



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2020 – 11:24 AM BST

PDB ID : 7C6V  
Title : Crystal structure of beta-glycosides-binding protein (W177X) of ABC transporter in a closed state bound to laminaritriose (Form II)  
Authors : Kanaujia, S.P.; Chandravanshi, M.; Samanta, R.  
Deposited on : 2020-05-22  
Resolution : 2.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.4.dev1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

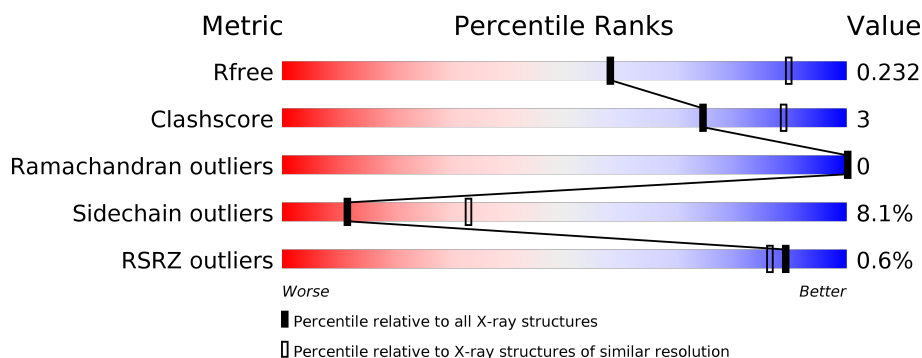
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	422	<div> <div style="width: 85%;"></div> <div style="width: 12%;"></div> <div style="width: 3%;"></div> <div style="width: 2%;"></div> </div> <div>85% 12% ..</div>
1	B	422	<div> <div style="width: 85%;"></div> <div style="width: 12%;"></div> <div style="width: 3%;"></div> <div style="width: 2%;"></div> </div> <div>85% 12% ..</div>
1	C	422	<div> <div style="width: 84%;"></div> <div style="width: 13%;"></div> <div style="width: 3%;"></div> <div style="width: 2%;"></div> </div> <div>84% 13% ..</div>
2	D	3	<div> <div style="width: 100%;"></div> </div> <div>100%</div>
2	E	3	<div> <div style="width: 33%;"></div> <div style="width: 67%;"></div> </div> <div>33% 67%</div>
2	F	3	<div> <div style="width: 33%;"></div> <div style="width: 67%;"></div> </div> <div>33% 67%</div>

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	EDO	A	504	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9672 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 Sugar ABC transporter, periplasmic sugar-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	1	0
			3160	2031	547	572	10			
1	B	413	Total	C	N	O	S	0	0	0
			3156	2027	548	571	10			
1	C	412	Total	C	N	O	S	0	1	0
			3151	2025	544	572	10			

There are 39 discrepancies between the modelled and reference sequences:

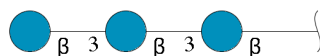
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q53W80
A	174	ARG	LYS	engineered mutation	UNP Q53W80
A	175	THR	ASN	engineered mutation	UNP Q53W80
A	176	PRO	SER	engineered mutation	UNP Q53W80
A	?	-	TRP	deletion	UNP Q53W80
A	177	ARG	ASP	engineered mutation	UNP Q53W80
A	178	THR	VAL	engineered mutation	UNP Q53W80
A	416	HIS	-	expression tag	UNP Q53W80
A	417	HIS	-	expression tag	UNP Q53W80
A	418	HIS	-	expression tag	UNP Q53W80
A	419	HIS	-	expression tag	UNP Q53W80
A	420	HIS	-	expression tag	UNP Q53W80
A	421	HIS	-	expression tag	UNP Q53W80
B	0	MET	-	initiating methionine	UNP Q53W80
B	174	ARG	LYS	engineered mutation	UNP Q53W80
B	175	THR	ASN	engineered mutation	UNP Q53W80
B	176	PRO	SER	engineered mutation	UNP Q53W80
B	?	-	TRP	deletion	UNP Q53W80
B	177	ARG	ASP	engineered mutation	UNP Q53W80
B	178	THR	VAL	engineered mutation	UNP Q53W80
B	416	HIS	-	expression tag	UNP Q53W80
B	417	HIS	-	expression tag	UNP Q53W80
B	418	HIS	-	expression tag	UNP Q53W80

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Chain	Residue	Modelled	Actual	Comment	Reference
B	419	HIS	-	expression tag	UNP Q53W80
B	420	HIS	-	expression tag	UNP Q53W80
B	421	HIS	-	expression tag	UNP Q53W80
C	0	MET	-	initiating methionine	UNP Q53W80
C	174	ARG	LYS	engineered mutation	UNP Q53W80
C	175	THR	ASN	engineered mutation	UNP Q53W80
C	176	PRO	SER	engineered mutation	UNP Q53W80
C	?	-	TRP	deletion	UNP Q53W80
C	177	ARG	ASP	engineered mutation	UNP Q53W80
C	178	THR	VAL	engineered mutation	UNP Q53W80
C	416	HIS	-	expression tag	UNP Q53W80
C	417	HIS	-	expression tag	UNP Q53W80
C	418	HIS	-	expression tag	UNP Q53W80
C	419	HIS	-	expression tag	UNP Q53W80
C	420	HIS	-	expression tag	UNP Q53W80
C	421	HIS	-	expression tag	UNP Q53W80

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	D	3	Total	C	O	0	0	0
			34	18	16			
2	E	3	Total	C	O	0	0	0
			34	18	16			
2	F	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



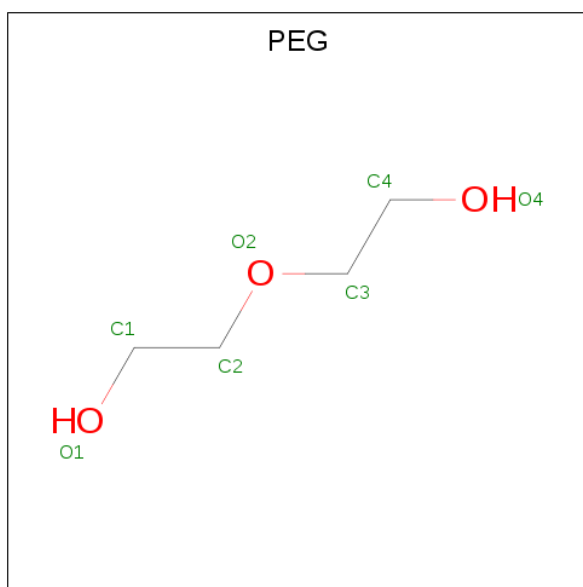
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



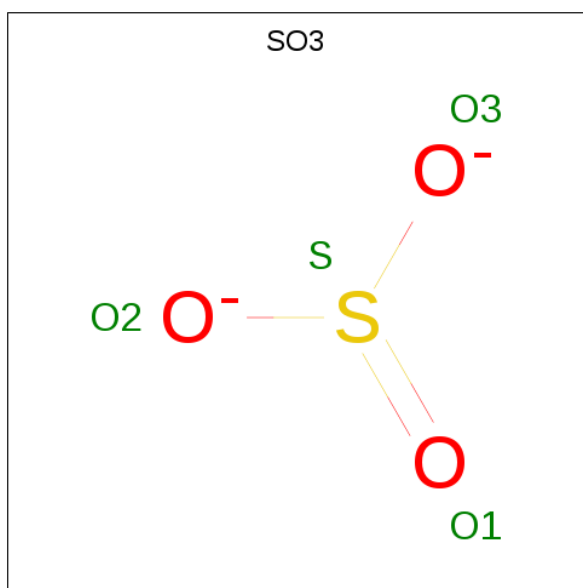
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



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

- Molecule 7 is SULFITE ION (three-letter code: SO3) (formula: O<sub>3</sub>S).



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

- Molecule 8 is water.

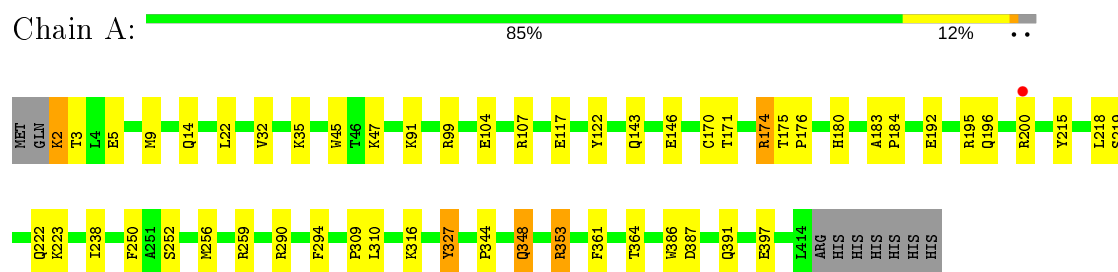
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	23	Total	O	0	0
			23	23		
8	B	12	Total	O	0	0
			12	12		
8	C	17	Total	O	0	0
			17	17		



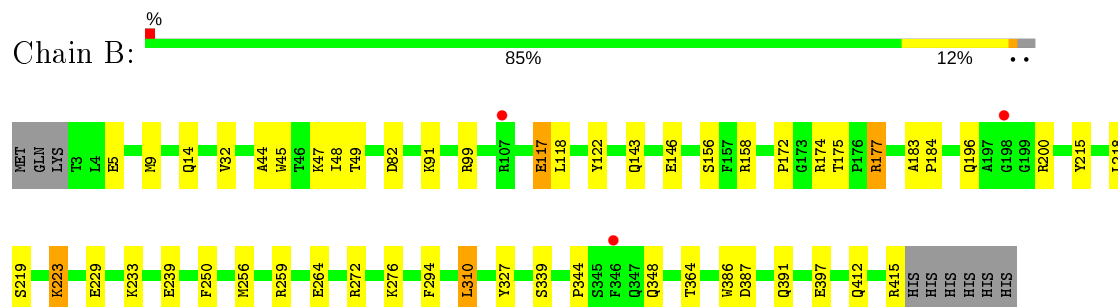
### 3 Residue-property plots [i](#)

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.

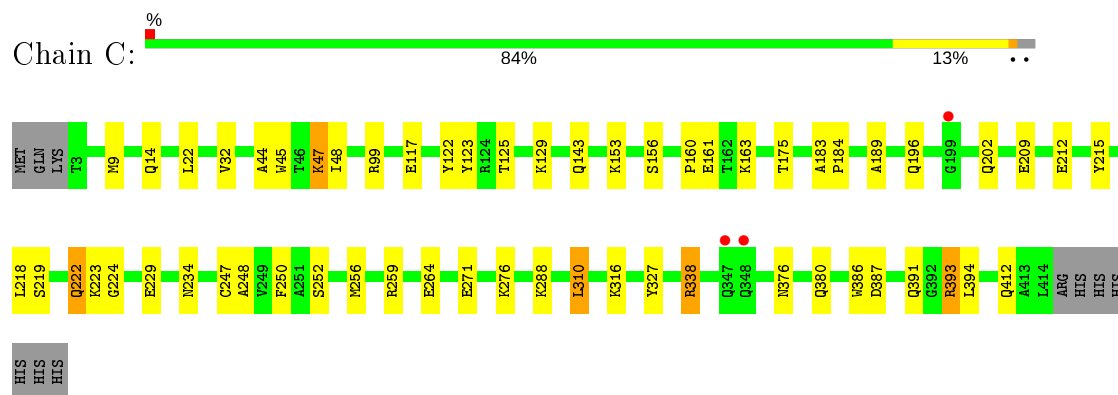
- Molecule 1: Sugar ABC transporter, periplasmic sugar-binding protein



- Molecule 1: Sugar ABC transporter, periplasmic sugar-binding protein



- Molecule 1: Sugar ABC transporter, periplasmic sugar-binding protein



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

Chain D:  100%

BGC1  
BGC2  
BGC3

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

Chain E:  33% 67%

BGC1  
BGC2  
BGC3

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

Chain F:  33% 67%

BGC1  
BGC2  
BGC3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	185.41 Å   185.41 Å   74.18 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	80.28 – 2.80 67.34 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (80.28-2.80) 99.9 (67.34-2.80)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.93 (at 2.81 Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.187 , 0.236 0.189 , 0.232	Depositor DCC
$R_{free}$ test set	1703 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.4	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 21.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9672	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: BGC, CL, EDO, SO3, SO4, PEG

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	0.83	2/3250 (0.1%)	0.96	1/4425 (0.0%)
1	B	0.85	5/3243 (0.2%)	0.96	0/4416
1	C	0.84	2/3241 (0.1%)	0.99	2/4414 (0.0%)
All	All	0.84	9/9734 (0.1%)	0.97	3/13255 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	146	GLU	CD-OE2	8.01	1.34	1.25
1	C	212	GLU	CD-OE2	7.02	1.33	1.25
1	A	397	GLU	CD-OE2	6.17	1.32	1.25
1	B	397	GLU	CD-OE2	6.10	1.32	1.25
1	B	229	GLU	CD-OE1	6.02	1.32	1.25
1	C	161	GLU	CD-OE1	5.42	1.31	1.25
1	B	229	GLU	CD-OE2	5.39	1.31	1.25
1	B	239	GLU	CD-OE2	5.22	1.31	1.25
1	B	117	GLU	CD-OE1	5.06	1.31	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	393	ARG	NE-CZ-NH1	-6.84	116.88	120.30
1	A	327	TYR	CB-CG-CD2	5.65	124.39	121.00
1	C	247	CYS	CB-CA-C	-5.13	100.15	110.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3160	0	3134	21	0
1	B	3156	0	3126	16	0
1	C	3151	0	3119	22	0
2	D	34	0	30	0	0
2	E	34	0	30	2	0
2	F	34	0	30	0	0
3	A	1	0	0	1	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	10	0	0	1	0
4	B	5	0	0	1	0
4	C	10	0	0	0	0
5	A	8	0	12	0	0
5	B	4	0	6	0	0
6	B	7	0	10	0	0
7	C	4	0	0	0	0
8	A	23	0	0	1	0
8	B	12	0	0	0	0
8	C	17	0	0	0	0
All	All	9672	0	9497	61	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 (61) 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:192:GLU:OE1	1:A:195:ARG:HD2	1.77	0.83
1:A:2:LYS:O	1:A:32:VAL:HG23	1.78	0.83
1:B:264:GLU:OE1	1:B:272:ARG:NH1	2.15	0.80
1:C:264:GLU:HB2	1:C:271:GLU:OE2	1.87	0.73
1:A:3:THR:HG21	1:A:35:LYS:HE2	1.70	0.72
1:A:170:CYS:HB3	1:A:238:ILE:HG23	1.73	0.70
1:B:344:PRO:O	1:B:348:GLN:HG3	1.93	0.67
1:C:175:THR:HG22	1:C:234:ASN:HB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:ASN:O	1:C:380:GLN:HG3	2.03	0.59
1:C:215:TYR:O	1:C:219:SER:HB3	2.04	0.58
1:B:174:ARG:NH1	1:B:387:ASP:OD2	2.38	0.57
1:C:153:LYS:HE2	1:C:224:GLY:O	2.05	0.57
1:B:215:TYR:O	1:B:219:SER:HB3	2.04	0.57
1:A:122:TYR:CZ	1:A:256:MET:HB2	2.41	0.56
1:A:215:TYR:O	1:A:219:SER:HB3	2.05	0.55
1:B:44:ALA:O	1:B:48:ILE:HD12	2.06	0.54
1:C:122:TYR:CZ	1:C:256:MET:HB2	2.42	0.54
1:A:353:ARG:HH11	1:A:353:ARG:HB3	1.72	0.54
1:C:160:PRO:O	1:C:163:LYS:HD3	2.08	0.53
1:B:122:TYR:CZ	1:B:256:MET:HB2	2.44	0.52
1:C:218:LEU:CD2	1:C:386:TRP:CZ2	2.92	0.52
1:B:387:ASP:O	1:B:391:GLN:HG3	2.12	0.50
1:A:180:HIS:ND1	4:A:502:SO4:O2	2.30	0.49
1:A:3:THR:CG2	1:A:35:LYS:HE2	2.40	0.49
1:B:218:LEU:HD23	1:B:386:TRP:CZ2	2.48	0.49
4:B:502:SO4:O4	2:E:2:BGC:H4	2.13	0.49
1:A:218:LEU:CD2	1:A:386:TRP:CZ2	2.97	0.48
1:C:218:LEU:HD23	1:C:386:TRP:CZ2	2.48	0.48
1:A:3:THR:HG21	1:A:35:LYS:CE	2.40	0.47
1:C:222:GLN:HE22	1:C:394:LEU:HB3	1.79	0.47
1:C:47:LYS:HE3	1:C:47:LYS:HB2	1.62	0.47
2:E:2:BGC:O4	2:E:3:BGC:O5	2.30	0.47
1:A:294:PHE:O	1:A:364:THR:HG22	2.14	0.47
1:C:387:ASP:O	1:C:391:GLN:HG3	2.15	0.47
1:C:44:ALA:O	1:C:48:ILE:HD12	2.15	0.47
1:A:387:ASP:O	1:A:391:GLN:HG3	2.15	0.46
1:B:218:LEU:CD2	1:B:386:TRP:CZ2	2.98	0.46
1:A:309:PRO:HG2	8:A:618:HOH:O	2.14	0.46
1:C:338:ARG:CG	1:C:338:ARG:HH21	2.28	0.46
1:B:294:PHE:O	1:B:364:THR:HG22	2.15	0.46
1:B:177:ARG:N	1:B:177:ARG:HD3	2.30	0.46
1:B:32:VAL:HG21	1:B:310:LEU:HD11	1.98	0.45
1:C:125:THR:O	1:C:129:LYS:HB2	2.17	0.45
1:C:189:ALA:O	1:C:209[B]:GLU:HG2	2.17	0.44
1:B:218:LEU:CD2	1:B:386:TRP:CE2	3.01	0.44
1:C:218:LEU:CD2	1:C:386:TRP:CE2	3.00	0.44
1:A:290:ARG:O	1:A:361:PHE:HB3	2.18	0.44
1:A:174:ARG:HD3	1:A:174:ARG:HA	1.42	0.43
1:C:22:LEU:HD22	1:C:327:TYR:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:VAL:HG21	1:C:310:LEU:HD11	2.00	0.43
1:B:172:PRO:HB3	1:B:233:LYS:O	2.18	0.43
1:A:176:PRO:HG3	3:A:501:CL:CL	2.55	0.43
1:C:163:LYS:HA	1:C:163:LYS:HD2	1.86	0.43
1:B:146:GLU:OE2	1:B:223:LYS:HE3	2.19	0.42
1:A:344:PRO:O	1:A:348:GLN:NE2	2.53	0.42
1:A:218:LEU:CD2	1:A:386:TRP:CE2	3.03	0.41
1:C:183:ALA:N	1:C:184:PRO:CD	2.83	0.41
1:A:22:LEU:HD22	1:A:327:TYR:CD1	2.55	0.41
1:A:183:ALA:N	1:A:184:PRO:CD	2.84	0.40
1:B:183:ALA:N	1:B:184:PRO:CD	2.84	0.40
1:C:123:TYR:HA	1:C:248:ALA:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	412/422 (98%)	400 (97%)	12 (3%)	0	100	100
1	B	411/422 (97%)	402 (98%)	9 (2%)	0	100	100
1	C	411/422 (97%)	404 (98%)	7 (2%)	0	100	100
All	All	1234/1266 (98%)	1206 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	313/321 (98%)	287 (92%)	26 (8%)	11	32
1	B	312/321 (97%)	285 (91%)	27 (9%)	10	30
1	C	312/321 (97%)	289 (93%)	23 (7%)	13	37
All	All	937/963 (97%)	861 (92%)	76 (8%)	11	33

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	5	GLU
1	A	9	MET
1	A	14	GLN
1	A	45	TRP
1	A	47	LYS
1	A	91	LYS
1	A	99	ARG
1	A	104	GLU
1	A	107	ARG
1	A	117	GLU
1	A	143	GLN
1	A	171	THR
1	A	174	ARG
1	A	175	THR
1	A	196	GLN
1	A	200	ARG
1	A	222	GLN
1	A	223	LYS
1	A	250	PHE
1	A	252	SER
1	A	259	ARG
1	A	310	LEU
1	A	316	LYS
1	A	348	GLN
1	A	353	ARG
1	B	5	GLU
1	B	9	MET
1	B	14	GLN
1	B	45	TRP
1	B	47	LYS

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Mol	Chain	Res	Type
1	B	49	THR
1	B	82	ASP
1	B	91	LYS
1	B	99	ARG
1	B	117	GLU
1	B	118	LEU
1	B	143	GLN
1	B	156	SER
1	B	158	ARG
1	B	175	THR
1	B	177	ARG
1	B	196	GLN
1	B	200	ARG
1	B	223	LYS
1	B	250	PHE
1	B	259	ARG
1	B	276	LYS
1	B	310	LEU
1	B	327	TYR
1	B	339	SER
1	B	412	GLN
1	B	415	ARG
1	C	9	MET
1	C	14	GLN
1	C	45	TRP
1	C	47	LYS
1	C	99	ARG
1	C	117	GLU
1	C	143	GLN
1	C	156	SER
1	C	196	GLN
1	C	202	GLN
1	C	222	GLN
1	C	223	LYS
1	C	229	GLU
1	C	250	PHE
1	C	252	SER
1	C	259	ARG
1	C	276	LYS
1	C	288	LYS
1	C	310	LEU
1	C	316	LYS

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Mol	Chain	Res	Type
1	C	338	ARG
1	C	393	ARG
1	C	412	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	14	GLN
1	C	412	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 ⓘ

9 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	D	1	2	12,12,12	0.60	0	17,17,17	1.42	2 (11%)
2	BGC	D	2	2	11,11,12	0.55	0	15,15,17	0.94	1 (6%)
2	BGC	D	3	2	11,11,12	0.57	0	15,15,17	1.24	2 (13%)
2	BGC	E	1	2	12,12,12	0.46	0	17,17,17	2.04	6 (35%)
2	BGC	E	2	2	11,11,12	0.72	0	15,15,17	1.41	1 (6%)
2	BGC	E	3	2	11,11,12	0.62	0	15,15,17	1.20	1 (6%)
2	BGC	F	1	2	12,12,12	0.64	0	17,17,17	1.80	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	BGC	F	2	2	11,11,12	0.67	0	15,15,17	0.64	0
2	BGC	F	3	2	11,11,12	0.56	0	15,15,17	1.83	5 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	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	E	1	2	-	0/2/22/22	0/1/1/1
2	BGC	E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	E	3	2	-	0/2/19/22	0/1/1/1
2	BGC	F	1	2	-	1/2/22/22	0/1/1/1
2	BGC	F	2	2	-	0/2/19/22	0/1/1/1
2	BGC	F	3	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	BGC	C1-O5-C5	4.40	118.15	112.19
2	F	1	BGC	C1-C2-C3	-4.39	101.20	110.31
2	E	1	BGC	C1-C2-C3	-4.30	101.39	110.31
2	E	1	BGC	C1-O5-C5	-4.01	106.10	113.66
2	E	1	BGC	O5-C1-C2	-3.72	103.64	110.28
2	F	3	BGC	O5-C5-C6	-3.68	101.43	107.20
2	D	1	BGC	C1-C2-C3	-3.47	103.12	110.31
2	E	3	BGC	O3-C3-C2	-3.43	103.43	109.99
2	F	3	BGC	O3-C3-C2	-2.95	104.34	109.99
2	F	3	BGC	O5-C5-C4	-2.84	103.92	110.83
2	D	1	BGC	O5-C5-C6	2.74	113.25	106.44
2	F	1	BGC	O5-C1-C2	-2.70	105.47	110.28
2	D	3	BGC	C1-C2-C3	2.57	112.83	109.67
2	E	1	BGC	O2-C2-C3	2.57	116.28	110.35
2	E	1	BGC	O6-C6-C5	-2.31	103.36	111.29
2	F	3	BGC	O4-C4-C5	2.30	115.00	109.30
2	D	2	BGC	C1-O5-C5	2.28	115.28	112.19
2	F	3	BGC	C6-C5-C4	2.26	118.30	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	BGC	O5-C5-C4	2.17	113.63	109.69
2	F	1	BGC	O2-C2-C1	2.13	114.11	109.16
2	E	1	BGC	O1-C1-O5	2.12	116.73	110.38
2	F	1	BGC	C1-O5-C5	-2.03	109.83	113.66
2	D	3	BGC	C2-C3-C4	2.02	114.38	110.89

There are no chirality outliers.

All (3) torsion outliers are listed below:

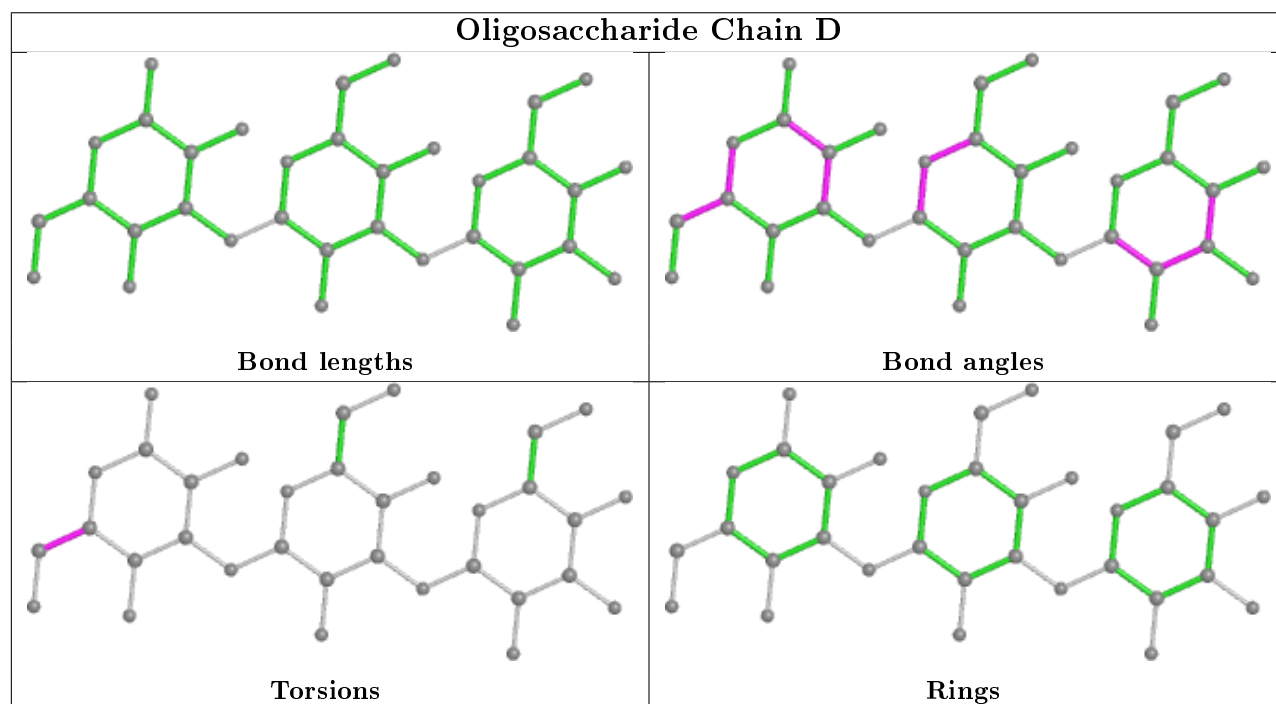
Mol	Chain	Res	Type	Atoms
2	D	1	BGC	O5-C5-C6-O6
2	D	1	BGC	C4-C5-C6-O6
2	F	1	BGC	O5-C5-C6-O6

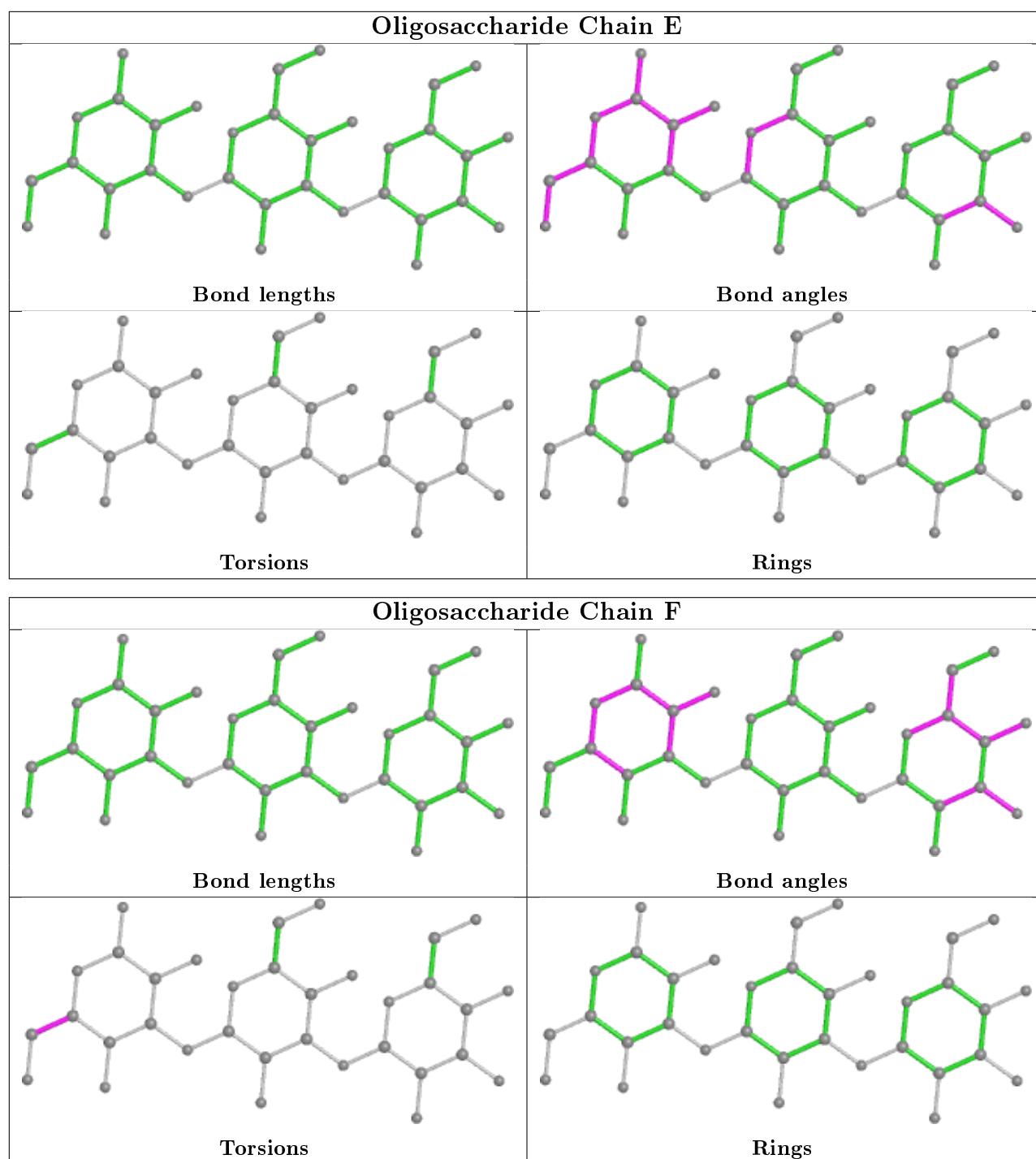
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	BGC	2	0
2	E	3	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 ⓘ

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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	$\# Z  > 2$
5	EDO	A	504	-	3,3,3	0.26	0	2,2,2	0.47	0
6	PEG	B	504	-	6,6,6	0.25	0	5,5,5	0.17	0
4	SO4	B	502	-	4,4,4	0.49	0	6,6,6	0.38	0
4	SO4	C	503	-	4,4,4	0.47	0	6,6,6	0.12	0
4	SO4	C	504	-	4,4,4	0.26	0	6,6,6	0.24	0
4	SO4	A	503	-	4,4,4	0.23	0	6,6,6	0.19	0
5	EDO	A	505	-	3,3,3	0.09	0	2,2,2	0.12	0
4	SO4	A	502	-	4,4,4	0.38	0	6,6,6	0.20	0
5	EDO	B	503	-	3,3,3	0.18	0	2,2,2	0.62	0
7	SO3	C	502	-	1,3,3	1.64	0	0,3,3	0.00	-

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	EDO	A	504	-	-	1/1/1/1	-
6	PEG	B	504	-	-	2/4/4/4	-
5	EDO	B	503	-	-	1/1/1/1	-
5	EDO	A	505	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	504	PEG	O1-C1-C2-O2
5	A	504	EDO	O1-C1-C2-O2
5	B	503	EDO	O1-C1-C2-O2
6	B	504	PEG	C4-C3-O2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	502	SO4	1	0
4	A	502	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	413/422 (97%)	-0.33	1 (0%) 95 94	29, 52, 86, 113	0
1	B	413/422 (97%)	-0.23	3 (0%) 87 84	27, 53, 98, 137	0
1	C	412/422 (97%)	-0.32	3 (0%) 87 84	30, 49, 81, 126	0
All	All	1238/1266 (97%)	-0.29	7 (0%) 89 86	27, 52, 90, 137	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	348	GLN	5.0
1	C	347	GLN	3.2
1	C	199	GLY	3.0
1	B	198	GLY	3.0
1	B	107	ARG	2.3
1	A	200	ARG	2.1
1	B	346	PHE	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	BGC	F	1	12/12	0.95	0.15	43,48,62,68	0

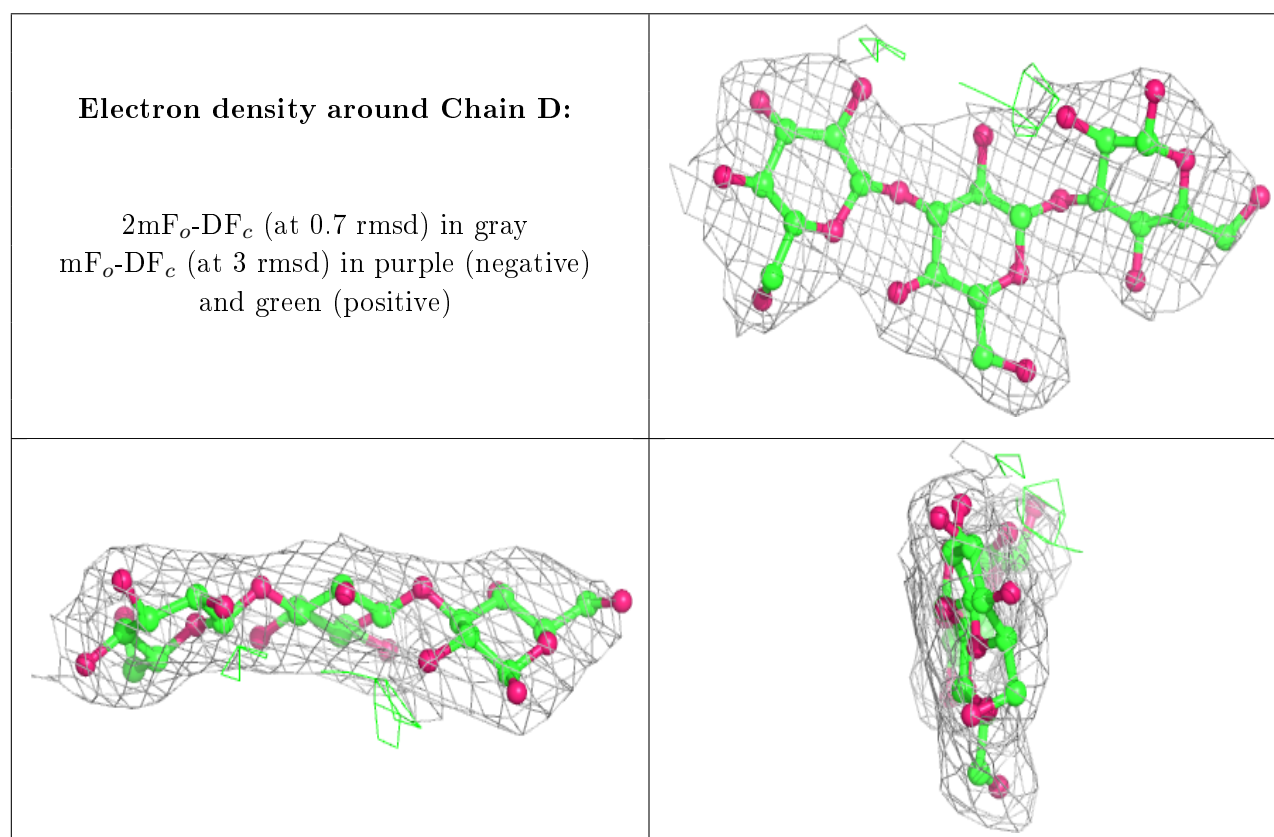
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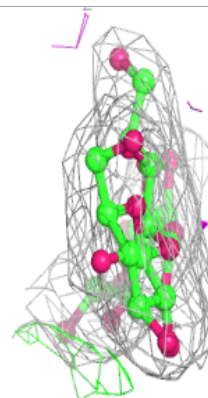
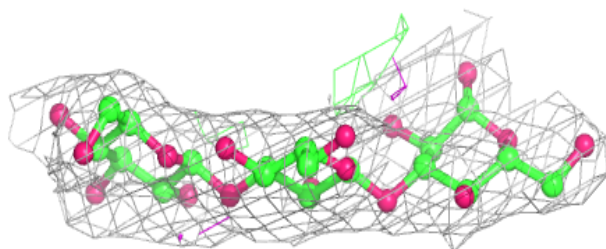
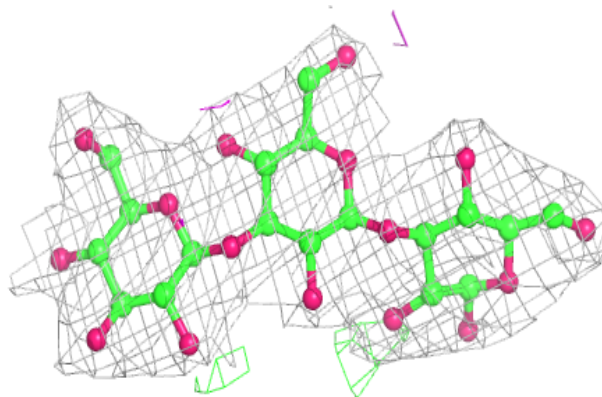
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BGC	E	1	12/12	0.96	0.12	44,49,58,64	0
2	BGC	E	2	11/12	0.97	0.17	38,39,41,43	0
2	BGC	D	2	11/12	0.97	0.15	43,44,47,50	0
2	BGC	D	1	12/12	0.97	0.18	51,60,77,85	0
2	BGC	D	3	11/12	0.98	0.14	44,47,52,55	0
2	BGC	F	3	11/12	0.98	0.12	29,35,38,39	0
2	BGC	F	2	11/12	0.98	0.12	34,38,40,40	0
2	BGC	E	3	11/12	0.98	0.12	31,33,36,39	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.

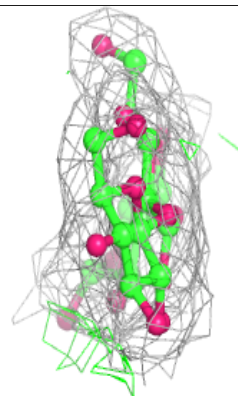
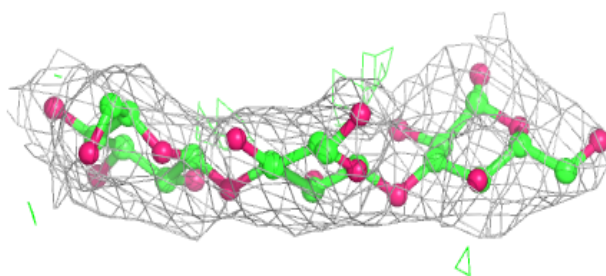
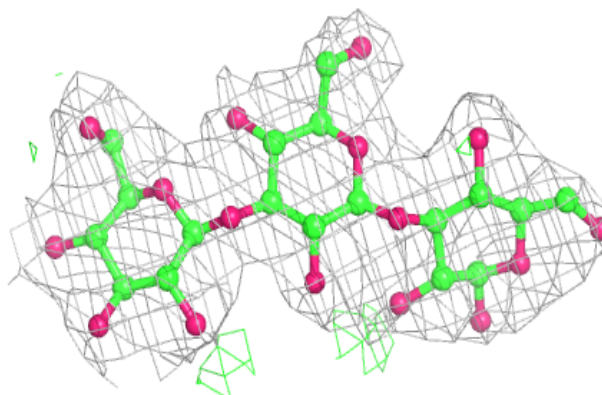


**Electron density around Chain E:**

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

**Electron density around Chain F:**

$2mF_o - DF_c$  (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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	EDO	A	504	4/4	0.79	0.43	60,67,68,71	0
6	PEG	B	504	7/7	0.85	0.25	66,73,75,81	0
7	SO3	C	502	4/4	0.89	0.18	74,84,88,96	0
4	SO4	C	504	5/5	0.93	0.15	65,72,81,85	0
3	CL	C	501	1/1	0.94	0.12	61,61,61,61	0
5	EDO	A	505	4/4	0.95	0.10	56,57,58,61	0
5	EDO	B	503	4/4	0.95	0.18	45,49,51,54	0
3	CL	A	501	1/1	0.95	0.10	57,57,57,57	0
4	SO4	A	503	5/5	0.96	0.12	52,57,77,77	0
3	CL	B	501	1/1	0.97	0.11	57,57,57,57	0
4	SO4	A	502	5/5	0.97	0.15	57,57,60,66	0
4	SO4	B	502	5/5	0.98	0.11	39,44,47,56	0
4	SO4	C	503	5/5	0.99	0.10	38,40,43,46	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.