



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:45 AM UTC

PDB ID : 6JFJ / pdb_00006jff
Title : Crystal structure of Pullulanase from *Paenibacillus barengoltzii* complex with maltohexaose and alpha-cyclodextrin
Authors : Wu, S.W.; Yang, S.Q.; Qin, Z.; You, X.; Huang, P.; Jiang, Z.Q.
Deposited on : 2019-02-09
Resolution : 1.93 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

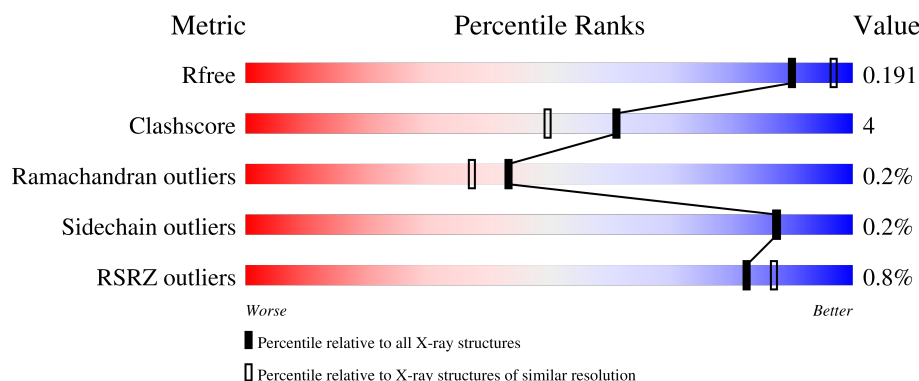
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	675	% 88% 7% .
2	B	3	100%
2	C	3	33% 33% 33%
3	D	5	20% 80%

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	PEG	A	722	-	-	X	-

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 5936 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 Pulullanase.

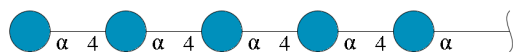
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	646	Total	C	N	O	S	0	8	0
			5190	3287	907	974	22			

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



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

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



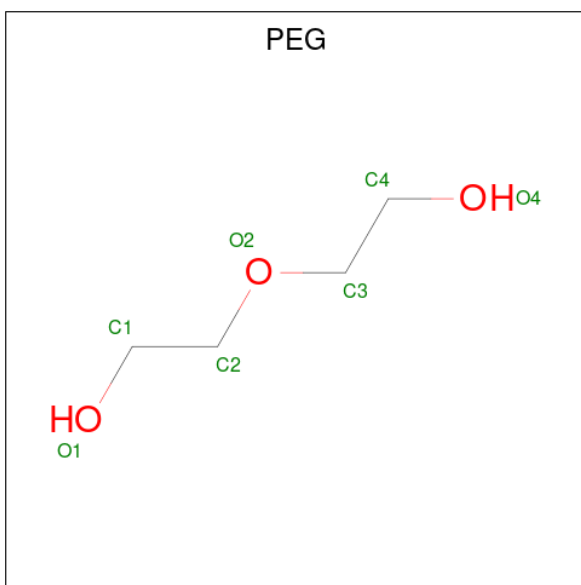
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	5	Total	C	O	0	0	0
			56	30	26			

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



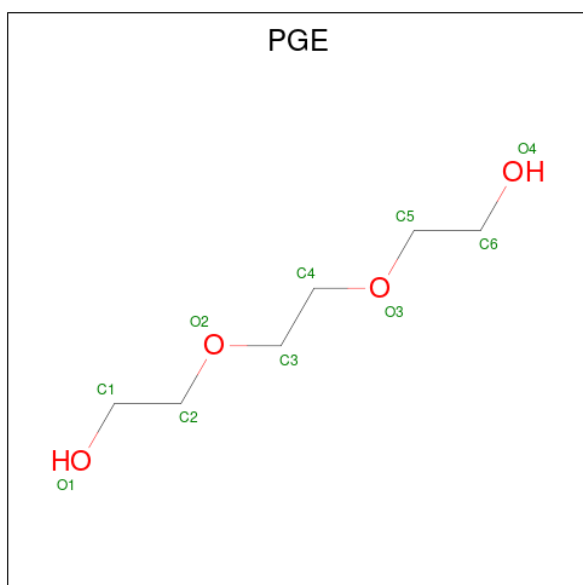
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



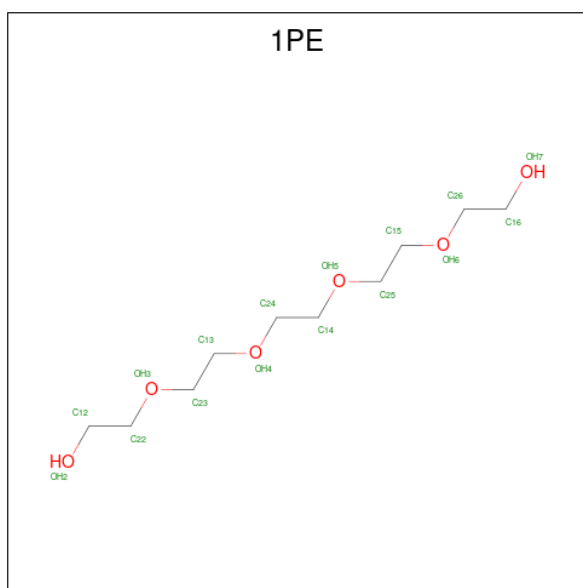
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



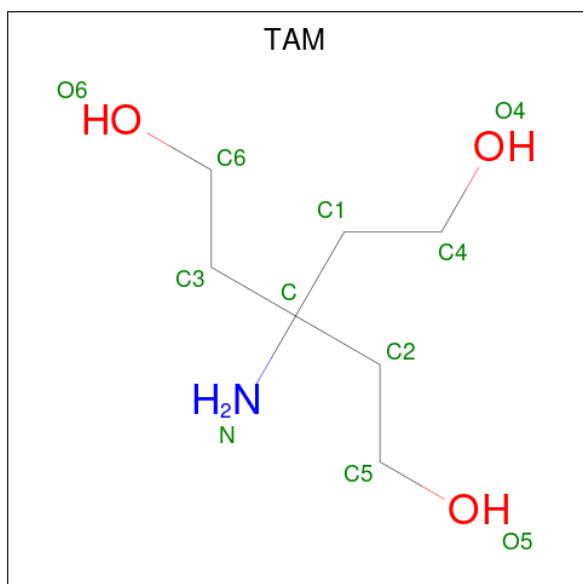
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 10 6 4	0	0
6	A	1	Total C O 10 6 4	0	0

- Molecule 7 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



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

- Molecule 8 is TRIS(HYDROXYETHYL)AMINOMETHANE (CCD ID: TAM) (formula: $C_7H_{17}NO_3$).



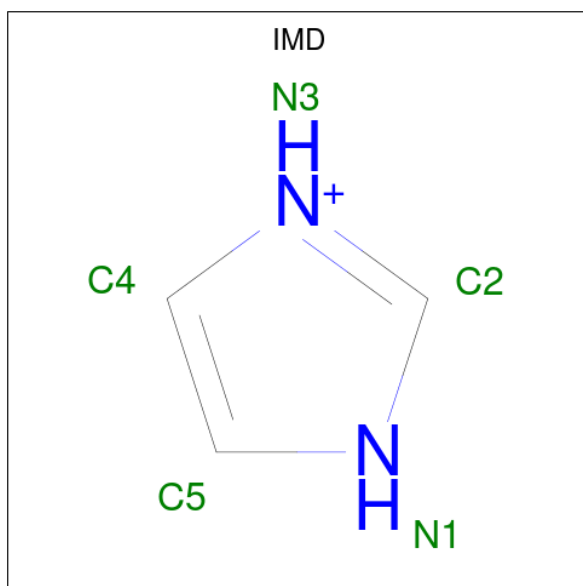
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			11	7	1	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			11	7	1	3		

- Molecule 9 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	N	0	0
			5	3	2		
9	A	1	Total	C	N	0	0
			5	3	2		
9	A	1	Total	C	N	0	0
			5	3	2		
9	A	1	Total	C	N	0	0
			5	3	2		

- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	2	Total	Ca	0	0
			2	2		

- Molecule 11 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	8	Total	Cl	0	0
			8	8		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	440	Total	O	0	0
			440	440		

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.91Å 98.18Å 140.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.09 – 1.93 49.09 – 1.93	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.09-1.93) 99.5 (49.09-1.93)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.69 (at 1.94Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.145 , 0.189 0.146 , 0.191	Depositor DCC
R_{free} test set	2607 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	18.0	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5936	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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, CL, GOL, GLC, CA, 1PE, TAM, IMD

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	0.29	0/5323	0.48	0/7225

There are no bond length outliers.

There are no bond angle outliers.

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	5190	0	5023	38	0
2	B	34	0	30	0	0
2	C	34	0	30	1	0
3	D	56	0	48	2	0
4	A	24	0	32	0	0
5	A	70	0	100	7	0
6	A	20	0	28	3	0
7	A	16	0	22	0	0
8	A	22	0	34	4	0
9	A	20	0	20	4	0
10	A	2	0	0	0	0
11	A	8	0	0	1	0
12	A	440	0	0	5	0
All	All	5936	0	5367	46	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 (46) 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:411[B]:MET:HE1	1:A:465:TYR:H	1.46	0.80
1:A:577:ARG:HE	9:A:732:IMD:H4	1.61	0.65
1:A:540:ARG:HH11	6:A:727:PGE:H62	1.60	0.65
1:A:577:ARG:HE	9:A:732:IMD:C4	2.15	0.59
6:A:727:PGE:H22	12:A:1126:HOH:O	2.03	0.58
1:A:573:ARG:O	9:A:732:IMD:H2	2.05	0.56
1:A:664:ARG:NH2	12:A:803:HOH:O	2.37	0.56
1:A:278[A]:MET:HG2	1:A:280:VAL:HG13	1.88	0.56
1:A:189[B]:ARG:NH2	12:A:805:HOH:O	2.38	0.55
1:A:278[B]:MET:HE1	1:A:338:TRP:CE2	2.41	0.55
1:A:214:ILE:HD11	1:A:278[A]:MET:HE2	1.89	0.54
1:A:362[A]:GLU:OE2	1:A:365:ARG:NH2	2.33	0.53
1:A:278[A]:MET:HE1	1:A:338:TRP:CE3	2.44	0.53
1:A:366:ARG:HH12	5:A:722:PEG:H42	1.74	0.53
1:A:411[B]:MET:HE3	1:A:412:ARG:N	2.26	0.50
1:A:675:ARG:HG3	11:A:739:CL:CL	2.50	0.49
1:A:213:PRO:HB3	1:A:215:TYR:CZ	2.49	0.48
5:A:722:PEG:H12	12:A:929:HOH:O	2.13	0.47
5:A:725:PEG:H11	3:D:3:GLC:H3	1.96	0.47
1:A:379:GLU:OE1	2:C:1:GLC:H1	2.14	0.47
1:A:106:LYS:NZ	8:A:729:TAM:H41	2.29	0.46
1:A:122:VAL:HG22	1:A:243[B]:VAL:HG11	1.97	0.46
1:A:366:ARG:NH1	5:A:722:PEG:H42	2.31	0.46
5:A:724:PEG:H12	3:D:3:GLC:H5	1.98	0.46
1:A:405:GLY:HA2	1:A:461:GLN:HA	1.97	0.46
1:A:46:ALA:HB1	1:A:48:GLU:OE1	2.16	0.46
8:A:730:TAM:H32	8:A:730:TAM:H51	1.42	0.46
1:A:365:ARG:NH1	1:A:369:GLU:OE2	2.50	0.45
8:A:729:TAM:H52	9:A:731:IMD:C4	2.47	0.45
1:A:65:VAL:HG22	1:A:77:GLU:HG2	1.98	0.44
1:A:26:PHE:CE2	1:A:308:ARG:HD2	2.54	0.43
1:A:453:ARG:HG2	1:A:454:GLN:N	2.34	0.43
1:A:303:ARG:HG3	1:A:321:ALA:HA	2.01	0.43
8:A:729:TAM:H42	8:A:729:TAM:H21	1.85	0.42
1:A:278[A]:MET:HE3	1:A:278[A]:MET:HB2	1.77	0.42
1:A:491:ARG:HG2	1:A:517[A]:MET:SD	2.60	0.42
1:A:411[A]:MET:SD	1:A:441:GLY:HA3	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:GLU:HB2	1:A:509:PHE:CZ	2.55	0.42
1:A:362[B]:GLU:OE1	5:A:722:PEG:O1	2.24	0.42
1:A:329:LYS:HB2	5:A:722:PEG:H21	2.02	0.42
1:A:661:LEU:HG	1:A:663:VAL:HG13	2.01	0.42
1:A:162:HIS:HB3	1:A:165:ASP:CG	2.45	0.41
1:A:143:GLU:H	1:A:143:GLU:CD	2.27	0.41
6:A:727:PGE:H6	12:A:866:HOH:O	2.19	0.41
1:A:184:THR:HG22	1:A:265:LEU:HA	2.02	0.41
1:A:234:TRP:CD2	1:A:527:TYR:HA	2.55	0.41

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	650/675 (96%)	635 (98%)	14 (2%)	1 (0%)	43	37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213	PRO

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	547/552 (99%)	545 (100%)	2 (0%)	84 84

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	517[A]	MET
1	A	517[B]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	ASN
1	A	464	ASN
1	A	631	HIS

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 ⓘ

11 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	GLC	B	1	2	12,12,12	0.51	0	17,17,17	0.61	0
2	GLC	B	2	2	11,11,12	0.33	0	15,15,17	0.76	0
2	GLC	B	3	2	11,11,12	0.28	0	15,15,17	0.85	0
2	GLC	C	1	2	12,12,12	0.66	0	17,17,17	1.53	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	C	2	2	11,11,12	0.45	0	15,15,17	0.83	0
2	GLC	C	3	2	11,11,12	0.31	0	15,15,17	0.85	1 (6%)
3	GLC	D	1	3	12,12,12	0.61	0	17,17,17	0.63	0
3	GLC	D	2	3	11,11,12	0.37	0	15,15,17	1.11	2 (13%)
3	GLC	D	3	3	11,11,12	0.31	0	15,15,17	0.77	0
3	GLC	D	4	3	11,11,12	0.44	0	15,15,17	1.04	2 (13%)
3	GLC	D	5	3	11,11,12	0.32	0	15,15,17	1.12	1 (6%)

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	GLC	B	1	2	-	0/2/22/22	0/1/1/1
2	GLC	B	2	2	-	0/2/19/22	0/1/1/1
2	GLC	B	3	2	-	1/2/19/22	0/1/1/1
2	GLC	C	1	2	-	2/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	C	3	2	-	2/2/19/22	0/1/1/1
3	GLC	D	1	3	-	0/2/22/22	0/1/1/1
3	GLC	D	2	3	-	0/2/19/22	0/1/1/1
3	GLC	D	3	3	-	0/2/19/22	0/1/1/1
3	GLC	D	4	3	-	0/2/19/22	0/1/1/1
3	GLC	D	5	3	-	1/2/19/22	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	1	GLC	O5-C5-C4	3.39	115.80	109.70
2	C	1	GLC	C1-O5-C5	2.70	118.88	113.65
3	D	2	GLC	O4-C4-C3	-2.60	104.25	110.38
3	D	2	GLC	O5-C1-C2	-2.51	104.80	110.79
3	D	4	GLC	C1-O5-C5	2.51	115.54	112.19
3	D	4	GLC	O4-C4-C3	-2.39	104.75	110.38
3	D	5	GLC	C6-C5-C4	-2.24	107.51	113.02
2	C	1	GLC	C4-C3-C2	-2.19	106.99	110.83
2	C	1	GLC	O2-C2-C3	2.07	115.25	110.38
2	C	1	GLC	O5-C1-C2	-2.05	106.69	110.30
2	C	3	GLC	C1-O5-C5	2.02	114.90	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

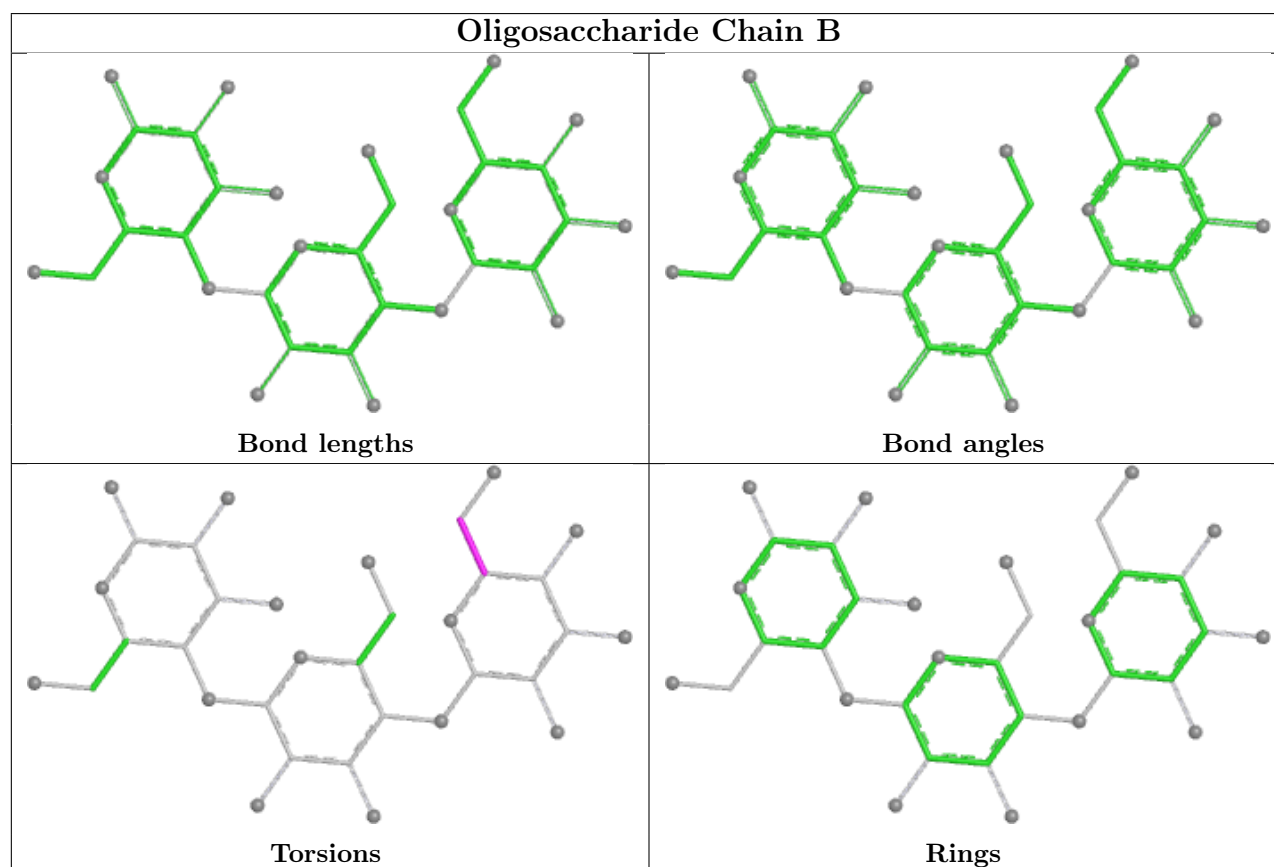
Mol	Chain	Res	Type	Atoms
2	C	3	GLC	O5-C5-C6-O6
2	C	1	GLC	C4-C5-C6-O6
2	B	3	GLC	O5-C5-C6-O6
2	C	3	GLC	C4-C5-C6-O6
2	C	1	GLC	O5-C5-C6-O6
3	D	5	GLC	C4-C5-C6-O6

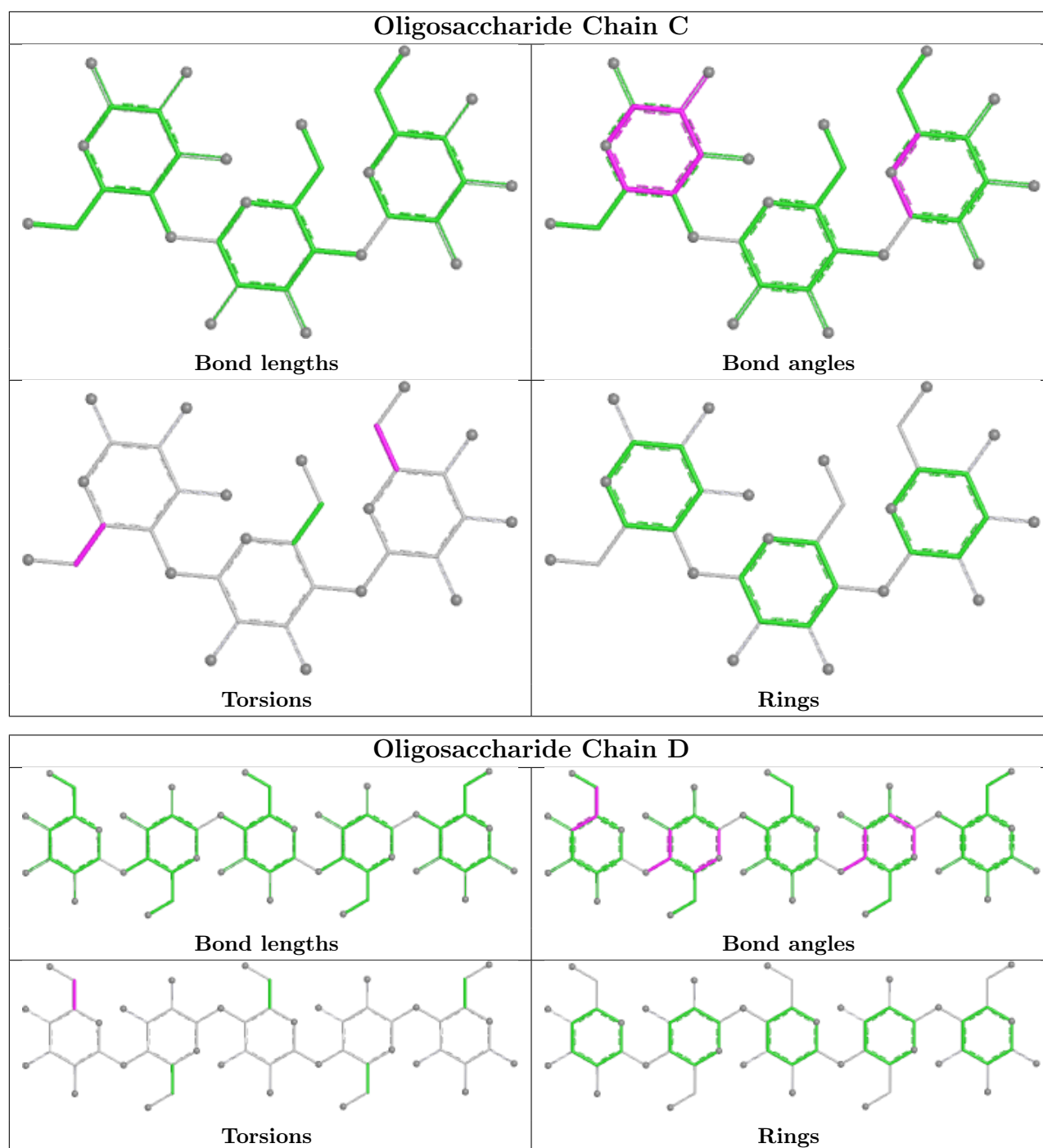
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3	GLC	2	0
2	C	1	GLC	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](#)

Of 33 ligands modelled in this entry, 10 are monoatomic - leaving 23 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	PEG	A	722	-	6,6,6	0.42	0	5,5,5	0.57	0
9	IMD	A	734	-	5,5,5	0.65	0	5,5,5	0.39	0
9	IMD	A	733	-	5,5,5	0.63	0	5,5,5	0.39	0
9	IMD	A	732	-	5,5,5	0.62	0	5,5,5	0.39	0
8	TAM	A	729	-	10,10,10	0.58	0	12,12,12	2.09	2 (16%)
4	GOL	A	712	-	5,5,5	0.93	0	5,5,5	1.11	0
4	GOL	A	715	-	5,5,5	0.94	0	5,5,5	1.08	0
5	PEG	A	723	-	6,6,6	0.48	0	5,5,5	0.29	0
5	PEG	A	717	-	6,6,6	0.38	0	5,5,5	0.46	0
9	IMD	A	731	-	5,5,5	0.65	0	5,5,5	0.46	0
5	PEG	A	716	-	6,6,6	0.46	0	5,5,5	0.43	0
4	GOL	A	713	-	5,5,5	0.81	0	5,5,5	1.06	0
5	PEG	A	721	-	6,6,6	0.44	0	5,5,5	0.38	0
6	PGE	A	727	-	9,9,9	0.33	0	8,8,8	0.69	0
7	1PE	A	728	-	15,15,15	0.45	0	14,14,14	0.49	0
5	PEG	A	725	-	6,6,6	0.45	0	5,5,5	0.27	0
4	GOL	A	714	-	5,5,5	0.97	0	5,5,5	1.05	0
5	PEG	A	718	-	6,6,6	0.47	0	5,5,5	0.28	0
5	PEG	A	720	-	6,6,6	0.45	0	5,5,5	0.39	0
5	PEG	A	719	-	6,6,6	0.41	0	5,5,5	0.44	0
8	TAM	A	730	-	10,10,10	0.55	0	12,12,12	1.63	2 (16%)
6	PGE	A	726	-	9,9,9	0.30	0	8,8,8	0.32	0
5	PEG	A	724	-	6,6,6	0.52	0	5,5,5	0.23	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	PEG	A	722	-	-	1/4/4/4	-
9	IMD	A	734	-	-	-	0/1/1/1
9	IMD	A	733	-	-	-	0/1/1/1
9	IMD	A	732	-	-	-	0/1/1/1
8	TAM	A	729	-	-	5/12/12/12	-
4	GOL	A	712	-	-	3/4/4/4	-
4	GOL	A	715	-	-	3/4/4/4	-
5	PEG	A	723	-	-	1/4/4/4	-
5	PEG	A	717	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	IMD	A	731	-	-	-	0/1/1/1
5	PEG	A	716	-	-	2/4/4/4	-
4	GOL	A	713	-	-	2/4/4/4	-
5	PEG	A	721	-	-	0/4/4/4	-
6	PGE	A	727	-	-	5/7/7/7	-
7	1PE	A	728	-	-	8/13/13/13	-
5	PEG	A	725	-	-	0/4/4/4	-
4	GOL	A	714	-	-	4/4/4/4	-
5	PEG	A	718	-	-	1/4/4/4	-
5	PEG	A	720	-	-	1/4/4/4	-
5	PEG	A	719	-	-	0/4/4/4	-
8	TAM	A	730	-	-	8/12/12/12	-
6	PGE	A	726	-	-	3/7/7/7	-
5	PEG	A	724	-	-	2/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	729	TAM	C4-C1-C	-5.49	109.50	115.97
8	A	729	TAM	C6-C3-C	-4.19	111.03	115.97
8	A	730	TAM	C6-C3-C	-3.69	111.62	115.97
8	A	730	TAM	C4-C1-C	-3.38	111.98	115.97

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	712	GOL	O1-C1-C2-C3
4	A	713	GOL	C1-C2-C3-O3
4	A	714	GOL	O1-C1-C2-C3
4	A	714	GOL	C1-C2-C3-O3
8	A	729	TAM	C1-C-C3-C6
8	A	729	TAM	C2-C-C3-C6
8	A	729	TAM	N-C-C3-C6
8	A	730	TAM	C1-C-C2-C5
8	A	730	TAM	C3-C-C2-C5
8	A	730	TAM	N-C-C2-C5
8	A	730	TAM	C1-C-C3-C6

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Mol	Chain	Res	Type	Atoms
8	A	730	TAM	C2-C-C3-C6
8	A	730	TAM	N-C-C3-C6
8	A	730	TAM	C-C1-C4-O4
8	A	730	TAM	C-C2-C5-O5
7	A	728	1PE	OH6-C15-C25-OH5
6	A	726	PGE	O1-C1-C2-O2
4	A	715	GOL	O1-C1-C2-C3
6	A	727	PGE	O1-C1-C2-O2
4	A	712	GOL	O1-C1-C2-O2
4	A	713	GOL	O2-C2-C3-O3
4	A	714	GOL	O1-C1-C2-O2
8	A	729	TAM	C-C1-C4-O4
4	A	714	GOL	O2-C2-C3-O3
6	A	727	PGE	C3-C4-O3-C5
4	A	715	GOL	O2-C2-C3-O3
7	A	728	1PE	C15-C25-OH5-C14
5	A	723	PEG	O2-C3-C4-O4
5	A	716	PEG	C4-C3-O2-C2
6	A	727	PGE	C6-C5-O3-C4
7	A	728	1PE	C23-C13-OH4-C24
8	A	729	TAM	C-C2-C5-O5
6	A	727	PGE	C1-C2-O2-C3
4	A	712	GOL	O2-C2-C3-O3
4	A	715	GOL	O1-C1-C2-O2
7	A	728	1PE	C13-C23-OH3-C22
5	A	722	PEG	C1-C2-O2-C3
7	A	728	1PE	C12-C22-OH3-C23
6	A	726	PGE	O3-C5-C6-O4
6	A	727	PGE	O2-C3-C4-O3
5	A	718	PEG	O1-C1-C2-O2
7	A	728	1PE	OH5-C14-C24-OH4
5	A	716	PEG	O2-C3-C4-O4
5	A	724	PEG	C1-C2-O2-C3
5	A	720	PEG	O2-C3-C4-O4
6	A	726	PGE	C4-C3-O2-C2
7	A	728	1PE	OH4-C13-C23-OH3
5	A	724	PEG	O1-C1-C2-O2
7	A	728	1PE	OH2-C12-C22-OH3

There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	722	PEG	5	0
9	A	732	IMD	3	0
8	A	729	TAM	3	0
9	A	731	IMD	1	0
6	A	727	PGE	3	0
5	A	725	PEG	1	0
8	A	730	TAM	1	0
5	A	724	PEG	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	646/675 (95%)	-0.49	5 (0%) 82 87	6, 16, 35, 52	8 (1%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	93	ALA	3.1
1	A	46	ALA	3.0
1	A	48	GLU	2.5
1	A	45	TYR	2.3
1	A	94	GLU	2.2

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.

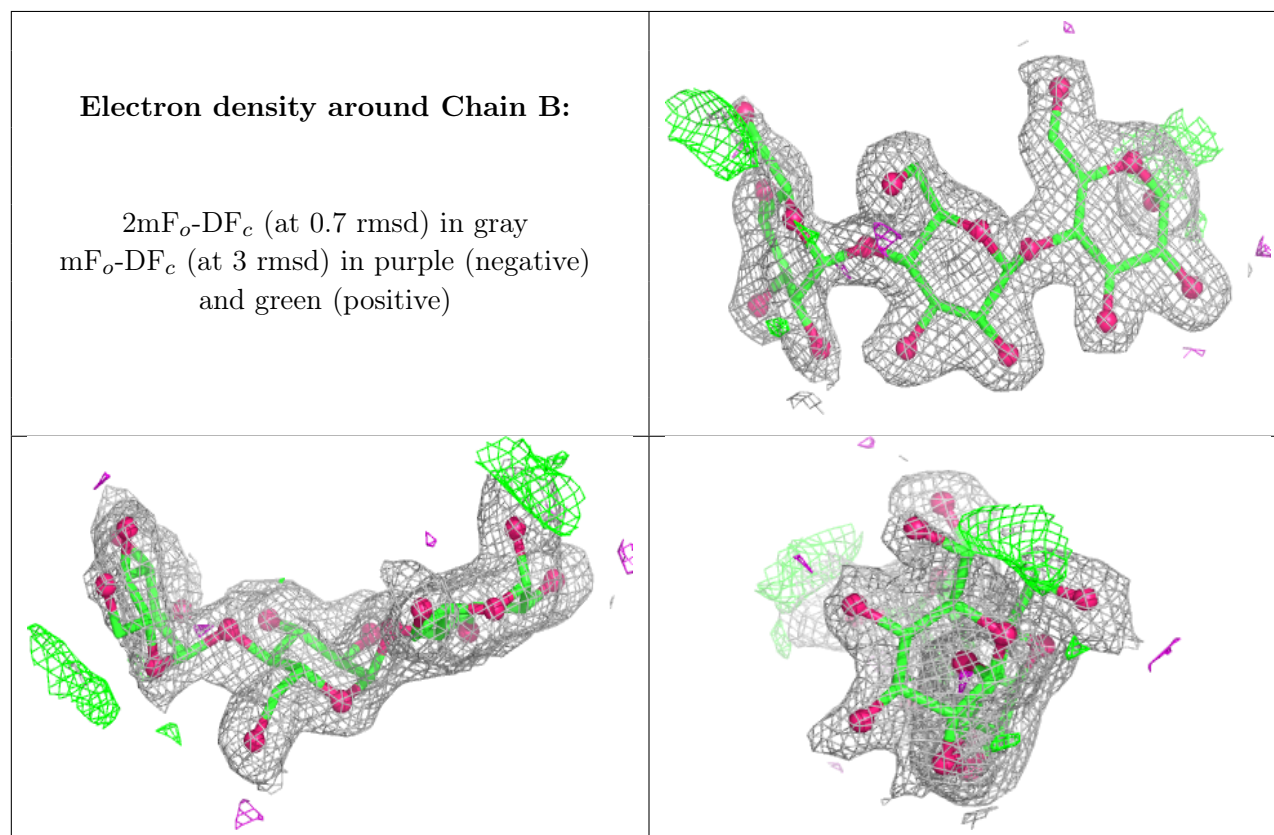
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	C	3	11/12	0.76	0.12	42,49,58,59	0
2	GLC	B	3	11/12	0.78	0.12	36,39,43,43	11
3	GLC	D	1	12/12	0.79	0.12	52,64,67,69	0
3	GLC	D	2	11/12	0.82	0.13	27,51,60,61	0
3	GLC	D	5	11/12	0.86	0.11	13,31,43,43	11
2	GLC	C	1	12/12	0.87	0.10	18,30,34,37	0
2	GLC	C	2	11/12	0.87	0.10	27,32,38,40	0

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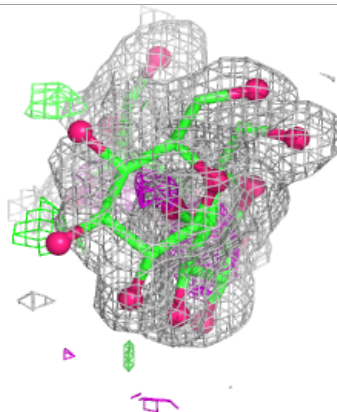
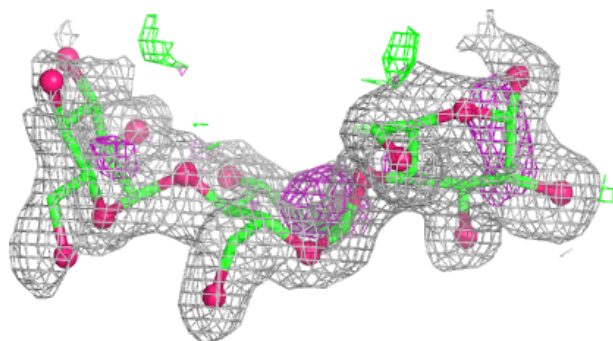
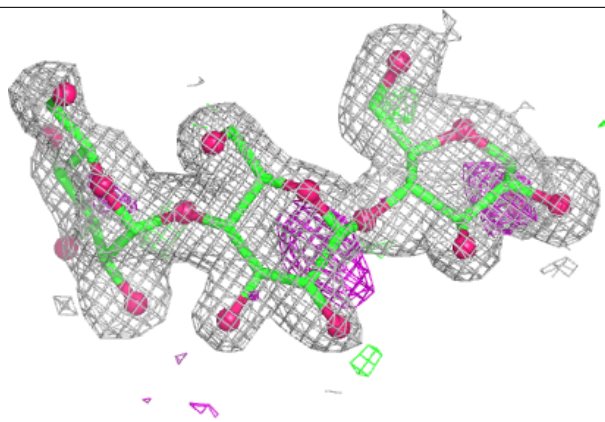
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	B	2	11/12	0.94	0.07	21,24,29,29	0
3	GLC	D	4	11/12	0.95	0.07	13,14,16,21	0
2	GLC	B	1	12/12	0.96	0.06	13,17,20,23	0
3	GLC	D	3	11/12	0.96	0.07	13,15,20,22	0

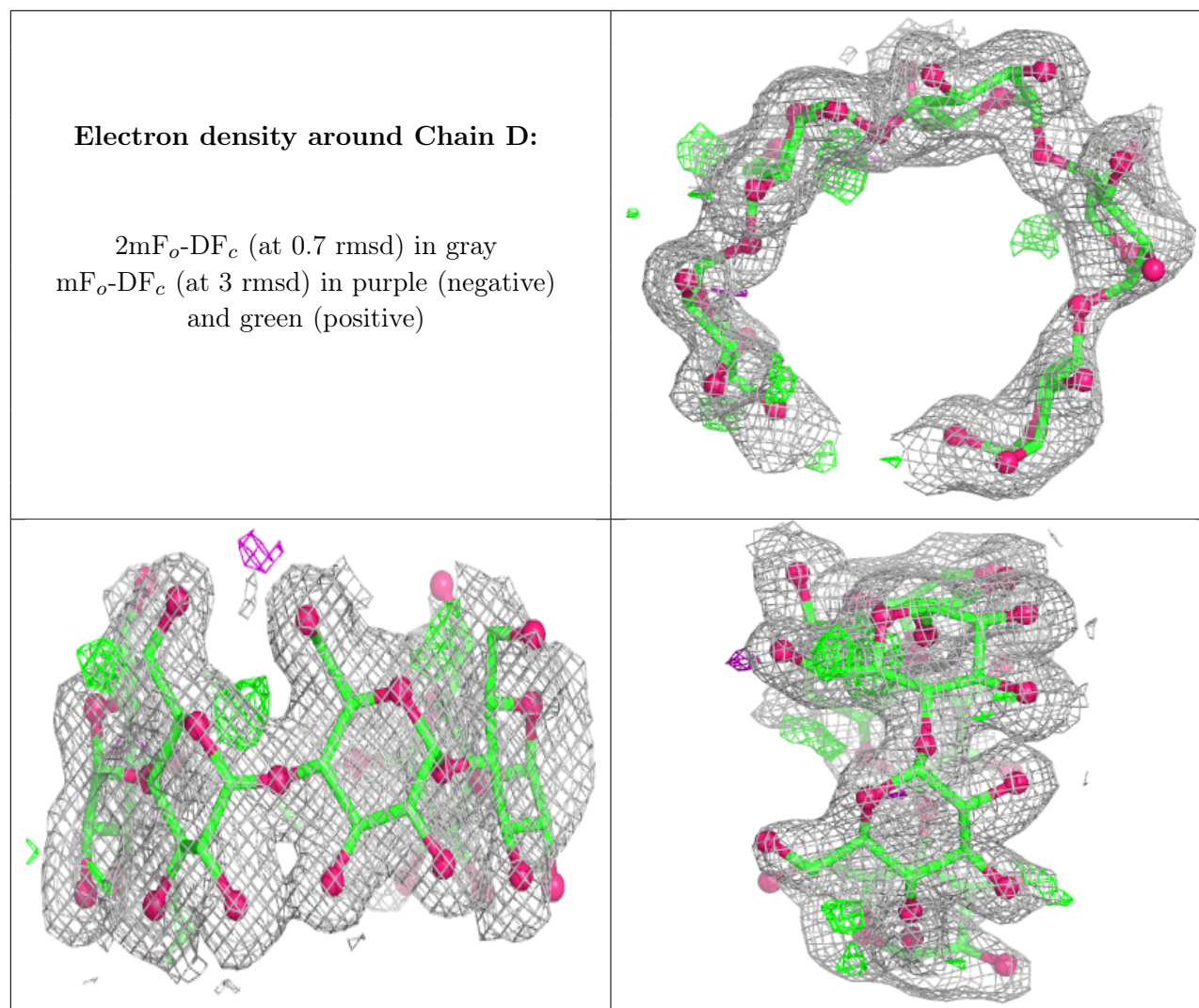
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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)





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
9	IMD	A	731	5/5	0.64	0.20	49,56,63,64	0
8	TAM	A	730	11/11	0.65	0.19	46,55,64,65	0
4	GOL	A	715	6/6	0.66	0.16	46,51,54,60	0
8	TAM	A	729	11/11	0.66	0.19	46,55,62,67	0
4	GOL	A	712	6/6	0.69	0.14	43,49,54,56	0
5	PEG	A	723	7/7	0.70	0.15	38,44,50,57	0
5	PEG	A	719	7/7	0.73	0.16	46,52,53,58	0
5	PEG	A	722	7/7	0.74	0.16	31,43,51,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PEG	A	725	7/7	0.75	0.18	39,49,56,58	0
5	PEG	A	717	7/7	0.75	0.17	33,43,51,54	0
4	GOL	A	714	6/6	0.76	0.15	49,55,57,57	0
6	PGE	A	727	10/10	0.78	0.14	23,39,46,52	0
5	PEG	A	716	7/7	0.79	0.16	45,51,56,58	0
5	PEG	A	720	7/7	0.80	0.13	40,46,49,49	0
9	IMD	A	733	5/5	0.80	0.14	38,44,49,53	0
7	1PE	A	728	16/16	0.81	0.15	22,43,56,61	0
5	PEG	A	724	7/7	0.82	0.14	35,48,51,56	0
9	IMD	A	734	5/5	0.82	0.15	40,43,48,49	0
5	PEG	A	721	7/7	0.84	0.14	39,44,54,59	0
10	CA	A	736	1/1	0.84	0.13	61,61,61,61	0
6	PGE	A	726	10/10	0.85	0.12	43,53,56,63	0
4	GOL	A	713	6/6	0.85	0.11	37,45,53,58	0
9	IMD	A	732	5/5	0.85	0.14	24,30,38,42	0
5	PEG	A	718	7/7	0.86	0.11	36,38,41,50	0
11	CL	A	740	1/1	0.96	0.12	37,37,37,37	0
11	CL	A	741	1/1	0.96	0.07	30,30,30,30	0
11	CL	A	739	1/1	0.98	0.07	23,23,23,23	0
11	CL	A	743	1/1	0.98	0.08	22,22,22,22	0
11	CL	A	744	1/1	0.98	0.05	31,31,31,31	0
11	CL	A	738	1/1	0.99	0.02	18,18,18,18	1
11	CL	A	742	1/1	0.99	0.16	37,37,37,37	0
10	CA	A	735	1/1	0.99	0.05	21,21,21,21	0
11	CL	A	737	1/1	0.99	0.05	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.