



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:55 AM UTC

PDB ID : 8X18 / pdb_00008x18
Title : Xanthomonas campestris pv. campestris OpgD mutant-D379N with beta-1,2-glucan
Authors : Motouchi, S.; Nakajima, M.
Deposited on : 2023-11-06
Resolution : 2.25 Å(reported)

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

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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

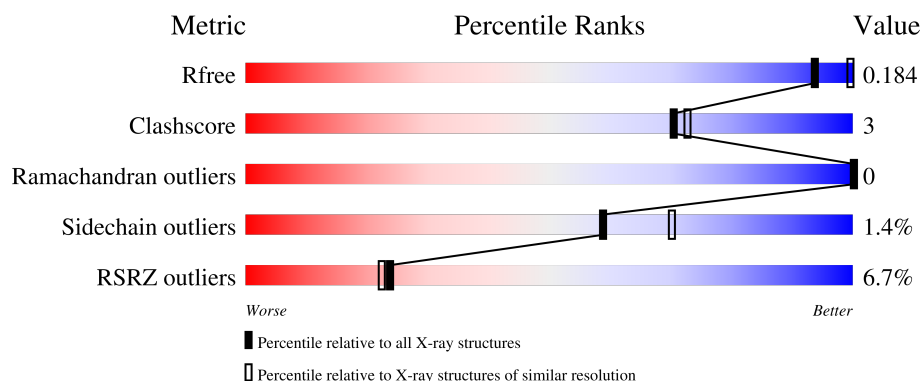
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	541	3% 85% 8% 7%
1	B	541	9% 81% 9% 9%
2	C	22	32% 64% 5%
3	D	11	73% 27%
4	E	10	70% 30%

i

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 Glucans biosynthesis protein D.

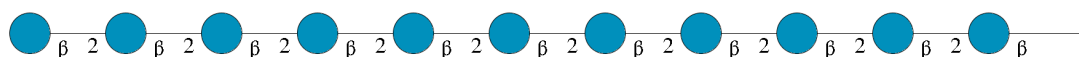
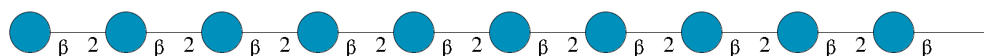
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total 4020	C 2577	N 705	O 727	S 11	0	0	0
1	B	490	Total 3927	C 2522	N 686	O 708	S 11	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	379	ASN	ASP	engineered mutation	UNP Q8P3C6
A	534	LEU	-	expression tag	UNP Q8P3C6
A	535	GLU	-	expression tag	UNP Q8P3C6
A	536	HIS	-	expression tag	UNP Q8P3C6
A	537	HIS	-	expression tag	UNP Q8P3C6
A	538	HIS	-	expression tag	UNP Q8P3C6
A	539	HIS	-	expression tag	UNP Q8P3C6
A	540	HIS	-	expression tag	UNP Q8P3C6
A	541	HIS	-	expression tag	UNP Q8P3C6
B	379	ASN	ASP	engineered mutation	UNP Q8P3C6
B	534	LEU	-	expression tag	UNP Q8P3C6
B	535	GLU	-	expression tag	UNP Q8P3C6
B	536	HIS	-	expression tag	UNP Q8P3C6
B	537	HIS	-	expression tag	UNP Q8P3C6
B	538	HIS	-	expression tag	UNP Q8P3C6
B	539	HIS	-	expression tag	UNP Q8P3C6
B	540	HIS	-	expression tag	UNP Q8P3C6
B	541	HIS	-	expression tag	UNP Q8P3C6

- [illegible]

A horizontal number line starting at 0 and ending at 16. There are blue circular markers at every integer value from 0 to 16.

[illegible][illegible]

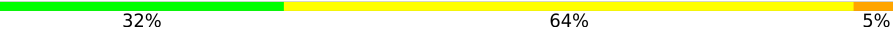
- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	298	Total	O	0	0
			298	298		
6	B	243	Total	O	0	0
			243	243		

Chain C:  32% 64% 5%

BGC1
BGC2
BGC3
BGC4
BGC5
BGC6
BGC7
BGC8
BGC9
BGC10
BGC11
BGC12
BGC13
BGC14
BGC15
BGC16
BGC17
BGC18
BGC19
BGC20
BGC21
BGC22

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

Chain D:  73% 27%

BGC1
BGC2
BGC3
BGC4
BGC5
BGC6
BGC7
BGC8
BGC9
BGC10
BGC11

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

Chain E:  70% 30%

BGC1
BGC2
BGC3
BGC4
BGC5
BGC6
BGC7
BGC8
BGC9
BGC10

4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	171.88Å 171.88Å 128.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.72 – 2.25 48.72 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.72-2.25) 100.0 (48.72-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0405	Depositor
R, R_{free}	0.173 , 0.176 0.181 , 0.184	Depositor DCC
R_{free} test set	5213 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9012	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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: GOL, BGC

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	0.67	0/4146	1.02	7/5634 (0.1%)
1	B	0.69	1/4050 (0.0%)	1.05	6/5504 (0.1%)
All	All	0.68	1/8196 (0.0%)	1.04	13/11138 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	6
All	All	0	12

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	79	TYR	C-N	-6.50	1.24	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	493	PRO	N-CA-CB	6.73	106.96	103.19
1	B	524	PRO	N-CA-CB	6.54	106.62	103.22
1	B	351	PRO	N-CA-C	6.36	121.17	111.19
1	A	257	ARG	N-CA-C	-6.08	106.19	113.97
1	B	504	ARG	CB-CA-C	5.95	120.04	110.16
1	A	493	PRO	N-CA-CB	5.92	106.50	103.19
1	B	165	ASP	CB-CA-C	5.69	119.61	109.38
1	A	249	ASP	CA-CB-CG	5.51	118.11	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	PRO	N-CA-CB	5.38	108.03	103.35
1	A	257	ARG	N-CA-CB	-5.24	103.39	110.67
1	A	87	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	324	ASN	CB-CA-C	5.14	115.55	110.71
1	B	372	PRO	N-CA-CB	5.04	107.80	103.31

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	237	ARG	Sidechain
1	A	326	ARG	Sidechain
1	A	36	ARG	Sidechain
1	A	468	ARG	Sidechain
1	A	508	ARG	Sidechain
1	A	53	ARG	Sidechain
1	B	279	ARG	Sidechain
1	B	350	ARG	Sidechain
1	B	36	ARG	Sidechain
1	B	402	ARG	Sidechain
1	B	53	ARG	Sidechain
1	B	85	ARG	Sidechain

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	4020	0	3870	22	0
1	B	3927	0	3774	34	0
2	C	243	0	201	3	0
3	D	122	0	102	0	0
4	E	111	0	93	0	0
5	A	36	0	48	9	0
5	B	12	0	16	2	0
6	A	298	0	0	0	0
6	B	243	0	0	3	0
All	All	9012	0	8104	57	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 (57) 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:B:433:ARG:HH11	1:B:433:ARG:HG3	1.41	0.86
1:A:104:HIS:HD2	1:A:105:LEU:O	1.70	0.74
5:A:605:GOL:O1	1:B:433:ARG:NH2	2.22	0.72
1:B:237:ARG:HD3	6:B:910:HOH:O	1.88	0.72
1:A:470:THR:HA	5:A:604:GOL:H2	1.74	0.69
1:A:104:HIS:HE1	1:A:128:TYR:OH	1.77	0.68
1:A:523:THR:H	5:A:603:GOL:H12	1.60	0.67
1:B:433:ARG:HH11	1:B:433:ARG:CG	2.11	0.63
1:B:347:TYR:HA	1:B:350:ARG:HD2	1.81	0.63
1:B:44:ASP:HB2	5:B:602:GOL:H31	1.79	0.62
1:A:36:ARG:HG2	1:A:124:GLN:CG	2.32	0.60
1:A:466:VAL:HG22	5:A:604:GOL:H11	1.84	0.58
1:B:379:ASN:ND2	2:C:7:BGC:H6C1	2.19	0.57
1:B:130:PRO:HB3	1:B:135:TYR:OH	2.06	0.55
1:A:392:GLN:N	1:A:395:GLN:OE1	2.39	0.52
1:A:379:ASN:O	5:A:601:GOL:H12	2.10	0.51
1:B:80:GLN:C	1:B:82:ILE:N	2.66	0.51
1:B:508:ARG:HD3	6:B:704:HOH:O	2.09	0.51
1:B:279:ARG:HD3	6:B:906:HOH:O	2.11	0.50
1:A:312:PRO:HA	5:A:603:GOL:C3	2.42	0.50
1:B:74:LEU:N	1:B:78:GLN:CD	2.70	0.50
1:B:379:ASN:HD22	2:C:7:BGC:H6C1	1.76	0.49
1:A:36:ARG:HG2	1:A:124:GLN:HG2	1.94	0.49
1:B:266:GLY:N	1:B:267:PRO:CD	2.76	0.48
1:B:75:ASN:H	1:B:78:GLN:NE2	2.13	0.47
1:B:45:TYR:HB3	5:B:602:GOL:H2	1.98	0.46
1:A:284:ASP:HB2	5:A:605:GOL:O3	2.16	0.46
1:A:463:VAL:O	1:A:505:LEU:HA	2.16	0.46
1:B:32:VAL:HG23	1:B:33:GLY:O	2.16	0.46
1:B:263:LEU:HD22	1:B:391:PRO:HG3	1.98	0.46
1:B:30:LYS:HD2	1:B:31:ALA:H	1.82	0.45
1:B:211:LEU:HD12	1:B:211:LEU:N	2.32	0.44
1:A:260:ILE:HB	1:A:391:PRO:HG2	1.99	0.44
1:A:471:THR:HA	1:A:490:ASP:O	2.18	0.44
1:B:80:GLN:O	1:B:81:SER:C	2.59	0.44
1:B:436:PHE:CD2	1:B:530:ARG:HD3	2.52	0.44
1:A:312:PRO:HA	5:A:603:GOL:H32	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:VAL:HG22	1:B:403:LEU:CD2	2.47	0.44
1:B:107:LEU:HD23	1:B:108:TYR:H	1.83	0.44
1:A:237:ARG:HH12	1:A:239:ALA:HB2	1.82	0.43
1:A:229:SER:O	1:A:230:PRO:C	2.61	0.43
5:A:605:GOL:C1	1:B:433:ARG:NH2	2.82	0.43
1:B:224:TYR:CE2	1:B:237:ARG:HG3	2.53	0.42
1:B:80:GLN:N	1:B:80:GLN:OE1	2.52	0.42
1:B:468:ARG:CZ	1:B:499:GLN:HB2	2.49	0.42
2:C:4:BGC:H3	2:C:6:BGC:H6C2	2.02	0.42
1:A:237:ARG:NH1	1:A:239:ALA:HB2	2.35	0.42
1:B:82:ILE:H	1:B:82:ILE:HG13	1.75	0.42
1:B:281:MET:O	1:B:281:MET:HG3	2.19	0.42
1:B:35:ARG:HG2	1:B:127:ALA:HB3	2.02	0.41
1:B:426:GLY:HA2	1:B:439:ARG:HB2	2.03	0.41
1:A:436:PHE:CD2	1:A:530:ARG:HD3	2.56	0.41
1:B:88:HIS:CE1	1:B:131:ALA:O	2.74	0.41
1:A:315:LEU:HD12	1:A:371:ILE:HG12	2.03	0.40
1:A:355:VAL:HG22	1:A:403:LEU:CD2	2.52	0.40
1:B:433:ARG:CG	1:B:433:ARG:NH1	2.76	0.40
1:A:455:ASP:HA	1:A:456:PRO:HD3	1.93	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	502/541 (93%)	486 (97%)	16 (3%)	0	100	100
1	B	484/541 (90%)	468 (97%)	16 (3%)	0	100	100
All	All	986/1082 (91%)	954 (97%)	32 (3%)	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	410/436 (94%)	403 (98%)	7 (2%)	53	65
1	B	401/436 (92%)	397 (99%)	4 (1%)	68	77
All	All	811/872 (93%)	800 (99%)	11 (1%)	59	70

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ARG
1	A	247	VAL
1	A	423	THR
1	A	457	LYS
1	A	468	ARG
1	A	508	ARG
1	A	531	LYS
1	B	32	VAL
1	B	82	ILE
1	B	107	LEU
1	B	157	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	HIS
1	A	273	GLN
1	A	314	HIS
1	A	318	ASN
1	A	367	GLN
1	A	379	ASN
1	A	500	GLN
1	B	78	GLN
1	B	125	GLN
1	B	183	GLN
1	B	318	ASN

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Mol	Chain	Res	Type
1	B	367	GLN
1	B	379	ASN
1	B	500	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 ⓘ

43 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	0.21	0	17,17,17	0.50	0
2	BGC	C	10	2	11,11,12	0.26	0	15,15,17	0.89	1 (6%)
2	BGC	C	11	2	11,11,12	0.32	0	15,15,17	0.67	1 (6%)
2	BGC	C	12	2	11,11,12	0.20	0	15,15,17	0.68	0
2	BGC	C	13	2	11,11,12	0.24	0	15,15,17	0.91	1 (6%)
2	BGC	C	14	2	11,11,12	0.36	0	15,15,17	1.08	1 (6%)
2	BGC	C	15	2	11,11,12	0.17	0	15,15,17	0.74	1 (6%)
2	BGC	C	16	2	11,11,12	0.31	0	15,15,17	1.11	1 (6%)
2	BGC	C	17	2	11,11,12	0.26	0	15,15,17	0.86	1 (6%)
2	BGC	C	18	2	11,11,12	0.24	0	15,15,17	0.56	0
2	BGC	C	19	2	11,11,12	0.27	0	15,15,17	0.62	0
2	BGC	C	2	2	11,11,12	0.30	0	15,15,17	0.79	1 (6%)
2	BGC	C	20	2	11,11,12	0.29	0	15,15,17	0.60	0
2	BGC	C	21	2	11,11,12	0.88	0	15,15,17	0.77	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	C	22	2	11,11,12	0.69	0	15,15,17	1.16	1 (6%)
2	BGC	C	3	2	11,11,12	0.27	0	15,15,17	0.73	1 (6%)
2	BGC	C	4	2	11,11,12	0.20	0	15,15,17	0.51	0
2	BGC	C	5	2	11,11,12	0.25	0	15,15,17	0.92	0
2	BGC	C	6	2	11,11,12	0.23	0	15,15,17	0.62	0
2	BGC	C	7	2	11,11,12	0.72	0	15,15,17	1.43	2 (13%)
2	BGC	C	8	2	11,11,12	0.32	0	15,15,17	0.45	0
2	BGC	C	9	2	11,11,12	0.31	0	15,15,17	1.34	1 (6%)
3	BGC	D	1	3	12,12,12	0.21	0	17,17,17	0.47	0
3	BGC	D	10	3	11,11,12	0.39	0	15,15,17	0.68	0
3	BGC	D	11	3	11,11,12	0.27	0	15,15,17	0.79	0
3	BGC	D	2	3	11,11,12	0.29	0	15,15,17	0.50	0
3	BGC	D	3	3	11,11,12	0.28	0	15,15,17	0.83	1 (6%)
3	BGC	D	4	3	11,11,12	0.45	0	15,15,17	0.94	1 (6%)
3	BGC	D	5	3	11,11,12	0.35	0	15,15,17	0.69	0
3	BGC	D	6	3	11,11,12	0.34	0	15,15,17	0.57	0
3	BGC	D	7	3	11,11,12	0.30	0	15,15,17	0.84	1 (6%)
3	BGC	D	8	3	11,11,12	0.33	0	15,15,17	0.64	0
3	BGC	D	9	3	11,11,12	0.44	0	15,15,17	0.71	0
4	BGC	E	1	4	12,12,12	0.17	0	17,17,17	0.27	0
4	BGC	E	10	4	11,11,12	0.21	0	15,15,17	0.65	0
4	BGC	E	2	4	11,11,12	0.26	0	15,15,17	0.94	1 (6%)
4	BGC	E	3	4	11,11,12	0.36	0	15,15,17	0.87	1 (6%)
4	BGC	E	4	4	11,11,12	0.34	0	15,15,17	0.73	1 (6%)
4	BGC	E	5	4	11,11,12	0.36	0	15,15,17	0.61	0
4	BGC	E	6	4	11,11,12	0.34	0	15,15,17	0.60	0
4	BGC	E	7	4	11,11,12	0.28	0	15,15,17	0.60	0
4	BGC	E	8	4	11,11,12	0.35	0	15,15,17	0.73	0
4	BGC	E	9	4	11,11,12	0.36	0	15,15,17	0.70	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	C	1	2	-	0/2/22/22	0/1/1/1
2	BGC	C	10	2	-	0/2/19/22	0/1/1/1
2	BGC	C	11	2	-	0/2/19/22	0/1/1/1
2	BGC	C	12	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	C	13	2	-	0/2/19/22	0/1/1/1
2	BGC	C	14	2	-	0/2/19/22	0/1/1/1
2	BGC	C	15	2	-	0/2/19/22	0/1/1/1
2	BGC	C	16	2	-	0/2/19/22	0/1/1/1
2	BGC	C	17	2	-	0/2/19/22	0/1/1/1
2	BGC	C	18	2	-	0/2/19/22	0/1/1/1
2	BGC	C	19	2	-	0/2/19/22	0/1/1/1
2	BGC	C	2	2	-	2/2/19/22	0/1/1/1
2	BGC	C	20	2	-	0/2/19/22	0/1/1/1
2	BGC	C	21	2	-	0/2/19/22	0/1/1/1
2	BGC	C	22	2	-	0/2/19/22	0/1/1/1
2	BGC	C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	C	4	2	-	0/2/19/22	0/1/1/1
2	BGC	C	5	2	-	0/2/19/22	0/1/1/1
2	BGC	C	6	2	-	0/2/19/22	0/1/1/1
2	BGC	C	7	2	-	0/2/19/22	0/1/1/1
2	BGC	C	8	2	-	0/2/19/22	0/1/1/1
2	BGC	C	9	2	-	0/2/19/22	0/1/1/1
3	BGC	D	1	3	-	0/2/22/22	0/1/1/1
3	BGC	D	10	3	-	0/2/19/22	0/1/1/1
3	BGC	D	11	3	-	0/2/19/22	0/1/1/1
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	BGC	D	5	3	-	0/2/19/22	0/1/1/1
3	BGC	D	6	3	-	0/2/19/22	0/1/1/1
3	BGC	D	7	3	-	0/2/19/22	0/1/1/1
3	BGC	D	8	3	-	0/2/19/22	0/1/1/1
3	BGC	D	9	3	-	2/2/19/22	0/1/1/1
4	BGC	E	1	4	-	0/2/22/22	0/1/1/1
4	BGC	E	10	4	-	0/2/19/22	0/1/1/1
4	BGC	E	2	4	-	0/2/19/22	0/1/1/1
4	BGC	E	3	4	-	0/2/19/22	0/1/1/1
4	BGC	E	4	4	-	0/2/19/22	0/1/1/1
4	BGC	E	5	4	-	0/2/19/22	0/1/1/1
4	BGC	E	6	4	-	2/2/19/22	0/1/1/1
4	BGC	E	7	4	-	0/2/19/22	0/1/1/1
4	BGC	E	8	4	-	1/2/19/22	0/1/1/1
4	BGC	E	9	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	9	BGC	C1-C2-C3	4.17	115.72	109.64
2	C	7	BGC	C1-O5-C5	4.13	117.72	112.19
2	C	16	BGC	C1-C2-C3	3.23	114.35	109.64
4	E	2	BGC	C1-C2-C3	3.02	114.04	109.64
2	C	14	BGC	C1-C2-C3	2.94	113.93	109.64
2	C	22	BGC	C1-O5-C5	2.88	116.04	112.19
3	D	4	BGC	C1-C2-C3	2.78	113.69	109.64
3	D	3	BGC	C1-C2-C3	2.67	113.54	109.64
2	C	13	BGC	C1-C2-C3	2.55	113.36	109.64
2	C	10	BGC	C1-C2-C3	2.41	113.15	109.64
4	E	3	BGC	C1-C2-C3	2.37	113.10	109.64
3	D	7	BGC	C1-C2-C3	2.32	113.02	109.64
2	C	11	BGC	C1-O5-C5	2.30	115.26	112.19
2	C	17	BGC	C1-C2-C3	2.24	112.90	109.64
2	C	15	BGC	C1-C2-C3	2.23	112.89	109.64
2	C	7	BGC	C1-C2-C3	2.15	112.78	109.64
2	C	2	BGC	C1-O5-C5	2.05	114.94	112.19
2	C	3	BGC	C1-O5-C5	2.05	114.93	112.19
4	E	4	BGC	C1-C2-C3	2.04	112.62	109.64
2	C	21	BGC	C1-C2-C3	2.04	112.61	109.64

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	BGC	O5-C5-C6-O6
2	C	2	BGC	C4-C5-C6-O6
3	D	9	BGC	C4-C5-C6-O6
3	D	9	BGC	O5-C5-C6-O6
4	E	6	BGC	C4-C5-C6-O6
4	E	6	BGC	O5-C5-C6-O6
4	E	8	BGC	C4-C5-C6-O6

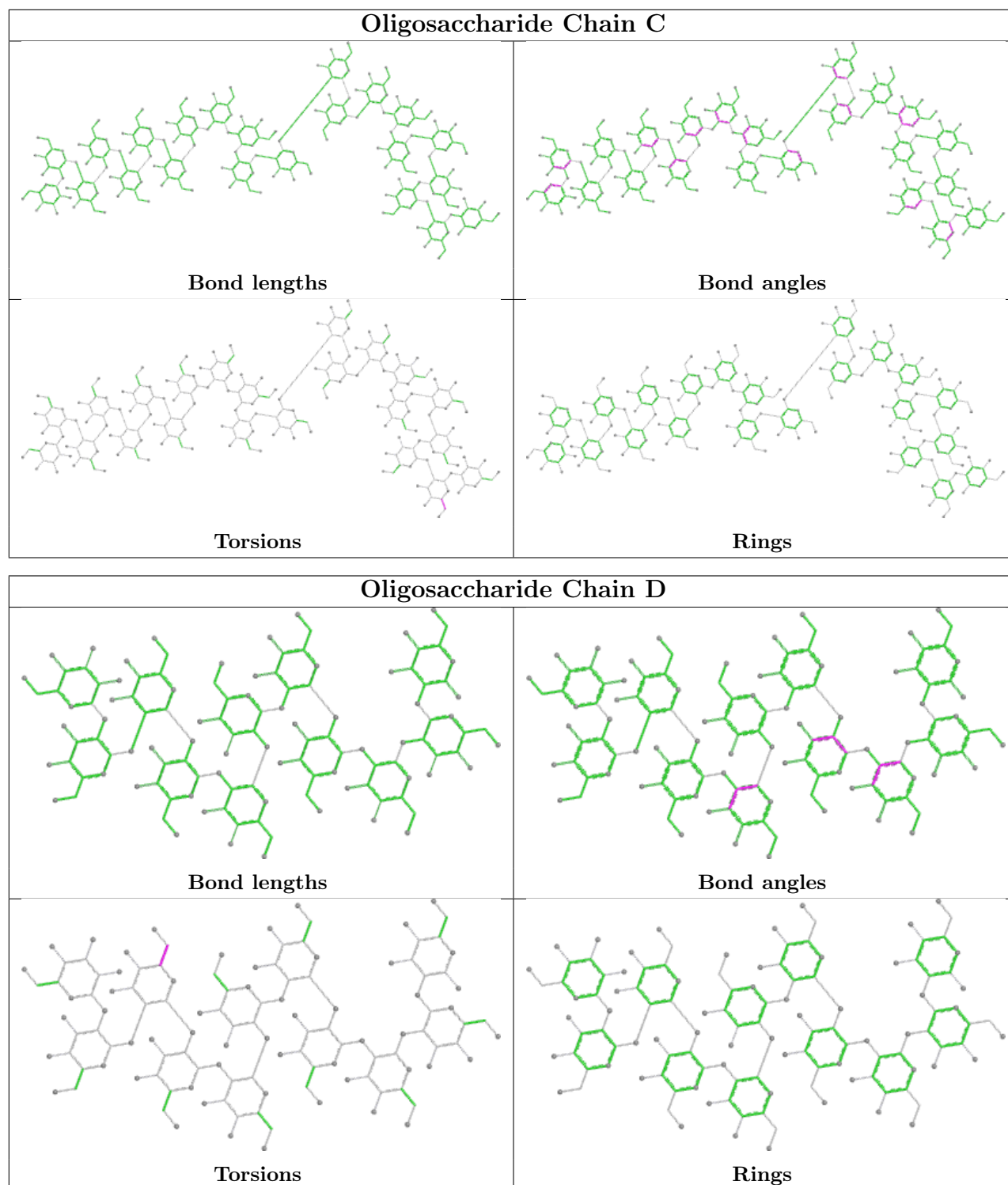
There are no ring outliers.

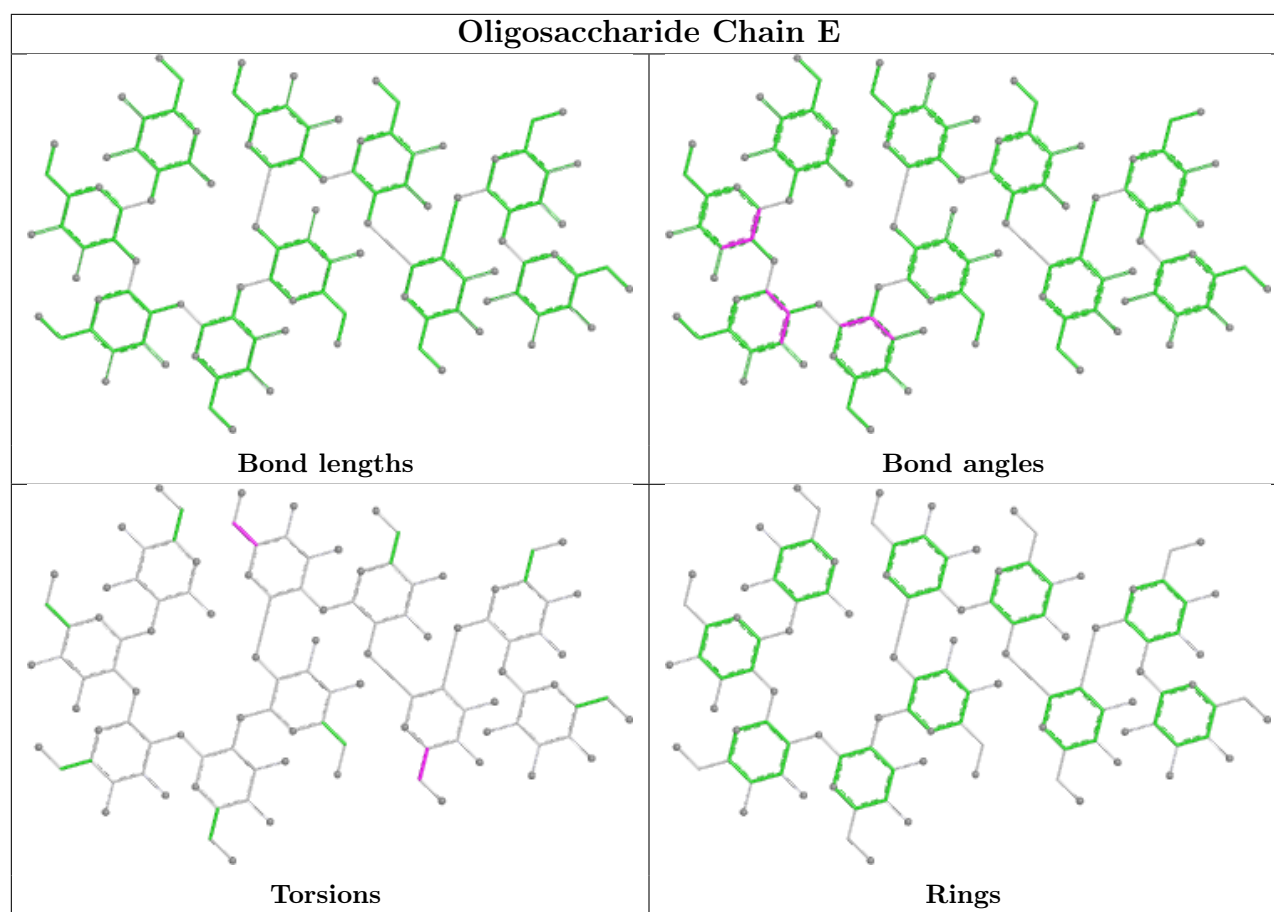
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	4	BGC	1	0
2	C	6	BGC	1	0
2	C	7	BGC	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

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	$\# Z > 2$
5	GOL	B	601	-	5,5,5	0.13	0	5,5,5	0.44	0
5	GOL	A	603	-	5,5,5	0.25	0	5,5,5	0.54	0
5	GOL	A	605	-	5,5,5	0.14	0	5,5,5	0.43	0
5	GOL	B	602	-	5,5,5	0.36	0	5,5,5	0.88	0
5	GOL	A	602	-	5,5,5	0.21	0	5,5,5	0.67	0
5	GOL	A	601	-	5,5,5	0.09	0	5,5,5	0.34	0
5	GOL	A	606	-	5,5,5	0.15	0	5,5,5	0.46	0
5	GOL	A	604	-	5,5,5	0.24	0	5,5,5	1.10	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	601	-	-	2/4/4/4	-
5	GOL	A	603	-	-	2/4/4/4	-
5	GOL	A	605	-	-	2/4/4/4	-
5	GOL	B	602	-	-	2/4/4/4	-
5	GOL	A	602	-	-	0/4/4/4	-
5	GOL	A	601	-	-	4/4/4/4	-
5	GOL	A	606	-	-	3/4/4/4	-
5	GOL	A	604	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	GOL	O1-C1-C2-C3
5	A	603	GOL	O1-C1-C2-C3
5	A	604	GOL	O1-C1-C2-C3
5	A	605	GOL	C1-C2-C3-O3
5	A	605	GOL	O2-C2-C3-O3
5	A	606	GOL	O1-C1-C2-C3
5	B	601	GOL	O1-C1-C2-C3
5	B	602	GOL	C1-C2-C3-O3
5	A	601	GOL	O2-C2-C3-O3
5	A	604	GOL	O1-C1-C2-O2
5	A	601	GOL	C1-C2-C3-O3
5	A	603	GOL	O1-C1-C2-O2
5	A	606	GOL	O1-C1-C2-O2
5	A	604	GOL	O2-C2-C3-O3
5	B	602	GOL	O2-C2-C3-O3
5	A	601	GOL	O1-C1-C2-O2
5	A	606	GOL	O2-C2-C3-O3
5	B	601	GOL	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	603	GOL	3	0
5	A	605	GOL	3	0
5	B	602	GOL	2	0
5	A	601	GOL	1	0
5	A	604	GOL	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	504/541 (93%)	-0.28	17 (3%)	48 48	19, 27, 54, 81	0
1	B	490/541 (90%)	0.03	50 (10%)	12 11	18, 28, 73, 107	0
All	All	994/1082 (91%)	-0.13	67 (6%)	24 22	18, 27, 65, 107	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	74	LEU	16.1
1	B	107	LEU	8.1
1	B	135	TYR	6.0
1	B	68	PRO	5.9
1	B	30	LYS	5.5
1	B	108	TYR	5.1
1	B	81	SER	4.4
1	A	509	ALA	4.3
1	B	75	ASN	4.2
1	B	36	ARG	4.0
1	B	110	HIS	3.9
1	A	36	ARG	3.9
1	B	78	GLN	3.9
1	A	459	LYS	3.9
1	A	432	LYS	3.8
1	B	79	TYR	3.7
1	A	30	LYS	3.6
1	B	83	ARG	3.6
1	B	76	TRP	3.5
1	B	430	GLY	3.5
1	B	80	GLN	3.4
1	B	39	GLN	3.4
1	B	67	LEU	3.3
1	B	160	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	457	LYS	3.3
1	B	454	LYS	3.2
1	B	66	VAL	3.2
1	B	105	LEU	3.2
1	B	82	ILE	3.1
1	B	31	ALA	3.1
1	B	145	LEU	3.1
1	A	457	LYS	3.1
1	B	95	ASN	3.1
1	A	160	LYS	3.1
1	B	432	LYS	3.1
1	A	454	LYS	3.0
1	A	512	LYS	3.0
1	B	131	ALA	3.0
1	A	531	LYS	2.9
1	B	64	LYS	2.9
1	B	456	PRO	2.8
1	B	33	GLY	2.8
1	B	531	LYS	2.8
1	A	39	GLN	2.7
1	A	456	PRO	2.7
1	B	164	ARG	2.7
1	B	459	LYS	2.6
1	B	77	ASP	2.6
1	A	468	ARG	2.4
1	B	32	VAL	2.4
1	A	395	GLN	2.4
1	A	143	LYS	2.3
1	B	279	ARG	2.3
1	A	511	GLY	2.3
1	B	496	GLU	2.3
1	B	87	ASP	2.3
1	A	142	GLY	2.3
1	B	468	ARG	2.2
1	B	281	MET	2.2
1	B	147	LYS	2.2
1	B	106	GLY	2.1
1	B	35	ARG	2.1
1	B	261	GLU	2.0
1	B	37	LEU	2.0
1	B	130	PRO	2.0
1	B	504	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	133	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, 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.

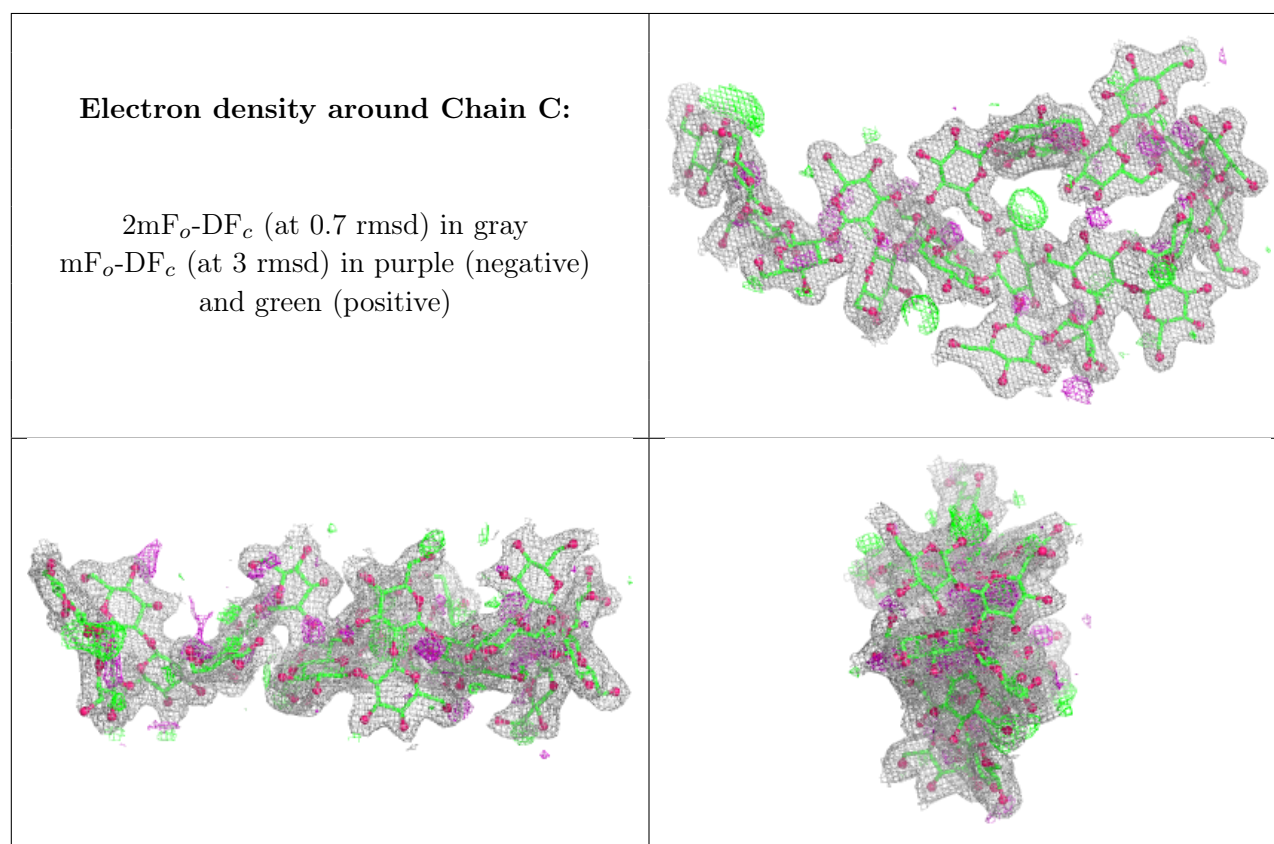
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BGC	D	1	12/12	0.82	0.17	45,54,65,74	0
2	BGC	C	2	11/12	0.84	0.15	41,53,67,70	0
4	BGC	E	3	11/12	0.84	0.14	35,49,51,53	0
2	BGC	C	13	11/12	0.85	0.13	42,48,53,56	0
2	BGC	C	1	12/12	0.87	0.11	37,45,48,48	0
3	BGC	D	4	11/12	0.88	0.13	39,47,51,53	0
2	BGC	C	14	11/12	0.88	0.12	43,46,55,59	0
3	BGC	D	6	11/12	0.89	0.12	37,41,46,46	0
4	BGC	E	6	11/12	0.89	0.12	33,36,43,49	0
2	BGC	C	19	11/12	0.90	0.13	40,48,52,52	0
3	BGC	D	7	11/12	0.90	0.12	40,46,55,58	0
2	BGC	C	16	11/12	0.91	0.11	39,44,49,50	0
4	BGC	E	1	12/12	0.91	0.11	35,41,50,56	0
3	BGC	D	5	11/12	0.92	0.10	29,32,35,39	0
2	BGC	C	18	11/12	0.92	0.10	31,37,41,43	0
4	BGC	E	5	11/12	0.92	0.10	35,37,43,46	0
2	BGC	C	21	11/12	0.92	0.10	45,48,52,54	0
2	BGC	C	15	11/12	0.93	0.09	41,44,45,46	0
2	BGC	C	20	11/12	0.93	0.09	30,35,40,40	0
2	BGC	C	5	11/12	0.93	0.09	29,32,37,37	0
3	BGC	D	8	11/12	0.93	0.09	26,32,35,36	0
3	BGC	D	9	11/12	0.93	0.09	25,29,34,34	0
2	BGC	C	17	11/12	0.93	0.10	34,41,42,43	0
3	BGC	D	2	11/12	0.93	0.09	34,36,44,45	0
4	BGC	E	4	11/12	0.93	0.10	33,36,38,40	0
3	BGC	D	3	11/12	0.93	0.09	32,36,41,42	0
2	BGC	C	12	11/12	0.93	0.09	41,44,47,49	0

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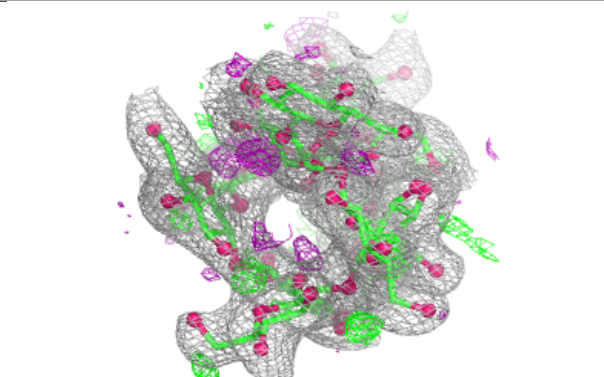
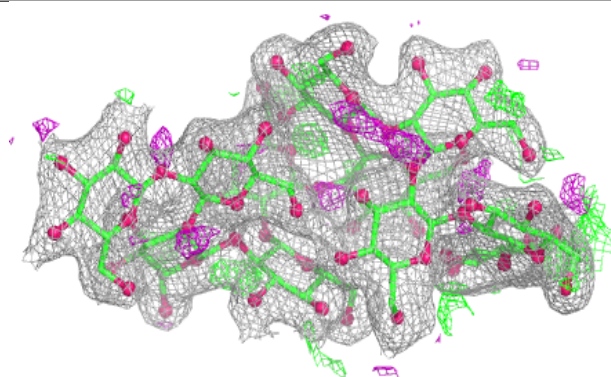
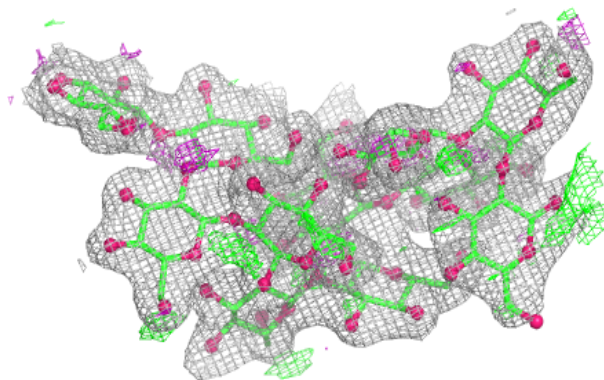
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BGC	D	11	11/12	0.94	0.10	28,32,36,37	0
2	BGC	C	11	11/12	0.94	0.08	29,36,40,42	0
2	BGC	C	4	11/12	0.94	0.08	30,34,35,37	0
2	BGC	C	7	11/12	0.94	0.09	26,29,33,36	0
2	BGC	C	8	11/12	0.94	0.08	31,37,38,39	0
2	BGC	C	10	11/12	0.94	0.08	27,33,34,34	0
4	BGC	E	10	11/12	0.94	0.08	26,29,32,33	0
4	BGC	E	2	11/12	0.95	0.07	28,30,32,34	0
4	BGC	E	7	11/12	0.95	0.08	26,31,34,39	0
4	BGC	E	8	11/12	0.95	0.08	24,28,33,36	0
4	BGC	E	9	11/12	0.95	0.07	26,29,31,32	0
2	BGC	C	22	11/12	0.95	0.08	41,46,49,49	0
3	BGC	D	10	11/12	0.96	0.07	29,30,33,33	0
2	BGC	C	6	11/12	0.96	0.07	24,30,33,33	0
2	BGC	C	9	11/12	0.96	0.07	25,31,32,33	0
2	BGC	C	3	11/12	0.97	0.06	21,24,30,30	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.

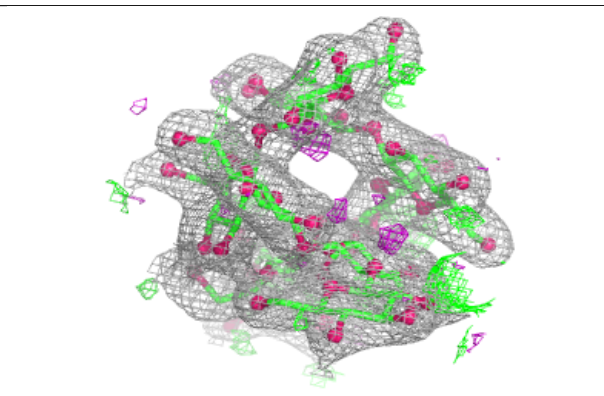
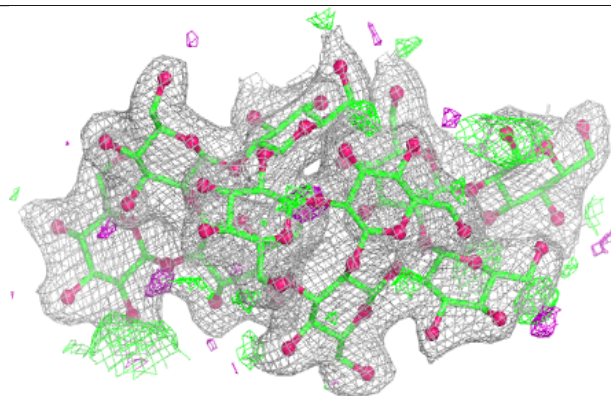
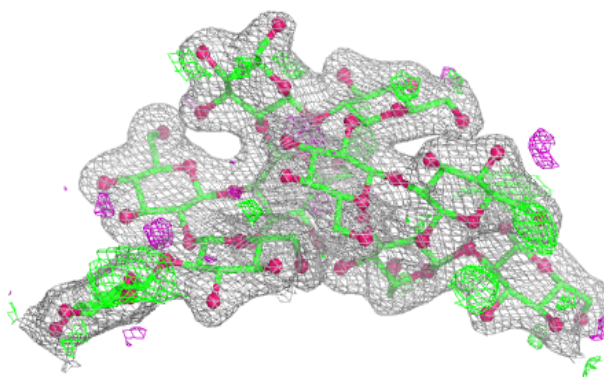


Electron density around Chain D:

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

**Electron density around Chain E:**

$2mF_o-DF_c$ (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
5	GOL	A	601	6/6	0.77	0.21	30,34,41,42	0
5	GOL	B	602	6/6	0.78	0.21	41,46,47,56	0
5	GOL	A	603	6/6	0.88	0.20	42,46,63,64	0
5	GOL	A	606	6/6	0.91	0.16	55,64,68,71	0
5	GOL	A	605	6/6	0.92	0.13	39,43,49,50	0
5	GOL	B	601	6/6	0.94	0.11	26,35,42,51	0
5	GOL	A	604	6/6	0.94	0.10	30,37,38,40	0
5	GOL	A	602	6/6	0.95	0.08	26,30,30,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.