



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:43 AM UTC

PDB ID : 8IP1 / pdb_00008ip1
Title : Escherichia coli OpgD mutant-D388N with beta-1,2-glucan
Authors : Motouchi, S.; Nakajima, M.
Deposited on : 2023-03-13
Resolution : 2.06 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

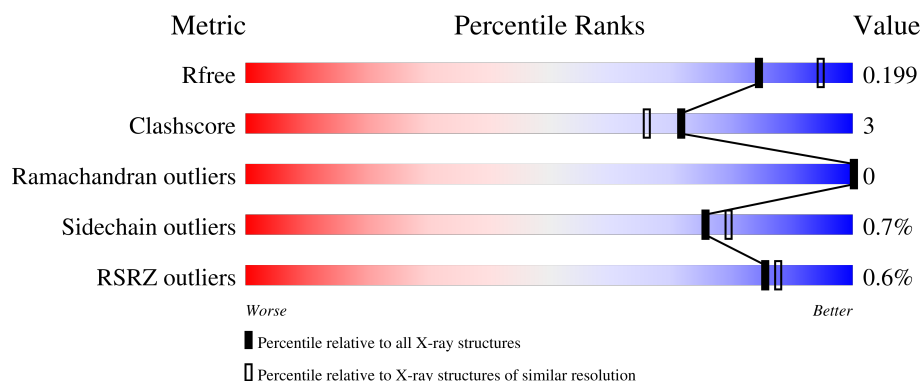
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	559	% 80% 9% 10%
1	B	559	% 82% 7% 10%
2	C	11	82% 18%
3	E	13	100%

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.

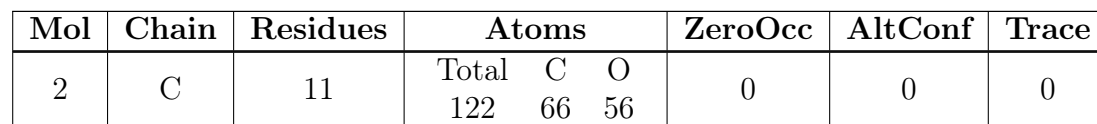
- Molecule 1 is a protein called Glucans biosynthesis protein D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	502	Total 4075	C 2604	N 704	O 744	S 23	0	0	0
1	B	503	Total 4082	C 2608	N 705	O 746	S 23	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	388	ASN	ASP	engineered mutation	UNP P40120
A	552	LEU	-	expression tag	UNP P40120
A	553	GLU	-	expression tag	UNP P40120
A	554	HIS	-	expression tag	UNP P40120
A	555	HIS	-	expression tag	UNP P40120
A	556	HIS	-	expression tag	UNP P40120
A	557	HIS	-	expression tag	UNP P40120
A	558	HIS	-	expression tag	UNP P40120
A	559	HIS	-	expression tag	UNP P40120
B	388	ASN	ASP	engineered mutation	UNP P40120
B	552	LEU	-	expression tag	UNP P40120
B	553	GLU	-	expression tag	UNP P40120
B	554	HIS	-	expression tag	UNP P40120
B	555	HIS	-	expression tag	UNP P40120
B	556	HIS	-	expression tag	UNP P40120
B	557	HIS	-	expression tag	UNP P40120
B	558	HIS	-	expression tag	UNP P40120
B	559	HIS	-	expression tag	UNP P40120

- [illegible]



- | Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|---------|---------|-------|
| 3 | E | 13 | Total | C | O | 0 | 0 | 0 |
| | | | 144 | 78 | 66 | | | |

- PEG
-
- The diagram illustrates the chemical structure of Polyethylene Glycol (PEG). It shows a zigzag chain of carbon atoms (C1, C2, C3, C4) and oxygen atoms (O1, O2). The chain starts with a hydroxyl group (HO) attached to C1 and ends with a hydroxyl group (OH) attached to C4. The oxygen atoms are labeled O1 and O2.

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

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

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



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

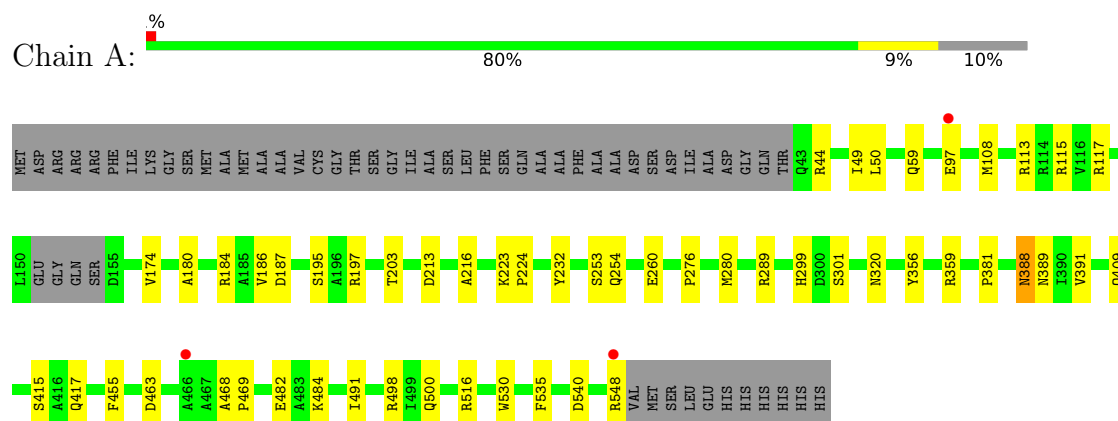
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	277	Total	O	0	0
			277	277		
6	B	289	Total	O	0	0
			289	289		

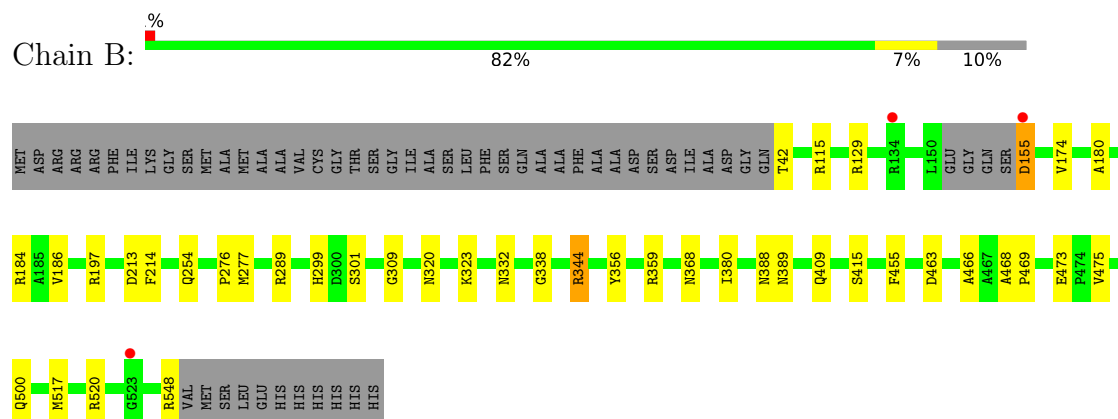
3 Residue-property plots [i](#)

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.

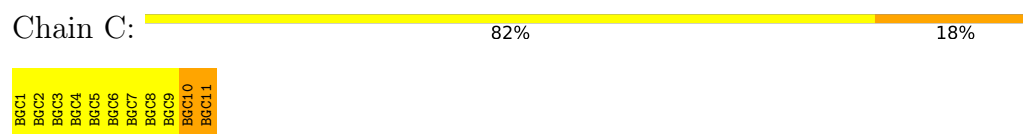
• Molecule 1: Glucans biosynthesis protein D



• Molecule 1: Glucans biosynthesis protein D



• Molecule 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-(1-2)-beta-D-glucopyranose



- 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-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose

Chain E:

100%

BGC1
BGC2
BGC3
BGC4
BGC5
BGC6
BGC7
BGC8
BGC9
BGC10
BGC11
BGC12
BGC13

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.09Å 87.10Å 110.85Å 90.00° 101.13° 90.00°	Depositor
Resolution (Å)	47.74 – 2.06 47.74 – 2.06	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.74-2.06) 99.2 (47.74-2.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.175 , 0.224 (Not available) , 0.199	Depositor DCC
R_{free} test set	3252 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9013	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, PEG, 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	0.99	0/4198	1.21	2/5697 (0.0%)
1	B	0.98	0/4205	1.22	1/5707 (0.0%)
All	All	0.99	0/8403	1.21	3/11404 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	388	ASN	CA-CB-CG	5.41	118.01	112.60
1	A	535	PHE	CB-CA-C	5.09	115.53	110.33
1	B	214	PHE	N-CA-C	-5.06	101.51	109.25

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4075	0	3892	31	0
1	B	4082	0	3899	23	0
2	C	122	0	102	1	0
3	E	144	0	120	1	0
4	A	14	0	20	2	0
5	B	10	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	277	0	0	2	0
6	B	289	0	0	2	0
All	All	9013	0	8047	54	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 (54) 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:463:ASP:OD1	1:B:466:ALA:HB3	1.78	0.84
1:A:59:GLN:HE22	4:A:602:PEG:H22	1.46	0.80
1:B:368:ASN:OD1	1:B:409:GLN:NE2	2.22	0.73
1:A:540:ASP:CG	6:A:704:HOH:O	2.42	0.63
1:A:59:GLN:HE22	4:A:602:PEG:C2	2.15	0.59
1:A:289:ARG:HD3	1:A:320:ASN:O	2.03	0.59
1:B:344:ARG:NH1	1:B:359:ARG:O	2.34	0.59
1:B:289:ARG:HD3	1:B:320:ASN:O	2.05	0.56
1:B:174:VAL:HA	1:B:186:VAL:HG22	1.87	0.56
1:A:491:ILE:HD11	1:A:498:ARG:HB2	1.87	0.56
1:B:180:ALA:HA	1:B:213:ASP:OD1	2.07	0.55
1:B:197:ARG:HB2	1:B:276:PRO:HG2	1.88	0.54
1:A:174:VAL:HA	1:A:186:VAL:HG22	1.90	0.54
1:A:180:ALA:HA	1:A:213:ASP:OD1	2.08	0.53
1:A:108:MET:HE1	1:A:115:ARG:HG2	1.90	0.53
1:A:356:TYR:HA	1:A:359:ARG:HD2	1.91	0.53
1:B:468:ALA:HB3	1:B:469:PRO:HD3	1.91	0.52
1:B:309:GLY:HA3	1:B:332:ASN:O	2.12	0.50
1:B:475:VAL:O	1:B:517:MET:HA	2.13	0.48
1:A:299:HIS:HB2	1:A:301:SER:O	2.13	0.48
1:A:117:ARG:O	1:A:216:ALA:HA	2.14	0.47
1:A:108:MET:HE2	1:A:113:ARG:O	2.14	0.47
1:B:299:HIS:HB2	1:B:301:SER:O	2.14	0.47
1:A:381:PRO:HB2	1:B:548:ARG:HD2	1.96	0.47
1:A:203:THR:HG21	1:A:391:VAL:HG11	1.97	0.47
1:B:184:ARG:CD	6:B:895:HOH:O	2.63	0.46
1:A:254:GLN:HB3	1:A:415:SER:HB3	1.98	0.46
1:B:254:GLN:HB3	1:B:415:SER:HB3	1.98	0.46
1:B:473:GLU:OE1	1:B:520:ARG:NH2	2.49	0.45
1:B:115:ARG:NH2	1:B:155:ASP:O	2.47	0.45
1:A:280:MET:HA	1:A:389:ASN:OD1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:PHE:O	1:B:500:GLN:HA	2.17	0.44
1:B:356:TYR:HA	1:B:359:ARG:HD2	2.00	0.43
1:A:223:LYS:HD2	1:A:224:PRO:HD2	2.01	0.43
1:A:417:GLN:NE2	6:A:701:HOH:O	2.36	0.43
1:A:44:ARG:HG3	1:A:49:ILE:CD1	2.48	0.43
1:B:42:THR:HG22	1:B:129:ARG:HG2	2.00	0.43
1:A:455:PHE:O	1:A:500:GLN:HA	2.19	0.43
1:A:482:GLU:OE1	1:A:484:LYS:NZ	2.36	0.43
1:B:380:ILE:HB	1:B:389:ASN:HB2	2.01	0.42
1:A:184:ARG:HG2	1:A:195:SER:HA	2.00	0.42
1:A:50:LEU:HD22	1:A:232:TYR:HB3	2.00	0.42
1:A:197:ARG:HB2	1:A:276:PRO:HG2	2.01	0.42
1:A:260:GLU:HG2	1:A:409:GLN:HG2	2.02	0.41
1:B:184:ARG:HD3	6:B:895:HOH:O	2.20	0.41
2:C:10:BGC:O2	2:C:11:BGC:H4	2.20	0.41
1:A:468:ALA:HB3	1:A:469:PRO:HD3	2.02	0.41
1:A:97:GLU:O	1:A:224:PRO:HB3	2.21	0.41
1:A:108:MET:HE1	1:A:115:ARG:CG	2.49	0.41
1:A:187:ASP:HB2	1:A:253:SER:O	2.21	0.41
1:A:108:MET:HE3	1:A:115:ARG:HA	2.03	0.41
1:B:277:MET:HE1	1:B:338:GLY:HA2	2.02	0.41
1:B:388:ASN:HB2	3:E:3:BGC:H3	2.03	0.41
1:A:516:ARG:HA	1:A:530:TRP: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	498/559 (89%)	483 (97%)	15 (3%)	0	100	100
1	B	499/559 (89%)	484 (97%)	15 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	997/1118 (89%)	967 (97%)	30 (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	427/470 (91%)	424 (99%)	3 (1%)	76	79
1	B	428/470 (91%)	425 (99%)	3 (1%)	76	79
All	All	855/940 (91%)	849 (99%)	6 (1%)	76	79

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	388	ASN
1	A	463	ASP
1	A	548	ARG
1	B	155	ASP
1	B	323	LYS
1	B	344	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	262	HIS
1	A	319	ASN
1	A	368	ASN
1	A	409	GLN
1	B	85	GLN
1	B	191	GLN
1	B	325	GLN
1	B	368	ASN

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Mol	Chain	Res	Type
1	B	409	GLN
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 ⓘ

24 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	1.22	1 (5%)
2	BGC	C	10	2	11,11,12	0.54	0	15,15,17	1.30	3 (20%)
2	BGC	C	11	2	11,11,12	0.56	0	15,15,17	1.37	3 (20%)
2	BGC	C	2	2	11,11,12	0.47	0	15,15,17	1.86	6 (40%)
2	BGC	C	3	2	11,11,12	0.66	0	15,15,17	1.39	1 (6%)
2	BGC	C	4	2	11,11,12	0.98	0	15,15,17	1.35	2 (13%)
2	BGC	C	5	2	11,11,12	0.82	1 (9%)	15,15,17	1.13	1 (6%)
2	BGC	C	6	2	11,11,12	0.74	0	15,15,17	1.61	3 (20%)
2	BGC	C	7	2	11,11,12	0.64	0	15,15,17	2.80	3 (20%)
2	BGC	C	8	2	11,11,12	0.69	0	15,15,17	1.49	2 (13%)
2	BGC	C	9	2	11,11,12	0.50	0	15,15,17	1.17	2 (13%)
3	BGC	E	1	3	12,12,12	0.52	0	17,17,17	1.41	4 (23%)
3	BGC	E	10	3	11,11,12	0.52	0	15,15,17	1.35	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BGC	E	11	3	11,11,12	0.89	0	15,15,17	1.29	1 (6%)
3	BGC	E	12	3	11,11,12	0.61	0	15,15,17	1.53	4 (26%)
3	BGC	E	13	3	11,11,12	0.57	0	15,15,17	0.79	1 (6%)
3	BGC	E	2	3	11,11,12	0.61	0	15,15,17	1.99	2 (13%)
3	BGC	E	3	3	11,11,12	0.72	0	15,15,17	0.75	0
3	BGC	E	4	3	11,11,12	0.62	0	15,15,17	1.44	2 (13%)
3	BGC	E	5	3	11,11,12	0.52	0	15,15,17	1.74	4 (26%)
3	BGC	E	6	3	11,11,12	0.55	0	15,15,17	1.20	2 (13%)
3	BGC	E	7	3	11,11,12	0.78	0	15,15,17	2.45	6 (40%)
3	BGC	E	8	3	11,11,12	1.59	2 (18%)	15,15,17	1.83	4 (26%)
3	BGC	E	9	3	11,11,12	0.67	0	15,15,17	1.61	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	-	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	2	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	-	1/2/19/22	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	-	1/2/19/22	0/1/1/1
2	BGC	C	9	2	-	0/2/19/22	0/1/1/1
3	BGC	E	1	3	-	0/2/22/22	0/1/1/1
3	BGC	E	10	3	-	0/2/19/22	0/1/1/1
3	BGC	E	11	3	-	0/2/19/22	0/1/1/1
3	BGC	E	12	3	-	2/2/19/22	0/1/1/1
3	BGC	E	13	3	-	0/2/19/22	0/1/1/1
3	BGC	E	2	3	-	2/2/19/22	0/1/1/1
3	BGC	E	3	3	-	0/2/19/22	0/1/1/1
3	BGC	E	4	3	-	0/2/19/22	0/1/1/1
3	BGC	E	5	3	-	0/2/19/22	0/1/1/1
3	BGC	E	6	3	-	0/2/19/22	0/1/1/1
3	BGC	E	7	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	E	8	3	-	0/2/19/22	0/1/1/1
3	BGC	E	9	3	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	8	BGC	O4-C4	3.43	1.51	1.43
3	E	8	BGC	C2-C3	2.85	1.56	1.52
2	C	5	BGC	O5-C1	2.10	1.47	1.43

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	7	BGC	C1-O5-C5	7.69	122.50	112.19
3	E	7	BGC	C1-O5-C5	6.06	120.31	112.19
3	E	2	BGC	C1-O5-C5	5.48	119.53	112.19
2	C	7	BGC	C1-C2-C3	4.58	116.32	109.64
2	C	7	BGC	O2-C2-C3	-4.24	101.38	110.15
3	E	8	BGC	C1-O5-C5	4.18	117.78	112.19
3	E	5	BGC	O2-C2-C3	-4.11	101.64	110.15
2	C	2	BGC	C6-C5-C4	-3.91	103.42	113.02
2	C	6	BGC	O3-C3-C2	-3.83	102.24	110.05
3	E	7	BGC	C6-C5-C4	-3.65	104.06	113.02
3	E	2	BGC	O6-C6-C5	-3.48	99.48	111.33
3	E	7	BGC	C1-C2-C3	3.45	114.67	109.64
2	C	3	BGC	C1-O5-C5	3.44	116.80	112.19
2	C	1	BGC	O6-C6-C5	-3.44	99.63	111.33
3	E	9	BGC	C1-O5-C5	3.33	116.65	112.19
2	C	2	BGC	O2-C2-C3	-3.24	103.43	110.15
3	E	12	BGC	O2-C2-C3	-3.15	103.63	110.15
3	E	9	BGC	O5-C5-C4	-3.13	103.20	110.83
3	E	5	BGC	O2-C2-C1	3.10	116.32	109.22
2	C	4	BGC	C1-C2-C3	-3.09	105.15	109.64
3	E	1	BGC	O6-C6-C5	-3.05	100.95	111.33
3	E	5	BGC	O4-C4-C5	3.04	116.81	109.32
3	E	8	BGC	C2-C3-C4	3.00	116.14	110.86
3	E	7	BGC	O5-C5-C6	3.00	113.50	107.66
3	E	11	BGC	C1-C2-C3	2.88	113.84	109.64
3	E	4	BGC	C1-C2-C3	-2.75	105.63	109.64
3	E	8	BGC	O5-C5-C4	2.72	117.44	110.83
3	E	12	BGC	C1-O5-C5	2.66	115.76	112.19
2	C	6	BGC	O4-C4-C5	2.66	115.88	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	8	BGC	O5-C1-C2	-2.66	104.45	110.79
2	C	10	BGC	C1-O5-C5	2.65	115.74	112.19
3	E	4	BGC	O4-C4-C5	-2.64	102.83	109.32
2	C	8	BGC	O2-C2-C3	-2.62	104.73	110.15
3	E	9	BGC	O2-C2-C1	-2.60	103.27	109.22
2	C	9	BGC	C1-C2-C3	2.58	113.40	109.64
3	E	6	BGC	O2-C2-C3	-2.57	104.82	110.15
3	E	7	BGC	O2-C2-C3	-2.57	104.83	110.15
2	C	2	BGC	C1-O5-C5	2.51	115.55	112.19
3	E	8	BGC	C1-C2-C3	2.50	113.28	109.64
2	C	5	BGC	O5-C5-C6	2.46	112.45	107.66
2	C	11	BGC	O2-C2-C3	2.42	115.16	110.15
3	E	6	BGC	O3-C3-C2	-2.41	105.13	110.05
3	E	12	BGC	C1-C2-C3	2.30	113.00	109.64
2	C	2	BGC	C3-C4-C5	2.30	114.40	110.23
3	E	1	BGC	O5-C1-C2	-2.25	106.34	110.30
2	C	4	BGC	O4-C4-C3	-2.24	105.09	110.38
3	E	9	BGC	C1-C2-C3	2.24	112.91	109.64
2	C	2	BGC	O3-C3-C4	-2.20	105.18	110.38
2	C	10	BGC	C1-C2-C3	2.18	112.82	109.64
2	C	11	BGC	O5-C5-C6	2.16	111.87	107.66
2	C	6	BGC	C1-O5-C5	2.15	115.06	112.19
3	E	7	BGC	O2-C2-C1	2.14	114.11	109.22
3	E	10	BGC	C1-O5-C5	2.12	115.03	112.19
2	C	11	BGC	O3-C3-C4	-2.09	105.45	110.38
3	E	13	BGC	O2-C2-C3	2.06	114.42	110.15
3	E	12	BGC	O6-C6-C5	-2.05	104.35	111.33
2	C	2	BGC	O5-C5-C6	2.05	111.65	107.66
2	C	9	BGC	O5-C5-C4	-2.02	105.92	110.83
3	E	5	BGC	C1-O5-C5	-2.02	109.48	112.19
2	C	10	BGC	O3-C3-C2	-2.01	105.95	110.05
3	E	1	BGC	C1-O5-C5	-2.00	109.78	113.65
3	E	1	BGC	C1-C2-C3	-2.00	106.27	110.36

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	12	BGC	C4-C5-C6-O6
3	E	2	BGC	C4-C5-C6-O6
3	E	12	BGC	O5-C5-C6-O6
3	E	2	BGC	O5-C5-C6-O6

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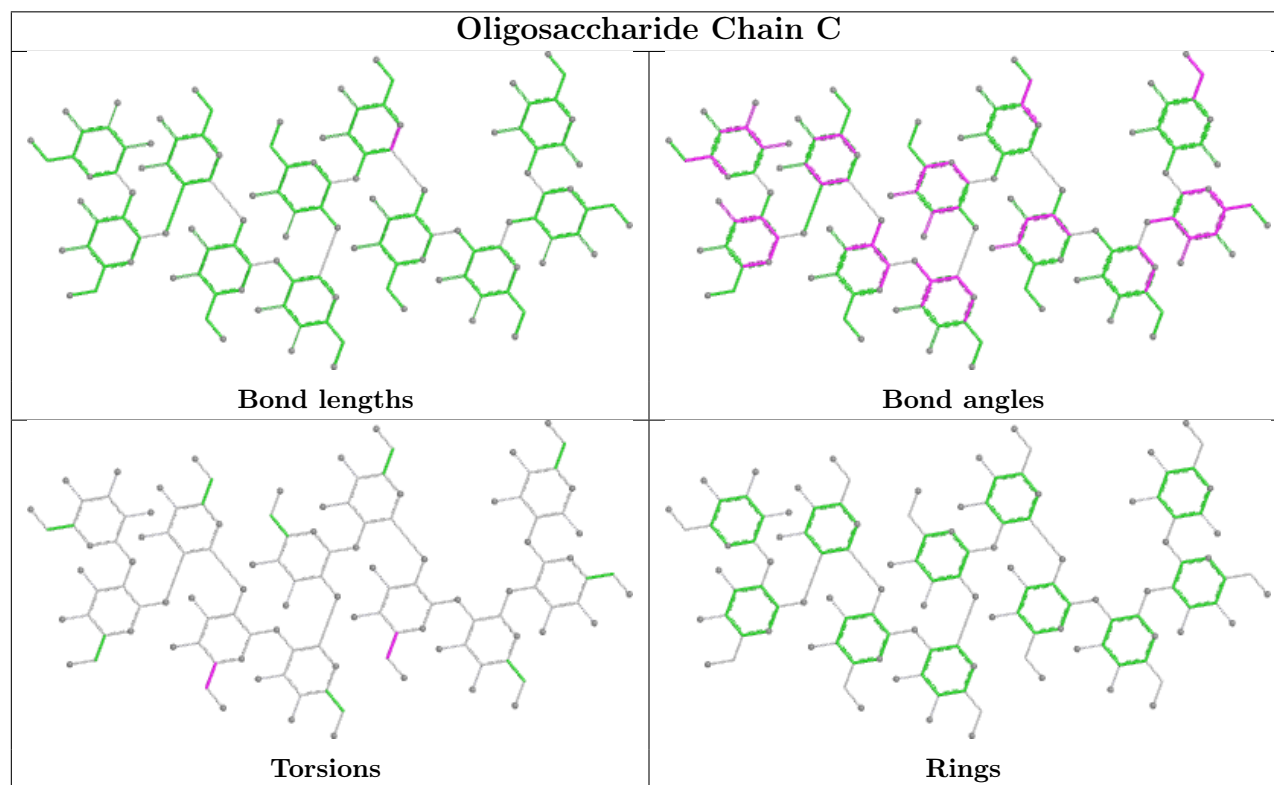
Mol	Chain	Res	Type	Atoms
2	C	4	BGC	C4-C5-C6-O6
2	C	8	BGC	O5-C5-C6-O6

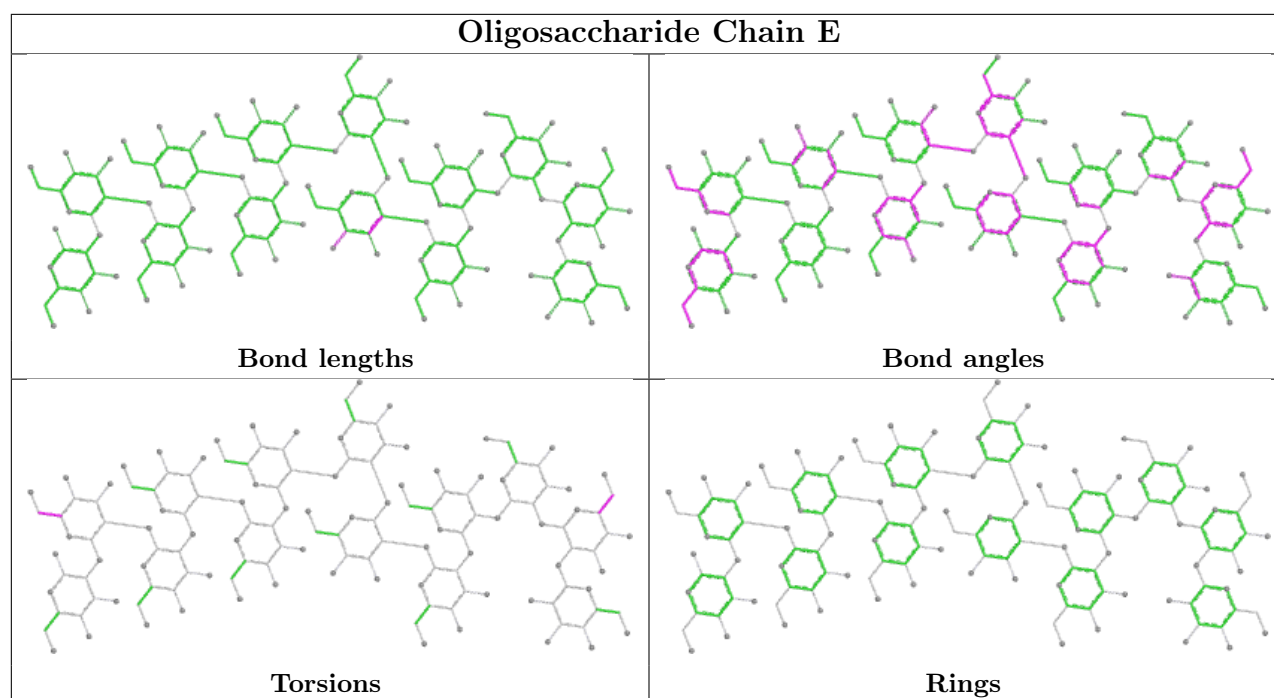
There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	10	BGC	1	0
2	C	11	BGC	1	0
3	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 [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PEG	A	601	-	6,6,6	0.11	0	5,5,5	0.20	0
4	PEG	A	602	-	6,6,6	0.14	0	5,5,5	0.11	0
5	PGE	B	601	-	9,9,9	0.15	0	8,8,8	0.18	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
4	PEG	A	601	-	-	2/4/4/4	-
4	PEG	A	602	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PGE	B	601	-	-	3/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	602	PEG	O1-C1-C2-O2
4	A	601	PEG	O2-C3-C4-O4
4	A	601	PEG	C1-C2-O2-C3
5	B	601	PGE	C6-C5-O3-C4
5	B	601	PGE	C3-C4-O3-C5
5	B	601	PGE	O3-C5-C6-O4

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	PEG	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 [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	502/559 (89%)	-0.26	3 (0%) 85 88	15, 22, 37, 55	0
1	B	503/559 (89%)	-0.23	3 (0%) 85 88	15, 22, 37, 58	0
All	All	1005/1118 (89%)	-0.25	6 (0%) 85 88	15, 22, 37, 58	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	155	ASP	3.1
1	A	466	ALA	2.3
1	A	548	ARG	2.2
1	A	97	GLU	2.2
1	B	134	ARG	2.1
1	B	523	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	0.91	0.08	19,21,24,24	0
2	BGC	C	2	11/12	0.94	0.07	18,21,26,30	0
2	BGC	C	11	11/12	0.94	0.07	21,22,23,23	0

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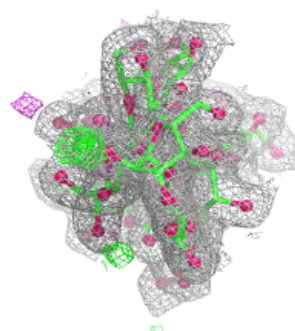
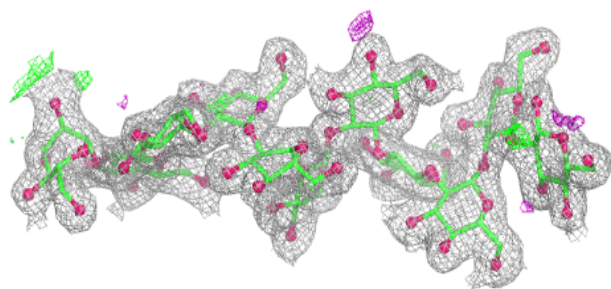
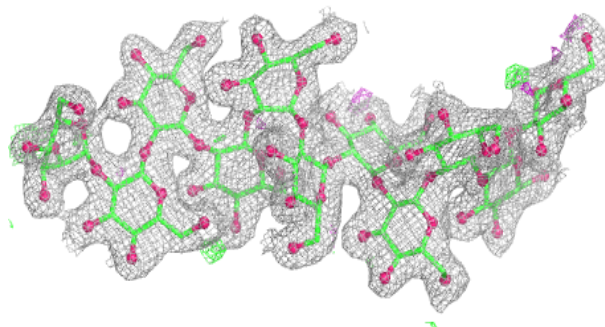
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BGC	C	8	11/12	0.95	0.06	17,19,21,23	0
2	BGC	C	4	11/12	0.96	0.05	16,17,18,19	0
2	BGC	C	7	11/12	0.96	0.06	14,16,17,17	0
2	BGC	C	5	11/12	0.97	0.04	14,15,16,18	0
2	BGC	C	9	11/12	0.97	0.05	18,18,20,21	0
2	BGC	C	10	11/12	0.97	0.05	15,18,20,21	0
2	BGC	C	3	11/12	0.97	0.05	14,15,16,16	0
2	BGC	C	6	11/12	0.98	0.04	15,16,17,18	0
3	BGC	E	1	12/12	-	-	21,23,29,30	0
3	BGC	E	2	11/12	-	-	21,23,29,33	0
3	BGC	E	3	11/12	-	-	16,17,18,18	0
3	BGC	E	4	11/12	-	-	16,17,18,19	0
3	BGC	E	5	11/12	-	-	15,16,17,18	0
3	BGC	E	6	11/12	-	-	14,15,16,16	0
3	BGC	E	7	11/12	-	-	15,16,17,17	0
3	BGC	E	8	11/12	-	-	18,21,24,25	0
3	BGC	E	9	11/12	-	-	17,17,18,21	0
3	BGC	E	10	11/12	-	-	18,18,20,20	0
3	BGC	E	11	11/12	-	-	19,22,25,26	0
3	BGC	E	12	11/12	-	-	30,34,39,39	0
3	BGC	E	13	11/12	-	-	30,34,37,40	0

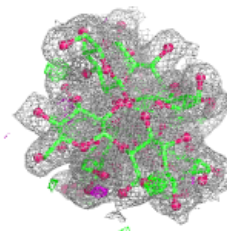
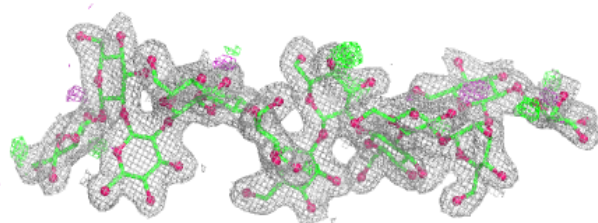
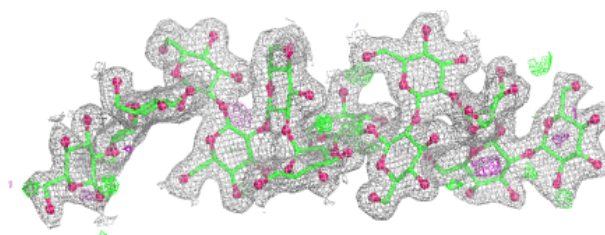
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

**Electron density around Chain 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
4	PEG	A	601	7/7	0.83	0.12	37,38,39,40	0
4	PEG	A	602	7/7	0.90	0.12	42,42,44,44	0
5	PGE	B	601	10/10	0.94	0.08	24,31,33,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.