



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 31, 2026 – 10:58 AM UTC

PDB ID : 7NOX / pdb_00007nox
Title : Structure of SGBP BO2743 from Bacteroides ovatus in complex with mixed-linked gluco-nonasaccharide
Authors : Correia, V.C.; Trovao, F.; Pinheiro, B.A.; Palma, A.S.; Carvalho, A.L.
Deposited on : 2021-02-26
Resolution : 1.43 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

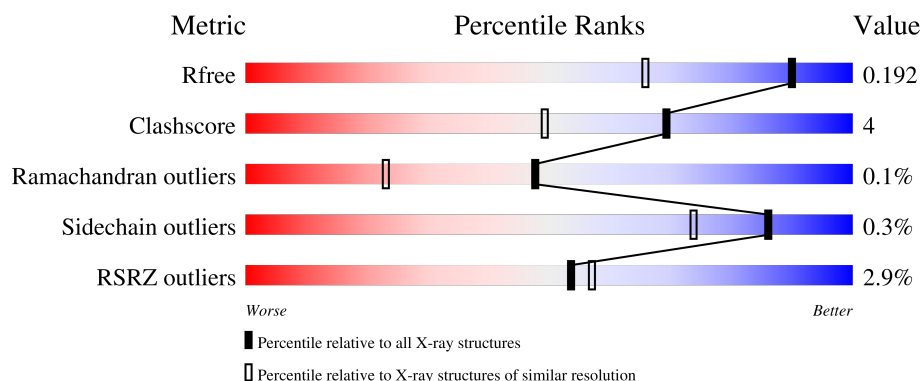
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.43 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	3234 (1.46-1.42)
Clashscore	190562	3289 (1.46-1.42)
Ramachandran outliers	187476	3248 (1.46-1.42)
Sidechain outliers	187428	3248 (1.46-1.42)
RSRZ outliers	180081	3234 (1.46-1.42)

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	598	2% 81% 6% 13%
1	B	598	3% 84% 13%
2	C	9	22% 67% 11%
2	D	9	33% 44% 22%

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
5	PGE	A	605	-	-	X	-
7	AZI	A	610	-	X	-	-
7	AZI	A	611	-	X	-	-
7	AZI	A	612	-	X	-	-
7	AZI	A	613	-	X	-	-
7	AZI	A	614	-	X	-	-
7	AZI	A	615	-	X	-	-
7	AZI	A	616	-	X	-	-
7	AZI	A	617	-	X	-	-
7	AZI	B	611	-	X	-	-
7	AZI	B	612	-	X	-	-
7	AZI	B	613	-	X	-	-
7	AZI	B	614	-	X	-	-
7	AZI	B	615	-	X	-	-
7	AZI	B	616	-	X	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9707 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 Surface glycan-binding protein BO2743.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	520	Total	C	N	O	S	0	17	0
			4196	2660	690	825	21			
1	B	520	Total	C	N	O	S	0	8	0
			4152	2625	690	816	21			

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-38	MET	-	initiating methionine	UNP A7LY27
A	-37	HIS	-	expression tag	UNP A7LY27
A	-36	HIS	-	expression tag	UNP A7LY27
A	-35	HIS	-	expression tag	UNP A7LY27
A	-34	HIS	-	expression tag	UNP A7LY27
A	-33	HIS	-	expression tag	UNP A7LY27
A	-32	HIS	-	expression tag	UNP A7LY27
A	-31	SER	-	expression tag	UNP A7LY27
A	-30	SER	-	expression tag	UNP A7LY27
A	-29	GLY	-	expression tag	UNP A7LY27
A	-28	VAL	-	expression tag	UNP A7LY27
A	-27	ASP	-	expression tag	UNP A7LY27
A	-26	ASN	-	expression tag	UNP A7LY27
A	-25	LYS	-	expression tag	UNP A7LY27
A	-24	PHE	-	expression tag	UNP A7LY27
A	-23	ASN	-	expression tag	UNP A7LY27
A	-22	LYS	-	expression tag	UNP A7LY27
A	-21	GLU	-	expression tag	UNP A7LY27
A	-20	ARG	-	expression tag	UNP A7LY27
A	-19	ARG	-	expression tag	UNP A7LY27
A	-18	ARG	-	expression tag	UNP A7LY27
A	-17	ALA	-	expression tag	UNP A7LY27
A	-16	ARG	-	expression tag	UNP A7LY27
A	-15	ARG	-	expression tag	UNP A7LY27
A	-14	GLU	-	expression tag	UNP A7LY27

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	ILE	-	expression tag	UNP A7LY27
A	-12	ARG	-	expression tag	UNP A7LY27
A	-11	HIS	-	expression tag	UNP A7LY27
A	-10	LEU	-	expression tag	UNP A7LY27
A	-9	PRO	-	expression tag	UNP A7LY27
A	-8	ASN	-	expression tag	UNP A7LY27
A	-7	LEU	-	expression tag	UNP A7LY27
A	-6	ASN	-	expression tag	UNP A7LY27
A	-5	ARG	-	expression tag	UNP A7LY27
A	-4	GLU	-	expression tag	UNP A7LY27
A	-3	GLN	-	expression tag	UNP A7LY27
A	-2	ARG	-	expression tag	UNP A7LY27
A	-1	ARG	-	expression tag	UNP A7LY27
A	0	ALA	-	expression tag	UNP A7LY27
A	1	PHE	-	expression tag	UNP A7LY27
A	2	ILE	-	expression tag	UNP A7LY27
A	3	ARG	-	expression tag	UNP A7LY27
A	4	SER	-	expression tag	UNP A7LY27
A	5	LEU	-	expression tag	UNP A7LY27
A	6	ARG	-	expression tag	UNP A7LY27
A	7	ASP	-	expression tag	UNP A7LY27
A	8	ASP	-	expression tag	UNP A7LY27
A	9	PRO	-	expression tag	UNP A7LY27
A	10	SER	-	expression tag	UNP A7LY27
A	11	GLN	-	expression tag	UNP A7LY27
A	12	SER	-	expression tag	UNP A7LY27
A	13	ALA	-	expression tag	UNP A7LY27
A	14	ASN	-	expression tag	UNP A7LY27
A	15	LEU	-	expression tag	UNP A7LY27
A	16	LEU	-	expression tag	UNP A7LY27
A	17	ALA	-	expression tag	UNP A7LY27
A	18	GLU	-	expression tag	UNP A7LY27
A	19	ALA	-	expression tag	UNP A7LY27
A	20	LYS	-	expression tag	UNP A7LY27
A	21	LYS	-	expression tag	UNP A7LY27
A	22	LEU	-	expression tag	UNP A7LY27
A	23	ASN	-	expression tag	UNP A7LY27
A	24	ASP	-	expression tag	UNP A7LY27
A	25	ALA	-	expression tag	UNP A7LY27
A	26	GLN	-	expression tag	UNP A7LY27
A	27	PRO	-	expression tag	UNP A7LY27
A	28	LYS	-	expression tag	UNP A7LY27

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Chain	Residue	Modelled	Actual	Comment	Reference
A	29	GLY	-	expression tag	UNP A7LY27
A	30	THR	-	expression tag	UNP A7LY27
A	31	GLU	-	expression tag	UNP A7LY27
A	32	ASN	-	expression tag	UNP A7LY27
A	33	LEU	-	expression tag	UNP A7LY27
A	34	TYR	-	expression tag	UNP A7LY27
A	35	PHE	-	expression tag	UNP A7LY27
A	36	GLN	-	expression tag	UNP A7LY27
A	37	SER	-	expression tag	UNP A7LY27
A	38	MET	-	expression tag	UNP A7LY27
A	559	GLN	-	expression tag	UNP A7LY27
B	-38	MET	-	initiating methionine	UNP A7LY27
B	-37	HIS	-	expression tag	UNP A7LY27
B	-36	HIS	-	expression tag	UNP A7LY27
B	-35	HIS	-	expression tag	UNP A7LY27
B	-34	HIS	-	expression tag	UNP A7LY27
B	-33	HIS	-	expression tag	UNP A7LY27
B	-32	HIS	-	expression tag	UNP A7LY27
B	-31	SER	-	expression tag	UNP A7LY27
B	-30	SER	-	expression tag	UNP A7LY27
B	-29	GLY	-	expression tag	UNP A7LY27
B	-28	VAL	-	expression tag	UNP A7LY27
B	-27	ASP	-	expression tag	UNP A7LY27
B	-26	ASN	-	expression tag	UNP A7LY27
B	-25	LYS	-	expression tag	UNP A7LY27
B	-24	PHE	-	expression tag	UNP A7LY27
B	-23	ASN	-	expression tag	UNP A7LY27
B	-22	LYS	-	expression tag	UNP A7LY27
B	-21	GLU	-	expression tag	UNP A7LY27
B	-20	ARG	-	expression tag	UNP A7LY27
B	-19	ARG	-	expression tag	UNP A7LY27
B	-18	ARG	-	expression tag	UNP A7LY27
B	-17	ALA	-	expression tag	UNP A7LY27
B	-16	ARG	-	expression tag	UNP A7LY27
B	-15	ARG	-	expression tag	UNP A7LY27
B	-14	GLU	-	expression tag	UNP A7LY27
B	-13	ILE	-	expression tag	UNP A7LY27
B	-12	ARG	-	expression tag	UNP A7LY27
B	-11	HIS	-	expression tag	UNP A7LY27
B	-10	LEU	-	expression tag	UNP A7LY27
B	-9	PRO	-	expression tag	UNP A7LY27
B	-8	ASN	-	expression tag	UNP A7LY27

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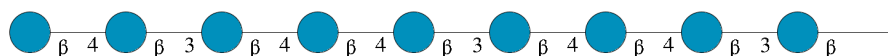
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	LEU	-	expression tag	UNP A7LY27
B	-6	ASN	-	expression tag	UNP A7LY27
B	-5	ARG	-	expression tag	UNP A7LY27
B	-4	GLU	-	expression tag	UNP A7LY27
B	-3	GLN	-	expression tag	UNP A7LY27
B	-2	ARG	-	expression tag	UNP A7LY27
B	-1	ARG	-	expression tag	UNP A7LY27
B	0	ALA	-	expression tag	UNP A7LY27
B	1	PHE	-	expression tag	UNP A7LY27
B	2	ILE	-	expression tag	UNP A7LY27
B	3	ARG	-	expression tag	UNP A7LY27
B	4	SER	-	expression tag	UNP A7LY27
B	5	LEU	-	expression tag	UNP A7LY27
B	6	ARG	-	expression tag	UNP A7LY27
B	7	ASP	-	expression tag	UNP A7LY27
B	8	ASP	-	expression tag	UNP A7LY27
B	9	PRO	-	expression tag	UNP A7LY27
B	10	SER	-	expression tag	UNP A7LY27
B	11	GLN	-	expression tag	UNP A7LY27
B	12	SER	-	expression tag	UNP A7LY27
B	13	ALA	-	expression tag	UNP A7LY27
B	14	ASN	-	expression tag	UNP A7LY27
B	15	LEU	-	expression tag	UNP A7LY27
B	16	LEU	-	expression tag	UNP A7LY27
B	17	ALA	-	expression tag	UNP A7LY27
B	18	GLU	-	expression tag	UNP A7LY27
B	19	ALA	-	expression tag	UNP A7LY27
B	20	LYS	-	expression tag	UNP A7LY27
B	21	LYS	-	expression tag	UNP A7LY27
B	22	LEU	-	expression tag	UNP A7LY27
B	23	ASN	-	expression tag	UNP A7LY27
B	24	ASP	-	expression tag	UNP A7LY27
B	25	ALA	-	expression tag	UNP A7LY27
B	26	GLN	-	expression tag	UNP A7LY27
B	27	PRO	-	expression tag	UNP A7LY27
B	28	LYS	-	expression tag	UNP A7LY27
B	29	GLY	-	expression tag	UNP A7LY27
B	30	THR	-	expression tag	UNP A7LY27
B	31	GLU	-	expression tag	UNP A7LY27
B	32	ASN	-	expression tag	UNP A7LY27
B	33	LEU	-	expression tag	UNP A7LY27
B	34	TYR	-	expression tag	UNP A7LY27

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Chain	Residue	Modelled	Actual	Comment	Reference
B	35	PHE	-	expression tag	UNP A7LY27
B	36	GLN	-	expression tag	UNP A7LY27
B	37	SER	-	expression tag	UNP A7LY27
B	38	MET	-	expression tag	UNP A7LY27
B	559	GLN	-	expression tag	UNP A7LY27

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	9	Total	C	O	0	0	0
			100	54	46			
2	D	9	Total	C	O	0	1	0
			101	54	47			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

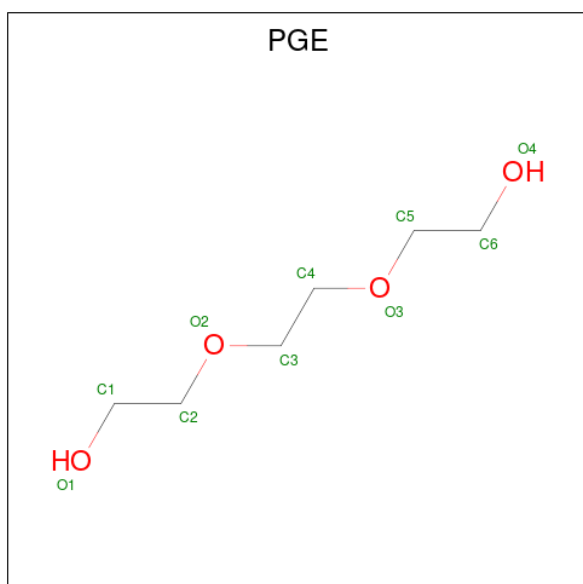
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).

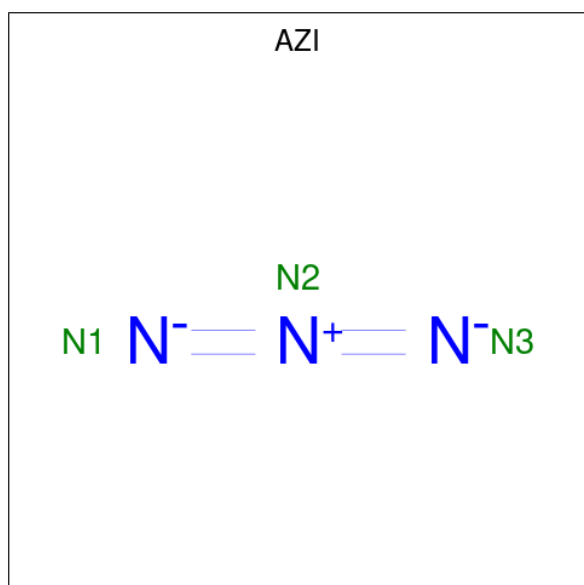


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 10 6 4	0	0
5	A	1	Total C O 10 6 4	0	0
5	A	1	Total C O 10 6 4	0	0
5	A	1	Total C O 10 6 4	0	0
5	B	1	Total C O 10 6 4	0	0
5	B	1	Total C O 10 6 4	0	0
5	B	1	Total C O 10 6 4	0	0
5	B	1	Total C O 10 6 4	0	0

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

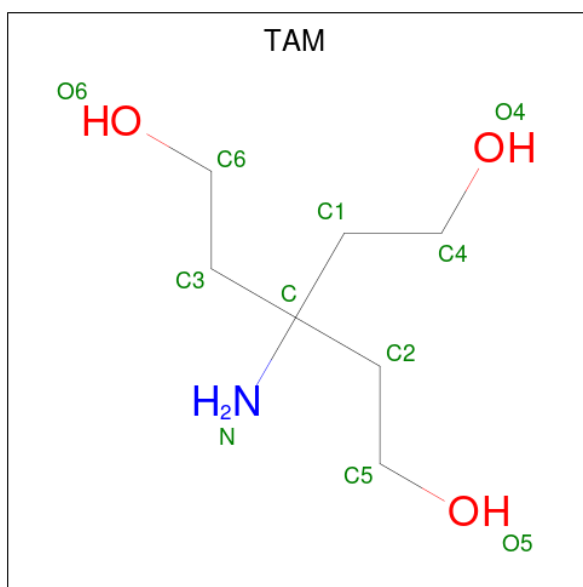
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Na 2 2	0	0
6	B	1	Total Na 1 1	0	0

- Molecule 7 is AZIDE ION (CCD ID: AZI) (formula: N₃).



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

- Molecule 8 is TRIS(HYDROXYETHYL)AMINOMETHANE (CCD ID: TAM) (formula: $C_7H_{17}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			11	7	1	3		

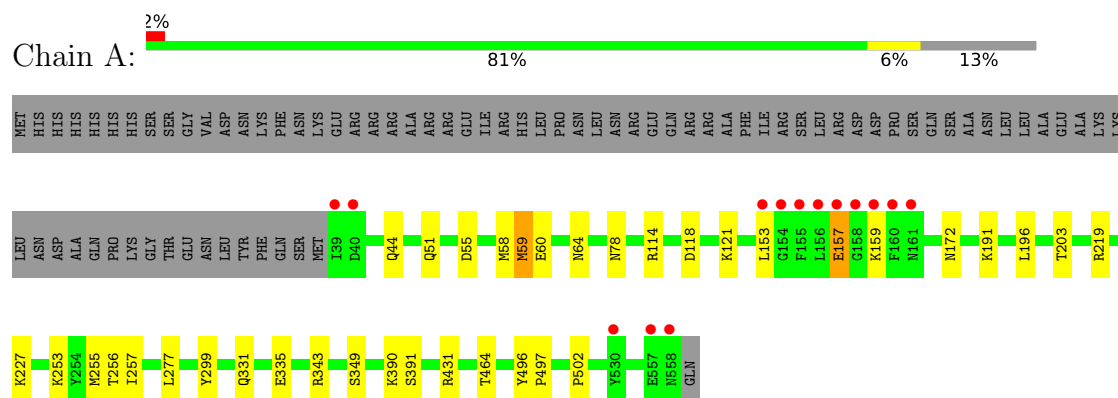
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	516	Total	O	0	0
			516	516		
9	B	474	Total	O	0	0
			474	474		

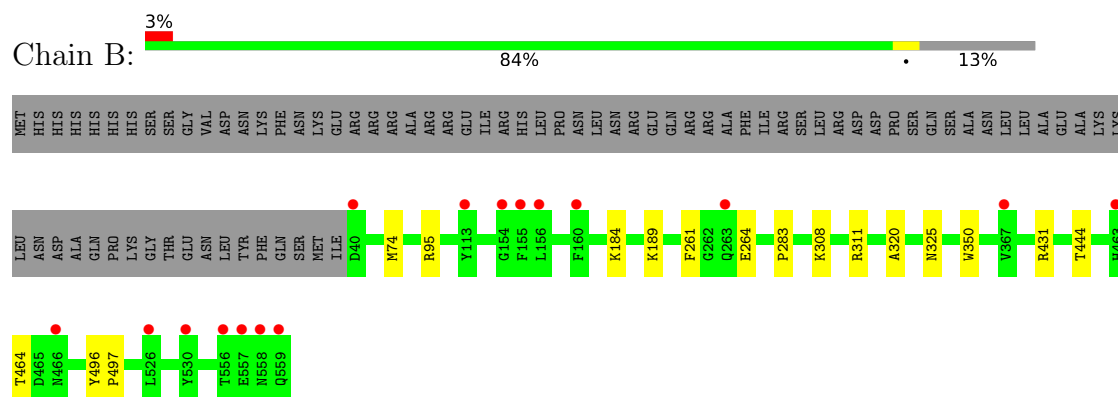
3 Residue-property plots [i](#)

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: Surface glycan-binding protein BO2743



- Molecule 1: Surface glycan-binding protein BO2743



- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain D: 33% 44% 22%

BCC1
BCC2
BCC3
BCC4
BCC5
BCC6
BCC7
BCC8
BCC9

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.84Å 88.44Å 156.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.86 – 1.43 44.86 – 1.43	Depositor EDS
% Data completeness (in resolution range)	78.3 (44.86-1.43) 78.3 (44.86-1.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 1.43Å)	Xtriage
Refinement program	PHENIX 1.19	Depositor
R, R_{free}	0.162 , 0.190 0.165 , 0.192	Depositor DCC
R_{free} test set	8680 reflections (3.88%)	wwPDB-VP
Wilson B-factor (Å ²)	17.5	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.001 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9707	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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: BGC, AZI, MG, NA, GOL, PGE, TAM

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	0.63	1/4349 (0.0%)	0.78	1/5911 (0.0%)
1	B	0.61	0/4276	0.73	0/5811
All	All	0.62	1/8625 (0.0%)	0.76	1/11722 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	MET	SD-CE	-5.46	1.65	1.79

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	LEU	CB-CA-C	5.45	121.26	110.42

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	4196	0	4019	33	0
1	B	4152	0	3961	16	0
2	C	100	0	84	2	0
2	D	101	0	80	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	12	0	14	1	0
4	B	18	0	22	1	0
5	A	40	0	56	18	0
5	B	40	0	56	7	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
7	A	24	0	0	1	0
7	B	18	0	0	1	0
8	B	11	0	17	0	0
9	A	516	0	0	10	0
9	B	474	0	0	5	0
All	All	9707	0	8309	60	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 4.

The worst 5 of 60 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:331:GLN:HE21	1:A:335:GLU:HG3	1.38	0.87
1:A:196:LEU:HA	5:A:606:PGE:H5	1.59	0.83
1:A:203:THR:HG23	7:A:611:AZI:N3	1.97	0.80
1:A:196:LEU:HD23	5:A:606:PGE:H42	1.65	0.76
1:B:264:GLU:N	1:B:264:GLU:OE2	2.22	0.72

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	535/598 (90%)	520 (97%)	14 (3%)	1 (0%)	43	22
1	B	526/598 (88%)	516 (98%)	10 (2%)	0	100	100
All	All	1061/1196 (89%)	1036 (98%)	24 (2%)	1 (0%)	48	23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	GLU

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	455/511 (89%)	451 (99%)	4 (1%)	70	44
1	B	446/511 (87%)	444 (100%)	2 (0%)	84	69
All	All	901/1022 (88%)	895 (99%)	6 (1%)	86	53

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	464[B]	THR
1	B	431[A]	ARG
1	B	431[B]	ARG
1	A	431[B]	ARG
1	A	431[A]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	81	ASN
1	B	91	ASN
1	B	428	GLN
1	B	325	ASN
1	B	331	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

19 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	0.29	0	17,17,17	0.84	1 (5%)
2	BGC	C	2	2	11,11,12	1.33	1 (9%)	15,15,17	1.24	2 (13%)
2	BGC	C	3	2	11,11,12	0.23	0	15,15,17	0.83	0
2	BGC	C	4	2	11,11,12	0.79	0	15,15,17	1.14	1 (6%)
2	BGC	C	5	2	11,11,12	0.65	0	15,15,17	1.05	1 (6%)
2	BGC	C	6	2	11,11,12	0.64	0	15,15,17	0.87	1 (6%)
2	BGC	C	7	2	11,11,12	0.99	1 (9%)	15,15,17	1.08	1 (6%)
2	BGC	C	8	2	11,11,12	0.42	0	15,15,17	0.58	0
2	BGC	C	9	2	11,11,12	0.34	0	15,15,17	0.61	0
2	BGC	D	1	2	12,12,12	0.35	0	17,17,17	0.83	1 (5%)
2	BGC	D	2	2	11,11,12	1.08	1 (9%)	15,15,17	0.87	1 (6%)
2	BGC	D	3	2	11,11,12	0.69	0	15,15,17	1.30	1 (6%)
2	BGC	D	4	2	11,11,12	0.58	0	15,15,17	1.56	2 (13%)
2	BGC	D	5[A]	-	11,11,12	0.43	0	15,15,17	0.97	0
2	BGC	D	5[B]	-	11,11,12	1.64	1 (9%)	15,15,17	1.32	1 (6%)
2	BGC	D	6	2	11,11,12	0.80	0	15,15,17	0.96	0
2	BGC	D	7	2	11,11,12	0.77	0	15,15,17	1.16	1 (6%)
2	BGC	D	8	2	11,11,12	0.38	0	15,15,17	0.63	0
2	BGC	D	9	2	11,11,12	0.57	0	15,15,17	0.59	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
2	BGC	C	1	2	-	2/2/22/22	0/1/1/1
2	BGC	C	2	2	-	1/2/19/22	0/1/1/1
2	BGC	C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	C	4	2	-	0/2/19/22	0/1/1/1
2	BGC	C	5	2	-	0/2/19/22	0/1/1/1
2	BGC	C	6	2	-	0/2/19/22	0/1/1/1
2	BGC	C	7	2	-	0/2/19/22	0/1/1/1
2	BGC	C	8	2	-	0/2/19/22	0/1/1/1
2	BGC	C	9	2	-	2/2/19/22	0/1/1/1
2	BGC	D	1	2	-	2/2/22/22	0/1/1/1
2	BGC	D	2	2	-	0/2/19/22	0/1/1/1
2	BGC	D	3	2	-	0/2/19/22	0/1/1/1
2	BGC	D	4	2	-	0/2/19/22	0/1/1/1
2	BGC	D	5[A]	-	-	1/2/19/22	0/1/1/1
2	BGC	D	5[B]	-	-	2/2/19/22	0/1/1/1
2	BGC	D	6	2	-	2/2/19/22	0/1/1/1
2	BGC	D	7	2	-	0/2/19/22	0/1/1/1
2	BGC	D	8	2	-	0/2/19/22	0/1/1/1
2	BGC	D	9	2	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	5[B]	BGC	O6-C6	-5.25	1.20	1.42
2	C	2	BGC	O5-C1	-4.28	1.36	1.43
2	D	2	BGC	O5-C1	-3.42	1.37	1.43
2	C	7	BGC	O5-C1	-2.95	1.38	1.43

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	5[B]	BGC	O6-C6-C5	3.85	124.45	111.33
2	D	4	BGC	O3-C3-C2	-3.79	102.33	110.05
2	C	5	BGC	O4-C4-C5	-3.23	101.38	109.32
2	C	2	BGC	C1-O5-C5	3.04	116.26	112.19
2	D	3	BGC	O3-C3-C2	-3.01	103.91	110.05

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

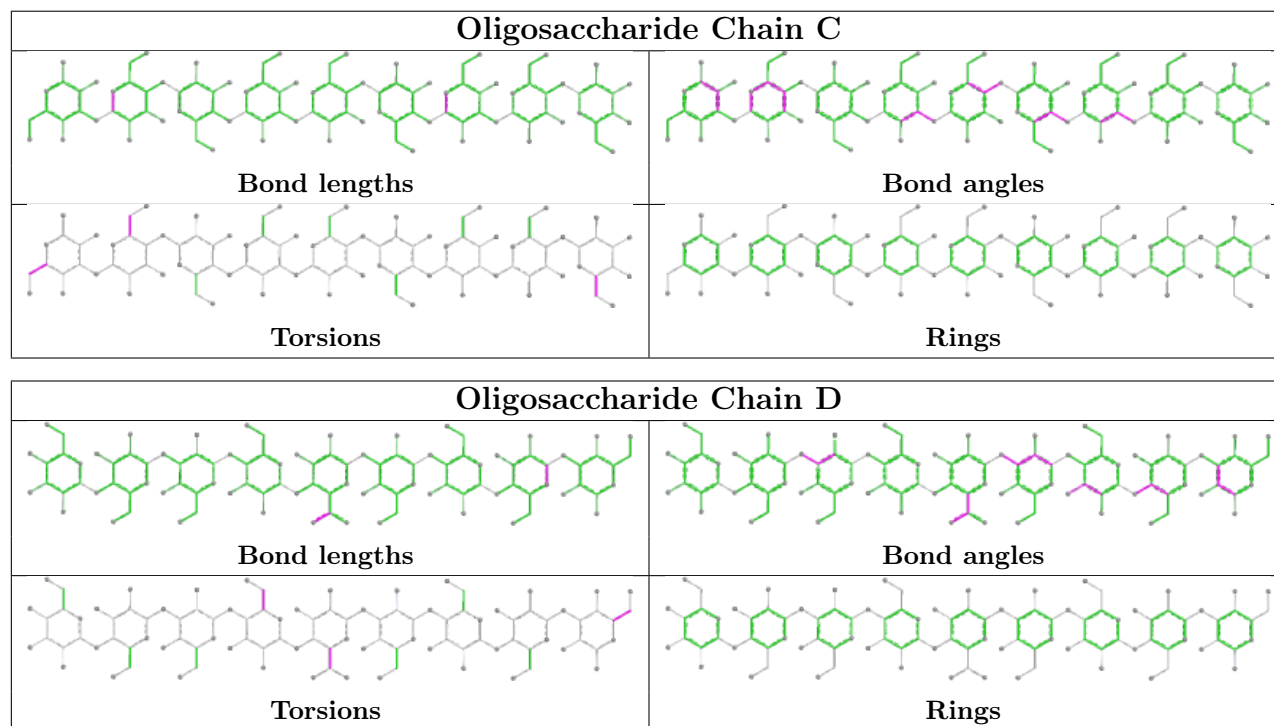
Mol	Chain	Res	Type	Atoms
2	D	5[B]	BGC	C4-C5-C6-O6
2	C	9	BGC	O5-C5-C6-O6
2	D	1	BGC	O5-C5-C6-O6
2	C	1	BGC	O5-C5-C6-O6
2	D	5[B]	BGC	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	9	BGC	1	0
2	C	1	BGC	1	0
2	D	5[A]	BGC	1	0
2	D	1	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 33 ligands modelled in this entry, 5 are monoatomic - leaving 28 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	GOL	A	603	-	5,5,5	3.08	3 (60%)	5,5,5	0.81	0
7	AZI	A	610	-	2,2,2	2.89	2 (100%)	0,1,1	-	-
7	AZI	B	613	-	2,2,2	3.41	2 (100%)	0,1,1	-	-
4	GOL	B	604	-	5,5,5	0.56	0	5,5,5	1.26	1 (20%)
7	AZI	A	612	-	2,2,2	3.72	2 (100%)	0,1,1	-	-
8	TAM	B	602	-	10,10,10	0.51	0	12,12,12	3.87	4 (33%)
7	AZI	A	616	-	2,2,2	2.74	2 (100%)	0,1,1	-	-
5	PGE	A	607	-	9,9,9	0.31	0	8,8,8	0.79	0
4	GOL	B	603	-	5,5,5	0.48	0	5,5,5	1.12	0
7	AZI	A	615	-	2,2,2	2.80	2 (100%)	0,1,1	-	-
5	PGE	B	608	-	9,9,9	0.53	0	8,8,8	0.23	0
7	AZI	B	614	-	2,2,2	2.65	2 (100%)	0,1,1	-	-
7	AZI	A	614	-	2,2,2	2.36	2 (100%)	0,1,1	-	-
4	GOL	A	602	-	5,5,5	1.01	0	5,5,5	0.88	0
7	AZI	A	617	-	2,2,2	3.78	2 (100%)	0,1,1	-	-
5	PGE	A	606	-	9,9,9	0.49	0	8,8,8	1.00	0
5	PGE	B	606	-	9,9,9	0.35	0	8,8,8	0.47	0
5	PGE	A	604	-	9,9,9	0.30	0	8,8,8	0.67	0
5	PGE	A	605	-	9,9,9	0.39	0	8,8,8	0.55	0
7	AZI	B	612	-	2,2,2	2.64	2 (100%)	0,1,1	-	-
5	PGE	B	607	-	9,9,9	0.37	0	8,8,8	0.34	0
4	GOL	B	605	-	5,5,5	2.66	3 (60%)	5,5,5	0.94	0
7	AZI	B	616	-	2,2,2	2.43	2 (100%)	0,1,1	-	-
7	AZI	A	611	-	2,2,2	2.95	2 (100%)	0,1,1	-	-
7	AZI	B	615	-	2,2,2	3.11	2 (100%)	0,1,1	-	-
5	PGE	B	609	-	9,9,9	0.51	0	8,8,8	0.74	0
7	AZI	A	613	-	2,2,2	2.94	2 (100%)	0,1,1	-	-
7	AZI	B	611	-	2,2,2	2.70	2 (100%)	0,1,1	-	-

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	GOL	B	603	-	-	0/4/4/4	-
4	GOL	A	603	-	-	1/4/4/4	-
5	PGE	A	606	-	-	6/7/7/7	-
5	PGE	B	607	-	-	3/7/7/7	-
4	GOL	B	605	-	-	0/4/4/4	-
4	GOL	B	604	-	-	2/4/4/4	-
5	PGE	B	606	-	-	2/7/7/7	-
5	PGE	A	604	-	-	2/7/7/7	-
5	PGE	B	608	-	-	5/7/7/7	-
8	TAM	B	602	-	-	9/12/12/12	-
5	PGE	A	605	-	-	5/7/7/7	-
5	PGE	A	607	-	-	4/7/7/7	-
5	PGE	B	609	-	-	6/7/7/7	-
4	GOL	A	602	-	-	1/4/4/4	-

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	GOL	O2-C2	-5.56	1.27	1.43
7	A	612	AZI	N3-N2	-3.97	1.15	1.23
4	B	605	GOL	O2-C2	-3.96	1.31	1.43
7	A	617	AZI	N3-N2	-3.81	1.15	1.23
7	A	617	AZI	N1-N2	-3.76	1.15	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	602	TAM	C6-C3-C	-8.82	105.56	115.97
8	B	602	TAM	C4-C1-C	-7.78	106.79	115.97
8	B	602	TAM	C5-C2-C	-5.17	109.87	115.97
8	B	602	TAM	C3-C-C1	-2.79	105.58	110.50
4	B	604	GOL	C3-C2-C1	-2.41	102.95	111.80

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	602	TAM	C2-C-C1-C4

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Mol	Chain	Res	Type	Atoms
8	B	602	TAM	N-C-C1-C4
8	B	602	TAM	C1-C-C2-C5
8	B	602	TAM	C3-C-C2-C5
8	B	602	TAM	N-C-C2-C5

There are no ring outliers.

11 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	GOL	1	0
7	B	613	AZI	1	0
5	A	607	PGE	5	0
4	B	603	GOL	1	0
5	B	608	PGE	1	0
5	A	606	PGE	5	0
5	B	606	PGE	1	0
5	A	604	PGE	2	0
5	A	605	PGE	6	0
7	A	611	AZI	1	0
5	B	609	PGE	5	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	520/598 (86%)	-0.15	14 (2%) 56 59	10, 18, 32, 51	17 (3%)
1	B	520/598 (86%)	0.04	16 (3%) 51 54	11, 20, 42, 60	8 (1%)
All	All	1040/1196 (86%)	-0.06	30 (2%) 53 57	10, 19, 38, 60	25 (2%)

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	159	LYS	7.7
1	A	158	GLY	7.4
1	A	160	PHE	6.8
1	A	156	LEU	6.3
1	B	559	GLN	6.2

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.

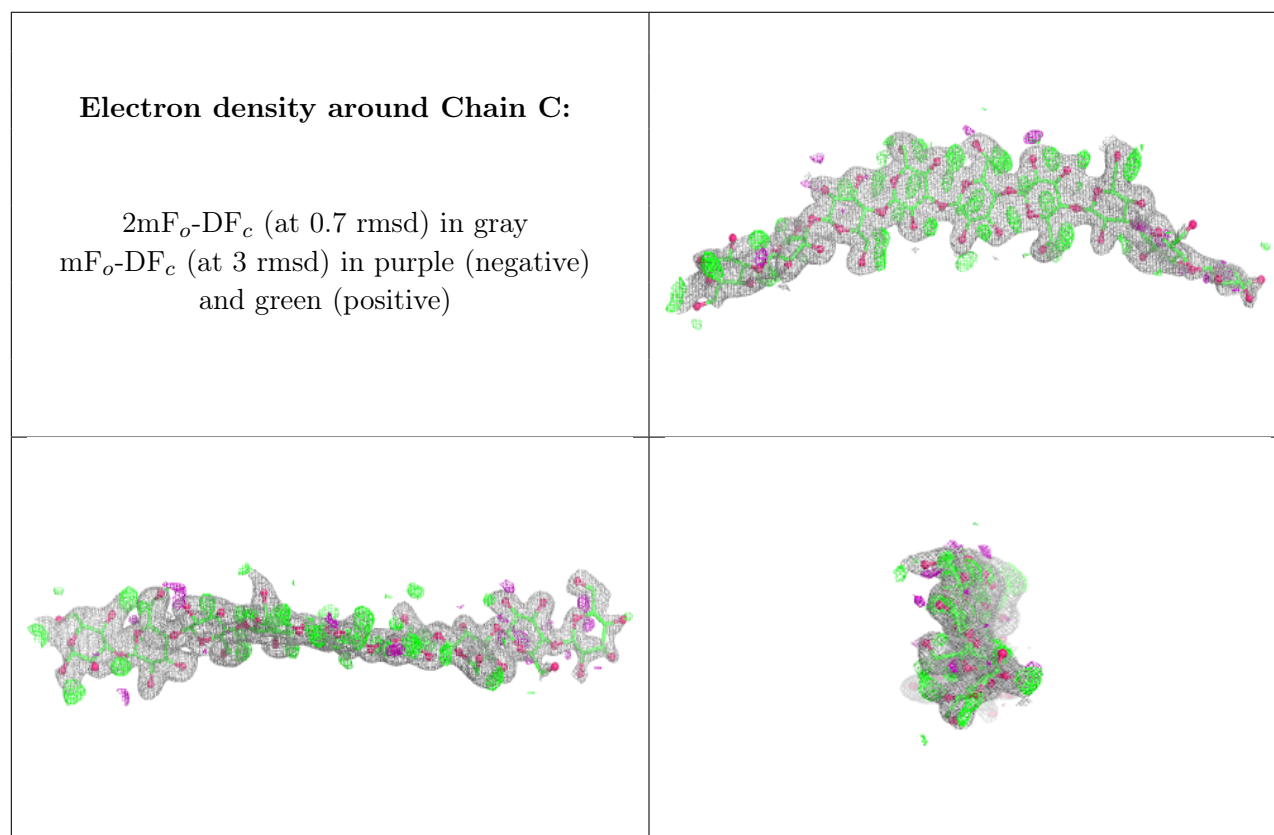
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BGC	C	1	12/12	0.68	0.17	49,59,64,72	0
2	BGC	D	1	12/12	0.78	0.14	43,51,59,60	0
2	BGC	D	9	11/12	0.78	0.16	35,54,65,65	0
2	BGC	C	9	11/12	0.81	0.16	44,60,65,66	0
2	BGC	D	8	11/12	0.85	0.15	30,40,48,61	0

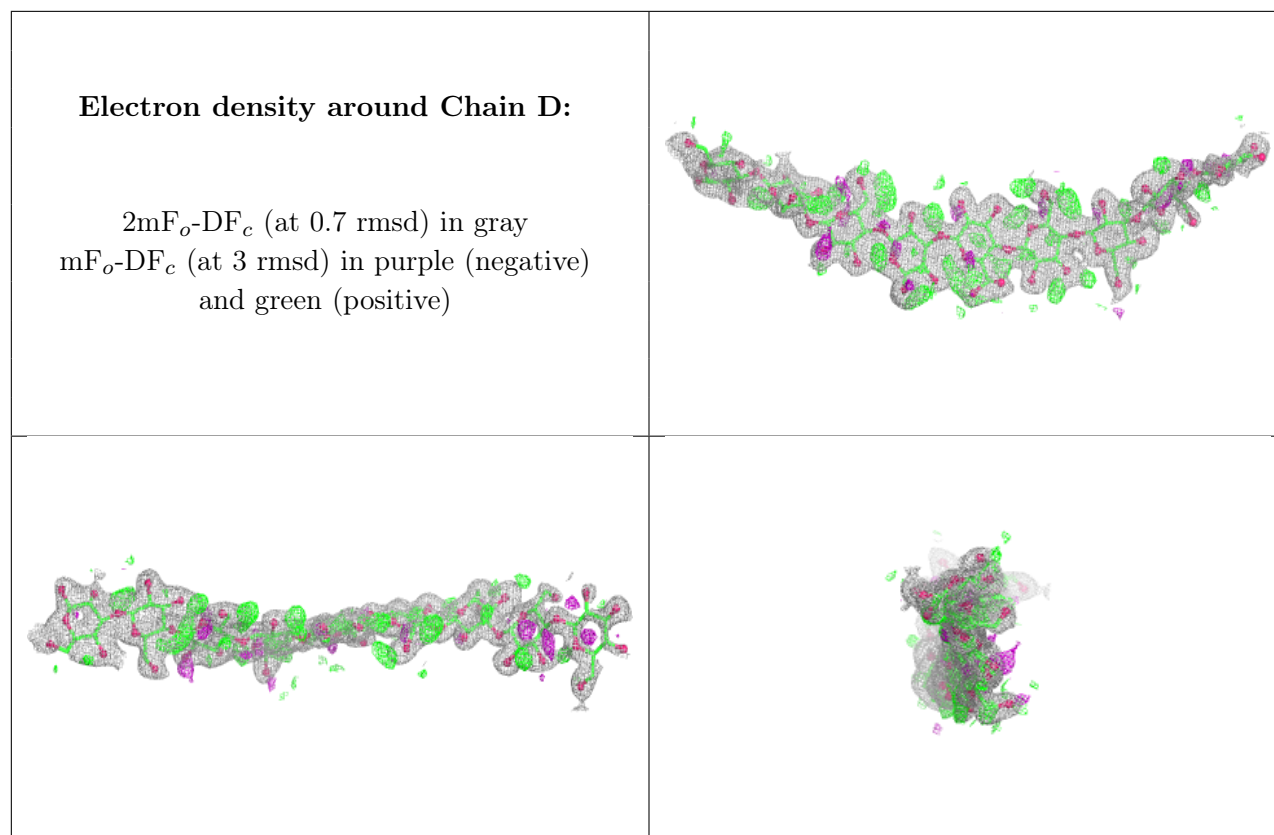
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BGC	C	8	11/12	0.85	0.14	33,37,54,60	0
2	BGC	D	5[B]	11/12	0.87	0.13	18,22,28,29	1
2	BGC	D	3	11/12	0.87	0.12	19,26,30,32	0
2	BGC	D	5[A]	11/12	0.87	0.13	18,22,29,31	1
2	BGC	D	7	11/12	0.88	0.12	23,27,29,37	0
2	BGC	D	4	11/12	0.89	0.10	15,21,24,30	0
2	BGC	D	2	11/12	0.89	0.12	25,32,45,45	0
2	BGC	C	5	11/12	0.89	0.12	15,23,29,31	0
2	BGC	C	4	11/12	0.90	0.10	17,20,24,30	0
2	BGC	C	7	11/12	0.90	0.10	21,27,32,34	0
2	BGC	D	6	11/12	0.90	0.11	15,21,30,30	0
2	BGC	C	6	11/12	0.91	0.10	18,23,28,31	0
2	BGC	C	2	11/12	0.91	0.11	21,28,43,48	0
2	BGC	C	3	11/12	0.92	0.09	16,22,27,28	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	PGE	B	608	10/10	0.53	0.26	31,52,65,66	0
7	AZI	A	614	3/3	0.72	0.14	34,34,36,38	0
7	AZI	A	611	3/3	0.74	0.17	38,38,39,55	0
5	PGE	A	607	10/10	0.74	0.20	36,49,54,57	0
7	AZI	A	616	3/3	0.77	0.13	41,41,45,48	0
7	AZI	B	614	3/3	0.77	0.14	43,43,50,52	0
5	PGE	A	605	10/10	0.79	0.18	28,48,55,63	0
8	TAM	B	602	11/11	0.79	0.17	26,48,69,79	0
7	AZI	A	615	3/3	0.81	0.12	42,42,42,60	0
5	PGE	A	606	10/10	0.81	0.17	23,38,55,57	0
5	PGE	A	604	10/10	0.82	0.17	30,37,68,78	0
7	AZI	B	612	3/3	0.82	0.11	39,39,46,48	0
5	PGE	B	607	10/10	0.83	0.15	41,52,58,65	0
7	AZI	A	612	3/3	0.83	0.13	33,33,40,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	602	6/6	0.83	0.14	29,36,44,45	0
5	PGE	B	609	10/10	0.83	0.16	28,39,55,58	0
7	AZI	B	616	3/3	0.85	0.32	26,26,34,34	0
7	AZI	A	613	3/3	0.85	0.12	40,40,57,59	0
7	AZI	B	613	3/3	0.86	0.12	32,32,35,40	0
4	GOL	B	603	6/6	0.86	0.12	27,39,44,54	0
7	AZI	B	611	3/3	0.87	0.12	27,27,31,49	0
7	AZI	B	615	3/3	0.87	0.11	44,44,46,57	0
5	PGE	B	606	10/10	0.87	0.13	34,39,52,52	0
4	GOL	B	604	6/6	0.87	0.15	27,47,55,59	0
7	AZI	A	617	3/3	0.89	0.10	32,32,44,46	0
7	AZI	A	610	3/3	0.89	0.12	29,29,31,51	0
6	NA	B	610	1/1	0.95	0.07	25,25,25,25	0
6	NA	A	609	1/1	0.96	0.07	28,28,28,28	0
4	GOL	A	603	6/6	0.97	0.08	15,18,27,31	0
6	NA	A	608	1/1	0.98	0.08	23,23,23,23	0
3	MG	B	601	1/1	0.98	0.04	16,16,16,16	0
4	GOL	B	605	6/6	0.98	0.06	18,23,24,29	0
3	MG	A	601	1/1	0.99	0.02	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.