



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:24 AM UTC

PDB ID : 6HA9 / pdb_00006ha9
Title : Structure of an endo-Xyloglucanase from Cellvibrio japonicus complexed with
XXXG(2F)-beta-DNP
Authors : Offen, W.A.; Davies, G.J.
Deposited on : 2018-08-07
Resolution : 2.00 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

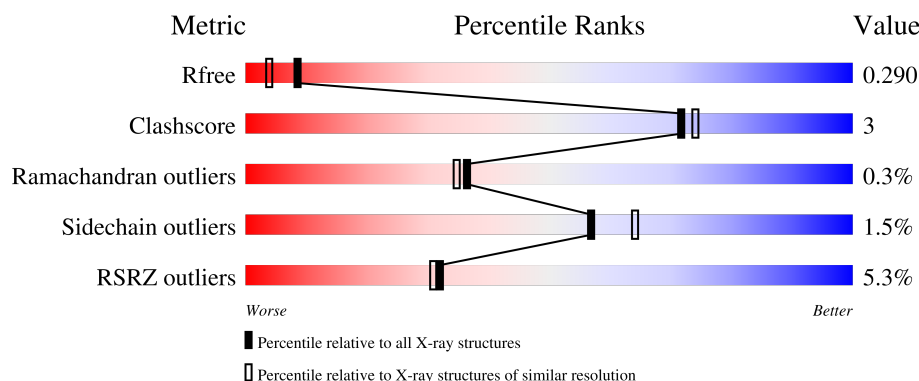
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	396	 3% 79% 13% • 7%
1	B	396	 7% 84% 9% • 7%
2	C	6	 100%
3	D	7	 100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6291 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 Cellulase, putative, cel5D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	4	0
			2954	1873	501	569	11			
1	B	370	Total	C	N	O	S	0	3	0
			2916	1848	496	562	10			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	MET	-	initiating methionine	UNP B3PD52
A	74	GLY	-	expression tag	UNP B3PD52
A	75	SER	-	expression tag	UNP B3PD52
A	76	SER	-	expression tag	UNP B3PD52
A	77	HIS	-	expression tag	UNP B3PD52
A	78	HIS	-	expression tag	UNP B3PD52
A	79	HIS	-	expression tag	UNP B3PD52
A	80	HIS	-	expression tag	UNP B3PD52
A	81	HIS	-	expression tag	UNP B3PD52
A	82	HIS	-	expression tag	UNP B3PD52
A	83	SER	-	expression tag	UNP B3PD52
A	84	SER	-	expression tag	UNP B3PD52
A	85	GLY	-	expression tag	UNP B3PD52
A	86	LEU	-	expression tag	UNP B3PD52
A	87	VAL	-	expression tag	UNP B3PD52
A	88	PRO	-	expression tag	UNP B3PD52
A	89	ARG	-	expression tag	UNP B3PD52
A	90	GLY	-	expression tag	UNP B3PD52
A	91	SER	-	expression tag	UNP B3PD52
A	92	HIS	-	expression tag	UNP B3PD52
A	93	MET	-	expression tag	UNP B3PD52
A	94	ALA	-	expression tag	UNP B3PD52
A	95	SER	-	expression tag	UNP B3PD52
A	255	ALA	GLU	engineered mutation	UNP B3PD52
B	73	MET	-	initiating methionine	UNP B3PD52

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Chain	Residue	Modelled	Actual	Comment	Reference
B	74	GLY	-	expression tag	UNP B3PD52
B	75	SER	-	expression tag	UNP B3PD52
B	76	SER	-	expression tag	UNP B3PD52
B	77	HIS	-	expression tag	UNP B3PD52
B	78	HIS	-	expression tag	UNP B3PD52
B	79	HIS	-	expression tag	UNP B3PD52
B	80	HIS	-	expression tag	UNP B3PD52
B	81	HIS	-	expression tag	UNP B3PD52
B	82	HIS	-	expression tag	UNP B3PD52
B	83	SER	-	expression tag	UNP B3PD52
B	84	SER	-	expression tag	UNP B3PD52
B	85	GLY	-	expression tag	UNP B3PD52
B	86	LEU	-	expression tag	UNP B3PD52
B	87	VAL	-	expression tag	UNP B3PD52
B	88	PRO	-	expression tag	UNP B3PD52
B	89	ARG	-	expression tag	UNP B3PD52
B	90	GLY	-	expression tag	UNP B3PD52
B	91	SER	-	expression tag	UNP B3PD52
B	92	HIS	-	expression tag	UNP B3PD52
B	93	MET	-	expression tag	UNP B3PD52
B	94	ALA	-	expression tag	UNP B3PD52
B	95	SER	-	expression tag	UNP B3PD52
B	255	ALA	GLU	engineered mutation	UNP B3PD52

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-2,4-dinitrophenyl 2-deoxy-2-fluoro-beta-D-glucopyranoside.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	6	Total	C	F	N	O	0	0	0
			75	40	1	2	32			

- Molecule 3 is an oligosaccharide called alpha-D-xylopyranose-(1-6)-beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-2,4-dinitrophenyl 2-deoxy-2-fluoro-beta-D-glucopyranoside.

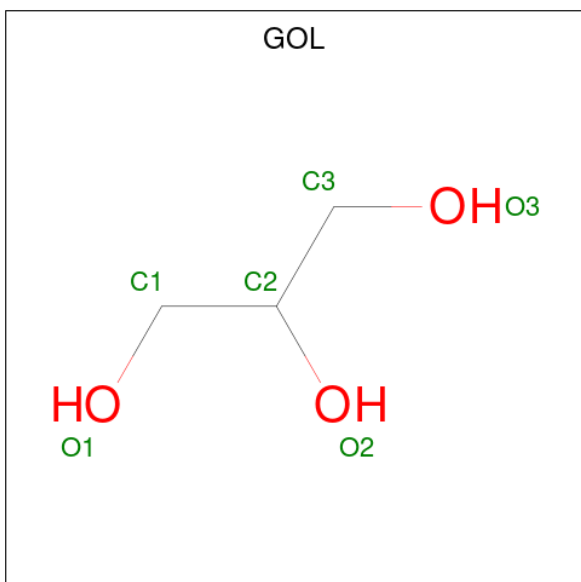
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	7	Total	C	F	N	O	0	0	0
			84	45	1	2	36			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



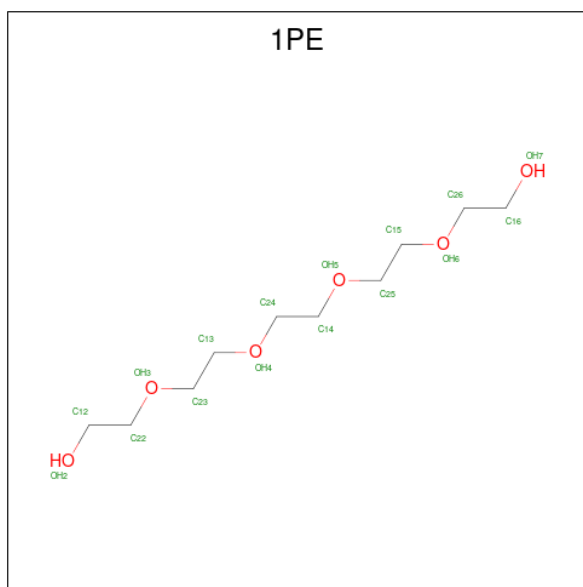
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			16	10	6		

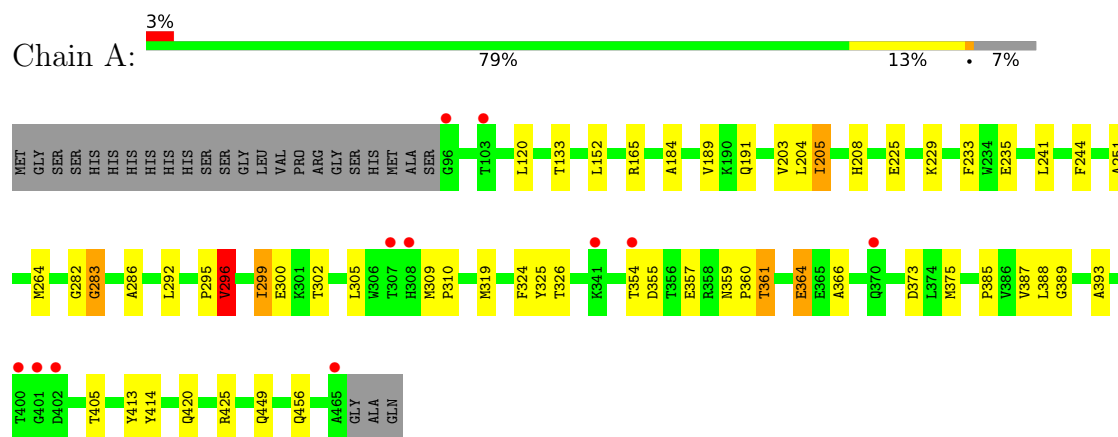
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	112	Total	O	0	0
			112	112		
7	B	97	Total	O	0	0
			97	97		

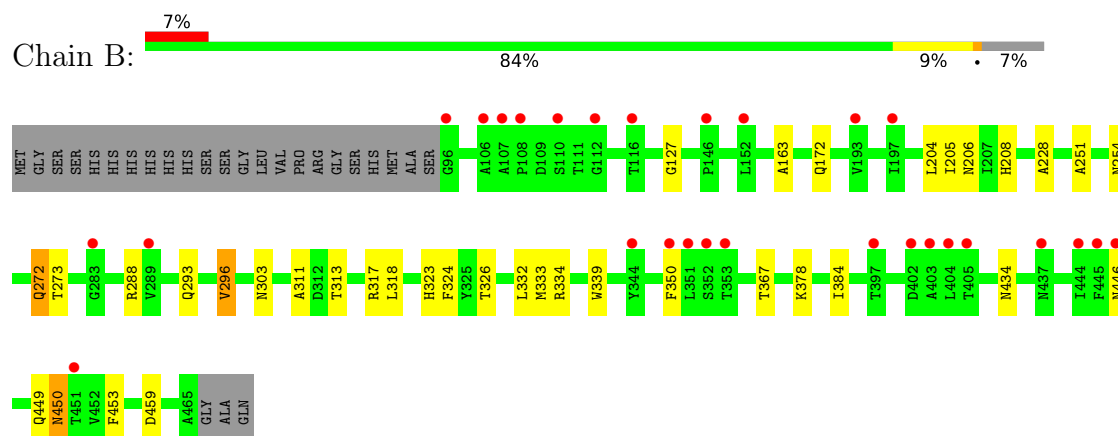
3 Residue-property plots [i](#)

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.

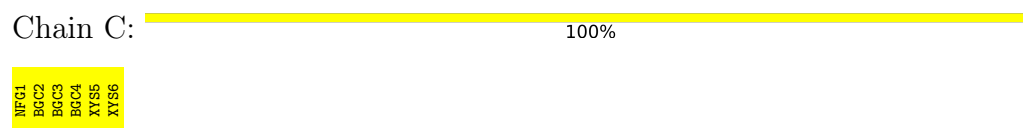
- Molecule 1: Cellulase, putative, cel5D



- Molecule 1: Cellulase, putative, cel5D



- Molecule 2: beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-2,4-dinitrophenyl 2-deoxy-2-fluoro-beta-D-glucopyranoside



- Molecule 3: alpha-D-xylopyranose-(1-6)-beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-2,4-dinitro phenyl 2-deoxy-2-fluoro-beta-D-glucopyranoside

Chain D:

100%

NEG1
BGC2
BGC3
BGC4
XYS5
XYS6
XYS7

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.48Å 97.81Å 158.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.19 – 2.00 79.19 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (79.19-2.00) 99.8 (79.19-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.219 , 0.287 0.227 , 0.290	Depositor DCC
R_{free} test set	2965 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6291	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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: 1PE, XYS, NFG, GOL, BGC, SO4

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	1.28	19/3027 (0.6%)	1.20	9/4124 (0.2%)
1	B	1.25	13/2989 (0.4%)	1.24	4/4078 (0.1%)
All	All	1.27	32/6016 (0.5%)	1.22	13/8202 (0.2%)

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	2
1	B	0	3
All	All	0	5

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	127	GLY	N-CA	10.56	1.55	1.44
1	B	172	GLN	N-CA	8.67	1.57	1.46
1	B	323	HIS	CE1-NE2	7.31	1.39	1.32
1	B	384	ILE	N-CA	7.30	1.51	1.46
1	A	366	ALA	C-O	6.79	1.32	1.24
1	A	456	GLN	C-O	6.72	1.31	1.24
1	A	184	ALA	C-O	-6.64	1.16	1.24
1	A	229	LYS	N-CA	6.59	1.54	1.46
1	A	325	TYR	N-CA	6.32	1.53	1.46
1	A	244	PHE	N-CA	5.91	1.53	1.45
1	A	235	GLU	N-CA	5.88	1.53	1.46
1	B	332	LEU	C-O	-5.85	1.17	1.23
1	A	286	ALA	N-CA	5.77	1.53	1.46
1	A	152	LEU	N-CA	5.58	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	225	GLU	N-CA	5.57	1.53	1.46
1	A	208	HIS	CE1-NE2	5.53	1.38	1.32
1	B	453	PHE	C-O	-5.51	1.17	1.24
1	A	191	GLN	C-O	5.49	1.30	1.24
1	B	318	LEU	N-CA	5.49	1.52	1.45
1	A	389	GLY	N-CA	5.46	1.53	1.45
1	B	205	ILE	N-CA	5.36	1.52	1.46
1	A	420	GLN	N-CA	5.35	1.52	1.46
1	A	299	ILE	N-CA	5.33	1.52	1.46
1	B	228	ALA	N-CA	5.32	1.52	1.46
1	B	163	ALA	N-CA	5.29	1.52	1.46
1	A	393	ALA	C-O	-5.28	1.17	1.24
1	B	313	THR	C-O	-5.09	1.17	1.24
1	B	273	THR	C-O	5.08	1.30	1.24
1	A	189	VAL	C-O	-5.03	1.18	1.24
1	B	272	GLN	N-CA	5.02	1.52	1.46
1	A	283	GLY	N-CA	5.01	1.52	1.45
1	A	241	LEU	C-O	5.00	1.30	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	350	PHE	CA-CB-CG	7.26	121.06	113.80
1	A	360	PRO	CB-CA-C	-6.38	102.72	111.21
1	A	300	GLU	CB-CG-CD	6.00	122.79	112.60
1	B	459	ASP	CA-CB-CG	5.53	118.13	112.60
1	A	282	GLY	O-C-N	-5.51	117.56	122.57
1	A	361	THR	N-CA-C	-5.50	106.61	113.38
1	A	233	PHE	CA-CB-CG	5.32	119.11	113.80
1	B	367	THR	N-CA-C	-5.17	105.83	111.82
1	B	434	ASN	CA-CB-CG	5.12	117.72	112.60
1	A	359	ASN	N-CA-CB	5.07	115.62	109.74
1	A	133	THR	CB-CA-C	5.03	120.42	110.42
1	A	282	GLY	CA-C-N	-5.00	111.60	121.41
1	A	282	GLY	C-N-CA	-5.00	111.60	121.41

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	ARG	Sidechain
1	A	283	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	B	288	ARG	Sidechain
1	B	317	ARG	Sidechain
1	B	334	ARG	Sidechain

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	2954	0	2784	27	0
1	B	2916	0	2717	12	0
2	C	75	0	54	0	0
3	D	84	0	61	0	0
4	A	5	0	0	0	0
4	B	20	0	0	0	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
6	B	16	0	22	2	0
7	A	112	0	0	3	0
7	B	97	0	0	0	0
All	All	6291	0	5654	39	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 3.

All (39) 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:309:MET:HG3	1:A:310:PRO:HD2	1.72	0.72
1:A:264:MET:HE1	1:A:295:PRO:CG	2.25	0.67
1:A:364:GLU:OE1	7:A:601:HOH:O	2.15	0.64
1:A:295:PRO:HD2	1:A:302:THR:OG1	1.99	0.63
1:A:264:MET:HE1	1:A:295:PRO:HD3	1.84	0.57
1:A:264:MET:HE3	1:A:305:LEU:HB2	1.90	0.53
1:A:264:MET:HE1	1:A:295:PRO:CD	2.38	0.53
1:A:264:MET:HE1	1:A:295:PRO:HG3	1.92	0.51
1:A:324:PHE:CZ	1:A:326:THR:HB	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:THR:OG1	7:A:602:HOH:O	2.19	0.51
1:A:355:ASP:OD1	1:A:357:GLU:OE2	2.29	0.51
1:B:324:PHE:CZ	1:B:326:THR:HB	2.46	0.51
1:A:319[A]:MET:HE2	1:A:387:VAL:HG23	1.95	0.49
1:B:206:ASN:OD1	1:B:206:ASN:C	2.54	0.48
1:A:203:VAL:HG12	1:A:205:ILE:HD12	1.96	0.47
1:A:373:ASP:OD1	1:A:425:ARG:NE	2.44	0.47
1:A:264:MET:HE1	1:A:295:PRO:HB3	1.96	0.47
1:A:373:ASP:OD2	7:A:603:HOH:O	2.20	0.47
1:B:272:GLN:NE2	1:B:311:ALA:O	2.40	0.47
1:A:264:MET:HE1	1:A:295:PRO:CB	2.45	0.46
1:B:204:LEU:HD11	1:B:251:ALA:HB2	1.96	0.46
1:A:319[A]:MET:HE3	1:A:385:PRO:HB2	1.98	0.46
1:B:293:GLN:N	1:B:293:GLN:CD	2.74	0.46
1:A:324:PHE:HB2	1:A:388:LEU:HD11	1.98	0.45
1:B:450:ASN:HD22	1:B:450:ASN:HA	1.68	0.45
1:A:357:GLU:H	1:A:357:GLU:CD	2.26	0.44
1:A:204:LEU:HD11	1:A:251:ALA:HB2	2.00	0.44
1:A:292:LEU:HD13	1:A:310:PRO:HD2	2.01	0.42
1:A:203:VAL:HG12	1:A:205:ILE:CD1	2.49	0.42
1:B:446:ASN:OD1	1:B:446:ASN:C	2.63	0.42
1:B:303:ASN:HA	1:B:378:LYS:HE3	2.02	0.42
1:A:299:ILE:HG23	1:A:375:MET:HE3	2.01	0.41
1:B:208:HIS:HA	1:B:254:ASN:HB2	2.01	0.41
1:A:120:LEU:HD12	1:A:120:LEU:HA	1.93	0.41
1:B:339:TRP:CE3	6:B:513:1PE:H122	2.56	0.41
1:A:295:PRO:C	1:A:296:VAL:HG23	2.45	0.41
1:A:413:TYR:O	1:A:414:TYR:C	2.64	0.41
1:B:339:TRP:CZ3	6:B:513:1PE:H122	2.56	0.40
1:B:333:MET:HE3	1:B:339:TRP:CH2	2.57	0.40

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	372/396 (94%)	350 (94%)	21 (6%)	1 (0%)	36	35
1	B	371/396 (94%)	350 (94%)	20 (5%)	1 (0%)	36	35
All	All	743/792 (94%)	700 (94%)	41 (6%)	2 (0%)	36	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	296	VAL
1	A	296	VAL

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	303/326 (93%)	297 (98%)	6 (2%)	48	54
1	B	294/326 (90%)	291 (99%)	3 (1%)	68	75
All	All	597/652 (92%)	588 (98%)	9 (2%)	57	64

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	ILE
1	A	296	VAL
1	A	354	THR
1	A	364	GLU
1	A	405	THR
1	A	449	GLN
1	B	296	VAL
1	B	449	GLN
1	B	450	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	ASN
1	A	199	ASN
1	A	217	ASN
1	A	247	HIS
1	A	450	ASN
1	B	114	GLN
1	B	194	GLN
1	B	217	ASN
1	B	382	GLN
1	B	437	ASN
1	B	450	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 ⓘ

13 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	NFG	C	1	2	25,25,25	3.24	7 (28%)	28,36,36	1.72	6 (21%)
2	BGC	C	2	2	11,11,12	1.42	2 (18%)	15,15,17	1.96	5 (33%)
2	BGC	C	3	2	11,11,12	1.37	2 (18%)	15,15,17	0.86	0
2	BGC	C	4	2	11,11,12	1.16	1 (9%)	15,15,17	1.91	5 (33%)
2	XYS	C	5	2	9,9,10	1.14	1 (11%)	10,12,14	1.88	4 (40%)
2	XYS	C	6	2	9,9,10	1.20	0	10,12,14	2.65	3 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NFG	D	1	3	25,25,25	2.95	7 (28%)	28,36,36	1.33	3 (10%)
3	BGC	D	2	3	11,11,12	1.62	3 (27%)	15,15,17	2.52	5 (33%)
3	BGC	D	3	3	11,11,12	1.32	2 (18%)	15,15,17	0.88	0
3	BGC	D	4	3	11,11,12	0.96	0	15,15,17	1.14	1 (6%)
3	XYS	D	5	3	9,9,10	0.67	0	10,12,14	2.37	4 (40%)
3	XYS	D	6	3	9,9,10	1.80	3 (33%)	10,12,14	1.38	1 (10%)
3	XYS	D	7	3	9,9,10	0.93	0	10,12,14	1.61	1 (10%)

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	NFG	C	1	2	-	0/10/34/34	0/2/2/2
2	BGC	C	2	2	-	0/2/19/22	0/1/1/1
2	BGC	C	3	2	-	1/2/19/22	0/1/1/1
2	BGC	C	4	2	-	0/2/19/22	0/1/1/1
2	XYS	C	5	2	-	-	0/1/1/1
2	XYS	C	6	2	-	-	0/1/1/1
3	NFG	D	1	3	-	0/10/34/34	0/2/2/2
3	BGC	D	2	3	-	0/2/19/22	0/1/1/1
3	BGC	D	3	3	-	0/2/19/22	0/1/1/1
3	BGC	D	4	3	-	0/2/19/22	0/1/1/1
3	XYS	D	5	3	-	-	0/1/1/1
3	XYS	D	6	3	-	-	0/1/1/1
3	XYS	D	7	3	-	-	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NFG	O22-N2	9.87	1.39	1.22
3	D	1	NFG	O12-N1	9.25	1.38	1.22
2	C	1	NFG	O12-N1	8.84	1.38	1.22
3	D	1	NFG	O22-N2	8.15	1.36	1.22
2	C	1	NFG	C12-C11	4.76	1.49	1.40
2	C	1	NFG	C12-N1	-4.04	1.38	1.45
2	C	1	NFG	C2-C3	3.93	1.56	1.52
3	D	1	NFG	C12-C11	3.73	1.47	1.40
3	D	2	BGC	C2-C3	3.21	1.57	1.52
3	D	3	BGC	O5-C1	3.14	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	6	XYS	O5-C5	3.09	1.48	1.43
2	C	2	BGC	C2-C3	2.96	1.57	1.52
3	D	1	NFG	O3-C3	2.89	1.50	1.43
2	C	4	BGC	C2-C3	2.89	1.56	1.52
3	D	6	XYS	C4-C3	2.81	1.56	1.52
3	D	2	BGC	O5-C5	2.77	1.48	1.43
3	D	1	NFG	C2-C1	2.67	1.55	1.52
3	D	1	NFG	C14-N2	-2.63	1.38	1.45
3	D	6	XYS	O2-C2	-2.51	1.38	1.43
2	C	2	BGC	O5-C1	2.50	1.47	1.43
3	D	3	BGC	C2-C3	2.47	1.56	1.52
2	C	5	XYS	O5-C1	2.37	1.47	1.43
2	C	1	NFG	O1-C1	2.36	1.44	1.41
2	C	3	BGC	O2-C2	2.24	1.48	1.43
2	C	3	BGC	C2-C3	2.18	1.55	1.52
3	D	1	NFG	C12-N1	-2.10	1.41	1.45
2	C	1	NFG	O3-C3	2.07	1.48	1.43
3	D	2	BGC	O4-C4	2.03	1.48	1.43

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	BGC	C1-O5-C5	6.53	120.94	112.19
2	C	6	XYS	C5-C4-C3	5.25	117.28	109.64
2	C	6	XYS	O3-C3-C2	-5.07	99.72	110.05
3	D	5	XYS	C5-O5-C1	5.06	119.58	111.42
2	C	2	BGC	C1-O5-C5	4.80	118.61	112.19
2	C	4	BGC	C1-C2-C3	4.64	116.40	109.64
3	D	2	BGC	C1-C2-C3	4.52	116.22	109.64
2	C	1	NFG	F-C2-C3	-3.84	105.48	108.81
3	D	2	BGC	O5-C1-C2	3.70	119.61	110.79
3	D	4	BGC	C1-O5-C5	3.58	116.99	112.19
2	C	5	XYS	C4-C3-C2	-3.52	106.73	110.92
2	C	1	NFG	O22-N2-C14	3.48	123.60	118.82
2	C	4	BGC	O2-C2-C1	-3.41	101.42	109.22
3	D	1	NFG	C15-C14-N2	3.28	122.20	119.34
3	D	1	NFG	C3-C4-C5	3.24	116.10	110.23
2	C	6	XYS	C4-C3-C2	3.19	114.71	110.92
3	D	5	XYS	O4-C4-C5	-2.95	102.47	109.22
2	C	2	BGC	O4-C4-C3	2.94	117.30	110.38
2	C	1	NFG	C1-C2-C3	2.90	114.78	110.54
3	D	7	XYS	O3-C3-C4	-2.82	104.30	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	6	XYS	O4-C4-C3	-2.72	104.52	110.15
2	C	5	XYS	O2-C2-C3	2.71	115.76	110.15
2	C	2	BGC	C1-C2-C3	2.67	113.54	109.64
2	C	1	NFG	C15-C14-N2	2.64	121.64	119.34
3	D	1	NFG	C13-C14-N2	-2.54	116.55	118.74
2	C	2	BGC	O5-C1-C2	2.53	116.83	110.79
3	D	5	XYS	C1-C2-C3	-2.49	106.02	109.64
2	C	1	NFG	O1-C1-C2	2.47	111.31	107.29
2	C	5	XYS	C5-C4-C3	2.39	113.12	109.64
3	D	5	XYS	O3-C3-C4	2.39	114.92	110.05
3	D	2	BGC	O4-C4-C5	2.38	115.19	109.32
2	C	1	NFG	C14-C13-C12	2.33	122.34	119.26
2	C	4	BGC	C1-O5-C5	-2.24	109.18	112.19
2	C	5	XYS	O4-C4-C5	2.04	113.89	109.22
2	C	4	BGC	O3-C3-C2	2.04	114.21	110.05
3	D	2	BGC	O2-C2-C1	-2.03	104.57	109.22
2	C	2	BGC	O3-C3-C2	-2.02	105.93	110.05
2	C	4	BGC	C2-C3-C4	-2.01	107.32	110.86

There are no chirality outliers.

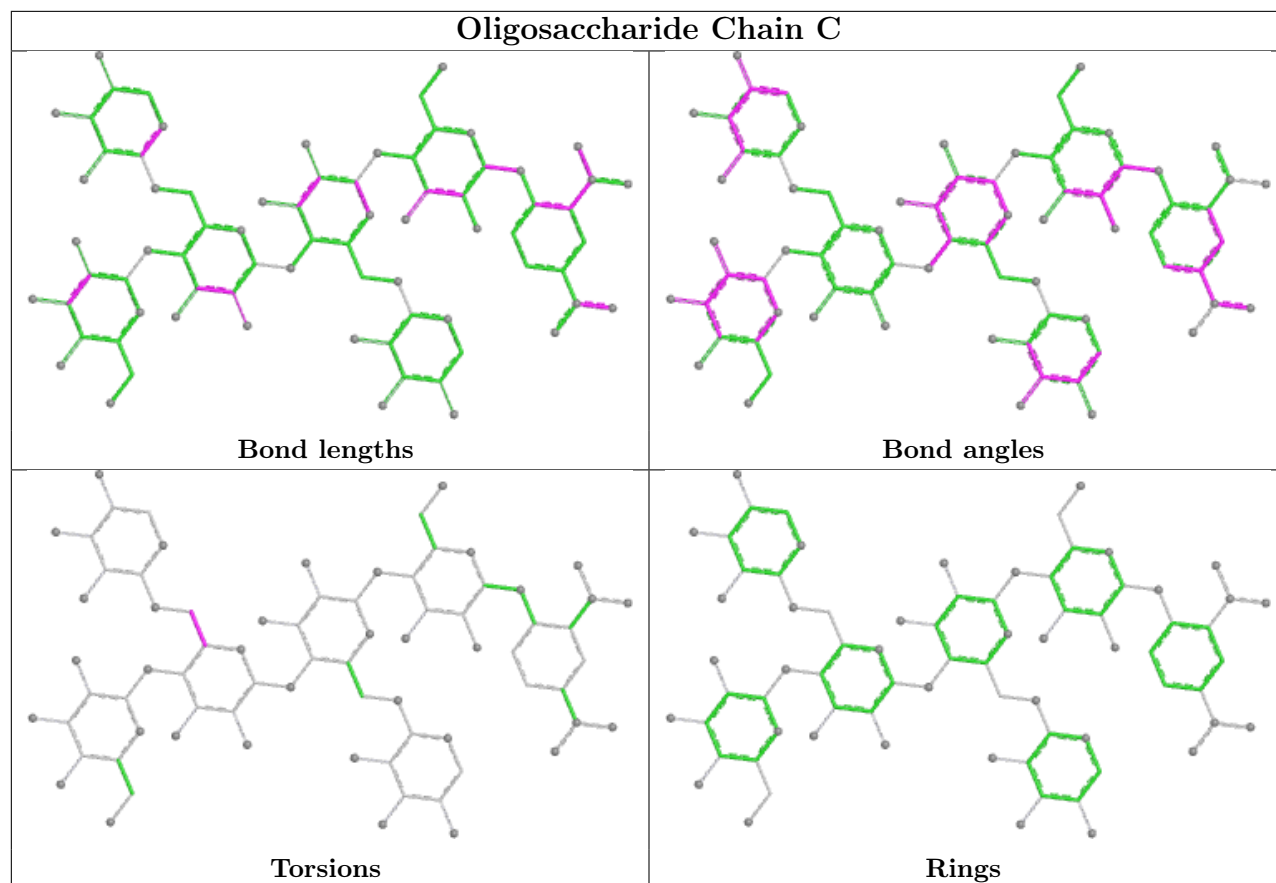
All (1) torsion outliers are listed below:

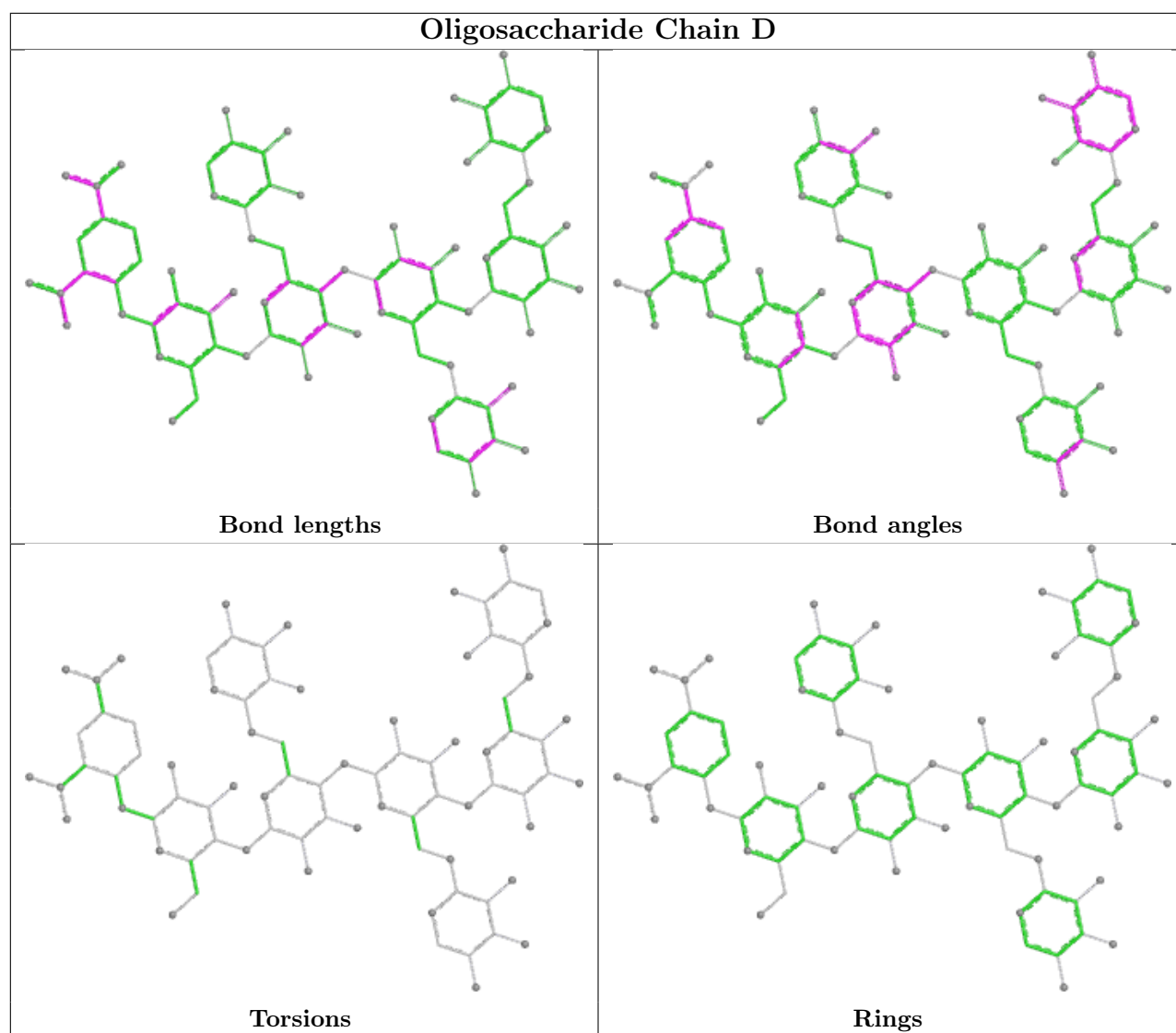
Mol	Chain	Res	Type	Atoms
2	C	3	BGC	C4-C5-C6-O6

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](#)

8 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	$\# Z > 2$
4	SO4	B	504	-	4,4,4	0.45	0	6,6,6	0.19	0
4	SO4	B	502	-	4,4,4	0.69	0	6,6,6	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	501	-	4,4,4	0.49	0	6,6,6	0.35	0
5	GOL	A	508	-	5,5,5	0.40	0	5,5,5	0.87	0
5	GOL	B	512	-	5,5,5	0.48	0	5,5,5	0.98	0
6	1PE	B	513	-	15,15,15	0.46	0	14,14,14	0.65	0
4	SO4	B	501	-	4,4,4	0.36	0	6,6,6	0.79	0
4	SO4	B	503	-	4,4,4	0.40	0	6,6,6	0.87	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	GOL	B	512	-	-	2/4/4/4	-
5	GOL	A	508	-	-	4/4/4/4	-
6	1PE	B	513	-	-	10/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	508	GOL	C1-C2-C3-O3
5	B	512	GOL	O1-C1-C2-O2
5	B	512	GOL	O1-C1-C2-C3
6	B	513	1PE	OH4-C13-C23-OH3
5	A	508	GOL	O1-C1-C2-C3
6	B	513	1PE	OH5-C14-C24-OH4
5	A	508	GOL	O2-C2-C3-O3
6	B	513	1PE	OH7-C16-C26-OH6
6	B	513	1PE	OH2-C12-C22-OH3
5	A	508	GOL	O1-C1-C2-O2
6	B	513	1PE	C16-C26-OH6-C15
6	B	513	1PE	C24-C14-OH5-C25
6	B	513	1PE	C15-C25-OH5-C14
6	B	513	1PE	C13-C23-OH3-C22
6	B	513	1PE	OH6-C15-C25-OH5
6	B	513	1PE	C12-C22-OH3-C23

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	513	1PE	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	370/396 (93%)	0.36	11 (2%) 52 51	17, 39, 52, 67	14 (3%)
1	B	370/396 (93%)	0.66	28 (7%) 20 18	20, 42, 59, 68	32 (8%)
All	All	740/792 (93%)	0.51	39 (5%) 32 31	17, 41, 57, 68	46 (6%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	352	SER	11.8
1	B	107	ALA	6.1
1	B	353	THR	5.1
1	A	103	THR	5.0
1	B	351	LEU	4.6
1	B	96	GLY	4.1
1	A	402	ASP	3.3
1	B	289	VAL	3.1
1	A	96	GLY	3.0
1	B	350	PHE	2.9
1	B	197	ILE	2.8
1	B	451	THR	2.7
1	A	308	HIS	2.7
1	B	112	GLY	2.5
1	B	444	ILE	2.5
1	A	465	ALA	2.5
1	B	108	PRO	2.5
1	A	354	THR	2.4
1	B	193	VAL	2.4
1	B	106	ALA	2.3
1	A	400	THR	2.3
1	A	341	LYS	2.3
1	A	307	THR	2.3
1	B	397	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	401	GLY	2.2
1	B	404	LEU	2.2
1	B	402	ASP	2.2
1	B	403	ALA	2.1
1	B	116	THR	2.1
1	A	370[A]	GLN	2.1
1	B	445	PHE	2.1
1	B	110	SER	2.1
1	B	344	TYR	2.1
1	B	437	ASN	2.1
1	B	146	PRO	2.1
1	B	405	THR	2.1
1	B	152	LEU	2.0
1	B	446	ASN	2.0
1	B	283	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

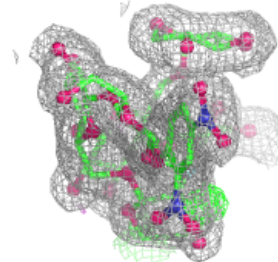
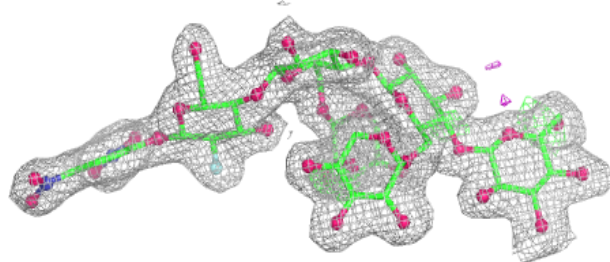
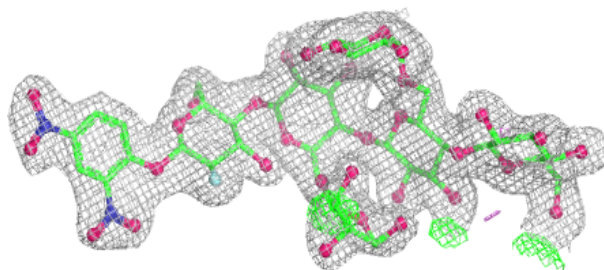
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	XYS	D	5	9/10	0.64	0.26	41,43,46,48	9
2	XYS	C	6	9/10	0.79	0.21	24,25,27,28	9
3	XYS	D	7	9/10	0.79	0.25	21,26,33,35	9
3	BGC	D	4	11/12	0.91	0.09	41,46,52,56	0
3	XYS	D	6	9/10	0.92	0.07	31,34,38,40	0
3	BGC	D	3	11/12	0.94	0.08	30,35,39,39	0
2	BGC	C	4	11/12	0.94	0.06	33,37,39,40	0
2	NFG	C	1	24/24	0.94	0.08	32,37,43,52	0
3	NFG	D	1	24/24	0.94	0.08	31,37,43,47	0
3	BGC	D	2	11/12	0.94	0.08	29,33,40,41	0
2	BGC	C	2	11/12	0.95	0.06	28,30,34,35	0
2	BGC	C	3	11/12	0.96	0.06	28,32,37,38	0
2	XYS	C	5	9/10	0.96	0.06	28,32,35,35	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.

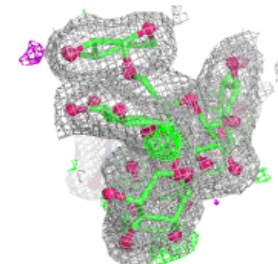
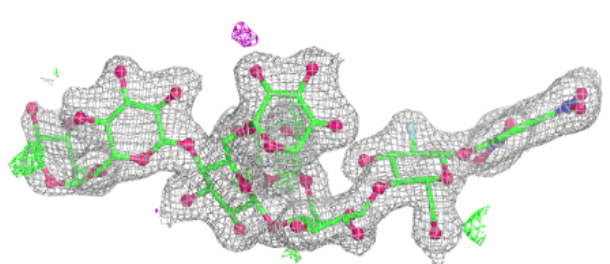
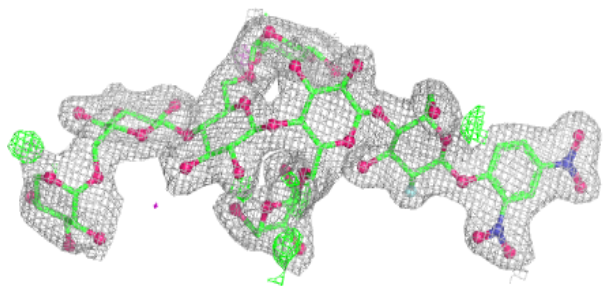
Electron density around Chain C:

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



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 [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	SO4	B	502	5/5	0.65	0.21	40,45,52,52	5
4	SO4	A	501	5/5	0.77	0.15	52,55,57,61	5
4	SO4	B	503	5/5	0.78	0.15	40,41,47,50	5
4	SO4	B	504	5/5	0.80	0.10	52,55,57,64	5
5	GOL	A	508	6/6	0.84	0.23	29,33,35,42	6
5	GOL	B	512	6/6	0.85	0.19	40,45,48,49	6
4	SO4	B	501	5/5	0.88	0.10	39,41,43,43	5
6	1PE	B	513	16/16	0.91	0.16	35,44,51,53	16

6.5 Other polymers [i](#)

There are no such residues in this entry.