



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2020 – 11:28 AM BST

PDB ID : 7C70
Title : Crystal structure of beta-glycosides-binding protein (W67A) of ABC transporter in an open-liganded state bound to gentiobiose
Authors : Kanaujia, S.P.; Chandravanshi, M.; Samanta, R.
Deposited on : 2020-05-22
Resolution : 1.63 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 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

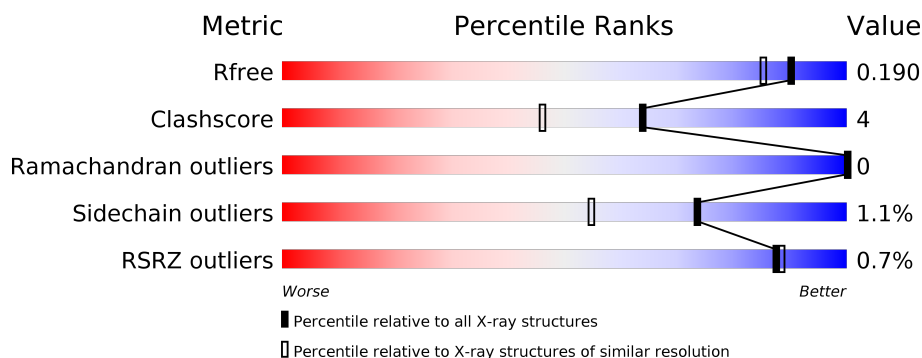
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.63 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	3122 (1.66-1.62)
Clashscore	141614	3268 (1.66-1.62)
Ramachandran outliers	138981	3215 (1.66-1.62)
Sidechain outliers	138945	3215 (1.66-1.62)
RSRZ outliers	127900	3079 (1.66-1.62)

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 ≥ 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	423	<div> <div>90%</div> <div>8%</div> </div>
1	B	423	<div> <div>%</div> <div>89%</div> <div>8%</div> </div>
2	C	2	<div> <div>50%</div> <div>50%</div> </div>
2	D	2	<div> <div>100%</div> </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PGO	A	504	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 7451 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.

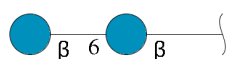
- Molecule 1 is a protein called Sugar ABC transporter, periplasmic sugar-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	16	0
			3274	2109	561	593	11			
1	B	415	Total	C	N	O	S	0	10	0
			3220	2074	556	580	10			

There are 16 discrepancies between the modelled and reference sequences:

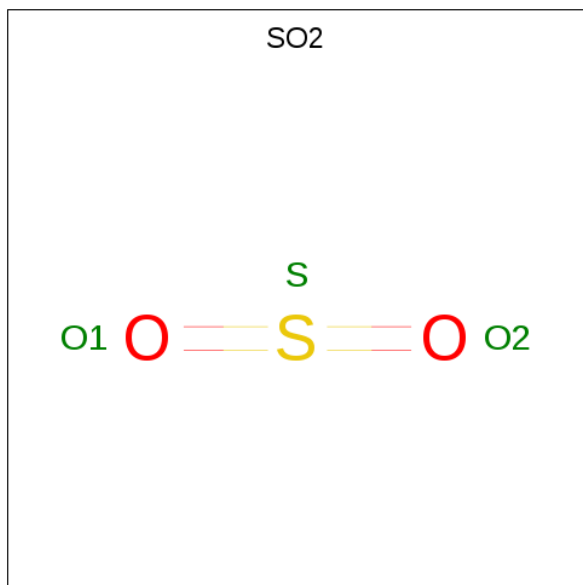
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q53W80
A	67	ALA	TRP	engineered mutation	UNP Q53W80
A	417	HIS	-	expression tag	UNP Q53W80
A	418	HIS	-	expression tag	UNP Q53W80
A	419	HIS	-	expression tag	UNP Q53W80
A	420	HIS	-	expression tag	UNP Q53W80
A	421	HIS	-	expression tag	UNP Q53W80
A	422	HIS	-	expression tag	UNP Q53W80
B	0	MET	-	initiating methionine	UNP Q53W80
B	67	ALA	TRP	engineered mutation	UNP Q53W80
B	417	HIS	-	expression tag	UNP Q53W80
B	418	HIS	-	expression tag	UNP Q53W80
B	419	HIS	-	expression tag	UNP Q53W80
B	420	HIS	-	expression tag	UNP Q53W80
B	421	HIS	-	expression tag	UNP Q53W80
B	422	HIS	-	expression tag	UNP Q53W80

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-6)-beta-D-glucopyranose.



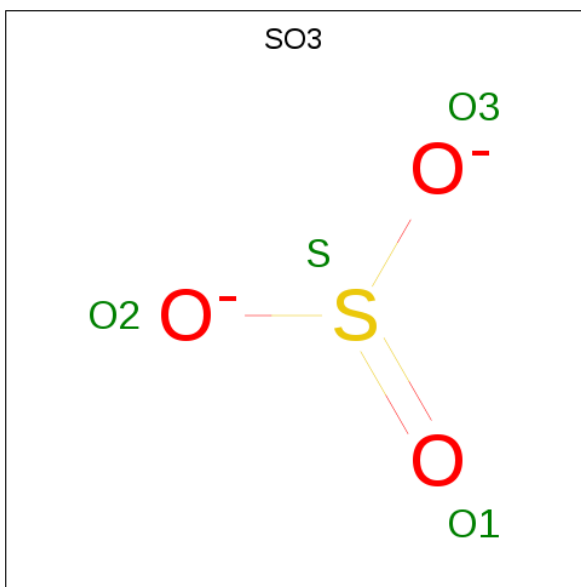
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	0	0
			23	12	11			
2	D	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is SULFUR DIOXIDE (three-letter code: SO₂) (formula: O₂S).



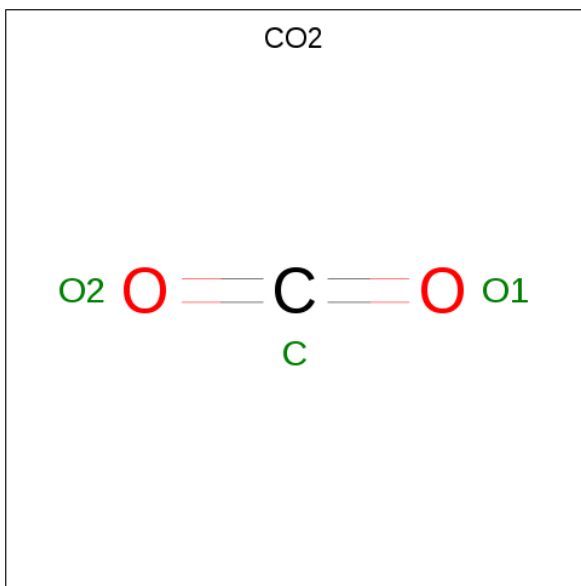
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			3	2	1		
3	B	1	Total	O	S	0	0
			3	2	1		
3	B	1	Total	O	S	0	0
			3	2	1		

- Molecule 4 is SULFITE ION (three-letter code: SO₃) (formula: O₃S).



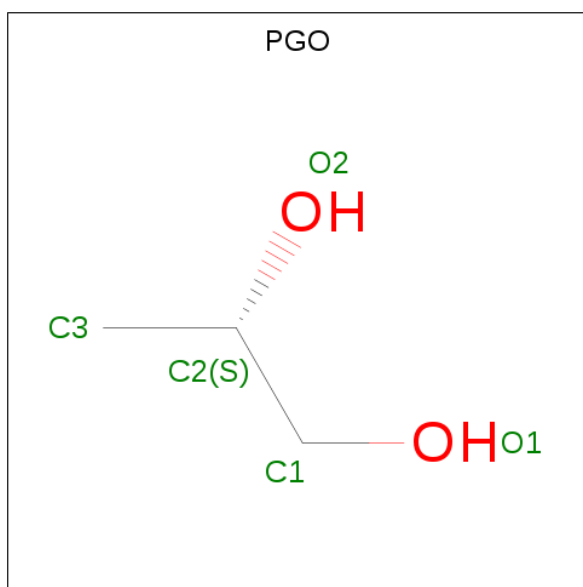
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			4	3	1		

- Molecule 5 is CARBON DIOXIDE (three-letter code: CO₂) (formula: CO₂).



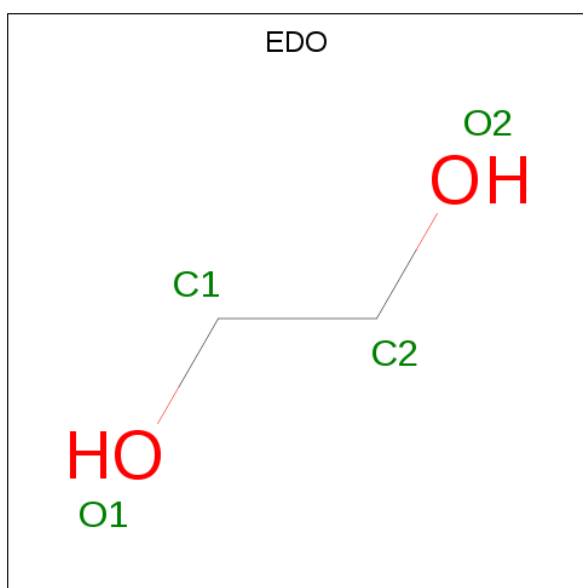
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	1	2		
5	B	1	Total	C	O	0	0
			3	1	2		

- Molecule 6 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula: C₃H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			5	3	2		
6	B	1	Total	C	O	0	0
			5	3	2		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



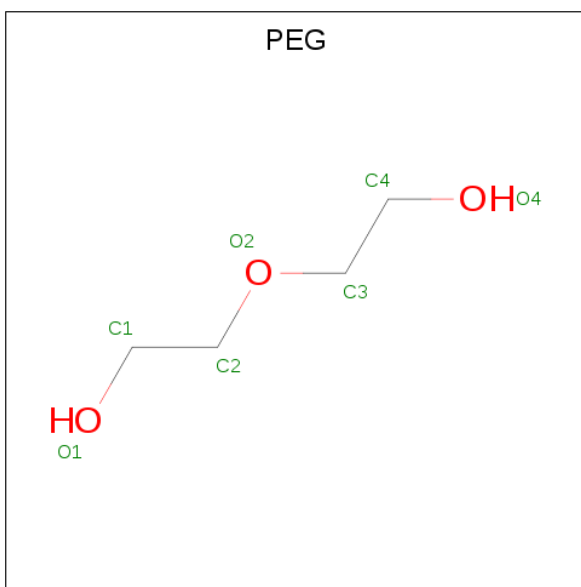
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

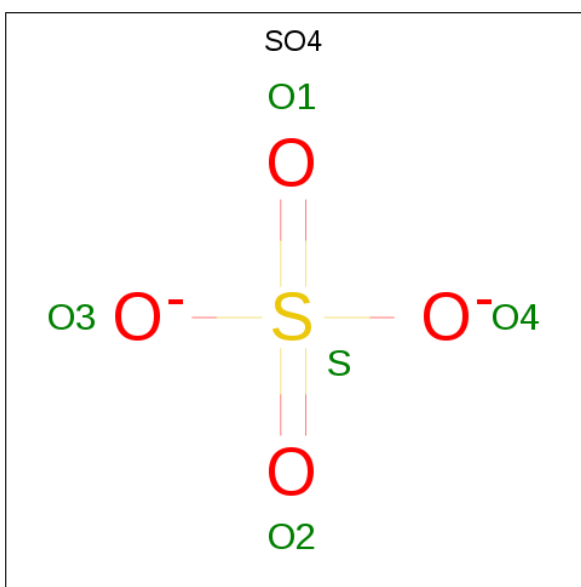
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



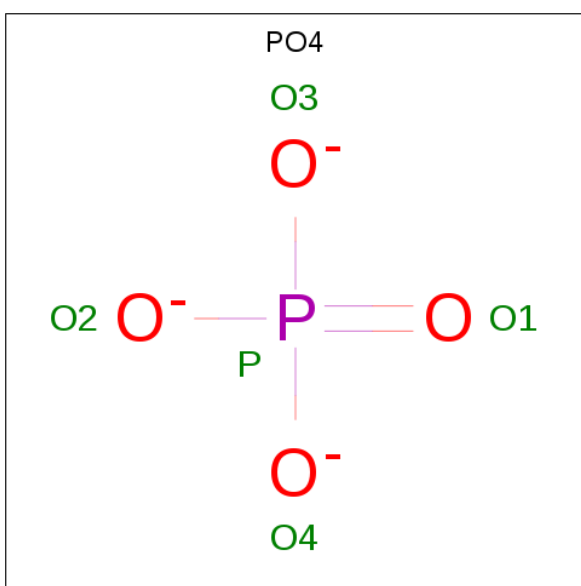
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			7	4	3		
8	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



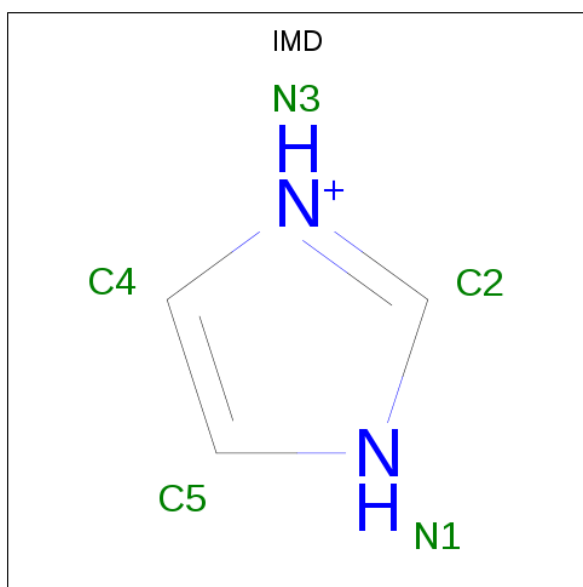
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 10 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 11 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	N	0	0
			5	3	2		

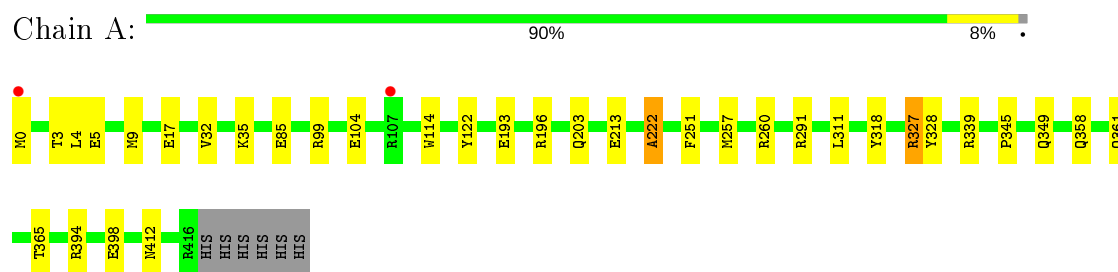
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	405	Total	O	0	0
			405	405		
12	B	427	Total	O	0	0
			427	427		

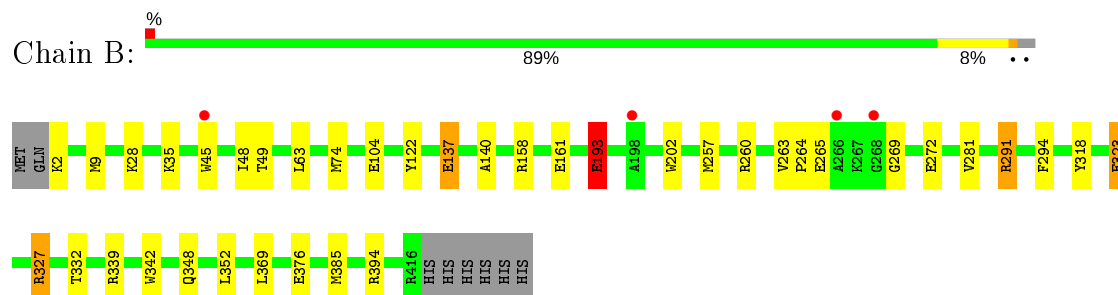
3 Residue-property plots [i](#)

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



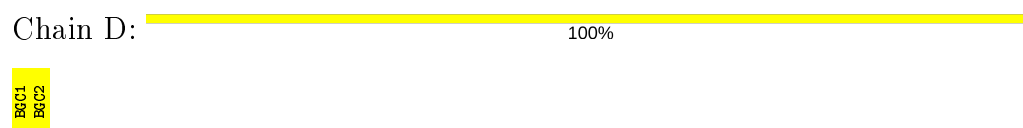
- Molecule 1: Sugar ABC transporter, periplasmic sugar-binding protein



- Molecule 2: beta-D-glucopyranose-(1-6)-beta-D-glucopyranose



- Molecule 2: beta-D-glucopyranose-(1-6)-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.24Å 98.96Å 66.56Å 90.00° 103.25° 90.00°	Depositor
Resolution (Å)	49.48 – 1.63 49.48 – 1.63	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.48-1.63) 98.9 (49.48-1.63)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.68 (at 1.63Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.140 , 0.178 0.153 , 0.190	Depositor DCC
R_{free} test set	4157 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	13.6	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7451	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CO2, IMD, PGO, PO4, EDO, SO2, SO3, BGC, 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	0.87	3/3405 (0.1%)	1.03	11/4631 (0.2%)
1	B	0.92	8/3336 (0.2%)	1.06	12/4540 (0.3%)
All	All	0.90	11/6741 (0.2%)	1.04	23/9171 (0.3%)

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	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	104	GLU	CD-OE1	11.62	1.38	1.25
1	B	193	GLU	CD-OE2	10.19	1.36	1.25
1	A	104	GLU	CD-OE1	9.10	1.35	1.25
1	A	398	GLU	CD-OE1	7.41	1.33	1.25
1	B	272	GLU	CD-OE2	5.62	1.31	1.25
1	B	137	GLU	CD-OE1	5.40	1.31	1.25
1	B	376	GLU	CD-OE1	5.37	1.31	1.25
1	A	5	GLU	CD-OE1	5.31	1.31	1.25
1	B	323[A]	GLU	C-O	5.25	1.33	1.23
1	B	323[B]	GLU	C-O	5.25	1.33	1.23
1	B	161	GLU	CD-OE2	5.20	1.31	1.25

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	260	ARG	NE-CZ-NH1	-14.24	113.18	120.30
1	B	291	ARG	NE-CZ-NH1	11.02	125.81	120.30
1	B	291	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	B	327[A]	ARG	NE-CZ-NH2	-8.70	115.95	120.30
1	B	327[B]	ARG	NE-CZ-NH2	-8.70	115.95	120.30
1	A	327	ARG	NE-CZ-NH2	8.29	124.44	120.30
1	B	260	ARG	NE-CZ-NH1	-8.06	116.27	120.30
1	A	260	ARG	NE-CZ-NH2	7.19	123.89	120.30
1	A	339	ARG	NE-CZ-NH1	-7.07	116.77	120.30
1	B	193	GLU	CG-CD-OE2	7.04	132.38	118.30
1	A	291	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	B	158	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	B	260	ARG	NE-CZ-NH2	6.35	123.47	120.30
1	A	196	ARG	CG-CD-NE	-5.75	99.73	111.80
1	A	327	ARG	NE-CZ-NH1	-5.67	117.46	120.30
1	A	196	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	260	ARG	CB-CG-CD	-5.46	97.42	111.60
1	A	291	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	B	394[A]	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	B	394[B]	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	B	193	GLU	CG-CD-OE1	-5.33	107.64	118.30
1	B	294	PHE	CB-CG-CD1	-5.22	117.15	120.80
1	A	394	ARG	NE-CZ-NH1	5.07	122.83	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	222	ALA	Mainchain

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	3274	0	3293	21	0
1	B	3220	0	3229	29	0
2	C	23	0	21	0	0
2	D	23	0	21	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	3	0	0	0	0
3	B	6	0	0	0	0
4	A	4	0	0	0	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0
6	A	5	0	8	4	0
6	B	5	0	8	1	0
7	A	12	0	18	1	0
7	B	4	0	6	0	0
8	A	7	0	10	1	0
8	B	7	0	10	3	0
9	B	10	0	0	0	0
10	B	5	0	0	0	0
11	B	5	0	5	0	0
12	A	405	0	0	18	0
12	B	427	0	0	10	0
All	All	7451	0	6629	55	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.

All (55) 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:358[B]:GLN:NE2	12:A:604:HOH:O	1.86	1.04
1:A:17[B]:GLU:OE2	12:A:602:HOH:O	1.81	0.96
6:A:504:PGO:C3	12:A:912:HOH:O	2.12	0.96
1:A:17[B]:GLU:OE2	12:A:603:HOH:O	1.82	0.96
1:B:323[B]:GLU:HG2	12:B:701:HOH:O	1.66	0.95
1:B:318:TYR:HE1	8:B:510:PEG:H32	1.37	0.87
1:A:365[A]:THR:OG1	12:A:601:HOH:O	1.69	0.85
6:A:504:PGO:H31	12:A:912:HOH:O	1.76	0.84
1:B:193:GLU:OE2	12:B:601:HOH:O	1.98	0.81
1:B:323[B]:GLU:CG	12:B:701:HOH:O	2.29	0.78
1:B:2:LYS:N	12:B:605:HOH:O	2.23	0.70
6:A:504:PGO:C1	12:A:867:HOH:O	2.39	0.70
1:B:265:GLU:O	12:B:603:HOH:O	2.13	0.66
6:A:504:PGO:H12	12:A:867:HOH:O	1.94	0.66
1:B:318:TYR:CE1	8:B:510:PEG:H32	2.26	0.65
1:A:412:ASN:HD22	7:A:507:EDO:H21	1.63	0.63
1:B:281[B]:VAL:HG12	1:B:352:LEU:HD22	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:TYR:OH	1:A:327:ARG:NH1	2.32	0.62
1:B:327[B]:ARG:HD2	12:B:951:HOH:O	2.04	0.58
1:A:222:ALA:HB2	12:A:681:HOH:O	2.04	0.57
1:A:222:ALA:CB	12:A:681:HOH:O	2.54	0.56
1:A:345:PRO:O	1:A:349:GLN:HG2	2.05	0.56
1:B:45:TRP:O	1:B:49[A]:THR:HG23	2.06	0.55
1:A:4:LEU:HD11	1:A:311[A]:LEU:HG	1.92	0.51
1:B:348:GLN:NE2	12:B:613:HOH:O	2.43	0.51
8:A:508:PEG:H12	12:A:910:HOH:O	2.10	0.50
1:A:358[B]:GLN:CD	12:A:604:HOH:O	2.36	0.50
1:A:213[B]:GLU:CD	12:A:610:HOH:O	2.50	0.48
1:B:137:GLU:HG2	12:B:962:HOH:O	2.13	0.48
1:B:28:LYS:HE3	12:B:991:HOH:O	2.12	0.48
1:B:49[B]:THR:HG22	12:B:899:HOH:O	2.12	0.48
1:B:318:TYR:HE1	8:B:510:PEG:C3	2.16	0.48
1:A:122:TYR:CZ	1:A:257:MET:HB2	2.49	0.47
1:B:332:THR:O	6:B:508:PGO:H12	2.14	0.47
1:A:203:GLN:NE2	12:A:605:HOH:O	2.25	0.47
1:B:49[A]:THR:HG22	1:B:74:MET:CE	2.44	0.47
1:B:385:MET:HE2	1:B:385:MET:HB2	1.81	0.47
1:A:327:ARG:HD3	12:A:754:HOH:O	2.15	0.47
1:B:281[A]:VAL:HG23	1:B:352:LEU:HD22	1.96	0.47
1:B:263:VAL:HG12	1:B:269:GLY:H	1.81	0.46
1:B:48:ILE:HD13	1:B:63:LEU:CD2	2.45	0.46
1:B:122:TYR:CZ	1:B:257:MET:HB2	2.52	0.45
1:A:85:GLU:HG2	12:A:656:HOH:O	2.17	0.44
1:B:263:VAL:O	1:B:264:PRO:C	2.56	0.44
1:A:32:VAL:HG11	1:A:311[A]:LEU:HD21	2.00	0.43
12:A:674:HOH:O	1:B:35:LYS:HE3	2.19	0.43
1:A:99:ARG:NH1	12:A:627:HOH:O	2.52	0.43
1:B:339:ARG:HG3	1:B:342:TRP:CZ3	2.54	0.42
1:A:114:TRP:CZ2	1:A:328:TYR:CE2	3.08	0.42
1:B:140:ALA:HA	1:B:291:ARG:HH22	1.85	0.41
1:A:3[B]:THR:HG21	1:A:35:LYS:HG3	2.02	0.41
1:B:263:VAL:O	1:B:269:GLY:HA3	2.19	0.41
1:B:202:TRP:CE2	1:B:369:LEU:HD21	2.56	0.41
1:B:48:ILE:HD13	1:B:63:LEU:HD23	2.03	0.40
1:A:318:TYR:HH	1:A:327:ARG:HH12	1.69	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	431/423 (102%)	427 (99%)	4 (1%)	0	100	100
1	B	423/423 (100%)	419 (99%)	4 (1%)	0	100	100
All	All	854/846 (101%)	846 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	331/321 (103%)	326 (98%)	5 (2%)	65	42
1	B	323/321 (101%)	321 (99%)	2 (1%)	86	75
All	All	654/642 (102%)	647 (99%)	7 (1%)	73	55

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	MET
1	A	9	MET
1	A	193	GLU
1	A	251	PHE
1	A	361	GLN
1	B	9	MET
1	B	193	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	308	ASN
1	B	348	GLN
1	B	361	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 ⓘ

4 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	0.64	0	17,17,17	0.57	0
2	BGC	C	2	2	11,11,12	0.90	0	15,15,17	2.23	5 (33%)
2	BGC	D	1	2	12,12,12	0.67	0	17,17,17	1.25	2 (11%)
2	BGC	D	2	2	11,11,12	0.71	0	15,15,17	1.67	4 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	C	1	2	-	2/2/22/22	0/1/1/1

Continued on next page...

Continued from previous page...

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

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	BGC	O2-C2-C1	4.53	118.42	109.15
2	C	2	BGC	O5-C5-C6	4.35	114.02	107.20
2	D	2	BGC	C1-O5-C5	3.21	116.55	112.19
2	D	1	BGC	C1-O5-C5	-3.15	107.72	113.66
2	D	2	BGC	O5-C1-C2	-3.01	106.12	110.77
2	D	2	BGC	O5-C5-C4	-2.97	103.61	110.83
2	C	2	BGC	C1-C2-C3	-2.68	106.37	109.67
2	C	2	BGC	O3-C3-C2	2.61	114.99	109.99
2	C	2	BGC	C2-C3-C4	-2.53	106.51	110.89
2	D	2	BGC	O2-C2-C3	2.02	114.18	110.14
2	D	1	BGC	C4-C3-C2	-2.01	107.32	110.82

There are no chirality outliers.

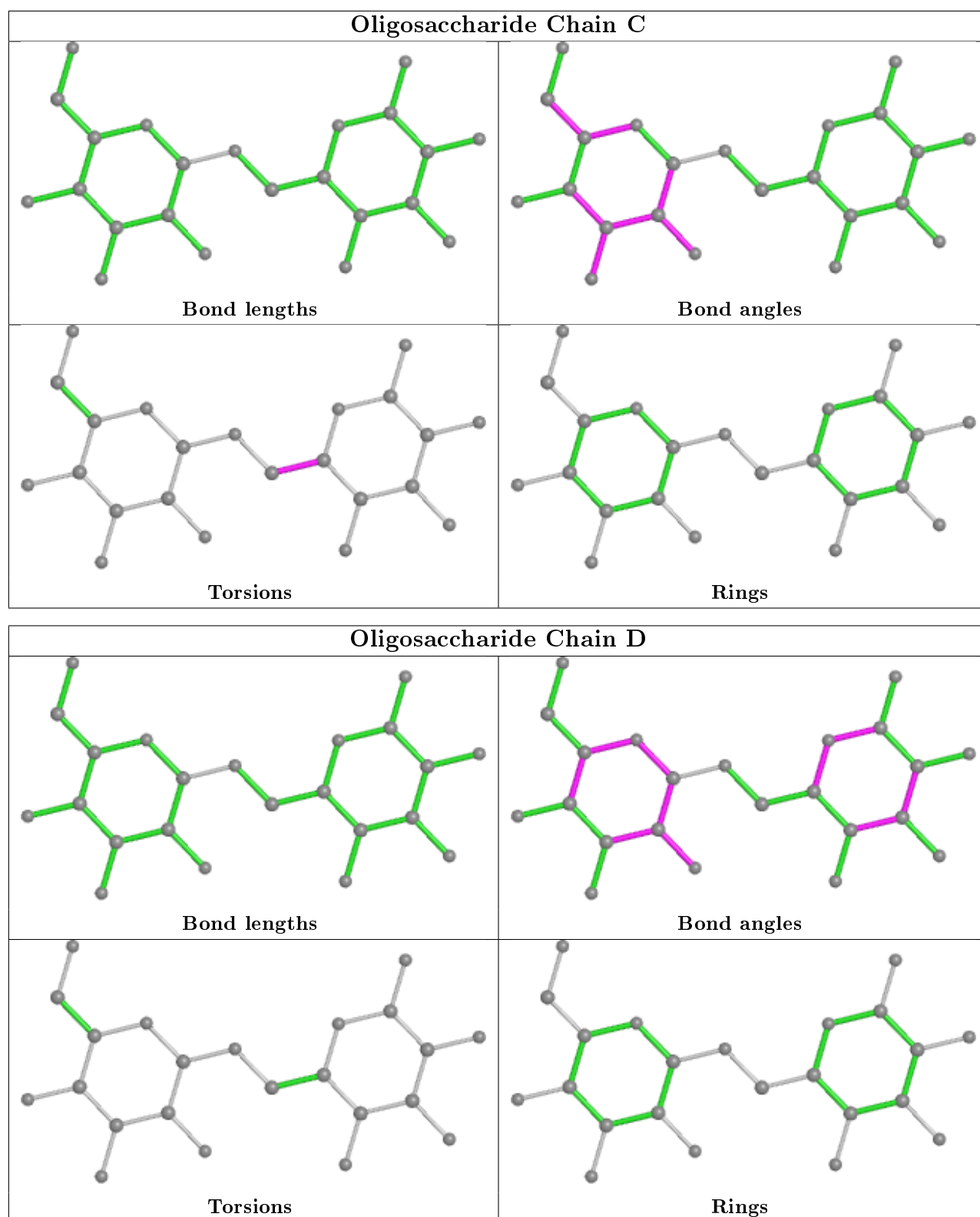
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	BGC	C4-C5-C6-O6
2	C	1	BGC	O5-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](#)

18 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	$\# Z > 2$
9	SO4	B	505	-	4,4,4	0.35	0	6,6,6	0.28	0
7	EDO	A	506	-	3,3,3	0.17	0	2,2,2	0.33	0
6	PGO	A	504	-	3,4,4	0.36	0	1,4,4	0.09	0
3	SO2	B	502	-	2,2,2	0.99	0	1,1,1	0.05	0
8	PEG	A	508	-	6,6,6	0.18	0	5,5,5	0.13	0
7	EDO	A	505	-	3,3,3	0.22	0	2,2,2	0.43	0
9	SO4	B	504	-	4,4,4	0.32	0	6,6,6	0.13	0
8	PEG	B	510	-	6,6,6	0.22	0	5,5,5	0.34	0
3	SO2	B	501	-	2,2,2	0.43	0	1,1,1	0.29	0
3	SO2	A	501	-	2,2,2	0.55	0	1,1,1	0.25	0
5	CO2	B	503	-	2,2,2	0.06	0	1,1,1	0.99	0
7	EDO	A	507	-	3,3,3	0.31	0	2,2,2	0.34	0
7	EDO	B	509	-	3,3,3	0.24	0	2,2,2	0.13	0
5	CO2	A	503	-	2,2,2	0.16	0	1,1,1	0.97	0
10	PO4	B	506	-	4,4,4	0.97	0	6,6,6	0.63	0
6	PGO	B	508	-	3,4,4	0.27	0	1,4,4	0.07	0
11	IMD	B	507	-	3,5,5	0.30	0	4,5,5	0.68	0
4	SO3	A	502	-	1,3,3	1.45	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
6	PGO	A	504	-	-	1/2/2/2	-
8	PEG	A	508	-	-	2/4/4/4	-
7	EDO	A	505	-	-	1/1/1/1	-
8	PEG	B	510	-	-	2/4/4/4	-
7	EDO	A	506	-	-	0/1/1/1	-
7	EDO	A	507	-	-	1/1/1/1	-
7	EDO	B	509	-	-	0/1/1/1	-
6	PGO	B	508	-	-	0/2/2/2	-
11	IMD	B	507	-	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	508	PEG	O2-C3-C4-O4
8	B	510	PEG	O2-C3-C4-O4
8	B	510	PEG	C1-C2-O2-C3
7	A	507	EDO	O1-C1-C2-O2
8	A	508	PEG	O1-C1-C2-O2
7	A	505	EDO	O1-C1-C2-O2
6	A	504	PGO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	504	PGO	4	0
8	A	508	PEG	1	0
8	B	510	PEG	3	0
7	A	507	EDO	1	0
6	B	508	PGO	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, 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	417/423 (98%)	-0.40	2 (0%) 91 91	7, 13, 24, 50	0
1	B	415/423 (98%)	-0.35	4 (0%) 82 83	7, 12, 25, 59	0
All	All	832/846 (98%)	-0.38	6 (0%) 87 88	7, 13, 24, 59	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	266	ALA	4.9
1	A	0	MET	2.7
1	B	198	ALA	2.6
1	B	45	TRP	2.4
1	A	107	ARG	2.3
1	B	268	GLY	2.0

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

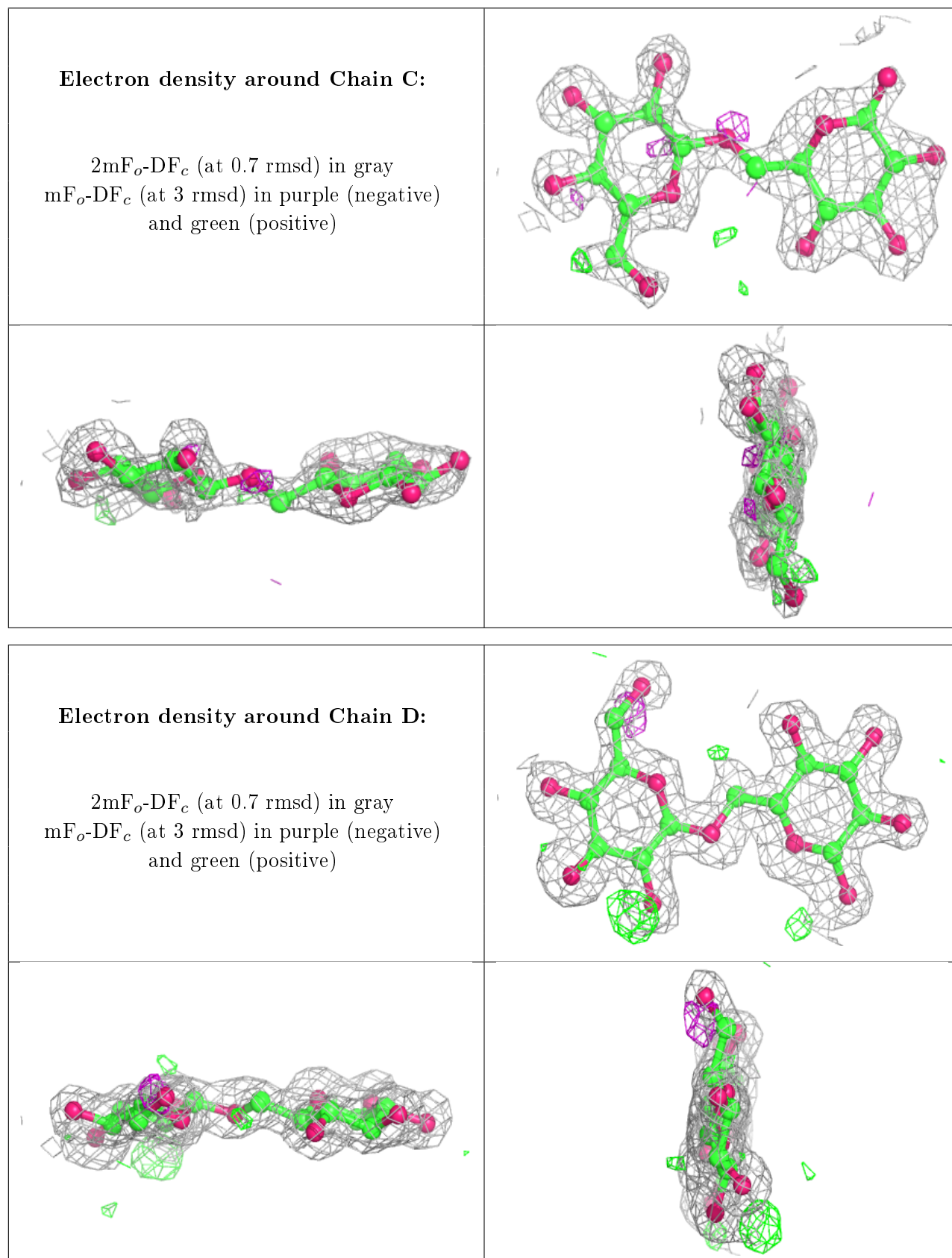
There are no non-standard protein/DNA/RNA residues in this entry.

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
2	BGC	C	1	12/12	0.76	0.18	38,40,44,47	0
2	BGC	C	2	11/12	0.80	0.27	25,33,39,43	0
2	BGC	D	1	12/12	0.90	0.12	23,25,28,30	0
2	BGC	D	2	11/12	0.92	0.15	18,21,23,26	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(Å ²)	Q<0.9
7	EDO	A	507	4/4	0.72	0.16	28,28,30,37	0
7	EDO	A	505	4/4	0.80	0.15	33,33,35,35	0
11	IMD	B	507	5/5	0.83	0.15	40,42,43,44	0
8	PEG	A	508	7/7	0.86	0.10	36,40,44,44	0
8	PEG	B	510	7/7	0.88	0.18	23,26,30,32	0
6	PGO	B	508	5/5	0.89	0.13	41,42,43,45	0
3	SO2	A	501	3/3	0.89	0.14	40,40,49,55	0
7	EDO	A	506	4/4	0.91	0.10	32,35,35,36	0
4	SO3	A	502	4/4	0.91	0.21	39,40,46,47	0
10	PO4	B	506	5/5	0.92	0.13	22,26,33,35	0
5	CO2	A	503	3/3	0.93	0.10	42,42,43,45	0
5	CO2	B	503	3/3	0.94	0.07	43,43,44,45	0
7	EDO	B	509	4/4	0.95	0.08	30,33,35,39	0
9	SO4	B	504	5/5	0.95	0.18	36,40,44,46	0
6	PGO	A	504	5/5	0.96	0.15	28,30,31,32	0
3	SO2	B	501	3/3	0.97	0.11	34,34,41,41	0
3	SO2	B	502	3/3	0.97	0.09	21,21,24,35	0
9	SO4	B	505	5/5	0.98	0.09	25,29,34,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.