	BGC	C	2[B]	3	11,11,12	1.28	2 (18%)	15,15,17	1.34	1 (6%)
4	BGC	D	1	4	12,12,12	0.95	0	17,17,17	1.65	3 (17%)
4	BGC	D	2[A]	-	11,11,12	1.14	1 (9%)	15,15,17	1.59	3 (20%)
4	BGC	D	2[B]	-	11,11,12	1.15	1 (9%)	15,15,17	1.86	4 (26%)
4	BGC	D	3	4	11,11,12	1.02	0	15,15,17	0.95	1 (6%)
4	BGC	D	4	4	11,11,12	0.71	0	15,15,17	0.95	1 (6%)
4	BGC	D	5	4	11,11,12	1.49	3 (27%)	15,15,17	1.69	3 (20%)
4	BGC	D	6	4	11,11,12	1.59	3 (27%)	15,15,17	2.19	4 (26%)

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	B	1[A]	2	-	0/2/22/22	0/1/1/1
2	BGC	B	2[A]	2	-	0/2/19/22	0/1/1/1
3	GLC	C	1[B]	3	-	0/2/22/22	0/1/1/1
3	BGC	C	2[B]	3	-	0/2/19/22	0/1/1/1
4	BGC	D	1	4	-	0/2/22/22	0/1/1/1
4	BGC	D	2[A]	-	-	1/2/19/22	0/1/1/1
4	BGC	D	2[B]	-	-	2/2/19/22	0/1/1/1
4	BGC	D	3	4	-	0/2/19/22	0/1/1/1
4	BGC	D	4	4	-	0/2/19/22	0/1/1/1
4	BGC	D	5	4	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BGC	D	6	4	-	2/2/19/22	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	6	BGC	O5-C5	3.06	1.49	1.43
4	D	6	BGC	O5-C1	2.88	1.48	1.43
3	C	2[B]	BGC	C4-C5	2.81	1.59	1.53
3	C	1[B]	GLC	O2-C2	2.80	1.49	1.43
4	D	5	BGC	O4-C4	2.80	1.49	1.43
2	B	1[A]	BGC	O1-C1	2.36	1.47	1.39
4	D	2[A]	BGC	C2-C3	-2.29	1.49	1.52
4	D	2[B]	BGC	C2-C3	-2.29	1.49	1.52
4	D	5	BGC	O5-C5	2.21	1.47	1.43
3	C	2[B]	BGC	C4-C3	2.12	1.57	1.52
4	D	6	BGC	O3-C3	2.12	1.48	1.43
4	D	5	BGC	O2-C2	-2.00	1.39	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	6	BGC	C1-O5-C5	-5.77	104.46	112.19
4	D	2[B]	BGC	O6-C6-C5	3.93	124.73	111.33
4	D	1	BGC	O4-C4-C3	-3.61	101.87	110.38
4	D	6	BGC	O6-C6-C5	-3.53	99.32	111.33
3	C	2[B]	BGC	O5-C5-C6	3.46	114.41	107.66
4	D	5	BGC	O4-C4-C5	-3.39	100.97	109.32
4	D	2[A]	BGC	C1-O5-C5	-3.01	108.15	112.19
4	D	2[B]	BGC	C1-O5-C5	-3.01	108.15	112.19
4	D	5	BGC	C1-O5-C5	-3.01	108.15	112.19
4	D	1	BGC	O5-C1-C2	2.92	115.44	110.30
4	D	6	BGC	O5-C5-C4	-2.82	103.96	110.83
2	B	1[A]	BGC	C3-C4-C5	2.81	115.32	110.23
2	B	2[A]	BGC	C1-O5-C5	2.55	115.61	112.19
2	B	1[A]	BGC	O2-C2-C3	-2.54	104.39	110.38
4	D	5	BGC	C6-C5-C4	2.48	119.11	113.02
4	D	2[A]	BGC	O5-C5-C6	2.47	112.47	107.66
4	D	2[B]	BGC	O5-C5-C6	2.47	112.47	107.66
4	D	2[A]	BGC	C3-C4-C5	-2.45	105.79	110.23
4	D	2[B]	BGC	C3-C4-C5	-2.45	105.79	110.23
3	C	1[B]	GLC	O2-C2-C3	-2.44	104.64	110.38
3	C	1[B]	GLC	O1-C1-C2	-2.33	102.22	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	BGC	C3-C4-C5	2.32	114.44	110.23
4	D	3	BGC	O4-C4-C3	-2.29	104.99	110.38
4	D	6	BGC	O2-C2-C3	-2.09	105.83	110.15
4	D	4	BGC	O5-C1-C2	-2.07	105.86	110.79
3	C	1[B]	GLC	C3-C4-C5	-2.04	106.54	110.23

There are no chirality outliers.

All (7) torsion outliers are listed below:

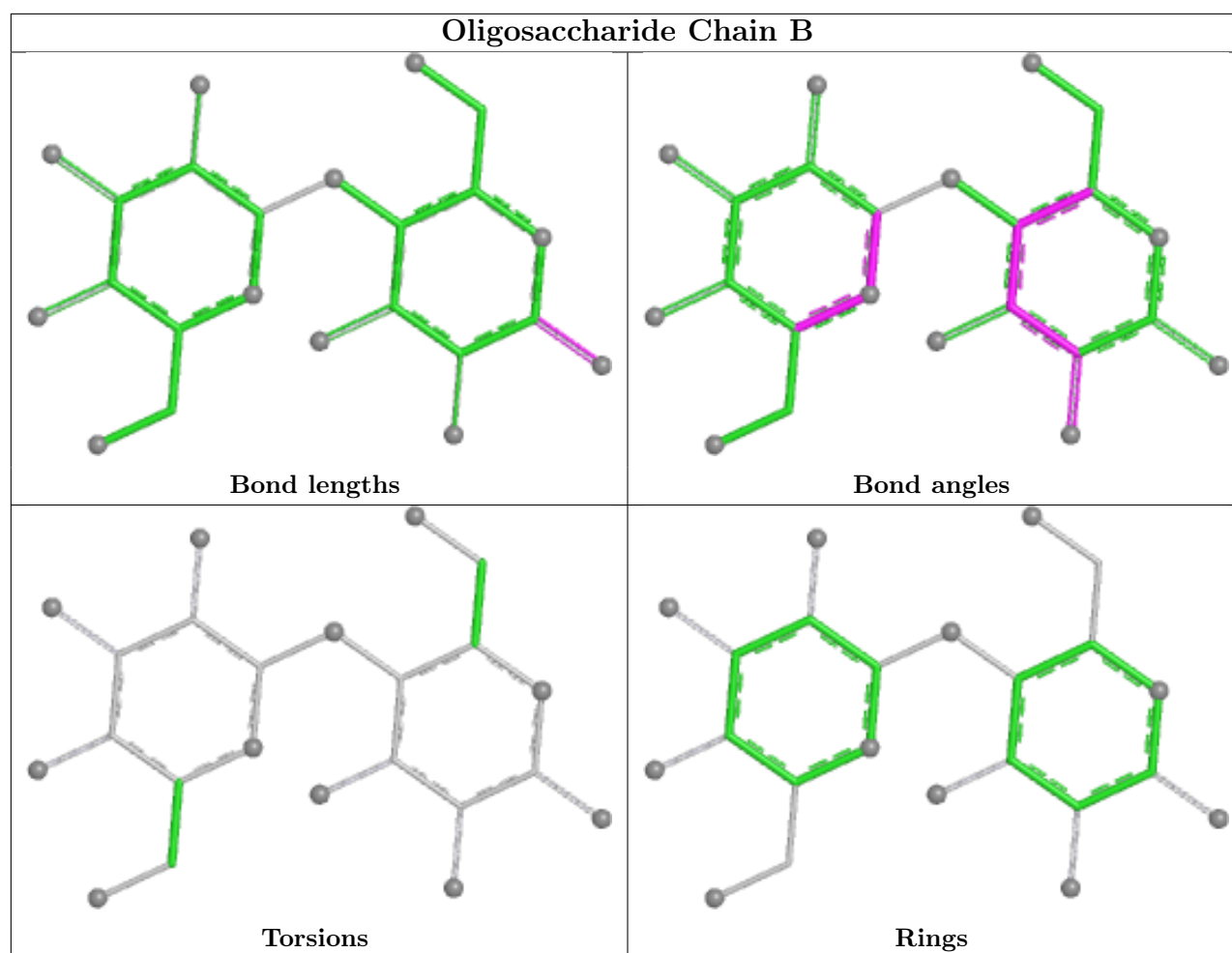
Mol	Chain	Res	Type	Atoms
4	D	2[B]	BGC	O5-C5-C6-O6
4	D	2[B]	BGC	C4-C5-C6-O6
4	D	5	BGC	C4-C5-C6-O6
4	D	5	BGC	O5-C5-C6-O6
4	D	6	BGC	O5-C5-C6-O6
4	D	2[A]	BGC	C4-C5-C6-O6
4	D	6	BGC	C4-C5-C6-O6

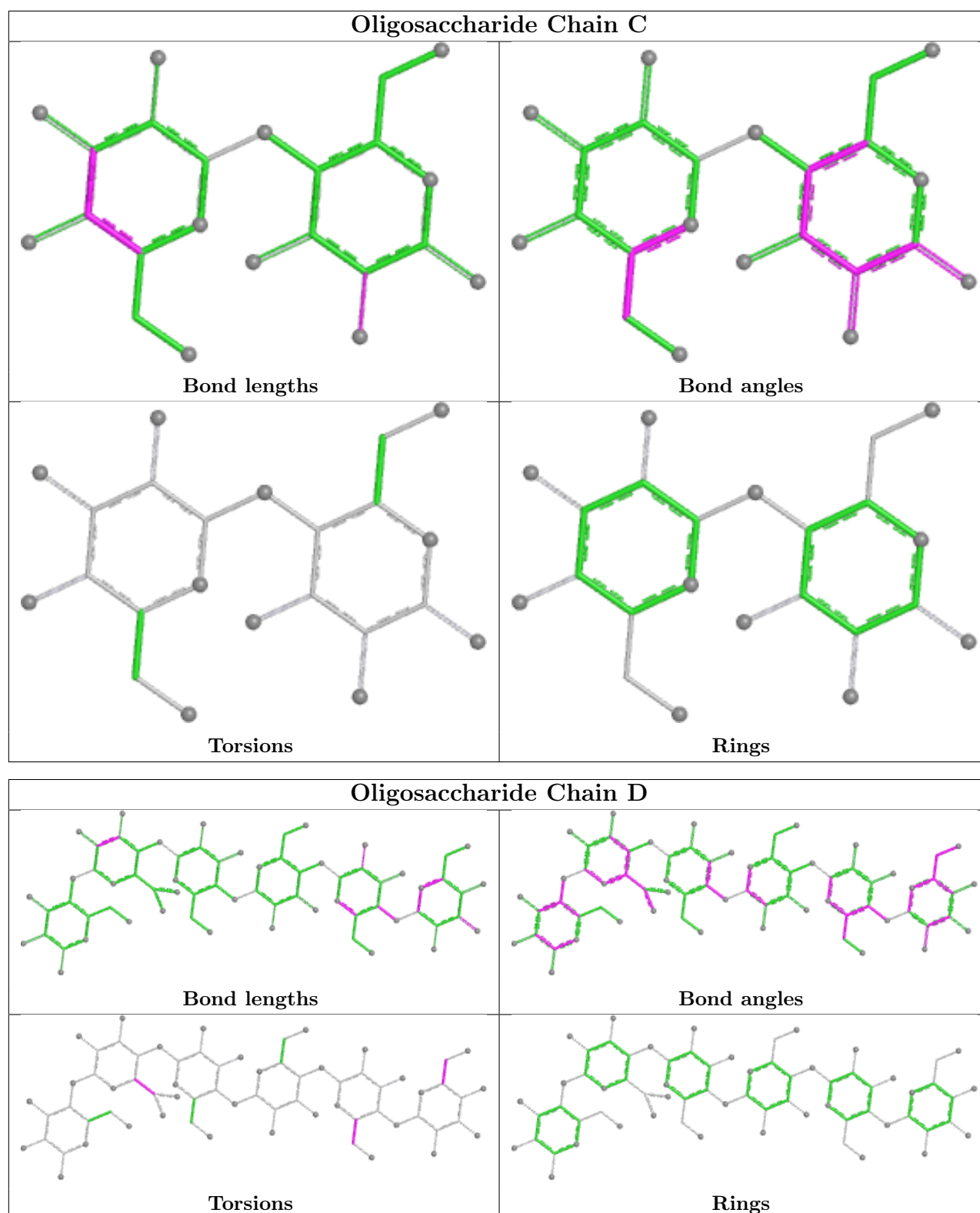
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1[A]	BGC	1	0
4	D	2[B]	BGC	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 [i](#)

Of 37 ligands modelled in this entry, 34 are monoatomic - leaving 3 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$
9	ACT	A	737	8	3,3,3	1.38	1 (33%)	3,3,3	1.72	2 (66%)
10	EDO	A	738	-	3,3,3	0.45	0	2,2,2	0.11	0
9	ACT	A	736	8	3,3,3	1.02	0	3,3,3	0.55	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
10	EDO	A	738	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	737	ACT	OXT-C	-2.35	1.20	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	737	ACT	OXT-C-CH3	2.18	124.19	115.05
9	A	737	ACT	OXT-C-O	-2.01	114.59	122.03

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	636/642 (99%)	-0.69	4 (0%) 85 88	2, 8, 18, 54	43 (6%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	311	SER	3.1
1	A	313	TRP	2.8
1	A	308	ASP	2.5
1	A	638	GLY	2.5

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.

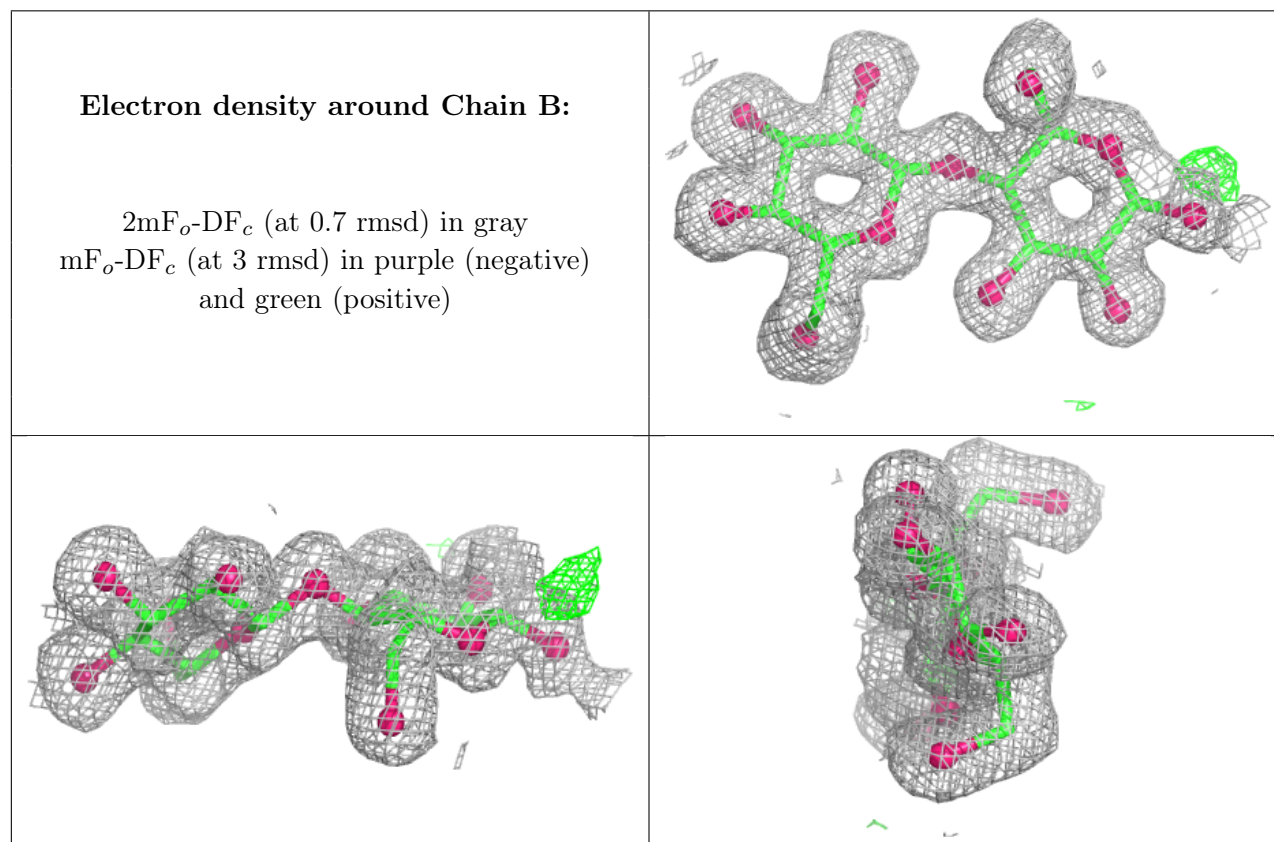
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BGC	D	6	11/12	0.84	0.11	21,25,30,31	0
4	BGC	D	5	11/12	0.94	0.07	10,14,17,19	0
3	GLC	C	1[B]	12/12	0.94	0.06	9,12,14,14	12
3	BGC	C	2[B]	11/12	0.96	0.04	7,8,8,9	11
4	BGC	D	4	11/12	0.97	0.04	8,9,11,11	0
4	BGC	D	2[B]	11/12	0.98	0.04	6,7,8,9	1
4	BGC	D	3	11/12	0.98	0.04	7,7,8,9	0
2	BGC	B	1[A]	12/12	0.98	0.04	3,5,6,9	12

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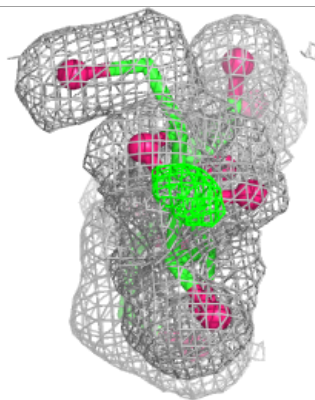
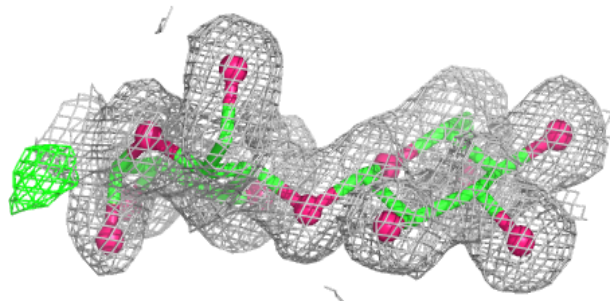
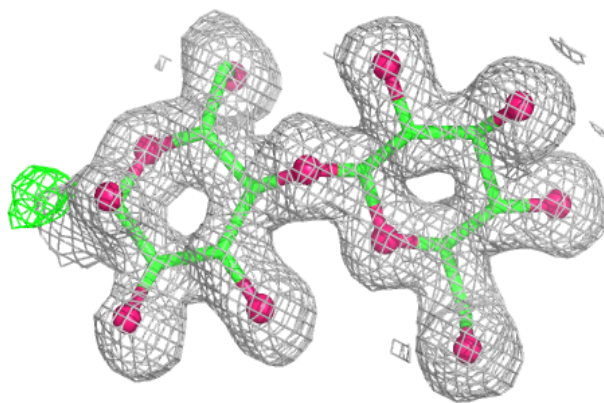
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BGC	D	1	12/12	0.98	0.04	4,5,7,8	0
4	BGC	D	2[A]	11/12	0.98	0.04	6,7,8,9	1
2	BGC	B	2[A]	11/12	0.99	0.03	2,2,2,3	11

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.

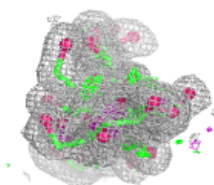
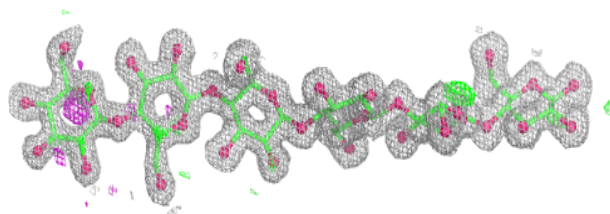
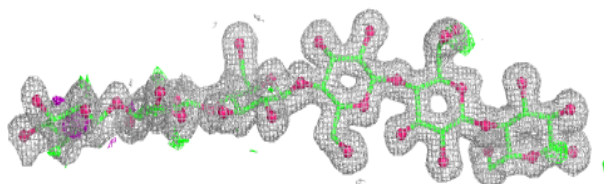


Electron density around Chain C:

$2mF_o-DF_c$ (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 ⓘ

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
7	FE	A	713	1/1	0.79	0.11	39,39,39,39	1
8	ZN	A	731	1/1	0.84	0.10	62,62,62,62	1
8	ZN	A	732	1/1	0.86	0.16	52,52,52,52	1
10	EDO	A	738	4/4	0.86	0.11	30,35,36,44	0
9	ACT	A	737	4/4	0.88	0.12	25,29,33,36	0
9	ACT	A	736	4/4	0.88	0.14	34,38,41,42	0
8	ZN	A	727	1/1	0.90	0.11	56,56,56,56	1
6	NA	A	709	1/1	0.92	0.09	27,27,27,27	0
6	NA	A	710	1/1	0.93	0.17	32,32,32,32	0
8	ZN	A	735	1/1	0.94	0.07	33,33,33,33	1
6	NA	A	708	1/1	0.94	0.07	35,35,35,35	0
8	ZN	A	734	1/1	0.95	0.09	35,35,35,35	1
5	CA	A	706	1/1	0.96	0.11	31,31,31,31	0
7	FE	A	712[A]	1/1	0.96	0.04	19,19,19,19	1
7	FE	A	712[B]	1/1	0.96	0.04	29,29,29,29	1
8	ZN	A	730[B]	1/1	0.97	0.13	25,25,25,25	1
5	CA	A	707	1/1	0.97	0.11	21,21,21,21	1
8	ZN	A	729	1/1	0.97	0.04	31,31,31,31	1
8	ZN	A	730[A]	1/1	0.97	0.13	28,28,28,28	1
8	ZN	A	722	1/1	0.98	0.06	18,18,18,18	1
8	ZN	A	728	1/1	0.99	0.04	14,14,14,14	1
8	ZN	A	716	1/1	0.99	0.02	16,16,16,16	0
8	ZN	A	717	1/1	0.99	0.02	13,13,13,13	1
8	ZN	A	718	1/1	0.99	0.03	16,16,16,16	0
8	ZN	A	720	1/1	0.99	0.06	17,17,17,17	1
8	ZN	A	721	1/1	0.99	0.08	22,22,22,22	1
8	ZN	A	733	1/1	0.99	0.02	16,16,16,16	1
7	FE	A	711	1/1	0.99	0.03	9,9,9,9	1
8	ZN	A	724	1/1	0.99	0.05	14,14,14,14	1
8	ZN	A	725	1/1	0.99	0.02	17,17,17,17	1
8	ZN	A	726	1/1	0.99	0.03	15,15,15,15	1
5	CA	A	705	1/1	0.99	0.06	15,15,15,15	0
5	CA	A	704	1/1	1.00	0.01	8,8,8,8	0
7	FE	A	714	1/1	1.00	0.08	16,16,16,16	0
8	ZN	A	715	1/1	1.00	0.02	7,7,7,7	0
8	ZN	A	723	1/1	1.00	0.04	13,13,13,13	1
8	ZN	A	719	1/1	1.00	0.02	8,8,8,8	0

6.5 Other polymers [i](#)

There are no such residues in this entry.